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Atoms and Peridynamic Continua

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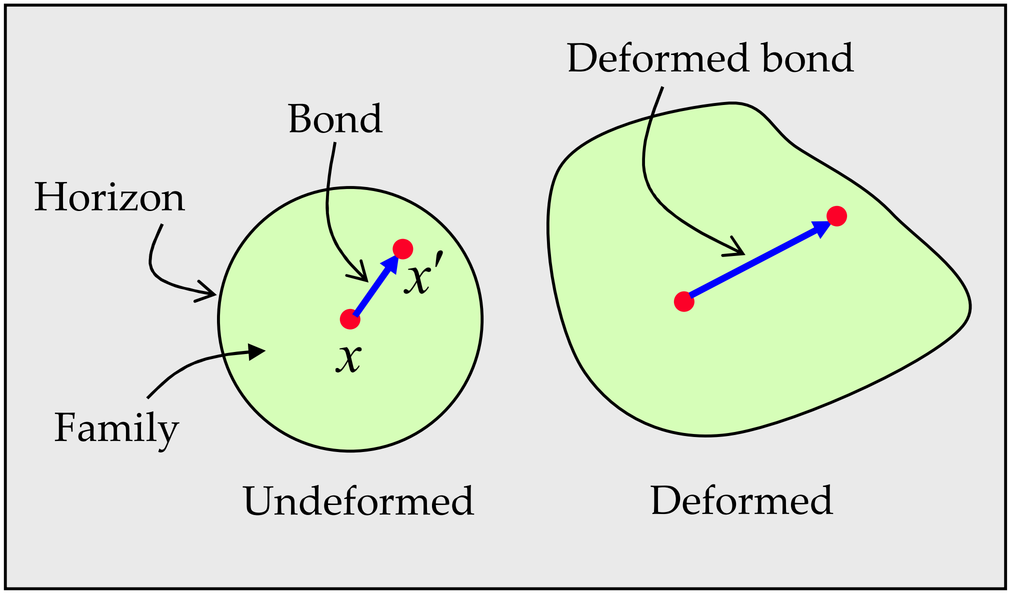
Horizon, family, and bonds

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



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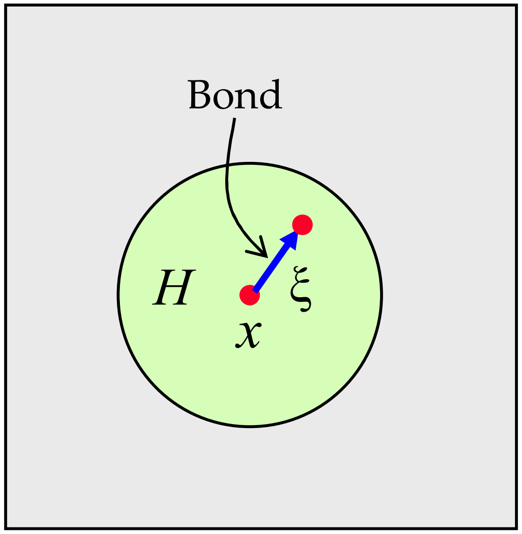
Vector states

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

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

- Example:

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



- Define the dot product of 2 vector states by

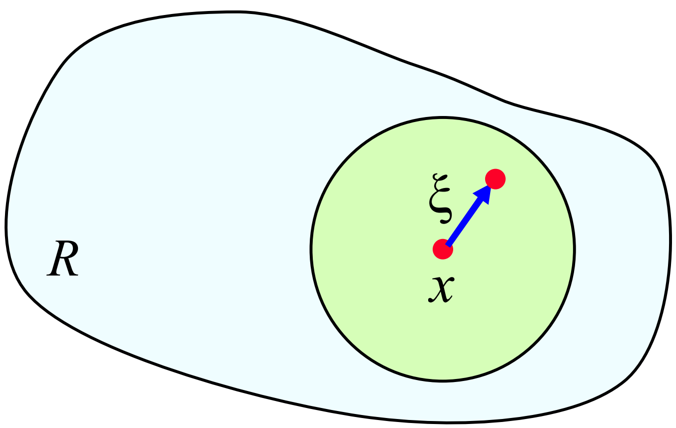
$$\underline{A} \bullet \underline{B} = \int_H \underline{A}\langle\xi\rangle \cdot \underline{B}\langle\xi\rangle dV_\xi$$

Usual scalar product of 2 vectors

Notation for vector state-valued fields

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

$\underline{A}[x,t]\langle\xi\rangle$ …the value (a vector) of this vector state for a bond ξ



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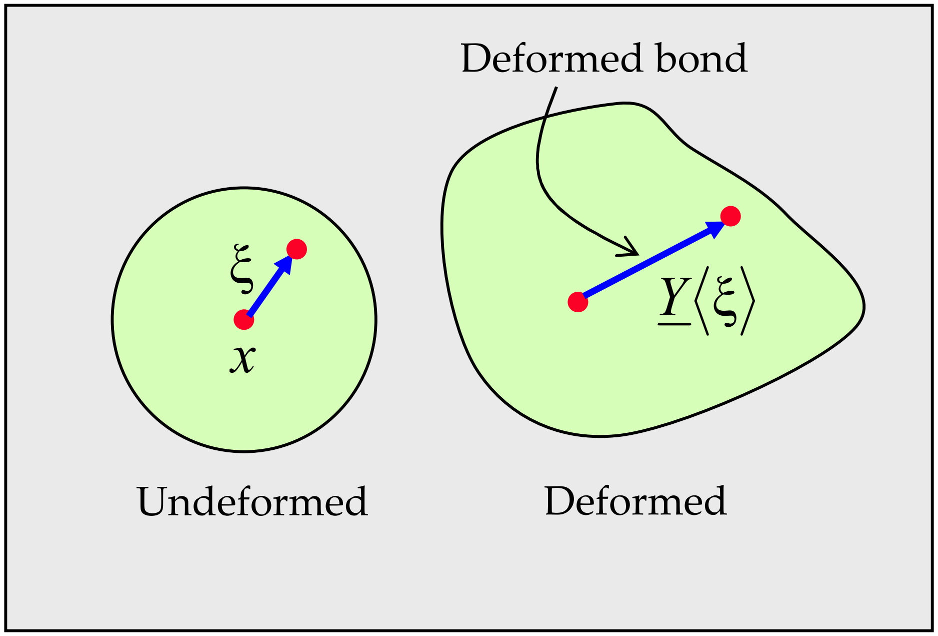
Deformation states

- 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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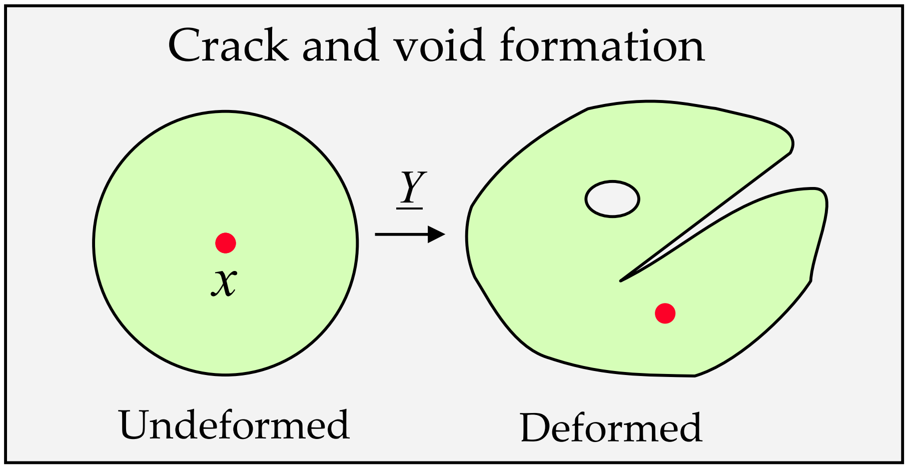
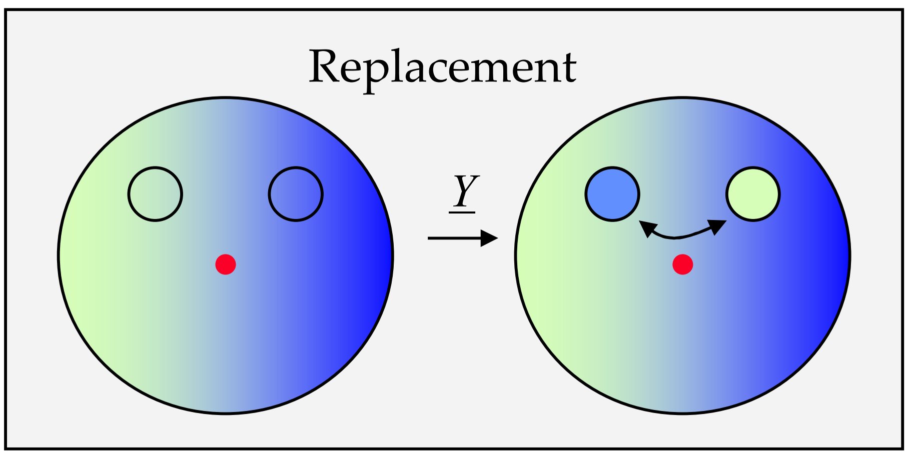
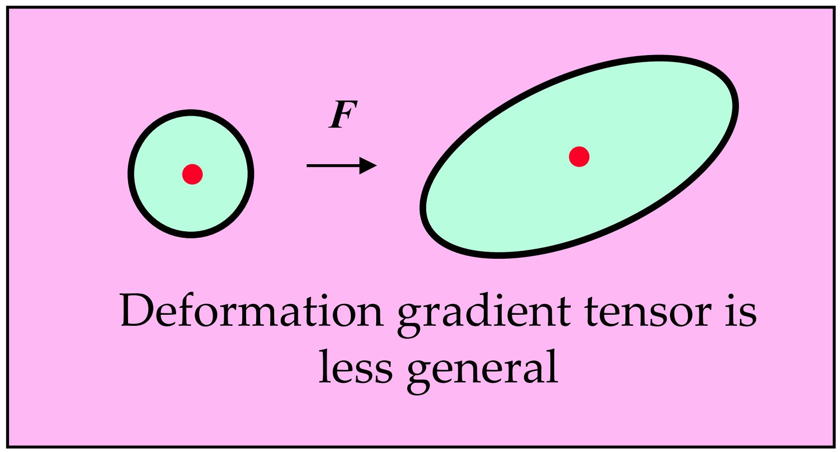
Deformation states can describe complex motions







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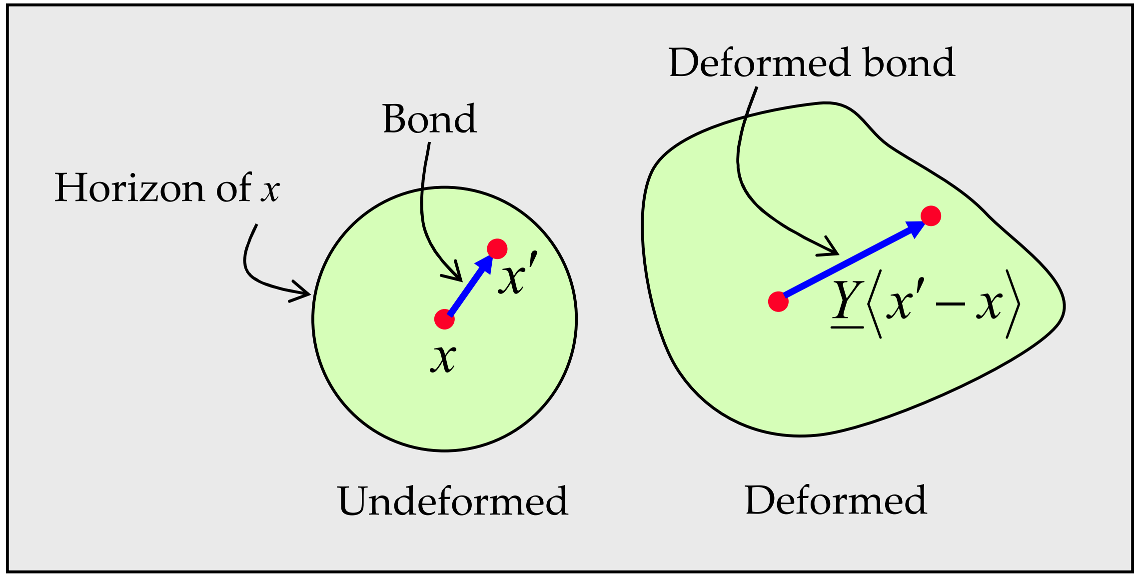
The basic assumption

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



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,

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

then $\underline{T}$ is the Frechet derivative 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:

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

$\underline{T}$ is called the force state.

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Equilibrium equation from stationary potential energy

Potential energy in a body:

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

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

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

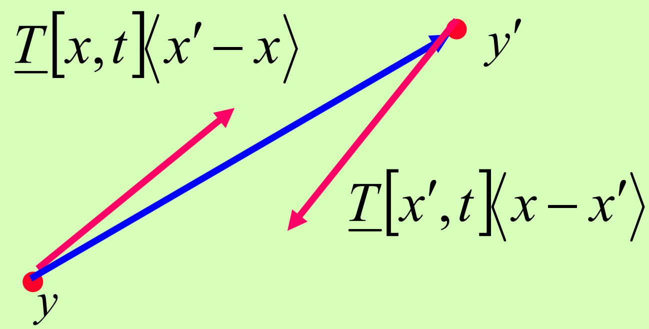
Internal forces

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.

Special case: Bonds independent of each other

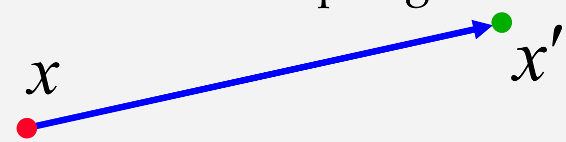
Suppose the strain energy density function is

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

w... scalar-valued "micropotential" function

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

Nonlinear spring



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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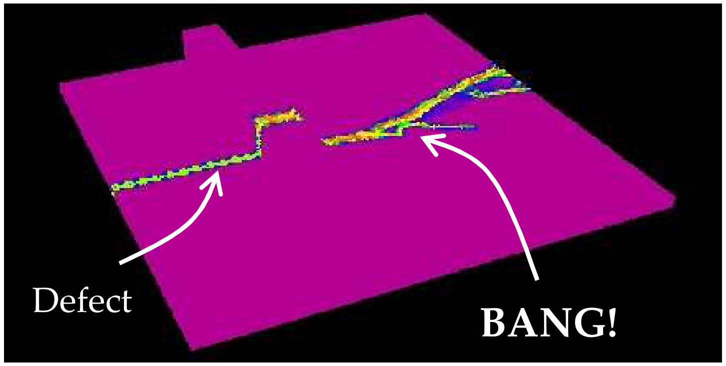
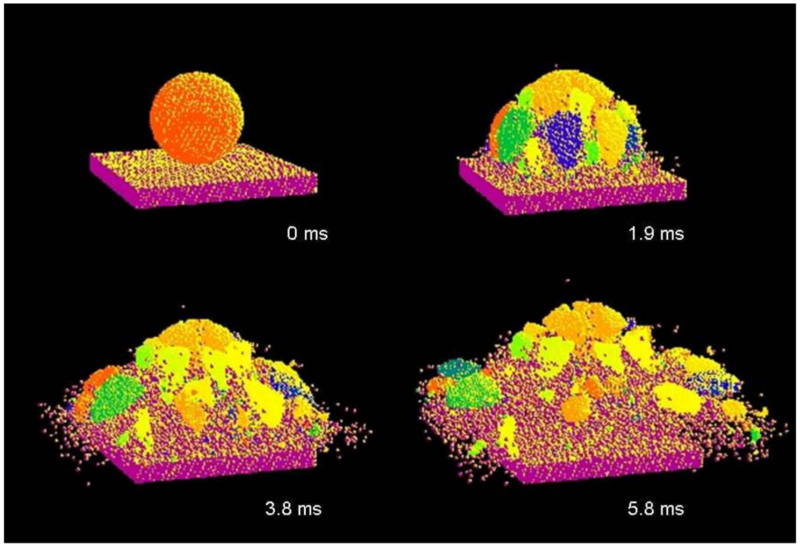
Some applications of the bond-based theory

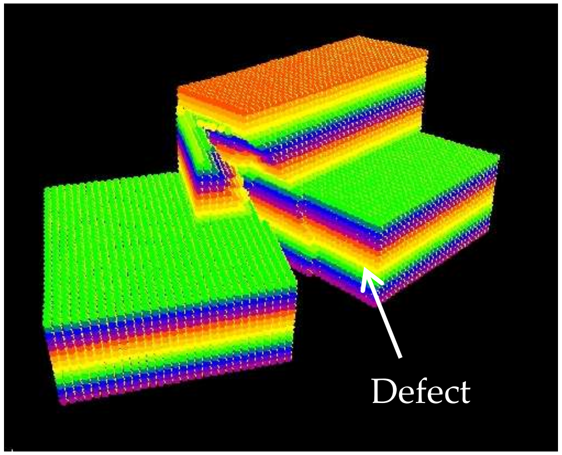
Results from the Emu computer code demonstrate the ability to model complex discontinuities



Transition to unstable crack growth



Impact and fragmentation



Crack turning in a 3D feature

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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

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

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

Some properties of peridynamic constitutive models

Define the composition of two vector states by

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

Condition for material frame indifference (objectivity):

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

for all orthogonal states $\underline{Q}$

Orthogonal states rigidly rotate bonds

Condition for isotropy:

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

for all orthogonal states $\underline{Q}$

What about stress?

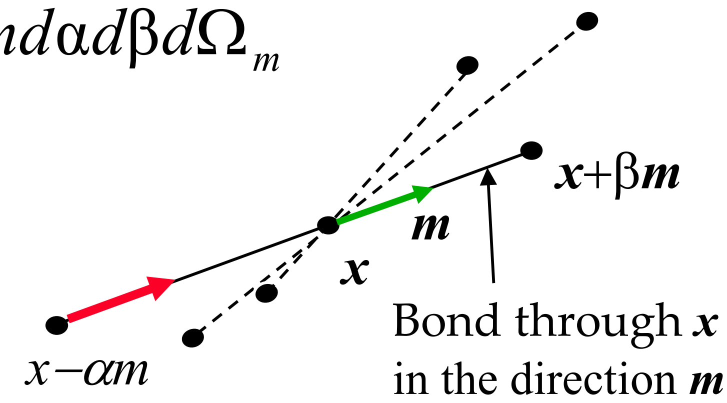
- How to eliminate stress from your life:

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

- But if you want stress in your life, define the peridynamic stress tensor:

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

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



Then:

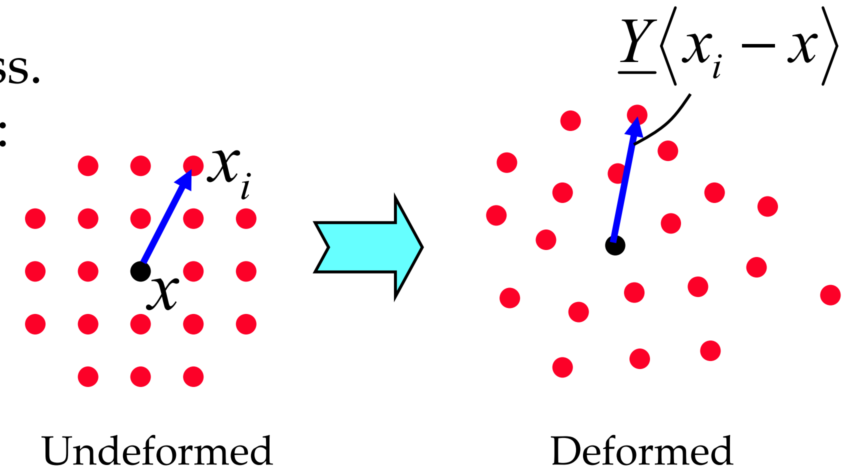
$$\nabla \cdot \nu = \int \left\{ \underline{T}[x]\langle x'-x\rangle - \underline{T}[x']\langle x-x'\rangle \right\} dV_{x'}$$

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.



Description of this system as a nonhomogeneous peridynamic body:

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

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

where x_i is the reference position of atom i.

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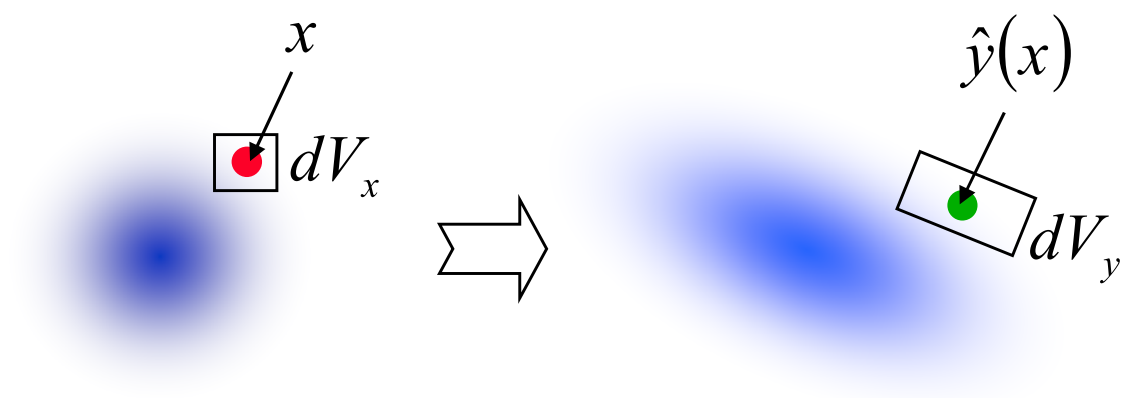
Statistical interpretation of a deformation



Undeformed probability distribution P_k

Deformed probability distribution 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

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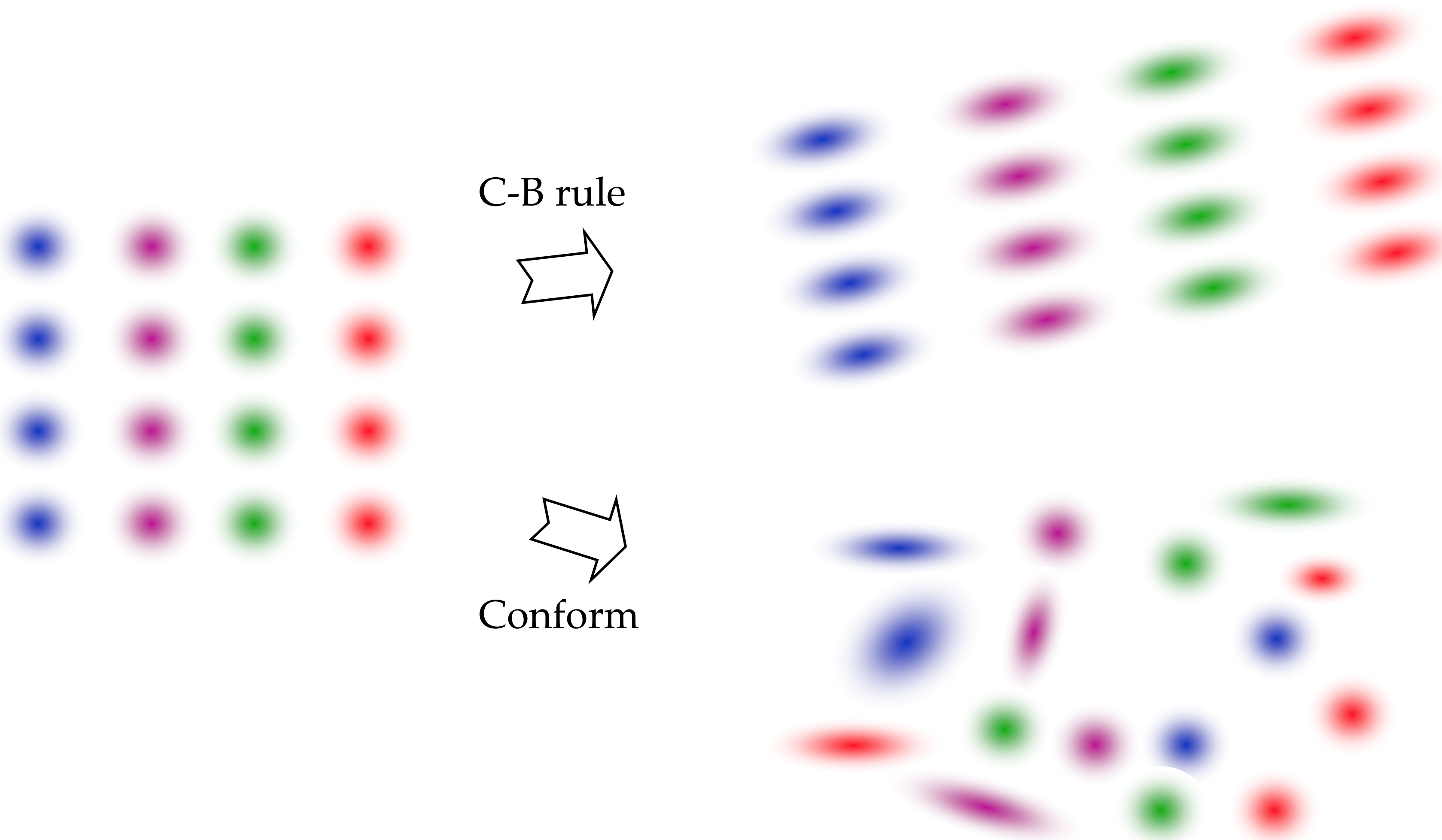
Resulting kinematics are less restrictive than the Cauchy-Born rule



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Peridynamic representation of a statistical distribution of atoms

Define a nonhomogeneous peridynamic body by

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

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

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

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If the atomic positions are known exactly

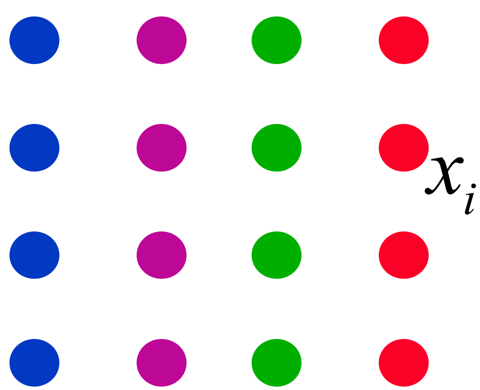
If the atomic positions $\boldsymbol{x}_i$ are known exactly:

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

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

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

Same as before



Total free energy in the statistical peridynamic body

$$U = \int \hat{W}\left(\underline{Y}\right) dV_x$$

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

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

$$= \sum_k \iint \ldots \int \psi\left(y_1 - y, y_2 - y, \ldots, y_N - y\right)$$

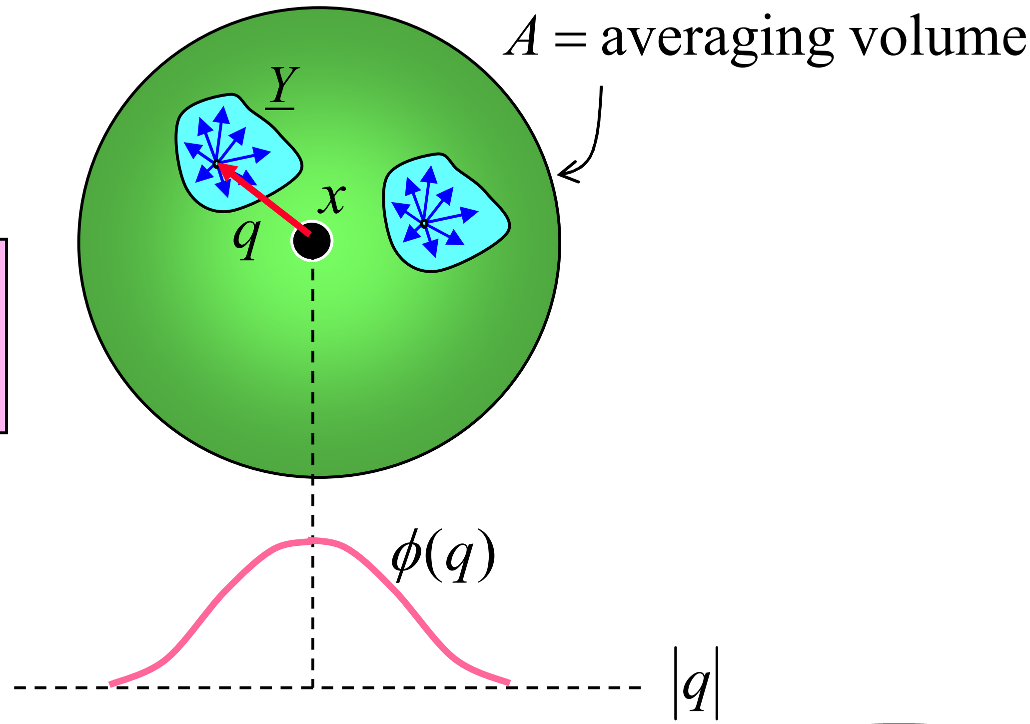
$$p_1(y_1) p_2(y_2) \ldots p_k(y) \ldots p_N(y_N) dV_{y_1} dV_{y_2} \ldots dV_y \ldots dV_{y_N}$$

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 $\phi(q)$ where q is a vector; $\int_A \phi(q)dV_q = 1.$
- Define a homogenized material model by

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



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

Homogenization

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

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

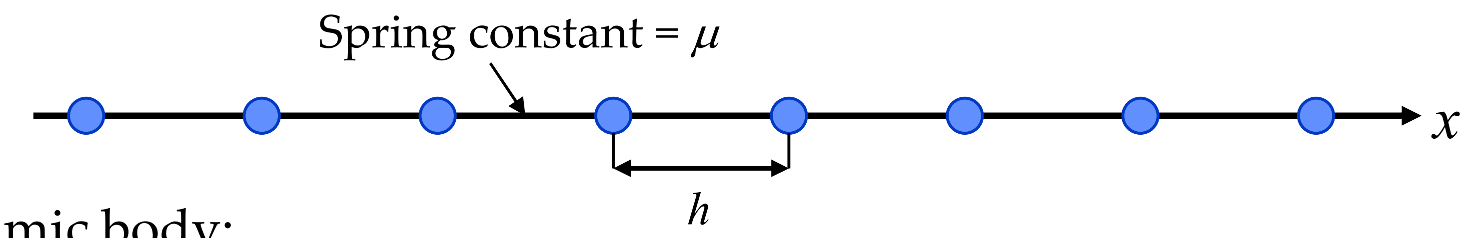
$$= \int_{R^3} \varphi(q) dV_q \int_{R^3} \hat{W}\left(\underline{Y}, z\right) dV_z$$

$$= \int_{R^3} \hat{W}\left(\underline{Y}, z\right) dV_z$$

$$= U$$

- Therefore the total strain energy is unchanged by homogenization.

Homogenization example: 1D spring-mass system

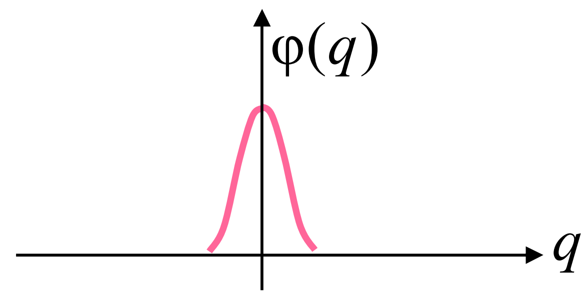


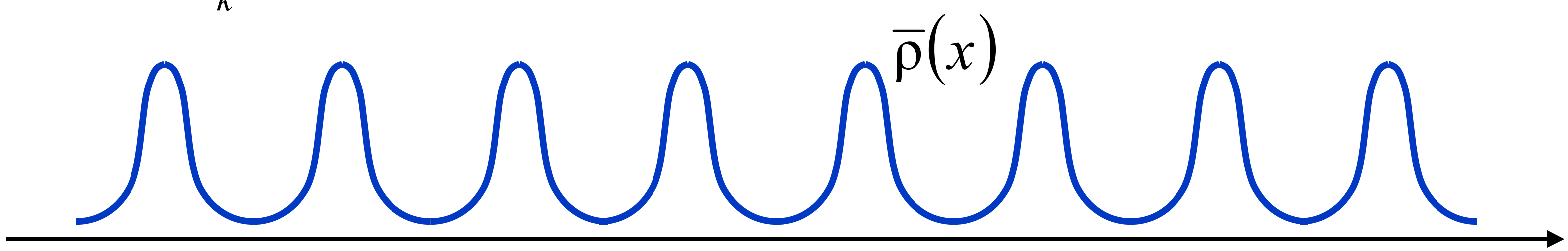
Peridynamic body:

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

Peridynamic body after homogenization:

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





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Homogenization example: 1D spring-mass system

Peridynamic body:

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

Peridynamic body after homogenization:

$$\overline{W}(\underline{Y}, x) = \frac{\mu}{4} \left(\int \sum_k \Delta(x + q - hk) \varphi(q) dq \right) \left\{ (\underline{Y}\langle h \rangle - h)^2 + (\underline{Y}\langle -h \rangle + h)^2 \right\}$$

$$= \frac{\mu}{4} \sum_k \varphi(x - hk) \left\{ (u(x + h) - u(x))^2 + (u(x - h) - u(x))^2 \right\}$$

Homogenization example: 1D spring-mass system

Equation of motion after homogenization boils down to:

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

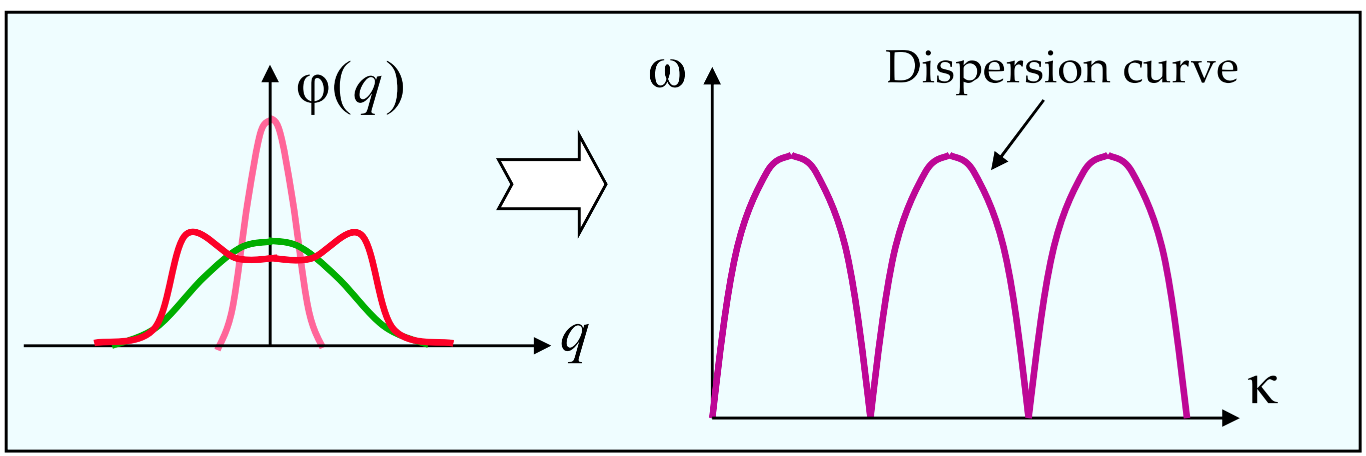
If we assume waves of the form

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

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

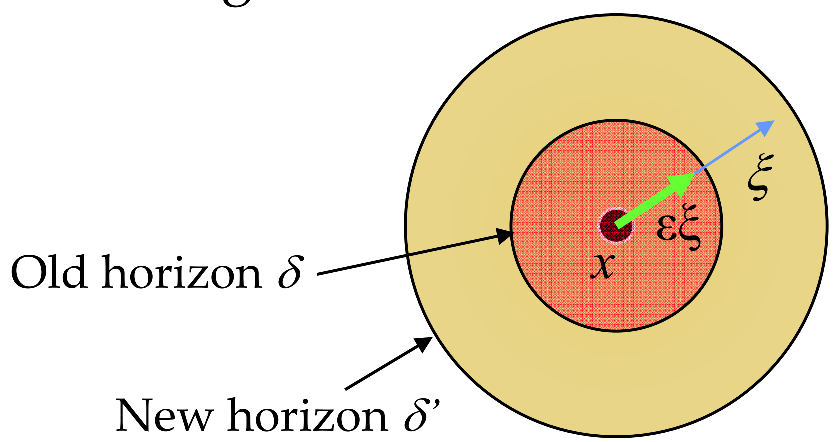


Rescaling:
Increase the length scale of a PD material model

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

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

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



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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.