

# CIVIL-408

## Multiscale Modeling in Mechanics

Prof. Kostas Karapiperis

### Week 4

Recall:

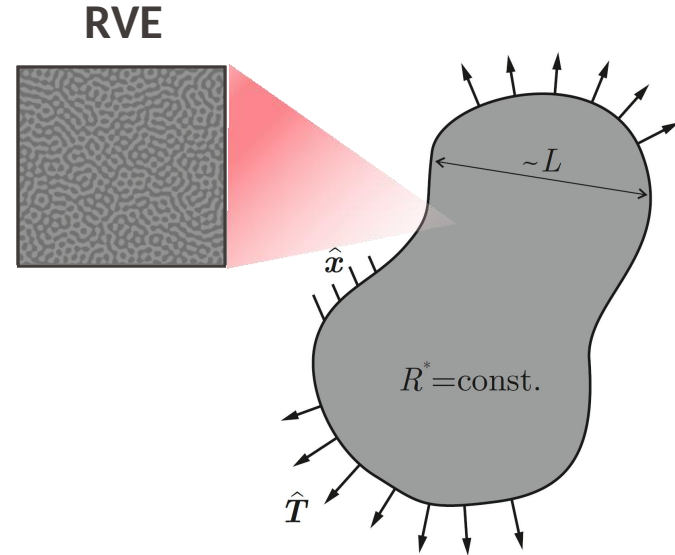
$$\mathbf{P}^* = \langle \mathbf{P} \rangle$$

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

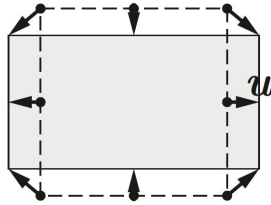
Requirements:

- Impose averages of stresses/strains
- Satisfy the Hill-Mandel condition:

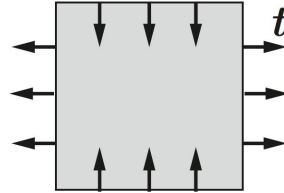
$$\mathbf{P}^* \cdot \delta \mathbf{F}^* = \langle \mathbf{P}(\mathbf{X}) \cdot \delta \mathbf{F}(\mathbf{X}) \rangle$$



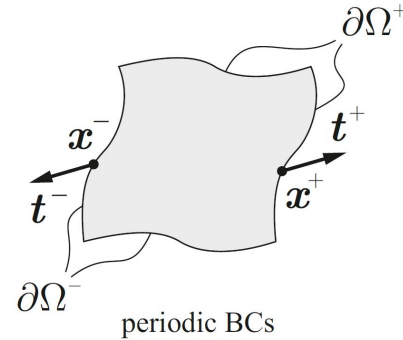
Different types of boundary conditions



affine displacement BCs



uniform traction BCs



periodic BCs

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

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

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

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

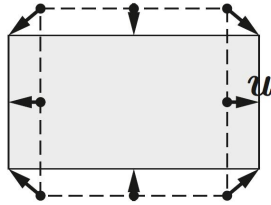
Linearized kin.:  $\mathbf{u} = \boldsymbol{\varepsilon}_0 \mathbf{x}$

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

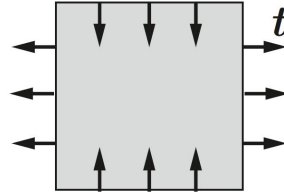
$$\mathbf{u}^+ = \mathbf{u}^- + \boldsymbol{\varepsilon}_0 (\mathbf{x}^+ - \mathbf{x}^-)$$

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

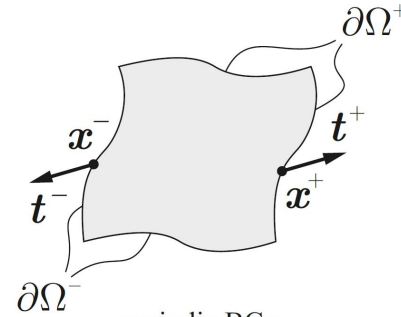
Different types of boundary conditions



affine displacement BCs



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

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

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

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

RVE averages:  $\langle \boldsymbol{F} \rangle = \boldsymbol{F}_0$

$$\langle \boldsymbol{P} \rangle = \boldsymbol{P}_0$$

$$\langle \boldsymbol{F} \rangle = \boldsymbol{F}_0$$

Ideal for: average-strain driven

average-stress driven

average-strain driven

# Consistency of affine displacement BCs

We impose

$$\boldsymbol{\varphi} = \mathbf{F}_0 \mathbf{X} \quad \text{on } \partial\Omega$$

Using the average strain theorem

$$\langle \mathbf{F} \rangle = \frac{1}{V} \int_{\partial\Omega} \boldsymbol{\varphi} \otimes \mathbf{N} \, dS = \frac{1}{V} \int_{\partial\Omega} \mathbf{F}_0 \mathbf{X} \otimes \mathbf{N} \, dS = \frac{\mathbf{F}_0}{V} \int_{\partial\Omega} \mathbf{X} \otimes \mathbf{N} \, dS = \mathbf{F}_0$$

Let us also verify the Hill-Mandel condition

$$\begin{aligned} \langle \mathbf{P} \cdot \mathbf{F} \rangle &= \frac{1}{V} \int_{\partial\Omega} \mathbf{T} \cdot \boldsymbol{\varphi} \, dS = \frac{1}{V} \int_{\partial\Omega} \mathbf{T} \cdot \mathbf{F}_0 \mathbf{X} \, dS = \frac{1}{V} \int_{\partial\Omega} T_i F_{iJ}^0 X_J \, dS \\ &= F_{iJ}^0 \frac{1}{V} \int_{\partial\Omega} T_i X_J \, dS = \mathbf{F}_0 \cdot \frac{1}{V} \int_{\partial\Omega} \mathbf{T} \otimes \mathbf{X} \, dS = \mathbf{F}_0 \cdot \langle \mathbf{P} \rangle, \end{aligned}$$

$$\text{Hence } \langle \mathbf{P} \cdot \mathbf{F} \rangle = \mathbf{F}_0 \cdot \langle \mathbf{P} \rangle = \langle \mathbf{F} \rangle \cdot \langle \mathbf{P} \rangle$$

We can show the same for **uniform traction** and **periodic BCs** (with a bit more work..)

# EPFL Implementing periodic boundary conditions

One possibility: **penalty potential**

$$I_C[\mathbf{u}] = \frac{1}{2\epsilon} \int_{\partial\Omega^+} \left\| (\mathbf{F}_0 - \mathbf{I})(\mathbf{X}^+ - \mathbf{X}^-) - (\mathbf{u}^+ - \mathbf{u}^-) \right\|^2 dS$$

so that

$$I[\mathbf{u}] = \int_{\Omega} W(\mathbf{F}) dV + I_C[\mathbf{u}]$$

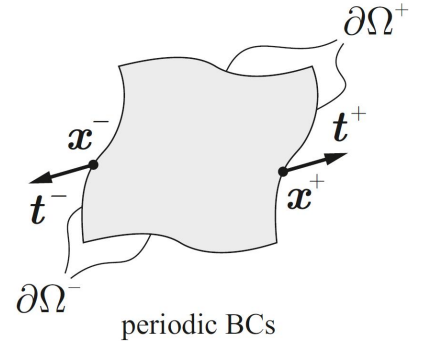
This effectively implements **penalty tractions** on the boundaries:

$$\mathbf{T}^+ = \frac{1}{\epsilon} \left[ (\mathbf{F}_0 - \mathbf{I})(\mathbf{X}^+ - \mathbf{X}^-) - (\mathbf{u}^+ - \mathbf{u}^-) \right] \quad \text{on } \partial\Omega^+$$

$$\mathbf{T}^- = -\frac{1}{\epsilon} \left[ (\mathbf{F}_0 - \mathbf{I})(\mathbf{X}^+ - \mathbf{X}^-) - (\mathbf{u}^+ - \mathbf{u}^-) \right] \quad \text{on } \partial\Omega^-$$

## Observations:

- Easy to implement
- Tricky to choose the penalty parameter  $\longrightarrow$  Let's look at a **practical alternative!**



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

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

# EPFL Implementing periodic boundary conditions

Starting point of FEM = equilibrium relations:

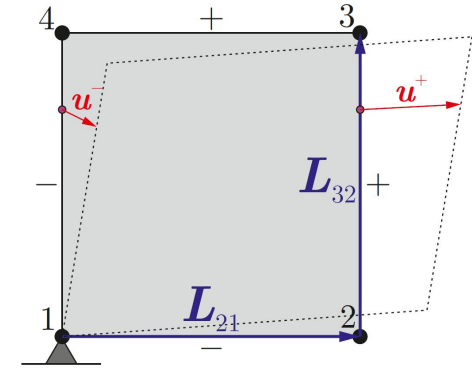
$$f(U) = F_{\text{int}}(U) - F_{\text{ext}} = 0$$

plus BCs in terms of some (linear) constraints on the nodal displacements:

$$f_c(U) = \sum_{a=1}^n \sum_{i=1}^d \alpha_i^a u_i^a - \delta = 0 \quad \text{e.g.} \quad f_c(U) = u_i^a - \delta = 0,$$

Periodic BCs:

$$f_c(U) = u^+ - u^- - (F^* - I)(X^+ - X^-) = 0$$



# Implementing periodic boundary conditions

Starting point of FEM = equilibrium relations:

$$\mathbf{f}(\mathbf{U}) = \mathbf{F}_{\text{int}}(\mathbf{U}) - \mathbf{F}_{\text{ext}} = \mathbf{0}$$

Periodic BCs:

$$\mathbf{f}_c(\mathbf{U}) = \mathbf{u}^+ - \mathbf{u}^- - (\mathbf{F}^* - \mathbf{I})(\mathbf{X}^+ - \mathbf{X}^-) = \mathbf{0}$$

Fix one corner to avoid rigid body motion:

$$\varphi^1 = \mathbf{X}_1 \quad \text{or} \quad \mathbf{u}^1 = \mathbf{0}$$

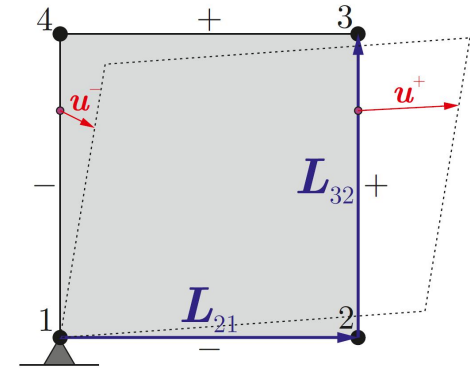
$$\text{so that } \mathbf{u}^2 = \mathbf{u}^1 + (\mathbf{F}^* - \mathbf{I})(\mathbf{X}^2 - \mathbf{X}^1) = (\mathbf{F}^* - \mathbf{I})\mathbf{L}_{21},$$

$$\mathbf{u}^4 = \mathbf{u}^1 + (\mathbf{F}^* - \mathbf{I})(\mathbf{X}^4 - \mathbf{X}^1) = (\mathbf{F}^* - \mathbf{I})\mathbf{L}_{41},$$

$$\mathbf{u}^3 = \mathbf{u}^1 + (\mathbf{F}^* - \mathbf{I})(\mathbf{X}^3 - \mathbf{X}^1) = (\mathbf{F}^* - \mathbf{I})(\mathbf{L}_{21} + \mathbf{L}_{41}) = \mathbf{u}^2 + \mathbf{u}^4.$$

$$\text{Left/right boundary: } \mathbf{u}^+ = \mathbf{u}^- + (\mathbf{F}^* - \mathbf{I})(\mathbf{X}^+ - \mathbf{X}^-) = \mathbf{u}^- + (\mathbf{F}^* - \mathbf{I})\mathbf{L}_{21} = \mathbf{u}^- + \mathbf{u}^2$$

$$\text{Top/bottom boundary: } \mathbf{u}^+ = \mathbf{u}^- + (\mathbf{F}^* - \mathbf{I})(\mathbf{X}^+ - \mathbf{X}^-) = \mathbf{u}^- + (\mathbf{F}^* - \mathbf{I})\mathbf{L}_{41} = \mathbf{u}^- + \mathbf{u}^4$$



$$\mathbf{L}_{21} = \mathbf{X}_2 - \mathbf{X}_1 = \mathbf{X}_3 - \mathbf{X}_4$$

$$\mathbf{L}_{41} = \mathbf{X}_4 - \mathbf{X}_1 = \mathbf{X}_3 - \mathbf{X}_2$$

# EPFL Implementing periodic boundary conditions

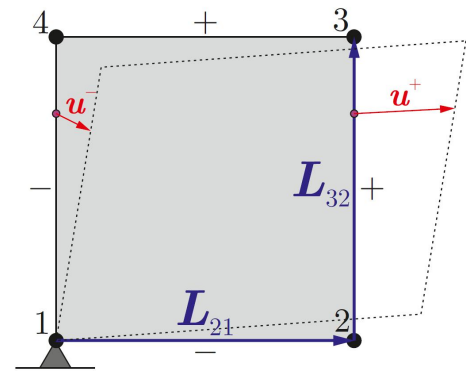
Altogether, periodic BCs imply:

$$f_1(U) = u^1 = 0,$$

$$f_3(U) = u^3 - u^2 - u^4 = 0,$$

$$f_+(U) = u^+ - u^- - u^2 = 0 \quad \text{for each left/right pair}$$

$$f_+(U) = u^+ - u^- - u^4 = 0 \quad \text{for each top/bottom pair}$$



A simple way of implementing constraints in a linear(ized) system, e.g.:

$$\begin{pmatrix} K_{11} & K_{12} & \dots & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \mathbf{0} & \mathbf{0} & \mathbf{1} & \mathbf{0} & \mathbf{0} \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & K_{55} \end{pmatrix} \begin{pmatrix} u^1 \\ u^2 \\ \mathbf{u^3} \\ u^4 \\ u^5 \end{pmatrix} = \begin{pmatrix} F_{\text{ext}}^1 \\ F_{\text{ext}}^2 \\ \hat{u}^3 \\ F_{\text{ext}}^4 \\ F_{\text{ext}}^5 \end{pmatrix}$$

# Implementing periodic boundary conditions

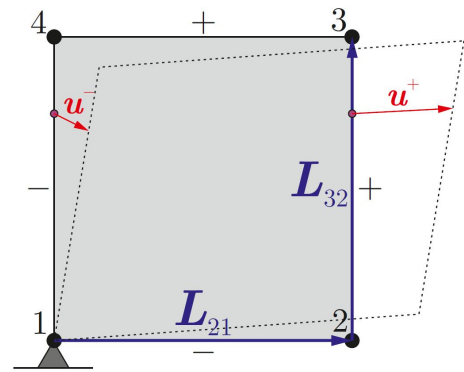
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$$L_{21} = X_2 - X_1 = X_3 - X_4$$

$$L_{41} = X_4 - X_1 = X_3 - X_2$$

Here:

$$\begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \dots \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \dots \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \dots \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \dots \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \dots \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \dots \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix} \begin{pmatrix} u^1 \\ u^2 \\ u^3 \\ u^4 \\ \vdots \\ u^+ \\ u^- \\ \vdots \end{pmatrix} = \begin{pmatrix} F_{\text{ext}}^1 \\ F_{\text{ext}}^2 \\ F_{\text{ext}}^3 \\ F_{\text{ext}}^4 \\ \vdots \\ F_{\text{ext}}^+ \\ F_{\text{ext}}^- \\ \vdots \end{pmatrix}$$

# Implementing periodic boundary conditions

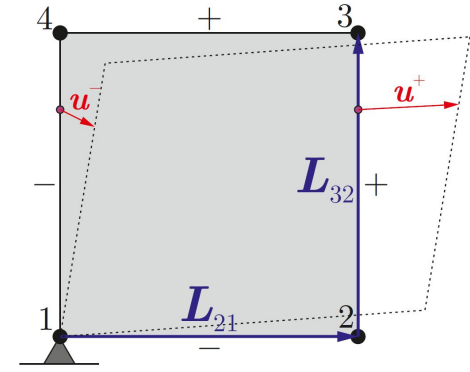
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Here:

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & \dots \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \dots \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \dots \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \dots \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \dots \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \dots \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix} \begin{pmatrix} u^1 \\ u^2 \\ u^3 \\ u^4 \\ \vdots \\ u^+ \\ u^- \\ \vdots \end{pmatrix} = \begin{pmatrix} 0 \\ F_{\text{ext}}^2 \\ F_{\text{ext}}^3 \\ F_{\text{ext}}^4 \\ \vdots \\ F_{\text{ext}}^+ \\ F_{\text{ext}}^- \\ \vdots \end{pmatrix}$$

# Implementing periodic boundary conditions

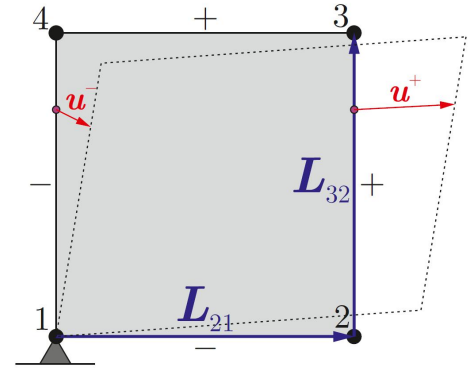
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Here:

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & \dots \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \dots \\ 0 & -1 & 1 & -1 & 0 & 0 & 0 & \dots \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \dots \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \dots \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \dots \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix} \begin{pmatrix} u^1 \\ u^2 \\ u^3 \\ u^4 \\ \vdots \\ u^+ \\ u^- \\ \vdots \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ F_{\text{ext}}^4 \\ \vdots \\ F_{\text{ext}}^+ \\ F_{\text{ext}}^- \\ \vdots \end{pmatrix}$$

# Implementing periodic boundary conditions

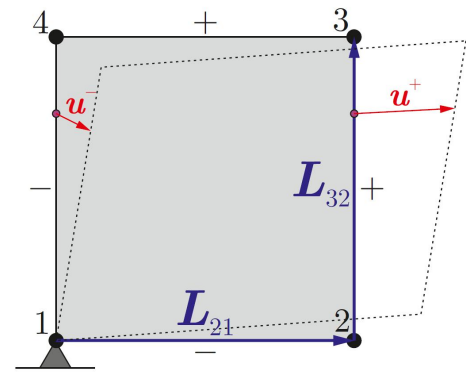
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# Implementing periodic boundary conditions

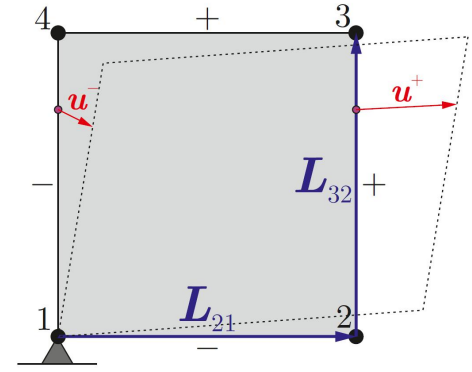
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Here:

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Need to replace this row by the sum of the original two +/- rows!



# Alternative implementation

formulate the full dof's (**master nodes**) in terms of a reduced set (**slave nodes**):

$$U = TU_{\text{red}} + c$$

FE problem:

$$I[U] = I[TU_{\text{red}} + c] \rightarrow \min_{U_{\text{red}}}$$

For the example on the right:

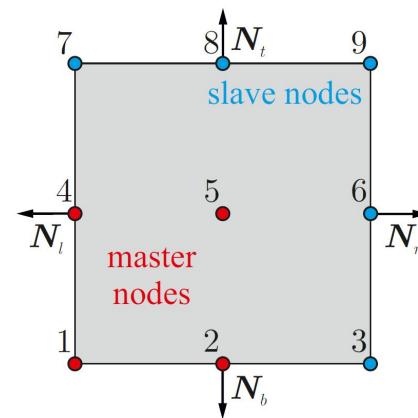
$$\underbrace{\begin{pmatrix} u^1 \\ u^2 \\ u^3 \\ u^4 \\ u^5 \\ u^6 \\ u^7 \\ u^8 \\ u^9 \end{pmatrix}}_{=U} = \underbrace{\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}}_{=T} \underbrace{\begin{pmatrix} u^1 \\ u^2 \\ u^4 \\ u^5 \end{pmatrix}}_{=U_{\text{red}}} + \underbrace{\begin{pmatrix} 0 \\ 0 \\ c^3 \\ 0 \\ 0 \\ c^6 \\ c^7 \\ c^8 \\ c^9 \end{pmatrix}}_{=c}$$



Resulting linear(ized) system:

$$F_{\text{red}} = T^T F_{\text{int}} \in \mathbb{R}^{dm}$$

$$T^T K T U_{\text{red}} = F_{\text{red,ext}}$$



# Enforcing average stress

Variational problem with constant surface tractions:

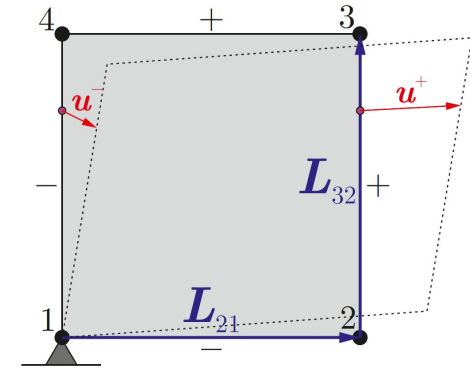
$$\begin{aligned}
 I[\varphi] &= \int_{\Omega} W(\mathbf{F}) dV - \int_{\partial\Omega} \hat{\mathbf{T}} \cdot \varphi dS \\
 &= \int_{\Omega} W(\mathbf{F}) dV - \int_{\partial\Omega} \mathbf{P}^* \mathbf{N} \cdot \varphi dS \\
 &= \int_{\Omega} W(\mathbf{F}) dV - \mathbf{P}^* \cdot \int_{\partial\Omega} \varphi \otimes \mathbf{N} dS
 \end{aligned}$$

After some math...

$$\begin{aligned}
 I[\varphi] &= \int_{\Omega} W(\mathbf{F}) dV - \mathbf{u}^4 \cdot \mathbf{P}^* \int_{\partial\Omega_t} \mathbf{N}_t dS - \mathbf{u}^2 \cdot \mathbf{P}^* \int_{\partial\Omega_r} \mathbf{N}_r dS \\
 \hat{\mathbf{F}}_4 &= \mathbf{P}^* \int_{\partial\Omega_t} \mathbf{N}_t dS \quad \text{and} \quad \hat{\mathbf{F}}_2 = \mathbf{P}^* \int_{\partial\Omega_r} \mathbf{N}_r dS
 \end{aligned}$$

If the average  $\mathbf{F}^*$  is known, impose  $\mathbf{u}^2$  and  $\mathbf{u}^4$ .

If the average  $\mathbf{P}^*$  is known, impose  $\mathbf{F}^2$  and  $\mathbf{F}^4$ .



recall:

$$\begin{aligned}
 \mathbf{f}_1(\mathbf{U}) &= \mathbf{u}^1 = \mathbf{0}, \\
 \mathbf{f}_3(\mathbf{U}) &= \mathbf{u}^3 - \mathbf{u}^2 - \mathbf{u}^4 = \mathbf{0}, \\
 \mathbf{f}_+( \mathbf{U}) &= \mathbf{u}^+ - \mathbf{u}^- - \mathbf{u}^2 = \mathbf{0} \\
 \mathbf{f}_+(\mathbf{U}) &= \mathbf{u}^+ - \mathbf{u}^- - \mathbf{u}^4 = \mathbf{0}
 \end{aligned}$$

and

$$\begin{aligned}
 \mathbf{u}^2 &= (\mathbf{F}^* - \mathbf{I}) \mathbf{L}_{21} \\
 \mathbf{u}^4 &= (\mathbf{F}^* - \mathbf{I}) \mathbf{L}_{41}
 \end{aligned}$$

# EPFL Enforcing mixed stress/strain - An example

Consider **uniaxial extension** (with free lateral boundaries):

$$\mathbf{F}^* = \begin{pmatrix} \lambda & F_{12} \\ F_{21} & F_{22} \end{pmatrix}, \quad \mathbf{P}^* = \begin{pmatrix} P_{11} & 0 \\ 0 & 0 \end{pmatrix}$$

Resulting forces:

$$\hat{\mathbf{F}}_2 = \mathbf{P}^* \mathbf{N}_r L_{r/l} = L_{r/l} \begin{pmatrix} P_{11}^* \\ P_{21}^* \end{pmatrix}, \quad \hat{\mathbf{F}}_4 = \mathbf{P}^* \mathbf{N}_t L_{t/b} = L_{t/b} \begin{pmatrix} P_{12}^* \\ P_{22}^* \end{pmatrix}$$

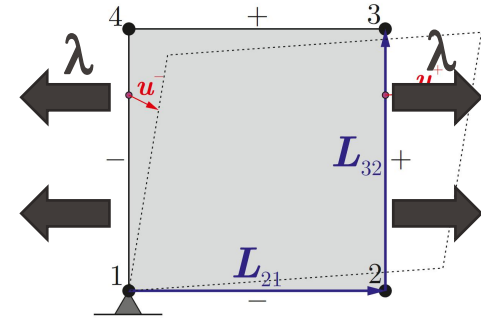
Resulting displacements:

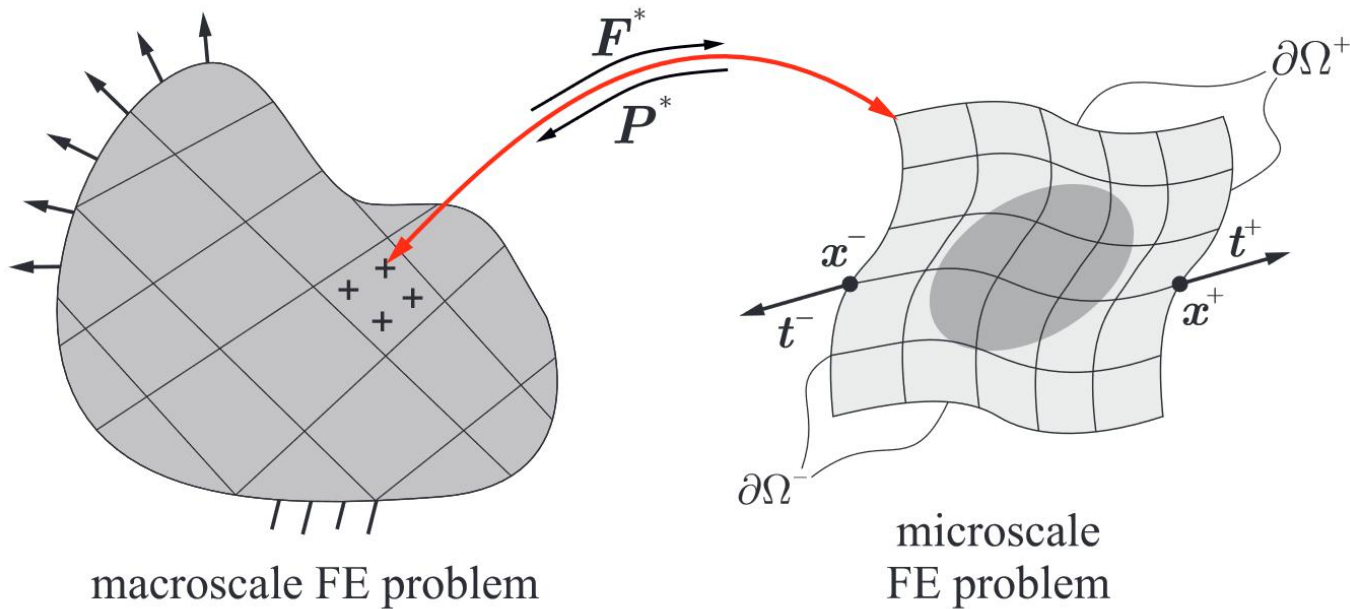
$$\mathbf{u}^2 = (\mathbf{F}^* - \mathbf{I}) \mathbf{N}_r L_{t/b} = \begin{pmatrix} F_{11}^* - 1 \\ F_{21}^* \end{pmatrix} L_{t/b}, \quad \mathbf{u}^4 = (\mathbf{F}^* - \mathbf{I}) \mathbf{N}_t L_{r/l} = \begin{pmatrix} F_{12}^* \\ F_{22}^* - 1 \end{pmatrix} L_{r/l}$$

In this example:

$$u_1^2 = (\lambda - 1)L_{r/l}, \quad F_2^2 = 0 \quad \text{and} \quad \hat{\mathbf{F}}_4 = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

Extensions to **3D** and to **linearized kinematics** are straight-forward.





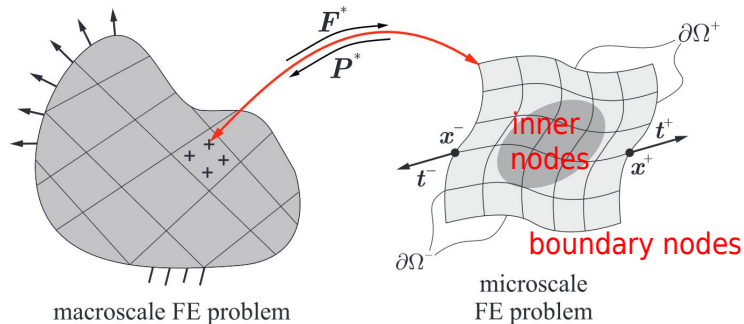
We learned how to obtain the effective stress, but that is not enough for Newton schemes ...

# Extracting the consistent tangent

Split into **i**nner and **b**oundary nodes:

$$\mathbf{U} = \begin{pmatrix} \mathbf{U}_i \\ \mathbf{U}_b \end{pmatrix}, \quad \mathbf{F} = \begin{pmatrix} \mathbf{F}_i \\ \mathbf{F}_b \end{pmatrix}$$

$$\Rightarrow \quad \mathbf{T} = \frac{\partial \mathbf{F}_{\text{int}}}{\partial \mathbf{U}^h} = \begin{pmatrix} \mathbf{K}_{ii} & \mathbf{K}_{ib} \\ \mathbf{K}_{bi} & \mathbf{K}_{bb} \end{pmatrix}$$



Equilibrium + BCs:

$$\begin{cases} \mathbf{F}_i(\mathbf{U}^h) = \mathbf{0} \\ \mathbf{F}_b(\mathbf{U}^h) - \mathbf{\Xi} = \mathbf{0} \\ \mathbf{U}_b - \mathbf{D}\mathbf{E}^* = \mathbf{0} \end{cases}$$

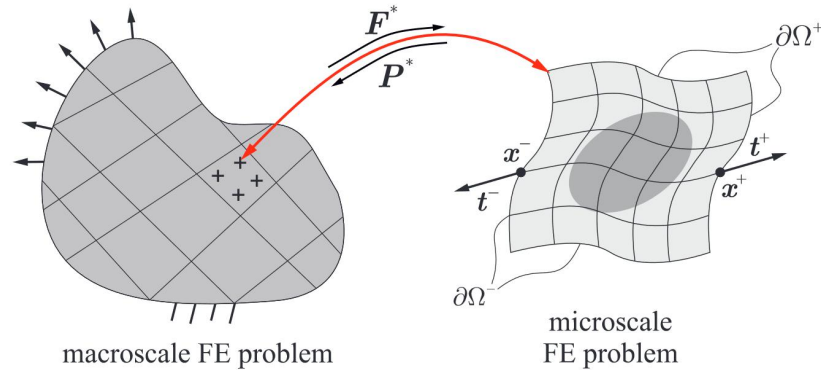
Taylor expansion about equilibrium:

$$\begin{cases} \mathbf{F}_i(\mathbf{U}_0^h) + \mathbf{K}_{ii}(\mathbf{U}_0^h)\Delta\mathbf{U}_i + \mathbf{K}_{ib}(\mathbf{U}_0^h)\Delta\mathbf{U}_b = \mathbf{0} \\ \mathbf{F}_b(\mathbf{U}_0^h) - \mathbf{\Xi} + \mathbf{K}_{bi}(\mathbf{U}_0^h)\Delta\mathbf{U}_i + \mathbf{K}_{bb}(\mathbf{U}_0^h)\Delta\mathbf{U}_b - \Delta\mathbf{\Xi} = \mathbf{0} \\ \mathbf{U}_{b,0} - \mathbf{D}\mathbf{E}^* + \Delta\mathbf{U}_b - \mathbf{D}\Delta\mathbf{E}^* = \mathbf{0} \end{cases}$$

Resulting consistent tangent:

$$\mathbb{C}^* = \frac{\partial \mathbf{P}^*}{\partial \mathbf{E}^*} = \frac{1}{V} \mathbf{D}^T \left[ \mathbf{K}_{bb}(\mathbf{U}_0^h) - \mathbf{K}_{bi}(\mathbf{U}_0^h) \mathbf{K}_{ii}^{-1}(\mathbf{U}_0^h) \mathbf{K}_{ib}(\mathbf{U}_0^h) \right] \mathbf{D}$$

Computational homogenization can be impractical (inefficient) for several problems



Can we approximate the stiffness of specific systems (e.g. matrix with inclusions) analytically?

**That's what I prepared for you today.**

**What would you like to discuss?**

# Reading for next class:

Multiscale Modeling, D.M. Kochmann

Chapter 9

# Reading for next class:

**Multiscale Modeling, D.M. Kochmann**

**Chapter 9**

Optionally:

**A Short Introduction to Basic Aspects of  
Continuum Micromechanics, H Bohm**

**Chapters 1,2,3**