Computational Homogenization and Multiscale Modeling

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Lecture 2: Contents

- Nested macro-micro computations (basis for FE^2)
  - Variationally consistent homogenization
  - Generalized macrohomogeneity (Hill-Mandel) condition
- Prolongation conditions - nonlinear SVE-problems
  - Boundary conditions versus macroscale strain or stress control – Overview (table)
  - Displacement Boundary Condition (nonlinear DBC-problem)
  - Traction Displacement Boundary Condition (nonlinear TBC-problem)
  - Weakly Periodic Boundary Condition (nonlinear PBC-problem) – generalization of classical strong displacement periodicity

Model-based homogenization

- Two separate scales *a priori* within each SVE. Local $\boldsymbol{u}(\bar{\boldsymbol{X}};\boldsymbol{X}) \in \mathbb{U}$, global $\bar{\boldsymbol{u}}(\bar{\boldsymbol{X}}) \in \bar{\mathbb{U}}$

$$\boldsymbol{u}(\bar{\boldsymbol{X}};\boldsymbol{X}) = \boldsymbol{u}^{\mathrm{M}}(\bar{\boldsymbol{X}};\boldsymbol{X}) + \boldsymbol{u}^{\mathrm{s}}(\bar{\boldsymbol{X}};\boldsymbol{X})$$

- Macroscale prolongation to $\Gamma_\square$. For given $\bar{\boldsymbol{X}} \in \Omega$:

$$\boldsymbol{u}^{\mathrm{M}}(\boldsymbol{X}) = \boldsymbol{u}^{\mathrm{M}}(\bar{\boldsymbol{H}}^{(0)} \stackrel{\mathrm{def}}{=} \bar{\boldsymbol{u}}, \bar{\boldsymbol{H}}^{(1)} \stackrel{\mathrm{def}}{=} \bar{\boldsymbol{H}}, \bar{\boldsymbol{H}}^{(2)}, ..., \bar{\boldsymbol{H}}^{(K)}; \boldsymbol{X})$$

with "higher order" gradients (K = order of homogenization):

$$\bar{\boldsymbol{H}}^{(k)} \stackrel{\mathrm{def}}{=} \bar{\boldsymbol{u}} \otimes \underbrace{\bar{\boldsymbol{\nabla}} \otimes \bar{\boldsymbol{\nabla}} \otimes ... \otimes \bar{\boldsymbol{\nabla}}}_{k}$$

  – 1st order (conventional): $\boldsymbol{u}^{\mathrm{M}}(\boldsymbol{X}) = \bar{\boldsymbol{u}} + \bar{\boldsymbol{H}} \cdot [\boldsymbol{X} - \bar{\boldsymbol{X}}]$

  – 2nd order: $\boldsymbol{u}^{\mathrm{M}}(\boldsymbol{X}) = \bar{\boldsymbol{u}} + \bar{\boldsymbol{H}} \cdot [\boldsymbol{X} - \bar{\boldsymbol{X}}] + \frac{1}{2}[\boldsymbol{X} - \bar{\boldsymbol{X}}] \cdot \bar{\boldsymbol{H}}^{(2)} \cdot [\boldsymbol{X} - \bar{\boldsymbol{X}}]$

    Note: $\bar{\boldsymbol{H}}^{(2)}$ 3rd order tensor (such as curvature), e.g. KUZNETSOVA ET AL. 2002

Model-based homogenization

- Prolongation condition defines (implicitly) how the fluctuation depends on the macro-solution: $\boldsymbol{u}^{\mathrm{s}}\{\boldsymbol{u}^{\mathrm{M}}\}, \forall \boldsymbol{u}^{\mathrm{M}} \in \mathbb{U}^{\mathrm{M}}$

$$\Rightarrow \quad \bar{\boldsymbol{u}}(\bar{\boldsymbol{X}}) \quad \overset{\text{SVE}}{\rightarrow} \quad \boldsymbol{u}^{\mathrm{M}}(\bar{\boldsymbol{X}}, \boldsymbol{X}) \quad \rightarrow \quad \boldsymbol{u}^{\mathrm{s}}\{\boldsymbol{u}^{\mathrm{M}}(\bar{\boldsymbol{X}}, \boldsymbol{X})\} \quad \rightarrow \quad \boldsymbol{u}\{\bar{\boldsymbol{u}}(\bar{\boldsymbol{X}}), \boldsymbol{X}\}$$

- Homogenized problem:

$$y(\bar{\boldsymbol{X}}) \mapsto \langle y \rangle_{\square}(\bar{\boldsymbol{X}}), \quad \bar{\boldsymbol{X}} \in \Omega$$

Note: Global boundary data assumed to vary "slowly" $\Rightarrow y(\bar{\boldsymbol{X}}) \approx \bar{y}(\bar{\boldsymbol{X}})$ on Γ

- Variational problem: Find $\boldsymbol{u}^{\mathrm{M}} \in \mathbb{U}^{\mathrm{M}}$ s. t.

$$R(\boldsymbol{u}\{\boldsymbol{u}^{\mathrm{M}}\}; \delta\boldsymbol{u}) \overset{\text{def}}{=} l(\delta\boldsymbol{u}) - a(\boldsymbol{u}\{\boldsymbol{u}^{\mathrm{M}}\}; \delta\boldsymbol{u}) = 0 \quad \forall \delta\boldsymbol{u}^{\mathrm{M}} \in \mathbb{U}^{\mathrm{M},0}.$$

where

$$a(\boldsymbol{u}; \delta\boldsymbol{u}) \overset{\text{def}}{=} \int_{\Omega} \langle \boldsymbol{P} : \delta\boldsymbol{H} \rangle_{\square} \, \mathrm{d}V, \quad l(\delta\boldsymbol{u}) \overset{\text{def}}{=} \int_{\Omega} \langle \boldsymbol{f} \cdot \delta\boldsymbol{u} \rangle_{\square} \, \mathrm{d}V + \int_{\Gamma_{\mathrm{N}}} \bar{\boldsymbol{t}}_{\mathrm{p}} \cdot \delta\bar{\boldsymbol{u}} \, \mathrm{d}S$$

VMS vs. Homogenization

- Single-scale problem: Find $\boldsymbol{u} \in \mathbb{U}$ such that

$$R(\boldsymbol{u};\delta\boldsymbol{u}) \stackrel{\text{def}}{=} l(\delta\boldsymbol{u}) - a(\boldsymbol{u};\delta\boldsymbol{u}) = 0 \quad \forall\delta\boldsymbol{u} \in \mathbb{U}^0$$

- Variational Multiscale Method (HUGHES 1995) $(\boldsymbol{u}^{\mathrm{M}}, \boldsymbol{u}^{\mathrm{s}}) \in \mathbb{U}^{\mathrm{M}} \times \mathbb{U}^{\mathrm{s}}$

$$\begin{aligned} R(\boldsymbol{u}^{\mathrm{M}} + \boldsymbol{u}^{\mathrm{s}};\delta\boldsymbol{u}^{\mathrm{M}}) &= 0 \quad \forall\delta\boldsymbol{u}^{\mathrm{M}} \in \mathbb{U}^{\mathrm{M},0} \subset \mathbb{U}^0 \\ R(\boldsymbol{u}^{\mathrm{M}} + \boldsymbol{u}^{\mathrm{s}};\delta\boldsymbol{u}^{\mathrm{s}}) &= 0 \quad \forall\delta\boldsymbol{u}^{\mathrm{s}} \quad \rightarrow \boldsymbol{u}^{\mathrm{s}}\{\boldsymbol{u}^{\mathrm{M}}\} \end{aligned}$$

- Localized problem for $\boldsymbol{u}^{\mathrm{s}} \Rightarrow$ We seek solutions $\tilde{\boldsymbol{u}}$

$$\rightsquigarrow \tilde{\boldsymbol{u}} \in \tilde{\mathbb{U}} \stackrel{\text{def}}{=} \{\mathbb{U} \ni \boldsymbol{u} = \boldsymbol{u}^{\mathrm{M}} + \boldsymbol{u}^{\mathrm{s}}\{\boldsymbol{u}^{\mathrm{M}}\},\ \boldsymbol{u}^{\mathrm{M}} \in \mathbb{U}^{\mathrm{M}}\}$$

- Issue: Due to approximations/restrictions

$$R(\tilde{\boldsymbol{u}};\delta\boldsymbol{u}) \neq 0$$

In general not even for $\delta\boldsymbol{u} = \delta\boldsymbol{u}^{\mathrm{M}} + \boldsymbol{u}^{\mathrm{s}}\{\delta\boldsymbol{u}^{\mathrm{M}}\}$

Two possible choices for weighted residuals

I Classical assumption (in VMS *and* Homogenization)

$$R(\boldsymbol{u}^{\mathrm{M}} + \boldsymbol{u}^{\mathrm{s}}; \delta\boldsymbol{u}^{\mathrm{M}}) = 0 \quad \forall \delta\boldsymbol{u}^{\mathrm{M}} \in \mathbb{U}^{\mathrm{M},0}$$

- Straightforward choice (presuming globally exact $\boldsymbol{u}^{\mathrm{s}}\{\bullet\}$, i.e. $\mathbb{U}^{\mathrm{s}} = \mathbb{U} \ominus \mathbb{U}^{\mathrm{M}}$)
- $\delta\boldsymbol{u}^{\mathrm{M}}$ "homogenizer" $\leadsto$ Balance of homogenized fluxes/stresses

II Generalized (non-linear) Galerkin-type

$$R(\underbrace{\boldsymbol{u}^{\mathrm{M}} + \boldsymbol{u}^{\mathrm{s}}}_{\tilde{\boldsymbol{u}}}; \underbrace{\delta\boldsymbol{u}^{\mathrm{M}} + (\boldsymbol{u}^{\mathrm{s}})' \{\boldsymbol{u}^{\mathrm{M}}; \delta\boldsymbol{u}^{\mathrm{M}}\}}_{\delta\tilde{\boldsymbol{u}}}) = 0 \quad \forall \delta\boldsymbol{u}^{\mathrm{M}} \in \mathbb{U}^{\mathrm{M},0}$$

Test space: tangent space to approximation space

$$\delta\tilde{\boldsymbol{u}} \in \tilde{\mathbb{U}}^0(\boldsymbol{u}^{\mathrm{M}}) \stackrel{\mathrm{def}}{=} \{\mathbb{U} \ni \delta\boldsymbol{u} = \delta\boldsymbol{u}^{\mathrm{M}} + \underbrace{(\boldsymbol{u}^{\mathrm{s}})' \{\boldsymbol{u}^{\mathrm{M}}; \delta\boldsymbol{u}^{\mathrm{M}}\}}_{\text{sensitivity}},\ \delta\boldsymbol{u}^{\mathrm{M}} \in \mathbb{U}^{\mathrm{M}}\}$$

- Variation of energy (if $\exists$)
- Preserves symmetry for $R'(\boldsymbol{u}; \delta\boldsymbol{u}, \delta\boldsymbol{u})$

Variationally Consistent Macrohomogeneity Condition (VCMC)

- By construction of local problems, i.e. by defining $\boldsymbol{u}^{\mathrm{s}}\{\bullet\}$

$$\underbrace{R(\boldsymbol{u}^{\mathrm{M}} + \boldsymbol{u}^{\mathrm{s}}; \delta\boldsymbol{u}^{\mathrm{M}})}_{\mathrm{I}} - \underbrace{R(\boldsymbol{u}^{\mathrm{M}} + \boldsymbol{u}^{\mathrm{s}}; \delta\boldsymbol{u}^{\mathrm{M}} + (\boldsymbol{u}^{\mathrm{s}})'\{\boldsymbol{u}^{\mathrm{M}}; \delta\boldsymbol{u}^{\mathrm{M}}\})}_{\mathrm{II}}$$
$$= \underbrace{R(\boldsymbol{u}^{\mathrm{M}} + \boldsymbol{u}^{\mathrm{s}}; (\boldsymbol{u}^{\mathrm{s}})'\{\boldsymbol{u}^{\mathrm{M}}; \delta\boldsymbol{u}^{\mathrm{M}}\})}_{\text{Fluctuation residual}} = 0 \quad \forall \delta\boldsymbol{u}^{\mathrm{M}} \in \mathbb{U}^{\mathrm{M},0}$$

- Solve I and get II "for free"
  - Energy equivalence (Hill-Mandel condition)
  - Symmetric VMS-problem

Macrohomogeneity condition

- "Local" version of VCMC in terms of SVE-residual

$$R(\boldsymbol{u};\delta\boldsymbol{u}^{\mathrm{s}}) \stackrel{\mathrm{def}}{=} \int_{\Omega} R_{\Box}(\boldsymbol{u};\delta\boldsymbol{u}^{\mathrm{s}})\,\mathrm{d}V$$

$$R_{\Box}\left(\boldsymbol{u};\delta\boldsymbol{u}^{\mathrm{s}}\right) \stackrel{\mathrm{def}}{=} \langle \boldsymbol{f}\cdot\delta\boldsymbol{u}^{\mathrm{s}}\rangle_{\Box} - \langle \boldsymbol{P}:\delta\boldsymbol{H}^{\mathrm{s}}\rangle_{\Box} = \frac{1}{|\Omega_{\Box}|}\int_{\Omega_{\Box}} \left[\boldsymbol{f}\cdot\delta\boldsymbol{u}^{\mathrm{s}} - \boldsymbol{P}:\delta\boldsymbol{H}^{\mathrm{s}}\right]\mathrm{d}V$$

$$= -\frac{1}{|\Omega_{\Box}|}\int_{\Gamma_{\Box}} \boldsymbol{t}\cdot\delta\boldsymbol{u}^{\mathrm{s}}\,\mathrm{d}S$$

- Sufficent condition for VCMC

$$R_{\Box}\left(\boldsymbol{u}\{u^{\mathrm{M}}\};(\boldsymbol{u}^{\mathrm{s}})'\{\boldsymbol{u}^{\mathrm{M}};\delta\boldsymbol{u}^{\mathrm{M}}\}\right) = 0, \quad \forall\delta\boldsymbol{u}^{\mathrm{M}} \in \mathbb{U}^{\mathrm{M},0}.$$

- **Note**: No need to solve for sensitivity fields

VCMC - 1st order homogenization

- VCMC $\equiv$ HMC (classical Hill-Mandel macrohomogeneity condition)

$$\boldsymbol{u}^{\mathrm{M}}(\boldsymbol{X}) = \bar{\boldsymbol{u}} + \bar{\boldsymbol{H}} \cdot [\boldsymbol{X} - \bar{\boldsymbol{X}}]$$

$$\Rightarrow \quad \delta\boldsymbol{u}^{\mathrm{M}}(\boldsymbol{X}) = \delta\bar{\boldsymbol{u}} + \delta\bar{\boldsymbol{H}} \cdot [\boldsymbol{X} - \bar{\boldsymbol{X}}], \quad \delta\boldsymbol{H}^{\mathrm{M}}(\boldsymbol{X}) = \delta\bar{\boldsymbol{H}}$$

$$\Rightarrow \quad \langle \boldsymbol{P} : \delta\boldsymbol{H} \rangle_{\square} = \langle \boldsymbol{P} \rangle_{\square} : \langle \delta\boldsymbol{H} \rangle_{\square} = \bar{\boldsymbol{P}} : \delta\bar{\boldsymbol{H}}, \quad \forall \delta\boldsymbol{u} \in \mathbb{U}_{\square}$$

- **Note**: HMC valid only if the condition $\langle \delta\boldsymbol{H} \rangle_{\square} = \delta\bar{\boldsymbol{H}}$ is satisfied:
  - automatically by the choice of test functions
  - imposed as part of the SVE-problem
- **Note**: Higher order homogenization "stresses" and "strains" on macro-level will appear in case of higher order homogenization, e.g. GEERS ET AL.

Explicit homogenization results

- Homogenized variational forms

$$a(\boldsymbol{u}\{\boldsymbol{u}^{\mathrm{M}}\};\delta\boldsymbol{u}^{\mathrm{M}}) = \int_{\Omega}\langle\boldsymbol{P}:\delta\boldsymbol{H}^{\mathrm{M}}\rangle_{\square}\,\mathrm{d}\bar{V},$$

$$l(\delta\boldsymbol{u}^{\mathrm{M}}) = \int_{\Omega}\langle\boldsymbol{f}\cdot\delta\boldsymbol{u}^{\mathrm{M}}\rangle_{\square}\,\mathrm{d}\bar{V} + \int_{\Gamma_{\mathrm{N}}}\bar{\boldsymbol{t}}_{\mathrm{p}}\cdot\delta\bar{\boldsymbol{u}}\,\mathrm{d}\bar{S}$$

SVE-forms: $\langle\boldsymbol{P}:\delta\boldsymbol{H}\rangle_{\square} = \bar{\boldsymbol{P}}\{\bar{\boldsymbol{H}}\}:\delta\bar{\boldsymbol{H}},\quad \langle\boldsymbol{f}\cdot\delta\boldsymbol{u}^{\mathrm{M}}\rangle_{\square} = \bar{\boldsymbol{f}}\cdot\delta\bar{\boldsymbol{u}} + \underbrace{\bar{\boldsymbol{f}}^{(2)}\cdot\delta\bar{\boldsymbol{H}}}_{\text{ignored}}$

- Macroscale problem: Find $\bar{\boldsymbol{u}}\in\bar{\mathbb{U}}$ s. t.

$$\bar{R}\{\bar{\boldsymbol{u}};\delta\bar{\boldsymbol{u}}\} \stackrel{\text{def}}{=} \bar{l}\{\delta\bar{\boldsymbol{u}}\} - \bar{a}\{\bar{\boldsymbol{u}};\delta\bar{\boldsymbol{u}}\} = 0 \quad \forall\delta\bar{\boldsymbol{u}}\in\bar{\mathbb{U}}^{0}.$$

$\bar{a}\{\bar{\boldsymbol{u}};\delta\bar{\boldsymbol{u}}\} \stackrel{\text{def}}{=} \int_{\Omega}\bar{\boldsymbol{P}}\{\bar{\boldsymbol{H}}\}:\delta\bar{\boldsymbol{H}}\,\mathrm{d}\bar{V},\quad \bar{l}\{\delta\bar{\boldsymbol{u}}\} \stackrel{\text{def}}{=} \int_{\Omega}\bar{\boldsymbol{f}}\cdot\delta\bar{\boldsymbol{u}}\,\mathrm{d}\bar{V} + \int_{\Gamma_{\mathrm{N}}}\bar{\boldsymbol{t}}_{\mathrm{p}}\cdot\delta\bar{\boldsymbol{u}}\,\mathrm{d}\bar{S}$

- **Note**: $\bar{a}$ may represent higher order continuum model

Nested FE^2-algorithm

- Solution via Newton iterations based on the tangent form

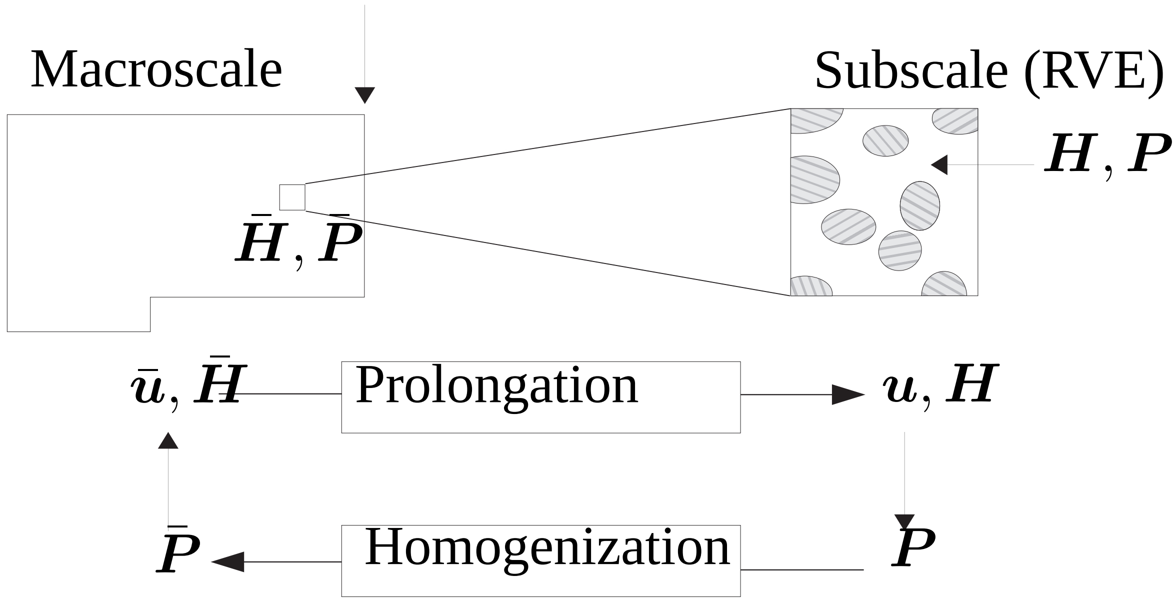
$$\bar{a}'\{\bar{\boldsymbol{u}};\delta\bar{\boldsymbol{u}},\Delta\bar{\boldsymbol{u}}\} \stackrel{\text{def}}{=} \int_\Omega a'_\Box(\boldsymbol{u}\{\boldsymbol{u}^{\mathrm{M}}\};\delta\boldsymbol{u}^{\mathrm{M}},\Delta\boldsymbol{u}^{\mathrm{M}}+(\boldsymbol{u}^{\mathrm{s}})'\{\boldsymbol{u}^{\mathrm{M}};\Delta\boldsymbol{u}^{\mathrm{M}}\})\,\mathrm{d}\,\bar{V}$$
$$= \int_\Omega \delta\bar{\boldsymbol{H}} : \bar{\mathsf{L}}_{\mathrm{AT}} : \Delta\bar{\boldsymbol{H}}\,\mathrm{d}\,\bar{V}$$

Macroscale Algorithmic Tangent (AT) stiffness $\bar{\mathsf{L}}_{\mathrm{AT}}$ defined from

$$\mathrm{d}\bar{\boldsymbol{P}}\{\bar{\boldsymbol{H}}\} = \bar{\mathsf{L}}_{\mathrm{AT}}\{\bar{\boldsymbol{H}}\} : \mathrm{d}\bar{\boldsymbol{H}}$$

- $\bar{\mathsf{L}}_{\mathrm{AT}}$ obtained from linearized SVE-problem (sensitivity problem)
- Sensitivity problem formulated for each choice of prolongation condition

Nested FE^2-algorithm



1. Assume (nonequilibrium) macroscale stress $\bar{\boldsymbol{P}}$, in the macroscale iteration, corresponding to given $\bar{\boldsymbol{u}}$ (and $\bar{\boldsymbol{H}}$).
2. **Prolongation-homogenization**: For given $\bar{\boldsymbol{H}} = \bar{\boldsymbol{H}}(\bar{\boldsymbol{X}}_i)$ in each macroscale (Gauss) quadrature point $\bar{\boldsymbol{X}}_i$, solve the nonlinear RVE-problem (with chosen prolongation conditions) for subscale $\boldsymbol{u}(\bar{\boldsymbol{X}}_i, \boldsymbol{X})$ and homogenized (macroscale) stress $\bar{\boldsymbol{P}}(\bar{\boldsymbol{X}}_i)$.
3. Check macroscale residual. If convergence, $|\bar{R}| < TOL$, then stop, else compute a new (updated) $\bar{\boldsymbol{u}}$ (while using $\bar{\mathsf{L}}_{\mathrm{AT}}$) and return to 1.

DBC – Macroscale strain control

- Appropriate subscale spaces

$$\begin{aligned}\mathbb{U}_{\square}^{\mathrm{D}} &= \{\boldsymbol{u} \in \mathbb{U}_{\square} |\ \exists \hat{\boldsymbol{H}} \in \mathbb{R}^{3\times 3} \text{ s.t. } \boldsymbol{u} = \hat{\boldsymbol{H}} \cdot [\boldsymbol{X} - \bar{\boldsymbol{X}}] \text{ on } \Gamma_{\square}\} \\ \mathbb{U}_{\square}^{\mathrm{D},0} &= \{\boldsymbol{u} \in \mathbb{U}_{\square} |\ \boldsymbol{u} = \boldsymbol{0} \text{ on } \Gamma_{\square}\}\end{aligned}$$

- SVE-problem: For given value of $\bar{\boldsymbol{H}} \in \mathbb{R}^{3\times 3}$, find $\boldsymbol{u}^{\mathrm{s}} \in \mathbb{U}_{\square}^{\mathrm{D},0}$ that solves

$$a_{\square}(\boldsymbol{u}^{\mathrm{M}}(\bar{\boldsymbol{H}}) + \boldsymbol{u}^{\mathrm{s}}; \delta \boldsymbol{u}^{\mathrm{s}}) = 0 \quad \forall \delta \boldsymbol{u}^{\mathrm{s}} \in \mathbb{U}_{\square}^{\mathrm{D},0}.$$

  with $\boldsymbol{u}^{\mathrm{M}}(\bar{\boldsymbol{H}}) = \bar{\boldsymbol{H}} \cdot \left[\boldsymbol{X} - \bar{\boldsymbol{X}}\right]$.
  Solved by Newton iterations in standard fashion

- Postprocessing: $\bar{\boldsymbol{P}} = \langle \boldsymbol{P} \rangle_{\square}$

DBC– Macroscale strain control: AT stiffness

- Macroscale Algorithmic Tangent (AT) stiffness tensor: Compute sensitivity in $\boldsymbol{u}^{\mathrm{s}}$ for change in $\bar{\boldsymbol{H}}$:

$$\mathrm{d}\bar{\boldsymbol{H}} \rightarrow \mathrm{d}\boldsymbol{u} = \mathrm{d}\boldsymbol{u}^{\mathrm{M}} + \mathrm{d}\boldsymbol{u}^{\mathrm{s}} = \mathrm{d}\boldsymbol{u}^{\mathrm{M}} + (\boldsymbol{u}^{\mathrm{s}})'\{\boldsymbol{u}^{\mathrm{M}}; \mathrm{d}\boldsymbol{u}^{\mathrm{M}}\}$$

- *Ansatz*: $\mathrm{d}\boldsymbol{u}^{\mathrm{s}} = \sum_{i,j} \hat{\boldsymbol{u}}^{\mathrm{s}(ij)}\, \mathrm{d}\bar{H}_{ij}$
- "Unit fluctuation fields" (sensitivity fields) $\hat{\boldsymbol{u}}^{\mathrm{s}(kl)}$ for $k, l = 1, 2, ..., NDIM$

$$(a_{\square})'(\bullet; \delta\boldsymbol{u}^{\mathrm{s}}, \hat{\boldsymbol{u}}^{\mathrm{s}(kl)}) = -(a_{\square})'(\bullet; \delta\boldsymbol{u}^{\mathrm{s}}, \hat{\boldsymbol{u}}^{\mathrm{M}(kl)}) \quad \forall \delta\boldsymbol{u}^{\mathrm{s}} \in \mathbb{U}_{\square}^{\mathrm{D,s}}$$

- Primal approach for computing AT-tensor

$$\bar{\mathsf{L}}_{\mathrm{AT}} = \langle \mathsf{L} \rangle_{\square} + \sum_{k,l=1}^{NDIM} \left\langle \mathsf{L} : \hat{\boldsymbol{H}}^{\mathrm{s}(kl)} \right\rangle_{\square} \otimes \boldsymbol{e}_k \otimes \boldsymbol{e}_l$$

- Dual approach for computing AT-tensor: Useful method in conjunction with goal-oriented error computation for subscale FE-discretization, LARSSON AND RUNESSON 2007, **"power of duality"**!

TBC – Macroscale strain control

- Appropriate subscale spaces

$$\begin{aligned} \mathbb{U}_{\square}^{\mathrm{N}} &= \{\boldsymbol{u} \in \mathbb{U}_{\square} \text{ s.t. } \boldsymbol{u}(\bar{\boldsymbol{X}}) = \boldsymbol{0}\} \\ \mathbb{U}_{\square}^{\mathrm{N,s}} &= \{\boldsymbol{u} \in \mathbb{U}_{\square} : \langle \boldsymbol{H} \rangle_{\square} = \boldsymbol{0}\} \end{aligned}$$

- SVE-problem: For given value of $\bar{\boldsymbol{H}} \in \mathbb{R}^{3\times 3}$, find $\boldsymbol{u} \in \mathbb{U}_{\square}^{\mathrm{N}}$ and $\bar{\boldsymbol{P}} \in \mathbb{R}^{3\times 3}$ that solve

$$\begin{aligned} a_{\square}(\boldsymbol{u};\delta\boldsymbol{u}) - c_{\square}^{(\mathrm{H})}(\delta\boldsymbol{u};\bar{\boldsymbol{P}}) &= 0 \quad \forall \delta\boldsymbol{u} \in \mathbb{U}_{\square}^{\mathrm{N}} \\ c_{\square}^{(\mathrm{H})}(\boldsymbol{u};\delta\bar{\boldsymbol{P}}) &= \delta\bar{\boldsymbol{P}} : \bar{\boldsymbol{H}} \quad \forall \delta\bar{\boldsymbol{P}} \in \mathbb{R}^{3\times 3} \end{aligned}$$

where

$$c_{\square}^{(\mathrm{H})}(\boldsymbol{u};\bar{\boldsymbol{P}}) \overset{\mathrm{def}}{=} \langle \boldsymbol{H} \rangle_{\square} : \bar{\boldsymbol{P}}$$

- **Note**: Term $c_{\square}^{(\mathrm{H})}(\delta\boldsymbol{u};\bar{\boldsymbol{P}})$ follows from model assumption

$$\boldsymbol{t} = \boldsymbol{P}\cdot\boldsymbol{N} = \bar{\boldsymbol{P}}\cdot\boldsymbol{N} \quad \text{in} \quad \Gamma_{\square}$$

- No postprocessing of $\bar{\boldsymbol{P}} = \langle \boldsymbol{P} \rangle_{\square}$, "built-in" property in variational format

TBC – Macroscale strain control: AT stiffness

- Macroscale Algorithmic Tangent (AT) stiffness tensor: Compute sensitivity in $\boldsymbol{u}$ and $\bar{\boldsymbol{P}}$ for change in $\bar{\boldsymbol{H}}$:

$$\mathrm{d}\bar{\boldsymbol{H}} \rightarrow \mathrm{d}\boldsymbol{u},\ \mathrm{d}\bar{\boldsymbol{P}}$$

- *Ansatz*: $\mathrm{d}\boldsymbol{u}^{\mathrm{s}} = \sum_{i,j} \hat{\boldsymbol{u}}^{\mathrm{s}(ij)}\, \mathrm{d}\bar{H}_{ij}$, $\mathrm{d}\bar{\boldsymbol{P}} = \sum_{i,j} \hat{\bar{\boldsymbol{P}}}^{(ij)}\, \mathrm{d}\bar{H}_{ij}$
- "Unit fluctuation fields" (sensitivity fields) $\hat{\boldsymbol{u}}^{\mathrm{s}(kl)}$ and $\hat{\bar{\boldsymbol{P}}}^{(ij)}$ for $k, l = 1, 2, ..., NDIM$

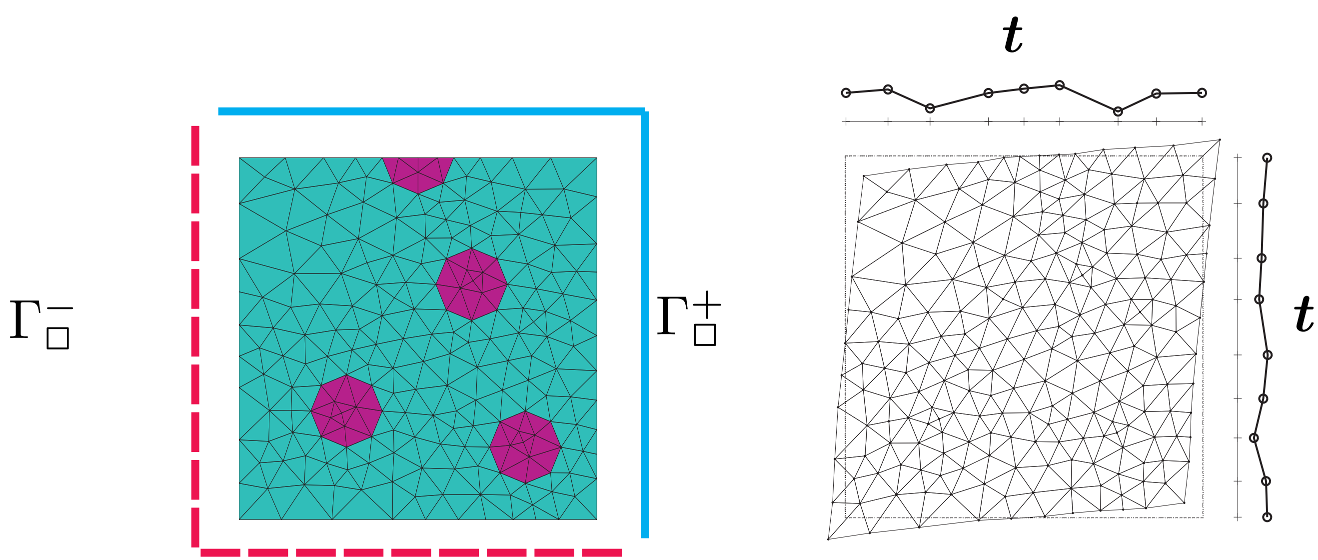
$$\begin{aligned} (a_\square)'(\bullet; \delta\boldsymbol{u}, \hat{\boldsymbol{u}}^{(kl)}) - c_\square^{(\mathrm{H})}(\delta\boldsymbol{u}, \hat{\bar{\boldsymbol{P}}}^{(kl)}) &= 0 \quad \forall \delta\boldsymbol{u} \in \mathbb{U}_\square^{\mathrm{N}} \\ c_\square^{(\mathrm{H})}(\hat{\boldsymbol{u}}^{(kl)}, \delta\bar{\boldsymbol{P}}) &= (\delta\bar{P})_{kl} \quad \forall \delta\bar{\boldsymbol{P}} \in \mathbb{R}^{3\times 3} \end{aligned}$$

- AT-tensor

$$\bar{\mathsf{L}}_{\mathrm{AT}} = \sum_{k,l=1}^{NDIM} \hat{\bar{\boldsymbol{P}}}^{(kl)} \otimes \boldsymbol{e}_k \otimes \boldsymbol{e}_l$$

- **Note**: MIEHE AND KOCH 2002 in the FE-discrete setting, LARSSON AND RUNESSON, 2007 in the continuous setting

WBC (weak periodicity) – Macroscale strain control



- Periodic boundary conditions using "mirroring" $(\boldsymbol{X}^- : \Gamma_\square^+ \rightarrow \Gamma_\square^-)$, $\Gamma_\square = \Gamma_\square^+ \bigcup \Gamma_\square^+$
- Periodic displacements and anti-periodic tractions

$$[\![\boldsymbol{u}]\!] \stackrel{\text{def}}{=} \boldsymbol{u}(\boldsymbol{X}) - \boldsymbol{u}(\boldsymbol{X}^-(\boldsymbol{X})) = \bar{\boldsymbol{H}} \cdot [\![\boldsymbol{X}]\!] \quad \text{on } \Gamma_\square^+$$

$$\boldsymbol{t} \stackrel{\text{def}}{=} \boldsymbol{t}(\boldsymbol{X}) = -\boldsymbol{t}(\boldsymbol{X}^-(\boldsymbol{X})) \quad \text{on } \Gamma_\square^+$$

WBC cont'd

- Appropriate subscale spaces

$$\begin{aligned} \mathbb{U}_\square &= \mathbb{U}_\square^{\mathrm{N}} = \{\boldsymbol{u} \in \mathbb{U}_\square \text{ s.t. } \boldsymbol{u}(\bar{\boldsymbol{X}}) = \mathbf{0}\} \\ \mathbb{T}_\square &= \{\boldsymbol{t} \text{ "suff. regular" }\} \quad \textbf{Note}\text{: Built-in self-equilibration} \end{aligned}$$

- Weak micro-periodicity formulation for SVE: For given value of $\bar{\boldsymbol{H}}$, find $\boldsymbol{u}, \boldsymbol{t} \in \mathbb{U}_\square \times \mathbb{T}_\square$ s.t.

$$\begin{aligned} a_\square(\boldsymbol{u}; \delta\boldsymbol{u}) - d_\square(\boldsymbol{t}, \delta\boldsymbol{u}) &= 0 & \forall \delta\boldsymbol{u} \in \mathbb{U}_\square \\ -d_\square(\delta\boldsymbol{t}, \boldsymbol{u}) &= -d_\square(\delta\boldsymbol{t}, \bar{\boldsymbol{H}} \cdot [\boldsymbol{X} - \bar{\boldsymbol{X}}] & \forall \delta\boldsymbol{t} \in \mathbb{T}_\square \end{aligned}$$

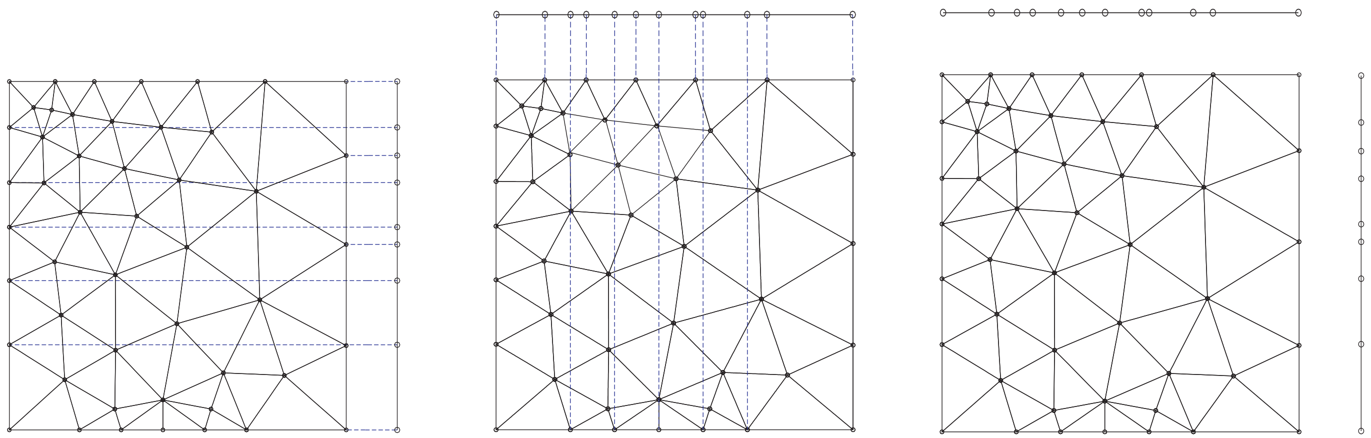
where

$$d_\square(\boldsymbol{t}, \boldsymbol{u}) \stackrel{\text{def}}{=} \frac{1}{|\Omega_\square|} \int_{\Gamma_\square^+} \boldsymbol{t} \cdot [\![\boldsymbol{u}]\!] \, \mathrm{d}\Gamma$$

- **Remark:** Variational framework guarantees Hill-Mandel condition for continuous or discrete $\mathbb{U}_\square$ and $\mathbb{T}_\square$. $\square$
- ATS-tensor LARSSON ET AL CMAME 2011

WPBC – Mixed FE-approximation

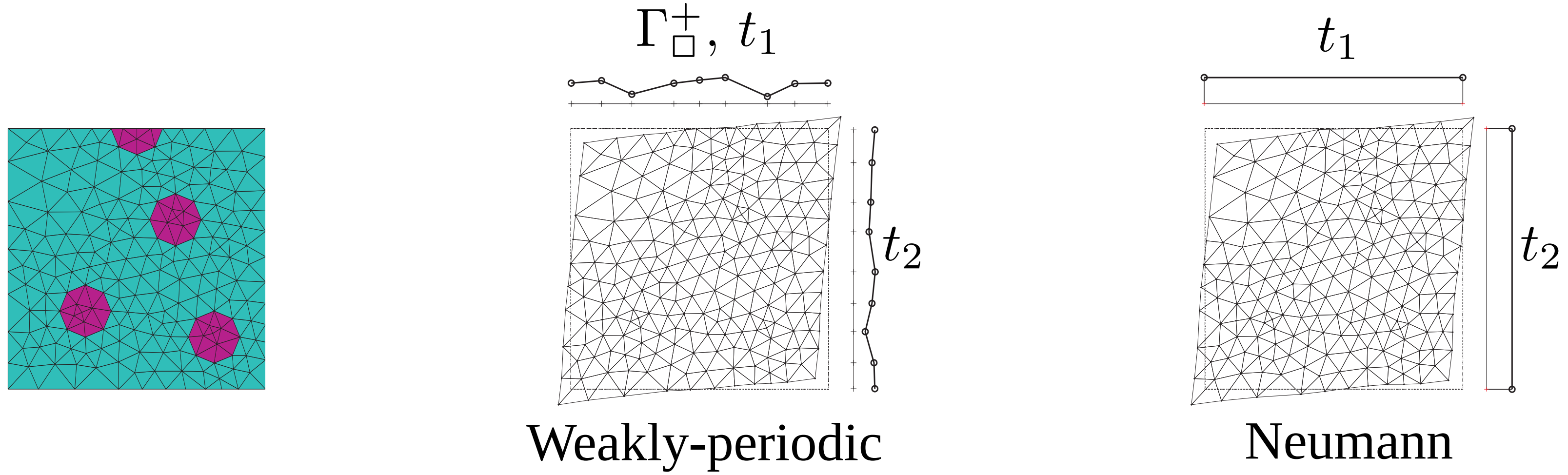
- Adopted FE: P.w. linear $\boldsymbol{u}$ and p.w. linear (continuous) $\boldsymbol{t}$ in 2D
- Construction of traction mesh



- No need for periodic mesh displacement $\rightarrow$ Advantageous for adaptive meshing!

WPBC – Mixed FE, cont'd

- **Remarks**:
  - Stable combination (in the sense of LBB-condition) for "complete" $\boldsymbol{t}$-mesh, follows from analysis of contact problems, cf. EL-ABBASI & BATHE 2001, WRIGGERS 2002.
  - Stable for arbitrarily coarsened $\boldsymbol{t}$-mesh; however, $\dim(\mathbb{T}_{\square,h})$ can not be too large
  - Special choice: Constant $\boldsymbol{t}$ on each side $\rightsquigarrow$ Standard TBC (Neumann b.c)
  - Possible to use p.w. constant $\boldsymbol{t}$ from regularity viewpoint



WPBC – Mixed FE, cont'd

- Weak format of periodicity

$$d_{\square}(\delta \boldsymbol{t}_h, \boldsymbol{u}_h^{\mathrm{s}}) = 0 \quad \forall \delta \boldsymbol{t}_h \in \mathbb{T}_{\square,h}$$

- Special case: **Strong periodicity**, $[|\boldsymbol{u}_h^{\mathrm{s}}|] = \mathbf{0}, \forall \boldsymbol{X} \in \Gamma_{\square}^{+}$
  - Increase $\dim(\mathbb{T}_{\square,h})$ *indefinitely*. Not feasable in practice due to instability unless $\mathbb{U}_{\square,h}$ is enlarged indefinitely
  - Introduce *strictly periodic mesh*, i. e. $\mathrm{trace}(\mathbb{U}_{\square,h})$ on $\Gamma_{\square}^{+}$ and $\mathrm{trace}(\mathbb{U}_{\square,h})$ on $\Gamma_{\square}^{-}$ are identical. Choose

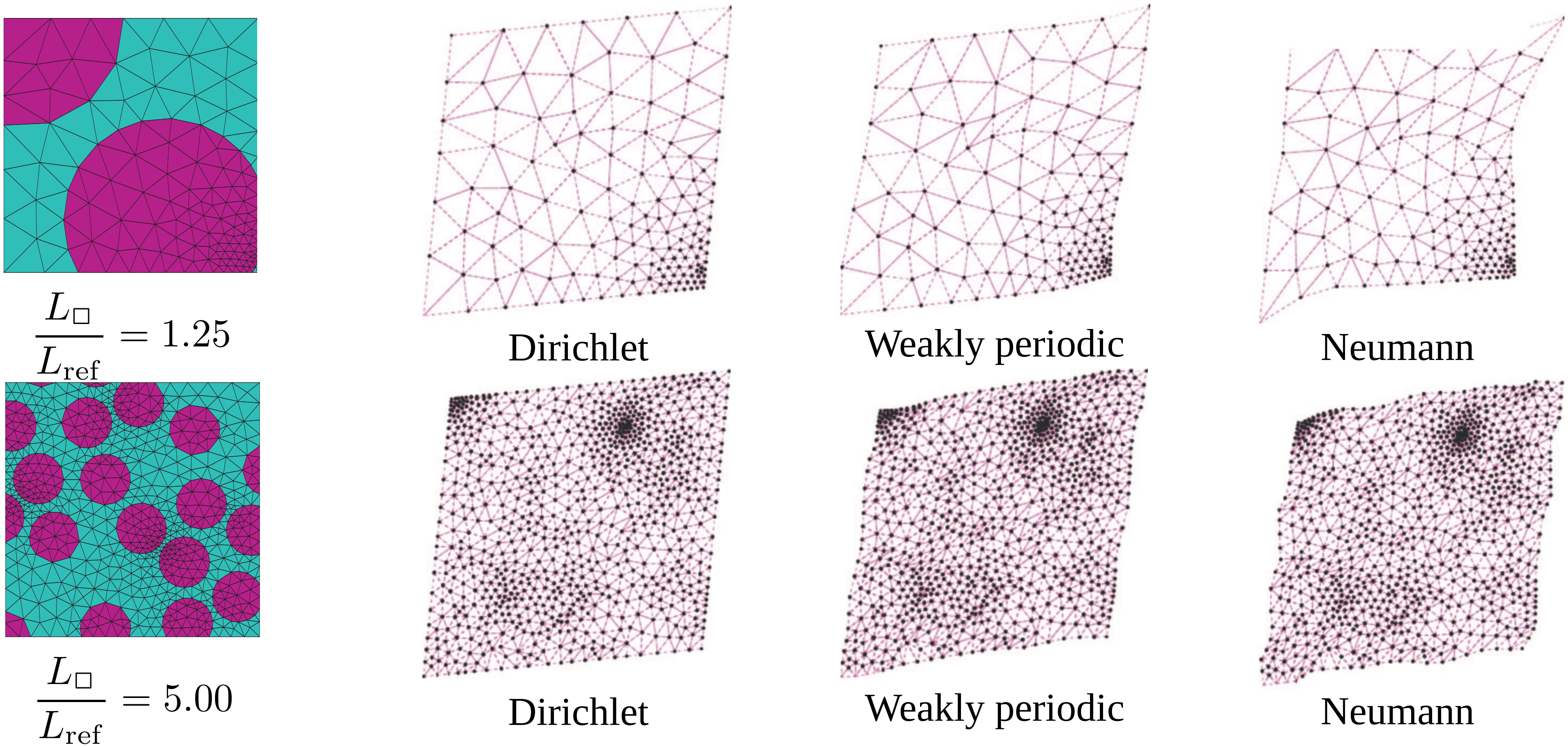
$$\mathbb{T}_{\square,h} = \mathrm{trace}(\mathbb{U}_{\square,h})_{\Gamma_{\square}^{+}} = \mathrm{trace}(\mathbb{U}_{\square,h})_{\Gamma_{\square}^{-}}$$

    Setting $\delta \boldsymbol{t}_h = [|\boldsymbol{u}_h^{\mathrm{s}}|] \in \mathbb{T}_{\square,h} \quad \Rightarrow \quad [|\boldsymbol{u}_h^{\mathrm{s}}|] = \mathbf{0}$, i. e. strong periodicity!

  - **Note**: Strong periodicity does not require any particular arrangement or precautions. It is merely considered as a special choice out of many possible meshes.

WPBC – Typical results

- Snapshots of deformed RVEs for single realization, from CMAME, in print



- **Remark:** Non-periodic mesh for weakly periodic bc! Suitable for adaptive meshing.

SVE-problems

- Displacement b.c. (DBC), Traction b.c. (TBC), Weak periodicity b.c. (WPBC)
- Macroscale data (input or output) for SVE-problem:
  - Macrostrain $\bar{\boldsymbol{H}} \in \mathbb{R}^{3\times 3}$ or Macrostress $\bar{\boldsymbol{P}} \in \mathbb{R}^{3\times 3}$
- Subscale variables (fields)
  - Displacement $\boldsymbol{u} \in \mathbb{U}_{\square}^{\mathrm{D}}, \mathbb{U}_{\square}^{\mathrm{P}}, \mathbb{U}_{\square}^{\mathrm{N}}$
  - Tractions $\boldsymbol{t} \in \mathbb{T}_{\square}$
- Classical versions: DBC with strain control, TBC with stress control

	DBC	WPBC	TBC
Strain control $\bar{\boldsymbol{H}}$	$\boldsymbol{u}$ $\bar{\boldsymbol{P}}$ from post-proc	$\boldsymbol{u}, \boldsymbol{t}$ $\bar{\boldsymbol{P}}$ from post-proc	$\boldsymbol{u}, \bar{\boldsymbol{P}}$
Stress control $\bar{\boldsymbol{P}}$	$\boldsymbol{u}, \bar{\boldsymbol{H}}$	$\boldsymbol{u}, \boldsymbol{t}, \bar{\boldsymbol{H}}$	$\boldsymbol{u}$ $\bar{\boldsymbol{H}}$ from post-proc