

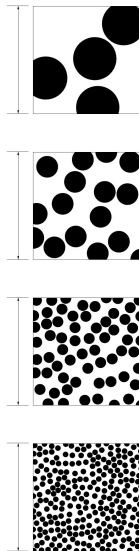
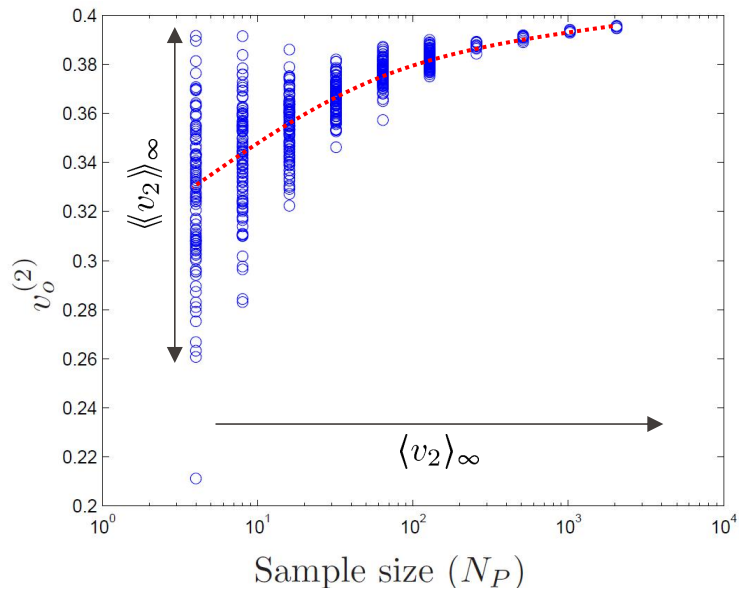
CIVIL-408

Multiscale Modeling in Mechanics

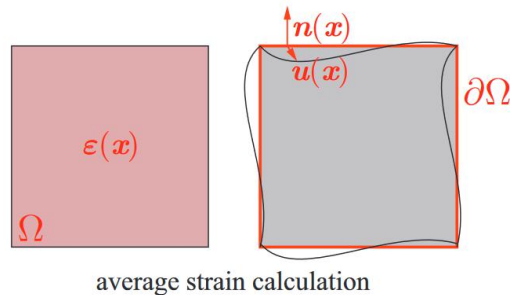
Prof. Kostas Karapiperis

Week 3

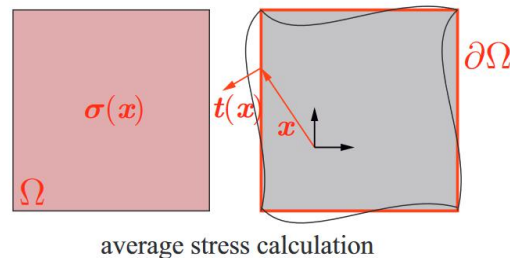
Representative Volume Elements



Averaging Theorems



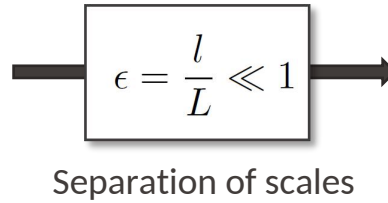
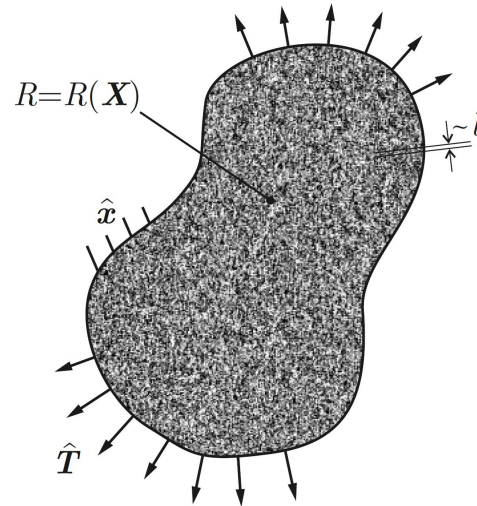
$$\langle \epsilon \rangle = \frac{1}{V} \int_{\partial\Omega} \text{sym}(u \otimes n) dS$$



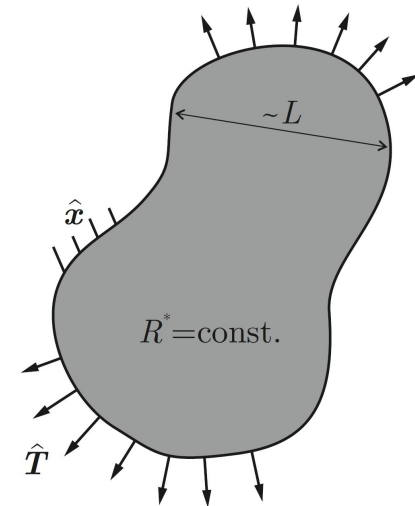
$$\langle \sigma \rangle = \frac{1}{V} \int_{\partial\Omega} t \otimes x dS$$

The homogenization problem

Heterogeneous problem:



Homogenized problem:



$$\begin{aligned}
 & \text{find } \varphi(\mathbf{X}) \text{ s.t.} \\
 & \text{Div } \mathbf{P}(\mathbf{X}, \mathbf{F}(\mathbf{X})) + R(\mathbf{X})\mathbf{B}(\mathbf{X}) = \mathbf{0} \quad \text{in } \Omega, \\
 & \quad \varphi(\mathbf{X}) = \hat{\mathbf{x}}(\mathbf{X}) \quad \text{on } \partial\Omega_D, \\
 & \quad \mathbf{P}(\mathbf{X}, \mathbf{F}(\mathbf{X}))\mathbf{N}(\mathbf{X}) = \hat{\mathbf{T}}(\mathbf{X}) \quad \text{on } \partial\Omega_N, \\
 & \quad \mathbf{P} = \mathbf{P}(\mathbf{X}, \mathbf{F}),
 \end{aligned}$$

$$\begin{aligned}
 & \text{find } \varphi^*(\mathbf{X}) \text{ s.t.} \\
 & \text{Div } \mathbf{P}^*(\mathbf{F}(\mathbf{X})) + R^*\mathbf{B}(\mathbf{X}) = \mathbf{0} \quad \text{in } \Omega, \\
 & \quad \varphi^*(\mathbf{X}) = \hat{\mathbf{x}}(\mathbf{X}) \quad \text{on } \partial\Omega_D, \\
 & \quad \mathbf{P}^*(\mathbf{F}(\mathbf{X}))\mathbf{N}(\mathbf{X}) = \hat{\mathbf{T}}(\mathbf{X}) \quad \text{on } \partial\Omega_N, \\
 & \quad \mathbf{P}^* = \mathbf{P}^*(\mathbf{F}).
 \end{aligned}$$

Define:

$$R^* = \frac{1}{V} \int_{\Omega} R(\mathbf{X}) dV = \langle R \rangle$$

$$\mathbf{P}^* = \langle \mathbf{P} \rangle$$

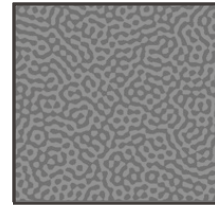
$$\mathbf{F}^* = \langle \mathbf{F} \rangle$$

Within the RVE, solve:

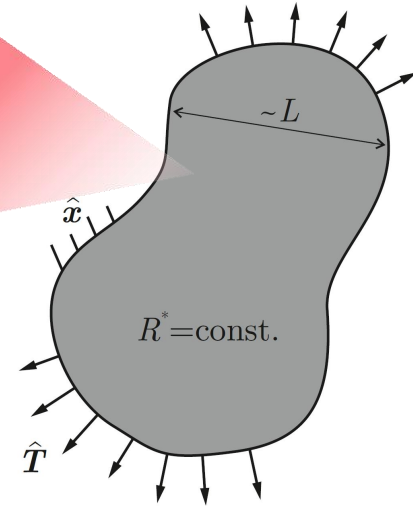
$$\text{Div } \mathbf{P}(\mathbf{X}, \mathbf{F}) = \mathbf{0} \quad (\text{Microscale problem})$$

... but what are the boundary conditions on the microscale?

RVE



Macroscale problem:



At the RVE level:

- no body forces
- no inertial effects

find $\varphi^*(\mathbf{X})$ s.t.

$$\text{Div } \mathbf{P}^*(\mathbf{F}(\mathbf{X})) + R^* \mathbf{B}(\mathbf{X}) = \mathbf{0} \quad \text{in } \Omega,$$

$$\varphi^*(\mathbf{X}) = \hat{\mathbf{x}}(\mathbf{X}) \quad \text{on } \partial\Omega_D,$$

$$\mathbf{P}^*(\mathbf{F}(\mathbf{X}))\mathbf{N}(\mathbf{X}) = \hat{\mathbf{T}}(\mathbf{X}) \quad \text{on } \partial\Omega_N,$$

$$\mathbf{P}^* = \mathbf{P}^*(\mathbf{F}).$$

The Hill-Mandel condition

Conservation of energy across scales (for elastic problems):

$$V W^*(\boldsymbol{\varepsilon}^*) = \int_{\Omega} W(\mathbf{x}, \boldsymbol{\varepsilon}(\mathbf{x})) dV$$

Alternative versions:

$$\mathbf{P}^* \cdot \delta \mathbf{F}^* = \langle \mathbf{P}(\mathbf{X}) \cdot \delta \mathbf{F}(\mathbf{X}) \rangle$$

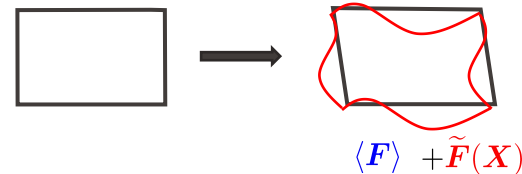
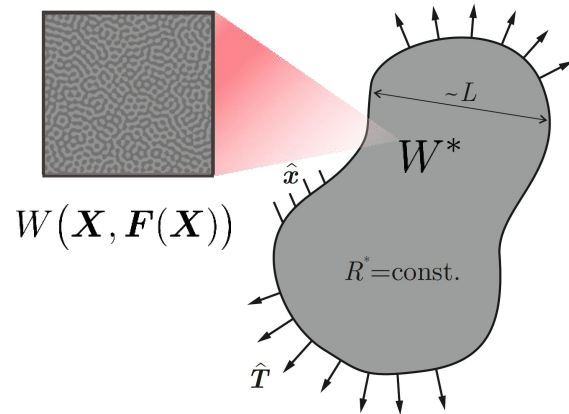
$$\mathbf{P}^* \cdot \dot{\mathbf{F}}^* = \langle \mathbf{P}(\mathbf{X}) \cdot \dot{\mathbf{F}}(\mathbf{X}) \rangle$$

Can re-formulate in terms of **mean + perturbation**:

$$\mathbf{P}(\mathbf{X}) = \langle \mathbf{P} \rangle + \tilde{\mathbf{P}}(\mathbf{X}), \quad \mathbf{F}(\mathbf{X}) = \langle \mathbf{F} \rangle + \tilde{\mathbf{F}}(\mathbf{X})$$

$$\langle \tilde{\mathbf{P}}(\mathbf{X}) \rangle = \mathbf{0}, \quad \langle \tilde{\mathbf{F}}(\mathbf{X}) \rangle = \mathbf{0},$$

$$\langle \tilde{\mathbf{P}} \cdot \tilde{\mathbf{F}} \rangle = 0$$



... still, how do we impose averages and what BCs to apply?

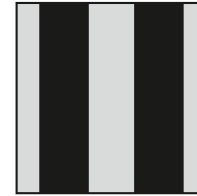
Example: Affine deformation

Let us apply **affine deformation** to **every point** inside the RVE:

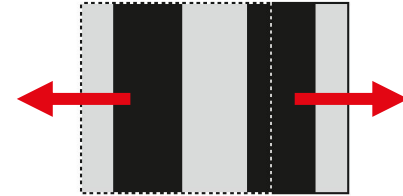
$$\varphi = \mathbf{F}^* \mathbf{X} \quad \text{or} \quad \mathbf{u} = \boldsymbol{\varepsilon}^* \mathbf{x}$$

Check **Hill-Mandel**:

$$\langle \mathbf{P} \cdot \mathbf{F} \rangle = \langle \mathbf{P} \cdot \mathbf{F}^* \rangle = \langle \mathbf{P} \rangle \cdot \mathbf{F}^* = \langle \mathbf{P} \rangle \cdot \langle \mathbf{F} \rangle$$



two-phase composite RVE



affine deformation

Average deformation:

$$\langle \mathbf{F} \rangle = \frac{1}{V} \int_{\Omega} \mathbf{F}(\mathbf{X}) dV = \frac{1}{V} \int_{\Omega} \mathbf{F}^* dV = \mathbf{F}^* \quad \text{or} \quad \langle \boldsymbol{\varepsilon} \rangle = \frac{1}{V} \int_{\Omega} \boldsymbol{\varepsilon}(\mathbf{x}) dv = \boldsymbol{\varepsilon}^*$$

Effective response (for a composite):

$$\langle \mathbf{P} \rangle = \frac{1}{V} \int_{\Omega} \mathbf{P}(\mathbf{X}, \mathbf{F}^*) = \frac{1}{V} \sum_i V_i \mathbf{P}_i(\mathbf{F}^*) = \sum_i v_i \mathbf{P}_i(\mathbf{F}^*)$$

Example: Elastic Composite

Consider a **linear elastic composite**:

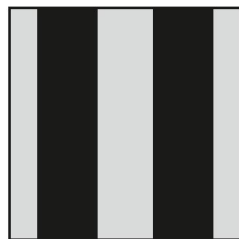
$$\boldsymbol{\sigma}(\boldsymbol{x}) = \mathbb{C}(\boldsymbol{x})\boldsymbol{\varepsilon}(\boldsymbol{x}),$$

Effective response:

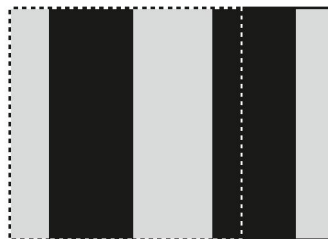
$$\langle \boldsymbol{\sigma}(\boldsymbol{x}) \rangle = \frac{1}{V} \sum_i V_i \mathbb{C}_i \boldsymbol{\varepsilon}^* = \mathbb{C}_{\text{Voigt}}^* \boldsymbol{\varepsilon}^* \quad \text{with}$$

$$\mathbb{C}_{\text{Voigt}}^* = \frac{1}{V} \sum_i V_i \mathbb{C}_i$$

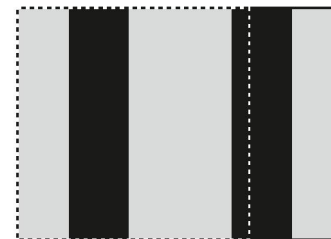
in general:



two-phase composite RVE



affine deformation



realistic deformation

Example: Elastic Composite

Consider a **linear elastic composite**:

$$\boldsymbol{\sigma}(\mathbf{x}, \boldsymbol{\varepsilon}(\mathbf{x})) = \mathbb{C}(\mathbf{x})\boldsymbol{\varepsilon}(\mathbf{x}),$$

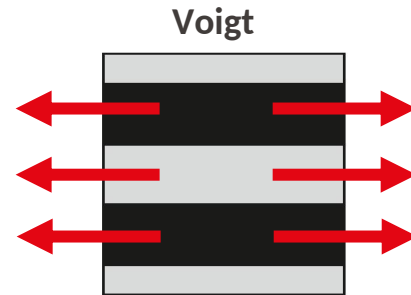
Effective response:

$$\langle \boldsymbol{\sigma}(\mathbf{x}) \rangle = \frac{1}{V} \sum_i V_i \mathbb{C}_i \boldsymbol{\varepsilon}^* = \mathbb{C}_{\text{Voigt}}^* \boldsymbol{\varepsilon}^*$$

with

$$\mathbb{C}_{\text{Voigt}}^* = \frac{1}{V} \sum_i V_i \mathbb{C}_i$$

Upper bound!



Let's perform a thought experiment and do the opposite, i.e., **prescribe uniform stresses**:

$$\langle \boldsymbol{\varepsilon}(\mathbf{x}) \rangle = \frac{1}{V} \sum_i V_i \mathbb{C}_i^{-1} \boldsymbol{\sigma}^* = (\mathbb{C}_{\text{Reuss}}^*)^{-1} \boldsymbol{\sigma}^*$$

with

$$\mathbb{C}_{\text{Reuss}} = \left(\frac{1}{V} \sum_i V_i \mathbb{C}_i^{-1} \right)^{-1}$$

In continuous systems:

$$\mathbb{C}_{\text{Reuss}} = \left(\frac{1}{V} \int_{\Omega} \mathbb{C}^{-1} \right)^{-1} = \langle \mathbb{C}^{-1} \rangle^{-1}$$

Lower bound!

Example: Two-phase Linear Elastic Composite

Generally:

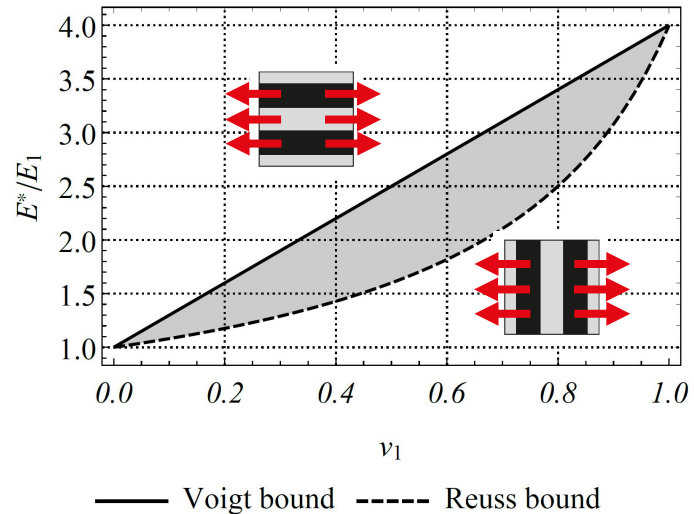
$$\mathbb{C}_{\text{Reuss}} = \langle \mathbb{C}^{-1} \rangle^{-1} \leq \mathbb{C}^* \leq \mathbb{C}_{\text{Voigt}} = \langle \mathbb{C} \rangle$$

Generally

$$\mathbb{C}_{\text{Reuss}} = \langle \mathbb{C}^{-1} \rangle^{-1} \leq \mathbb{C}^* \leq \mathbb{C}_{\text{Voigt}} = \langle \mathbb{C} \rangle$$

Example of a two-phase composite with **isotropic** phases:

$$\left(\frac{v_1}{E_1} + \frac{v_2}{E_2} \right)^{-1} \leq E^* \leq v_1 E_1 + v_2 E_2$$



EPFL Energetic explanation of the Voigt bound

Recall the variational problem (minimization of potential energy)

$$\mathbf{u}(\mathbf{x}) = \arg \min I[\mathbf{u}] = \arg \min \frac{1}{2} \int_{\Omega} \boldsymbol{\varepsilon} \cdot \mathbb{C} \boldsymbol{\varepsilon} dV \quad \text{s.t.} \quad \langle \boldsymbol{\varepsilon} \rangle = \left\langle \frac{1}{2} (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) \right\rangle = \boldsymbol{\varepsilon}^*$$

Expand the displacement field into affine deformation + perturbation

$$\mathbf{u}(\mathbf{x}) = \boldsymbol{\varepsilon}^* \mathbf{x} + \tilde{\mathbf{u}}(\mathbf{x}) \quad \Rightarrow \quad \boldsymbol{\varepsilon}(\mathbf{x}) = \boldsymbol{\varepsilon}^* + \tilde{\boldsymbol{\varepsilon}}(\mathbf{x}) \quad \text{and} \quad \langle \tilde{\boldsymbol{\varepsilon}}(\mathbf{x}) \rangle = \mathbf{0}$$

We can rewrite the potential energy

$$I[\mathbf{u}] = \frac{1}{2} \boldsymbol{\varepsilon}^* \cdot \int_{\Omega} \mathbb{C} dV \boldsymbol{\varepsilon}^* + \boldsymbol{\varepsilon}^* \cdot \int_{\Omega} \mathbb{C} \tilde{\boldsymbol{\varepsilon}} dV + \frac{1}{2} \int_{\Omega} \tilde{\boldsymbol{\varepsilon}} \cdot \mathbb{C} \tilde{\boldsymbol{\varepsilon}} dV$$

such that equilibrium corresponds to the minimizer

$$\tilde{\mathbf{u}}(\mathbf{x}) = \arg \min \left[\frac{1}{2} \boldsymbol{\varepsilon}^* \cdot V \langle \mathbb{C} \rangle \boldsymbol{\varepsilon}^* + \boldsymbol{\varepsilon}^* \cdot \int_{\Omega} \mathbb{C} \tilde{\boldsymbol{\varepsilon}} dV + \frac{1}{2} \int_{\Omega} \tilde{\boldsymbol{\varepsilon}} \cdot \mathbb{C} \tilde{\boldsymbol{\varepsilon}} dV \right] \quad \text{s.t.} \quad \langle \tilde{\boldsymbol{\varepsilon}} \rangle = \mathbf{0}$$

EPFL Energetic explanation of the Voigt bound

The energy of the equilibrated RVE must match that of the effective medium i.e.

$$\begin{aligned}\min_{\mathbf{u}(\mathbf{x})} I[\mathbf{u}(\mathbf{x})] &= \min_{\tilde{\mathbf{u}}(\mathbf{x})} I[\boldsymbol{\varepsilon}^* \mathbf{x} + \tilde{\mathbf{u}}(\mathbf{x})] = \min_{\tilde{\mathbf{u}}(\mathbf{x})} \left[\frac{V}{2} \boldsymbol{\varepsilon}^* \cdot \langle \mathbb{C} \rangle \boldsymbol{\varepsilon}^* + \boldsymbol{\varepsilon}^* \cdot \int_{\Omega} \mathbb{C} \tilde{\boldsymbol{\varepsilon}} dV + \frac{1}{2} \int_{\Omega} \tilde{\boldsymbol{\varepsilon}} \cdot \mathbb{C} \tilde{\boldsymbol{\varepsilon}} dV \right] \\ &= \frac{V}{2} \boldsymbol{\varepsilon}^* \cdot \langle \mathbb{C} \rangle \boldsymbol{\varepsilon}^* + \min_{\tilde{\mathbf{u}}(\mathbf{x})} \left[\boldsymbol{\varepsilon}^* \cdot \int_{\Omega} \mathbb{C} \tilde{\boldsymbol{\varepsilon}} dV + \frac{1}{2} \int_{\Omega} \tilde{\boldsymbol{\varepsilon}} \cdot \mathbb{C} \tilde{\boldsymbol{\varepsilon}} dV \right] = \frac{V}{2} \boldsymbol{\varepsilon}^* \cdot \mathbb{C}^* \boldsymbol{\varepsilon}^*\end{aligned}$$

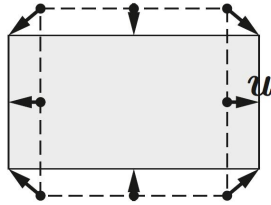
Choosing a particular perturbation field (zero field) suggests:

$$\min_{\tilde{\mathbf{u}}(\mathbf{x})} \left[\boldsymbol{\varepsilon}^* \cdot \int_{\Omega} \mathbb{C} \tilde{\boldsymbol{\varepsilon}} dV + \frac{1}{2} \int_{\Omega} \tilde{\boldsymbol{\varepsilon}} \cdot \mathbb{C} \tilde{\boldsymbol{\varepsilon}} dV \right] \leq \left[\boldsymbol{\varepsilon}^* \cdot \int_{\Omega} \mathbb{C} \tilde{\boldsymbol{\varepsilon}} dV + \frac{1}{2} \int_{\Omega} \tilde{\boldsymbol{\varepsilon}} \cdot \mathbb{C} \tilde{\boldsymbol{\varepsilon}} dV \right]_{\tilde{\boldsymbol{\varepsilon}}=\mathbf{0}} = 0$$

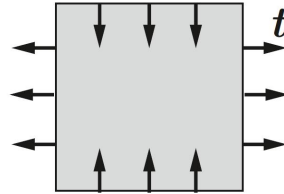
Hence

$$\boldsymbol{\varepsilon}^* \cdot \mathbb{C}^* \boldsymbol{\varepsilon}^* \leq \boldsymbol{\varepsilon}^* \cdot \langle \mathbb{C} \rangle \boldsymbol{\varepsilon}^* \quad \text{for all symmetric strain tensors } \boldsymbol{\varepsilon}^*$$

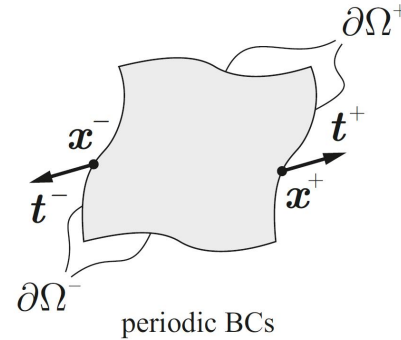
Different types of boundary conditions



affine displacement BCs



uniform traction BCs



periodic BCs

Finite strains: $\mathbf{x} = \mathbf{F}_0 \mathbf{X}$

$$\mathbf{T} = \mathbf{P}_0 \mathbf{N}$$

$$\mathbf{x}^+ = \mathbf{x}^- + \mathbf{F}_0 (\mathbf{X}^+ - \mathbf{X}^-)$$

$$\mathbf{T}^+ = -\mathbf{T}^-$$

Linearized kin.: $\mathbf{u} = \boldsymbol{\varepsilon}_0 \mathbf{x}$

$$\mathbf{t} = \boldsymbol{\sigma}_0 \mathbf{n}$$

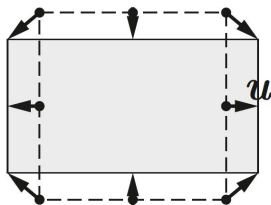
$$\mathbf{u}^+ = \mathbf{u}^- + \boldsymbol{\varepsilon}_0 (\mathbf{x}^+ - \mathbf{x}^-)$$

$$\mathbf{t}^+ = -\mathbf{t}^-$$

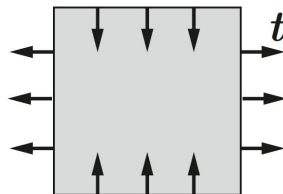
As you will see, these three satisfy the Hill-Mandel criterion.

Outlook: RVE Boundary Conditions

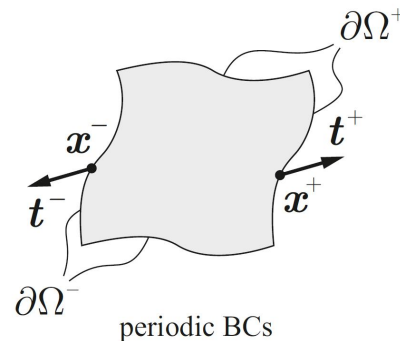
Different types of boundary conditions



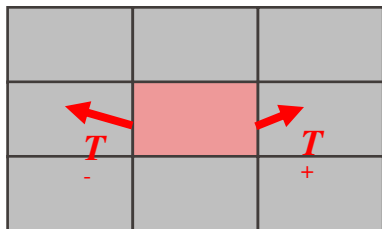
affine displacement BCs



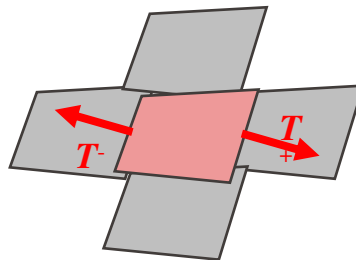
uniform traction BCs



periodic BCs



geometrically compatible,
not equilibrated

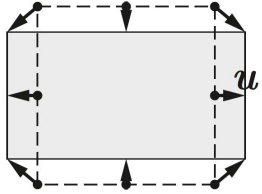


not compatible,
equilibrated

compatible &
equilibrated

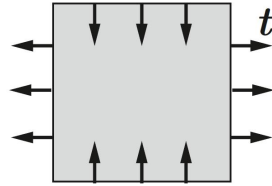
Different types of boundary conditions

Remember: equilibrium means
the energy is minimized



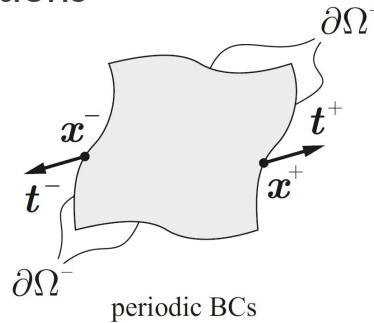
affine displacement BCs

(1)



uniform traction BCs

(2)



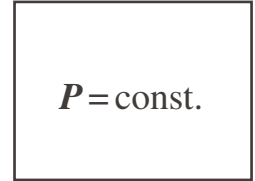
periodic BCs

(3)



affine deformation

(4)



uniform stresses

(5)

What freedom does the RVE have to accommodate the imposed deformation?

Only interior points are free to deform in equilibrium.

Not even the average deformation is fixed, but in equilibrium.

Lots of freedom (in equilibrium), while the **average is fixed**.

None! All points move in an affine manner.

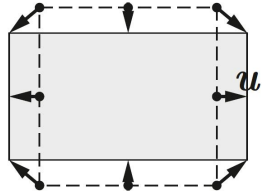
All! No constraint on deformation.

Let's order their stiffnesses from lowest to highest!

Outlook: RVE Boundary Conditions

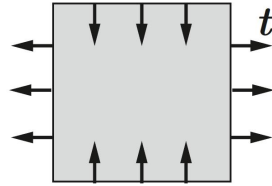
Different types of boundary conditions

Remember: equilibrium means the energy is minimized



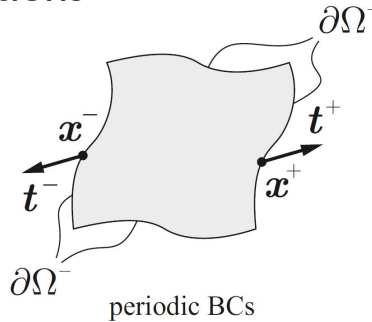
affine displacement BCs

(1)



uniform traction BCs

(2)



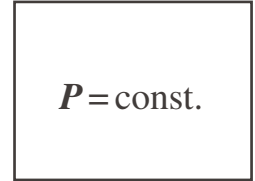
periodic BCs

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Lots of freedom (in equilibrium), while the average is fixed.

None! All points move in an affine manner.

All! No constraint on deformation.

Reuss \leq uniform traction BC \leq periodic BCs \leq affine displacement BCs \leq Voigt

(5)

(2)

(3)

(1)

(4)

That's what I prepared for you today.

What would you like to discuss?

Reading for next class:

Multiscale Modeling, D.M. Kochmann
Chapters 6-8