Computational Homogenization in Material Mechanics

by

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Preface

In recent years the research field of *computational multiscale material modeling* has grown tremendously in popularity and importance on the international scene within the field of Solid Mechanics. It is fair to say that a new paradigm has been created that allows for unification of and interaction between computational quantum physics, continuum mechanics and computational mathematics. Hence, the field is strongly interdisciplinary. In particular, classical ideas of homogenization in mathematics and mechanics have been put in a new perspective, and they have been generalized within the framework of Variational Multiscale Modeling. In particular, this framework constitutes the foundation of Variationally Consistent Homogenization, by which it is possible to establish the macroscale and subscale problems for a wide class of mechanics and physics phenomena that are relevant for micro-heterogenous materials. The unifying variational framework has also opened up for the application of adaptive modeling based on reliable estimation of various types of model, discretization and other solution errors. It is our intention to describe some of these aspects in the present Lecture Notes, which we believe can not (at least not presently) be found elsewhere in a single volume.

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Chapter 1

INTRODUCTION

1.1 Motivation for multiscale modeling

The mechanical properties of all engineering and natural materials depend on the physical structure of the material on various subscales (below the macroscopic or continuum) scale. Consequently, any macroscopic model represents (in some way) the averaged properties of the substructure on the subscale(s), and this averaging can be carried out *a priori* in many cases. The relevant number of subscales, as well as the characteristics of the heterogeneous structure on any given scale, differ strongly from one material to the other. For example, for polycrystalline metals the next subscale below the macroscale (mesoscale) is determined by the grain size, and the properties within the grain are defined by the phase structure and the pertinent assumption on constitutive relations (typically crystal plasticity) within each phase.

In the classical approach of developing phenomenological constitutive relations for the macroscale response, no explicit account is taken for the heterogeneous subscale structure(s). Rather, the material parameters are determined directly via the calibration against experimental results on specimens that are macroscopically homogeneous and subjected to macroscopically homogeneous stress and strain states (at least in theory). However, a more fundamental approach is to carry out some sort of homogenization to obtain the *effective* properties. In many cases, in particular when the subscale stress-strain relation is linear, it is possible to carry out the homogenization *a priori* (once and for all), whereas the homogenization must be carried out in a nested fashion when the subscale relations are nonlinear. In such a case we speak about *computational homogenization*. Of particular interest is to establish *bounds* for the effective properties.

1.2 Literature – Historical remarks

Part I

CLASSICAL AND COMPUTATIONAL HOMOGENIZATION - THE FOUNDATION

Chapter 2

CLASSICAL HOMOGENIZATION - LINEAR ELASTICITY

2.1 Subscale linear elasticity

2.1.1 Linear elasticity - Strong format of boundary value problem

Consider the standard problem of a body occupying the spatial domain Ω with boundary $\partial\Omega$ in the (undeformed) reference configuration. The quasistatic equilibrium problem for linear elasticity is then defined by the equilibrium equation

$$-\boldsymbol{\sigma} \cdot \boldsymbol{\nabla} = \boldsymbol{f} \text{ in } \Omega, \tag{2.1}$$ {eq:2-1}

and the constitutive equation representing linear elasticity[1] reads

$$\boldsymbol{\sigma} = \mathsf{E} : \boldsymbol{\epsilon}\ , \quad \boldsymbol{\epsilon} = \boldsymbol{\epsilon}[\boldsymbol{u}] \stackrel{\text{def}}{=} (\boldsymbol{u} \otimes \boldsymbol{\nabla})^{\text{sym}}, \tag{2.2}$$ {eq:2-2}

where E is the subscale (constant) stiffness tensor that possesses (in particular) first and second minor symmetry, e.g. $E_{ijkl} = E_{jikl} = E_{ijlk}$. For completeness we give the explicit expressions for[2] $\mathsf{E} = \mathsf{C}^{-1}$ and $\mathsf{C} = \mathsf{E}^{-1}$ in the special case of isotropic response:

$$\mathsf{E} = 2G\mathsf{I}^{\text{sym}}_{\text{dev}} + K\boldsymbol{I} \otimes \boldsymbol{I}, \quad \mathsf{C} = \frac{1}{2G}\mathsf{I}^{\text{sym}}_{\text{dev}} + \frac{1}{9K}\boldsymbol{I} \otimes \boldsymbol{I} \tag{2.3}$$ {eq:2-3}

with

$$\mathsf{I}^{\text{sym}}_{\text{dev}} \stackrel{\text{def}}{=} \mathsf{I}^{\text{sym}} - \frac{1}{3}\boldsymbol{I} \otimes \boldsymbol{I}, \quad \mathsf{I}^{\text{sym}} \stackrel{\text{def}}{=} \frac{1}{2}\left[\boldsymbol{I} \overline{\otimes} \boldsymbol{I} + \boldsymbol{I} \underline{\otimes} \boldsymbol{I}\right] \tag{2.4}$$ {eq:2-4}

where G and K are the shear and bulk modulus, respectively.

The standard boundary conditions on $\partial\Omega = \partial\Omega_{\text{D}} \cup \partial\Omega_{\text{N}}$ are:

$$\boldsymbol{u} = \boldsymbol{u}_{\text{P}} \text{ on } \partial\Omega_{\text{D}}, \tag{2.5a}$$ {eq:2-5a}

$$\boldsymbol{t} \stackrel{\text{def}}{=} \boldsymbol{\sigma} \cdot \boldsymbol{n} = \boldsymbol{t}_{\text{P}} \text{ on } \partial\Omega_{\text{N}}. \tag{2.5b}$$ {eq:2-5b}

Upon eliminating $\boldsymbol{\sigma}$ in (2.1) via (2.2), we obtain the classical strong format of the elasticity problem with the displacement field $\boldsymbol{u}$ as the primary unknown field. {eq:2-5}

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[1] The notation $\boldsymbol{\epsilon}[\bullet]$ denotes the "strain operator" on a displacement field.

[2] Note that the fourth order tensor E is singular with respect to rigid body rotation. Here, we define the inverse by considering the fourth order tensors as linear mappings between symmetric second order tensors, e.g. $\mathsf{E} : \mathbb{R}^{3\times3,\text{sym}} \rightarrow \mathbb{R}^{3\times3,\text{sym}}$.

2.1.2 Displacement-based variational formulations

Introduce the spaces {eq:2-6}

$$\mathbb{U} = \{\boldsymbol{u} \text{ suff. regular}|\ \boldsymbol{u} = \boldsymbol{u}_{\mathrm{P}} \text{ on } \partial\Omega_{\mathrm{D}}\}, \tag{2.6a}$$ {eq:2-6a}

$$\mathbb{U}^0 = \{\boldsymbol{u} \text{ suff. regular}|\ \boldsymbol{u} = \boldsymbol{0} \text{ on } \partial\Omega_{\mathrm{D}}\}. \tag{2.6b}$$ {eq:2-6b}

The corresponding weak format of (2.1) to (2.5) is: Find $\boldsymbol{u} \in \mathbb{U}$ that solves

{eq:2-7}
$$a(\boldsymbol{u}, \delta\boldsymbol{u}) = l(\delta\boldsymbol{u}) \quad \forall \delta\boldsymbol{u} \in \mathbb{U}^0, \tag{2.7}$$

where we introduced the symmetric and bilinear form $a(\boldsymbol{u}, \boldsymbol{v})$ and the linear functional $l(\boldsymbol{v})$ as

{eq:2-8a}
$$a(\boldsymbol{u}, \delta\boldsymbol{u}) \stackrel{\text{def}}{=} \int_\Omega \boldsymbol{\epsilon}[\boldsymbol{u}] : \mathsf{E} : \boldsymbol{\epsilon}[\delta\boldsymbol{u}] \, \mathrm{d}\Omega, \tag{2.8}$$

{eq:2-8b}
$$l(\delta\boldsymbol{u}) \stackrel{\text{def}}{=} \int_\Omega \boldsymbol{f} \cdot \delta\boldsymbol{u} \, \mathrm{d}\Omega + \int_{\partial\Omega_{\mathrm{N}}} \boldsymbol{t}_{\mathrm{P}} \cdot \delta\boldsymbol{u} \, \mathrm{d}\Gamma. \tag{2.9}$$

The weak format (2.7) is obtained upon multiplying (2.1) by $\delta\boldsymbol{u} \in \mathbb{U}^0$, integrating by parts and using the natural boundary condition (2.5b).

The elastic stiffness tensor E is positive definite in the sense that

{eq:2-11}
$$\boldsymbol{\delta\epsilon} \colon \mathsf{E} \colon \boldsymbol{\delta\epsilon} > 0 \quad \forall \delta\boldsymbol{\epsilon} \in \mathbb{R}^{3\times3,\text{sym}} \setminus \{\boldsymbol{0}\} \tag{2.10}$$

which infers that

{eq:2-12}
$$a(\delta\boldsymbol{u}, \delta\boldsymbol{u}) > 0 \quad \forall \delta\boldsymbol{u} \in \mathbb{U}^0 \setminus \{\boldsymbol{0}\} \tag{2.11}$$

We also introduce the strain energy density $\psi(\boldsymbol{\epsilon})$

{eq:2-13}
$$\psi(\boldsymbol{\epsilon}) = \frac{1}{2}\boldsymbol{\epsilon} \colon \mathsf{E} \colon \boldsymbol{\epsilon} \quad \Rightarrow \quad \boldsymbol{\sigma}(\boldsymbol{\epsilon}) = \frac{\partial\psi(\boldsymbol{\epsilon})}{\partial\boldsymbol{\epsilon}} = \mathsf{E} \colon \boldsymbol{\epsilon}, \tag{2.12}$$

and from the positive definiteness of E follows that $\psi(\boldsymbol{\epsilon}) > 0$ for all $\boldsymbol{\epsilon} \neq \boldsymbol{0}$. Moreover, $\psi(\boldsymbol{\epsilon})$ is strictly convex in the sense that, for any distinct $\boldsymbol{\epsilon}_1 \neq \boldsymbol{\epsilon}_2$, we have the inequality

{eq:2-14}
$$\psi(\boldsymbol{\epsilon}_2) - \psi(\boldsymbol{\epsilon}_1) > \frac{\partial\psi}{\partial\boldsymbol{\epsilon}}(\boldsymbol{\epsilon}_1) : [\boldsymbol{\epsilon}_2 - \boldsymbol{\epsilon}_1] = \boldsymbol{\sigma}(\boldsymbol{\epsilon}_1) : [\boldsymbol{\epsilon}_2 - \boldsymbol{\epsilon}_1] = \boldsymbol{\epsilon}_1 : \mathsf{E} : [\boldsymbol{\epsilon}_2 - \boldsymbol{\epsilon}_1]. \tag{2.13}$$

Show this inequality as HW!

Next, we introduce the potential energy $\Pi(\hat{\boldsymbol{u}})$ of any $\hat{\boldsymbol{u}} \in \mathbb{U}$ as follows:

{eq:2-15}
$$\Pi(\hat{\boldsymbol{u}}) = \frac{1}{2}a(\hat{\boldsymbol{u}}, \hat{\boldsymbol{u}}) - l(\hat{\boldsymbol{u}}) \tag{2.14}$$

The directional derivative of Π at any point $\hat{\boldsymbol{u}} \in \mathbb{U}$ in the direction $\delta\boldsymbol{u} \in \mathbb{U}^0$ is given as

{eq:2-16}
$$\Pi'_u(\hat{\boldsymbol{u}}; \delta\boldsymbol{u}) \stackrel{\text{def}}{=} \frac{\mathrm{d}}{\mathrm{d}\gamma}\Pi(\hat{\boldsymbol{u}} + \gamma\delta\boldsymbol{u})|_{\gamma=0} = a(\hat{\boldsymbol{u}}, \delta\boldsymbol{u}) - l(\delta\boldsymbol{u}) \tag{2.15}$$

From the convexity of ψ, we conclude that Π is convex in the sense that, for any given pair $\boldsymbol{u}_1 \in \mathbb{U}$ and $\boldsymbol{u}_2 \in \mathbb{U}$, we have the inequality

{eq:2-17}
$$\begin{aligned}
\Pi(\boldsymbol{u}_2) - \Pi(\boldsymbol{u}_1) &= \frac{1}{2}[a(\boldsymbol{u}_2, \boldsymbol{u}_2) - a(\boldsymbol{u}_1, \boldsymbol{u}_1)] - l(\boldsymbol{u}_2 - \boldsymbol{u}_1) \\
&= \int_\Omega [\psi(\boldsymbol{\epsilon}_2) - \psi(\boldsymbol{\epsilon}_1)] \, \mathrm{d}\Omega - l(\boldsymbol{u}_2 - \boldsymbol{u}_1) \\
&\geq \int_\Omega \boldsymbol{\epsilon}_1 : \mathsf{E} : [\boldsymbol{\epsilon}_2 - \boldsymbol{\epsilon}_1] \, \mathrm{d}\Omega - l(\boldsymbol{u}_2 - \boldsymbol{u}_1) = a(\boldsymbol{u}_1, \boldsymbol{u}_2 - \boldsymbol{u}_1) - l(\boldsymbol{u}_2 - \boldsymbol{u}_1) \\
&= \Pi'_u(\boldsymbol{u}_1; \boldsymbol{u}_2 - \boldsymbol{u}_1)
\end{aligned} \tag{2.16}$$

The solution $\boldsymbol{u} \in \mathbb{U}$ of the weak problem (2.7) is also the minimizer of $\Pi(\hat{\boldsymbol{u}})$, i.e.

{eq:2-18}
$$\boldsymbol{u} = \arg\left[\min_{\hat{\boldsymbol{u}}\in\mathbb{U}} \Pi(\hat{\boldsymbol{u}})\right]. \tag{2.17}$$

In other words,

$$\Pi(\boldsymbol{u}) \leq \Pi(\hat{\boldsymbol{u}}) \quad \forall \hat{\boldsymbol{u}} \in \mathbb{U} \quad \text{or} \quad \Pi(\boldsymbol{u}) = \min_{\hat{\boldsymbol{u}}\in\mathbb{U}} \Pi(\hat{\boldsymbol{u}}) \tag{2.18}$$ {eq:2-19}

which is the *Principle of Minimum Potential Energy (MPE-principle).*

Proof: Firstly, we establish the equation for a stationary point of $\Pi(\hat{\boldsymbol{u}})$. To this end, consider the directional derivative in the direction $\delta\boldsymbol{u}$ at any arbitrary point $\hat{\boldsymbol{u}}$. Obviously, the equation

$$\Pi'_u(\boldsymbol{u};\delta\boldsymbol{u}) = a(\boldsymbol{u};\delta\boldsymbol{u}) - l(\delta\boldsymbol{u}) = 0 \quad \forall \delta\boldsymbol{u} \in \mathbb{U}^0 \tag{2.19}$$ {eq:2-20}

is identical to the weak format (2.7); hence, the condition that $\boldsymbol{u}$ is a stationary point is precisely the weak format.

Secondly, we set out to show the stationary point is, indeed, a minimizer of Π'_u. For any $\hat{\boldsymbol{u}} \in \mathbb{U}$, due to the convexity of Π, we obtain the inequality

$$\Pi(\hat{\boldsymbol{u}}) - \Pi(\boldsymbol{u}) \geq \Pi'_u(\boldsymbol{u};\hat{\boldsymbol{u}} - \boldsymbol{u}) = 0 \tag{2.20}$$ {eq:2-21}

The last identity is obtained from the stationarity condition (2.19) upon noting that $\hat{\boldsymbol{u}} - \boldsymbol{u} \in \mathbb{U}^0$. $\square$

The minimum value of Π can be computed as follows: Introduce any displacement field $\bar{\boldsymbol{u}} \in \mathbb{U}$ and the complement $\boldsymbol{u}' \overset{\text{def}}{=} \boldsymbol{u} - \bar{\boldsymbol{u}} \in \mathbb{U}^0$. In particular, $\boldsymbol{u}'$ satisfies homogenous displacement boundary conditions on Γ_{D}. Upon inserting $\boldsymbol{u} = \bar{\boldsymbol{u}} + \boldsymbol{u}'$ into $\Pi(\boldsymbol{u})$ and using (2.7) to obtain

$$a(\boldsymbol{u},\boldsymbol{u}') - l(\boldsymbol{u}') = 0 \tag{2.21}$$ {eq:2-22}

we conclude that the minimum value, $\Pi(\boldsymbol{u})$, can be computed as

$$\Pi(\boldsymbol{u}) = \Pi(\bar{\boldsymbol{u}}) - \frac{1}{2}a(\boldsymbol{u}',\boldsymbol{u}') \tag{2.22}$$ {eq:2-23}

Finally, in the special case that $\boldsymbol{u}_{\text{P}} = \boldsymbol{0}$, then it is possible to choose $\bar{\boldsymbol{u}} = \boldsymbol{0}$, which gives $\boldsymbol{u}' = \boldsymbol{u}$. The result in (2.22) then reduces to

$$\Pi(\boldsymbol{u}) = -\frac{1}{2}a(\boldsymbol{u},\boldsymbol{u}) \tag{2.23}$$ {eq:2-24}

2.1.3 Stress-based (complementary) variational formulations

Introduce the spaces {eq:2-31}

$$\mathbb{S} = \{\boldsymbol{\sigma} \text{ suff. regular} | -\boldsymbol{\sigma}\cdot\boldsymbol{\nabla} = \boldsymbol{f} \text{ in } \Omega, \quad \boldsymbol{t} \overset{\text{def}}{=} \boldsymbol{\sigma}\cdot\boldsymbol{n} = \boldsymbol{t}_{\text{P}} \text{ on } \partial\Omega_{\text{N}}\} \tag{2.24a}$$ {eq:2-31a}

$$\mathbb{S}^0 = \{\boldsymbol{\sigma} \text{ suff. regular} | -\boldsymbol{\sigma}\cdot\boldsymbol{\nabla} = \boldsymbol{0} \text{ in } \Omega, \quad \boldsymbol{t} = \boldsymbol{0} \text{ on } \partial\Omega_{\text{N}}\} \tag{2.24b}$$ {eq:2-32b}

The complementary weak format of (2.1) to (2.5b) is: Find $\boldsymbol{\sigma} \in \mathbb{S}$ that solves

$$a^*(\boldsymbol{\sigma},\delta\boldsymbol{\sigma}) = l^*(\delta\boldsymbol{\sigma}) \quad \forall \delta\boldsymbol{\sigma} \in \mathbb{S}^0 \tag{2.25}$$ {eq:2-33}

where we introduced the complementary variational forms {eq:2-34}

$$a^*(\boldsymbol{\sigma}, \delta\boldsymbol{\sigma}) \overset{\text{def}}{=} \int_\Omega \boldsymbol{\sigma} : \mathsf{C} : \delta\boldsymbol{\sigma} \; \mathrm{d}\Omega \tag{2.26a}$$ {eq:2-34a}

$$l^*(\delta\boldsymbol{\sigma}) \overset{\text{def}}{=} \int_{\partial\Omega_\mathrm{D}} \boldsymbol{u}_\mathrm{P} \cdot \delta\boldsymbol{t} \; \mathrm{d}\Gamma \tag{2.26b}$$ {eq:2-34b}

In (2.26b), we used the relation $\delta\boldsymbol{t} \overset{\text{def}}{=} \delta\boldsymbol{\sigma}\cdot\boldsymbol{n}$.

The complementary weak format (2.25) is obtained as follows: Consider the constitutive relation (2.12) in the compliance format

{eq:2-35}
$$\boldsymbol{\epsilon} = \mathsf{C} : \boldsymbol{\sigma} \tag{2.27}$$

where $\mathsf{C} = \mathsf{E}^{-1}$ is the positive definite compliance tensor. Upon multiplying (2.27) by $\delta\boldsymbol{\sigma} \in \mathbb{S}^0$, and integrating by parts we obtain

{eq:2-36}
$$\int_\Omega \boldsymbol{\sigma} : \mathsf{C} : \delta\boldsymbol{\sigma} \; \mathrm{d}\Omega = \int_\Omega \boldsymbol{\epsilon} : \delta\boldsymbol{\sigma} \; \mathrm{d}\Omega = -\int_\Omega [\delta\boldsymbol{\sigma}\cdot\boldsymbol{\nabla}]\cdot\boldsymbol{u} \; \mathrm{d}\Omega + \int_{\partial\Omega} \delta\boldsymbol{t}\cdot\boldsymbol{u} \; \mathrm{d}\Gamma \tag{2.28}$$

Now using the properties of $\mathbb{S}^0$, i.e.

{eq:2-37}
$$\delta\boldsymbol{\sigma}\cdot\boldsymbol{\nabla} = \boldsymbol{0} \text{ in } \Omega \text{ and } \delta\boldsymbol{t} = \boldsymbol{0} \text{ on } \partial\Omega_\mathrm{N} \tag{2.29}$$

and using the boundary conditions on the Dirichlet part of the boundary, as expressed in (**??**), we obtain from (2.28)

{eq:2-38}
$$\int_\Omega \boldsymbol{\sigma} : \mathsf{C} : \delta\boldsymbol{\sigma} \; \mathrm{d}\Omega = \int_{\partial\Omega_\mathrm{D}} \delta\boldsymbol{t}\cdot\boldsymbol{u}^\mathrm{P} \; \mathrm{d}\Gamma \quad \forall\delta\boldsymbol{\sigma} \in \mathbb{S}^0 \tag{2.30}$$

which is precisely (2.25).

In analogy to the strain energy $\psi(\boldsymbol{\epsilon})$ density, we introduce the stress energy density (or complementary strain energy density) $\psi^*(\boldsymbol{\sigma})$

{eq:2-39}
$$\psi^*(\boldsymbol{\sigma}) = \frac{1}{2}\boldsymbol{\sigma} : \mathsf{C} : \boldsymbol{\sigma} \quad \Rightarrow \quad \boldsymbol{\epsilon}(\boldsymbol{\sigma}) = \frac{\partial\psi^*(\boldsymbol{\sigma})}{\partial\boldsymbol{\sigma}} = \mathsf{C} : \boldsymbol{\sigma} \tag{2.31}$$

and from the positive definiteness of C follows that $\psi^*(\boldsymbol{\sigma}) > 0$ for all $\boldsymbol{\sigma} \neq \boldsymbol{0}$. Moreover, $\psi^*(\boldsymbol{\sigma})$ is strictly convex in the sense that, for any any two $\boldsymbol{\sigma}_1$ and $\boldsymbol{\sigma}_2$, we have the inequality

{eq:2-41}
$$\psi^*(\boldsymbol{\sigma}_2) - \psi^*(\boldsymbol{\sigma}_1) \geq \frac{\partial\psi^*}{\partial\boldsymbol{\sigma}}(\boldsymbol{\sigma}_1) : [\boldsymbol{\sigma}_2 - \boldsymbol{\sigma}_1] = \boldsymbol{\sigma}(\boldsymbol{\sigma}_1) : [\boldsymbol{\sigma}_2 - \boldsymbol{\sigma}_1] = \boldsymbol{\sigma}_1 : \mathsf{C} : [\boldsymbol{\sigma}_2 - \boldsymbol{\sigma}_1] \tag{2.32}$$

Next, we introduce the complementary potential energy $\Pi^*(\hat{\boldsymbol{\sigma}})$ of any $\hat{\boldsymbol{\sigma}} \in \mathbb{S}$ as follows:

{eq:2-42}
$$\Pi^*(\hat{\boldsymbol{\sigma}}) = l^*(\hat{\boldsymbol{\sigma}}) - \frac{1}{2}a^*(\hat{\boldsymbol{\sigma}}, \hat{\boldsymbol{\sigma}}) \tag{2.33}$$

The directional derivative of Π^* at any point $\hat{\boldsymbol{\sigma}} \in \mathbb{S}$ in the direction $\delta\boldsymbol{\sigma} \in \mathbb{S}^0$ is given as

{eq:2-43}
$$(\Pi^*)'_\sigma(\hat{\boldsymbol{\sigma}}; \delta\boldsymbol{\sigma}) = l^*(\delta\boldsymbol{\sigma}) - a^*(\hat{\boldsymbol{\sigma}}, \delta\boldsymbol{\sigma}) \tag{2.34}$$

From the convexity of ψ^*, we conclude that Π^* is concave in the sense that, for any given pair $\boldsymbol{\sigma}_1 \in \mathbb{S}$ and $\boldsymbol{\sigma}_2 \in \mathbb{S}$, we have the inequality

{eq:2-44}

$$\begin{aligned}
\Pi^*(\boldsymbol{\sigma}_2) - \Pi^*(\boldsymbol{\sigma}_1) &= l^*(\boldsymbol{\sigma}_2 - \boldsymbol{\sigma}_1) - \frac{1}{2}\left[a^*(\boldsymbol{\sigma}_2, \boldsymbol{\sigma}_2) - a^*(\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_1)\right] \\
&= l^*(\boldsymbol{\sigma}_2 - \boldsymbol{\sigma}_1) - \int_\Omega [\psi^*(\boldsymbol{\sigma}_2) - \psi^*(\boldsymbol{\sigma}_1)] \, \mathrm{d}\Omega \\
&\geq l^*(\boldsymbol{\sigma}_2 - \boldsymbol{\sigma}_1) - \int_\Omega \boldsymbol{\sigma}_1 : \mathsf{C} : [\boldsymbol{\sigma}_2 - \boldsymbol{\sigma}_1] \, \mathrm{d}\Omega \\
&= l^*(\boldsymbol{\sigma}_2 - \boldsymbol{\sigma}_1) - a^*(\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2 - \boldsymbol{\sigma}_1) \\
&= (\Pi^*)'_\sigma(\boldsymbol{\sigma}_1; \boldsymbol{\sigma}_2 - \boldsymbol{\sigma}_1) \qquad (2.35)
\end{aligned}$$

The solution $\boldsymbol{\sigma} \in \mathbb{S}$ of (2.25) is also the maximizer of $\Pi^*(\hat{\boldsymbol{\sigma}})$, i.e.

$$\boldsymbol{\sigma} = \arg\left[\max_{\hat{\boldsymbol{\sigma}} \in \mathbb{S}} \Pi^*(\hat{\boldsymbol{\sigma}})\right] \qquad (2.36)$$ {eq:2-45}

In other words,

$$\Pi^*(\boldsymbol{\sigma}) \geq \Pi^*(\hat{\boldsymbol{\sigma}}) \quad \forall \hat{\boldsymbol{\sigma}} \in \mathbb{S} \quad \text{or} \quad \Pi^*(\boldsymbol{\sigma}) = \max_{\hat{\boldsymbol{\sigma}} \in \mathbb{S}} \Pi^*(\hat{\boldsymbol{\sigma}}) \qquad (2.37)$$ {eq:2-46}

which is the *Principle of Maximum Complementary Potential Energy (MCPE-principle).*

Proof: The proof follows the same line of reasoning as for the MPE-principle and is left as HW to the reader. □

Now, introduce any given stress field $\bar{\boldsymbol{\sigma}} \in \mathbb{S}$ and the complement $\boldsymbol{\sigma}' \stackrel{\text{def}}{=} \boldsymbol{\sigma} - \bar{\boldsymbol{\sigma}} \in \mathbb{S}^0$. In particular, $\boldsymbol{\sigma}'$ satisfies the homogeneous equilibrium equation and homogeneous traction boundary condition on $\partial\Omega_\mathrm{N}$. Upon introducing $\boldsymbol{\sigma} = \bar{\boldsymbol{\sigma}} + \boldsymbol{\sigma}'$ into $\Pi^*(\boldsymbol{\sigma})$ and using (2.25) to obtain

$$a^*(\boldsymbol{\sigma}, \boldsymbol{\sigma}') - l^*(\boldsymbol{\sigma}') = 0 \qquad (2.38)$$ {eq:2-51}

we conclude that the maximum value, $\Pi^*(\boldsymbol{\sigma})$, can be computed as

$$\Pi^*(\boldsymbol{\sigma}) = \Pi^*(\bar{\boldsymbol{\sigma}}) + \frac{1}{2} a^*(\boldsymbol{\sigma}', \boldsymbol{\sigma}') \qquad (2.39)$$ {eq:2-52}

Finally, in the special case when $\boldsymbol{t}_\mathrm{P} = \mathbf{0}$, then it is possible to choose $\bar{\boldsymbol{\sigma}} = \mathbf{0}$, which gives $\boldsymbol{\sigma}' = \boldsymbol{\sigma}$. The result in (2.39) then reduces to

$$\Pi^*(\boldsymbol{\sigma}) = \frac{1}{2} a^*(\boldsymbol{\sigma}', \boldsymbol{\sigma}') \qquad (2.40)$$ {eq:2-53}

2.2 Basic concepts and assumptions within the theory of homogenization

2.2.1 Macroscale properties – Upscaling

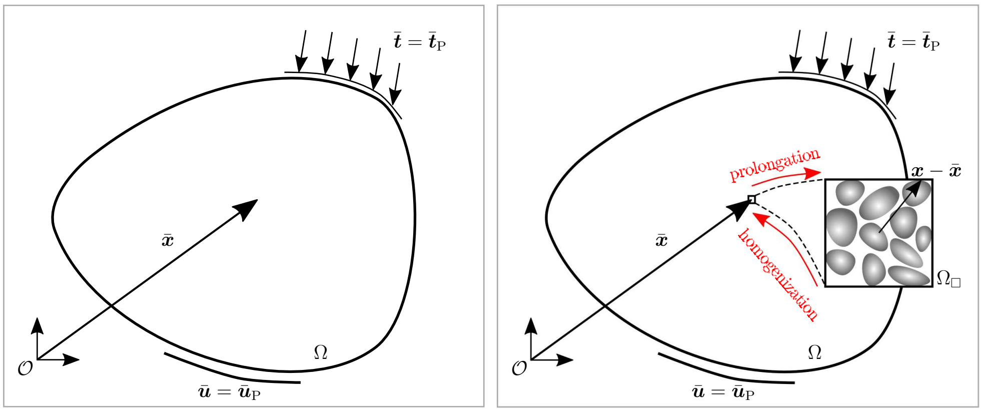


Figure 2.1: *(a) Fine-scale (resolved) boundary value problem. (b) Upscaling via computational homogenization/FE*^{2}. {fig:2-1}

The purpose of homogenization is to replace the fine-scale (microscale) representation of elasticity with a macroscale problem in terms of *smoother* fields[3] $\bar{\boldsymbol{u}}, \bar{\boldsymbol{\sigma}}$ etc. For the considered prototype model of linear elasticity, we then postulate the macroscale equilibrium equation

{eq:2-54} $$-\bar{\boldsymbol{\sigma}} \cdot \boldsymbol{\nabla} = \bar{\boldsymbol{f}} \text{ in } \Omega, \tag{2.41}$$

the constitutive equation representing the "effective relation" of linear elasticity

{eq:2-55} $$\bar{\boldsymbol{\sigma}} = \bar{\mathbf{E}} : \bar{\boldsymbol{\epsilon}} \ , \quad \bar{\boldsymbol{\epsilon}} = \boldsymbol{\epsilon}[\bar{\boldsymbol{u}}] \overset{\text{def}}{=} (\bar{\boldsymbol{u}} \otimes \boldsymbol{\nabla})^{\text{sym}} \tag{2.42}$$

{eq:2-56} and the boundary conditions on $\partial\Omega = \partial\Omega_{\text{D}} \cup \partial\Omega_{\text{N}}$:

{eq:2-56a} $$\bar{\boldsymbol{u}} = \bar{\boldsymbol{u}}_{\text{P}} \text{ on } \partial\Omega_{\text{D}} \tag{2.43a}$$

{eq:2-56b} $$\bar{\boldsymbol{t}} \overset{\text{def}}{=} \bar{\boldsymbol{\sigma}} \cdot \boldsymbol{n} = \bar{\boldsymbol{t}}_{\text{P}} \text{ on } \partial\Omega_{\text{N}} \tag{2.43b}$$

Obviously, the key issue is to derive the effective elastic stiffness tensor $\bar{\mathbf{E}}(\bar{\boldsymbol{x}})$[4] at any given macroscale point $\bar{\boldsymbol{x}} \in \Omega$ based on the fine-scale variation of $\mathbf{E}(\boldsymbol{x})$ in a neighborhood of $\bar{\boldsymbol{x}} \in \Omega$. This is what homogenization is about.

The corresponding weak format of (2.41) to (2.43) is: Find $\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}$ that solves

{eq:2-57} $$\bar{a}(\bar{\boldsymbol{u}}, \delta\bar{\boldsymbol{u}}) = \bar{l}(\delta\bar{\boldsymbol{u}}) \quad \forall \delta\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}^0 \tag{2.44}$$

where we introduced the symmetric and bilinear form $\bar{a}(\bar{\boldsymbol{u}}, \bar{\boldsymbol{v}})$ and the linear functional $\bar{l}(\bar{\boldsymbol{v}})$

{eq:2-58} $$\bar{a}(\bar{\boldsymbol{u}}, \delta\bar{\boldsymbol{u}}) \overset{\text{def}}{=} \int_\Omega \bar{\boldsymbol{\epsilon}} : \bar{\mathbf{E}} : \delta\bar{\boldsymbol{\epsilon}} \ \text{d}\Omega = \int_\Omega \boldsymbol{\epsilon}[\bar{\boldsymbol{u}}] : \bar{\mathbf{E}} : \boldsymbol{\epsilon}[\delta\bar{\boldsymbol{u}}] \ \text{d}\Omega \tag{2.45}$$

{eq:2-59} $$\bar{l}(\delta\bar{\boldsymbol{u}}) \overset{\text{def}}{=} \int_\Omega \bar{\boldsymbol{f}} \cdot \delta\bar{\boldsymbol{u}} \ \text{d}\Omega + \int_{\partial\Omega_{\text{N}}} \bar{\boldsymbol{t}}_{\text{P}} \cdot \delta\bar{\boldsymbol{u}} \ \text{d}\Gamma \tag{2.46}$$

[3] An overbar denotes macroscale variable.
[4] Essentially, there is only one single scale involved in the sense that we interpret $\bar{\mathbf{E}}(\bar{\boldsymbol{x}}) = \bar{\mathbf{E}}(\boldsymbol{x})|_{\boldsymbol{x}=\bar{\boldsymbol{x}}}$.

In terms of a "constitutive driver", that represents the algorithmic implementation of a macroscale constitutive model in a standard FE-code, we may view $\bar{\boldsymbol{\epsilon}}$ as the "input" and $\bar{\boldsymbol{\sigma}}$ as the "output". The operations involved in the homogenization process that maps the fine-scale field $\bar{\mathbf{E}}(\boldsymbol{x})$ to the macroscale field $\bar{\mathbf{E}}(\boldsymbol{x})$ is thus equivalant to the evaluation of the macroscale constitutive model. For a linear problem this may be denoted *direct upscaling* to compute the material parameters, since the linearity is preserved at the homogenization. However, when the fine-scale problem has a nonlinear character, such as nonlinear elasticity (or an incremental step for a dissipative material model), the situation is less simple. Firstly, $\bar{\boldsymbol{\sigma}}$ depends implicitly on $\bar{\boldsymbol{\epsilon}}$ in a nonlinear fashion. Secondly, there are (at least) two different routes as to the role of homogenization.

- Linear problem
  - *Direct upscaling* gives the components of $\bar{\mathbf{E}}$
- Nonlinear problem
  - *Indirect upscaling* gives parameter values in the *a priori* defined macroscale constitutive model. This represents a calibration (parameter identification) procedure, where the corresponding values of $\bar{\boldsymbol{\sigma}}$ are computed via homogenization for a given set of values of $\bar{\boldsymbol{\epsilon}}$ pertinent to increasing loading levels. In other words, these "virtual test/experimental data" will thus replace the physical experimental data in the calibration procedure.
  - It is possible to circumvent the need for a macroscopic model by solving a "subscale boundary/intial value problem" and using FE-discretization on both scales (macroscale and microscale); hence the notion *FE*^{2}.

2.2.2 Concept of Representative Volume Element (RVE) and Statistical Volume Element (SVE)

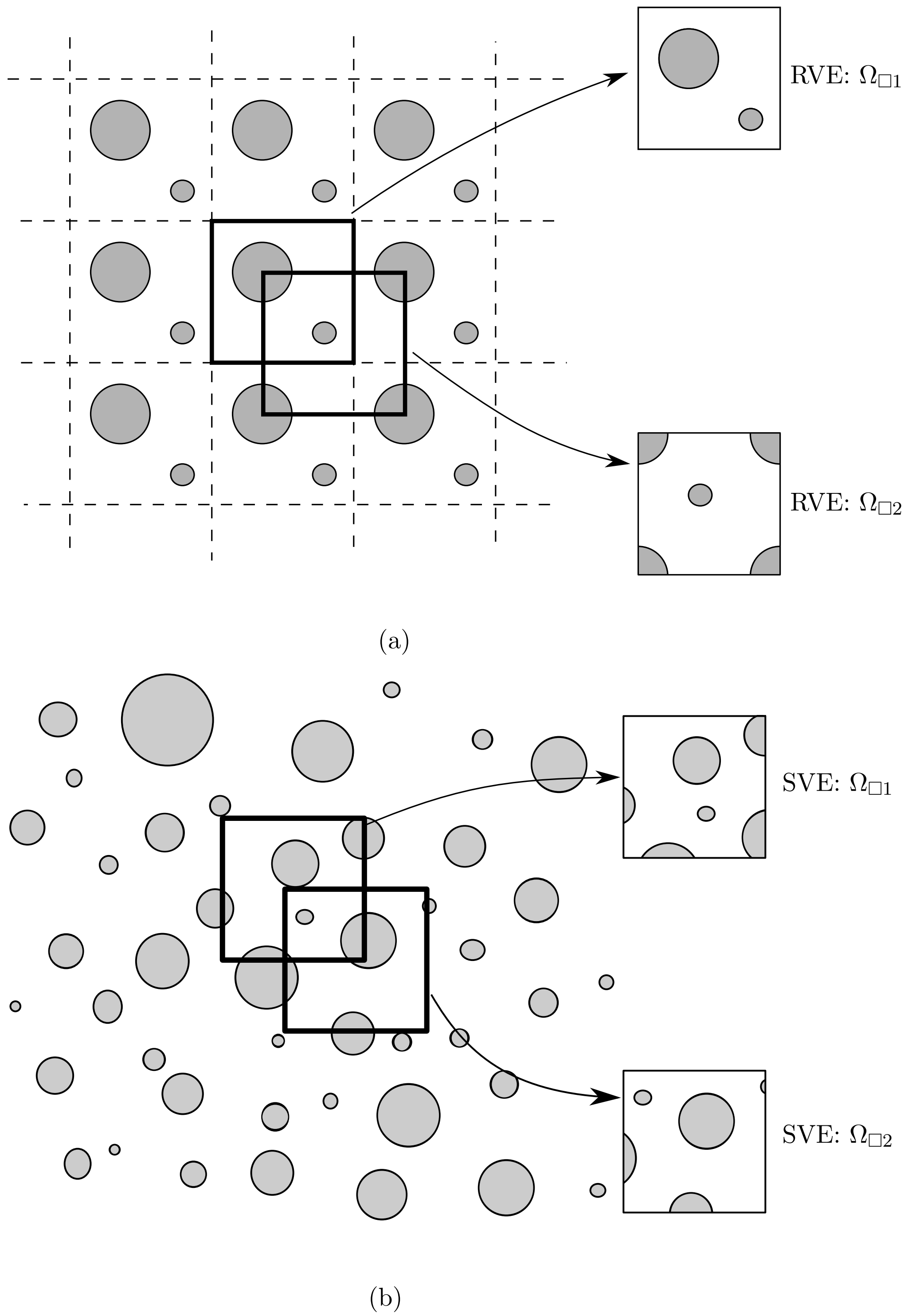
The macroscopic (or effective, overall) properties of any material, such as the elasticity modulus tensor $\bar{\mathbf{E}}$, are obtained upon averaging (or homogenizing) on a socalled "computational volume" of the (micro)heterogeneous subscale structure. If this subscale domain is "sufficiently large" (the precise meaning of which is somewhat arbitrary), it is commonly denoted a Representative Volume Element (RVE). Theoretically, the RVE should have infinite size for a completely irregular (aperiodic) microstructure. In practice, it is clear that any computational volume must be finite-sized; hence, it is assumed to occupy the (sub)domain $\Omega_\square$ with boundary $\Gamma_\square$ and having a typical diameter $L_\square$.

Although it is quite common that each micro-constituent (phase, particle, etc) is isotropic, the resulting macroscopic property may be isotropic or anisotropic depending on the geometric (directional) properties of the constituents.

Two major characteristics of the microstructure can be identified:

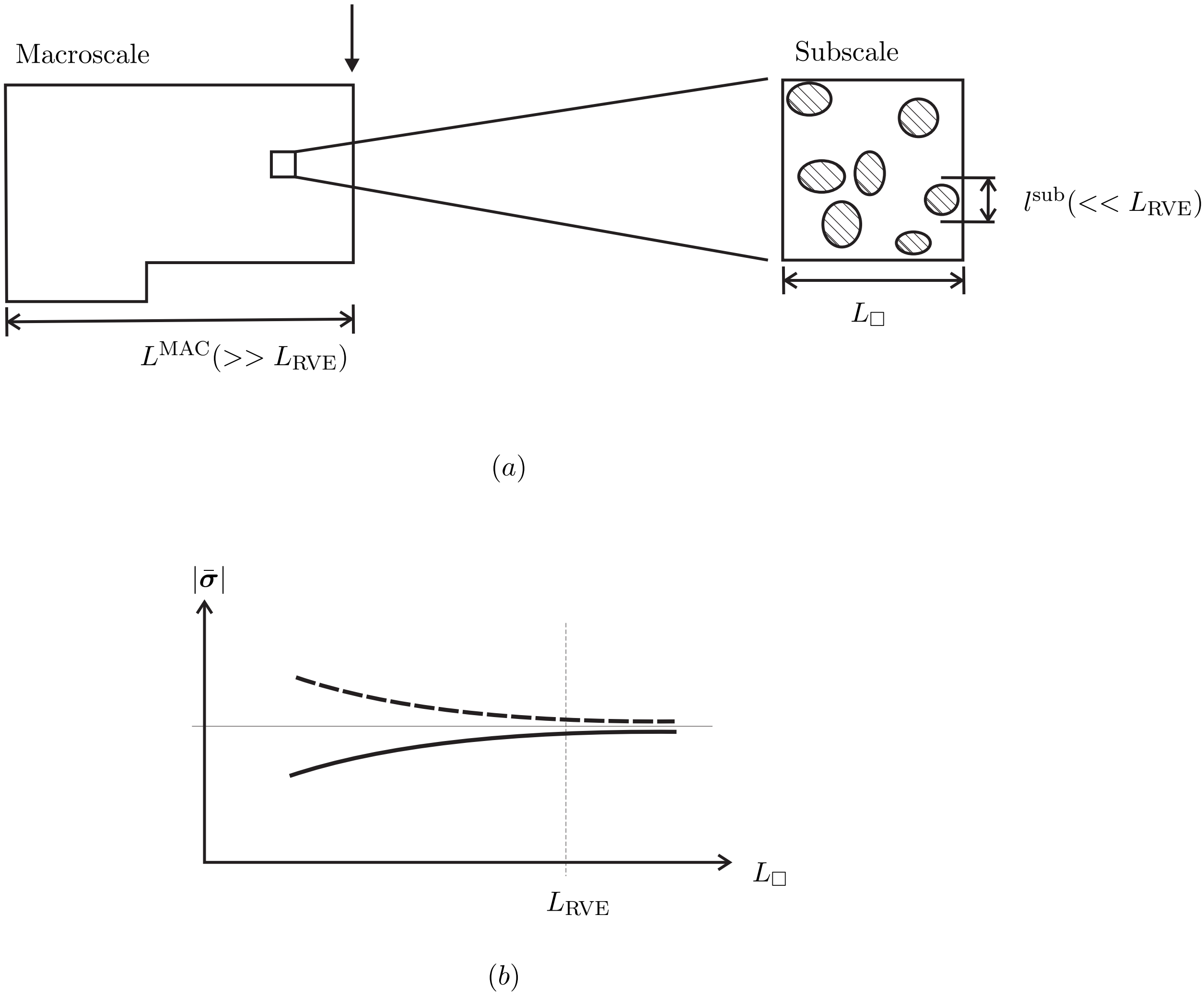
- Truly periodic microstructure, period L_{per}, as shown schematically in Figure **??**(a). In this case the proper choice of computational domain is $L_\square = L_{\text{per}}$, and any resulting computational domain $\Omega_\square$ will constitute an RVE. In combination with truly periodic, denoted "strongly periodic" in what follows, boundary conditions (as discussed in Section 2.4), the exact value of $\bar{\mathbf{E}}$ is obtainable for any choice of $\Omega_\square$ representing the true periodicity. Hence, $\bar{\mathbf{E}}_{\square 1} = \bar{\mathbf{E}}_{\square 2} = \bar{\mathbf{E}}$ for the two selected RVE's in Figure 2.2(a).

- Aperiodic microstructure with random characteristics, as shown schematically in Figure 2.2(b). It is normally assumed that the random properties are "statistically homogeneous", by which is meant that (loosely speaking) the homogenized result will not be affected by the choice of the centroid of $\Omega_\square$, as long as it is sufficiently large. In this general case of a truly random microstructure, the computational domain is denoted Statistical Volume Element (SVE), and we expect that $\bar{\mathbf{E}}_{\square 1} \neq \bar{\mathbf{E}}_{\square 2} \neq \bar{\mathbf{E}}$ for any feasible boundary conditions (as defined later) on the SVE.



{fig:2-3} Figure 2.2: *Illustration of particle-reinforced matrix (a) Periodic micro-structure with two selected RVE's obtained by "translation" of the centroid. (b) Aperiodic micro-structure with two different SVE's taken from a single realization of the random microstructure, which is characterized by the same average volume fractions of matrix and particles as the periodic structure.*

Henceforth we shall focus (essentially) on the general situation of a truly aperiodic microstructure. In such a case the shape of the computational volume is irrelevant in principle, and it is often taken as a cube in 3D (square in 2D) for computational simplicity. We shall also think of the situation that the microstructural features are random variables in a given macroscopic "point", which further motivates the notion Statistical Volume Element (SVE) for any realization. It is then possible to use the results from a large (but finite) number of individual realizations when $L_\square < \infty$ towards obtaining bounds for the expected value of $\bar{\mathbf{E}}$. Such a Virtual Testing strategy is based on statistical sampling and "windowing", known as "ensemble averaging", and it is described later in this text.



{fig:2-4} Figure 2.3: *(a) Requirements on the RVE-size in the case of complete scale separation visavi typical macroscale and subscale dimensions. (b) Convergence of the magnitude of the macroscopic stress* $\bar{\boldsymbol{\sigma}}$ *with increasing size of the computational volume, represented by* $L_\square$.

Remark: Normally, the measure L^{MAC} represents the macroscopic size of the considered structure (component); however, it is then presumed that the macroscopic fields are sufficiently smooth. This is not the case in the event of incipient macroscale fracture that is manifested by strong localization of the macroscale strain to a localization zone (or band). This situation is considered in Chapter 13. □

2.2.3 Average strain and stress representations

We introduce the volume average on the RVE of a given variable (or property) as

$$\langle \bullet \rangle_\square \overset{\text{def}}{=} \frac{1}{|\Omega_\square|} \int_{\Omega_\square} \bullet \, \mathrm{d}\Omega \tag{2.47}$$ {eq:2-61}

For the strain average, $\bar{\boldsymbol{\epsilon}} \overset{\text{def}}{=} \langle \boldsymbol{\epsilon} \rangle_\square$, and the stress average, $\bar{\boldsymbol{\sigma}} \overset{\text{def}}{=} \langle \boldsymbol{\sigma} \rangle_\square$, it is possible to replace the volume integral in (2.47) with expressions that involve surface integrals on the RVE. This will be shown subsequently.

For the strain average, we first make use of Gauss' theorem to obtain the identity for the displacement gradient:

$$\int_{\Omega_\square} \boldsymbol{u} \otimes \boldsymbol{\nabla} \, \mathrm{d}\Omega = \int_{\Gamma_\square} \boldsymbol{u} \otimes \boldsymbol{n} \, \mathrm{d}\Gamma \tag{2.48}$$ {eq:2-63}

where $\boldsymbol{n}$ is the outward unit normal on $\Gamma_\square$. Hence, we obtain

$$\begin{aligned} \langle \boldsymbol{\epsilon} \rangle_\square &= \frac{1}{|\Omega_\square|} \int_{\Omega_\square} \boldsymbol{\epsilon} \, \mathrm{d}\Omega = \frac{1}{|\Omega_\square|} \int_{\Omega_\square} (\boldsymbol{u} \otimes \boldsymbol{\nabla})^{\text{sym}} \, \mathrm{d}\Omega \\ &= \frac{1}{|\Omega_\square|} \int_{\Gamma_\square} (\boldsymbol{u} \otimes \boldsymbol{n})^{\text{sym}} \, \mathrm{d}\Gamma = \left(\frac{1}{|\Omega_\square|} \int_{\Gamma_\square} \boldsymbol{u} \otimes \boldsymbol{n} \, \mathrm{d}\Gamma \right)^{\text{sym}} \end{aligned} \tag{2.49}$$ {eq:2-64}

For the stress average, we first consider the identity[5]

$$\boldsymbol{\nabla} \cdot [\boldsymbol{\sigma}^{\mathrm{T}} \otimes \boldsymbol{x}] = \boldsymbol{\sigma} \cdot \boldsymbol{I} + [\boldsymbol{\sigma} \cdot \boldsymbol{\nabla}] \otimes \boldsymbol{x} = \boldsymbol{\sigma} - \boldsymbol{f} \otimes \boldsymbol{x} \tag{2.50}$$ {eq:2-65}

where we used the identity[6] $\boldsymbol{x} \otimes \boldsymbol{\nabla} = \boldsymbol{I}$ and the static equilibrium equation[7] expressed as

$$-\boldsymbol{\sigma} \cdot \boldsymbol{\nabla} = \boldsymbol{f} \ \text{ in } \ \Omega_\square \tag{2.51}$$ {eq:2-66}

Hence, we obtain with Gauss' theorem

$$\begin{aligned} \langle \boldsymbol{\sigma} \rangle_\square &= \frac{1}{|\Omega_\square|} \int_{\Omega_\square} \boldsymbol{\sigma} \, \mathrm{d}\Omega = \frac{1}{|\Omega_\square|} \int_{\Omega_\square} \boldsymbol{\nabla} \cdot [\boldsymbol{\sigma}^{\mathrm{T}} \otimes \boldsymbol{x}] \, \mathrm{d}\Omega + \frac{1}{|\Omega_\square|} \int_{\Omega_\square} \boldsymbol{f} \otimes \boldsymbol{x} \, \mathrm{d}\Omega \\ &= \frac{1}{|\Omega_\square|} \int_{\Gamma_\square} \underbrace{\boldsymbol{n} \cdot \boldsymbol{\sigma}^{\mathrm{T}}}_{=\boldsymbol{t}} \otimes \boldsymbol{x} \, \mathrm{d}\Gamma + \frac{1}{|\Omega_\square|} \int_{\Omega_\square} \boldsymbol{f} \otimes \boldsymbol{x} \, \mathrm{d}\Omega \end{aligned} \tag{2.52}$$ {eq:2-67}

where it was used that $\boldsymbol{t} = \boldsymbol{\sigma} \cdot \boldsymbol{n} = \boldsymbol{n} \cdot \boldsymbol{\sigma}^{\mathrm{T}}$. In the *special case* of vanishing volume load, $\boldsymbol{f} = \boldsymbol{0}$, we obtain

$$\langle \boldsymbol{\sigma} \rangle_\square = \frac{1}{|\Omega_\square|} \int_{\Gamma_\square} \boldsymbol{t} \otimes \boldsymbol{x} \, \mathrm{d}\Gamma = \left(\frac{1}{|\Omega_\square|} \int_{\Gamma_\square} \boldsymbol{t} \otimes \boldsymbol{x} \, \mathrm{d}\Gamma \right)^{\text{sym}} \tag{2.53}$$ {eq:ch2_11}

where the last identity follows from the symmetry of $\boldsymbol{\sigma}$. Henceforth in this Chapter, we make the significant assumption that $\boldsymbol{f} = \boldsymbol{0}$, which has a profound importance for classical homogenization results.

[5] $(\boldsymbol{\nabla} \cdot [\boldsymbol{\sigma}^{\mathrm{T}} \otimes \boldsymbol{x}])_{iI} = (\sigma^{\mathrm{T}}_{Ji} x_I)_{,J} = \sigma_{iJ,J} x_I + \sigma_{iJ} \delta_{IJ} = \sigma_{iI} - f_i x_I$

[6] $(\boldsymbol{x} \otimes \boldsymbol{\nabla})_{IJ} = x_{I,J} = \delta_{IJ}$

[7] $-\sigma_{iJ,J} = f_i$

2.2.4 Average strain and stress representations in the presence of cracks/pores

Include!!!

2.2.5 First order homogenization

According to the classical assumption of *first order homogenization*, we introduce the additive split of the displacement field $\boldsymbol{u}(\boldsymbol{x})$ into the macroscale field $\boldsymbol{u}^{\mathrm{M}}(\boldsymbol{x})$ and the fluctuation field $\boldsymbol{u}^{\mu}(\boldsymbol{x})$[8] within a given RVE occupying $\Omega_{\square}$:

{eq:2-68}
$$\boldsymbol{u}(\boldsymbol{x}) = \boldsymbol{u}^{\mathrm{M}}(\boldsymbol{x}) + \boldsymbol{u}^{\mu}(\boldsymbol{x}), \quad \boldsymbol{u}^{\mathrm{M}}(\boldsymbol{x}) = \bar{\boldsymbol{\epsilon}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}], \quad \boldsymbol{x} \in \Omega_{\square} \tag{2.54}$$

which means that the strain is decomposed as

{eq:2-69}
$$\boldsymbol{\epsilon}(\boldsymbol{x}) = \bar{\boldsymbol{\epsilon}} + \boldsymbol{\epsilon}^{\mu}(\boldsymbol{x}), \quad \boldsymbol{\epsilon}^{\mu} = \boldsymbol{\epsilon}[\boldsymbol{u}^{\mu}] \quad \boldsymbol{x} \in \Omega_{\square} \tag{2.55}$$

It is noted that $\bar{\boldsymbol{\epsilon}}$ is a truly constant field within $\Omega_{\square}$.

Remark: The choice of the "reference point" $\bar{\boldsymbol{x}}$ is arbitrary and is a matter of convenience. A common choice is the volume center of the SVE, i.e. $\bar{\boldsymbol{x}} = \langle \boldsymbol{x} \rangle_{\square}$. □

2.2.6 The Hill-Mandel macrohomogeneity condition - Classical version

l version}

So far we have not established the link between the macroscale strain and stress variables, $\bar{\boldsymbol{\epsilon}}$ and $\bar{\boldsymbol{\sigma}}$, and the corresponding fine-scale fields $\boldsymbol{\epsilon}$ and $\boldsymbol{\sigma}$ within a given SVE. The missing link is established via the so-called *Hill-Mandel macrohomogeneity condition(s)*. In this Chapter, we give the classical statements of the H-M condition[9] in a form that is valid for subscale linear elasticity, cf. SUQUET [1987][10], NEMAT-NASSER AND HORI [1993][11]. However, we shall also briefly extend to the situation of nonlinear material properties.

In establishing the H-M condition it is illuminating to separately consider the two situations of macroscale strain control ($\bar{\boldsymbol{\epsilon}}$ is prescribed) and macroscale stress control ($\bar{\boldsymbol{\sigma}}$ is prescribed).

H-M condition for macroscale strain control

For given $\bar{\boldsymbol{\epsilon}}$ the task is to compute the resulting subscale fields $\boldsymbol{u}(\boldsymbol{x}) \rightarrow \boldsymbol{\epsilon}(\boldsymbol{x})$ and $\boldsymbol{\sigma}(\boldsymbol{x})$ for $\boldsymbol{x} \in \Omega_{\square}$. The problem formulation for the RVE must then be posed such that the following two types of identities (constraints) hold:

- Strain identity:

{eq:2-71}
$$\langle \boldsymbol{\epsilon} \rangle_{\square} = \bar{\boldsymbol{\epsilon}} \tag{2.56}$$

- Work identity:

{eq:2-72}
$$\langle \boldsymbol{\sigma} : \boldsymbol{\epsilon} \rangle_{\square} = \langle \boldsymbol{\sigma} \rangle_{\square} : \langle \boldsymbol{\epsilon} \rangle_{\square} \, [= \langle \boldsymbol{\sigma} \rangle_{\square} : \bar{\boldsymbol{\epsilon}}] \tag{2.57}$$

[8] To indicate the two-scale dependence, we may write (2.54) as $\boldsymbol{u}(\boldsymbol{x};\bar{\boldsymbol{x}}) = \bar{\boldsymbol{u}}(\bar{\boldsymbol{x}}) + \bar{\boldsymbol{\epsilon}}(\bar{\boldsymbol{x}}) \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}] + \boldsymbol{u}^{\mu}(\boldsymbol{x})$, where $\bar{\boldsymbol{x}}$ is now considered as the macroscale independent spatial coordinate.

[9] We shall later elaborate on the H-M condition in the context of Variationally Consistent Homogenization, where it is shown that the classical statements are, in fact, unnecessarily restrictive.

[10] Suequet [1987] Springer Lecture Notes: Homogenization techniques for composite media

[11] Nemat-Nasser and Hori [1993] Micromechanics: Overall Properties of Heterogeneous Materials

The macroscale stress is computed as $\bar{\boldsymbol{\sigma}} := \langle \boldsymbol{\sigma} \rangle_\square$ in a "postprocessing" step; hence, this identity is *not a constraint* that must be satisfied a priori as part of the problem solution.

Remark: In the general case of nonlinear material properties, e.g. nonlinear elasticity, we consider a linearization of the solution w.r.t. $\bar{\boldsymbol{\epsilon}}$. In other words, we consider the differential fields $\mathrm{d}\boldsymbol{u}(\boldsymbol{x}) \to \mathrm{d}\boldsymbol{\epsilon}(\boldsymbol{x})$ and $\mathrm{d}\boldsymbol{\sigma}(\boldsymbol{x})$ for $\boldsymbol{x} \in \Omega_\square$ due to the change $\mathrm{d}\bar{\boldsymbol{\epsilon}}$. The constraints (2.56-2.57) are then replaced by

$$\langle \boldsymbol{\epsilon} \rangle_\square = \bar{\boldsymbol{\epsilon}} \quad \Rightarrow \quad \langle \mathrm{d}\boldsymbol{\epsilon} \rangle_\square = \mathrm{d}\bar{\boldsymbol{\epsilon}} \tag{2.58}$$ {eq:2-73}

$$\langle \boldsymbol{\sigma} : \mathrm{d}\boldsymbol{\epsilon} \rangle_\square = \langle \boldsymbol{\sigma} \rangle_\square : \langle \mathrm{d}\boldsymbol{\epsilon} \rangle_\square \, [= \langle \boldsymbol{\sigma} \rangle_\square : \mathrm{d}\bar{\boldsymbol{\epsilon}}] \tag{2.59}$$ {eq:2-74}

Again, the macroscale stress can be computed as $\bar{\boldsymbol{\sigma}} := \langle \boldsymbol{\sigma} \rangle_\square$ in a "postprocessing" step; hence, we must note that this identity is *not a constraint* that must be satisfied a priori as part of the problem solution. □

H-M condition for macroscale stress control

For given $\bar{\boldsymbol{\sigma}}$ the task is to compute the resulting subscale fields $\boldsymbol{u}(\boldsymbol{x}) \to \boldsymbol{\epsilon}(\boldsymbol{x})$ and $\boldsymbol{\sigma}(\boldsymbol{x})$ for $\boldsymbol{x} \in \Omega_\square$. The problem formulation for the RVE must then be posed such that the following two types of identities (constraints) hold:

- Stress identity:

$$\langle \boldsymbol{\sigma} \rangle_\square = \bar{\boldsymbol{\sigma}} \tag{2.60}$$ {eq:2-75}

- Work identity:

$$\langle \boldsymbol{\epsilon} : \boldsymbol{\sigma} \rangle_\square = \langle \boldsymbol{\epsilon} \rangle_\square : \langle \boldsymbol{\sigma} \rangle_\square \, [= \langle \boldsymbol{\epsilon} \rangle_\square : \bar{\boldsymbol{\sigma}}] \tag{2.61}$$ {eq:2-76}

The macroscale strain is computed as $\bar{\boldsymbol{\epsilon}} := \langle \boldsymbol{\epsilon} \rangle_\square$ in a "postprocessing" step; hence, this identity is *not a constraint* that must be satisfied a priori as part of the problem solution.

The conditions (2.57) and (2.59) state that the *internal work*, or the *internal complementary work*, on the macroscale equals that of the subscale. In order to check if this condition is satisfied for different (approximate) assumptions of $\boldsymbol{\epsilon}$ and/or $\boldsymbol{\sigma}$ on $\Gamma_\square$, we note the following useful relation between properties in on $\Omega_\square$ and on $\Gamma_\square$ (that is obtained using Gauss' theorem):

$$\langle \boldsymbol{\sigma} : \boldsymbol{\epsilon} \rangle_\square \;=\; \frac{1}{|\Omega_\square|} \int_{\Omega_\square} \boldsymbol{\sigma} : \boldsymbol{\epsilon} \, \mathrm{d}\Omega = \frac{1}{|\Omega_\square|} \int_{\Gamma_\square} \boldsymbol{t} \cdot \boldsymbol{u} \, \mathrm{d}\Gamma \tag{2.62}$$ {eq:2-77}

where we used the assumption $\boldsymbol{f} = \boldsymbol{0}$, and where $\boldsymbol{t} = \boldsymbol{\sigma} \cdot \boldsymbol{n}$ on $\Gamma_\square$.

Remark: A more general formulation of the Hill-Mandel macrohomogeneity condition that is valid also in the case of non-vanishing volume-specific load, $\boldsymbol{f} \neq \boldsymbol{0}$, is discussed later. □

Let us next introduce the additive decomposition into macroscale and subscale fluctuation fields for the stresses and displacements (and strains) inside an SVE, i.e. for $\boldsymbol{x} \in \Omega_\square$:

$$\boldsymbol{u}(\boldsymbol{x}) \;=\; \bar{\boldsymbol{\epsilon}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}] + \boldsymbol{u}^\mu(\boldsymbol{x}) \quad \Rightarrow \quad \boldsymbol{\epsilon}(\boldsymbol{x}) = \bar{\boldsymbol{\epsilon}} + \boldsymbol{\epsilon}^\mu(\boldsymbol{x}), \quad \langle \boldsymbol{\epsilon}^\mu \rangle_\square = \boldsymbol{0} \tag{2.63}$$ {eq:2-78}

$$\boldsymbol{\sigma}(\boldsymbol{x}) \;=\; \bar{\boldsymbol{\sigma}} + \boldsymbol{\sigma}^\mu(\boldsymbol{x}) \quad \langle \boldsymbol{\sigma}^\mu \rangle_\square = \boldsymbol{0} \tag{2.64}$$ {eq:2-79}

where we used the strain and stress identities/conditions. With these decompositions, we may write

$$\begin{aligned}\langle \boldsymbol{\sigma} : \boldsymbol{\epsilon} \rangle_\square &= \langle [\bar{\boldsymbol{\sigma}} + \boldsymbol{\sigma}^\mu] : [\bar{\boldsymbol{\epsilon}} + \boldsymbol{\epsilon}^\mu] \rangle_\square \\ &= \bar{\boldsymbol{\sigma}} : \bar{\boldsymbol{\epsilon}} + \bar{\boldsymbol{\sigma}} : \underbrace{\langle \boldsymbol{\epsilon}^\mu \rangle_\square}_{=\mathbf{0}} + \underbrace{\langle \boldsymbol{\sigma}^\mu \rangle_\square}_{=\mathbf{0}} : \bar{\boldsymbol{\epsilon}} + \langle \boldsymbol{\sigma}^\mu : \boldsymbol{\epsilon}^\mu \rangle_\square \\ &= \bar{\boldsymbol{\sigma}} : \bar{\boldsymbol{\epsilon}} + \langle \boldsymbol{\sigma}^\mu : \boldsymbol{\epsilon}^\mu \rangle_\square \end{aligned} \tag{2.65}$$ {eq:2-81}

Hence, we may express the macrohomogeneity condition as

{eq:2-82}
$$\langle \boldsymbol{\sigma}^\mu : \boldsymbol{\epsilon}^\mu \rangle_\square = 0 \tag{2.66}$$

Using the boundary representation in (2.62), we may reformulate (2.66) as the condition

{eq:2-83}
$$\int_{\Gamma_\square} \boldsymbol{t}^\mu \cdot \boldsymbol{u}^\mu \, \mathrm{d}\Gamma = 0 \tag{2.67}$$

or, alternatively,

{eq:2-85}
$$\int_{\Gamma_\square} [\boldsymbol{t} - \bar{\boldsymbol{\sigma}} \cdot \boldsymbol{n}] \cdot [\boldsymbol{u} - \bar{\boldsymbol{\epsilon}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}]] \, \mathrm{d}\Gamma = 0 \tag{2.68}$$

This expression is commonly found in the literature, e.g. Zohdi and Wriggers [2008][12].

2.2.7 Macroscale strain energy

Consider (for the sake of brevity) the situation of macroscale strain control. It is of considerable interest that the H-M condition can be used to identify a macroscale strain energy density, denoted $\bar{\psi}(\bar{\boldsymbol{\epsilon}})$, that serves as a potential for $\bar{\boldsymbol{\sigma}}$, and that $\bar{\psi}(\bar{\boldsymbol{\epsilon}})$ is defined as the volume-average of the corresponding fine-scale energy density $\psi(\boldsymbol{\epsilon})$. In the case of linear elasticity, we have $\psi(\boldsymbol{\epsilon}) = \frac{1}{2}\boldsymbol{\epsilon} : \mathsf{E} : \boldsymbol{\epsilon}$. To show this, we use the H-M condition to obtain the identity

{eq:2-87}
$$\underbrace{\langle \frac{1}{2}\boldsymbol{\epsilon} : \mathsf{E} : \boldsymbol{\epsilon} \rangle_\square}_{=\psi(\boldsymbol{\epsilon})} = \underbrace{\frac{1}{2}\bar{\boldsymbol{\epsilon}} : \bar{\mathsf{E}} : \bar{\boldsymbol{\epsilon}}}_{:=\bar{\psi}(\bar{\boldsymbol{\epsilon}})} \tag{2.69}$$

We thus conclude that

{eq:2-88}
$$\bar{\boldsymbol{\sigma}}(\bar{\boldsymbol{\epsilon}}) = \frac{\partial \bar{\psi}(\bar{\boldsymbol{\epsilon}})}{\partial \bar{\boldsymbol{\epsilon}}} \quad \text{with} \quad \bar{\psi}(\bar{\boldsymbol{\epsilon}}) \stackrel{\text{def}}{=} \langle \psi(\boldsymbol{\epsilon}\{\bar{\boldsymbol{\epsilon}}\}) \rangle_\square, \tag{2.70}$$

where it was used that

{eq:2-89}
$$\mathrm{d}\bar{\psi}(\bar{\boldsymbol{\epsilon}}) = \mathrm{d}\left(\frac{1}{2}\bar{\boldsymbol{\epsilon}} : \bar{\mathsf{E}} : \bar{\boldsymbol{\epsilon}}\right) = \bar{\boldsymbol{\epsilon}} : \bar{\mathsf{E}} : \mathrm{d}\bar{\boldsymbol{\epsilon}} = \bar{\boldsymbol{\sigma}}(\bar{\boldsymbol{\epsilon}}) : \mathrm{d}\bar{\boldsymbol{\epsilon}} \tag{2.71}$$

Remark: In the case of nonlinear properties, we argue as follows. Firstly, we assume that there exists a strain density $\psi(\boldsymbol{\epsilon})$ (which may be of algorithmic character; the simplest being nonlinear elasticity) such that $\boldsymbol{\sigma}(\boldsymbol{\epsilon}) = \frac{\partial \psi(\boldsymbol{\epsilon})}{\partial \boldsymbol{\epsilon}}$. From the H-M condition we now obtain

{eq:2-91}
$$\langle \boldsymbol{\sigma}(\boldsymbol{\epsilon}) : \mathrm{d}\boldsymbol{\epsilon} \rangle_\square = \bar{\boldsymbol{\sigma}} : \mathrm{d}\bar{\boldsymbol{\epsilon}} \tag{2.72}$$

Once again we arrive at (2.70) upon noting that the LHS of (2.72) can be evaluated as

{eq:2-92}
$$\langle \boldsymbol{\sigma}(\boldsymbol{\epsilon}) : \mathrm{d}\boldsymbol{\epsilon} \rangle_\square = \langle \frac{\partial \psi(\boldsymbol{\epsilon})}{\partial \boldsymbol{\epsilon}} : \mathrm{d}\boldsymbol{\epsilon} \rangle_\square = \mathrm{d}\langle \psi(\boldsymbol{\epsilon}) \rangle_\square = \langle \boldsymbol{\sigma}(\boldsymbol{\epsilon}) \rangle_\square : \langle \mathrm{d}\boldsymbol{\epsilon} \rangle_\square \tag{2.73}$$

where $\mathrm{d}\boldsymbol{\epsilon} \stackrel{\text{def}}{=} \boldsymbol{\epsilon}'\{\bar{\boldsymbol{\epsilon}}; \mathrm{d}\bar{\boldsymbol{\epsilon}}\}$ is the sensitivity of $\boldsymbol{\epsilon}$ for change of $\bar{\boldsymbol{\epsilon}}$. $\square$

[12] Zohdi and Wriggers [2008]: An Introduction to Computational Micromechanics

2.2.8 Effective linear elastic stiffness and compliance tensors

The issue is how to obtain the effective material response in terms of $\bar{\mathbf{E}}$ for given fine-scale distribution of $\mathbf{E}$. [The arguments for $\bar{\mathbf{C}}$ are completely analogous and, therefore, omitted here.] It is recalled that $\bar{\mathbf{E}} = \bar{\mathbf{E}}_\square$ for sufficiently large $L_\square$. The basic challenge is then to extract the (generally non-symmetric) 4th order "strain concentration tensor" $\mathbf{A}(\boldsymbol{x}) = \mathbf{A}_\epsilon(\boldsymbol{x})$ for $\boldsymbol{x} \in \Omega_\square$ in the relation

$$\boldsymbol{\epsilon}(\boldsymbol{x}) = \mathbf{A}(\boldsymbol{x}) : \bar{\boldsymbol{\epsilon}}, \quad \boldsymbol{x} \in \Omega_\square \tag{2.74}$$ {eq:2-94}

and using the conditions $\langle \boldsymbol{\epsilon} \rangle_\square = \bar{\boldsymbol{\epsilon}}$ and $\langle \boldsymbol{\sigma} \rangle_\square = \bar{\boldsymbol{\sigma}}$ to obtain

$$\bar{\boldsymbol{\epsilon}} = \langle \boldsymbol{\epsilon} \rangle_\square = \langle \mathbf{A} \rangle_\square : \bar{\boldsymbol{\epsilon}} \quad \Rightarrow \quad \langle \mathbf{A} \rangle_\square = \mathbf{I} \tag{2.75}$$ {eq:2-95}

$$\bar{\boldsymbol{\sigma}} = \langle \boldsymbol{\sigma} \rangle_\square = \langle \mathbf{E} \colon \boldsymbol{\epsilon} \rangle_\square = \langle \mathbf{E} \colon \mathbf{A} \rangle_\square \colon \bar{\boldsymbol{\epsilon}} \quad \Rightarrow \quad \bar{\mathbf{E}} = \langle \mathbf{E} \colon \mathbf{A} \rangle_\square \tag{2.76}$$ {eq:2-96}

where $\mathbf{I}$ is the 4th order identity tensor[13]. Note that it is not possible to make any conclusions as regarding the major symmetry of $\bar{\mathbf{E}}$ based on (2.76). To do this, we introduce the Hill-Mandel condition in the form

$$\bar{\boldsymbol{\sigma}} : \bar{\boldsymbol{\epsilon}} = \langle \boldsymbol{\sigma} : \boldsymbol{\epsilon} \rangle_\square = \langle \boldsymbol{\epsilon} : \mathbf{E} : \boldsymbol{\epsilon} \rangle_\square \tag{2.77}$$ {eq:2-97}

Upon introducing the relation (2.74) into (2.77), we obtain

$$\bar{\mathbf{E}} = \langle \mathbf{A}^{\mathrm{T}} : \mathbf{E} : \mathbf{A} \rangle_\square \tag{2.78}$$ {eq:2-98}

This expression shows that $\bar{\mathbf{E}}$ possesses major symmetry, in view of the symmetry of the subscale constitutive tensor $\mathbf{E}$.

We note that $\bar{\mathbf{E}}$ is never computable exactly in practice, since this would require the *exact* solution of the strain concentration field $\mathbf{A}$ within the RVE. Obviously, this would require the true resolution of the subscale properties within an infinitely large RVE (for a random medium). Rather, it is common to opt for techniques to obtain

- bounds on (the eigenvalues) of $\bar{\mathbf{E}}$, or
- a good approximation of $\bar{\mathbf{E}}$

As to the issue of computing an accurate value of $\bar{\mathbf{E}}$ for an arbitrary subscale structure (without any particular features that simplify the computation of sharp bounds), we note that $\bar{\mathbf{E}}$ can be expressed in closed-form and computed a priori *independent of* $\bar{\boldsymbol{\epsilon}}$ only when the subscale material properties are linear elastic and static loading conditions are assumed (inertia forces ignored). Moreover, it is necessary to make "clever" approximations of the strain and stress fields within the RVE. However, for a complex substructure the most versatile approach is to (i) choose the boundary conditions on the SVE in such a way that the Hill-Mandel condition is satisfied and to (ii) use FE-discretization of the subscale, which motivates the notion of *computational homogenization*. Two conceptually different strategies can thus be identified:

Classical mean-field approaches

In the literature on classical (non-computational) homogenization, a variety of methods have been proposed for obtaining a good approximation of $\bar{\mathbf{E}}$ via "clever" approximation of the strain concentration field $\mathbf{A}$ within a sufficiently large SVE. Such estimates are preferably carried out under the assumptions/constraints:

[13] $(\mathbf{I})_{ijkl} = \delta_{ik}\delta_{jl}$

- Minimal (or no) knowledge about the actual topology of the subscale constituents are used
- Simplified closed-form solutions of the field $\mathbf{A}$ are sought for homogeneous inclusions (or particles) in a homogeneous matrix material

The most important of these simplified, socalled "mean-field", approaches are discussed subsequently in Section 2.3.

Computational homogenization based on FE-analysis

By "computational homogenization" we denote the strategy to compute the field $\mathbf{A}$ using FE-analysis of a "SVE-problem" for a finite-sized SVE. The following assumptions, or constraints, are then introduced:

- Boundary conditions are specified on the SVE so as to satisfy the Hill-Mandel macrohomogenity condition(s).
- The solution to the SVE-problem, in terms of the strain concentration field $\mathbf{A}$, is computed for sufficiently many realizations of the random-field fine-scale features that are defined by the field $\mathbf{E}$. Ideally, it is necessary (or at least strongly desirable) to represent the true 3D-character of the fine-scale topology and material properties in order to obtain predictive results. The appropriate socalled Virtual Testing strategy is presented in Chapter 7.

We remark that the quality of the homogenized response critically depends on, not only the boundary conditions and the accuracy of the subscale representation, but also on the FE-resolution of the subscale features.

Remark: All types of error in establishing the true strain concentration field $\mathbf{A}$ that emanate from the fine-scale approximations (including the FE-discretization within the SVE) can be treated as model errors in the context of adaptive modeling, as discussed in Chapter 9. $\square$

2.3 Classical estimates of effective properties

properties}

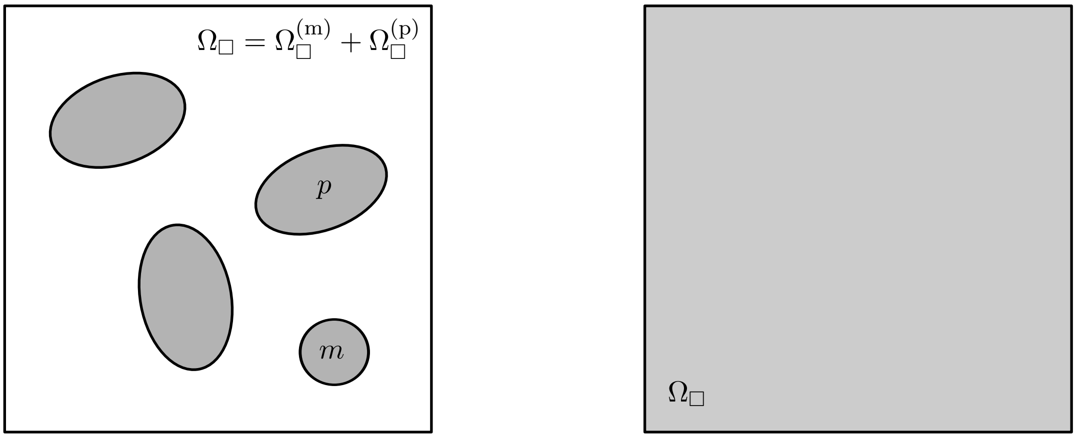
2.3.1 Mean-field models – Preliminaries

Classical estimates of the effective properties are based on socalled "mean-field models". No information about the actual subscale topology is used, and RVE is assumed to have infinite size.

Consider the ideal composite that consists of two distinct phases: The homogeneous contiguous matrix occupying the domain $\Omega_\square^{(\mathrm{m})}$ and the embedded microinclusions (particles) that may be arbitrarily shaped and distributed in the matrix and collectively occupy the subdomain $\Omega_\square^{(\mathrm{p})}$, as shown in Figure 2.5(a). Most importantly, both the matrix and the inclusions are assumed to be *homogeneous* with constant elasticity tensors $\mathbf{E}^{(\mathrm{m})}$ and $\mathbf{E}^{(\mathrm{p})}$, respectively. The corresponding volume fractions are

{eq:2-101}

$$n^{(\mathrm{m})} \overset{\mathrm{def}}{=} \frac{|\Omega_\square^{(\mathrm{m})}|}{|\Omega_\square|}, \quad n^{(\mathrm{p})} \overset{\mathrm{def}}{=} \frac{|\Omega_\square^{(\mathrm{p})}|}{|\Omega_\square|}, \quad n^{(\mathrm{m})} + n^{(\mathrm{p})} = 1 \tag{2.79}$$



(a) (b)

{fig:2-5} Figure 2.4: *(a) RVE with two distinct phases: homogeneous matrix (m):* $\Omega_\Box^{(\mathrm{m})}, \mathsf{E}^{(\mathrm{m})}$ *and distributed homogeneous particles (microinclusions) (p):* $\Omega_\Box^{(\mathrm{p})}, \mathsf{E}^{(\mathrm{p})}$*. (b) Comparison-RVE with one single homogenous comparison material,* E_0*, subjected to eigenstrains in* $\Omega_\Box^{(\mathrm{p})}$*.*

Here we shall consider only the DBC-problem with macroscale strain control (prescribed boundary displacements). [The dual case of the NBC-problem with macroscale stress control (prescribed boundary tractions) can be treated in a similar fashion and is, therefore, omitted]. We thus consider the case

$$\boldsymbol{u}(\boldsymbol{x}) = \bar{\boldsymbol{\epsilon}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}] + \boldsymbol{u}^\mu(\boldsymbol{x}), \quad \boldsymbol{x} \in \Gamma_\Box \tag{2.80}$$ {eq:2-102}

for given value of $\bar{\boldsymbol{\epsilon}}$. In the general case, both strain and stress fields vary locally (fluctuate) within each phase: For example, the strain fluctuation can be expressed via the strain concentration tensor given in (2.74)

$$\boldsymbol{\epsilon}(\boldsymbol{x}) = \mathsf{A}(\boldsymbol{x}) : \bar{\boldsymbol{\epsilon}}, \quad \boldsymbol{x} \in \Omega_\Box \tag{2.81}$$ {eq:2-103}

The stress field in the two phase can be expressed as

$$\boldsymbol{\sigma}(\boldsymbol{x}) = \mathsf{E}^{(\alpha)} : \boldsymbol{\epsilon}(\boldsymbol{x}), \quad \boldsymbol{x} \in \Omega_\Box^{(\alpha)} \quad \alpha = \mathrm{m}, \mathrm{p} \tag{2.82}$$ {eq:2-104}

Due to the piecewise homogenous microstructure, it turns out useful to introduce phase averages, or *mean fields*, as follows

$$\bar{\boldsymbol{\epsilon}}^{(\alpha)} \stackrel{\mathrm{def}}{=} \langle \boldsymbol{\epsilon} \rangle_\Box^{(\alpha)}, \quad \bar{\boldsymbol{\sigma}}^{(\alpha)} \stackrel{\mathrm{def}}{=} \langle \boldsymbol{\sigma} \rangle_\Box^{(\alpha)} \quad \alpha = \mathrm{m}, \mathrm{p} \tag{2.83}$$ {eq:2-105}

where we introduced the phase volume average

$$\langle \bullet \rangle_\Box^{(\alpha)} \stackrel{\mathrm{def}}{=} \frac{1}{|\Omega_\Box^{(\alpha)}|} \int_{\Omega_\Box^{(\alpha)}} \bullet \, \mathrm{d}\Omega \quad \alpha = \mathrm{m}, \mathrm{p} \tag{2.84}$$ {eq:2-106}

We then define phase concentrations

$$\bar{\boldsymbol{\epsilon}}^{(\alpha)} = \bar{\mathsf{A}}^{(\alpha)} : \bar{\boldsymbol{\epsilon}} \quad \text{with } \bar{\mathsf{A}}^{(\alpha)} \stackrel{\mathrm{def}}{=} \langle \mathsf{A} \rangle_\Box^{(\alpha)}, \quad \alpha = \mathrm{m}, \mathrm{p} \tag{2.85}$$ {eq:2-107}

The identity

$$n^{(\mathrm{m})} \bar{\boldsymbol{\epsilon}}^{(\mathrm{m})} + n^{(\mathrm{p})} \bar{\boldsymbol{\epsilon}}^{(\mathrm{p})} = \bar{\boldsymbol{\epsilon}} \tag{2.86}$$ {eq:2-108}

gives, together with (2.85), the relation

$$n^{(\mathrm{m})}\bar{\mathbf{A}}^{(\mathrm{m})} + n^{(\mathrm{p})}\bar{\mathbf{A}}^{(\mathrm{p})} = \mathbf{I} \tag{2.87}$$ {eq:2-109}

The effective elastic stiffness can thus be expressed as

$$\bar{\mathbf{E}} = n^{(\mathrm{m})}\mathbf{E}^{(\mathrm{m})} : \bar{\mathbf{A}}^{(\mathrm{m})} + n^{(\mathrm{p})}\mathbf{E}^{(\mathrm{p})} : \bar{\mathbf{A}}^{(\mathrm{p})} = \mathbf{E}^{(\mathrm{m})} + n^{(\mathrm{p})}\Delta\mathbf{E} : \bar{\mathbf{A}}^{(\mathrm{p})} \tag{2.88}$$ {eq:2-110}

with $\Delta\mathbf{E} \stackrel{\mathrm{def}}{=} \mathbf{E}^{(\mathrm{p})} - \mathbf{E}^{(\mathrm{m})}$.

Remark: The relation (2.88) is exact, independent on the shape and distribution of the inclusions. □

2.3.2 Voigt upper bound and Reuss lower bounds

Two extreme assumptions on the strain and stress fields within the RVE are commonly adopted.

Voigt (Taylor) assumption: The subscale strain field $\boldsymbol{\epsilon}$ is uniform, i.e. $\boldsymbol{\epsilon} = \bar{\boldsymbol{\epsilon}}$ in $\Omega_\square$. We then obtain

{eq:2-111}
$$\bar{\boldsymbol{\sigma}} = \langle\boldsymbol{\sigma}\rangle_\square = \langle\mathbf{E}\rangle_\square : \bar{\boldsymbol{\epsilon}} \quad \Rightarrow \quad \bar{\mathbf{E}}_\square = \bar{\mathbf{E}}_\square^{\mathrm{V}} := \langle\mathbf{E}\rangle_\square \tag{2.89}$$

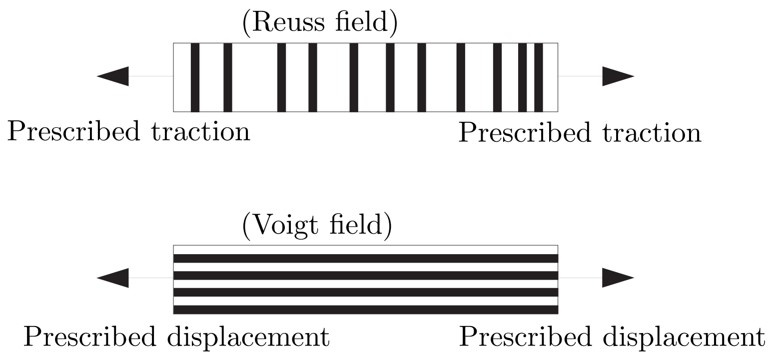
where superscript (V) stands for Voigt.

Reuss (Hill-Sachs) assumption: The subscale stress field $\boldsymbol{\sigma}$ is uniform, i.e. $\boldsymbol{\sigma} = \bar{\boldsymbol{\sigma}}$ in $\Omega_\square$, whereby we obtain[14]

{eq:2-112}
$$\bar{\boldsymbol{\epsilon}} = \langle\boldsymbol{\epsilon}\rangle_\square = \langle\mathbf{C}\rangle_\square : \bar{\boldsymbol{\sigma}} \quad \Rightarrow \quad \bar{\mathbf{E}}_\square = \bar{\mathbf{E}}_\square^{\mathrm{R}} = \langle\mathbf{C}\rangle_\square^{-1} \tag{2.90}$$

where superscript (R) stands for Reuss.

The two situations associated with the Voigt and Reuss assumption, respectively, are illustrated in Figure 2.5. We note that the only information used in computing $\bar{\mathbf{E}}_\square^{\mathrm{V}}$ is the material



{fig:2-5} Figure 2.5: *One-dimensional representation of the Voigt and Reuss assumptions.*

micro-heterogeneity, e.g. volume fractions of homogeneous micro-constituents (such as particle-reinforced matrix), and no information about the strain concentration is needed. It thus follows

[14] $\mathbf{C} := \mathbf{E}^{-1}$ denotes the inverse of the operator $\mathbf{E} : \mathbb{R}^{(3\times3)}_{\mathrm{sym}} \to \mathbb{R}^{(3\times3)}_{\mathrm{sym}}$. For the commonly adopted matrix (or Voigt) notation, where the elastic stiffness is expressed in terms of the 6×6 matrix $\underline{\mathbf{E}}$, the matrix notation of the Reuss average is obtained as the straightforward counterpart $\underline{\bar{\mathbf{E}}}^{\mathrm{R}} = \langle\underline{\mathbf{C}}\rangle_\square^{-1}$.

that the result is independent on the size of the SVE if each such SVE is statistically homogeneous. e.g. it is generated with the same volume fractions of the micro-constituents; hence, $\bar{\mathsf{E}}^{\mathrm{V}}_{\square} = \bar{\mathsf{E}}^{\mathrm{V}}$ corresponding to $L_{\square} \to \infty$.

Next, we shall establish that $\bar{\mathsf{E}}^{\mathrm{V}}$ and $\bar{\mathsf{E}}^{\mathrm{R}}$ are, in fact, upper and lower bounds on the exact value of $\bar{\mathsf{E}}$.

The upper bound: We may always split $\boldsymbol{\epsilon}(\boldsymbol{x})$, $\boldsymbol{x} \in \Omega_{\square}$, additively into the constant field $\bar{\boldsymbol{\epsilon}}$ and the fluctuation field $\boldsymbol{\epsilon}^{\mu}(\boldsymbol{x})$:

$$\boldsymbol{\epsilon}(\boldsymbol{x}) = \bar{\boldsymbol{\epsilon}} + \boldsymbol{\epsilon}^{\mu}(\boldsymbol{x}), \quad \boldsymbol{x} \in \Omega_{\square} \tag{2.91}$$ {eq:2-113}

where we have, by definition, the condition

$$\langle \boldsymbol{\epsilon} \rangle_{\square} = \bar{\boldsymbol{\epsilon}} + \langle \boldsymbol{\epsilon}^{\mu} \rangle_{\square} = \bar{\boldsymbol{\epsilon}} \quad \Rightarrow \quad \langle \boldsymbol{\epsilon}^{\mu} \rangle_{\square} = \mathbf{0} \tag{2.92}$$ {eq:2-114}

Since E is positive definite, we derive

$$\begin{aligned} 0 &\leq \langle \boldsymbol{\epsilon}^{\mu} : \mathsf{E} : \boldsymbol{\epsilon}^{\mu} \rangle_{\square} = \langle [\boldsymbol{\epsilon} - \bar{\boldsymbol{\epsilon}}] : \mathsf{E} : [\boldsymbol{\epsilon} - \bar{\boldsymbol{\epsilon}}] \rangle_{\square} \\ &= \langle \boldsymbol{\epsilon} : \mathsf{E} : \boldsymbol{\epsilon} \rangle_{\square} - 2\bar{\boldsymbol{\epsilon}} : \underbrace{\langle \mathsf{E} : \boldsymbol{\epsilon} \rangle_{\square}}_{=\bar{\boldsymbol{\sigma}} = \bar{\mathsf{E}} : \bar{\boldsymbol{\epsilon}}} + \bar{\boldsymbol{\epsilon}} : \langle \mathsf{E} \rangle_{\square} : \bar{\boldsymbol{\epsilon}} \\ &= \{\text{H-M condition}\} = \bar{\boldsymbol{\epsilon}} : \bar{\mathsf{E}} : \bar{\boldsymbol{\epsilon}} - 2\bar{\boldsymbol{\epsilon}} : \bar{\mathsf{E}} : \bar{\boldsymbol{\epsilon}} + \bar{\boldsymbol{\epsilon}} : \bar{\mathsf{E}}^{\mathrm{V}} : \bar{\boldsymbol{\epsilon}} = \bar{\boldsymbol{\epsilon}} : \left[\bar{\mathsf{E}}^{\mathrm{V}} - \bar{\mathsf{E}}\right] : \bar{\boldsymbol{\epsilon}} \end{aligned} \tag{2.93}$$ {eq:2-115}

where we also used that $\bar{\boldsymbol{\sigma}} = \bar{\mathsf{E}} : \bar{\boldsymbol{\epsilon}}$. Since (2.93) must hold for *any* possible value of $\bar{\boldsymbol{\epsilon}}$, we conclude that the eigenvalues of $\bar{\mathsf{E}}^{\mathrm{V}}$ are *larger* than (or equal to) those of $\bar{\mathsf{E}}$. We may write this condition symbolically as

$$\bar{\mathsf{E}} \leq \bar{\mathsf{E}}^{\mathrm{V}} \tag{2.94}$$ {eq:2-116}

In other words, the Voigt assumption leads to an upper bound of the homogenized stiffness tensor.

The lower bound: We may split $\boldsymbol{\sigma}(\boldsymbol{x})$, $\boldsymbol{x} \in \Omega_{\square}$, additively into $\bar{\boldsymbol{\sigma}}$ and $\boldsymbol{\sigma}^{\mu}(\boldsymbol{x})$ in a fashion that is completely analogous to $\boldsymbol{\epsilon}(\boldsymbol{x})$:

$$\boldsymbol{\sigma}(\boldsymbol{x}) = \bar{\boldsymbol{\sigma}} + \boldsymbol{\sigma}^{\mu}(\boldsymbol{x}), \quad \boldsymbol{x} \in \Omega_{\square} \tag{2.95}$$ {eq:2-117}

where we have, by definition, that

$$\langle \boldsymbol{\sigma} \rangle_{\square} = \bar{\boldsymbol{\sigma}} + \langle \boldsymbol{\sigma}^{\mathrm{s}} \rangle_{\square} = \bar{\boldsymbol{\sigma}} \quad \Rightarrow \quad \langle \boldsymbol{\sigma}^{\mathrm{s}} \rangle_{\square} = \mathbf{0} \tag{2.96}$$ {eq:2-118}

In a fashion that is completely analogeous to the upper bound, we now derive

$$0 \leq \bar{\boldsymbol{\sigma}} : \left[\bar{\mathsf{C}}^{\mathrm{R}} - \bar{\mathsf{C}}\right] : \bar{\boldsymbol{\sigma}} = \bar{\boldsymbol{\sigma}} : \left[[\bar{\mathsf{E}}^{\mathrm{R}}]^{-1} - [\bar{\mathsf{E}}]^{-1}\right] : \bar{\boldsymbol{\sigma}} \tag{2.97}$$ {eq:2-119}

Since (2.97) must hold for *any* possible $\bar{\boldsymbol{\sigma}}$, we conclude that the eigenvalues of $[\bar{\mathsf{E}}^{\mathrm{R}}]^{-1}$ are *larger* than (or equal to) those of $\bar{\mathsf{E}}^{-1}$. Hence, the eigenvalues of $\bar{\mathsf{E}}^{\mathrm{R}}$ are *smaller* than (or equal to) those of $\bar{\mathsf{E}}$, which can be written symbolically as

$$\bar{\mathsf{E}}^{\mathrm{R}} \leq \bar{\mathsf{E}} \tag{2.98}$$ {eq:2-120}

In other words, the Reuss assumption leads to a lower bound of the homogenized stiffness tensor.

Finally, we may summarize (2.94) and (2.98) as the "Hill-Reuss-Voigt" bounds

$$\bar{\mathsf{E}}^{\mathrm{R}} \leq \bar{\mathsf{E}} \leq \bar{\mathsf{E}}^{\mathrm{V}} \tag{2.99}$$ {eq:2-121}

2.3.3 Eshelby's solution for single inclusion in an infinite body

The main issue is how to compute the mean fields $\bar{\mathbf{A}}^{(\alpha)}$ with good approximation. As a preliminary to a number of different socalled "mean field models" that are based on analytical estimates for idealized geometries of the inclusions/particles, we shall in this Subsection consider Eshelby's solution to the problem of an elliptic-shaped inclusion, occupying the domain Ω, that is embedded in an infinite medium and subject to the (constant) far-field strain $\boldsymbol{\epsilon}^0$. Both the inclusion/particle and the embedding matrix are assumed linear elastic and *homogeneous* with elastic stiffness $\mathbf{E}^{(\mathrm{p})}$ and $\mathbf{E}^0$, respectively.

The static stress problem of finding the displacement field $\boldsymbol{u}(\boldsymbol{x})$ for $\boldsymbol{x} \in \mathbb{R}^3$ can be stated as follows:

{eq:2-122}
$$-\boldsymbol{\sigma} \cdot \boldsymbol{\nabla} = \mathbf{0} \text{ in } \Omega, \tag{2.100}$$

subjected to the conditions

{eq:2-123}
$$|\boldsymbol{u} - \boldsymbol{\epsilon}^0 \cdot \boldsymbol{x}| \to 0 \quad \text{as} \quad |\boldsymbol{x}| \to \infty \tag{2.101}$$

{eq:2-124}
$$\boldsymbol{\sigma} = \begin{cases} \mathbf{E}^{(\mathrm{p})} : \boldsymbol{\epsilon}[\boldsymbol{u}] & \text{in } \Omega \\ \mathbf{E}^0 : \boldsymbol{\epsilon}[\boldsymbol{u}] & \text{in } \mathbb{R}^3 \setminus \Omega \end{cases} \tag{2.102}$$

We assume, for simplicity, that the elliptic-shaped region Ω is centered at $\boldsymbol{x} = \mathbf{0}$.

Our aim is to solve for $\boldsymbol{u} = \boldsymbol{u}^{(\mathrm{p})}$ or, rather, the strain field $\boldsymbol{\epsilon}^{(\mathrm{p})} = \boldsymbol{\epsilon}[\boldsymbol{u}^{(\mathrm{p})}]$, in terms of the given "load" $\boldsymbol{\epsilon}^0$. Now, for an elliptic inclusion, the strain field will be *constant* in Ω, i.e. $\boldsymbol{\epsilon}^{(\mathrm{p})} = \bar{\boldsymbol{\epsilon}}^{(\mathrm{p})}$, which has a profound importance.

In order to determine the solution, we introduce the concept of a "comparison-medium" with eigenstrains. This is a classical approach, originally suggested by Hill. The purpose is to restate the original problem as a problem with uniform elasticity stiffness $\mathbf{E}^0$, as shown in Figure 2.5(b), whereby analytical solution technique(s) can be exploited. Upon decomposing the displacement and stress fields as

{eq:2-125}
$$\boldsymbol{u}(\boldsymbol{x}) = \boldsymbol{\epsilon}^0 \cdot \boldsymbol{x} + \boldsymbol{u}'(\boldsymbol{x}), \quad \boldsymbol{\sigma}(\boldsymbol{x}) = \mathbf{E}^0 : \boldsymbol{\epsilon}^0 + \boldsymbol{\sigma}'(\boldsymbol{x}), \tag{2.103}$$

and noting that $\boldsymbol{\sigma}^0 := \mathbf{E}^0 : \boldsymbol{\epsilon}^0$ is a constant field, we may restate Eqs. (2.100), (2.101) as

{eq:2-126}
$$-\boldsymbol{\sigma}' \cdot \boldsymbol{\nabla} = \mathbf{0} \text{ in } \mathbb{R}^3, \tag{2.104}$$

subjected to the conditions

{eq:2-127}
$$|\boldsymbol{u}'| \to 0 \quad \text{as} \quad |\boldsymbol{x}| \to \infty \tag{2.105}$$

Further, we introduce a (fictitious) socalled "eigenstrain" field $\boldsymbol{\epsilon}^*(\boldsymbol{x})$ and postulate that the actual stress field can be represented in the comparison-medium as follows:

{eq:2-128}
$$\boldsymbol{\sigma}' = \begin{cases} \mathbf{E}^0 : [\boldsymbol{\epsilon}[\boldsymbol{u}'] - \boldsymbol{\epsilon}^*] & \text{in } \Omega \\ \mathbf{E}^0 : \boldsymbol{\epsilon}[\boldsymbol{u}'] & \text{in } \mathbb{R}^3 \setminus \Omega \end{cases} \tag{2.106}$$

In order to satisfy (2.102), we identify the "consistency condition"

{eq:2-129}
$$\mathbf{E}^{(\mathrm{p})} : \left[\boldsymbol{\epsilon}^0 + \boldsymbol{\epsilon}'\{\boldsymbol{\epsilon}^*\}\right] = \mathbf{E}^0 : \left[\boldsymbol{\epsilon}^0 + \boldsymbol{\epsilon}'\{\boldsymbol{\epsilon}^*\} - \boldsymbol{\epsilon}^*\right] \quad \text{in } \Omega_\square \tag{2.107}$$

which may be rewritten as

{eq:2-131}
$$\Delta\mathbf{E} : \boldsymbol{\epsilon}' = -\Delta\mathbf{E} : \boldsymbol{\epsilon}^0 - \mathbf{E}^0 : \boldsymbol{\epsilon}^* \quad \text{with } \Delta\mathbf{E} := \mathbf{E}^{(\mathrm{p})} - \mathbf{E}^0 \quad \text{in } \Omega_\square \tag{2.108}$$

Now, we shall assume that it s possible to solve for $\boldsymbol{u}'\{\boldsymbol{\epsilon}^*\}$, and thus $\boldsymbol{\epsilon}'\{\boldsymbol{\epsilon}^*\}$, analytically from (2.89), (**??**)???, (**??**)???, where $\boldsymbol{\epsilon}^*$ is considered as the "loading" to this problem of the comparison medium. Due to the linearity, it is then possible to express the solution for the constant strain field $\boldsymbol{\epsilon}'$ as

{eq:2-132}
$$\boldsymbol{\epsilon}' = \mathbf{S}(\mathbf{E}^0, \Omega) : \boldsymbol{\epsilon}^* \tag{2.109}$$

The explicit expression for $\mathbf{S}(\mathbf{E}^0, \Omega)$ is

{eq:2-133}
$$\mathbf{S}(\mathbf{E}^0, \Omega) = \sum_{i,j,k,l} \int_\Omega \boldsymbol{\epsilon}[\boldsymbol{\varphi}^{ij}(\boldsymbol{x})] \otimes \boldsymbol{e}_k \otimes \boldsymbol{e}_l \, \mathrm{d}\Omega \tag{2.110}$$

where $\boldsymbol{\varphi}^{ij}(\boldsymbol{x})$ is the Green's function that solves {eq:2-134}

$$-\left[\mathbf{E}^0 : \left[\boldsymbol{\epsilon}[\boldsymbol{\varphi}^{ij}(\boldsymbol{x})] - \boldsymbol{e}_i \otimes \boldsymbol{e}_j \delta(\boldsymbol{x})\right]\right] \cdot \boldsymbol{\nabla} = \mathbf{0} \quad \text{in } \mathbb{R}^3 \tag{2.111a}$$ {eq:2-134a}

$$|\boldsymbol{\varphi}^{ij}| \to 0 \quad \text{as} \quad |\boldsymbol{x}| \to \infty \tag{2.111b}$$ {eq:2-134b}

where $\delta(\boldsymbol{x})$ denotes the Dirac delta distribution. We shall not elaborate on the solution any further but simply note that $\boldsymbol{\varphi}^{ij}$ depends on $\mathbf{E}^0$ and that $\mathbf{S}$, in addition to $\mathbf{E}^0$, depends on the shape of the elliptic inclusion via the integration on Ω.

Remark: The expression for $\mathbf{S}$ in (2.111) corresponds to evaluating $\boldsymbol{\epsilon}[\boldsymbol{u}']$ at $\boldsymbol{x} = \mathbf{0}$. □

Remark: In the special case of (i) isotropic elasticity and (ii) spherical inclusions, then $\mathbf{S}$ takes the simple explicit form

$$\mathbf{S} = \alpha_{\mathrm{G}} \mathbf{I}^{\mathrm{sym}}_{\mathrm{dev}} + \alpha_{\mathrm{K}} \boldsymbol{I} \otimes \boldsymbol{I} \tag{2.112}$$ {eq:2-135}

where the non-dimensional coefficients depend only on the elastic moduli of the (homogeneous) matrix material as follows: {eq:2-136}

$$\alpha_{\mathrm{G}} = \frac{2\left[K^{(\mathrm{m})} + 2G^{(\mathrm{m})}\right]}{5\left[3K^{(\mathrm{m})} + 4G^{(\mathrm{m})}\right]} = \frac{2\left[4 - 5\nu^{(\mathrm{m})}\right]}{15\left[1 - \nu^{(\mathrm{m})}\right]} \tag{2.113a}$$ {eq:2-136a}

$$\alpha_{\mathrm{K}} = \frac{K^{(\mathrm{m})}}{3K^{(\mathrm{m})} + 4G^{(\mathrm{m})}} = \frac{1 + \nu^{(\mathrm{m})}}{9\left[1 - \nu^{(\mathrm{m})}\right]} \tag{2.113b}$$ {eq:2-136b}

A more complicated expression for $\mathbf{S}$, showing anisotropy, applies in the case of non-spherical (e.g. penny-shaped, needle-shaped) inclusions. □

Upon combining the the consistency condition in (2.108) with the solution in (2.111), we may eliminate the eigenstrain $\boldsymbol{\epsilon}^*$ and solve for $\boldsymbol{\epsilon}'$ in terms of the farfield strain $\boldsymbol{\epsilon}^0$ as follows:

$$\boldsymbol{\epsilon}' = -\left[\mathbf{E}^0 : \mathbf{S}^{-1} + \Delta\mathbf{E}\right]^{-1} : \Delta\mathbf{E} : \boldsymbol{\epsilon}^0 \tag{2.114}$$ {eq:2-137}

Finally, we obtain the strain field $\bar{\boldsymbol{\epsilon}}^{(\mathrm{p})}$ inside the inclusion/particle, which occupies the domain Ω, as follows

$$\begin{aligned} \bar{\boldsymbol{\epsilon}}^{(\mathrm{p})} &= \boldsymbol{\epsilon}^0 + \boldsymbol{\epsilon}' \\ &= \bar{\mathbf{A}}^{(\mathrm{p})} : \boldsymbol{\epsilon}^0, \quad \bar{\mathbf{A}}^{(\mathrm{p})} \stackrel{\mathrm{def}}{=} \left[\mathbf{I} + \mathbf{S} : \left[\mathbf{E}^0\right]^{-1} : \Delta\mathbf{E}\right]^{-1} \end{aligned} \tag{2.115}$$ {eq:2-138}

2.3.4 Mean field model based on dilute concentration of inclusions

In the case that $n^{(\mathrm{p})}$ is very small (dilute concentration of inclusions/particles) and inclusions have elliptical shape, then it is possible to directly apply Eshelby's solution for a single homogeneous inclusion in an infinite homogeneous matrix, as presented in the previous Subsection.

Applied to the RVE, we then use the solution in (2.96) upon setting $\boldsymbol{\epsilon}^0 = \bar{\boldsymbol{\epsilon}}$ and $\mathbf{E}^0 = \mathbf{E}^{(\mathrm{m})}$. We thus obtain

$$\bar{\boldsymbol{\epsilon}}^{(\mathrm{p})} = \bar{\mathbf{A}}^{(\mathrm{p})}_{\mathrm{DIL}} : \bar{\boldsymbol{\epsilon}}, \quad \text{with } \bar{\mathbf{A}}^{(\mathrm{p})}_{\mathrm{DIL}} \stackrel{\text{def}}{=} \left[\mathbf{I} + \mathbf{S} : \left[\mathbf{E}^{(\mathrm{m})}\right]^{-1} : \Delta\mathbf{E}\right]^{-1} \tag{2.116}$$ {eq:2-141}

The expression for $\bar{\mathbf{A}}^{(\mathrm{p})}_{\mathrm{DIL}}$ is introduced in $(2.88)_2$ to, finally, give $\bar{\mathbf{E}} = \bar{\mathbf{E}}_{\mathrm{DIL}}$.

2.3.5 Mori-Tanaka mean field model for non-dilute inclusions

When the concentration of inclusions is not dilute, then Eshelby's solution is no longer a good approximation. In such a case, a strategy to account for the interaction of particles, attributed to Mori and Tanaka **?**, is to apply Eshelby's solution in principle; however, to replace the "far-field" strain $\bar{\boldsymbol{\epsilon}}$ by the "effective" strain that is the (homogeneous) mean-field matrix strain $\bar{\boldsymbol{\epsilon}}^{(\mathrm{m})}$. We thus set $\boldsymbol{\epsilon}^0 = \bar{\boldsymbol{\epsilon}}^{(\mathrm{m})}$ and $\mathbf{E}^0 = \mathbf{E}^{(\mathrm{m})}$. Hence, we have the relation

{eq:2-142}
$$\bar{\boldsymbol{\epsilon}}^{(\mathrm{p})}\{\boldsymbol{\epsilon}^*\} = \bar{\boldsymbol{\epsilon}}^{(\mathrm{m})} + \mathbf{S}_{\mathrm{DIL}} : \boldsymbol{\epsilon}^* \tag{2.117}$$

Upon inserting (2.117) into (2.88), we obtain

{eq:2-143}
$$\bar{\boldsymbol{\epsilon}}^{(\mathrm{p})}\{\boldsymbol{\epsilon}^*\} = \bar{\boldsymbol{\epsilon}}^{(\mathrm{m})} + \mathbf{S}_{\mathrm{MT}} : \boldsymbol{\epsilon}^*, \quad \mathbf{S}_{\mathrm{MT}} \stackrel{\text{def}}{=} n^{(\mathrm{m})}\mathbf{S}_{\mathrm{DIL}} \tag{2.118}$$

In this case the consistency condition (2.107) gives

{eq:2-144}
$$\boldsymbol{\epsilon}^* = \mathbf{R}_{\mathrm{MT}} : \bar{\boldsymbol{\epsilon}}, \quad \text{with } \mathbf{R}_{\mathrm{MT}} \stackrel{\text{def}}{=} -\left[[\Delta\mathbf{E}]^{-1} : \mathbf{E}^{(\mathrm{m})} + \mathbf{S}_{\mathrm{MT}}\right]^{-1} \tag{2.119}$$

in complete analogy with the case of dilute concentration. Next, (2.119) is inserted into (2.117) to give

{eq:2-145}
$$\bar{\boldsymbol{\epsilon}}^{(\mathrm{p})} = \bar{\mathbf{A}}^{(\mathrm{p})}_{\mathrm{MT}} : \bar{\boldsymbol{\epsilon}}, \quad \bar{\mathbf{A}}^{(\mathrm{p})}_{\mathrm{MT}} \stackrel{\text{def}}{=} \left[\mathbf{I} + \mathbf{S}_{\mathrm{MT}} : \left[\mathbf{E}^{(\mathrm{m})}\right]^{-1} : \Delta\mathbf{E}\right]^{-1} \tag{2.120}$$

which is introduced in $(2.88)_2$ to, finally, give $\bar{\mathbf{E}} = \bar{\mathbf{E}}_{\mathrm{MT}}$.

Remark: It is possible to rephrase the Mori-Tanaka-assumption by assuming, as the point of departure for the derivations, that

{eq:2-146}
$$\bar{\boldsymbol{\epsilon}}^{(\mathrm{p})} = \bar{\mathbf{A}}^{(\mathrm{p})}_{\mathrm{DIL}} : \bar{\boldsymbol{\epsilon}}^{(\mathrm{m})} \quad \text{with } \bar{\mathbf{A}}^{(\mathrm{p})}_{\mathrm{DIL}} = \left[\mathbf{I} + \mathbf{S}_{\mathrm{DIL}} : \left[\mathbf{E}^{(\mathrm{m})}\right]^{-1} : \Delta\mathbf{E}\right]^{-1} \tag{2.121}$$

This assumption is equivalent to (2.117), which is shown as follows: Upon inserting the assumption for $\bar{\boldsymbol{\epsilon}}^{(\mathrm{p})}\{\boldsymbol{\epsilon}^*\}$, given in (2.117), into the consistency condition (2.107), we obtain the alternative expression

{eq:2-147}
$$\boldsymbol{\epsilon}^* = \mathbf{R}_{\mathrm{DIL}} : \bar{\boldsymbol{\epsilon}}^{(\mathrm{m})} \tag{2.122}$$

which can be inserted back into (2.117) to give the alternative representation

{eq:2-148}
$$\bar{\boldsymbol{\epsilon}}^{(\mathrm{p})} = \left[\mathbf{I} - \mathbf{S}_{\mathrm{DIL}} : \left[[\Delta\mathbf{E}]^{-1} : \mathbf{E}^{(\mathrm{m})} + \mathbf{S}_{\mathrm{DIL}}\right]^{-1}\right] : \bar{\boldsymbol{\epsilon}}^{(\mathrm{m})} \tag{2.123}$$

This expression is identical to (2.121): Show as homework! □

2.3.6 Self-consistent mean field model for non-dilute inclusions

An alternative strategy to deal with non-dilute concentration of inclusions is to reuse Eshelby's solution but replace the matrix material (stiffness tensor $\mathbf{E}^{(\mathrm{m})}$) with the effective material (stiffness tensor $\bar{\mathbf{E}}$) in evaluating the strain concentration in the inclusions. We thus set $\boldsymbol{\epsilon}^0 = \bar{\boldsymbol{\epsilon}}$ and $\mathbf{E}^0 = \bar{\mathbf{E}}$. Hence, $\bar{\mathbf{A}}^{(\mathrm{p})}_{\mathrm{DIL}}$ in (2.116) is replaced by the (approximate) expression

{eq:2-148}
$$\bar{\mathbf{A}}^{(\mathrm{p})}_{\mathrm{SC}}(\bar{\mathbf{E}}) = \left[\mathbf{I} + \mathbf{S}(\bar{\mathbf{E}}) : \bar{\mathbf{E}}^{-1} : \left[\mathbf{E}^{(\mathrm{p})} - \bar{\mathbf{E}}\right]\right]^{-1} \tag{2.124}$$

where the dependence $\mathbf{S}(\bar{\mathbf{E}})$ is noted. However, (2.87) is still valid with the adjusted mean-field strain concentration given in (2.124), i. e.

$$\bar{\mathbf{E}} = \mathbf{E}^{(\mathrm{m})} + n^{(\mathrm{p})} \Delta \mathbf{E} : \bar{\mathbf{A}}^{(\mathrm{p})}_{\mathrm{SC}}(\bar{\mathbf{E}}) \tag{2.125}$$ {eq:2-149}

Now, since $\bar{\mathbf{A}}^{(\mathrm{p})}_{\mathrm{SC}}$ depends on $\bar{\mathbf{E}}$, the sought stiffness $\bar{\mathbf{E}} = \bar{\mathbf{E}}_{\mathrm{SC}}$ is the solution of (2.125) with (2.124). This system can conveniently be solved using fixed-point iterations as follows: For iterations $k = 1, 2, ...$, solve for $\bar{\mathbf{E}}_k$ from

$$\bar{\mathbf{E}}_k = \mathbf{E}^{(\mathrm{m})} + n^{(\mathrm{p})} \Delta \mathbf{E} : \bar{\mathbf{A}}^{(\mathrm{p})}_{\mathrm{SC}}(\bar{\mathbf{E}}_{k-1}) \tag{2.126}$$ {eq:2-150}

until convergence.

2.3.7 Hashin-Shtrikman mean field model for non-dilute inclusions. Hashin-Shtrikman bounds

Hashin and Shtrikman ? provided the tightest possible bounds on $\bar{\mathbf{E}}$ for isotropic linear elastic subscale material response in the absence of information on the actual substructural toplogy; hence, volume fractions and phase properties are the only data. Since it is assumed that the RVE is infinitely large, the effective elastic properties are isotropic as well. It is then possible to use the Hashin-Shtrikman variational principles (as described in Appendix A) for prescribed boundary displacements or boundary tractions together with (a suitable modification of) Eshelby's solution for a single inclusion in an infinite homogeneous matrix in order to obtain upper and lower bounds on the effective stiffness tensor $\bar{\mathbf{E}}$. Below we consider the case of prescribed boundary displacements (for the sake of brevity). To obtain explicit results, we shall assume that the inclusions are spherical.

Lower bound on elastic stiffness moduli

To obtain lower bounds, we consider the homogeneous comparison solid and set $\mathbf{E}^0 = \mathbf{E}^{(\mathrm{m})}$. For a given homogeneous "eigenstrain" field inside the inclusions, $\boldsymbol{\epsilon}^*$, we assume that the solution in the comparison-RVE is represented as

$$\bar{\boldsymbol{\epsilon}}^{(\mathrm{p})} = \bar{\boldsymbol{\epsilon}} + \mathbf{S} : \boldsymbol{\epsilon}^* \tag{2.127}$$ {eq:2-151}

where $\mathbf{S}$ is a *constant* 4'th order tensor (with major as well as minor symmetry) that depends only on the properties of $\mathbf{E}^{(\mathrm{m})}$ and the volume fraction of matrix and inclusions.

Upon introducing the notation $\boldsymbol{\sigma}^* \stackrel{\mathrm{def}}{=} -\mathbf{E}^{(\mathrm{m})} : \boldsymbol{\epsilon}^*$, we may rewrite the solution in the inclusions as

$$\bar{\boldsymbol{\epsilon}}^{(\mathrm{p})} = \bar{\boldsymbol{\epsilon}} - \boldsymbol{\Gamma}^{(\mathrm{m})} : \boldsymbol{\sigma}^*, \quad \boldsymbol{\Gamma}^{(\mathrm{m})} \stackrel{\mathrm{def}}{=} \mathbf{S} : \left[\mathbf{E}^{(\mathrm{m})}\right]^{-1} \tag{2.128}$$ {eq:2-152}

where the *constant* 4'th order tensor $\mathbf{\Gamma}^{(\mathrm{m})}$ is denoted the "correlation tensor" by NEMAT-NASSER AND HORI **?**.

It now remains to introduce the (approximative) ansatz for the fluctuation field $\hat{\bar{\boldsymbol{\epsilon}}}'$ expressed in terms of the *constant* tensor $\hat{\boldsymbol{\sigma}}^*$:

{eq:2-153}
$$\hat{\bar{\boldsymbol{\epsilon}}}'(\hat{\boldsymbol{\sigma}}^*) = -\mathbf{\Gamma}^{(\mathrm{m})} : \hat{\boldsymbol{\sigma}}^*, \quad \boldsymbol{x} \in \Omega_\square^{(\mathrm{p})} \tag{2.129}$$

{eq:2-154}
$$= \mathbf{0}, \quad \boldsymbol{x} \in \Omega_\square^{(\mathrm{m})} \tag{2.130}$$

into the HS-functional $\Pi_{\mathrm{HS}}^{(\mathrm{D})}$ to obtain

{eq:2-155}
$$\begin{aligned}\Pi_{\mathrm{HS}}^{(\mathrm{D})}(\hat{\boldsymbol{\sigma}}^*) &= \frac{1}{2}\langle \hat{\boldsymbol{\sigma}}^* : \hat{\bar{\boldsymbol{\epsilon}}}'(\hat{\boldsymbol{\sigma}}^*)\rangle_\square - \frac{1}{2}\langle \hat{\boldsymbol{\sigma}}^* : [\Delta\mathbf{E}]^{-1} : \hat{\boldsymbol{\sigma}}^*\rangle_\square + \bar{\boldsymbol{\epsilon}} : \langle \hat{\boldsymbol{\sigma}}^*\rangle_\square \\ &= -\frac{1}{2} n^{(\mathrm{p})} \hat{\boldsymbol{\sigma}}^* : \left[\mathbf{J}^{(\mathrm{m})}\right]^{-1} : \hat{\boldsymbol{\sigma}}^* + n^{(\mathrm{p})} \bar{\boldsymbol{\epsilon}} : \hat{\boldsymbol{\sigma}}^* \end{aligned} \tag{2.131}$$

where the 4th order tensor $\mathbf{J}^{(\mathrm{m})}$ is given as

{eq:2-156}
$$\mathbf{J}^{(\mathrm{m})} \stackrel{\mathrm{def}}{=} \left[[\Delta\mathbf{E}]^{-1} + \mathbf{\Gamma}^{(\mathrm{m})}\right]^{-1} \tag{2.132}$$

The stationary condition of $\Pi_{\mathrm{HS}}^{(\mathrm{D})}$ gives the solution

{eq:2-157}
$$\boldsymbol{\sigma}^* = \mathbf{J}^{(\mathrm{m})} : \bar{\boldsymbol{\epsilon}} \tag{2.133}$$

Since we assumed that $\Delta\mathbf{E}$ is positive (semi-)definite, it is concluded that $\boldsymbol{\sigma}^*$ is a maximizer of $\Pi_{\mathrm{HS}}^{(\mathrm{D})}(\hat{\boldsymbol{\sigma}}^*)$ for all ansatz-stresses $\hat{\boldsymbol{\sigma}}^* \in \mathbb{R}^{3\times 3}$, and this maximum value is obtained as

{eq:2-158}
$$\Pi_{\mathrm{HS}}^{(\mathrm{D})}(\boldsymbol{\sigma}^*) = \frac{1}{2} n^{(\mathrm{p})} \bar{\boldsymbol{\epsilon}} : \mathbf{J}^{(\mathrm{m})} : \bar{\boldsymbol{\epsilon}} \tag{2.134}$$

Since this maximum is always lower than the exact maximum value, i.e.

{eq:2-159}
$$\Pi_{\mathrm{HS}}^{(\mathrm{D})}(\boldsymbol{\sigma}^*) \leq (\Pi_{\mathrm{HS}}^{(\mathrm{D})})_{\max} \tag{2.135}$$

where

{eq:2-160}
$$(\Pi_{\mathrm{HS}}^{(\mathrm{D})})_{\max} = \frac{1}{2}\bar{\boldsymbol{\epsilon}} : \left[\bar{\mathbf{E}} - \mathbf{E}^{(\mathrm{m})}\right] : \bar{\boldsymbol{\epsilon}} \tag{2.136}$$

we obtain the energy bounds

{eq:2-161}
$$\frac{1}{2}\bar{\boldsymbol{\epsilon}} : \left[\mathbf{E}^{(\mathrm{m})} + n^{(\mathrm{p})}\mathbf{J}^{(\mathrm{m})}\right] : \bar{\boldsymbol{\epsilon}} \leq \frac{1}{2}\bar{\boldsymbol{\epsilon}} : \bar{\mathbf{E}} : \bar{\boldsymbol{\epsilon}} \tag{2.137}$$

In order to obtain the sharpest possible bound it is desirable to choose $\mathbf{\Gamma}^{(\mathrm{m})}$ such that it resembles the true solution of the eigenstrain problem as close as possible. The classical HS-estimates rely on the particular choice pertinent to the MT-assumption discussed in Subsection 3.4.3???, i.e.

{eq:2-162}
$$\mathbf{S} = \mathbf{S}_{\mathrm{MT}} \stackrel{\mathrm{def}}{=} n^{(\mathrm{m})}\mathbf{S}_{\mathrm{DIL}} \tag{2.138}$$

In this case we obtain $\mathbf{\Gamma}^{(\mathrm{m})} = n^{(\mathrm{m})}\mathbf{S}_{\mathrm{DIL}} : \left[\mathbf{E}^{(\mathrm{m})}\right]^{-1}$, which gives

{eq:2-163}
$$\mathbf{J}^{(\mathrm{m})} = \left[[\Delta\mathbf{E}]^{-1} + n^{(\mathrm{m})}\mathbf{S}_{\mathrm{DIL}} : \left[\mathbf{E}^{(\mathrm{m})}\right]^{-1}\right]^{-1} \tag{2.139}$$

{eq:2-164} Upon exploiting the explicit relations for $\mathsf{E}^{(\mathrm{m})}$, $\Delta\mathsf{E}$ and $\mathsf{S}_{\mathrm{DIL}}$:

{eq:2-164a}
$$\mathsf{E}^{(\alpha)} = 2G^{(\alpha)}\mathsf{I}^{\mathrm{sym}}_{\mathrm{dev}} + K^{(\alpha)}\boldsymbol{I}\otimes\boldsymbol{I}, \quad \alpha = \mathrm{m}, \mathrm{p} \tag{2.140a}$$

{eq:2-164b}
$$\mathsf{S}_{\mathrm{DIL}} = \alpha_{\mathrm{G}}\mathsf{I}^{\mathrm{sym}}_{\mathrm{dev}} + \alpha_{\mathrm{K}}\boldsymbol{I}\otimes\boldsymbol{I} \tag{2.140b}$$

we obtain the explicit expression

{eq:2-166}
$$\mathsf{J}^{(\mathrm{m})} = 2G^{(\mathrm{m})}\left[\frac{G^{(\mathrm{m})}}{\Delta G} + n^{(\mathrm{m})}\alpha_{\mathrm{G}}\right]^{-1}\mathsf{I}^{\mathrm{sym}}_{\mathrm{dev}} + K^{(\mathrm{m})}\left[\frac{K^{(\mathrm{m})}}{\Delta K} + 3n^{(\mathrm{m})}\alpha_{\mathrm{K}}\right]^{-1}\boldsymbol{I}\otimes\boldsymbol{I} \tag{2.141}$$

This expression is inserted into (2.137) to yield the lower bounds on the effective moduli {eq:2-167}

$$\bar{G} \geq \bar{G}^{-} \stackrel{\mathrm{def}}{=} G^{(\mathrm{m})}\left[1 + \frac{n^{(\mathrm{p})}}{\frac{G^{(\mathrm{m})}}{\Delta G} + n^{(\mathrm{m})}\alpha_{\mathrm{G}}}\right] \tag{2.142a}$$ {eq:2-167a}

$$\bar{K} \geq \bar{K}^{-} \stackrel{\mathrm{def}}{=} K^{(\mathrm{m})}\left[1 + \frac{n^{(\mathrm{p})}}{\frac{K^{(\mathrm{m})}}{\Delta K} + 3n^{(\mathrm{m})}\alpha_{\mathrm{K}}}\right] \tag{2.142b}$$ {eq:2-167b}

Upper bound on elastic stiffness moduli

To obtain upper bounds, we consider the homogeneous comparison solid and set $\mathsf{E}^0 = \mathsf{E}^{(\mathrm{p})}$.

2.4 The classical RVE-problems

{The classi

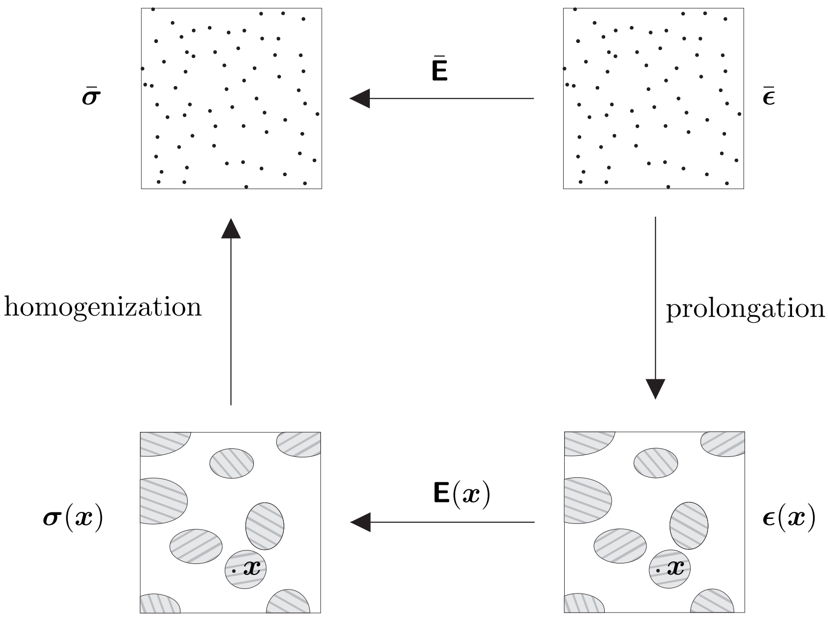


Figure 2.6: *Sketch of the computation of* $\bar{\mathsf{E}}$. {fig:2-7}

2.4.1 Preliminaries

For any given finite-sized SVE, the major issue is how to assign boundary conditions on $\Gamma_\square$ on either displacements, traction, or both, in order to obtain the "best possible" approximation of $\bar{\mathsf{E}}$. The standard choices are:

- Linear boundary displacements (Dirichlet boundary conditions) – denoted the DBC-problem
- Uniform boundary tractions (Neumann boundary conditions) – denoted the NBC-problem
- Periodic boundary displacements and antiperiodic tractions – denoted the PBC-problem, which is realizable in practice only for a cubic SVE in 3D (square in 2D)

For either choice, it is possible to formulate the SVE-problem, either with (i) imposed macroscale strain (strain control), whereby $\bar{\boldsymbol{\epsilon}} = \langle \boldsymbol{\epsilon} \rangle_\square$ is prescribed, or with (ii) imposed macroscale stress (stress control), whereby $\bar{\boldsymbol{\sigma}} = \langle \boldsymbol{\sigma} \rangle_\square$ is prescribed. The *standard* problem formulation for macroscale strain control is that of DBC, whereas the *standard* problem formulation for macroscale stress control is that of NBC. The reason is that it is only for these combinations of boundary conditions and "loading" that a standard displacement formulation can be established, whereas *mixed methods* are necessary for DBC with macroscale stress control and for NBC with macroscale strain control. All these problems are discussed in some depth for the general nonlinear SVE-problem in Chapter 4.

If the chosen SVE is considered as a "windowed" subdomain of a larger RVE, then it is clear that the actual boundary values on the SVE are neither of the three idealized ones listed above. The actual variation of displacements and tractions along $\Gamma_\square$ depend strongly on both the "mode of macroscale control" and, most importantly, on the "degree of heterogeneity" inside the SVE. This is shown in Figure **??** for a particular mode of macroscopic deformation. The degree to which the solutions of the DBC- and NBC-problems agree (for a given type of macroscale control) may be regarded as a measure of how close the solution of the SVE-problem is to the actual RVE-solution. In other words, it is a measure of how close the *apparent stiffness* tensor $\bar{\mathsf{E}}_\square$ is to the actual effective stiffness tensor $\bar{\mathsf{E}}$.

Remark: It is not possible to know in advance which of the prolongation conditions that produce the best approximation of $\bar{\mathsf{E}}$ for a given $L_\square < \infty$ and a given realization. Hence, hierarchical models can not be established. It is merely known that $\bar{\mathsf{E}}_\square \to \bar{\mathsf{E}}$ when $L_\square \to \infty$.

2.4.2 Dirichlet boundary conditions (DBC-problem)

Dirichlet boundary conditions on the RVE are introduced via the *modeling assumption* for the boundary displacements

{eq:2-171}
$$\boldsymbol{u}(\boldsymbol{x}) = \bar{\boldsymbol{\epsilon}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}] \quad \text{or} \quad \boldsymbol{u}^\mu(\boldsymbol{x}) = \boldsymbol{0}, \quad \boldsymbol{x} \in \Gamma_\square \tag{2.143}$$

The assumption (2.121) means that the displacements vary in a linear fashion along any boundary that is straight. Since this is the case in practice it is common to speak about *linear displacement boundary conditions*. This model assumption means that the relation $\langle \boldsymbol{\epsilon} \rangle_\square = \bar{\boldsymbol{\epsilon}}$ is satisfied a priori (automatically by construction), which is shown as follows:

$$\langle \boldsymbol{\epsilon} \rangle_\square = \left(\frac{1}{|\Omega_\square|} \int_{\Gamma_\square} \boldsymbol{u} \otimes \boldsymbol{n} \, \mathrm{d}\Gamma \right)^{\mathrm{sym}} = \bar{\boldsymbol{\epsilon}} \cdot \underbrace{\left(\frac{1}{|\Omega_\square|} \int_{\Gamma_\square} \boldsymbol{n} \otimes [\boldsymbol{x} - \bar{\boldsymbol{x}}] \, \mathrm{d}\Gamma \right)^{\mathrm{sym}}}_{=\boldsymbol{I}} = \bar{\boldsymbol{\epsilon}}$$

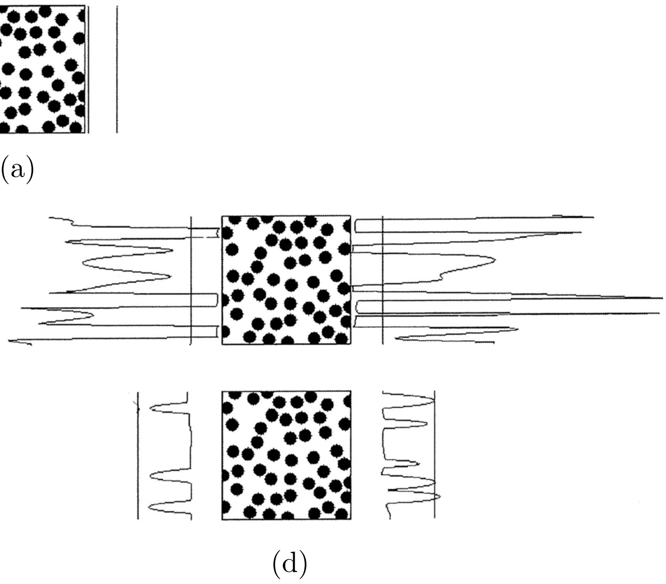
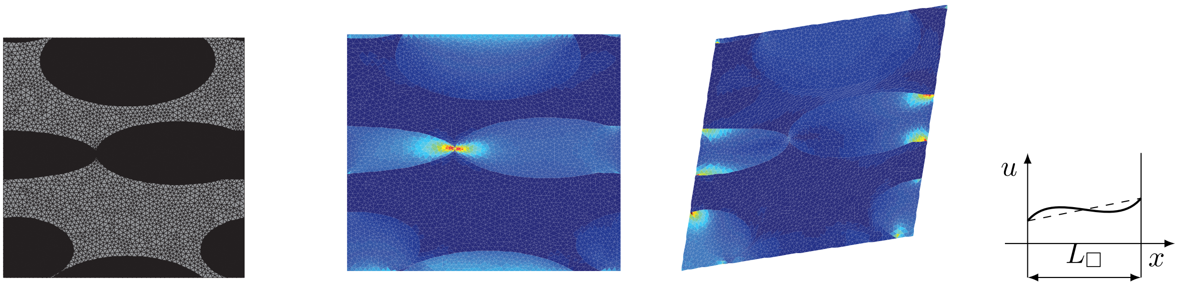


Figure 2.7: *Illustration of how fluctuations of boundary fields increase for an SVE with increasing mismatch of the shear modulus G for a matrix(m)-particle(p) composite with 35% volume fraction of particles. The SVE is subjected to macroscopic anti-plane shear. (a) Homogenous:* $G^{(p)}/G^{(m)} = 1$. *(b)* $G^{(p)}/G^{(m)} = 0.2$. *(c)*$G^{(p)}/G^{(m)} = 0.05$. *(d)* $G^{(p)}/G^{(m)} = 0.02$. The first row shows the fluctuation of tractions from DBC, whereas the second row shows the fluctuation of displacements from NBC. [From Ostoja-Starzewski **?**]

{fig:2-8}

Moreover, this relation holds automatically for strain as well as for stress control.

Figure 2.8 shows the deformed shape of a square RVE in 2D, representing a particle-reinforced matrix, for the two cases of pure normal strain ($\bar{\epsilon}_{11} \neq 0$) and pure shear strain ($\bar{\epsilon}_{12} = \bar{\epsilon}_{21} \neq 0$).



{fig:2-9} Figure 2.8: *Examples of deformed shapes of square RVE with particles in matrix subjected to DBC. Left: Undeformed RVE. Middle: Normal strain: Only $\bar{\epsilon}_{11}$ is non-zero. Right: Shear strain: Only $\bar{\epsilon}_{12} = \bar{\epsilon}_{21}$ is non-zero.*

Next, we show that the choice in (2.143) is sufficient to ensure that the corresponding fine-scale fields $\boldsymbol{\epsilon}$ and $\boldsymbol{\sigma}$ do, indeed, satisfy the Hill-Mandel condition. In order to do so, we use (2.68) together with (2.143) to obtain

{eq:2-173}
$$\int_{\Gamma_\Box} [\boldsymbol{t} - \bar{\boldsymbol{\sigma}} \cdot \boldsymbol{n}] \cdot \underbrace{\boldsymbol{u}^\mu}_{=\boldsymbol{0}} \, \mathrm{d}\Gamma = 0 \tag{2.144}$$

2.4.3 Strongly periodic boundary conditions (SPBC-problem)

A classical model *assumption* is that the subscale fluctuation field $\boldsymbol{u}^\mu$ is periodic w.r.t. the chosen local coordinate axes with periodicity of the size of the SVE, which is taken as a cube in 3D (square in 2D). This assumption of "micro-periodicity", which is a key ingredient (and frequently adopted) in the literature on mathematical homogenization, is tacitly based on the perception that the micro-structure is built up by repetitive cells of identical shape and content. It is important to note that it is not the total displacement $\boldsymbol{u}$ that is periodic, but only the fluctuation part $\boldsymbol{u}^\mu$. Periodicity is indeed the proper characteristics of such a repetitive substructure composed of identical subcells. In the more general case, the assumption can be viewed as an approximation between the (stiffer) Dirichlet and the (flexible) Neumann boundary conditions, which fact is elaborated later.

Remark: Indeed, the Dirichlet boundary conditions represent a special case of periodicity since $\boldsymbol{u}^\mu = \boldsymbol{0}$ is periodic! $\Box$

Figure 2.9 shows the deformed shape of a square RVE in 2D, representing a particle-reinforced matrix, for the two cases of pure normal strain ($\bar{\epsilon}_{11} \neq 0$) and pure shear strain ($\bar{\epsilon}_{12} = \bar{\epsilon}_{21} \neq 0$).

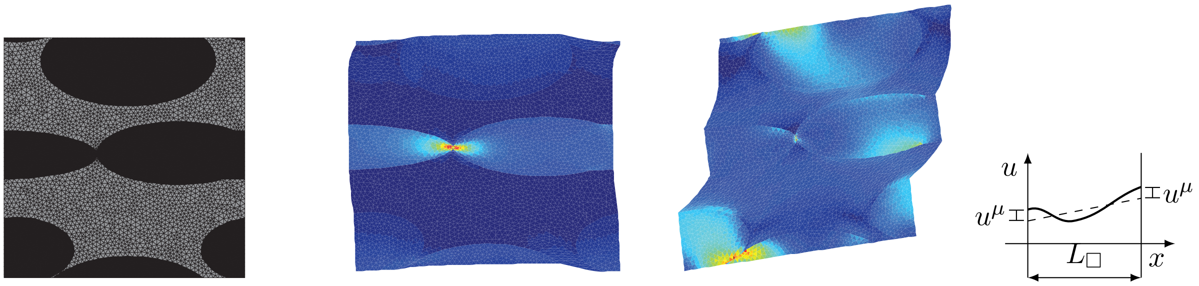


Figure 2.9: *Examples of deformed shapes of square RVE with particles in matrix subjected to SPBC. Left: Undeformed RVE. Middle: Normal strain: Only $\bar{\epsilon}_{11}$ is non-zero. Right: Shear strain: Only $\bar{\epsilon}_{12} = \bar{\epsilon}_{21}$ is non-zero.* {fig:2-10}

It is possible to show that the Hill-Mandel macrohomogeneity condition is identically satisfied in this case as well. However, the technical details are postponed until Chapter 3.

2.4.4 Neumann boundary conditions (NBC-problem)

Neumann boundary conditions on the RVE are introduced via the *model assumption* for the boundary traction

$$\boldsymbol{t}(\boldsymbol{x}) = \bar{\boldsymbol{\sigma}} \cdot \boldsymbol{n}(\boldsymbol{x}), \quad \boldsymbol{x} \in \Gamma_\square \tag{2.145}$$ {eq:2-174}

The assumption (2.145) means that the tractions are constant along any boundary part that is straight. Since it is common to choose a cubical shape of the RVE in practice, it is thus relevant to speak about *constant traction boundary conditions*. This model assumption means that the relation $\langle \boldsymbol{\sigma} \rangle_\square = \bar{\boldsymbol{\sigma}}$ is satisfied a priori (automatically by construction), which is shown as follows:

$$\langle \boldsymbol{\sigma} \rangle_\square = \left(\frac{1}{|\Omega_\square|} \int_{\Gamma_\square} \boldsymbol{t} \otimes \boldsymbol{x} \, \mathrm{d}\Gamma \right)^{\mathrm{sym}} = \bar{\boldsymbol{\sigma}} \cdot \underbrace{\left(\frac{1}{|\Omega_\square|} \int_{\Gamma_\square} \boldsymbol{n} \otimes \boldsymbol{x} \, \mathrm{d}\Gamma \right)^{\mathrm{sym}}}_{=\boldsymbol{I}} = \bar{\boldsymbol{\sigma}} \tag{2.146}$$ {eq:2-175}

Moreover, this relation holds automatically for strain as well as for stress control.

Figure 2.10 shows the deformed shape of a square RVE in 2D, representing a particle-reinforced matrix, for the two cases of pure normal strain ($\bar{\epsilon}_{11} \neq 0$) and pure shear strain ($\bar{\epsilon}_{12} = \bar{\epsilon}_{21} \neq 0$).

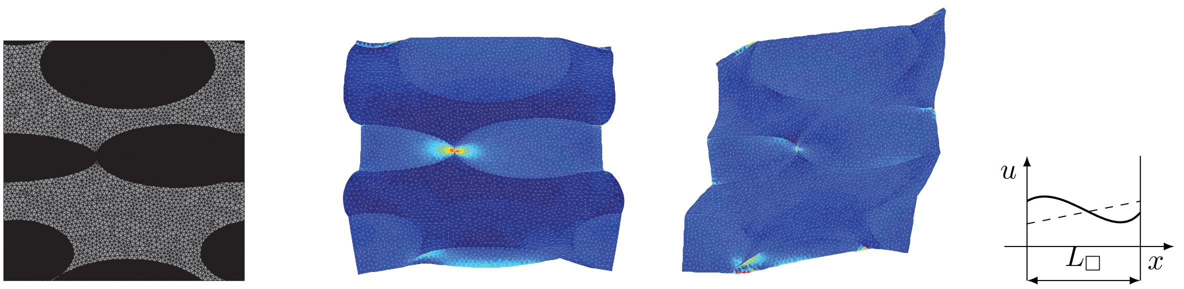


Figure 2.10: *Examples of deformed shapes of square RVE with particles in matrix subjected to NBC. Left: Undeformed RVE. Middle: Normal strain: Only $\bar{\epsilon}_{11}$ is non-zero. Right: Shear strain: Only $\bar{\epsilon}_{12} = \bar{\epsilon}_{21}$ is non-zero.* {fig:2-11}

Next, we show that this condition is sufficient to ensure that the Hill-Mandel condition holds. We then use (2.68) together with (2.145) to obtain

$$\int_{\Gamma_\square} \underbrace{[\boldsymbol{t} - \bar{\boldsymbol{\sigma}} \cdot \boldsymbol{n}]}_{=\mathbf{0}} \cdot [\boldsymbol{u} - \bar{\boldsymbol{\epsilon}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}]] \, \mathrm{d}\Gamma = 0 \tag{2.147}$$ {eq:2-177}

Chapter 3

COMPUTATIONAL HOMOGENIZATION - LINEAR ELASTICITY - UPSCALING

3.1 Canonical format of the SVE-problem

3.1.1 Preliminaries

As a preliminary for establishing the proper variational format, we first consider the most general weak form of the quasi-static equilibrium equation that is pertinent to the subscale (local) problem on a given SVE in the special case of neglected body forces ($\boldsymbol{f} = \boldsymbol{0}$) :

$$\langle \boldsymbol{\epsilon}[\boldsymbol{u}] : \mathsf{E} : \boldsymbol{\epsilon}[\delta \boldsymbol{u}] \rangle_\square - \frac{1}{|\Omega_\square|} \int_{\Gamma_\square} \boldsymbol{t} \cdot \delta \boldsymbol{u} \, \mathrm{d}\Gamma = 0 \tag{3.1}$$ {eq:3-1}

where the test function $\delta \boldsymbol{u}$ is so far not specified. Here, the (total) displacement field $\boldsymbol{u}$ and the boundary traction field $\boldsymbol{t}$ are *a priori* both potentially unknowns; however, at this stage their properties are not further specified. For example, no boundary values or other restrictions on the displacements $\boldsymbol{u}$ are imposed a priori. In conclusion, the problem (3.1) is not uniquely solvable for a single RVE without further model assumptions.

Our first task is to identify the appropriate properties of the solution spaces for the solutions $\boldsymbol{u}$ and $\boldsymbol{t}$ and for the test space pertinent to $\delta \boldsymbol{u}$. To this end we test (3.1) with rigid body modes as follows: (i) $\delta \boldsymbol{u} = \delta \hat{\boldsymbol{u}} \in \mathbb{R}^3$ and (ii) $\delta \boldsymbol{u} = \delta \hat{\boldsymbol{h}}^{\mathrm{skw}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}]$ with $\delta \hat{\boldsymbol{h}}^{\mathrm{skw}} \in \mathbb{R}^{3\times 3}_{\mathrm{skw}}$, respectively. In both cases we note that $\boldsymbol{\epsilon}[\delta \boldsymbol{u}] = \boldsymbol{0}$ and we obtain the equations {eq:3-3}

$$\left[-\frac{1}{|\Omega_\square|} \int_{\Gamma_\square} \boldsymbol{t} \, \mathrm{d}\Gamma \right] \cdot \delta \hat{\boldsymbol{u}} = 0, \quad \forall \delta \hat{\boldsymbol{u}} \in \mathbb{R}^3 \tag{3.2a}$$ {eq:3-3a}

$$\left[-\frac{1}{|\Omega_\square|} \int_{\Gamma_\square} \boldsymbol{t} \otimes [\boldsymbol{x} - \bar{\boldsymbol{x}}] \, \mathrm{d}\Gamma \right] : \delta \hat{\boldsymbol{h}}^{\mathrm{skw}} = 0, \quad \forall \delta \hat{\boldsymbol{h}}^{\mathrm{skw}} \in \mathbb{R}^{3\times 3}_{\mathrm{skw}} \tag{3.2b}$$ {eq:3-3b}

from which follows that we must require $\boldsymbol{t} \in \mathbb{T}_\square$, where we introduced the space of "self-equilibrating tractions"

$$\mathbb{T}_\square = \{\boldsymbol{t} \text{ sufficiently regular on } \Gamma_\square, \int_{\Gamma_\square} \boldsymbol{t} \, \mathrm{d}\Gamma = \boldsymbol{0}, \left(\int_{\Gamma_\square} \boldsymbol{t} \otimes [\boldsymbol{x} - \bar{\boldsymbol{x}}] \, \mathrm{d}\Gamma \right)^{\mathrm{skw}} = \boldsymbol{0}\} \tag{3.3}$$ {eq:3-4}

Next, we show the invariance of (3.1) for Rigid Body Motion (RBM). If we choose $\boldsymbol{t} \in \mathbb{T}_\Box$, it is clear that (3.1) is trivially satisfied for those $\delta\boldsymbol{u}$ that represent translation and rotation (as used above). Hence, such modes (functions) need not be included in the space of test functions. Moreover, we see that if $\boldsymbol{u}$ is a solution, then $\boldsymbol{u} + \boldsymbol{u}^{\mathrm{RBM}}$ is also a solution. Similarly, since $\boldsymbol{\epsilon}[\boldsymbol{u}] = \boldsymbol{\epsilon}[\boldsymbol{u} + \boldsymbol{u}^{\mathrm{RBM}}]$ it follows that the macroscale stress $\bar{\boldsymbol{\sigma}} := \langle \boldsymbol{\sigma}(\boldsymbol{\epsilon}[\boldsymbol{u}])\rangle_\Box$ is invariant to the superpositon of any rigid mode $\boldsymbol{u}^{\mathrm{RBM}}$. Hence, we may (and must) prescribe any RBM-part of the solution to (3.1) in order to ensure that the solution is unique. In conclusion, we have $\boldsymbol{u} \in \mathbb{U}_\Box$ and choose $\delta\boldsymbol{u} \in \mathbb{U}_\Box$, where

{eq:3-5}

$$\mathbb{U}_\Box = \{\boldsymbol{u} \text{ sufficiently regular in } \Omega_\Box,\ \int_{\Omega_\Box} \boldsymbol{u}\, \mathrm{d}\Omega = \boldsymbol{0},\ \left(\int_{\Gamma_\Box} \boldsymbol{u} \otimes \boldsymbol{n}\, \mathrm{d}\Gamma\right)^{\mathrm{skw}} = \boldsymbol{0}\} \tag{3.4}$$

Remark: The invariance to RBM motivates the choice

{eq:3-6}

$$\boldsymbol{u}^{\mathrm{M}}(\boldsymbol{x}) = \bar{\boldsymbol{\epsilon}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}] \tag{3.5}$$

with $\bar{\boldsymbol{u}} = \boldsymbol{0}$, i.e. the constant $\bar{\boldsymbol{u}}$ in the original expression can be dropped and the macroscale displacement gradient $\bar{\boldsymbol{h}}$ can be replaced by its symmetric part $\bar{\boldsymbol{\epsilon}}$. Indeed, this is done henceforth in this Chapter at the explicit presentation of various RVE-problems. □

It is clear that (3.1) is (still) not solvable without imposing further condition(s) that link the displacement field, $\boldsymbol{u}$, (rather the fluctuation part $\boldsymbol{u}^\mu$) and the traction field, $\boldsymbol{t}$, to the condition that either (i) the macroscale strain $\bar{\boldsymbol{\epsilon}}$ is prescribed or (ii) the macroscale stress $\bar{\boldsymbol{\sigma}}$ is prescribed. Hence, both $\boldsymbol{u}$ and $\boldsymbol{t}$ are considered as implicit functions of $\bar{\boldsymbol{\epsilon}}$ or $\bar{\boldsymbol{\sigma}}$. Next, we consider the canonical format of the SVE-problem for these two "loading" cases before specifying further the modeling of $\boldsymbol{u}^\mu$ and/or $\boldsymbol{t}$.

Finally in this preliminary Subsection, we state the H-M condition that must be satisfied by the solution fields $\boldsymbol{u}$ and $\boldsymbol{t}$:

{eq:3-7}

$$\frac{1}{|\Omega_\Box|} \int_{\Gamma_\Box} [\boldsymbol{t} - \bar{\boldsymbol{\sigma}}_\Box\{\boldsymbol{t}\}] \cdot [\boldsymbol{u} - \bar{\boldsymbol{\epsilon}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}]]\, \mathrm{d}\Gamma = 0 \tag{3.6}$$

where we introduced the mean stress operator

{eq:3-8}

$$\bar{\boldsymbol{\sigma}}_\Box\{\boldsymbol{t}\} := \left(\frac{1}{|\Omega_\Box|} \int_{\Gamma_\Box} \boldsymbol{t} \otimes [\boldsymbol{x} - \bar{\boldsymbol{x}}]\, \mathrm{d}\Gamma\right)^{\mathrm{sym}} \tag{3.7}$$

3.1.2 Canonical format of SVE-problem for macroscale strain control

In the (standard) case of complete *macroscale strain control*, $\bar{\boldsymbol{\epsilon}}$ is supposed to be a known quantity at the solution of the SVE-problem, and $\boldsymbol{u} \in \mathbb{U}_\Box$, $\boldsymbol{t} \in \mathbb{T}_\Box$ are solved from the system:

{eq:3-9a}

$$\langle \boldsymbol{\epsilon}[\boldsymbol{u}] : \mathbf{E} : \boldsymbol{\epsilon}[\delta\boldsymbol{u}]\rangle_\Box - \frac{1}{|\Omega_\Box|} \int_{\Gamma_\Box} \boldsymbol{t} \cdot \delta\boldsymbol{u}\, \mathrm{d}\Gamma = 0 \qquad \forall \delta\boldsymbol{u} \in \mathbb{U}_\Box \tag{3.8a}$$

{eq:3-9b}

$$-\frac{1}{|\Omega_\Box|} \int_{\Gamma_\Box} \delta\boldsymbol{t} \cdot \boldsymbol{u}\, \mathrm{d}\Gamma = -\bar{\boldsymbol{\epsilon}} : \left[\frac{1}{|\Omega_\Box|} \int_{\Gamma_\Box} \delta\boldsymbol{t} \otimes [\boldsymbol{x} - \bar{\boldsymbol{x}}]\, \mathrm{d}\Gamma\right] \qquad \forall \delta\boldsymbol{t} \in \mathbb{T}_\Box \tag{3.8b}$$

{eq:3-9} We remark that the strain identity (2.56) as well as the H-M condition in (3.7) are embedded in the canonical formulation of the RVE-problem and are, thus, guaranteed by its solution. This {eq:3-10} is shown as follows: Decompose $\mathbb{T}_\square$ hierarchically as $\mathbb{T}_\square = \bar{\mathbb{T}}_\square \oplus \mathbb{T}'_\square$, where

{eq:3-10a}
$$\bar{\mathbb{T}}_\square = \{\boldsymbol{t} \in \mathbb{T}_\square |\ \exists \bar{\boldsymbol{\sigma}} \in \mathbb{R}^{3\times 3}_{\mathrm{sym}} \text{ s. t. } \boldsymbol{t} = \bar{\boldsymbol{\sigma}} \cdot \boldsymbol{n} \text{ on } \Gamma_\square\} \tag{3.9a}$$

{eq:3-10b}
$$\mathbb{T}'_\square = \{\boldsymbol{t} \in \mathbb{T}_\square |\ \left(\int_{\Gamma_\square} \boldsymbol{t} \otimes [\boldsymbol{x} - \bar{\boldsymbol{x}}] \,\mathrm{d}\Gamma\right)^{\mathrm{sym}} = \boldsymbol{0}\} \tag{3.9b}$$

We may thus choose, for any $\boldsymbol{t} \in \mathbb{T}_\square$, the decomposition $\boldsymbol{t} = \bar{\boldsymbol{t}} + \boldsymbol{t}'$ with $\bar{\boldsymbol{t}} \in \bar{\mathbb{T}}_\square$ and $\boldsymbol{t}' \in \mathbb{T}'_\square$.

- Test (3.8b) by $\delta\boldsymbol{t} = \delta\bar{\boldsymbol{\sigma}} \cdot \boldsymbol{n} \in \bar{\mathbb{T}}_\square$ for all possible $\delta\bar{\boldsymbol{\sigma}} \in \mathbb{R}^{3\times 3}_{\mathrm{sym}}$. The LHS and RHS of (3.8b) then become, respectively,

$$-\frac{1}{|\Omega_\square|}\int_{\Gamma_\square} \delta\boldsymbol{t} \cdot \boldsymbol{u} \,\mathrm{d}\Gamma = -\left[\frac{1}{|\Omega_\square|}\int_{\Gamma_\square} \boldsymbol{u} \otimes \boldsymbol{n} \,\mathrm{d}\Gamma\right] : \delta\bar{\boldsymbol{\sigma}} = -\langle \boldsymbol{\epsilon}[\boldsymbol{u}]\rangle_\square : \delta\bar{\boldsymbol{\sigma}}$$

$$-\bar{\boldsymbol{\epsilon}} : \frac{1}{|\Omega_\square|}\int_{\Gamma_\square} \delta\boldsymbol{t} \otimes [\boldsymbol{x} - \bar{\boldsymbol{x}}] \,\mathrm{d}\Gamma = -\bar{\boldsymbol{\epsilon}} : \left[\delta\bar{\boldsymbol{\sigma}} \cdot \underbrace{\frac{1}{|\Omega_\square|}\int_{\Gamma_\square} \boldsymbol{n} \otimes [\boldsymbol{x} - \bar{\boldsymbol{x}}] \,\mathrm{d}\Gamma}_{=\boldsymbol{I}}\right] = -\bar{\boldsymbol{\epsilon}} : \delta\bar{\boldsymbol{\sigma}}$$

  Upon noting that the LHS and RHS must be the same for any possible $\delta\bar{\boldsymbol{\sigma}} \in \mathbb{R}^{3\times 3}_{\mathrm{sym}}$, we then conclude that the strain identity is satisfied:

$$\langle \boldsymbol{\epsilon}[\boldsymbol{u}]\rangle_\square = \bar{\boldsymbol{\epsilon}} \tag{3.10}$$ {eq:3-12}

- Test (3.8b) by $\delta\boldsymbol{t} = \boldsymbol{t}' \in \mathbb{T}'_\square$. However, the solution $\boldsymbol{t}' \in \mathbb{T}'_\square$ can be written as $\boldsymbol{t}' = \boldsymbol{t} - \bar{\boldsymbol{\sigma}}_\square \cdot \boldsymbol{n}$ with $\boldsymbol{t} \in \mathbb{T}_\square$ due to the unique decomposition, and inserting this expression in (3.8b) is precisely the H-M condition given in (3.6).

In a post-processing step, $\bar{\boldsymbol{\sigma}}$ is computed as the volume average of the computed field $\boldsymbol{\sigma}$. We remark that it is possible to obtain the appropriate expression from (3.8a) with the choice of test function $\delta\boldsymbol{u} = \delta\bar{\boldsymbol{\epsilon}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}] \in \mathbb{U}_\square$ for all possible $\delta\bar{\boldsymbol{\epsilon}} \in \mathbb{R}^{3\times 3}_{\mathrm{sym}}$: Check!

$$\underbrace{\langle \boldsymbol{\epsilon}[\boldsymbol{u}] : \mathsf{E}\rangle_\square}_{=\bar{\boldsymbol{\sigma}}} = \frac{1}{|\Omega_\square|}\int_{\Gamma_\square} \boldsymbol{t} \otimes [\boldsymbol{x} - \bar{\boldsymbol{x}}] \,\mathrm{d}\Gamma \tag{3.11}$$ {eq:3-13}

3.1.3 Canonical format of SVE-problem for macroscale stress control

We also give the canonical format for the (non-standard) case of complete *macroscale stress control*. In such a case, $\bar{\boldsymbol{\sigma}}$ is supposed to be a known quantity at the solution of the RVE-problem, and $\boldsymbol{u} \in \mathbb{U}_\square$, $\boldsymbol{t} \in \mathbb{T}_\square$, $\bar{\boldsymbol{\epsilon}} \in \mathbb{R}^{3\times 3}_{\mathrm{sym}}$ are solved from the system:

$$\langle \boldsymbol{\epsilon}[\boldsymbol{u}] : \mathsf{E} : \boldsymbol{\epsilon}[\delta\boldsymbol{u}]\rangle_\square - \frac{1}{|\Omega_\square|}\int_{\Gamma_\square} \boldsymbol{t} \cdot \delta\boldsymbol{u} \,\mathrm{d}\Gamma = 0 \qquad \forall \delta\boldsymbol{u} \in \mathbb{U}_\square \tag{3.12a}$$ {eq:3-14a}

$$-\frac{1}{|\Omega_\square|}\int_{\Gamma_\square} \delta\boldsymbol{t} \cdot \boldsymbol{u} \,\mathrm{d}\Gamma + \bar{\boldsymbol{\epsilon}} : \frac{1}{|\Omega_\square|}\int_{\Gamma_\square} \delta\boldsymbol{t} \otimes [\boldsymbol{x} - \bar{\boldsymbol{x}}] \,\mathrm{d}\Gamma = 0 \qquad \forall \delta\boldsymbol{t} \in \mathbb{T}_\square \tag{3.12b}$$ {eq:3-14b}

$$\left[\frac{1}{|\Omega_\square|}\int_{\Gamma_\square} \boldsymbol{t} \otimes [\boldsymbol{x} - \bar{\boldsymbol{x}}] \,\mathrm{d}\Gamma\right] : \delta\bar{\boldsymbol{\epsilon}} = \bar{\boldsymbol{\sigma}} : \delta\bar{\boldsymbol{\epsilon}} \qquad \forall \delta\bar{\boldsymbol{\epsilon}} \in \mathbb{R}^{3\times 3} \tag{3.12c}$$ {eq:3-14c}

It is noted that $\bar{\boldsymbol{\epsilon}}$ is now part of the solution, such that the strain identity becomes satisfied by $\boldsymbol{u}$ and $\bar{\boldsymbol{\epsilon}}$. Moreover, the stress identity is ensured by (3.12c). Finally, that the H-M condition is embedded in the formulation can be shown exactly as for the situation of macroscale strain control. {eq:3-14}

3.1.4 Specification of canonical SVE-problem – Preliminary remarks

In order to define a uniquely solvable SVE-problem, it is necessary to introduce further model assumptions as regards the displacement field $\boldsymbol{u}$ and/or the traction field $\boldsymbol{t}$, which is manifested by the appropriate restrictions of $\mathbb{U}_\square$ and $\mathbb{T}_\square$. The classical boundary conditions

- Dirichlet boundary conditions (DBC-problem)
- Strongly Periodic boundary conditions (SPBC-problem)
- Neumann boundary conditions (NBC-problem)

were discussed in Chapter 2. In addition we shall discuss the non-classical

- Weakly Periodic boundary conditions (WPBC-problem)

It is possible to deduce the SVE-problems with the classical boundary conditions (DBC, NBC, and SPBC) as special cases of the WPBC-problem. This is the approach that is taken in Chapter 4 dealing with bounds on the effective properties. In this Chapter and in Chapter 5, however, we shall consider the formulation of the different SVE-problems as independent.

In the remainder of this Chapter, we consider all these boundary conditions in conjunction with both macroscale strain control ($\bar{\boldsymbol{\epsilon}}$ is prescribed) and macroscale stress control ($\bar{\boldsymbol{\sigma}}$ is prescribed). However, we focus on the former situation and establish the computational procedure for obtaining the apparant stiffness tensor $\bar{\mathbf{E}}_\square$ for any given realization SVE. As a general outline, we then need to establish

- the strain concentration tensor $\mathbf{A}(\boldsymbol{x})$, $\boldsymbol{x} \in \Omega_\square$, in the relation $\boldsymbol{\epsilon}(\boldsymbol{x}) = \mathbf{A}(\boldsymbol{x}) : \bar{\boldsymbol{\epsilon}}$ in terms of "unit fluctuation fields",
- the SVE-problem from which the pertinent unit fluctuation fields can be computed,
- $\bar{\mathbf{E}}_\square$ using the fields $\mathbf{E}(\boldsymbol{x})$ and $\mathbf{A}(\boldsymbol{x})$. For linear problems $\mathbf{A}(\boldsymbol{x})$ is independent of the actual $\bar{\boldsymbol{\epsilon}}$; hence, $\bar{\mathbf{E}}_\square$ can be established once and for all (for a given realization SVE).

Finally, we remark that it is only the macroscale strain control that is relevant in a "strain-controlled macroscale constitutive driver", which is the "heart" of any FE-code for nonlinear material response. In such cases direct upscaling is no longer possible. Issues related to nonlinear response are discussed in Chapter 4.

3.2 Dirichlet boundary conditions (DBC-problem)

3.2.1 Preliminaries

In order to establish a suitable variational setting we recall the basic space $\mathbb{U}_\square$ from (3.5), that contains sufficiently regular[1] (displacement) functions. We introduce the more restrictive spaces

{eq:3-15}
$$\mathbb{U}_\square^{\mathrm{D}} = \{\boldsymbol{u} \in \mathbb{U}_\square | \; \exists \hat{\boldsymbol{u}} \in \mathbb{R}^3,\, \hat{\boldsymbol{\epsilon}} \in \mathbb{R}^{3\times 3}_{\mathrm{sym}} \text{ s.t. } \boldsymbol{u} = \hat{\boldsymbol{u}} + \hat{\boldsymbol{\epsilon}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}] \text{ on } \Gamma_\square\} \tag{3.13}$$

[1] The notion "sufficiently regular" is used frequently in order to avoid specific discussion of which derivatives that are involved. Usually, this means a Hilbert space with sufficiently smooth functions.

Here, it appears that $\mathbb{U}_\square^{\mathrm{D}}$ is the subset of $\mathbb{U}_\square$ that can accomodate an arbitrary affine displacement on $\Gamma_\square$. Since a pure translation displacement represents a rigid body motion and does not affect
{eq:3-16} the stress response, it is convenient to exploit the spaces

{eq:3-16a}
$$\mathbb{U}_\square^{\mathrm{D}}(\bar{\boldsymbol{\epsilon}}) = \{\boldsymbol{u} \in \mathbb{U}_\square |\ \boldsymbol{u} = \bar{\boldsymbol{\epsilon}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}] \text{ on } \Gamma_\square\} \tag{3.14a}$$

{eq:3-16b}
$$\mathbb{U}_\square^{\mathrm{D},0} = \{\boldsymbol{u} \in \mathbb{U}_\square |\ \boldsymbol{u} = \boldsymbol{0} \text{ on } \Gamma_\square\} \tag{3.14b}$$

In the case of (macroscale) strain control, we require that $\boldsymbol{u} \in \mathbb{U}_\square^{\mathrm{D}}(\bar{\boldsymbol{\epsilon}})$. Further, it is clear that $\boldsymbol{u}^{\mathrm{M}}(\bar{\boldsymbol{\epsilon}}) \in \mathbb{U}_\square^{\mathrm{D}}(\bar{\boldsymbol{\epsilon}})$; hence, the fluctuation part $\boldsymbol{u}^\mu \in \mathbb{U}_\square^{\mathrm{D},0}$.

Remark: The restriction $\boldsymbol{u} \in \mathbb{U}_\square^{\mathrm{D}}$ is *imposed explicitly* in the case of macroscale *strain control*, i. e. when the value $\bar{\boldsymbol{\epsilon}}$ is prescribed as input data. However, in the case of macroscale *stress control*, i. e. when the value $\bar{\boldsymbol{\sigma}}$ is prescribed as input data, then the value $\bar{\boldsymbol{\epsilon}}$ is part of the solution of a mixed problem with $\boldsymbol{u}$ and $\bar{\boldsymbol{\epsilon}}$ as the variables. □

3.2.2 DBC-problem for macroscale strain control

Upon introducing the test function $\delta\boldsymbol{u} \in \mathbb{U}_\square^{\mathrm{D},0}$, which means that $\delta\boldsymbol{u} = \boldsymbol{0}$ on $\Gamma_\square$ for *given (fixed)* $\bar{\boldsymbol{\epsilon}}$, the bounday integral in (3.8a) vanishes. Moreover, choosing $\boldsymbol{u} \in \mathbb{U}_\square^{\mathrm{D}}(\bar{\boldsymbol{\epsilon}})$, we note that (3.8b) is an identity; i.e. it is trivially satisfied. In conclusion, the weak format of the DBC-problem for a SVE under macroscale strain control can be phrased as follows:

For given value of the macroscale strain $\bar{\boldsymbol{\epsilon}}$, find the fluctuation displacement field $\boldsymbol{u}^\mu \in \mathbb{U}_\square^{\mathrm{D},0}$ which solves

$$\langle \bar{\boldsymbol{\epsilon}} + \boldsymbol{\epsilon}[\boldsymbol{u}^\mu] : \mathsf{E} : \boldsymbol{\epsilon}[\delta\boldsymbol{u}] \rangle_\square = 0 \quad \forall \delta\boldsymbol{u} \in \mathbb{U}_\square^{\mathrm{D},0} \tag{3.15}$$ {eq:3-17}

This problem can be rewritten as

$$\langle \boldsymbol{\epsilon}[\boldsymbol{u}^\mu] : \mathsf{E} : \boldsymbol{\epsilon}[\delta\boldsymbol{u}] \rangle_\square = -\bar{\boldsymbol{\epsilon}} : \langle \mathsf{E} : \boldsymbol{\epsilon}[\delta\boldsymbol{u}] \rangle_\square \quad \forall \delta\boldsymbol{u} \in \mathbb{U}_\square^{\mathrm{D},0} \tag{3.16}$$ {eq:3-18}

where the RHS is known. Hence, the DBC-problem is driven directly by $\bar{\boldsymbol{\epsilon}}$ as the data.

3.2.3 Macroscale stiffness tensor

Sensitivity fields

The aim is to compute the entries of $\bar{\mathsf{E}}_\square$ once and for all (due to linearity). This is accomplished by first computing "unit displacement fluctuation fields" or, rather, *sensitivity fields*, corresponding to unit change of each of the Cartesian components of $\bar{\boldsymbol{\epsilon}}$. In 3D there are 6 independent components $\bar{\epsilon}_{ij}$; hence, 6 unit displacement fields are sought.

The macroscale displacement field $\boldsymbol{u}^{\mathrm{M}}$ can be represented as follows:

$$\boldsymbol{u}^{\mathrm{M}}(\boldsymbol{x}) = \bar{\boldsymbol{\epsilon}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}] = \sum_{i,j=1}^{NDIM} \hat{\boldsymbol{u}}^{\mathrm{M}(ij)}(\boldsymbol{x})\bar{\epsilon}_{ij} \quad \Rightarrow \quad \hat{\boldsymbol{u}}^{\mathrm{M}(ij)} = \boldsymbol{e}_i \otimes \boldsymbol{e}_j \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}] \tag{3.17}$$ {eq:3-21}

Clearly, the "unit displacement fields" $\hat{\boldsymbol{u}}^{\mathrm{M}(ij)}$ represent the value of $\boldsymbol{u}^{\mathrm{M}}$ for unit values of $\bar{\epsilon}_{ij}$. The strain corresponding to $\boldsymbol{u}^{\mathrm{M}}$ can be written, using (3.17), as

$$\boldsymbol{\epsilon}[\boldsymbol{u}^{\mathrm{M}}] = (\boldsymbol{u}^{\mathrm{M}} \otimes \boldsymbol{\nabla})^{\mathrm{sym}} = \bar{\boldsymbol{\epsilon}} = \sum_{i,j} \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{\mathrm{M}(ij)}]\bar{\epsilon}_{ij}, \quad \text{with} \quad \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{\mathrm{M}(ij)}] = (\boldsymbol{e}_i \otimes \boldsymbol{e}_j)^{\mathrm{sym}} \tag{3.18}$$ {eq:3-22}

Remark: Upon combining (3.18) with the identity $\bar{\epsilon}_{ij} = \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{\mathrm{M}(ij)}] : \bar{\boldsymbol{\epsilon}}$, we obtain the representation

$$\bar{\boldsymbol{\epsilon}} = \left[\sum_{i,j} \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{\mathrm{M}(ij)}] \otimes \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{\mathrm{M}(ij)}] \right] : \bar{\boldsymbol{\epsilon}} \tag{3.19}$$ {eq:3-23}

From this identity we conclude that

{eq:3-24} $$\mathbf{I}^{\mathrm{SYM}} = \sum_{i,j} \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{\mathrm{M}(ij)}] \otimes \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{\mathrm{M}(ij)}] = \sum_{i,j} (\boldsymbol{e}_i \otimes \boldsymbol{e}_j)^{\mathrm{sym}} \otimes (\boldsymbol{e}_i \otimes \boldsymbol{e}_j)^{\mathrm{sym}} \tag{3.20}$$

which is an alternative way of expressing the 4th order identity tensor. □

Next, we aim at expressing the fluctuation displacement $\boldsymbol{u}^{\mu}(\boldsymbol{x})$ as a linear function of $\bar{\boldsymbol{\epsilon}}$, in a fashion that is similar to (3.18), via the *ansatz*:

{eq:3-25} $$\boldsymbol{u}^{\mu}(\boldsymbol{x}) = \sum_{i,j} \hat{\boldsymbol{u}}^{\mu(ij)}(\boldsymbol{x}) \bar{\epsilon}_{ij} \tag{3.21}$$

whereby

{eq:3-26} $$\boldsymbol{u}(\boldsymbol{x}) = \sum_{i,j} \hat{\boldsymbol{u}}^{(ij)}(\boldsymbol{x}) \bar{\epsilon}_{ij} \quad \text{with} \quad \hat{\boldsymbol{u}}^{(ij)} \stackrel{\text{def}}{=} \hat{\boldsymbol{u}}^{\mathrm{M}(ij)} + \hat{\boldsymbol{u}}^{\mu(ij)} \tag{3.22}$$

To compute the "unit macroscale displacement fields" $\hat{\boldsymbol{u}}^{\mu(ij)}$ is the next task. Upon inserting the representations of $\boldsymbol{\epsilon}[\boldsymbol{u}^{\mathrm{M}}]$ in (3.18) and $\boldsymbol{u}^{\mu}$ in (3.21) into (3.16), while noting that this relation must hold for any given values $\bar{\epsilon}_{ij}$, we obtain the RVE-problem for each one of the "unit fluctuation displacement" fields: Find $\hat{\boldsymbol{u}}^{\mu(ij)} \in \mathbb{U}_{\square}^{\mathrm{D},0}$ for $i, j = 1, 2, NDIM$ as the solution of

{eq:3-526} $$\begin{aligned} \langle \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{\mu(ij)}] : \mathbf{E} : \boldsymbol{\epsilon}[\delta \boldsymbol{u}] \rangle_{\square} &= -\langle \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{\mathrm{M}(ij)}] : \mathbf{E} : \boldsymbol{\epsilon}[\delta \boldsymbol{u}] \rangle_{\square} \\ &= -\langle [\boldsymbol{e}_i \otimes \boldsymbol{e}_j] : \mathbf{E} : \boldsymbol{\epsilon}[\delta \boldsymbol{u}] \rangle_{\square} \quad \forall \delta \boldsymbol{u} \in \mathbb{U}_{\square}^{\mathrm{D},0} \end{aligned} \tag{3.23}$$

where we used the minor symmetry of $\mathbf{E}$ to obtain the last identity of the RHS.

Macroscale (apparent) stiffness tensor: "Nonsymmetric" version

We use the identity $\bar{\boldsymbol{\sigma}} = \langle \boldsymbol{\sigma} \rangle_{\square}$ to obtain

{eq:3-27} $$\bar{\sigma}_{ij} = \langle \boldsymbol{e}_i \cdot \boldsymbol{\sigma} \cdot \boldsymbol{e}_j \rangle_{\square} = \langle \boldsymbol{\sigma} : [\boldsymbol{e}_i \otimes \boldsymbol{e}_j] \rangle_{\square} = \langle \boldsymbol{\epsilon}[\boldsymbol{u}] : \mathbf{E} : \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{\mathrm{M}(ij)}] \rangle_{\square} \tag{3.24}$$

where it was utilized that $\boldsymbol{\sigma}$ is symmetrical. Upon introducing the representation of $\boldsymbol{u}$ in terms of sensitivities, as given i (3.22), into (3.24), we obtain

{eq:3-28} $$\bar{\sigma}_{ij} = \sum_{k,l} \underbrace{\langle \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{\mathrm{M}(ij)}] : \mathbf{E} : \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{(kl)}] \rangle_{\square}}_{(\bar{\mathbf{E}}_{\square})_{ijkl}} : \bar{\epsilon}_{kl} \tag{3.25}$$

i.e. it is shown that

{eq:3-29} $$(\bar{\mathbf{E}}_{\square})_{ijkl} = \langle \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{\mathrm{M}(ij)}] : \mathbf{E} : \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{(kl)}] \rangle_{\square} \tag{3.26}$$

Macroscale (apparent) stiffness tensor: "Symmetric" version

From the Hill-Mandel macrohomogeneity condition $\bar{\boldsymbol{\sigma}} : \bar{\boldsymbol{\epsilon}} = \langle \boldsymbol{\sigma} : \boldsymbol{\epsilon} \rangle_\square$, we first conclude that

{eq:3-31} $$\bar{\boldsymbol{\epsilon}} : \bar{\mathbf{E}}_\square : \bar{\boldsymbol{\epsilon}} = \langle \boldsymbol{\epsilon}[\boldsymbol{u}] : \mathbf{E} : \boldsymbol{\epsilon}[\boldsymbol{u}] \rangle_\square \tag{3.27}$$

which holds true for any given $\bar{\boldsymbol{\epsilon}}$. Now, upon introducing the representation of $\boldsymbol{u}$ in terms of sensitivities, as given in (3.22), into (3.27), we obtain

{eq:3-32} $$\sum_{ijkl} \bar{\epsilon}_{ij} (\bar{\mathbf{E}}_\square)_{ijkl} \bar{\epsilon}_{kl} = \sum_{ijkl} \bar{\epsilon}_{ij} \langle \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{(ij)}] : \mathbf{E} : \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{(kl)}] \rangle_\square \bar{\epsilon}_{kl} \tag{3.28}$$

and we conclude that

$$(\bar{\mathbf{E}}_\square)_{ijkl} = \langle \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{(ij)}] : \mathbf{E} : \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{(kl)}] \rangle_\square \tag{3.29}$$ {eq:3-33}

Remark: It is possible to arrive at the result in (3.29) by using the strain concentration tensor $\mathbf{A}$, as defined by the relation $\boldsymbol{\epsilon} = \mathbf{A} : \bar{\boldsymbol{\epsilon}}$. We first conclude that

$$\bar{\epsilon}_{ij} = \bar{\boldsymbol{\epsilon}} : [\boldsymbol{e}_i \otimes \boldsymbol{e}_j] = \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{\mathrm{M}(ij)}] : \bar{\boldsymbol{\epsilon}} \tag{3.30}$$ {eq:3-34}

which can be combined with the representation of $\boldsymbol{u}$ in terms of sensitivities, as given in (3.22), to give

$$\boldsymbol{\epsilon} = \sum_{i,j} \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{(ij)}] \bar{\epsilon}_{ij} = \underbrace{\sum_{i,j} \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{(ij)}] \otimes \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{\mathrm{M}(ij)}]}_{=\mathbf{A}} : \bar{\boldsymbol{\epsilon}} \tag{3.31}$$ {eq:3-35}

For known $\mathbf{A}$, it is possible to compute the (apparent) macroscale stiffness $\bar{\mathbf{E}}_\square$ via the definition

$$\begin{aligned} \bar{\mathbf{E}}_\square &= \langle \mathbf{A}^{\mathrm{T}} : \mathbf{E} : \mathbf{A} \rangle_\square \\ &= \sum_{m,n,p,q} \langle \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{\mathrm{M}(mn)}] \otimes \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{(mn)}] : \mathbf{E} : \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{(pq)}] \otimes \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{\mathrm{M}(pq)}] \rangle_\square \\ &= \sum_{m,n,p,q} (\boldsymbol{e}_m \otimes \boldsymbol{e}_n)^{\mathrm{sym}} \otimes \langle \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{(mn)}] : \mathbf{E} : \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{(pq)}] \rangle_\square \otimes (\boldsymbol{e}_p \otimes \boldsymbol{e}_q)^{\mathrm{sym}} \end{aligned} \tag{3.32}$$ {eq:3-37}

The components of $\bar{\mathbf{E}}_\square$ can then be computed explicitly as

$$\begin{aligned} (\bar{\mathbf{E}}_\square)_{ijkl} &= [\boldsymbol{e}_i \otimes \boldsymbol{e}_j] : \bar{\mathbf{E}}_\square : [\boldsymbol{e}_k \otimes \boldsymbol{e}_l] \\ &= \sum_{m,n,p,q} \underbrace{[\boldsymbol{e}_i \otimes \boldsymbol{e}_j] : (\boldsymbol{e}_m \otimes \boldsymbol{e}_n)^{\mathrm{sym}}}_{\substack{=1 \text{ if } m=i, n=j \\ =0 \text{ if else}}} \otimes \langle \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{(mn)}] : \mathbf{E} : \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{(pq)}] \rangle_\square \otimes \underbrace{(\boldsymbol{e}_p \otimes \boldsymbol{e}_q)^{\mathrm{sym}} : [\boldsymbol{e}_k \otimes \boldsymbol{e}_l]}_{\substack{=1 \text{ if } p=k, q=l \\ =0 \text{ if else}}} \\ &= \langle \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{(ij)}] : \mathbf{E} : \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{(kl)}] \rangle_\square \quad i,j,k,l = 1,2,...,NDIM \end{aligned} \tag{3.33}$$ {eq:3-38}

which is the same expression as in (3.29). $\square$

When the fluctuation part of the displacement field is ignored, i.e. $\hat{\boldsymbol{u}}^{\mu(ij)} = \mathbf{0}$, then the stiffness is pertinent to the Voigt (or Taylor) assumption, i.e. $\bar{\mathbf{E}}_\square = \bar{\mathbf{E}}_\square^{\mathrm{V}} \stackrel{\mathrm{def}}{=} \langle \mathbf{E} \rangle_\square$.

3.2.4 FE-approximation – Matrix format (in 2D)

Preliminaries

The spatial FE-discretization on $\Omega_\square$ is defined by basis functions $\{\boldsymbol{N}_k\}_{k=1}^{\mathrm{NVAR}}$ that are conveniently split into

- $\{\boldsymbol{N}_k^{\mathrm{i}}\}_{k=1}^{\mathrm{NVAR_i}}$ corresponding to $\mathrm{NVAR_i}$ internal nodal variables
- $\{\boldsymbol{N}_k^{\mathrm{b}}\}_{k=1}^{\mathrm{NVAR_b}}$ corresponding to $\mathrm{NVAR_b}$ boundary nodal variables,

where $\mathrm{NVAR} = \mathrm{NVAR_i} + \mathrm{NVAR_b}$. Hence, any displacement field $\boldsymbol{u}(\boldsymbol{x})$, for $\boldsymbol{x} \in \Omega_\square$, can be represented as the FE-approximation $\boldsymbol{u}_h(\boldsymbol{x})$:

{eq:3-41}
$$\boldsymbol{u}_h = \sum_{k=1}^{\mathrm{NVAR}} \boldsymbol{N}_k (\underline{\boldsymbol{u}})_k = \sum_{k=1}^{\mathrm{NVAR_i}} \boldsymbol{N}_k^{\mathrm{i}} (\underline{\boldsymbol{u}}^{\mathrm{i}})_k + \sum_{k=1}^{\mathrm{NVAR_b}} \boldsymbol{N}_k^{\mathrm{b}} (\underline{\boldsymbol{u}}^{\mathrm{b}})_k \tag{3.34}$$

whereby the corresponding strain field becomes

{eq:3-42}
$$\boldsymbol{\epsilon}[\boldsymbol{u}_h] = \sum_{k=1}^{\mathrm{NVAR}} (\boldsymbol{N}_k \otimes \boldsymbol{\nabla})^{\mathrm{sym}} (\underline{\boldsymbol{u}})_k = \sum_{k=1}^{\mathrm{NVAR}} \boldsymbol{B}_k (\underline{\boldsymbol{u}})_k \quad \text{with } \boldsymbol{B}_k \overset{\mathrm{def}}{=} (\boldsymbol{N}_k \otimes \boldsymbol{\nabla})^{\mathrm{sym}} \tag{3.35}$$

Here, $\underline{\boldsymbol{u}}^{\mathrm{i}}$ and $\underline{\boldsymbol{u}}^{\mathrm{b}}$ are column vectors containing all *internal* and *boundary* variables, respectively, such that the complete set of nodal variables are thus

{eq:3-43}
$$\underline{\boldsymbol{u}} = \begin{bmatrix} \underline{\boldsymbol{u}}^{\mathrm{i}} \\ \underline{\boldsymbol{u}}^{\mathrm{b}} \end{bmatrix}. \tag{3.36}$$

We note that the macroscopic (in-plane) strain and the work-conjugated stress can be organized in the Voigt matrix notation as follows:

{eq:3-44}
$$\underline{\bar{\boldsymbol{\epsilon}}} = \begin{bmatrix} \bar{\epsilon}_{11} \\ \bar{\epsilon}_{22} \\ 2\bar{\epsilon}_{12} \end{bmatrix} = \begin{bmatrix} \bar{\epsilon}_{11} \\ \bar{\epsilon}_{22} \\ \bar{\gamma}_{12} \end{bmatrix}, \quad \underline{\bar{\boldsymbol{\sigma}}} = \begin{bmatrix} \bar{\sigma}_{11} \\ \bar{\sigma}_{22} \\ \bar{\sigma}_{12} \end{bmatrix} \tag{3.37}$$

where $\bar{\gamma}_{12}$ is the engineering shear strain that accounts for the symmetry of $\bar{\boldsymbol{\epsilon}}$.

We split the nodal variables into "macroscale" and "fluctuation" parts as follows:

{eq:3-45}
$$\underline{\boldsymbol{u}} = \begin{bmatrix} \underline{\boldsymbol{u}}^{\mathrm{i}} \\ \underline{\boldsymbol{u}}^{\mathrm{b}} \end{bmatrix} = \begin{bmatrix} \underline{\boldsymbol{u}}^{\mathrm{M,i}} + \underline{\boldsymbol{u}}^{\mu,\mathrm{i}} \\ \underline{\boldsymbol{u}}^{\mathrm{M,b}} + \underbrace{\underline{\boldsymbol{u}}^{\mu,\mathrm{b}}}_{=\underline{\boldsymbol{0}}} \end{bmatrix} = \begin{bmatrix} \hat{\underline{\boldsymbol{u}}}^{\mathrm{M,i}} + \hat{\underline{\boldsymbol{u}}}^{\mu,\mathrm{i}} \\ \hat{\underline{\boldsymbol{u}}}^{\mathrm{M,b}} \end{bmatrix} \underline{\bar{\boldsymbol{\epsilon}}} \tag{3.38}$$

In (3.38), we introduced nodal variables $\hat{\underline{\boldsymbol{u}}}^{\mathrm{M,i}(ij)}$, $\hat{\underline{\boldsymbol{u}}}^{\mu,\mathrm{i}(ij)}$ and $\hat{\underline{\boldsymbol{u}}}^{\mathrm{M,b}(ij)}$ that correspond to "unit macroscale deformations", i. e. nodal displacements that correspond to $\bar{\epsilon}_{ij} = 1$ for $i, j = 1, 2, ..., NDIM$. In the 2D-case, we have

{eq:3-46}
$$\underline{\boldsymbol{u}}^{\mathrm{M,i}} = \hat{\underline{\boldsymbol{u}}}^{\mathrm{M,i}} \underline{\bar{\boldsymbol{\epsilon}}} = \begin{bmatrix} \hat{\underline{\boldsymbol{u}}}^{\mathrm{M,i}(11)}, \hat{\underline{\boldsymbol{u}}}^{\mathrm{M,i}(22)}, \hat{\underline{\boldsymbol{u}}}^{\mathrm{M,i}(12)} \end{bmatrix} \begin{bmatrix} \bar{\epsilon}_{11} \\ \bar{\epsilon}_{22} \\ \bar{\gamma}_{12} \end{bmatrix} \tag{3.39}$$

{eq:3-47}
$$\underline{\boldsymbol{u}}^{\mathrm{M,b}} = \underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}}\underline{\bar{\boldsymbol{\epsilon}}} = \left[\ \underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b(11)}}, \underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b(22)}}, \underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b(12)}}\ \right] \begin{bmatrix} \bar{\epsilon}_{11} \\ \bar{\epsilon}_{22} \\ \bar{\gamma}_{12} \end{bmatrix} \tag{3.40}$$

{eq:3-48}
$$\underline{\boldsymbol{u}}^{\mu,\mathrm{i}} = \underline{\hat{\boldsymbol{u}}}^{\mu,\mathrm{i}}\underline{\bar{\boldsymbol{\epsilon}}} = \left[\ \underline{\hat{\boldsymbol{u}}}^{\mu,\mathrm{i(11)}}, \underline{\hat{\boldsymbol{u}}}^{\mu,\mathrm{i(22)}}, \underline{\hat{\boldsymbol{u}}}^{\mu,\mathrm{i(12)}}\ \right] \begin{bmatrix} \bar{\epsilon}_{11} \\ \bar{\epsilon}_{22} \\ \bar{\gamma}_{12} \end{bmatrix} \tag{3.41}$$

In the 2D-case the dimensions are

$$\begin{aligned} dim(\underline{\boldsymbol{u}}^{\mathrm{M,i}}) &= \mathrm{NVAR_i} \times 1, \quad \dim(\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,i}}) = \mathrm{NVAR_i} \times 3 \\ dim(\underline{\boldsymbol{u}}^{\mu,\mathrm{i}}) &= \mathrm{NVAR_i} \times 1, \quad \dim(\underline{\hat{\boldsymbol{u}}}^{\mu,\mathrm{i}}) = \mathrm{NVAR_i} \times 3 \\ dim(\underline{\boldsymbol{u}}^{\mathrm{M,b}}) &= \mathrm{NVAR_b} \times 1, \quad \dim(\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}}) = \mathrm{NVAR_b} \times 3 \end{aligned} \tag{3.42}$$ {eq:3-49}

It must be noted that *a*ll components in $\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,i}}$ are $\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}}$ are *prescribed*, i.e. not only the boundary values $\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}}$; it is only for convenience of notation that the subdivision in (3.39) into internal and boundary variables is introduced. Indeed, the values of $\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,i}(ij)}$ and $\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}(ij)}$ are *given explicitly* from the coordinates of the nodal points. Consider a typical node located at the local position $\boldsymbol{x}_P$ and a nodal variable $\hat{u}^{\mathrm{M},\bullet(ij)}$ associated with a displacement in the direction of $\boldsymbol{e}_l$ for $l \in \{1, 2, ..., NDIM\}$. The value of $\hat{u}^{\mathrm{M},\bullet(ij)}$ is then computed explicitly as {eq:3-51}

$$\hat{u}^{\mathrm{M},\bullet(ii)} = [(x_P)_i - \bar{x}_i]\, \boldsymbol{e}_i \cdot \boldsymbol{e}_l, \quad i = 1, 2, \ldots, NDIM \tag{3.43a}$$ {eq:3-51a}

$$\hat{u}^{\mathrm{M},\bullet(ij)} = [(x_P)_i - \bar{x}_i]\, \boldsymbol{e}_j \cdot \boldsymbol{e}_l + [(x_P)_j - \bar{x}_j]\, \boldsymbol{e}_i \cdot \boldsymbol{e}_l, \quad i \neq j \in 1, 2, \ldots, NDIM \tag{3.43b}$$ {eq:3-51b}

For example, if the variable represents the 1-direction, then (3.43) becomes

$$\begin{aligned} \hat{u}^{\mathrm{M},\bullet(11)} &= [(x_P)_1 - \bar{x}_1] \\ \hat{u}^{\mathrm{M},\bullet(12)} &= [(x_P)_2 - \bar{x}_2] \\ \hat{u}^{\mathrm{M},\bullet(22)} &= 0 \end{aligned} \tag{3.44}$$ {eq:3-52}

SVE-problem – Formulation and solution

In order to define the subscale stiffness $\underline{\boldsymbol{K}}$ for the subscale FE-problem on the RVE, we consider

$$\begin{aligned} \langle \boldsymbol{\epsilon}[\delta \boldsymbol{u}_h] : \mathsf{E} : \boldsymbol{\epsilon}[\boldsymbol{u}_h] \rangle_\square &= \sum_{i,j=1}^{\mathrm{NVAR}} (\delta \underline{\boldsymbol{u}})_i \langle \boldsymbol{B}_i : \mathsf{E} : \boldsymbol{B}_j \rangle_\square (\underline{\boldsymbol{u}})_j = \sum_{i,j=1}^{\mathrm{NVAR}} (\delta \underline{\boldsymbol{u}})_i (\underline{\boldsymbol{K}})_{ij} (\underline{\boldsymbol{u}})_j \\ &= [\delta \underline{\boldsymbol{u}}]^{\mathrm{T}} \underline{\boldsymbol{K}} \underline{\boldsymbol{u}} \end{aligned} \tag{3.45}$$ {eq:3-53}

whereby we used that the stiffness matrix elements $(\underline{\boldsymbol{K}})_{ij}$ are given as

$$(\underline{\boldsymbol{K}})_{ij} = \langle \boldsymbol{B}_i : \mathsf{E} : \boldsymbol{B}_j \rangle_\square \quad i, j = 1, 2, ..., \mathrm{NVAR} \tag{3.46}$$ {eq:3-54}

The total stiffness matrix $\underline{\boldsymbol{K}}$ may be partitioned as follows corresponding to the free and prescribed variables:

$$\underline{\boldsymbol{K}} = \begin{bmatrix} \underline{\boldsymbol{K}}^{\mathrm{ii}} & \underline{\boldsymbol{K}}^{\mathrm{ib}} \\ \underline{\boldsymbol{K}}^{\mathrm{bi}} & \underline{\boldsymbol{K}}^{\mathrm{bb}} \end{bmatrix}, \quad \underline{\boldsymbol{K}}^{\mathrm{bi}} = [\underline{\boldsymbol{K}}^{\mathrm{ib}}]^{\mathrm{T}} \tag{3.47}$$ {eq:3-55}

We are now in the position to formulate the RVE-problem in (3.16) in matrix format as follows:

$$\left[\ \underline{\boldsymbol{K}}^{\mathrm{ii}} \quad \underline{\boldsymbol{K}}^{\mathrm{ib}}\ \right] \begin{bmatrix} \underline{\hat{\boldsymbol{u}}}^{\mathrm{i}} \\ \underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}} \end{bmatrix} = \underline{\boldsymbol{0}} \tag{3.48}$$ {eq:3-56}

or, corresponding to (3.16)???, as

$$\underline{\boldsymbol{K}}^{\mathrm{ii}}\underline{\hat{\boldsymbol{u}}}^{\mu,\mathrm{i}} = -\begin{bmatrix} \underline{\boldsymbol{K}}^{\mathrm{ii}} & \underline{\boldsymbol{K}}^{\mathrm{ib}} \end{bmatrix} \begin{bmatrix} \underline{\hat{\boldsymbol{u}}}^{\mathrm{M,i}} \\ \underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}} \end{bmatrix} \tag{3.49}$$
{eq:3-57}

Upon rewriting (3.48) in terms of the unknown (total) displacement vector $\underline{\hat{\boldsymbol{u}}}^{\mathrm{i}}$, we obtain the matrix equation

{eq:3-58}
$$\underline{\boldsymbol{K}}^{\mathrm{ii}}\underline{\hat{\boldsymbol{u}}}^{\mathrm{i}} = -\underline{\boldsymbol{K}}^{\mathrm{ib}}\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}} \tag{3.50}$$

This equation is readily seen to correspond exactly to that of solving three FE-problems on the RVE with different prescribed boundary displacements corresponding to the three unit deformation fields, or rather, their corresponding load vector that is obtained by the pre-multiplication by $-\underline{\boldsymbol{K}}^{\mathrm{ib}}$. Formally, the solution of (3.50) can be written as

{eq:3-59}
$$\underline{\hat{\boldsymbol{u}}}^{\mathrm{i}} = -\left[\underline{\boldsymbol{K}}^{\mathrm{ii}}\right]^{-1}\underline{\boldsymbol{K}}^{\mathrm{ib}}\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}} \tag{3.51}$$

Computing the stiffness matrix in practice

Next, we establish the macroscale stiffness matrix from the component expression in (**??**). Firstly, in analogy with (3.35), we have the FE-representation

{eq:3-61}
$$\boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{(ij)}] = \sum_{k=1}^{\mathrm{NVAR}} \boldsymbol{B}_k(\underline{\hat{\boldsymbol{u}}}^{(ij)})_k \quad \text{with } \boldsymbol{B}_k \stackrel{\mathrm{def}}{=} (\boldsymbol{N}_k \otimes \boldsymbol{\nabla})^{\mathrm{sym}} \tag{3.52}$$

whereby the components of $\bar{\mathsf{E}}_\square$ can be computed as

{eq:3-62}
$$(\bar{\mathsf{E}}_\square)_{ijkl} = \langle \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{(ij)}] : \mathsf{E} : \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{(kl)}]\rangle_\square = \left[\underline{\hat{\boldsymbol{u}}}^{(ij)}\right]^{\mathrm{T}} \underline{\boldsymbol{K}}\underline{\hat{\boldsymbol{u}}}^{(kl)} \tag{3.53}$$

Hence, we obtain the Voigt matrix representation

{eq:3-64}
$$\underline{\bar{\mathsf{E}}}_\square = \underline{\hat{\boldsymbol{u}}}^{\mathrm{T}}\underline{\boldsymbol{K}}\underline{\hat{\boldsymbol{u}}} = \begin{bmatrix} \left[\underline{\hat{\boldsymbol{u}}}^{\mathrm{i}}\right]^{\mathrm{T}}, & \left[\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}}\right]^{\mathrm{T}} \end{bmatrix} \begin{bmatrix} \underline{\boldsymbol{K}}^{\mathrm{ii}} & \underline{\boldsymbol{K}}^{\mathrm{ib}} \\ \underline{\boldsymbol{K}}^{\mathrm{bi}} & \underline{\boldsymbol{K}}^{\mathrm{bb}} \end{bmatrix} \begin{bmatrix} \underline{\hat{\boldsymbol{u}}}^{\mathrm{i}} \\ \underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}} \end{bmatrix} \tag{3.54}$$

Upon using the identity in (3.48), we may simplify (3.54) as follows:

{eq:3-65}
$$\underline{\bar{\mathsf{E}}}_\square = \left[\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}}\right]^{\mathrm{T}} \begin{bmatrix} \underline{\boldsymbol{K}}^{\mathrm{bi}} & \underline{\boldsymbol{K}}^{\mathrm{bb}} \end{bmatrix} \begin{bmatrix} \underline{\hat{\boldsymbol{u}}}^{\mathrm{i}} \\ \underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}} \end{bmatrix} = \left[\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}}\right]^{\mathrm{T}} \left[\underline{\boldsymbol{K}}^{\mathrm{bb}}\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}} + \underline{\boldsymbol{K}}^{\mathrm{bi}}\underline{\hat{\boldsymbol{u}}}^{\mathrm{i}}\right] \tag{3.55}$$

This is the operational format of $\underline{\bar{\mathsf{E}}}_\square$ in practice when $\underline{\hat{\boldsymbol{u}}}^{\mathrm{i}}$ is solved for from (3.50).

Remark: Formally, we may introduce (3.51) into (3.55) to obtain

{eq:3-66}
$$\underline{\bar{\mathsf{E}}}_\square = \left[\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}}\right]^{\mathrm{T}} \underline{\tilde{\boldsymbol{K}}}^{\mathrm{bb}}\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}} \tag{3.56}$$

where $\underline{\tilde{\boldsymbol{K}}}^{\mathrm{bb}}$ is the part-inverted matrix defined as follows

{eq:3-67}
$$\underline{\tilde{\boldsymbol{K}}}^{\mathrm{bb}} \stackrel{\mathrm{def}}{=} \underline{\boldsymbol{K}}^{\mathrm{bb}} - \underline{\boldsymbol{K}}^{\mathrm{bi}}\left[\underline{\boldsymbol{K}}^{\mathrm{ii}}\right]^{-1}\underline{\boldsymbol{K}}^{\mathrm{ib}} \tag{3.57}$$

However, this is a non-operational expression due to the presence of $\left[\underline{\boldsymbol{K}}^{\mathrm{ii}}\right]^{-1}$. $\square$

Remark: If the "nonsymmetric" expression $\bar{\mathsf{E}}_\square = \langle \mathsf{E} : \mathsf{A} \rangle_\square$ is used, then the expression in (3.54) would be replaced by

{eq:3-68}
$$\underline{\bar{\mathsf{E}}}_\square = \left[\underline{\hat{\boldsymbol{u}}}^{\mathrm{M}}\right]^{\mathrm{T}} \underline{\boldsymbol{K}\hat{\boldsymbol{u}}} = \begin{bmatrix} \left[\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,i}}\right]^{\mathrm{T}}, & \left[\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}}\right]^{\mathrm{T}} \end{bmatrix} \begin{bmatrix} \underline{\boldsymbol{K}}^{\mathrm{ii}} & \underline{\boldsymbol{K}}^{\mathrm{ib}} \\ \underline{\boldsymbol{K}}^{\mathrm{bi}} & \underline{\boldsymbol{K}}^{\mathrm{bb}} \end{bmatrix} \begin{bmatrix} \underline{\hat{\boldsymbol{u}}}^{\mathrm{i}} \\ \underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}} \end{bmatrix} \tag{3.58}$$

However, it can readily be concluded that this difference does not influence the operational expression given in (3.55). □

As to the dimensions of the matrices involved, we have in the 2D-case:

{eq:3-69}
$$\begin{aligned} dim(\underline{\hat{\boldsymbol{u}}}^{\mathrm{i}}) &= \mathrm{NVAR_i} \times 3 \\ dim(\underline{\hat{\boldsymbol{u}}}^{\mathrm{b}}) &= \mathrm{NVAR_b} \times 3 \\ dim(\underline{\boldsymbol{K}}^{\mathrm{ii}}) &= \mathrm{NVAR_i} \times \mathrm{NVAR_i} \\ dim(\underline{\boldsymbol{K}}^{\mathrm{ib}}) &= \mathrm{NVAR_i} \times \mathrm{NVAR_b} = dim(\left[\underline{\boldsymbol{K}}^{\mathrm{bi}}\right]^{\mathrm{T}}) \\ dim(\underline{\boldsymbol{K}}^{\mathrm{bb}}) &= \mathrm{NVAR_b} \times \mathrm{NVAR_b} = dim(\underline{\tilde{\boldsymbol{K}}}^{\mathrm{bb}}) \\ dim(\underline{\bar{\mathsf{E}}}_\square) &= 3 \times 3 \end{aligned} \tag{3.59}$$

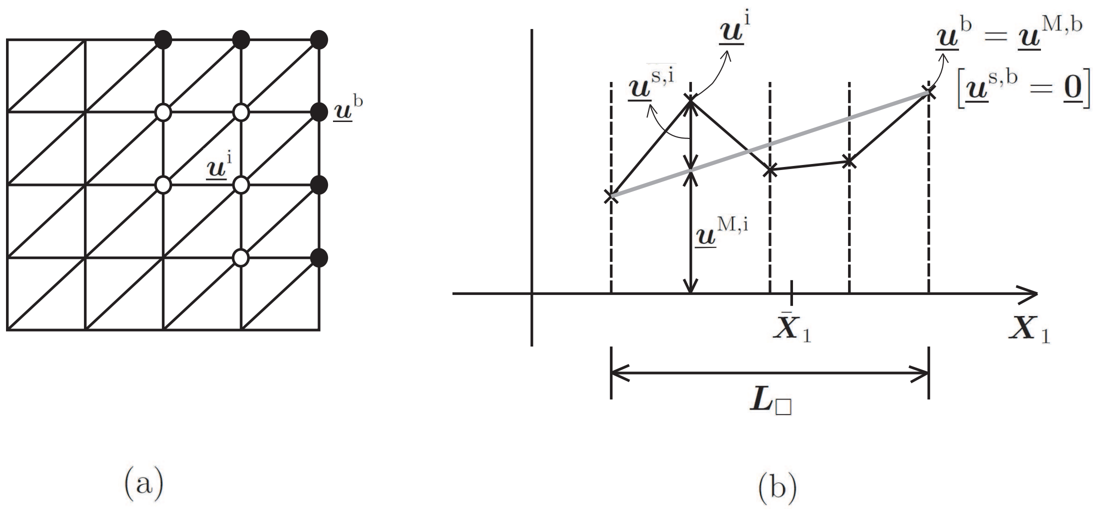


Figure 3.1: *(a) FE-mesh in SVE with internal nodes (open rings) and boundary nodes (filled rings). (b) Split of nodal values $\underline{\boldsymbol{u}}$ into $\underline{\boldsymbol{u}}^{\mathrm{M}}$ and $\underline{\boldsymbol{u}}^{\mu}$ for internal and boundary nodes. For the boundary nodes, $\underline{\boldsymbol{u}}^{\mu,\mathrm{b}} = \underline{\boldsymbol{0}}$ in the DBC-problem.* {fig:3-1}

3.2.5 DBC-problem for macroscale stress control

In the previous Subsection, we considered the (basic) case of determining the macroscale stress $\bar{\boldsymbol{\sigma}}$ for known macroscale displacement gradient $\bar{\boldsymbol{\epsilon}}$. We shall now consider the "inverse problem" of determining $\bar{\boldsymbol{\epsilon}}$ for a known $\bar{\boldsymbol{\sigma}}$.

The pertinent subscale space-variational problem on the SVE can then be phrased as follows:
{eq:3-71} For given value of the macroscale stress $\bar{\boldsymbol{\sigma}} \in \mathbb{R}^{3\times 3}$, find $\boldsymbol{u}^\mu \in \mathbb{U}_\square^{\mathrm{D},0}$ and $\bar{\boldsymbol{\epsilon}} \in \mathbb{R}^{3\times 3}_{\mathrm{sym}}$ that solve

{eq:3-71a}
$$\langle [\bar{\boldsymbol{\epsilon}} + \boldsymbol{\epsilon}[\boldsymbol{u}^\mu]] : \mathsf{E} : \boldsymbol{\epsilon}[\delta \boldsymbol{u}] \rangle_\square = 0 \qquad \forall \delta \boldsymbol{u} \in \mathbb{U}_\square^{\mathrm{D},0} \tag{3.60a}$$

{eq:3-71b}
$$\langle \mathsf{E} : [\bar{\boldsymbol{\epsilon}} + \boldsymbol{\epsilon}[\boldsymbol{u}^\mu]] \rangle_\square : \delta\bar{\boldsymbol{\epsilon}} = \bar{\boldsymbol{\sigma}} : \delta\bar{\boldsymbol{\epsilon}} \qquad \forall \delta\bar{\boldsymbol{\epsilon}} \in \mathbb{R}^{3\times 3}_{\mathrm{sym}} \tag{3.60b}$$

It is noted that (3.60b) can be interpreted as an auxiliary constraint equation.

Remark: Pure stress control is of interest mainly if the macroscale stress-strain response function is sought; hence, it is not relevant for a displacement-based macroscale FE-formulation. $\square$

3.3 Strongly periodic boundary conditions (SPBC-problem)

3.3.1 Preliminaries

In order to formulate the conditions on micro-periodicity, we consider the SVE in Figure **??**, where the boundary $\Gamma_\square$ has been split into two parts: $\Gamma_\square = \Gamma_\square^- \cup \Gamma_\square^+$. Here, $\Gamma_\square^+$ is the *image boundary* (which is also chosen as the computational domain for boundary integration), whereas Γ^- is the *mirror boundary.* The corner points on $\Gamma_\square$ are defined as $\boldsymbol{x}_{\mathrm{c}}^{(i,j,k)} \stackrel{\mathrm{def}}{=} \bar{\boldsymbol{x}} + \frac{L_\square}{2}[i\boldsymbol{e}_1 + j\boldsymbol{e}_2 + k\boldsymbol{e}_3]$, where $i, j, k = 1$ or -1.

We shall now introduce the proper mapping $\boldsymbol{\varphi}_{\mathrm{per}} : \Gamma^+ \to \Gamma^-$ such that any point $\boldsymbol{x}^+ \in \Gamma_\square^+$ is mirrored in a self-similar fashion to the corresponding point $\boldsymbol{x}^- \in \Gamma_\square^-$; hence, $\boldsymbol{x}^- = \boldsymbol{\varphi}_{\mathrm{per}}(\boldsymbol{x}^+)$. We note that there is a unique mirror point for each $\boldsymbol{x}^+ \in \Gamma_\square^+$ except for the corner point (in 3D) $\boldsymbol{x}^+ = \boldsymbol{x}_{\mathrm{c}}^{(1,1,1)}$, which has three mirror points $\boldsymbol{x}_{\mathrm{c}}^{(-1,1,1)}, \boldsymbol{x}_{\mathrm{c}}^{(1,-1,1)}$ and $\boldsymbol{x}_{\mathrm{c}}^{(1,1,-1)}$.

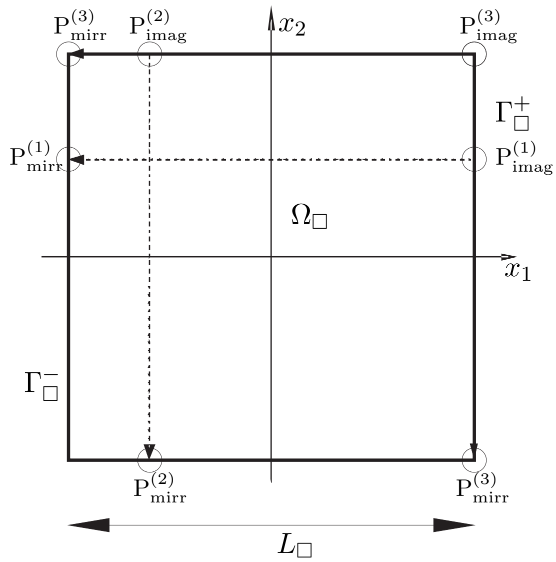


Figure 3.2: *SVE in 2D with "image" and "mirror" boundaries. Note that the corner point* $P^{(3)}_{\rm imag}$ *has two mirror points (corners).* {fig:3-2}

Based on these preliminaries, we express periodicity of the displacement fluctuation field as

$$\boldsymbol{u}^\mu(\boldsymbol{x}) = \boldsymbol{u}^\mu(\boldsymbol{\varphi}_{\rm per}(\boldsymbol{x})), \quad \forall \boldsymbol{x} \in \Gamma^+_\square \tag{3.61}$$ {eq:3-73}

or, equivalently, in terms of the "jump" between the fluctuation fields on the image and mirror parts of the boundary as follows:

$$[\![\boldsymbol{u}^\mu]\!]_\square = \boldsymbol{0} \quad \text{on } \Gamma^+_\square, \quad [\![\boldsymbol{u}^\mu]\!]_\square(\boldsymbol{x}) \overset{\rm def}{=} \boldsymbol{u}^\mu(\boldsymbol{x}) - \boldsymbol{u}^\mu(\boldsymbol{\varphi}_{\rm per}(\boldsymbol{x})) \tag{3.62}$$ {eq:3-74}

We shall also assume that the boundary tractions $\boldsymbol{t} \overset{\rm def}{=} \boldsymbol{\sigma}\cdot\boldsymbol{n}$ satisfy the following *anti-periodicity condition* for any mirror point (that is not a corner point)

$$\boldsymbol{t}(\boldsymbol{x}) = -\boldsymbol{t}(\boldsymbol{\varphi}_{\rm per}(\boldsymbol{x})), \quad \forall \boldsymbol{x} \in \Gamma^+_\square \tag{3.63}$$ {eq:3-75}

Moreover, for the corner point $\boldsymbol{x}_{\rm c}^{(1,1,1)}$ we obtain the *symmetry conditions* with respect to mirror points on the same coordinate surface defined by the given normal $\boldsymbol{n}$, as follows:

$$\begin{array}{lllll}
\boldsymbol{u}^\mu(\boldsymbol{x}_{\rm c}^{(1,1,1)}) & = & \boldsymbol{u}^\mu(\boldsymbol{x}_{\rm c}^{(1,1,-1)}) & = & \boldsymbol{u}^\mu(\boldsymbol{x}_{\rm c}^{(1,-1,1)}), \quad \boldsymbol{n} = \boldsymbol{e}_1 \\
\boldsymbol{u}^\mu(\boldsymbol{x}_{\rm c}^{(1,1,1)}) & = & \boldsymbol{u}^\mu(\boldsymbol{x}_{\rm c}^{(1,1,-1)}) & = & \boldsymbol{u}^\mu(\boldsymbol{x}_{\rm c}^{(-1,1,1)}), \quad \boldsymbol{n} = \boldsymbol{e}_2 \\
\boldsymbol{u}^\mu(\boldsymbol{x}_{\rm c}^{(1,1,1)}) & = & \boldsymbol{u}^\mu(\boldsymbol{x}_{\rm c}^{(1,-1,1)}) & = & \boldsymbol{u}^\mu(\boldsymbol{x}_{\rm c}^{(-1,1,1)}), \quad \boldsymbol{n} = \boldsymbol{e}_3
\end{array} \tag{3.64}$$ {eq:3-76}

as depicted in Figure **??**.

In conclusion, we introduce the solution (and test) space

$$\mathbb{U}^{\rm P,0}_\square = \{\boldsymbol{u} \in \mathbb{U}_\square |\ [\![\boldsymbol{u}]\!]_\square = \boldsymbol{0} \text{ on } \Gamma^+_\square\} \tag{3.65}$$ {eq:3-77}

and we shall require that the fluctuation part $\boldsymbol{u}^\mu \in \mathbb{U}^{\rm P,0}_\square$.

Finally, using the periodicity in (**??**) and the antiperiodicity in (**??**), we obtain from (**??**) that the Hill-Mandel macrohomogeneity condition is identically satisfied:

$$\int_{\Gamma_\square} [\boldsymbol{t} - \bar{\boldsymbol{\sigma}}_\square\{\boldsymbol{t}\} \cdot \boldsymbol{n}] \cdot \boldsymbol{u}^\mu \, \mathrm{d}\Gamma = \int_{\Gamma_\square^+} [\boldsymbol{t} - \bar{\boldsymbol{\sigma}}_\square\{\boldsymbol{t}\} \cdot \boldsymbol{n}] \cdot \underbrace{[\![\boldsymbol{u}^\mu]\!]_\square}_{=\boldsymbol{0}} \, \mathrm{d}\Gamma = 0 \tag{3.66}$$ {eq:3-78}

In order to obtain the last identity, we used that not only is $\boldsymbol{t}$ antiperiodic, but also that $\boldsymbol{t}^{\mathrm{M}} \overset{\mathrm{def}}{=} \bar{\boldsymbol{\sigma}}_\square\{\boldsymbol{t}\} \cdot \boldsymbol{n}$ is antiperiodic. That $\boldsymbol{t}^{\mathrm{M}}$ is antiperiodic follows from (i) $\bar{\boldsymbol{\sigma}} = \bar{\boldsymbol{\sigma}}_\square\{\boldsymbol{t}\}$ is a constant and (ii) $\boldsymbol{n}$ is antiperiodic.

3.3.2 SPBC-problem for macroscale strain control

Upon introducing the test function $\delta\boldsymbol{u} \in \mathbb{U}_\square^{\mathrm{P},0}$, which means that $[\![\delta\boldsymbol{u}]\!]_\square = \boldsymbol{0}$ on the boundary $\Gamma_\square^+$ for *given (fixed)* $\bar{\boldsymbol{\epsilon}}$, the boundary integral in (**??**a) vanishes, which is shown as follows:

$$\frac{1}{|\Omega_\square|} \int_{\Gamma_\square} \boldsymbol{t} \cdot \delta\boldsymbol{u} \, \mathrm{d}\Gamma = \{[\![\delta\boldsymbol{u}]\!]_\square = \boldsymbol{0} \text{ on } \Gamma_\square^+\} = \frac{1}{|\Omega_\square|} \int_{\Gamma_\square^+} \underbrace{[\boldsymbol{t}^+ + \boldsymbol{t}^-]}_{=\boldsymbol{0}} \cdot \delta\boldsymbol{u} \, \mathrm{d}\Gamma = 0$$

where we used the assumption that $\boldsymbol{t}$ is strongly antiperiodic. Moreover, choosing $\boldsymbol{u} = \boldsymbol{u}^{\mathrm{M}}(\bar{\boldsymbol{\epsilon}}) + \boldsymbol{u}^\mu$ with $\boldsymbol{u}^{\mathrm{M}}(\bar{\boldsymbol{\epsilon}}) = \bar{\boldsymbol{\epsilon}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}]$ on $\Gamma_\square$ and $\boldsymbol{u}^\mu \in \mathbb{U}_\square^{\mathrm{P},0}$, we may conclude that the LHS of (**??**b) becomes

$$-\frac{1}{|\Omega_\square|} \int_{\Gamma_\square} \delta\boldsymbol{t} \cdot \boldsymbol{u} \, \mathrm{d}\Gamma = -\bar{\boldsymbol{\epsilon}} : \left[\frac{1}{|\Omega_\square|} \int_{\Gamma_\square} \delta\boldsymbol{t} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}] \, \mathrm{d}\Gamma\right] - \frac{1}{|\Omega_\square|} \int_{\Gamma_\square^+} \delta\boldsymbol{t} \cdot \underbrace{[\![\boldsymbol{u}^\mu]\!]_\square}_{=\boldsymbol{0}} \, \mathrm{d}\Gamma$$

It thus follows that (**??**b) is trivially satisfied. In other words, the condition $\langle\boldsymbol{\epsilon}\rangle_\square = \bar{\boldsymbol{\epsilon}}$ is thus satisfied *a priori*.

In conclusion, the weak format of the SPBC-problem for a SVE under macroscale strain control can be phrased as follows: For given value of the macroscale strain $\bar{\boldsymbol{\epsilon}}$, find the fluctuation displacement field $\boldsymbol{u}^\mu \in \mathbb{U}_\square^{\mathrm{P},0}$ which solves

{eq:3-82} $$\langle(\bar{\boldsymbol{\epsilon}} + \boldsymbol{\epsilon}[\boldsymbol{u}^\mu]) : \mathsf{E} : \boldsymbol{\epsilon}[\delta\boldsymbol{u}]\rangle_\square = 0 \quad \forall\delta\boldsymbol{u} \in \mathbb{U}_\square^{\mathrm{P},0} \tag{3.67}$$

This problem can be rewritten as

{eq:3-83} $$\langle\boldsymbol{\epsilon}[\boldsymbol{u}^\mu] : \mathsf{E} : \boldsymbol{\epsilon}[\delta\boldsymbol{u}]\rangle_\square = -\bar{\boldsymbol{\epsilon}} : \langle\mathsf{E} : \boldsymbol{\epsilon}[\delta\boldsymbol{u}]\rangle_\square \quad \forall\delta\boldsymbol{u} \in \mathbb{U}_\square^{\mathrm{P},0} \tag{3.68}$$

where the RHS is known. Hence, the SPBC-problem is driven directly by $\bar{\boldsymbol{\epsilon}}$ as the data.

Obviously, the format of the SPBC-problem is formally the same as the DBC-problem with the difference that $\mathbb{U}_\square^{\mathrm{P},0}$ replaces $\mathbb{U}_\square^{\mathrm{D},0}$. The reader is referred to the previous Section on the DBC-problem for the formal discussion of how to compute $\bar{\mathsf{E}}_\square$.

The major additional issue from a computational viewpoint is to ensure that the displacements in $\mathbb{U}_\square^{\mathrm{P},0}$ do indeed possess the required strong periodicity. In a FE-context (see next Subsection), this requirement is satisfied by

- a completely periodic mesh along $\Gamma_\square^+$ and $\Gamma_\square^-$
- completely periodic FE-approximation of the displacement fluctuation along $\Gamma_\square^+$ and $\Gamma_\square^-$

3.3.3 FE-approximation – Matrix format (in 2D)

Preliminaries

The issue of preventing rigid body motion is trivially resolved, since the condition $[\![\boldsymbol{u}^{\mu}]\!] = \mathbf{0}$ removes rotation, whereas the condition $\boldsymbol{u}$ =?? removes translation. The starting point for the operational formulation is the following system of FE-equations:

$$\begin{bmatrix} \underline{\underline{\boldsymbol{K}}}^{\mathrm{ii}} & \underline{\underline{\boldsymbol{K}}}^{\mathrm{ib}} \\ \underline{\underline{\boldsymbol{K}}}^{\mathrm{bi}} & \underline{\underline{\boldsymbol{K}}}^{\mathrm{bb}} \end{bmatrix} \begin{bmatrix} \underline{\boldsymbol{u}}^{\mathrm{i}} \\ \underline{\boldsymbol{u}}^{\mathrm{b}} \end{bmatrix} = \begin{bmatrix} \underline{\mathbf{0}} \\ \underline{\boldsymbol{g}}^{\mathrm{b}} \end{bmatrix} \tag{3.69}$$ {eq:3-81}

where the nodal column matrix $\underline{\boldsymbol{g}}^{\mathrm{b}}$ represents loading from the tractions on $\Gamma_{\square}$ (that may be considered as "reaction forces" at the outset). In order to formulate the periodicity condition and account for removed RBM, the column matrices pertinent to the boundary are split as follows:

$$\underline{\boldsymbol{u}}^{\mathrm{b}} = \begin{bmatrix} \underline{\boldsymbol{u}}^{\mathrm{b}}_{+} \\ \underline{\boldsymbol{u}}^{\mathrm{b}}_{-} \\ \underline{\boldsymbol{u}}^{\mathrm{c}} \end{bmatrix}, \quad \underline{\boldsymbol{g}}^{\mathrm{b}} = \begin{bmatrix} \underline{\boldsymbol{g}}^{\mathrm{b}}_{+} \\ \underline{\boldsymbol{g}}^{\mathrm{b}}_{-} \\ \underline{\boldsymbol{g}}^{\mathrm{c}} \end{bmatrix} \tag{3.70}$$ {eq:3-82}

The displacements on the image and mirror boundary parts are denoted $\underline{\boldsymbol{u}}^{\mathrm{b}}_{+}$ and $\underline{\boldsymbol{u}}^{\mathrm{b}}_{-}$, respectively (as shown in Figure **??**). The exception is the corner variables (4 corners in 2D) that are collected separately in $\underline{\boldsymbol{u}}^{\mathrm{c}}$ in order to provide for removed RBM.

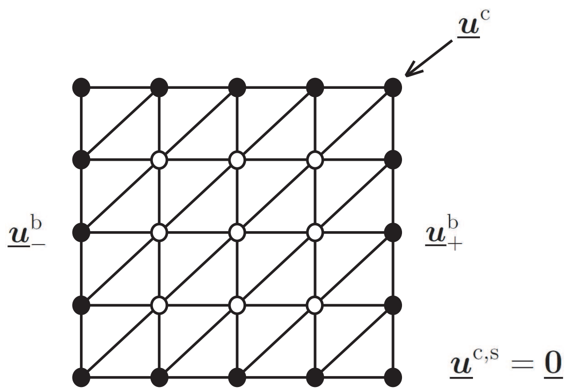


Figure 3.3: *Strongly periodic FE-mesh in SVE with internal nodes (open rings) and boundary nodes (filled rings). Decomposition of boundary nodal values $\underline{\boldsymbol{u}}^{\mathrm{b}}$ into (i) $\underline{\boldsymbol{u}}^{\mathrm{b}}_{+}$ on image boundary $\Gamma^{+}_{\square}$, (ii) $\underline{\boldsymbol{u}}^{\mathrm{b}}_{-}$ on mirror boundary $\Gamma^{-}_{\square}$ and (iii) $\underline{\boldsymbol{u}}^{\mathrm{c}}$ in the corners.* {fig:3-3}

Accordingly, the system of equations (**??**) is expanded as follows:

$$\begin{bmatrix} \underline{\boldsymbol{K}}^{\mathrm{ii}} & \underline{\boldsymbol{K}}^{\mathrm{ib}}_{+} & \underline{\boldsymbol{K}}^{\mathrm{ib}}_{-} & \underline{\boldsymbol{K}}^{\mathrm{ic}} \\ \underline{\boldsymbol{K}}^{\mathrm{bi}}_{+} & \underline{\boldsymbol{K}}^{\mathrm{bb}}_{++} & \underline{\boldsymbol{K}}^{\mathrm{bb}}_{+-} & \underline{\boldsymbol{K}}^{\mathrm{bc}}_{+} \\ \underline{\boldsymbol{K}}^{\mathrm{bi}}_{-} & \underline{\boldsymbol{K}}^{\mathrm{bb}}_{-+} & \underline{\boldsymbol{K}}^{\mathrm{bb}}_{--} & \underline{\boldsymbol{K}}^{\mathrm{bc}}_{-} \\ \underline{\boldsymbol{K}}^{\mathrm{ci}} & \underline{\boldsymbol{K}}^{\mathrm{cb}}_{+} & \underline{\boldsymbol{K}}^{\mathrm{cb}}_{-} & \underline{\boldsymbol{K}}^{\mathrm{cc}} \end{bmatrix} \begin{bmatrix} \underline{\boldsymbol{u}}^{\mathrm{i}} \\ \underline{\boldsymbol{u}}^{\mathrm{b}}_{+} \\ \underline{\boldsymbol{u}}^{\mathrm{b}}_{-} \\ \underline{\boldsymbol{u}}^{\mathrm{c}} \end{bmatrix} = \begin{bmatrix} \underline{\boldsymbol{0}} \\ \underline{\boldsymbol{g}}^{\mathrm{b}}_{+} \\ \underline{\boldsymbol{g}}^{\mathrm{b}}_{-} \\ \underline{\boldsymbol{g}}^{\mathrm{c}} \end{bmatrix} \tag{3.71}$$ {eq:3-83}

A comparison with (**??**) shows that we have introduced the decomposition

{eq:3-84} $$\underline{\boldsymbol{K}}^{\mathrm{ib}} = \begin{bmatrix} \underline{\boldsymbol{K}}^{\mathrm{ib}}_{+} & \underline{\boldsymbol{K}}^{\mathrm{ib}}_{-} & \underline{\boldsymbol{K}}^{\mathrm{ic}} \end{bmatrix}, \quad \underline{\boldsymbol{K}}^{\mathrm{bi}} = \begin{bmatrix} \underline{\boldsymbol{K}}^{\mathrm{bi}}_{+} \\ \underline{\boldsymbol{K}}^{\mathrm{bi}}_{-} \\ \underline{\boldsymbol{K}}^{\mathrm{ci}} \end{bmatrix}, \quad \underline{\boldsymbol{K}}^{\mathrm{bb}} = \begin{bmatrix} \underline{\boldsymbol{K}}^{\mathrm{bb}}_{++} & \underline{\boldsymbol{K}}^{\mathrm{bb}}_{+-} & \underline{\boldsymbol{K}}^{\mathrm{bc}}_{+} \\ \underline{\boldsymbol{K}}^{\mathrm{bb}}_{-+} & \underline{\boldsymbol{K}}^{\mathrm{bb}}_{--} & \underline{\boldsymbol{K}}^{\mathrm{bc}}_{-} \\ \underline{\boldsymbol{K}}^{\mathrm{cb}}_{+} & \underline{\boldsymbol{K}}^{\mathrm{cb}}_{-} & \underline{\boldsymbol{K}}^{\mathrm{cc}} \end{bmatrix}, \tag{3.72}$$

SVE-problem – Formulation and solution

Periodicity of the nodal displacement fluctuations and anti-periodicity of the nodal traction forces on $\Gamma_{\square}$ can be expressed as the constraints

{eq:3-85} $$\underline{\boldsymbol{u}}^{\mu,\mathrm{b}}_{+} = \underline{\boldsymbol{u}}^{\mu,\mathrm{b}}_{-} \stackrel{\mathrm{def}}{=} \underline{\boldsymbol{u}}^{\mu,\mathrm{b}} \quad \Rightarrow \quad \underline{\boldsymbol{u}}^{\mathrm{b}}_{+} = \underline{\boldsymbol{u}}^{\mathrm{M,b}}_{+} + \underline{\boldsymbol{u}}^{\mu,\mathrm{b}}, \quad \underline{\boldsymbol{u}}^{\mathrm{b}}_{-} = \underline{\boldsymbol{u}}^{\mathrm{M,b}}_{-} + \underline{\boldsymbol{u}}^{\mu,\mathrm{b}} \tag{3.73}$$

{eq:3-86} $$\underline{\boldsymbol{g}}^{\mathrm{b}}_{+} + \underline{\boldsymbol{g}}^{\mathrm{b}}_{-} = \underline{\boldsymbol{0}} \tag{3.74}$$

We choose to set the displacement fluctuation in all coordinate directions to zero at any (arbitrarily chosen) corner node. However, due to periodicity this means that the fluctuation in all corner nodes will vanish, i.e.

{eq:3-87} $$\underline{\boldsymbol{u}}^{\mu,\mathrm{c}} = \underline{\boldsymbol{0}} \quad \Rightarrow \quad \underline{\boldsymbol{u}}^{\mathrm{c}} = \underline{\boldsymbol{u}}^{\mathrm{M,c}} \tag{3.75}$$

The SVE-problem is then formulated in matrix format as the reduced version of (**??**):

{eq:3-88} $$\begin{bmatrix} \underline{\boldsymbol{K}}^{\mathrm{ii}} & \underline{\boldsymbol{K}}^{\mathrm{ib}}_{\substack{+\\-}} \\ \underline{\boldsymbol{K}}^{\mathrm{bi}}_{\substack{+\\-}} & \underline{\boldsymbol{K}}^{\mathrm{bb}}_{\substack{+\\-}} \end{bmatrix} \begin{bmatrix} \underline{\boldsymbol{u}}^{\mathrm{i}} \\ \underline{\boldsymbol{u}}^{\mu,\mathrm{b}} \end{bmatrix} = \begin{bmatrix} \underline{\boldsymbol{f}}^{\mathrm{i}} \\ \underline{\boldsymbol{f}}^{\mathrm{b}}_{\substack{+\\-}} \end{bmatrix} \tag{3.76}$$

{eq:appB_109} where we introduced the notation

{eq:3-89a} $$\underline{\boldsymbol{K}}^{\mathrm{ib}}_{\substack{+\\-}} = \underline{\boldsymbol{K}}^{\mathrm{ib}}_{+} + \underline{\boldsymbol{K}}^{\mathrm{ib}}_{-} \tag{3.77a}$$

{eq:3-89b} $$\underline{\boldsymbol{K}}^{\mathrm{bi}}_{\substack{+\\-}} = \underline{\boldsymbol{K}}^{\mathrm{bi}}_{+} + \underline{\boldsymbol{K}}^{\mathrm{bi}}_{-} \tag{3.77b}$$

{eq:3-89} $$\underline{\boldsymbol{K}}^{\mathrm{bb}}_{\substack{+\\-}} = \underline{\boldsymbol{K}}^{\mathrm{bb}}_{++} + \underline{\boldsymbol{K}}^{\mathrm{bb}}_{+-} + \underline{\boldsymbol{K}}^{\mathrm{bb}}_{-+} + \underline{\boldsymbol{K}}^{\mathrm{bb}}_{--} \tag{3.77c}$$

{eq:appB_110} and

{eq:appB_110a} $$\underline{\boldsymbol{f}}^{\mathrm{i}} = -\underline{\boldsymbol{K}}^{\mathrm{ib}}_{+}\underline{\boldsymbol{u}}^{\mathrm{M,b}}_{+} - \underline{\boldsymbol{K}}^{\mathrm{ib}}_{-}\underline{\boldsymbol{u}}^{\mathrm{M,b}}_{-} - \underline{\boldsymbol{K}}^{\mathrm{ic}}\underline{\boldsymbol{u}}^{\mathrm{M,c}} \tag{3.78a}$$

{eq:3-91} $$\underline{\boldsymbol{f}}^{\mathrm{b}}_{\substack{+\\-}} = -\left[\underline{\boldsymbol{K}}^{\mathrm{bb}}_{++} + \underline{\boldsymbol{K}}^{\mathrm{bb}}_{-+}\right]\underline{\boldsymbol{u}}^{\mathrm{M,b}}_{+} - \left[\underline{\boldsymbol{K}}^{\mathrm{bb}}_{+-} + \underline{\boldsymbol{K}}^{\mathrm{bb}}_{--}\right]\underline{\boldsymbol{u}}^{\mathrm{M,b}}_{-} - \left[\underline{\boldsymbol{K}}^{\mathrm{bc}}_{+} + \underline{\boldsymbol{K}}^{\mathrm{bc}}_{-}\right]\underline{\boldsymbol{u}}^{\mathrm{M,c}} \tag{3.78b}$$

Computing the stiffness matrix in practice

Like in the case of DBC, we have the component identity

{eq:3-91} $$(\bar{\mathsf{E}}_{\square})_{ijkl} = \left[\underline{\hat{\boldsymbol{u}}}^{(ij)}\right]^{\mathrm{T}} \underline{\boldsymbol{K}}\,\underline{\hat{\boldsymbol{u}}}^{(kl)} \tag{3.79}$$

Voigt matrix notation:

{eq:3-92} $$\bar{\mathsf{E}}_{\square} = \underline{\hat{\boldsymbol{u}}}^{\mathrm{T}}\underline{\boldsymbol{K}}\,\underline{\hat{\boldsymbol{u}}} = \left[\begin{array}{cc} \left[\underline{\hat{\boldsymbol{u}}}^{\mathrm{i}}\right]^{\mathrm{T}} & \left[\underline{\hat{\boldsymbol{u}}}^{\mathrm{b}}\right]^{\mathrm{T}} \end{array}\right] \left[\begin{array}{cc} \underline{\boldsymbol{K}}^{\mathrm{ii}} & \underline{\boldsymbol{K}}^{\mathrm{ib}} \\ \underline{\boldsymbol{K}}^{\mathrm{bi}} & \underline{\boldsymbol{K}}^{\mathrm{bb}} \end{array}\right] \left[\begin{array}{c} \underline{\hat{\boldsymbol{u}}}^{\mathrm{i}} \\ \underline{\hat{\boldsymbol{u}}}^{\mathrm{b}} \end{array}\right] \tag{3.80}$$

where we used the decomposition of $\underline{\boldsymbol{K}}$ as given in (**??**). Now, using the first row of (**??**) in (**??**), i.e.

{eq:3-93} $$\underline{\boldsymbol{K}}^{\mathrm{ii}}\underline{\boldsymbol{u}}^{\mathrm{i}} + \underline{\boldsymbol{K}}^{\mathrm{ib}}\underline{\boldsymbol{u}}^{\mathrm{b}} = \underline{\boldsymbol{0}}, \tag{3.81}$$

we obtain the operational expression

$$\bar{\mathsf{E}}_{\square} = \left[\underline{\hat{\boldsymbol{u}}}^{\mathrm{b}}\right]^{\mathrm{T}} \left[\begin{array}{cc} \underline{\boldsymbol{K}}^{\mathrm{bi}} & \underline{\boldsymbol{K}}^{\mathrm{bb}} \end{array}\right] \left[\begin{array}{c} \underline{\hat{\boldsymbol{u}}}^{\mathrm{i}} \\ \underline{\hat{\boldsymbol{u}}}^{\mathrm{b}} \end{array}\right] = \left[\underline{\hat{\boldsymbol{u}}}^{\mathrm{b}}\right]^{\mathrm{T}} \underline{\hat{\boldsymbol{g}}}^{\mathrm{b}} \tag{3.82}$$ {eq:3-94}

where we recall the decomposition of $\underline{\boldsymbol{K}}^{\mathrm{bi}}$, $\underline{\boldsymbol{K}}^{\mathrm{bb}}$, $\underline{\hat{\boldsymbol{u}}}^{\mathrm{b}}$ and $\underline{\hat{\boldsymbol{g}}}^{\mathrm{b}}$ as

$$\underline{\boldsymbol{K}}^{\mathrm{bi}} = \left[\begin{array}{c} \underline{\boldsymbol{K}}^{\mathrm{bi}}_{+} \\ \underline{\boldsymbol{K}}^{\mathrm{bi}}_{-} \\ \underline{\boldsymbol{K}}^{\mathrm{ci}} \end{array}\right], \quad \underline{\boldsymbol{K}}^{\mathrm{bb}} = \left[\begin{array}{ccc} \underline{\boldsymbol{K}}^{\mathrm{bb}}_{++} & \underline{\boldsymbol{K}}^{\mathrm{bb}}_{+-} & \underline{\boldsymbol{K}}^{\mathrm{bc}}_{+} \\ \underline{\boldsymbol{K}}^{\mathrm{bb}}_{-+} & \underline{\boldsymbol{K}}^{\mathrm{bb}}_{--} & \underline{\boldsymbol{K}}^{\mathrm{bc}}_{-} \\ \underline{\boldsymbol{K}}^{\mathrm{cb}}_{+} & \underline{\boldsymbol{K}}^{\mathrm{cb}}_{-} & \underline{\boldsymbol{K}}^{\mathrm{cc}} \end{array}\right], \quad \underline{\hat{\boldsymbol{u}}}^{\mathrm{b}} = \left[\begin{array}{c} \underline{\hat{\boldsymbol{u}}}^{\mathrm{b}}_{+} \\ \underline{\hat{\boldsymbol{u}}}^{\mathrm{b}}_{-} \\ \underline{\hat{\boldsymbol{u}}}^{\mathrm{c}} \end{array}\right], \quad \underline{\hat{\boldsymbol{g}}}^{\mathrm{b}} = \left[\begin{array}{c} \underline{\hat{\boldsymbol{g}}}^{\mathrm{b}}_{+} \\ \underline{\hat{\boldsymbol{g}}}^{\mathrm{b}}_{-} \\ \underline{\hat{\boldsymbol{g}}}^{\mathrm{c}} \end{array}\right] \tag{3.83}$$ {eq:3-95}

Here, $\underline{\hat{\boldsymbol{g}}}^{\mathrm{b}(ij)}$ are sensitivities that occur in the identity

$$\underline{\boldsymbol{g}}^{\mathrm{b}} = \sum_{ij} \underline{\hat{\boldsymbol{g}}}^{\mathrm{b}(ij)}\bar{\epsilon}_{ij} \tag{3.84}$$ {eq:3-96}

As to the dimensions of the matrices involved, we have in the 2D-case:

$$\begin{aligned} dim(\underline{\hat{\boldsymbol{u}}}^{\mathrm{b}}) = dim(\underline{\hat{\boldsymbol{g}}}^{\mathrm{b}}) &= \mathrm{NVAR_b} \times 3 \\ dim(\underline{\boldsymbol{K}}^{\mathrm{bi}}) &= \mathrm{NVAR_b} \times \mathrm{NVAR_i} \\ dim(\underline{\boldsymbol{K}}^{\mathrm{bb}}) &= \mathrm{NVAR_b} \times \mathrm{NVAR_b} \\ dim(\bar{\mathsf{E}}_{\square}) &= 3 \times 3 \end{aligned} \tag{3.85}$$ {eq:3-97}

3.4 Neumann boundary conditions (NBC-problem)

3.4.1 Preliminaries

We shall now consider the case where the prolongation is defined by the "weak" assumption on RVE-boundary tractions generated from the constant stress tensor $\bar{\boldsymbol{\sigma}}$. In order to establish a suitable variational setting, we introduce the spaces of admissible displacements as

$$\mathbb{U}^{\mathrm{N}}_{\square} = \mathbb{U}_{\square} \tag{3.86}$$ {eq:3-99}

Further, by assumption of the traction along $\Gamma_\square$, we obtain

$$\frac{1}{|\Omega_\square|}\int_{\Gamma_\square} \hat{\boldsymbol{t}} \cdot \delta \boldsymbol{u} \, \mathrm{d}\Gamma = \hat{\boldsymbol{\sigma}} : \langle \boldsymbol{\epsilon}[\delta \boldsymbol{u}] \rangle_\square \,, \quad \forall \delta \boldsymbol{u} \in \mathbb{U}_\square^{\mathrm{N}} \tag{3.87}$$ {eq:3-101}

for any $\hat{\boldsymbol{\sigma}} \in \mathbb{R}^{3\times 3}_{\mathrm{sym}}$ and $\hat{\boldsymbol{t}} \overset{\mathrm{def}}{=} \hat{\boldsymbol{\sigma}} \cdot \boldsymbol{n}$ on $\Gamma_\square$. This identity is used in the canonical format (**??**) with the choice $\hat{\boldsymbol{\sigma}} = \bar{\boldsymbol{\sigma}}$.

Remark: The expression in (**??**) is *imposed explicitly* as the boundary condition in the case of *macroscale stress control*, i. e. when the value $\bar{\boldsymbol{\sigma}}$ is prescribed as input data. However, in the case of macroscale strain control, i. e. when the value $\bar{\boldsymbol{\epsilon}}$ is prescribed as input data, then the value $\bar{\boldsymbol{\sigma}}$ is part of the solution of a mixed problem with $\boldsymbol{u}$ and $\bar{\boldsymbol{\sigma}}$ as the variables. $\square$

3.4.2 NBC-problem for macroscale strain control

{eq:3-102} For given value of the macroscale strain $\bar{\boldsymbol{\epsilon}} \in \mathbb{R}^{3\times 3}_{\mathrm{sym}}$, find $\boldsymbol{u} \in \mathbb{U}_\square^{\mathrm{N}}$ and $\bar{\boldsymbol{\sigma}} \in \mathbb{R}^{3\times 3}_{\mathrm{sym}}$ that solve

{eq:3-102a} $$\langle \boldsymbol{\epsilon}[\boldsymbol{u}] : \mathsf{E} : \boldsymbol{\epsilon}[\delta \boldsymbol{u}] \rangle_\square - \bar{\boldsymbol{\sigma}} : \langle \boldsymbol{\epsilon}[\delta \boldsymbol{u}] \rangle_\square = 0 \qquad \forall \delta \boldsymbol{u} \in \mathbb{U}_\square^{\mathrm{N}} \tag{3.88a}$$

{eq:3-102b} $$-\langle \boldsymbol{\epsilon}[\boldsymbol{u}] \rangle_\square : \delta\bar{\boldsymbol{\sigma}} = -\bar{\boldsymbol{\epsilon}} : \delta\bar{\boldsymbol{\sigma}} \qquad \forall \delta\bar{\boldsymbol{\sigma}} \in \mathbb{R}^{3\times 3}_{\mathrm{sym}} \tag{3.88b}$$

3.4.3 Macroscale stiffness tensor

Sensitivity fields

Like for the DBC-problem, we introduce sensitivities in terms of the "unit displacement fields" $\hat{\boldsymbol{u}}^{(ij)}$ and the "unit macrostresses" $\hat{\bar{\boldsymbol{\sigma}}}^{(ij)}$, due to a unit value of the components $\bar{\epsilon}_{ij}$, via the *ansatz*:

{eq:3-103} $$\boldsymbol{u} = \sum_{i,j} \hat{\boldsymbol{u}}^{(ij)} \bar{\epsilon}_{ij}, \quad \bar{\boldsymbol{\sigma}} = \sum_{i,j} \hat{\bar{\boldsymbol{\sigma}}}^{(ij)} \bar{\epsilon}_{ij} \tag{3.89}$$

Upon introducing these expressions into (**??**) and (**??**), we obtain the RVE-problems: Find
{eq:3-104} $\hat{\boldsymbol{u}}^{(ij)} \in \mathbb{U}_\square^{\mathrm{N}}$ and $\bar{\boldsymbol{\sigma}}^{(ij)} \in \mathbb{R}^{3\times 3}_{\mathrm{sym}}$ for $i, j = 1, 2, NDIM$ that solve

{eq:3-104a} $$\langle \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{(ij)}] : \mathsf{E} : \boldsymbol{\epsilon}[\delta \boldsymbol{u}] \rangle_\square - \hat{\bar{\boldsymbol{\sigma}}}^{(ij)} : \langle \boldsymbol{\epsilon}[\delta \boldsymbol{u}] \rangle_\square = 0 \qquad \forall \delta \boldsymbol{u} \in \mathbb{U}_\square^{\mathrm{N}} \tag{3.90a}$$

{eq:3-104b} $$-\langle \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{(ij)}] \rangle_\square : \delta\bar{\boldsymbol{\sigma}} = -(\delta\bar{\boldsymbol{\sigma}})_{ij} \qquad \forall \delta\bar{\boldsymbol{\sigma}} \in \mathbb{R}^{3\times 3}_{\mathrm{sym}} \tag{3.90b}$$

Macroscale (apparent) stiffness tensor

It is possible to directly use the ansatz for $\bar{\boldsymbol{\sigma}}$ in $(\textbf{??})_2$ to obtain

{eq:3-105} $$\bar{\mathsf{E}}_\square = \sum_{i,j} \hat{\bar{\boldsymbol{\sigma}}}^{(ij)} \otimes \boldsymbol{e}_i \otimes \boldsymbol{e}_j \tag{3.91}$$

or, in terms of components, as follows:

{eq:3-106} $$(\bar{\mathsf{E}}_\square)_{ijkl} = [\boldsymbol{e}_i \otimes \boldsymbol{e}_j] : \hat{\bar{\boldsymbol{\sigma}}}^{(kl)} \quad i, j, k, l = 1, 2, ..., NDIM \tag{3.92}$$

Remark: An alternative "naive" approach is to adopt the expression

{eq:3-107} $$(\bar{\mathsf{E}}_\square)_{ijkl} = \langle \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{\mathrm{M}(ij)}] : \mathsf{E} : \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{(kl)}] \rangle_\square \quad i, j, k, l = 1, 2, ..., NDIM \tag{3.93}$$

that was given already in (??) pertinent to the DBC-problem. However, (??) and (??) give completely identical numerical results, which can be shown as follows: Firstly, due to the symmetry of the tensors $\hat{\bar{\boldsymbol{\sigma}}}^{(kl)}$, we may rephrase (??) as

{eq:3-108}
$$(\bar{\mathsf{E}}_{\Box})_{ijkl} = \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{\mathrm{M}(ij)}] : \hat{\bar{\boldsymbol{\sigma}}}^{(kl)} \quad i,j,k,l = 1,2,...,NDIM \tag{3.94}$$

Secondly, upon setting $\delta \boldsymbol{u} = \hat{\boldsymbol{u}}^{\mathrm{M}(kl)}$ in (??) and noting that $\boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{\mathrm{M}(ij)}]$ are constant tensors, we obtain

$$\langle \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{(kl)}] : \mathsf{E} : \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{\mathrm{M}(ij)}] \rangle_{\Box} = \hat{\bar{\boldsymbol{\sigma}}}^{(kl)} : \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{\mathrm{M}(ij)}]. \tag{3.95}$$ {eq:3-109}

Finally, combining (??) and (??), we obtain the expression in ??. $\Box$

3.4.4 FE-approximation – Matrix format (in 2D)

Preliminaries

We express the pertinent forms in matrix format as {eq:3-111}

$$\bar{\boldsymbol{\sigma}} : \langle \boldsymbol{\epsilon}[\delta \boldsymbol{u}_h] \rangle_{\Box} = \left[\frac{1}{|\Omega_{\Box}|} \int_{\Gamma_{\Box}} \delta \boldsymbol{u}_h \otimes \boldsymbol{n} \, \mathrm{d}\Gamma \right] : \bar{\boldsymbol{\sigma}} = \sum_{k=1}^{\mathrm{NVAR_b}} (\delta \underline{\boldsymbol{u}}^{\mathrm{b}})_k \left[\underbrace{\frac{1}{|\Omega_{\Box}|} \int_{\Gamma_{\Box}} \boldsymbol{N}_k^{\mathrm{b}} \otimes \boldsymbol{n} \, \mathrm{d}\Gamma}_{\boldsymbol{C}_k} \right] : \bar{\boldsymbol{\sigma}}$$

$$= \sum_{k=1}^{\mathrm{NVAR_b}} (\delta \underline{\boldsymbol{u}}^{\mathrm{b}})_k \underline{\boldsymbol{C}}_k \underline{\bar{\boldsymbol{\sigma}}} = [\delta \underline{\boldsymbol{u}}^{\mathrm{b}}]^{\mathrm{T}} \underline{\boldsymbol{C}} \underline{\bar{\boldsymbol{\sigma}}} \tag{3.96a}$$ {eq:3-111a}

$$\langle \boldsymbol{\epsilon}[\boldsymbol{u}_h] \rangle_{\Box} : \delta \bar{\boldsymbol{\sigma}} = [\delta \underline{\bar{\boldsymbol{\sigma}}}]^{\mathrm{T}} \underline{\boldsymbol{C}}^{\mathrm{T}} \underline{\boldsymbol{u}}^{\mathrm{b}} \tag{3.96b}$$ {eq:3-111b}

where we introduced the Voigt matrix representation of $\boldsymbol{C}_k \stackrel{\mathrm{def}}{=} \frac{1}{|\Omega_{\Box}|} \int_{\Gamma_{\Box}} \boldsymbol{N}_k^{\mathrm{b}} \otimes \boldsymbol{n} \, \mathrm{d}\Gamma$ with the row matrix

$$\underline{\boldsymbol{C}}_k = \left[\begin{array}{ccc} (\boldsymbol{C}_k)_{11} & (\boldsymbol{C}_k)_{12} & (\boldsymbol{C}_k)_{22} \end{array} \right] \tag{3.97}$$ {eq:3-112}

Moreover, the matrix $\underline{\boldsymbol{C}}$ is defined as

$$\underline{\boldsymbol{C}} = \left[\begin{array}{ccc} (\boldsymbol{C}_1)_{11} & (\boldsymbol{C}_1)_{12} & (\boldsymbol{C}_1)_{22} \\ (\boldsymbol{C}_2)_{11} & (\boldsymbol{C}_2)_{12} & (\boldsymbol{C}_2)_{22} \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ (\boldsymbol{C}_{\mathrm{NVAR_b}})_{11} & (\boldsymbol{C}_{\mathrm{NVAR_b}})_{12} & (\boldsymbol{C}_{\mathrm{NVAR_b}})_{22} \end{array} \right] \tag{3.98}$$ {eq:3-113}

Each of the 3 columns in $\underline{\boldsymbol{C}}$ can be assembled elementwise like a "load vector" from line loading along element edges.

SVE-problem – Formulation and solution

All nodal displacement variables are free variables that are determined as part of the solution. The SVE-problem is then formulated in matrix format as: {eq:3-114}

$$\underline{\boldsymbol{K}}^{\mathrm{ii}} \underline{\boldsymbol{u}}^{\mathrm{i}} + \underline{\boldsymbol{K}}^{\mathrm{ib}} \underline{\boldsymbol{u}}^{\mathrm{b}} = \underline{\boldsymbol{0}} \tag{3.99a}$$ {eq:3-114a}

$$\underline{\boldsymbol{K}}^{\mathrm{bi}} \underline{\boldsymbol{u}}^{\mathrm{i}} + \underline{\boldsymbol{K}}^{\mathrm{bb}} \underline{\boldsymbol{u}}^{\mathrm{b}} - \underline{\boldsymbol{C}} \underline{\bar{\boldsymbol{\sigma}}} = \underline{\boldsymbol{0}} \tag{3.99b}$$ {eq:3-114b}

$$-\underline{\boldsymbol{C}}^{\mathrm{T}} \underline{\boldsymbol{u}}^{\mathrm{b}} = -\underline{\bar{\boldsymbol{\epsilon}}} \tag{3.99c}$$ {eq:3-114c}

We note that the solution as well as the test functions for the continuous counterpart (3.99) belong to $\mathbb{U}_{\square}^{\mathrm{N}} = \mathbb{U}_{\square}$, where rigid body motion is preveneted. This must also be considered in the present discrete forms. However, we are free to replace the integrals in (3.99) by any constraints that remove any (superimposed) RBM, while not affecting the state of deformation. In 2D, a simple way of enforcing this constraint is to set, e.g.,

{eq:3-115}
$$\begin{array}{ccc} u_1 = u_2 = 0 & \text{at} & (x_1, x_2) = (-\frac{l_\square}{2}, -\frac{l_\square}{2}) \\ u_2 = 0 & \text{at} & (x_1, x_2) = (\frac{l_\square}{2}, -\frac{l_\square}{2}) \end{array} \tag{3.100}$$

where $l_\square$ is the size of the RVE. In (**??**), such a constraint is imposed, whereby $\underline{\boldsymbol{u}}^{\mathrm{i}}, \underline{\boldsymbol{u}}^{\mathrm{b}}$ remove ?? the free dofs ?????

Summarizing, we are faced with the problem of computing $\underline{\boldsymbol{u}}^{\mathrm{i}}, \underline{\boldsymbol{u}}^{\mathrm{b}}$ and $\underline{\bar{\boldsymbol{\sigma}}}$ from the system of equations

{eq:3-116}
$$\begin{bmatrix} \underline{\boldsymbol{K}}^{\mathrm{ii}} & \underline{\boldsymbol{K}}^{\mathrm{ib}} & \underline{\mathbf{0}} \\ \underline{\boldsymbol{K}}^{\mathrm{bi}} & \underline{\boldsymbol{K}}^{\mathrm{bb}} & -\underline{\boldsymbol{C}} \\ \underline{\mathbf{0}} & -\underline{\boldsymbol{C}}^{\mathrm{T}} & \underline{\mathbf{0}} \end{bmatrix} \begin{bmatrix} \underline{\boldsymbol{u}}^{\mathrm{i}} \\ \underline{\boldsymbol{u}}^{\mathrm{b}} \\ \underline{\bar{\boldsymbol{\sigma}}} \end{bmatrix} = \begin{bmatrix} \underline{\mathbf{0}} \\ \underline{\mathbf{0}} \\ -\underline{\bar{\boldsymbol{\epsilon}}} \end{bmatrix} \tag{3.101}$$

Computing the (appparent) macroscale stiffness matrix in practice

To solve (**??**), while preserving the the "FE-structure" of the tangent stiffness matrix $\underline{\boldsymbol{K}}$, we introduce the decomposition via sensitivities w.r.t. to (a perturbation of) $\underline{\bar{\boldsymbol{\sigma}}}$:

{eq:3-117}
$$\underline{\boldsymbol{u}}^{\mathrm{i}} = \underline{\hat{\boldsymbol{u}}}^{\mathrm{i}}_{\bar{\mathrm{P}}} \underline{\bar{\boldsymbol{\sigma}}} + \underline{\boldsymbol{u}}^{\mathrm{i}}_{\mathrm{R}}, \quad \underline{\boldsymbol{u}}^{\mathrm{b}} = \underline{\hat{\boldsymbol{u}}}^{\mathrm{b}}_{\bar{\mathrm{P}}} \underline{\bar{\boldsymbol{\sigma}}} + \underline{\boldsymbol{u}}^{\mathrm{b}}_{\mathrm{R}} \tag{3.102}$$

Upon inserting into the two first equations of (**??**), we obtain the two sets of FE-equations

{eq:3-118}
$$\begin{bmatrix} \underline{\boldsymbol{K}}^{\mathrm{ii}} & \underline{\boldsymbol{K}}^{\mathrm{ib}} \\ \underline{\boldsymbol{K}}^{\mathrm{bi}} & \underline{\boldsymbol{K}}^{\mathrm{bb}} \end{bmatrix} \begin{bmatrix} \underline{\boldsymbol{u}}^{\mathrm{i}}_{\mathrm{R}} \\ \underline{\boldsymbol{u}}^{\mathrm{b}}_{\mathrm{R}} \end{bmatrix} = \begin{bmatrix} \underline{\mathbf{0}} \\ \underline{\mathbf{0}} \end{bmatrix} \tag{3.103}$$

{eq:3-119}
$$\begin{bmatrix} \underline{\boldsymbol{K}}^{\mathrm{ii}} & \underline{\boldsymbol{K}}^{\mathrm{ib}} \\ \underline{\boldsymbol{K}}^{\mathrm{bi}} & \underline{\boldsymbol{K}}^{\mathrm{bb}} \end{bmatrix} \begin{bmatrix} \underline{\hat{\boldsymbol{u}}}^{\mathrm{i}}_{\bar{\mathrm{P}}} \\ \underline{\hat{\boldsymbol{u}}}^{\mathrm{b}}_{\bar{\mathrm{P}}} \end{bmatrix} = \begin{bmatrix} \underline{\mathbf{0}} \\ \underline{\boldsymbol{C}} \end{bmatrix} \tag{3.104}$$

Firstly, it appears that the solution to (5.125) is the homogeneous solution $\underline{\boldsymbol{u}}^{\mathrm{i}}_{\mathrm{R}} = \underline{\mathbf{0}}$ and $\underline{\boldsymbol{u}}^{\mathrm{b}}_{\mathrm{R}} = \underline{\mathbf{0}}$, i.e.

{eq:3-121}
$$\underline{\boldsymbol{u}}^{\mathrm{i}} = \underline{\hat{\boldsymbol{u}}}^{\mathrm{i}}_{\bar{\mathrm{P}}} \underline{\bar{\boldsymbol{\sigma}}}, \quad \underline{\boldsymbol{u}}^{\mathrm{b}} = \underline{\hat{\boldsymbol{u}}}^{\mathrm{b}}_{\bar{\mathrm{P}}} \underline{\bar{\boldsymbol{\sigma}}} \tag{3.105}$$

Finally, we may solve for $\underline{\bar{\boldsymbol{\sigma}}}$ from the last equation in (**??**) while noting that $\underline{\boldsymbol{u}}^{\mathrm{b}} = \underline{\hat{\boldsymbol{u}}}^{\mathrm{b}}_{\bar{\mathrm{P}}} \underline{\bar{\boldsymbol{\sigma}}}$:

{eq:3-122}
$$\underline{\bar{\boldsymbol{\sigma}}} = \underbrace{\left[\underline{\boldsymbol{C}}^{\mathrm{T}} \underline{\hat{\boldsymbol{u}}}^{\mathrm{b}}_{\bar{\mathrm{P}}}\right]^{-1}}_{\underline{\bar{\mathbf{E}}}_\square} \underline{\bar{\boldsymbol{\epsilon}}} \tag{3.106}$$

i.e. we have deduced the operational expression for $\underline{\bar{\mathbf{E}}}_\square$

{eq:3-123}
$$\underline{\bar{\mathbf{E}}}_\square = \left[\underline{\boldsymbol{C}}^{\mathrm{T}} \underline{\hat{\boldsymbol{u}}}^{\mathrm{b}}_{\bar{\mathrm{P}}}\right]^{-1} \tag{3.107}$$

In the 2D-case this means to solve for 3 RHS:s in (**??**) corresponding to each one of the 3 columns of the identity matrix $\underline{\boldsymbol{I}}$.

Non-operational format: Possible to eliminate $\underline{\hat{\boldsymbol{u}}}^{\mathrm{i}}_{\mathrm{P}}$ in (??) to obtain

{eq:3-124} $$\underline{\tilde{\boldsymbol{K}}}^{\mathrm{bb}}\underline{\hat{\boldsymbol{u}}}^{\mathrm{b}}_{\mathrm{P}} = \underline{\boldsymbol{C}} \quad \Rightarrow \quad \underline{\hat{\boldsymbol{u}}}^{\mathrm{b}}_{\mathrm{P}} = \left[\underline{\tilde{\boldsymbol{K}}}^{\mathrm{bb}}\right]^{-1}\underline{\boldsymbol{C}} \tag{3.108}$$

where $\underline{\tilde{\boldsymbol{K}}}^{\mathrm{bb}}$ is the part-inverted matrix defined (for the DBC-problem) as follows:

{eq:3-125} $$\underline{\tilde{\boldsymbol{K}}}^{\mathrm{bb}} = \underline{\boldsymbol{K}}^{\mathrm{bb}} - \underline{\boldsymbol{K}}^{\mathrm{bi}}\left[\underline{\boldsymbol{K}}^{\mathrm{ii}}\right]^{-1}\underline{\boldsymbol{K}}^{\mathrm{ib}} \tag{3.109}$$

Inserting into (5.134):

$$\underline{\bar{\mathsf{E}}}_{\square} = \left[\underline{\boldsymbol{C}}^{\mathrm{T}}\left[\underline{\tilde{\boldsymbol{K}}}^{\mathrm{bb}}\right]^{-1}\underline{\boldsymbol{C}}\right]^{-1} \tag{3.110}$$ {eq:3-126}

As to the dimensions of the matrices involved, we have in the 2D-case:

$$\begin{aligned} dim(\underline{\hat{\boldsymbol{u}}}^{\mathrm{i}}) &= \mathrm{NVAR}_{\mathrm{i}} \times 3 \\ dim(\underline{\hat{\boldsymbol{u}}}^{\mathrm{b}}) &= \mathrm{NVAR}_{\mathrm{b}} \times 3 \\ dim(\underline{\boldsymbol{C}}) &= \mathrm{NVAR}_{\mathrm{b}} \times 3 \\ dim(\underline{\bar{\mathsf{E}}}_{\square}) &= 3 \times 3 \end{aligned} \tag{3.111}$$ {eq:3-127}

3.4.5 NBC-problem for macroscale stress control

We now turn to the situation when the macroscale stress $\bar{\boldsymbol{\sigma}}$ is prescribed: For given value of $\bar{\boldsymbol{\sigma}} \in \mathbb{R}^{3\times 3}_{\mathrm{sym}}$, find $\boldsymbol{u} \in \mathbb{U}^{\mathrm{N}}_{\square}$ that solves

$$\langle \boldsymbol{\epsilon}[\boldsymbol{u}] : \mathsf{E} : \boldsymbol{\epsilon}[\delta\boldsymbol{u}]\rangle_{\square} = \langle \boldsymbol{\epsilon}[\delta\boldsymbol{u}]\rangle_{\square} : \bar{\boldsymbol{\sigma}} \quad \forall \delta\boldsymbol{u} \in \mathbb{U}^{\mathrm{N}}_{\square} \tag{3.112}$$ {eq:3-128}

When the solution has been found it is possible to compute $\bar{\boldsymbol{\epsilon}}$ in a "post-processing step": $\bar{\boldsymbol{\epsilon}} = \langle \boldsymbol{\epsilon} \rangle_{\square}$. As to the interpretation of $\bar{\boldsymbol{\sigma}}$ in this case, we may choose $\delta\boldsymbol{u}$ in (??) such that $\boldsymbol{\epsilon}[\delta\boldsymbol{u}] = \delta\bar{\boldsymbol{\epsilon}}$ is constant, whereby the relation $\bar{\boldsymbol{\sigma}} = \langle \boldsymbol{\sigma} \rangle_{\square}$ is obtained. Hence, this relation is "built-in" the variational formulation from the construction of solution and test spaces.

Remark: This formulation represents the most straight-forward setting of the Neumann problem; hence, it is perhaps the most natural one when using "upscaling" strategy to calibrate a macroscale stress-strain relation, cf. LÖHNERT AND WRIGGERS ??. □

3.5 Weakly periodic boundary conditions (WPBC-problem)

3.5.1 Preliminaries – The concept of weak periodicity

For the sake of completeness, we reiterate the basic arguments of micro-periodicity as put forward in Subsection 3.3 for the case of SPBC. We thus recall that any subscale property on the mirror boundary, $\Gamma^{-}_{\square}$ is computed in terms of the property on the corresponding image boundary, $\Gamma^{+}_{\square}$. In particular, we express periodicity of the displacement fluctuation field as

$$\boldsymbol{u}^{\mu}(\boldsymbol{x}) = \boldsymbol{u}^{\mu}(\boldsymbol{\varphi}_{\mathrm{per}}(\boldsymbol{x})), \quad \forall \boldsymbol{x} \in \Gamma^{+}_{\square} \tag{3.113}$$ {eq:3-129}

Equivalently, we use the jump operator $[\![\bullet]\!]_{\square}$ to express the periodicity condition as follows:

$$[\![\boldsymbol{u}^{\mu}]\!]_{\square} = \boldsymbol{0} \quad \text{on } \Gamma^{+}_{\square}, \quad [\![\boldsymbol{u}^{\mu}]\!]_{\square}(\boldsymbol{x}) \stackrel{\text{def}}{=} \boldsymbol{u}^{\mu}(\boldsymbol{x}) - \boldsymbol{u}^{\mu}(\boldsymbol{\varphi}_{\mathrm{per}}(\boldsymbol{x})) \tag{3.114}$$ {eq:3-131}

Subsequently, we shall not enforce the condition (**??**) strongly as the point of departure; rather it is done weakly. To this end, we first assume that $\boldsymbol{\sigma}$ satisfies the *symmetry condition*

$$\boldsymbol{\sigma}(\boldsymbol{x}) = \boldsymbol{\sigma}(\boldsymbol{\varphi}_{\text{per}}(\boldsymbol{x})), \quad \forall \boldsymbol{x} \in \Gamma_{\square}^{+} \tag{3.115}$$ {eq:3-132}

As an immediate consequence of this symmetry assumption, we obtain that the boundary tractions $\boldsymbol{t} \overset{\text{def}}{=} \boldsymbol{\sigma} \cdot \boldsymbol{n}$ satisfy the following *anti-symmetry condition* for any mirror point that is not a corner point

{eq:3-133} $$\boldsymbol{t}(\boldsymbol{x}) = -\boldsymbol{t}(\boldsymbol{\varphi}_{\text{per}}(\boldsymbol{x})), \quad \forall \boldsymbol{x} \in \Gamma_{\square}^{+}. \tag{3.116}$$

It is noted that $\boldsymbol{t} \in \mathbb{T}_{\square}$ (the space of self-equilibrating tractions) in view of the assumption (**??**).

We now evaluate, upon using (**??**), the boundary term in (**??**) as follows:

{eq:3-134} $$\frac{1}{|\Omega_{\square}|} \int_{\Gamma_{\square}} \boldsymbol{t} \cdot \delta \boldsymbol{u} \, \mathrm{d}\Gamma = \frac{1}{|\Omega_{\square}|} \int_{\Gamma_{\square}^{+}} \boldsymbol{t} \cdot [\![\delta \boldsymbol{u}]\!]_{\square} \, \mathrm{d}\Gamma \tag{3.117}$$

A variational (weak) statement of the micro-periodicity constraint, that was previously given in (**??**) in the strong format, can now be formulated as

{eq:3-135} $$\frac{1}{|\Omega_{\square}|} \int_{\Gamma_{\square}^{+}} \delta \boldsymbol{\lambda} \cdot [\![\boldsymbol{u}^{\mu}]\!] \, \mathrm{d}\Gamma = 0, \quad \forall \delta \boldsymbol{\lambda} \in \mathbb{T}_{\square}^{+} \tag{3.118}$$

where $\mathbb{T}_{\square}^{+}$ is a suitable set of functions on the image boundary $\Gamma_{\square}^{+}$. Hence, all tractions of any concern live on $\Gamma_{\square}^{+}$ only. It is thus clear that $\boldsymbol{\lambda} \in \mathbb{T}_{\square}^{+}$ are Lagrangian multiplier fields that play the role of tractions on $\Gamma_{\square}^{+}$. Converesely, the tractions on the mirror part $\Gamma_{\square}^{-}$ is $-\boldsymbol{\lambda}(\varphi_{\text{per}}(\boldsymbol{x}))$???? for $\boldsymbol{x} \in \Gamma_{\square}^{+}$.

In the most general case the space $\mathbb{T}_{\square}^{+}$ is infinite-dimensional (and with sufficient regularity). Indeed, it is the particular choice of this space that defines the prolongation condition (model assumption).

Finally, we introduce the auxiliary variational form

{eq:3-136} $$d_{\square}(\boldsymbol{\lambda}, \boldsymbol{u}) \overset{\text{def}}{=} \frac{1}{|\Omega_{\square}|} \int_{\Gamma_{\square}^{+}} \boldsymbol{\lambda} \cdot [\![\boldsymbol{u}]\!]_{\square} \, \mathrm{d}\Gamma \tag{3.119}$$

in order to abbreviate the condition (**??**) in what follows.

3.5.2 WPBC-problem for macroscale strain control

Based on the developments in the previous Subsection, the variational form of the subscale problem for weakly imposed microperiodicity in the displacements can now be formulated for the case of macrostrain control as follows: Find $\boldsymbol{u} \in \mathbb{U}_{\square}$, and $\boldsymbol{\lambda} \in \mathbb{T}_{\square}^{+}$ that, for given value of
{eq:3-137} the macroscale displacement gradient $\bar{\boldsymbol{\epsilon}}$, solve the system

{eq:3-137a} $$\langle \boldsymbol{\epsilon}[\boldsymbol{u}] : \mathsf{E} : \boldsymbol{\epsilon}[\delta \boldsymbol{u}] \rangle_{\square} - d_{\square}(\boldsymbol{\lambda}, \delta \boldsymbol{u}) = 0 \qquad \forall \delta \boldsymbol{u} \in \mathbb{U}_{\square} \tag{3.120a}$$
{eq:3-137b} $$-d_{\square}(\delta \boldsymbol{\lambda}, \boldsymbol{u}) = -d_{\square}(\delta \boldsymbol{\lambda}, \bar{\boldsymbol{\epsilon}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}]) \qquad \forall \delta \boldsymbol{\lambda} \in \mathbb{T}_{\square}^{+} \tag{3.120b}$$

3.5.3 Macroscale stiffness tensor

Sensitivity fields

We introduce the "unit fields", or sensitivities, $\hat{\boldsymbol{u}}^{(ij)}$ and $\hat{\boldsymbol{\lambda}}^{(ij)}$, due to a unit value of the components $\bar{\epsilon}_{ij}$, via the *ansatz*

{eq:3-138}
$$\boldsymbol{u} = \sum_{i,j} \hat{\boldsymbol{u}}^{(ij)} \bar{\epsilon}_{ij}, \quad \boldsymbol{\lambda} = \sum_{i,j} \hat{\boldsymbol{\lambda}}^{(ij)} \bar{\epsilon}_{ij} \tag{3.121}$$

which may be inserted into (**??**) to give the equations that must hold for $k, l = 1, 2, ..., NDIM$:
{eq:3-139}

$$\langle \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{(kl)}] : \mathbf{E} : \boldsymbol{\epsilon}[\delta \boldsymbol{u}] \rangle_\square - d_\square(\hat{\boldsymbol{\lambda}}^{(kl)}, \delta \boldsymbol{u}) = 0 \qquad \forall \delta \boldsymbol{u} \in \mathbb{U}_\square \tag{3.122a}$$
{eq:3-139a}

$$-d_\square(\delta \boldsymbol{\lambda}, \hat{\boldsymbol{u}}^{(kl)}) = -d_\square(\delta \boldsymbol{\lambda}, \hat{\boldsymbol{u}}^{\mathrm{M}(kl)}) \qquad \forall \delta \boldsymbol{\lambda} \in \mathbb{T}_\square^+ \tag{3.122b}$$
{eq:3-139b}

Macroscale (apparent) stiffness tensor

Upon choosing $\delta \boldsymbol{u} = \hat{\boldsymbol{u}}^{\mathrm{M}(ij)}$ in (**??**), we obtain

$$\underbrace{\langle \boldsymbol{\epsilon}[\boldsymbol{u}] : \mathbf{E} \rangle_\square}_{=\bar{\boldsymbol{\sigma}}} : \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{\mathrm{M}(ij)}] = d_\square(\boldsymbol{\lambda}, \hat{\boldsymbol{u}}^{\mathrm{M}(ij)}) \tag{3.123}$$
{eq:3-141}

and, with the representation of $\boldsymbol{\lambda}$ in $(\mathbf{??})_2$,

$$\bar{\sigma}_{ij} = d_\square(\boldsymbol{\lambda}, \hat{\boldsymbol{u}}^{\mathrm{M}(ij)}) = \sum_{k,l} \underbrace{d_\square(\hat{\boldsymbol{\lambda}}^{(kl)}, \hat{\boldsymbol{u}}^{\mathrm{M}(ij)})}_{=(\bar{\mathbf{E}}_\square)_{ijkl}} \bar{\epsilon}_{kl} \tag{3.124}$$
{eq:3-142}

We thus conclude that

$$(\bar{\mathbf{E}}_\square)_{ijkl} = d_\square(\hat{\boldsymbol{\lambda}}^{(kl)}, \hat{\boldsymbol{u}}^{\mathrm{M}(ij)}) = \frac{1}{|\Omega_\square|} \int_{\Gamma_\square^+} \hat{\boldsymbol{\lambda}}^{(kl)} \cdot [\![\hat{\boldsymbol{u}}^{\mathrm{M}(ij)}]\!]_\square \, \mathrm{d}\Gamma \tag{3.125}$$
{eq:3-143}

Remark: The Neumann condition represents the weakest possible way of enforcing the micro-periodicity condition. Here it is considered as a *model assumption*; however, it is also possible to view this choice as a (crude) FE-approximation of the traction field, cf. discussion below. □

3.5.4 Mixed FE-approximation UPDATE

Variational format

The straightforward FE-formulation of the subscale problem is as follows: Find $\boldsymbol{u}_h \in \mathbb{U}_{\square,h} \subseteq \mathbb{U}_\square$, and $\boldsymbol{\lambda}_h \in \mathbb{T}_{\square,h}^+ \subseteq \mathbb{T}_\square^+$ that, for given value of the macroscale displacement gradient $\bar{\boldsymbol{\epsilon}}$, solve the system

$$\begin{aligned} a_\square(\boldsymbol{u}_h; \delta \boldsymbol{u}_h) - d_\square(\boldsymbol{\lambda}_h, \delta \boldsymbol{u}_h) &= 0 && \forall \delta \boldsymbol{u}_h \in \mathbb{U}_{\square,h}, \\ -d_\square(\delta \boldsymbol{\lambda}_h, \boldsymbol{u}_h) &= -d_\square(\delta \boldsymbol{\lambda}_h, \bar{\boldsymbol{\epsilon}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}]) && \forall \delta \boldsymbol{\lambda}_h \in \mathbb{T}_{\square,h}^+. \end{aligned} \tag{3.126}$$
{eq:3-144}

As to the particular choice of the FE-approximations for boundary tractions $\boldsymbol{\lambda}_h \in \mathbb{T}_{\square,h}^+$, we first note that no special regularity requirements are present; it is thus (at least in theory) possible to choose piecewise constant tractions along $\Gamma_\square^+$. However, it is always necessary to satisfy (i) the periodicity condition along any given coordinate surface on $\Gamma_\square^+$, and (ii) a stability criterion in the sense that the dimension of the traction space $\mathbb{T}_{\square,h}$ cannot be too large in comparison with the dimension of $\mathbb{U}_{\square,h}$. The precise requirement is expressed by the LBB-condition, cf. below. Henceforth, we shall restrict to the case when $\mathbb{T}_{\square,h}$ contains *continuous* functions on each coordinate surface of $\Gamma_\square^+$.

Construction of traction mesh

Next, we discuss the construction of the traction mesh $\mathcal{M}_h^{(\lambda)}$ in practice. Firstly, all the nodes in $\mathcal{M}_h^{(\mathrm{u})}$ on both the image boundary $\Gamma_\square^+$ and the mirror boundary $\Gamma_\square^-$ are "projected onto $\Gamma_\square^+$ to produce an "unprocessed" version of $\mathcal{M}_h^{(\lambda)}$ as illustrated in Figure **??**. However, it is possible, and indeed quite likely, that this mesh will contain elements that are too small, i.e. the projected nodes come extremely close. To overcome this situation, a procedure has been implemented according to which nodes closer than a predefined minimal distance are eliminated. Two methods for defining the minimal distance are introduced: (1) It is chosen *a priori* as a fixed measure, for instance, a fraction of $L_\square$. (2) It is chosen adaptively as the smallest element length divided by a factor less than (or equal to) unity. Clearly, if the factor is unity only the smallest element is eliminated. The resulting mesh is called the Standard mesh, and an example is depicted in Figure **??**(a).

For the Standard mesh it is possible to show that the LBB-condition is satisfied for piecewise linear functions in $\mathbb{U}_{\square,h}$ and in $\mathbb{T}_{\square,h}^+$, cf. the analogous problem of elastic contact discussed by El-Abbasi and Bathe **?**, Wriggers **?**. To be more specific, using the periodicity of the traction approximation as expressed in (**??**), we identify a special case of the analogeous contact situation analyzed in the literature. In fact, the very reason for imposing (**??**), which is not necessary from a regularity point of view (since the tractions need not be continuous) is to utilize these lowest order stable approximations. As a viable alternative, one would adopt a penalty formulation, cf. Heintz and Hansbo **?**.

Starting from the Standard traction mesh, we may reduce the number of elements in $\mathcal{M}_h^{(\lambda)}$ by choosing different tolerances. Such a Reduced traction mesh is illustrated in Figure **??**(b). Clearly, when $\mathcal{M}_h^{(\lambda)}$ has been reduced to one single element, then the problem is reduced to a constant traction on each coordinate face (since the two remaining nodes must have the same traction intensity due to stress periodicity). Hence, this case is equivalent to the *a priori* defined Neumann boundary conditions.

For the purpose of illustration, typical deformation fields and distribution of boundary tractions (tangential component) are shown in Figure **??** for a reduced traction mesh and the extreme case of Neumann conditions.

3.5.5 Mixed FE-approximation for strong micro-periodicity

A trivial conclusion is that the situation of strong micro-periodicity, defined by the condition $[\![\boldsymbol{u}_h^\mu]\!]_\square = \mathbf{0}$, $\forall \boldsymbol{x} \in \Gamma_\square^+$, is approached when the dimension of $\mathbb{T}_{\square,h}^+$ is *increased indefinitely.* In practice, this means that $\mathbb{U}_{\square,h}$ must also be enlarged indefinitely.

The classical situation of strong micro-periodicity is obtained by introducing strictly periodic meshes, i.e. the nodal positions are mirrored exactly from $\Gamma_\square^+$ to $\Gamma_\square^-$. In fact, this is the standard

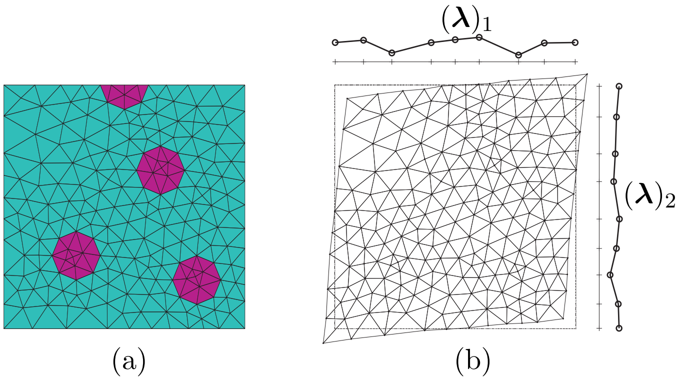


Figure 3.4: *(a) Typical particle-matrix composite in 2D. Typical deformation fields (macroscale shear deformation) and distribution of boundary tractions (tangential component) for (b) Periodic, (c) Neumann boundary conditions.* {fig:3-4}

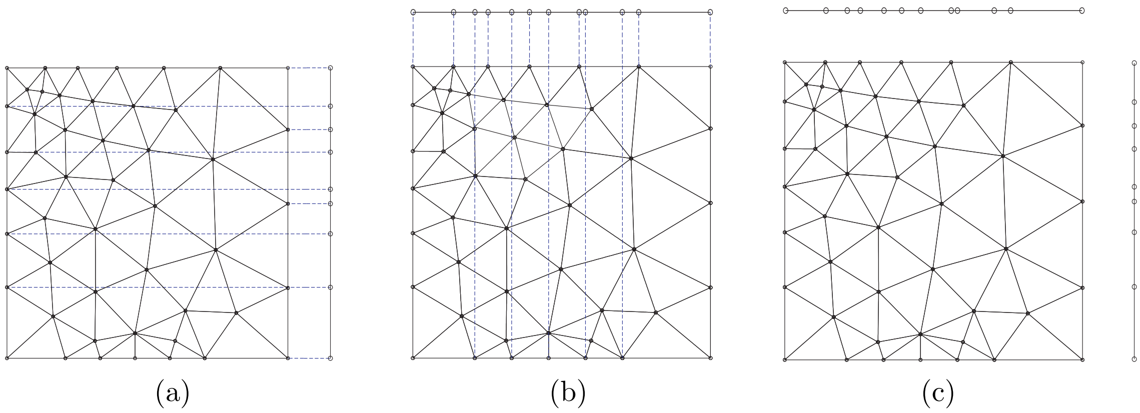


Figure 3.5: *Illustration in 2D of generic method to obtain the (unprocessed) traction mesh $\mathcal{M}_h^{(\lambda)}$ on $\Gamma_\square^+$ via "node projection" from the displacement mesh $\mathcal{M}_h^{(\mathrm{u})}$ in (a) x_1-direction, (b) x_2-direction. (c) Resulting "unprocessed" mesh.* {fig:3-5}

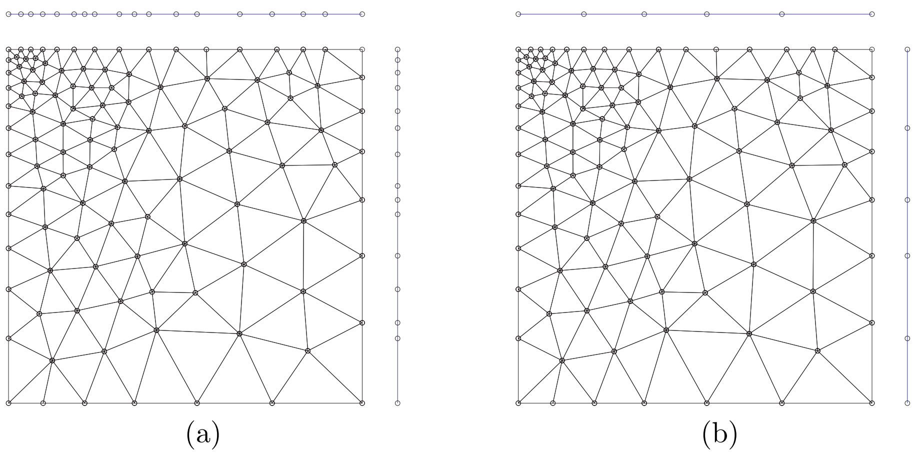


Figure 3.6: *(a) Standard traction mesh (obtained after processing), (b) Reduced traction mesh (with constant traction along each coordinate face as the extreme case = Neumann condition).* {fig:3-6}

approach widely used in the literature on computational homogenization, see e.g. MIEHE AND KOCH **?**, KOUZNETSOVA ET AL. **?**. Within the present variational framework, this situation is encountered as follows:

First, we note that (**??**)$_2$ can be rewritten as

{eq:3-145}
$$d_\Box(\delta\boldsymbol{\lambda}_h, \boldsymbol{u}_h^\mu) \quad = \quad 0 \qquad \forall \delta\boldsymbol{\lambda}_h \in \mathbb{T}^+_{\Box,h}. \tag{3.127}$$

Let us now choose the FE-spaces such that the trace of $\mathbb{U}_{\Box,h}$ on $\Gamma^+_\Box$ and on $\Gamma^-_\Box$ is identical and equals the traction space $\mathbb{T}^+_{\Box,h}$, i.e. $[\![\boldsymbol{u}_h^\mu]\!]_\Box \in \mathbb{T}^+_{\Box,h}$, $\forall \boldsymbol{x} \in \Gamma^+_\Box$. In such a case it is possible to choose $\delta\boldsymbol{\lambda}_h = [\![\boldsymbol{u}_h^\mu]\!]_\Box \in \mathbb{T}^+_{\Box,h}$ in (**??**), and it is trivially concluded that the only possible solution is $[\![\boldsymbol{u}_h^\mu]\!]_\Box = \boldsymbol{0}$. In other words, strong micro-periodicity on the fluctuation field is ensured along the whole RVE-boundary.

Remark: In practice, this case does not require any particular arrangement or precautions. It is merely considered as a special choice out of many possible meshes. □

3.5.6 Mixed FE-approximation – Matrix format (in 2D)

Preliminaries

The FE-discretization $\boldsymbol{u}_h$ on $\Omega_\Box$ is defined by the set of basis functions $\{\boldsymbol{N}_k^{\mathrm{u}}\}_{k=1}^{\mathrm{NVAR_u}}$. Similarly, the FE-discretization $\boldsymbol{\lambda}_h$ on $\Omega_\Box$ is defined by the set of basis functions $\{\boldsymbol{N}_k^{\lambda}\}_{k=1}^{\mathrm{NVAR}_\lambda}$. Moreover, both discretizations are expanded in internal nodal variables and boundary nodal variables.
{eq:3-1460} Hence, $\boldsymbol{u}_h(\boldsymbol{x})$ and $\boldsymbol{\lambda}_h(\boldsymbol{x})$ for $\boldsymbol{x} \in \Omega_\Box$, can be represented as

{eq:3-146a}
$$\boldsymbol{u}_h = \sum_{k=1}^{\mathrm{NVAR_u}} \boldsymbol{N}_k^{\mathrm{u}}(\underline{\boldsymbol{\lambda}})_k = \sum_{k=1}^{\mathrm{NVAR_{u,i}}} \boldsymbol{N}_k^{\mathrm{u,i}}(\underline{\boldsymbol{\lambda}}^{\mathrm{i}})_k + \sum_{k=1}^{\mathrm{NVAR_{u,b}}} \boldsymbol{N}_k^{\mathrm{u,b}}(\underline{\boldsymbol{\lambda}}^{\mathrm{b}})_k \tag{3.128a}$$

{eq:3-146b}
$$\boldsymbol{\lambda}_h = \sum_{k=1}^{\mathrm{NVAR}_\lambda} \boldsymbol{N}_k^{\lambda}(\underline{\boldsymbol{\lambda}})_k = \sum_{k=1}^{\mathrm{NVAR}_{\lambda,\mathrm{i}}} \boldsymbol{N}_k^{\lambda,\mathrm{i}}(\underline{\boldsymbol{\lambda}}^{\mathrm{i}})_k + \sum_{k=1}^{\mathrm{NVAR}_{\lambda,\mathrm{b}}} \boldsymbol{N}_k^{\lambda,\mathrm{b}}(\underline{\boldsymbol{\lambda}}^{\mathrm{b}})_k \tag{3.128b}$$

We express the form $d_{\square}(\boldsymbol{\lambda}_h, \delta\boldsymbol{u}_h)$ in matrix format as

$$
\begin{aligned}
d_{\square}(\boldsymbol{\lambda}_h, \delta\boldsymbol{u}_h) &\overset{\text{def}}{=} \frac{1}{|\Omega_{\square}|}\int_{\Gamma_{\square}^{+}} [\![\delta\boldsymbol{u}_h]\!]_{\square} \cdot \boldsymbol{\lambda}_h \,\mathrm{d}\Gamma = \frac{1}{|\Omega_{\square}|}\int_{\Gamma_{\square}^{+}} \delta\boldsymbol{u}_{+,h} \cdot \boldsymbol{\lambda}_h \,\mathrm{d}\Gamma - \frac{1}{|\Omega_{\square}|}\int_{\Gamma_{\square}^{+}} \delta\boldsymbol{u}_{-,h} \cdot \boldsymbol{\lambda}_h \,\mathrm{d}\Gamma \\
&= \sum_{k=1}^{\mathrm{NVAR}_{\mathrm{u,b+}}} (\delta\underline{\boldsymbol{u}}_{+}^{\mathrm{b}})_k \left[\frac{1}{|\Omega_{\square}|}\int_{\Gamma_{\square}^{+}} \boldsymbol{N}_k^{\mathrm{u,b+}} \cdot \boldsymbol{\lambda}_h \,\mathrm{d}\Gamma\right] - \sum_{k=1}^{\mathrm{NVAR}_{\mathrm{u,b-}}} (\delta\underline{\boldsymbol{u}}_{-}^{\mathrm{b}})_k \left[\frac{1}{|\Omega_{\square}|}\int_{\Gamma_{\square}^{+}} \boldsymbol{N}_k^{\mathrm{u,b-}} \cdot \boldsymbol{\lambda}_h \,\mathrm{d}\Gamma\right] \\
&= \sum_{k=1}^{\mathrm{NVAR}_{\mathrm{u,b+}}} \sum_{l=1}^{\mathrm{NVAR}_{\lambda}} (\delta\underline{\boldsymbol{u}}_{+}^{\mathrm{b}})_k \left[\underbrace{\frac{1}{|\Omega_{\square}|}\int_{\Gamma_{\square}^{+}} \boldsymbol{N}_k^{\mathrm{u,b+}} \cdot \boldsymbol{N}_l^{\lambda} \,\mathrm{d}\Gamma}_{(\underline{\boldsymbol{D}}_{+})_{kl}}\right] (\underline{\boldsymbol{\lambda}})_l \\
&\quad - \sum_{k=1}^{\mathrm{NVAR}_{\mathrm{u,b-}}} \sum_{l=1}^{\mathrm{NVAR}_{\lambda}} (\delta\underline{\boldsymbol{u}}_{+}^{\mathrm{b}})_k \left[\underbrace{\frac{1}{|\Omega_{\square}|}\int_{\Gamma_{\square}^{+}} \boldsymbol{N}_k^{\mathrm{u,b-}} \cdot \boldsymbol{N}_l^{\lambda} \,\mathrm{d}\Gamma}_{(\underline{\boldsymbol{D}}_{-})_{kl}}\right] (\underline{\boldsymbol{\lambda}})_l \\
&= \sum_{k=1}^{\mathrm{NVAR}_{\mathrm{u,b+}}} \sum_{l=1}^{\mathrm{NVAR}_{\lambda}} (\delta\underline{\boldsymbol{u}}_{+}^{\mathrm{b}})_k (\underline{\boldsymbol{D}}_{+})_{kl} (\underline{\boldsymbol{\lambda}})_l - \sum_{k=1}^{\mathrm{NVAR}_{\mathrm{u,b-}}} \sum_{l=1}^{\mathrm{NVAR}_{\lambda}} (\delta\underline{\boldsymbol{u}}_{-}^{\mathrm{b}})_k (\underline{\boldsymbol{D}}_{-})_{kl} (\underline{\boldsymbol{\lambda}})_l \\
&= [\delta\underline{\boldsymbol{u}}_{+}^{\mathrm{b}}]^{\mathrm{T}} \underline{\boldsymbol{D}}_{+} \underline{\boldsymbol{\lambda}} - [\delta\underline{\boldsymbol{u}}_{-}^{\mathrm{b}}]^{\mathrm{T}} \underline{\boldsymbol{D}}_{-} \underline{\boldsymbol{\lambda}} \qquad (3.129)
\end{aligned}
$$

{eq:3-147}

where $\underline{\boldsymbol{D}}_{+}$ and $\underline{\boldsymbol{D}}_{-}$ are defined as {eq:3-148}

$$(\underline{\boldsymbol{D}}_{+})_{kl} = \frac{1}{|\Omega_{\square}|}\int_{\Gamma_{\square}^{+}} \boldsymbol{N}_k^{\mathrm{u,b+}} \cdot \boldsymbol{N}_l^{\lambda} \,\mathrm{d}\Gamma \qquad (3.130a)$$ {eq:3-148a}

$$(\underline{\boldsymbol{D}}_{-})_{kl} = \frac{1}{|\Omega_{\square}|}\int_{\Gamma_{\square}^{+}} \boldsymbol{N}_k^{\mathrm{u,b-}} \cdot \boldsymbol{N}_l^{\lambda} \,\mathrm{d}\Gamma \qquad (3.130b)$$ {eq:3-148b}

We introduce

$$\underline{\boldsymbol{u}}^{\mathrm{b}} = \begin{bmatrix} \underline{\boldsymbol{u}}_{+}^{\mathrm{b}} \\ \underline{\boldsymbol{u}}_{-}^{\mathrm{b}} \end{bmatrix}, \quad \underline{\boldsymbol{D}} = \begin{bmatrix} \underline{\boldsymbol{D}}_{+} \\ -\underline{\boldsymbol{D}}_{-} \end{bmatrix} \qquad (3.131)$$ {eq:3-149}

whereby {eq:3-151}

$$
\begin{aligned}
d_{\square}(\boldsymbol{\lambda}_h, \delta\boldsymbol{u}_h) &= [\delta\underline{\boldsymbol{u}}_{+}^{\mathrm{b}}]^{\mathrm{T}} \underline{\boldsymbol{D}}_{+} \underline{\boldsymbol{\lambda}} - [\delta\underline{\boldsymbol{u}}_{-}^{\mathrm{b}}]^{\mathrm{T}} \underline{\boldsymbol{D}}_{-} \underline{\boldsymbol{\lambda}} \\
&= [\delta\underline{\boldsymbol{u}}^{\mathrm{b}}]^{\mathrm{T}} \underline{\boldsymbol{D}} \underline{\boldsymbol{\lambda}} \qquad (3.132a) \\
d_{\square}(\delta\boldsymbol{\lambda}_h, \boldsymbol{u}_h) &= [\delta\underline{\boldsymbol{\lambda}}]^{\mathrm{T}} \underline{\boldsymbol{D}}_{+}^{\mathrm{T}} \underline{\boldsymbol{u}}_{+}^{\mathrm{b}} - [\delta\underline{\boldsymbol{\lambda}}]^{\mathrm{T}} \underline{\boldsymbol{D}}_{-}^{\mathrm{T}} \underline{\boldsymbol{u}}_{-}^{\mathrm{b}} \\
&= [\delta\underline{\boldsymbol{\lambda}}]^{\mathrm{T}} \underline{\boldsymbol{D}}^{\mathrm{T}} \underline{\boldsymbol{u}}^{\mathrm{b}} \qquad (3.132b)
\end{aligned}
$$

{eq:3-151a} {eq:3-151b}

We also obtain

$$d_{\square}(\delta\boldsymbol{\lambda}_h, \bar{\boldsymbol{\epsilon}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}]) = [\delta\underline{\boldsymbol{\lambda}}]^{\mathrm{T}} \underline{\boldsymbol{D}}^{\mathrm{T}} \underline{\boldsymbol{u}}^{\mathrm{M,b}} = [\delta\underline{\boldsymbol{\lambda}}]^{\mathrm{T}} \underline{\boldsymbol{D}}^{\mathrm{T}} \underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}} \underline{\bar{\boldsymbol{\epsilon}}} \qquad (3.133)$$ {eq:appB_52

SVE-problem – Formulation and solution

The issue of preventing RBM is handled as follows: Microperiodicity prevents any rotation. Translation is most easily prevented by setting the displacements to zero in a single (arbitrarily chosen) node. All remaining nodal displacement variables are free variables that are determined as part of the solution. The SVE-problem is then formulated in matrix format as: {eq:3-152}

$$\underline{\boldsymbol{K}}^{\mathrm{ii}}\underline{\boldsymbol{u}}^{\mathrm{i}} + \underline{\boldsymbol{K}}^{\mathrm{ib}}\underline{\boldsymbol{u}}^{\mathrm{b}} = \underline{\boldsymbol{0}} \tag{3.134a}$$ {eq:3-152a}

$$\underline{\boldsymbol{K}}^{\mathrm{bi}}\underline{\boldsymbol{u}}^{\mathrm{i}} + \underline{\boldsymbol{K}}^{\mathrm{bb}}\underline{\boldsymbol{u}}^{\mathrm{b}} - \underline{\boldsymbol{D}}\underline{\boldsymbol{\lambda}} = \underline{\boldsymbol{0}} \tag{3.134b}$$ {eq:3-152b}

$$-\underline{\boldsymbol{D}}^{\mathrm{T}}\underline{\boldsymbol{u}}^{\mathrm{b}} = -\underline{\boldsymbol{D}}^{\mathrm{T}}\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}}\underline{\bar{\boldsymbol{\epsilon}}} \tag{3.134c}$$ {eq:3-152c}

$\underline{\boldsymbol{u}}^{\mathrm{i}}, \underline{\boldsymbol{u}}^{\mathrm{b}}$ and $\underline{\boldsymbol{\lambda}}$ are solved from the system of equations

{eq:3-153}
$$\begin{bmatrix} \underline{\boldsymbol{K}}^{\mathrm{ii}} & \underline{\boldsymbol{K}}^{\mathrm{ib}} & \underline{\boldsymbol{0}} \\ \underline{\boldsymbol{K}}^{\mathrm{bi}} & \underline{\boldsymbol{K}}^{\mathrm{bb}} & -\underline{\boldsymbol{D}} \\ \underline{\boldsymbol{0}} & -\underline{\boldsymbol{D}}^{\mathrm{T}} & \underline{\boldsymbol{0}} \end{bmatrix} \begin{bmatrix} \underline{\boldsymbol{u}}^{\mathrm{i}} \\ \underline{\boldsymbol{u}}^{\mathrm{b}} \\ \underline{\boldsymbol{\lambda}} \end{bmatrix} = \begin{bmatrix} \underline{\boldsymbol{0}} \\ \underline{\boldsymbol{0}} \\ -\underline{\boldsymbol{D}}^{\mathrm{T}}\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}}\underline{\bar{\boldsymbol{\epsilon}}} \end{bmatrix} \tag{3.135}$$

To solve (5.158), while preserving the "FE-structure" of the tangent stiffness matrix $\underline{\boldsymbol{K}}$, introduce the decomposition via sensitivities w.r.t. to (a perturbation of) $\underline{\boldsymbol{\lambda}}$:

{eq:3-154}
$$\underline{\boldsymbol{u}}^{\mathrm{i}} = \underline{\hat{\boldsymbol{u}}}^{\mathrm{i}}_{\lambda}\underline{\boldsymbol{\lambda}} + \underline{\boldsymbol{u}}^{\mathrm{i}}_{\mathrm{R}}, \quad \underline{\boldsymbol{u}}^{\mathrm{b}} = \underline{\hat{\boldsymbol{u}}}^{\mathrm{b}}_{\lambda}\underline{\boldsymbol{\lambda}} + \underline{\boldsymbol{u}}^{\mathrm{b}}_{\mathrm{R}} \tag{3.136}$$

Upon inserting into (5.158), we obtain the two sets of FE-equations

{eq:3-155}
$$\begin{bmatrix} \underline{\boldsymbol{K}}^{\mathrm{ii}} & \underline{\boldsymbol{K}}^{\mathrm{ib}} \\ \underline{\boldsymbol{K}}^{\mathrm{bi}} & \underline{\boldsymbol{K}}^{\mathrm{bb}} \end{bmatrix} \begin{bmatrix} \underline{\boldsymbol{u}}^{\mathrm{i}}_{\mathrm{R}} \\ \underline{\boldsymbol{u}}^{\mathrm{b}}_{\mathrm{R}} \end{bmatrix} = \begin{bmatrix} \underline{\boldsymbol{0}} \\ \underline{\boldsymbol{0}} \end{bmatrix} \tag{3.137}$$

{eq:3-156}
$$\begin{bmatrix} \underline{\boldsymbol{K}}^{\mathrm{ii}} & \underline{\boldsymbol{K}}^{\mathrm{ib}} \\ \underline{\boldsymbol{K}}^{\mathrm{bi}} & \underline{\boldsymbol{K}}^{\mathrm{bb}} \end{bmatrix} \begin{bmatrix} \underline{\hat{\boldsymbol{u}}}^{\mathrm{i}}_{\lambda} \\ \underline{\hat{\boldsymbol{u}}}^{\mathrm{b}}_{\lambda} \end{bmatrix} = \begin{bmatrix} \underline{\boldsymbol{0}} \\ \underline{\boldsymbol{D}} \end{bmatrix} \tag{3.138}$$

Firstly, it appears that the solution to (5.160) is the homogeneous solution $\underline{\boldsymbol{u}}^{\mathrm{i}}_{\mathrm{R}} = \underline{\boldsymbol{0}}$, $\underline{\boldsymbol{u}}^{\mathrm{b}}_{\mathrm{R}} = \underline{\boldsymbol{0}}$, i.e.

{eq:3-157}
$$\underline{\boldsymbol{u}}^{\mathrm{i}} = \underline{\hat{\boldsymbol{u}}}^{\mathrm{i}}_{\lambda}\underline{\boldsymbol{\lambda}}, \quad \underline{\boldsymbol{u}}^{\mathrm{b}} = \underline{\hat{\boldsymbol{u}}}^{\mathrm{b}}_{\lambda}\underline{\boldsymbol{\lambda}} \tag{3.139}$$

Now, upon using the ansatz $\underline{\boldsymbol{\lambda}} = \underline{\hat{\boldsymbol{\lambda}}}\underline{\bar{\boldsymbol{\epsilon}}}$, we may the solve for $\underline{\hat{\boldsymbol{\lambda}}}$ from the last equation in (5.158)

{eq:3-158}
$$\underline{\hat{\boldsymbol{\lambda}}} = \left[\underline{\boldsymbol{D}}^{\mathrm{T}}\underline{\hat{\boldsymbol{u}}}^{\mathrm{b}}_{\lambda}\right]^{-1}\underline{\boldsymbol{D}}^{\mathrm{T}}\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}} \tag{3.140}$$

As a postprocessing step, compute the macroscale stress $\underline{\bar{\boldsymbol{\sigma}}}$ from

{eq:3-159}
$$\underline{\bar{\boldsymbol{\sigma}}} = \left[\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}}\right]^{\mathrm{T}}\underline{\boldsymbol{D}}\underline{\boldsymbol{\lambda}} = \underbrace{\left[\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}}\right]^{\mathrm{T}}\underline{\boldsymbol{D}}\,\underline{\hat{\boldsymbol{\lambda}}}}_{=\underline{\bar{\mathsf{E}}}_{\square}}\underline{\bar{\boldsymbol{\epsilon}}} \tag{3.141}$$

Proof: Choosing $\delta\boldsymbol{u}_h = \delta\boldsymbol{u}^{\mathrm{M}} = \delta\bar{\boldsymbol{\epsilon}}\cdot[\boldsymbol{x}-\bar{\boldsymbol{x}}]$ in xxx gives:

{eq:3-161}
$$\underline{\bar{\boldsymbol{\sigma}}}^{\mathrm{T}}\delta\underline{\bar{\boldsymbol{\epsilon}}} = \underline{\boldsymbol{\lambda}}^{\mathrm{T}}\underline{\boldsymbol{D}}^{\mathrm{T}}\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}}\delta\underline{\bar{\boldsymbol{\epsilon}}} \tag{3.142}$$

Since this identity must hold for any choice of $\delta\underline{\bar{\boldsymbol{\epsilon}}}$, the relation (5.163) follows. □

We have thus derived the stiffness in the operational format

{eq:3-162}
$$\underline{\bar{\mathsf{E}}}_{\square} = \left[\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}}\right]^{\mathrm{T}}\underline{\boldsymbol{D}}\,\underline{\hat{\boldsymbol{\lambda}}}. \tag{3.143}$$

Non-operational format: It is possible to eliminate $\underline{\hat{\boldsymbol{u}}}_\lambda^{\mathrm{i}}$ in (**??**) to obtain

{eq:3-163}
$$\underline{\tilde{\boldsymbol{K}}}^{\mathrm{bb}}\underline{\hat{\boldsymbol{u}}}_\lambda^{\mathrm{b}} = \underline{\boldsymbol{D}} \quad \Rightarrow \quad \underline{\hat{\boldsymbol{u}}}_\lambda^{\mathrm{b}} = \left[\underline{\tilde{\boldsymbol{K}}}^{\mathrm{bb}}\right]^{-1} \underline{\boldsymbol{D}} \tag{3.144}$$

where $\underline{\tilde{\boldsymbol{K}}}^{\mathrm{bb}}$ is the part-inverted matrix defined (for the DBC-problem) as follows:

{eq:3-164}
$$\underline{\tilde{\boldsymbol{K}}}^{\mathrm{bb}} = \underline{\boldsymbol{K}}^{\mathrm{bb}} - \underline{\boldsymbol{K}}^{\mathrm{bi}} \left[\underline{\boldsymbol{K}}^{\mathrm{ii}}\right]^{-1} \underline{\boldsymbol{K}}^{\mathrm{ib}} \tag{3.145}$$

Inserting into (5.168) gives:

{eq:3-165}
$$\underline{\hat{\boldsymbol{\lambda}}} = \left[\underline{\boldsymbol{D}}^{\mathrm{T}} \left[\underline{\tilde{\boldsymbol{K}}}^{\mathrm{bb}}\right]^{-1} \underline{\boldsymbol{D}}\right]^{-1} \underline{\boldsymbol{D}}^{\mathrm{T}} \underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}} \bar{\boldsymbol{\epsilon}} \tag{3.146}$$

Finally, upon combining (**??**) with the relation (5.170), we obtain $\underline{\bar{\boldsymbol{\sigma}}} = \bar{\mathsf{E}}_\square \underline{\bar{\boldsymbol{\epsilon}}}$ with

$$\bar{\mathsf{E}}_\square = \left[\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}}\right]^{\mathrm{T}} \underline{\boldsymbol{D}} \left[\underline{\boldsymbol{D}}^{\mathrm{T}} \left[\underline{\tilde{\boldsymbol{K}}}^{\mathrm{bb}}\right]^{-1} \underline{\boldsymbol{D}}\right]^{-1} \underline{\boldsymbol{D}}^{\mathrm{T}} \underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}} \tag{3.147}$$
{eq:3- 166}

As to the dimensions of the matrices involved, we have in the 2D-case **UPDATE**:

$$\begin{aligned}
dim(\underline{\boldsymbol{D}}_+) &= \mathrm{NVAR}_{\mathrm{u,b+}} \times \mathrm{NVAR}_\lambda \\
dim(\underline{\boldsymbol{D}}_-) &= \mathrm{NVAR}_{\mathrm{u,b-}} \times \mathrm{NVAR}_\lambda \\
dim(\underline{\boldsymbol{D}}) &= \mathrm{NVAR}_{\mathrm{u,b}} \times \mathrm{NVAR}_\lambda \\
dim(\bar{\mathsf{E}}_\square) &= 3 \times 3
\end{aligned} \tag{3.148}$$
{eq:3-167}

□

Special case: Strong periodicity

Expand (5.156a) to (5.156c): {eq:3-168}

$$\underline{\boldsymbol{f}}^{\mathrm{i}}(\underline{\boldsymbol{u}}^{\mathrm{i}}, \underline{\boldsymbol{u}}_+^{\mathrm{b}}, \underline{\boldsymbol{u}}_-^{\mathrm{b}}) = \underline{\boldsymbol{0}} \tag{3.149a}$$
{eq:3-168a

$$\underline{\boldsymbol{f}}_+^{\mathrm{b}}(\underline{\boldsymbol{u}}^{\mathrm{i}}, \underline{\boldsymbol{u}}_+^{\mathrm{b}}, \underline{\boldsymbol{u}}_-^{\mathrm{b}}) - \underline{\boldsymbol{D}}_+ \underline{\boldsymbol{\lambda}} = \underline{\boldsymbol{0}} \tag{3.149b}$$
{eq:3-1683b

$$\underline{\boldsymbol{f}}_-^{\mathrm{b}}(\underline{\boldsymbol{u}}^{\mathrm{i}}, \underline{\boldsymbol{u}}_+^{\mathrm{b}}, \underline{\boldsymbol{u}}_-^{\mathrm{b}}) + \underline{\boldsymbol{D}}_- \underline{\boldsymbol{\lambda}} = \underline{\boldsymbol{0}} \tag{3.149c}$$
{eq:3-168c

$$\underline{\boldsymbol{D}}_+^{\mathrm{T}} \underline{\boldsymbol{u}}_+^{\mathrm{b}} - \underline{\boldsymbol{D}}_-^{\mathrm{T}} \underline{\boldsymbol{u}}_-^{\mathrm{b}} = \left[\underline{\boldsymbol{D}}_+^{\mathrm{T}} \underline{\hat{\boldsymbol{u}}}_+^{\mathrm{M,b}} - \underline{\boldsymbol{D}}_-^{\mathrm{T}} \underline{\hat{\boldsymbol{u}}}_-^{\mathrm{M,b}}\right] \underline{\bar{\boldsymbol{H}}} \tag{3.149d}$$
{eq:3-168d

A periodic FE-mesh is characterized by the identity $\underline{\boldsymbol{D}}_+ = \underline{\boldsymbol{D}}_-$, which is inserted in (**??**) to give the equation

$$\underline{\boldsymbol{D}}_+^{\mathrm{T}} \left[\underline{\boldsymbol{u}}_+^{\mathrm{b}} - \underline{\boldsymbol{u}}_-^{\mathrm{b}}\right] = \underline{\boldsymbol{D}}_+^{\mathrm{T}} \left[\underline{\hat{\boldsymbol{u}}}_+^{\mathrm{M,b}} - \underline{\hat{\boldsymbol{u}}}_-^{\mathrm{M,b}}\right] \underline{\bar{\boldsymbol{H}}} \tag{3.150}$$
{eq:3-169}

If $\underline{\boldsymbol{D}}_+$ is non-singular, a possible solution to (**??**) is

$$\underline{\boldsymbol{u}}_+^{\mathrm{b}} - \underline{\boldsymbol{u}}_-^{\mathrm{b}} = \left[\underline{\hat{\boldsymbol{u}}}_+^{\mathrm{M,b}} - \underline{\hat{\boldsymbol{u}}}_-^{\mathrm{M,b}}\right] \underline{\bar{\boldsymbol{H}}} \quad \text{or} \quad \underline{\boldsymbol{u}}_+^{\mathrm{s,b}} = \underline{\boldsymbol{u}}_-^{\mathrm{s,b}} \overset{\mathrm{def}}{=} \underline{\boldsymbol{u}}^{\mathrm{s,b}} \tag{3.151}$$
{eq:3-171}

which is the classical condition of strong periodicity. Finally, adding the equations (**??**) and (**??**) while using (**??**), we obtain the reduced set of equations {eq:3-172}

$$\underline{\boldsymbol{f}}^{\mathrm{i}}(\underline{\boldsymbol{u}}^{\mathrm{i}}, \underline{\boldsymbol{u}}^{\mathrm{b}}) = \underline{\boldsymbol{0}} \tag{3.152a}$$
{eq:3-172a

$$\underline{\boldsymbol{f}}_{\pm}^{\mathrm{b}}(\underline{\boldsymbol{u}}^{\mathrm{i}}, \underline{\boldsymbol{u}}^{\mathrm{b}}) = \underline{\boldsymbol{0}} \quad \text{with} \quad \underline{\boldsymbol{f}}_{\pm}^{\mathrm{b}} \overset{\mathrm{def}}{=} \underline{\boldsymbol{f}}_+^{\mathrm{b}} + \underline{\boldsymbol{f}}_-^{\mathrm{b}} \tag{3.152b}$$
{eq:3-172b

It appears that there is no need to solve for $\underline{\boldsymbol{\lambda}}$ when this reduced system is adopted.

3.5.7 WPBC-problem for macroscale stress control

Find $\boldsymbol{u} \in \mathbb{U}_\square$, $\boldsymbol{\lambda} \in \mathbb{T}_\square^+$ and $\bar{\boldsymbol{\epsilon}} \in \mathbb{R}^{3\times3}_{\text{sym}}$ that, for given value of the macroscale stress $\bar{\boldsymbol{\sigma}}$, solve the system {eq:3-173}

$$\langle \boldsymbol{\epsilon}[\boldsymbol{u}] : \mathsf{E} : \boldsymbol{\epsilon}[\delta \boldsymbol{u}] \rangle_\square - d_\square(\boldsymbol{\lambda}, \delta \boldsymbol{u}) = 0 \qquad \forall \delta \boldsymbol{u} \in \mathbb{U}_\square, \tag{3.153a}$$
{eq:3-173a}

$$-d_\square(\delta \boldsymbol{\lambda}, \boldsymbol{u}) + d_\square(\delta \boldsymbol{\lambda}, \bar{\boldsymbol{\epsilon}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}]) = 0 \qquad \forall \delta \boldsymbol{\lambda} \in \mathbb{T}_\square^+ \tag{3.153b}$$
{eq:3-173b}

$$d_\square(\boldsymbol{\lambda}, \delta \bar{\boldsymbol{\epsilon}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}]) = \bar{\boldsymbol{\sigma}} : \delta \bar{\boldsymbol{\epsilon}} \qquad \forall \delta \bar{\boldsymbol{\epsilon}} \in \mathbb{R}^{3\times3}_{\text{sym}} \tag{3.153c}$$
{eq:3-173c}

Chapter 4

EFFECTIVE PROPERTIES – LINEAR ELASTICITY – BOUNDS FROM VIRTUAL TESTING

{Bounds fro

4.1 Introduction

We consider the situation that we want to model the microstructure in order to estimate the macroscopic response without concurrently solving a macroscopic problem. The goal could, for instance, be to estimate material parameters related to an assumed (empirical) model on the macroscale[1] In that sense, the microscale problem replaces a physical experiment, motivating the notion of "virtual testing".

Adopting first order homogenization, as described in previous Chapters, we conclude the following:

- For *periodic microstructures*, periodic boundary conditions will allow for setting up a finite size RVE defining the effective properties.
- For *random microstructures*, the RVE is not finite, and has to replaced by Statical Volume Elements (SVE) of finite size.

This Chapter presents a methodology for estimating the effective properties of random media using statistical techniques for sampling SVEs with suitable boundary conditions.

4.2 Bounds on apparent stiffness and compliance tensors for a single SVE-realization

4.2.1 Preliminaries

The strategy for deriving bounds on the apparent macroscale stiffness tensor $\bar{\mathbf{E}}_\square$ for any given SVE-realization hinges on the following "building blocks":

[1] The most straight forward application is estimating effective elastic properties in the linear setting.

- Utilize the WPPC-problem and its properties as the "work-horse" for the analysis.
- Establish the SVE-potentials $\Pi_\square^{\mathrm{WP}}$ and $\Pi_\square^{*\mathrm{WP}}$ for macroscale strain and stress control, respectively. The stationarity conditions of these potentials will be identified as those given in 3.123 and 3.160, respectively.
- Identify the macroscale strain energy and the stress energy, respectively, from the stationary value of $\Pi_\square^{\mathrm{WP}}$ and $\Pi_\square^{*\mathrm{WP}}$ for prescribed $\bar{\boldsymbol{\epsilon}}$ and $\bar{\boldsymbol{\sigma}}$, respectively.
- Establish the hierarchy of solution spaces for displacements $\boldsymbol{u}$ and tractions $\boldsymbol{\lambda}$, and use the min-max properties of the SVE-potentials to bound the energy values.

4.2.2 Macroscale strain energy associated with the WPBC-problem

For the considered SVE, we introduce the SVE-functional

{eq:3-174}
$$\Psi_\square(\hat{\boldsymbol{u}}) \overset{\text{def}}{=} \langle \psi(\boldsymbol{\epsilon}[\hat{\boldsymbol{u}}])\rangle_\square = \frac{1}{2}\langle \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}] : \mathbf{E} : \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}]\rangle_\square \tag{4.1}$$

We also introduce the Hellinger-Reissner type of SVE-potential

{eq:3-175}
$$\Pi_\square^{\mathrm{WP}}(\bar{\boldsymbol{\epsilon}}; \hat{\boldsymbol{u}}, \hat{\boldsymbol{\lambda}}) \overset{\text{def}}{=} \Psi_\square(\hat{\boldsymbol{u}}) - d_\square(\hat{\boldsymbol{\lambda}}, \hat{\boldsymbol{u}} - \bar{\boldsymbol{\epsilon}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}]) \tag{4.2}$$

Now, consider the saddle-point (min-max in the present case) problem with solution $(\boldsymbol{u}\{\bar{\boldsymbol{\epsilon}}\}, \boldsymbol{\lambda}\{\bar{\boldsymbol{\epsilon}}\})$

{eq:3-176}
$$(\boldsymbol{u}, \boldsymbol{\lambda}) = \arg\left[\min_{\hat{\boldsymbol{u}}\in\mathbb{U}_\square} \max_{\hat{\boldsymbol{\lambda}}\in\mathbb{T}_\square^+} \Pi_\square^{\mathrm{WP}}(\bar{\boldsymbol{\epsilon}}; \hat{\boldsymbol{u}}, \hat{\boldsymbol{\lambda}})\right] \tag{4.3}$$

{eq:3-177} whose corresponding stationarity conditions are

{eq:3-177a}
$$(\Pi_\square^{\mathrm{WP}})'_u(\bar{\boldsymbol{\epsilon}}; \boldsymbol{u}, \boldsymbol{\lambda}; \delta\boldsymbol{u}) = \langle \boldsymbol{\epsilon}[\boldsymbol{u}] : \mathbf{E} : \boldsymbol{\epsilon}[\delta\boldsymbol{u}]\rangle_\square - d_\square(\boldsymbol{\lambda}, \delta\boldsymbol{u}) = 0 \quad \forall \delta\boldsymbol{u} \in \mathbb{U}_\square \tag{4.4a}$$

{eq:3-177b}
$$(\Pi_\square^{\mathrm{WP}})'_\lambda(\bar{\boldsymbol{\epsilon}}; \boldsymbol{u}, \boldsymbol{\lambda}; \delta\boldsymbol{\lambda}) = -d_\square(\delta\boldsymbol{\lambda}, \boldsymbol{u} - \bar{\boldsymbol{\epsilon}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}]) = 0 \quad \forall \delta\boldsymbol{\lambda} \in \mathbb{T}_\square^+ \tag{4.4b}$$

Indeed, these conditions are precisely those given in 3.123??.

Next, we note that, upon setting $\delta\boldsymbol{\lambda} = \boldsymbol{\lambda}\{\bar{\boldsymbol{\epsilon}}\}$ in 3.123b, we obtain

{eq:3-178}
$$d_\square(\boldsymbol{\lambda}\{\bar{\boldsymbol{\epsilon}}\}, \boldsymbol{u}\{\bar{\boldsymbol{\epsilon}}\} - \bar{\boldsymbol{\epsilon}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}]) = 0 \tag{4.5}$$

The value of $\Pi_\square^{\mathrm{WP}}$ at the saddle-point value is identical to the macroscale (volume-specific) strain energy density $\bar{\psi}_\square^{\mathrm{WP}}\{\bar{\boldsymbol{\epsilon}}\}$,

{eq:3-179}
$$\begin{aligned}\bar{\psi}_\square^{\mathrm{WP}}\{\bar{\boldsymbol{\epsilon}}\} &\overset{\text{def}}{=} \Pi_\square^{\mathrm{WP}}(\bar{\boldsymbol{\epsilon}}; \boldsymbol{u}\{\bar{\boldsymbol{\epsilon}}\}, \boldsymbol{\lambda}\{\bar{\boldsymbol{\epsilon}}\}) = \Psi_\square(\boldsymbol{u}\{\bar{\boldsymbol{\epsilon}}\}) \\ &= \frac{1}{2}\langle \boldsymbol{\epsilon}[\boldsymbol{u}\{\bar{\boldsymbol{\epsilon}}\}] : \mathbf{E} : \boldsymbol{\epsilon}[\boldsymbol{u}\{\bar{\boldsymbol{\epsilon}}\}]\rangle_\square = \frac{1}{2}\bar{\boldsymbol{\epsilon}} : \mathbf{E}_\square^{\mathrm{WP}} : \bar{\boldsymbol{\epsilon}}\end{aligned} \tag{4.6}$$

where the result in (**??**) was used. Moreover, $\bar{\psi}_\square^{\mathrm{WP}}\{\bar{\boldsymbol{\epsilon}}\}$ is a potential for $\bar{\boldsymbol{\sigma}}$ in the classical sense, i.e. $\bar{\boldsymbol{\sigma}}$ can be obtained as

{eq:3-181}
$$\bar{\boldsymbol{\sigma}}\{\bar{\boldsymbol{\epsilon}}\} = \frac{\mathrm{d}\bar{\psi}_\square^{\mathrm{WP}}\{\bar{\boldsymbol{\epsilon}}\}}{\mathrm{d}\bar{\boldsymbol{\epsilon}}} = \bar{\mathbf{E}}_\square^{\mathrm{WP}} : \bar{\boldsymbol{\epsilon}} \tag{4.7}$$

which follows directly from (**??**).

4.2.3 Macroscale stress energy associated with the WPBC-problem

Introduce the SVE-potential

{eq:3-183}
$$\Pi^{*\mathrm{WP}}_{\square}(\bar{\boldsymbol{\sigma}};\hat{\boldsymbol{u}},\hat{\boldsymbol{\lambda}},\hat{\bar{\boldsymbol{\epsilon}}}) \overset{\mathrm{def}}{=} -\Psi_{\square}(\hat{\boldsymbol{u}}) + d_{\square}(\hat{\boldsymbol{\lambda}},\hat{\boldsymbol{u}} - \hat{\bar{\boldsymbol{\epsilon}}}\cdot[\boldsymbol{x}-\bar{\boldsymbol{x}}]) + \bar{\boldsymbol{\sigma}} : \hat{\bar{\boldsymbol{\epsilon}}} \tag{4.8}$$

Now, consider the saddle-point (min-max in the present case) problem with solution $(\boldsymbol{u}\{\bar{\boldsymbol{\sigma}}\},\boldsymbol{\lambda}\{\bar{\boldsymbol{\sigma}}\},\bar{\boldsymbol{\epsilon}}\{\bar{\boldsymbol{\sigma}}\})$

$$(\boldsymbol{u},\boldsymbol{\lambda},\bar{\boldsymbol{\epsilon}}) = \arg\left[\max_{\hat{\boldsymbol{u}}\in\mathbb{U}_{\square}}\ \min_{\hat{\boldsymbol{\lambda}}\in\mathbb{T}^{+}_{\square}}\ \min_{\hat{\bar{\boldsymbol{\epsilon}}}\in\mathbb{R}^{3\times3}_{\mathrm{sym}}} \Pi^{*\mathrm{WP}}_{\square}(\bar{\boldsymbol{\sigma}};\hat{\boldsymbol{u}},\hat{\boldsymbol{\lambda}},\hat{\bar{\boldsymbol{\epsilon}}})\right] \tag{4.9}$$ {eq:3-184}

whose corresponding stationarity conditions are {eq:3-185}

$$(\Pi^{*\mathrm{WP}}_{\square})'_{u}(\bar{\boldsymbol{\sigma}};\boldsymbol{u},\boldsymbol{\lambda},\bar{\boldsymbol{\epsilon}};\delta\boldsymbol{u}) = -\langle\boldsymbol{\epsilon}[\boldsymbol{u}] : \mathbf{E} : \boldsymbol{\epsilon}[\delta\boldsymbol{u}]\rangle_{\square} + d_{\square}(\boldsymbol{\lambda},\delta\boldsymbol{u}) = 0 \quad \forall\delta\boldsymbol{u}\in\mathbb{U}_{\square} \tag{4.10a}$$ {eq:3-185a}

$$(\Pi^{*\mathrm{WP}}_{\square})'_{\lambda}(\bar{\boldsymbol{\sigma}};\boldsymbol{u},\boldsymbol{\lambda},\bar{\boldsymbol{\epsilon}};\delta\boldsymbol{\lambda}) = d_{\square}(\delta\boldsymbol{\lambda},\boldsymbol{u}-\bar{\boldsymbol{\epsilon}}\cdot[\boldsymbol{x}-\bar{\boldsymbol{x}}]) = 0 \quad \forall\delta\boldsymbol{\lambda}\in\mathbb{T}^{+}_{\square} \tag{4.10b}$$ {eq:3-185b}

$$(\Pi^{*\mathrm{WP}}_{\square})'_{\bar{\epsilon}}(\bar{\boldsymbol{\sigma}};\boldsymbol{u},\boldsymbol{\lambda},\bar{\boldsymbol{\epsilon}};\delta\bar{\boldsymbol{\epsilon}}) = -d_{\square}(\boldsymbol{\lambda},\delta\bar{\boldsymbol{\epsilon}}\cdot[\boldsymbol{x}-\bar{\boldsymbol{x}}]) + \bar{\boldsymbol{\sigma}} : \delta\bar{\boldsymbol{\epsilon}} = 0 \quad \forall\delta\bar{\boldsymbol{\epsilon}}\in\mathbb{R}^{3\times3}_{\mathrm{sym}} \tag{4.10c}$$ {eq:3-185c}

Indeed, these conditions are precisely those given in 3.160??.

Next, we note that, upon setting $\delta\boldsymbol{\lambda} = \boldsymbol{\lambda}\{\bar{\boldsymbol{\sigma}}\}$ in 3.160b, we obtain (in this case as well)

$$d_{\square}(\boldsymbol{\lambda}\{\bar{\boldsymbol{\epsilon}}\},\boldsymbol{u}\{\bar{\boldsymbol{\epsilon}}\} - \bar{\boldsymbol{\epsilon}}\cdot[\boldsymbol{x}-\bar{\boldsymbol{x}}]) = 0 \tag{4.11}$$ {eq:3-186}

The value of $\Pi^{*\mathrm{WP}}_{\square}$ at the saddle-point value is identical to the macroscale (volume-specific) stress energy density $\bar{\psi}^{*\mathrm{WP}}_{\square}\{\bar{\boldsymbol{\sigma}}\}$,

$$\begin{aligned}
\bar{\psi}^{*\mathrm{WP}}_{\square}\{\bar{\boldsymbol{\sigma}}\} &\overset{\mathrm{def}}{=} \Pi^{*\mathrm{WP}}_{\square}(\bar{\boldsymbol{\sigma}};\boldsymbol{u}\{\bar{\boldsymbol{\sigma}}\},\boldsymbol{\lambda}\{\bar{\boldsymbol{\sigma}}\},\bar{\boldsymbol{\epsilon}}\{\bar{\boldsymbol{\sigma}}\}) = -\Psi_{\square}(\boldsymbol{u}\{\bar{\boldsymbol{\sigma}}\}) + \bar{\boldsymbol{\sigma}} : \bar{\boldsymbol{\epsilon}}\{\bar{\boldsymbol{\sigma}}\} \\
&= -\frac{1}{2}\langle\boldsymbol{\epsilon}[\boldsymbol{u}\{\boldsymbol{\sigma}\}] : \mathbf{E} : \boldsymbol{\epsilon}[\boldsymbol{u}\{\boldsymbol{\sigma}\}]\rangle_{\square} + \bar{\boldsymbol{\sigma}} : \mathbf{C}^{\mathrm{WP}}_{\square} : \bar{\boldsymbol{\sigma}} \\
&= \frac{1}{2}\bar{\boldsymbol{\sigma}} : \mathbf{C}^{\mathrm{WP}}_{\square} : \bar{\boldsymbol{\sigma}}
\end{aligned} \tag{4.12}$$ {eq:3-187}

where the result in (**??**) was used. Moreover, $\bar{\psi}^{*\mathrm{WP}}_{\square}\{\bar{\boldsymbol{\sigma}}\}$ is a potential for $\bar{\boldsymbol{\epsilon}}$ in the classical sense, i.e. $\bar{\boldsymbol{\epsilon}}$ can be obtained as

$$\bar{\boldsymbol{\epsilon}}\{\bar{\boldsymbol{\sigma}}\} = \frac{\mathrm{d}\bar{\psi}^{*\mathrm{WP}}_{\square}\{\bar{\boldsymbol{\sigma}}\}}{\mathrm{d}\bar{\boldsymbol{\sigma}}} = \bar{\mathbf{C}}^{\mathrm{WP}}_{\square} : \bar{\boldsymbol{\sigma}}. \tag{4.13}$$ {eq:3-188}

where, once again, we note that $\bar{\mathbf{C}}^{\mathrm{WP}}_{\square} = \left[\bar{\mathbf{E}}^{\mathrm{WP}}_{\square}\right]^{-1}$.

Show as homework. Hint: **?????**

4.2.4 Bounds on macroscale stiffness and compliance tensors

It is possible to establish bounds on $\bar{\psi}^{\mathrm{WP}}_{\square}$ and $\bar{\psi}^{*\mathrm{WP}}_{\square}$ based on the particular restrictions of the solution spaces, i.e. subspaces of $\mathbb{U}_{\square}$ and $\mathbb{T}^{+}_{\square}$ that are pertinent to the various prolongation conditions discussed in this Chapter.

$$\begin{array}{ccccccccc}
 & & & & \mathbb{U}^{\mathrm{N}}_{\square}[=\mathbb{U}_{\square}] & = & \mathbb{U}^{\mathrm{WP}}_{\square}[=\mathbb{U}_{\square}] & \supseteq & \mathbb{U}^{\mathrm{SP}}_{\square} \supseteq \mathbb{U}^{\mathrm{D}}_{\square} \supseteq \mathbb{U}^{\mathrm{V}}_{\square} \\
\mathbb{T}^{\mathrm{V}}_{\square}[=\mathbb{T}^{+}_{\square}] & = & \mathbb{T}^{\mathrm{D}}_{\square}[=\mathbb{T}^{+}_{\square}] & \supseteq & \mathbb{T}^{\mathrm{SP}}_{\square}[=\mathbb{T}^{+}_{\square}] & \supseteq & \mathbb{T}^{\mathrm{WP}}_{\square} & \supseteq & \mathbb{T}^{\mathrm{N}}_{\square}
\end{array} \tag{4.14}$$ {eq:3-189}

$$\begin{array}{ccccccccc} & & \bar{\psi}^{\mathrm{N}}_{\square}\{\bar{\boldsymbol{\epsilon}}\} & \leq & \bar{\psi}^{\mathrm{WP}}_{\square}\{\bar{\boldsymbol{\epsilon}}\} & \leq & \bar{\psi}^{\mathrm{SP}}_{\square}\{\bar{\boldsymbol{\epsilon}}\} & \leq & \bar{\psi}^{\mathrm{D}}_{\square}\{\bar{\boldsymbol{\epsilon}}\} \leq \bar{\psi}^{\mathrm{V}}_{\square}\{\bar{\boldsymbol{\epsilon}}\} \\ \bar{\psi}^{*\mathrm{V}}_{\square}\{\bar{\boldsymbol{\sigma}}\} & \leq & \bar{\psi}^{*\mathrm{D}}_{\square}\{\bar{\boldsymbol{\sigma}}\} \leq \bar{\psi}^{*\mathrm{SP}}_{\square}\{\bar{\boldsymbol{\sigma}}\} & \leq & \bar{\psi}^{*\mathrm{WP}}_{\square}\{\bar{\boldsymbol{\sigma}}\} & \leq & \bar{\psi}^{*\mathrm{N}}_{\square}\{\bar{\boldsymbol{\sigma}}\} & & \end{array} \tag{4.15}$$ {eq:3-191}

Completed bounds: The Reuss bound is missing above, since it is based on a stress space that is not a subset of $\mathbb{T}^{\mathrm{N}}_{\square}$. However, in accordance with the analysis of Voigt-Reuss bounds in Chapter 2, it is concluded that

{eq:3-192}
$$0 \leq \bar{\boldsymbol{\sigma}} : \left[\bar{\mathsf{C}}^{\mathrm{R}}_{\square} - \bar{\mathsf{C}}_{\square}\right] : \bar{\boldsymbol{\sigma}} = \bar{\boldsymbol{\sigma}} : \left[[\bar{\mathsf{E}}^{\mathrm{R}}_{\square}]^{-1} - [\bar{\mathsf{E}}_{\square}]^{-1}\right] : \bar{\boldsymbol{\sigma}} \tag{4.16}$$

where $\bar{\mathsf{C}}_{\square}$ does, in fact, represent the apparent compliance for any choice of stress field as long as the H-M condition is satisfied. In particular, we may choose $\bar{\mathsf{C}}_{\square} = \bar{\mathsf{C}}^{\mathrm{N}}_{\square}$, whereby we conclude that

{eq:3-193}
$$\bar{\boldsymbol{\sigma}} : \bar{\mathsf{C}}^{\mathrm{R}}_{\square} : \bar{\boldsymbol{\sigma}} \geq \bar{\boldsymbol{\sigma}} : \bar{\mathsf{C}}^{\mathrm{N}}_{\square} : \bar{\boldsymbol{\sigma}} \quad \text{and} \quad \bar{\boldsymbol{\epsilon}} : \bar{\mathsf{E}}^{\mathrm{N}}_{\square} : \bar{\boldsymbol{\epsilon}} \geq \bar{\boldsymbol{\epsilon}} : \bar{\mathsf{E}}^{\mathrm{R}}_{\square} : \bar{\boldsymbol{\epsilon}} \tag{4.17}$$

where $\bar{\boldsymbol{\epsilon}}$ and $\bar{\boldsymbol{\sigma}}$ are related via ????????.

In conclusion, we give the completed bounds:

$$\begin{array}{ccccccccccc} & & \bar{\psi}^{\mathrm{R}}_{\square}\{\bar{\boldsymbol{\epsilon}}\} & \leq & \bar{\psi}^{\mathrm{N}}_{\square}\{\bar{\boldsymbol{\epsilon}}\} & \leq & \bar{\psi}^{\mathrm{WP}}_{\square}\{\bar{\boldsymbol{\epsilon}}\} & \leq & \bar{\psi}^{\mathrm{SP}}_{\square}\{\bar{\boldsymbol{\epsilon}}\} & \leq & \bar{\psi}^{\mathrm{D}}_{\square}\{\bar{\boldsymbol{\epsilon}}\} \leq \bar{\psi}^{\mathrm{V}}_{\square}\{\bar{\boldsymbol{\epsilon}}\} \\ \bar{\psi}^{*\mathrm{V}}_{\square}\{\bar{\boldsymbol{\sigma}}\} & \leq & \bar{\psi}^{*\mathrm{D}}_{\square}\{\bar{\boldsymbol{\sigma}}\} & \leq & \bar{\psi}^{*\mathrm{SP}}_{\square}\{\bar{\boldsymbol{\sigma}}\} & \leq & \bar{\psi}^{*\mathrm{WP}}_{\square}\{\bar{\boldsymbol{\sigma}}\} & \leq & \bar{\psi}^{*\mathrm{N}}_{\square}\{\bar{\boldsymbol{\sigma}}\} & \leq & \bar{\psi}^{*\mathrm{R}}_{\square}\{\bar{\boldsymbol{\sigma}}\} \end{array} \tag{4.18}$$ {eq:3-194}

Equivalently, we may write the inequalities for the strain energies in terms of eigenvalues of the corresponding (constant) stiffness tensors:

{eq:3-195}
$$\bar{\mathsf{E}}^{\mathrm{R}}_{\square} \leq \bar{\mathsf{E}}^{\mathrm{N}}_{\square} \leq \bar{\mathsf{E}}^{\mathrm{WP}}_{\square} \leq \bar{\mathsf{E}}^{\mathrm{SP}}_{\square} \leq \bar{\mathsf{E}}^{\mathrm{D}}_{\square} \leq \bar{\mathsf{E}}^{\mathrm{V}}_{\square} \tag{4.19}$$

It is clear that the corresponding inequalities for the compliance tensors can be established.

4.3 Virtual Statistical Testing

4.3.1 Computational strategy - Preliminaries

In the previous Section we considered an RVE which has to be "sufficiently large" in order to give representative results. By "representative" we thus mean that the solution is independent of (i) the considered (single) realization of the random microhetereogenous material structure and (ii) the choice of boundary conditions, as long as the Hill-Mandel condition is satisfied. However, in practice, it is convenient to adopt a strategy based on "domain decomposition" and "ergodicity", cf. Haznov & Huet (1995), Zohdi & Wriggers (2005) or Ostoja (2007) , whereby computations are carried out on Statistical Volume Elements (SVE) that occupy subdomains of the RVE. In particular, this strategy is useful for computing upper and lower bounds on the effective energy $\bar{\psi}\{\bar{\boldsymbol{\epsilon}}\}$. We thus outline the strategy as follows:

1. Decompose the RVE into K (which is large) non-overlapping domains $\Omega_{\square,i}$ of equal size, with boundaries $\Gamma_{\square,i}$, as shown in Figure 4.1, whereby each $\Omega_{\square,i}$ is occupied by an SVE, for any given realization. It should be noted that, while the RVE is assumed to possess a periodic microstructure, the SVEs do not posses such periodicity, in general. The "skeleton" of $\Omega_{\square}$, i.e. the union of all surfaces of the SVEs that are not part of the RVE-boundary, is denoted $\Gamma^{\mathrm{int}}_{\square}$.

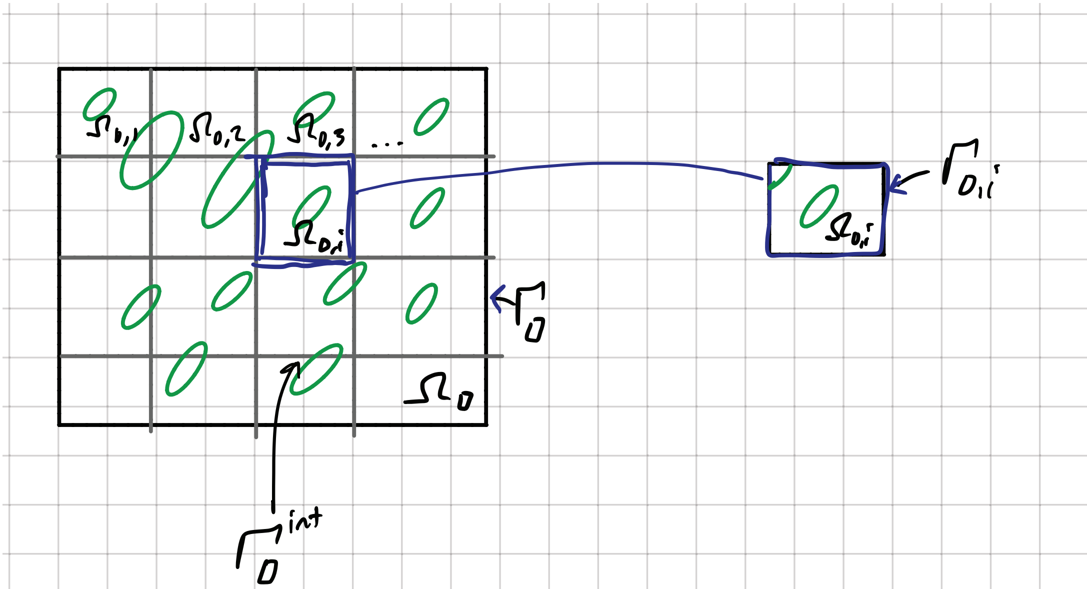


Figure 4.1: (a) A (large) RVE, occupying the domain $\Omega_\square$, cut into a (large) number of SVEs of the same size. The set of inner boundaries of the SVEs is denoted as $\Gamma_\square^{\text{int}}$ (b) A single SVE occupying the domain $\Omega_{\square,i}$ with boundary $\Gamma_{\square,i}$. {fig:4-1}

2. Replace the original RVE-problem by a "relaxed problem" by allowing the fields to be discontinuous across the SVE-boundaries. A corresponding incremental potential $\tilde{\Pi}_\square$ can be forumlated (assuming a valid potential $\Pi_\square$ for the original problem without discontinuities). Most importantly, the value of the effective energy that is obtained at the stationary point of $\tilde{\Pi}_\square$ is shown to be identical to $\bar{\psi}$.

3. Obtain upper and lower bounds on $\bar{\psi}\{\bar{\boldsymbol{\epsilon}}\}$ and $\bar{\psi}^*\{\bar{\boldsymbol{\sigma}}\}$ by suitable restriction of the pertinent function spaces on which the stationary point of $\tilde{\Pi}_\square$ is defined. As it turns out, these restrictions correspond to Dirichlet and Neumann boundary conditions. Depending on whether $\tilde{\Pi}_\square$ is minimized or maximized on the restricted function space, the resulting value at the stationary point represents an upper or lower bound, respectively. Furthermore, the restricted function spaces are constructed in such a fashion that it becomes possible to solve completely uncoupled SVE-problems (on each subdomain $\Omega_{\square,i}$).

4. Use an ergodicity argument to conclude that the bounds on $\bar{\psi}\{\bar{\boldsymbol{\epsilon}}\}$ and $\bar{\psi}^*\{\bar{\boldsymbol{\sigma}}\}$ can be computed as the mean value for sufficiently many random realizations of a given SVE-domain.

4.3.2 Decomposition of RVE

With a view towards decoupling the SVEs from each other, we now introduce the "trick" of relaxing the requirements on continuity along the inter-domain boundaries, via the "broken spaces" {eq:4-1}

$$\tilde{\mathbb{U}}_\square = \{\hat{\boldsymbol{u}} \in \mathbb{L}_2(\Omega_\square)^3,\ \hat{\boldsymbol{u}}|_{\Omega_{\square,i}} \in \mathbb{H}^1(\Omega_{\square,i})^3,\ \text{ for } i = 1,\dots,K\} \tag{4.20a}$$ {eq:4-1a}

$$\tilde{\mathbb{L}}_\square = \{\hat{\boldsymbol{\lambda}} \in \mathbb{L}_2(\Gamma_\square^{\text{int}} \cup \Gamma_{\square,i}^{+})^3,\ i = 1,\dots,K\} \tag{4.20b}$$ {eq:4-1b}

The displacements in $\tilde{\mathbb{U}}_\square$ may thus be discontinuous across the SVE-boundaries inside the RVE. We may generalize the definition of the jump symbol $[\![\bullet]\!]_\square$ as follows:

$$[\![\bullet]\!]_\square(\boldsymbol{x}) \overset{\text{def}}{=} \begin{cases} \lim_{\epsilon\to 0} \bullet(\boldsymbol{x}+\epsilon\boldsymbol{n}) - \bullet(\boldsymbol{x}-\epsilon\boldsymbol{n}), & \boldsymbol{x}\in\Gamma_\square^{\text{int}} \\ \bullet(\boldsymbol{x}) - \bullet(\boldsymbol{\varphi}_{\text{per}}(\boldsymbol{x})), & \boldsymbol{x}\in\Gamma_\square^{+} \end{cases} \tag{4.21}$$ {eq:4-2}

where we introduced the normal $\boldsymbol{n}$ on each positive boundary $\Gamma^+_{\square,i}$.

By introducing "relaxed" version of the of the form $d_\square$ as follows:

{eq:4-3} $$\tilde{d}_\square(\boldsymbol{\lambda},\boldsymbol{u}) \overset{\text{def}}{=} \frac{1}{K}\frac{1}{|\Omega_\square|}\int_{\Gamma_\square^+\cup\Gamma_\square^{\text{int}}} \boldsymbol{\lambda}\cdot[\![\boldsymbol{u}]\!]_\square \,\mathrm{d}S, \tag{4.22}$$

we may rephrase the micro-periodicity conditions in xxx by the weaker constraint condition

{eq:4-4} $$\tilde{d}_\square(\delta\boldsymbol{\lambda},\boldsymbol{u}-\boldsymbol{u}^{\mathrm{M}}(\bar{\boldsymbol{\epsilon}})) = 0, \quad \forall\delta\boldsymbol{\lambda}\in\tilde{\mathbb{L}}_\square, \tag{4.23}$$

4.4 Nonlinear material model – Bounds on effective strain energy

4.4.1 Preliminaries

4.4.2 Macroscale strain control – Canonical format of decomposed RVE-problem

We are now in the position to define the relaxed SVE-functional as

{eq:4-10} $$\tilde{\Pi}_\square(\bar{\boldsymbol{\epsilon}};\boldsymbol{u},\boldsymbol{\lambda}) = \frac{1}{K}\sum_{i=1}^{K}\Psi_{\square,i}(\boldsymbol{u}) - \tilde{d}_\square(\boldsymbol{\lambda},\boldsymbol{u}-\boldsymbol{u}^{\mathrm{M}}(\bar{\boldsymbol{\epsilon}})) \tag{4.24}$$

where

{eq:4-11} $$\Psi_{\square,i}(\boldsymbol{u}) := \langle\psi(\boldsymbol{\epsilon}[\boldsymbol{u}])\rangle_{\square,i}. \tag{4.25}$$

The RVE-problem in, e.g., eq521b is then replaced by: For given value of the macroscale strain $\bar{\boldsymbol{\epsilon}}$, find $(\tilde{\boldsymbol{u}},\tilde{\boldsymbol{\lambda}})\in\tilde{\mathbb{U}}_\square\times\tilde{\mathbb{L}}_\square$ such that

{eq:4-12} $$(\tilde{\boldsymbol{u}},\tilde{\boldsymbol{\lambda}}) = \arg\left\{\min_{\hat{\boldsymbol{u}}\in\tilde{\mathbb{U}}_\square}\max_{\hat{\boldsymbol{\lambda}}\in\tilde{\mathbb{L}}_\square}\tilde{\Pi}_\square(\bar{\boldsymbol{\epsilon}};\hat{\boldsymbol{u}},\hat{\boldsymbol{\lambda}})\right\} \tag{4.26}$$

It should be noticed that the solution depends implicitly on the "control" variable $\bar{\boldsymbol{\epsilon}}$. Upon using (4.26), we conclude that the stationarity solution satisfies the conditions

{eq:4-13} $$\tilde{d}_\square(\tilde{\boldsymbol{\lambda}}\{\bar{\boldsymbol{\epsilon}}\},\tilde{\boldsymbol{u}}\{\bar{\boldsymbol{\epsilon}}\}-\boldsymbol{u}^{\mathrm{M}}(\bar{\boldsymbol{\epsilon}})) = 0. \tag{4.27}$$

The stationary point thus takes the value

{eq:4-14} $$\tilde{\tilde{\psi}}_\square\{\bar{\boldsymbol{\epsilon}}\} := \tilde{\Pi}_\square(\bar{\boldsymbol{\epsilon}};\tilde{\boldsymbol{u}}\{\bar{\boldsymbol{\epsilon}}\},\tilde{\boldsymbol{\lambda}}\{\bar{\boldsymbol{\epsilon}}\}) = \frac{1}{K}\sum_{i=1}^{K}\Psi_{\square,i}(\tilde{\boldsymbol{u}}\{\bar{\boldsymbol{\epsilon}}\}), \tag{4.28}$$

We make the important observation that $\tilde{\Pi}_\square(\bar{\boldsymbol{\epsilon}};\tilde{\boldsymbol{u}}\{\bar{\boldsymbol{\epsilon}}\},\tilde{\boldsymbol{\lambda}}\{\bar{\boldsymbol{\epsilon}}\}) = \Pi_\square(\bar{\boldsymbol{\epsilon}};\tilde{\boldsymbol{u}}\{\bar{\boldsymbol{\epsilon}}\},\tilde{\boldsymbol{\lambda}}\{\bar{\boldsymbol{\epsilon}}\})$, which identity follows since $\tilde{\Pi}_\square$ is invariant to rigid body translation. We thus conclude that

{eq:4-15}
$$\bar{\psi}_\square\{\bar{\boldsymbol{\epsilon}}\} = \tilde{\bar{\psi}}_\square\{\bar{\boldsymbol{\epsilon}}\} = \frac{1}{K}\sum_{i=1}^{K}\Psi_{\square,i}(\tilde{u}\{\bar{\boldsymbol{\epsilon}}\}). \tag{4.29}$$

Finally, we consider $\bar{\psi}_\square\{\bar{\boldsymbol{\epsilon}},\omega\} : \omega \to \mathbb{R}$ as a stochastic process for given $\bar{\boldsymbol{\epsilon}}$ and given RVE-realization, ω, of the microstructure within $\Omega_\square$[2], whereby we define the effective energy as the limit

$$\bar{\psi}\{\bar{\boldsymbol{\epsilon}}\} = \lim_{|\Omega_\square|\to\infty}\bar{\psi}_\square\{\bar{\boldsymbol{\epsilon}},\omega\} \tag{4.30}$$ {eq:4-16}

Our aim is now to bound $\bar{\psi}$ by restricting the appropriate function space(s). Depending on whether the field corresponding to the function space is minimized or maximized when solving (4.26), a restriction of that function space will bound $\bar{\psi}$ from above or from below, respectively.

4.4.3 Upper bound on effective (incremental) strain energy

An upper bound of $\bar{\psi}$ may be found by restricting the function space(s) on which the corresponding field(s) are minimized in (4.26), while leaving the other fields unrestricted. Hence, we introduce the restricted spaces $\tilde{\mathbb{U}}_\square^{\mathrm{D}} \subseteq \tilde{\mathbb{U}}_\square$ for displacements as follows: {eq:4-17}

$$\tilde{\mathbb{U}}_\square^{\mathrm{D}} = \{\hat{\boldsymbol{u}} \in \tilde{\mathbb{U}}_\square \,|\, \hat{\boldsymbol{u}} = \boldsymbol{u}^{\mathrm{M}}(\bar{\boldsymbol{\epsilon}}) \text{ on } \Gamma_{\square,i},\ i = 1,\dots,K\} \tag{4.31a}$$ {eq:4-17a}

For $\hat{\boldsymbol{u}} \in \tilde{\mathbb{U}}_\square^{\mathrm{D}}$ we obviously have $\tilde{d}_\square(\boldsymbol{\lambda},\hat{\boldsymbol{u}} - \bar{\boldsymbol{\epsilon}}\cdot[\boldsymbol{x}-\bar{\boldsymbol{x}}]) = 0$ for any choice of $\boldsymbol{\lambda}$. Corresponding to this choice of Dirichlet-type of condition, we define the following minimum problem pertinent to the RVE for given value of the macroscale strain $\bar{\boldsymbol{\epsilon}}$: Find $\boldsymbol{u} \in \tilde{\mathbb{U}}_\square^{\mathrm{D}}$ that is the solution of the minimum problem

$$\min_{\hat{\boldsymbol{u}}\in\tilde{\mathbb{U}}_\square^{\mathrm{D}}}\frac{1}{K}\sum_{i=1}^{K}\Psi_{\square,i}(\hat{\boldsymbol{u}}) \tag{4.32}$$ {eq:4-18}

From (4.31), it is clear that there is no longer any coupling between SVEs; hence, the minimizing operation can be moved inside the sum over SVE:s by introducing the new spaces $\mathbb{U}_{\square,i}^{\mathrm{D}}$, which are localized to the SVE occupying $\Omega_{\square,i}$. We may now write the effective strain energy as

$$\begin{aligned}\bar{\psi}_\square\{\bar{\boldsymbol{\epsilon}}\} &\leq \frac{1}{K}\sum_{i=1}^{K}\underbrace{\min_{\hat{\boldsymbol{u}}\in\mathbb{U}_{\square,i}^{\mathrm{D}}}\Psi_{\square,i}(\hat{\boldsymbol{u}})}_{:=\bar{\psi}_{\square,i}^{\mathrm{D}}\{\bar{\boldsymbol{\epsilon}}\}} \\ &= \frac{1}{K}\sum_{i=1}^{K}\bar{\psi}_{\square,i}^{\mathrm{D}}\{\bar{\boldsymbol{\epsilon}}\}\end{aligned} \tag{4.33}$$ {eq:4-19}

where we introduced the notation

$$\bar{\psi}_{\square,i}^{\mathrm{D}}\{\bar{\boldsymbol{\epsilon}}\} := \Psi_{\square,i}(\boldsymbol{u}\{\bar{\boldsymbol{\epsilon}}\}) \tag{4.34}$$ {eq:4-19b}

[2]Henceforth, the argument that indicates a specific realization is dropped for brevity.

where $\boldsymbol{u}\{\bar{\boldsymbol{\epsilon}}\}$ is the solution of the minimization problem (corresponding to DBC) for prescribed value of $\bar{\boldsymbol{\epsilon}}$. The inequality in (4.33) follows from the restricted set on which the minimization is carried out.

To proceed, we need an argument of ergodicity. More specifically, it is assumed that the sequence $\{\Omega_{\square,i}(\omega)\}_{i=1}^{\infty}$ is statistically equivalent to $\{\Omega_{\square,1}(\omega_i)\}_{i=1}^{\infty}$, i.e. the sum in (4.33) can be replaced by a sum on different SVE-realizations. We thus obtain the final result

{eq:4-20}
$$\begin{aligned}\bar{\psi}\{\bar{\boldsymbol{\epsilon}}\} &\leq \lim_{K\to\infty}\frac{1}{K}\sum_{i}^{K}\bar{\psi}^{\mathrm{D}}_{\square,i}\{\bar{\boldsymbol{\epsilon}}\} \overset{\text{ergodicity}}{=} E[\bar{\psi}^{\mathrm{D}}_{\square}\{\bar{\boldsymbol{\epsilon}},\omega\}] \\ &= \bar{\psi}^{\mathrm{ub}}\{\bar{\boldsymbol{\epsilon}}\}\end{aligned} \tag{4.35}$$

where $E[\bullet]$ defines the expected value. The computational effort thus consists of solving a sufficiently large number of (uncoupled) SVE-problems with Dirichlet b.c. on $\boldsymbol{u}$ for prescribed $\bar{\boldsymbol{\epsilon}}$.

Operational format

The precise formulation of the operational format of a DBC-problem was outlined in Chapter 3; however, for completeness it is recalled here. Firstly, it is convenient to introduce the displacement space that is pertinent to the Dirichlet condition:

{eq:4-21}
$$\mathbb{U}_{\square}^{\mathrm{D},0} = \{\hat{\boldsymbol{u}} \in \mathbb{U}_{\square} \,|\, \hat{\boldsymbol{u}} = \boldsymbol{0} \text{ on } \Gamma_{\square,i},\ i = 1,\ldots,K\} \tag{4.36}$$

The operational format (suitable for implementation) for computing $\bar{\psi}^{\mathrm{D}}_{\square,}\{\bar{\boldsymbol{\epsilon}},\omega_i\}$ for any given ω_i (SVE-realization) is then formulated as follows[3]: For prescribed value of $\bar{\boldsymbol{\epsilon}}$, find $\boldsymbol{u}^{\mu} \in \mathbb{U}_{\square}^{\mathrm{D},0}$ that solves

{eq:4-22}
$$\langle \boldsymbol{\sigma}(\bar{\boldsymbol{\epsilon}} + \boldsymbol{\epsilon}[\boldsymbol{u}^{\mu}]) : \boldsymbol{\epsilon}[\delta\boldsymbol{u}]\rangle_{\square} = 0 \quad \forall \delta\boldsymbol{u} \in \mathbb{U}_{\square}^{\mathrm{D},0}. \tag{4.37}$$

After (4.37) has been solved for multiple realizations, $\bar{\psi}^{\mathrm{D}}\{\bar{\boldsymbol{\epsilon}}\}$, i.e. $\bar{\psi}^{\mathrm{ub}}\{\bar{\boldsymbol{\epsilon}}\}$, can be estimated.

4.4.4 Lower bound on effective (incremental) strain energy

A lower bound on $\bar{\psi}$ may be found by restricting the function spaces for which the corresponding fields are maximized in (4.26), while leaving the other fields unrestricted. Hence, we introduce the restricted spaces $\tilde{\mathbb{L}}_{\square}^{\mathrm{N}} \subseteq \tilde{\mathbb{L}}_{\square}$ for the Lagrange multiplier, representing tractions, as follows:

{eq:4-23a}
$$\tilde{\mathbb{L}}_{\square}^{\mathrm{N}} = \{\hat{\boldsymbol{\lambda}} \in \tilde{\mathbb{L}}_{\square} \,|\, \hat{\boldsymbol{\lambda}} = \hat{\bar{\boldsymbol{\sigma}}}\cdot\boldsymbol{n} \text{ on } \Gamma_{\square,i},\ i = 1,\ldots,K,\ \text{for some } \hat{\bar{\boldsymbol{\sigma}}} \in \mathbb{R}^{3\times3}_{\mathrm{sym}}\} \tag{4.38}$$

We may reformulate $\tilde{d}_{\square}$ (after some manipulations) for any choice of $\boldsymbol{\lambda}$ as

{eq:4-24}
$$\tilde{d}_{\square}(\boldsymbol{\lambda},\boldsymbol{u}) = \bar{\boldsymbol{\sigma}} : \frac{1}{K}\sum_{i=1}^{K}\langle\boldsymbol{\epsilon}[\boldsymbol{u}]\rangle_{\square,i} \tag{4.39}$$

Corresponding to this choice of Neumann type of condition, we define the following saddle-point problem pertinent to the RVE for given value of the macroscale strain $\bar{\boldsymbol{\epsilon}}$: Find $\boldsymbol{u} \in \tilde{\mathbb{U}}_{\square}$, $\bar{\boldsymbol{\sigma}} \in \mathbb{R}^{3\times3}_{\mathrm{sym}}$ that is the solution of the saddle-point problem

{eq:4-25}
$$\min_{\hat{\boldsymbol{u}}\in\tilde{\mathbb{U}}_{\square}}\ \max_{\hat{\bar{\boldsymbol{\sigma}}}\in\mathbb{R}^{3\times3}_{\mathrm{sym}}}\left[\frac{1}{K}\sum_{i=1}^{K}\left[\Psi_{\square,i}(\hat{\boldsymbol{u}}) - \hat{\bar{\boldsymbol{\sigma}}} : \langle\boldsymbol{\epsilon}[\hat{\boldsymbol{u}}]\rangle_{\square,i}\right] + \hat{\bar{\boldsymbol{\sigma}}} : \bar{\boldsymbol{\epsilon}}\right] \tag{4.40}$$

[3] We have here dropped the subscript i on the function spaces, for brevity.

Since $\min_x \max_y f(x,y) \geq \max_y \min_x f(x,y)$ always holds, we may shift the arguments of the saddlepoint problem and obtain the bound from (4.40) as

$$\begin{aligned}\bar{\psi}_\Box\{\bar{\boldsymbol{\epsilon}}\} &\geq \max_{\hat{\bar{\boldsymbol{\sigma}}}\in\mathbb{R}^{3\times3}_{\text{sym}}} \left[\frac{1}{K}\sum_{i=1}^{K} \underbrace{\min_{\hat{\boldsymbol{u}}\in\mathbb{U}_{\Box,i}} \left[\Psi_{\Box,i}(\hat{\boldsymbol{u}}) - \hat{\bar{\boldsymbol{\sigma}}}:\langle\boldsymbol{\epsilon}[\hat{\boldsymbol{u}}]\rangle_{\Box,i}\right]}_{=-\bar{\psi}^{*,\text{N}}_{\Box,i}\{\hat{\bar{\boldsymbol{\sigma}}}\}} + \hat{\bar{\boldsymbol{\sigma}}}:\bar{\boldsymbol{\epsilon}} \right] \\ &= \max_{\hat{\bar{\boldsymbol{\sigma}}}\in\mathbb{R}^{3\times3}_{\text{sym}}} \left[\hat{\bar{\boldsymbol{\sigma}}}:\bar{\boldsymbol{\epsilon}} - \frac{1}{K}\sum_{i=1}^{K} \bar{\psi}^{*,\text{N}}_{\Box,i}\{\hat{\bar{\boldsymbol{\sigma}}}\} \right]\end{aligned} \qquad (4.41) \quad \texttt{\{eq:4-26\}}$$

where we introduced

$$\bar{\psi}^{*,\text{N}}_{\Box,i}\{\hat{\bar{\boldsymbol{\sigma}}}\} := -\left[\Psi_{\Box,i}(\hat{\boldsymbol{u}}\{\hat{\bar{\boldsymbol{\sigma}}}\}) - \hat{\bar{\boldsymbol{\sigma}}}:\langle\boldsymbol{\epsilon}[\hat{\boldsymbol{u}}\{\hat{\bar{\boldsymbol{\sigma}}}\}]\rangle_{\Box,i}\right] \qquad (4.42) \quad \texttt{\{eq:4-26a\}}$$

where $\boldsymbol{u}\{\hat{\bar{\boldsymbol{\sigma}}}\}$ is the solution of the minimization problem (corresponding to NBC) for prescribed value of $\hat{\bar{\boldsymbol{\sigma}}}$. The inequality (4.41) follows from the restricted sets in (4.38) on which maximization is carried out.

For a fixed value of $\hat{\bar{\boldsymbol{sigma}}}$, it is clear that there is no longer any coupling between SVEs; hence, the min-max problem can be moved inside the sum over SVEs by introducing new spaces, e.g. $\mathbb{U}_{\Box,i}$, which are localized to the SVE occupying $\Omega_{\Box,i}$.

Using the same argument of ergodicity as in (4.35), we obtain

$$\begin{aligned}\bar{\psi}\{\bar{\boldsymbol{\epsilon}}\} &\geq \max_{\hat{\bar{\boldsymbol{\sigma}}}\in\mathbb{R}^{3\times3}_{\text{sym}}} \left[\hat{\bar{\boldsymbol{\sigma}}}:\bar{\boldsymbol{\epsilon}} - \lim_{K\to\infty}\frac{1}{K}\sum_{i=1}^{K} \bar{\psi}^{*\text{N}}_{\Box,i}\{\hat{\bar{\boldsymbol{\sigma}}},\omega\} \right] \\ &\overset{\text{ergodicity}}{=} \max_{\hat{\bar{\boldsymbol{\sigma}}}\in\mathbb{R}^{3\times3}_{\text{sym}}} \left[\hat{\bar{\boldsymbol{\sigma}}}:\bar{\boldsymbol{\epsilon}} - E\left[\bar{\psi}^{*\text{N}}_{\Box}\{\hat{\bar{\boldsymbol{\sigma}}},\tilde{\omega}\}\right]\right] \\ &= \bar{\psi}^{\text{lb}}\{\bar{\boldsymbol{\epsilon}}\}\end{aligned} \qquad (4.43) \quad \texttt{\{eq:4-27\}}$$

However, to compute the optimal value of $\bar{\boldsymbol{\sigma}}$ from the last expression in (4.43) is computationally intractable in practice, since it would require an iteration procedure that involves a large number of different SVE-problems that correspond to different realizations. Indeed, it is only in the special case of linear elasticity that no iteration is required, which case will be considered later in this Chapter. It is, therefore, useful in practice to look for a "good approximation" of $\bar{\boldsymbol{\sigma}} = \bar{\boldsymbol{\sigma}}^{\text{opt}}$ since the lower bound obviously holds true for *any* given choice $\bar{\boldsymbol{\sigma}} \neq \bar{\boldsymbol{\sigma}}^{\text{opt}}$, no matter how crude this approximation (or even guess) is. Obviously, the better the approximation, the sharper the lower bound.

Remark: Note that the condition $\langle\boldsymbol{\epsilon}[\boldsymbol{u}]\rangle_\Box = \bar{\boldsymbol{\epsilon}}$ is no longer guaranteed for an approximate (non-optimal) value of $\bar{\boldsymbol{\sigma}}$. □

When $\bar{\boldsymbol{\sigma}}$ has been computed, it is obviously possible to compute $\bar{\psi}^{\text{lb}}\{\bar{\boldsymbol{\epsilon}}\}$ from (4.43) as

$$\bar{\psi}^{\text{lb}}\{\bar{\boldsymbol{\epsilon}}\} \approx \bar{\boldsymbol{\sigma}}:\bar{\boldsymbol{\epsilon}} - E[\bar{\psi}^{*\text{N}}_{\Box}\{\bar{\boldsymbol{\sigma}},\tilde{\omega}\}] \qquad (4.44) \quad \texttt{\{eq:4-28\}}$$

Clearly, to compute $E[\bar{\psi}^{*\text{N}}_{\Box}\{\bar{\boldsymbol{\sigma}},\tilde{\omega}\}]$ corresponds to solving a large number of independent SVE-problems with Neumann boundary conditions for prescribed $\bar{\boldsymbol{\sigma}}$ (macroscale stress control), each of which is defined by the saddle-point problem

$$\bar{\psi}^{*\text{N}}_{\Box}\{\boldsymbol{\sigma},\bar{\boldsymbol{\omega}}_{\boldsymbol{i}}\} = -\min_{\hat{\boldsymbol{u}}\in\mathbb{U}_\Box}\left[\Psi_\Box(\hat{\boldsymbol{u}}) - \bar{\boldsymbol{\sigma}}:\langle\boldsymbol{\epsilon}[\hat{\boldsymbol{u}}]\rangle_\Box\right] \qquad (4.45) \quad \texttt{\{eq:4-29\}}$$

Operational format

The precise formulation of the operational format of an NBC-problem was outlined in Chapter 3 for the spexial case of linear elasticity. The operational format (suitable for implementation) for any given ω_i (SVE-realization) is then formulated as follows[4]: For given value of $\bar{\boldsymbol{\sigma}}$, find $\boldsymbol{u} \in \mathbb{U}_\square$ that solves

{eq:4-30a}
$$\langle \boldsymbol{\sigma}(\boldsymbol{\epsilon}[\boldsymbol{u}]) : \boldsymbol{\epsilon}[\delta \boldsymbol{u}] \rangle_\square = \bar{\boldsymbol{\sigma}} : \langle \boldsymbol{\epsilon}[\delta \boldsymbol{u}] \rangle_\square \quad \forall \delta \boldsymbol{u} \in \mathbb{U}_\square \tag{4.46}$$

Guaranteed lower bound based on non-optimal macroscale stress

In order to motivate a good approximation for the optimal stress, we argue as follows: Firstly, note that the condition

{eq:4-31}
$$\frac{1}{K} \sum_{1}^{K} \langle \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}] \rangle_{\square,i} = \bar{\boldsymbol{\epsilon}} \tag{4.47}$$

follows as part of the stationarity conditions that correspond to the problem in (4.41). A significant simplication is introduced if we replace (4.47) with the stronger requirement

{eq:4-32}
$$\langle \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}] \rangle_{\square,i} = \bar{\boldsymbol{\epsilon}}, \quad i = 1, \ldots, K. \tag{4.48}$$

The corresponding variational problem, that replaces (4.40), then becomes (for each realization): For given $\bar{\boldsymbol{\epsilon}}$, solve the individual SVE-problems

{eq:4-33}
$$\max_{\hat{\bar{\boldsymbol{\sigma}}} \in \mathbb{R}^{3\times3}} \min_{\hat{\boldsymbol{u}} \in \mathbb{U}_\square} \left[\Psi_\square(\hat{\boldsymbol{u}}) - \hat{\bar{\boldsymbol{\sigma}}} \colon \langle \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}] \rangle_\square + \hat{\bar{\boldsymbol{\sigma}}} \colon \bar{\boldsymbol{\epsilon}} \right] \tag{4.49}$$

The operational format of the stationarity conditions that correspond to the saddle-point problem in (4.49) reads: For given value of the macrostrain $\bar{\boldsymbol{\epsilon}}$, find $\bar{\boldsymbol{\sigma}}^{\mathrm{N}} \in \mathbb{R}^{3\times3}$, $\boldsymbol{u} \in \mathbb{U}_\square$ that solve {eq:4-34}

{eq:4-34a}
$$\langle \boldsymbol{\sigma}(\boldsymbol{\epsilon}[\boldsymbol{u}]) \colon \boldsymbol{\epsilon}[\delta \boldsymbol{u}] \rangle_\square - \bar{\boldsymbol{\sigma}}^{\mathrm{N}} \colon \langle \boldsymbol{\epsilon}[\delta \boldsymbol{u}] \rangle_\square = 0 \qquad \forall \delta \boldsymbol{u} \in \mathbb{U}_\square \tag{4.50a}$$

{eq:4-34b}
$$-\delta \bar{\boldsymbol{\sigma}} \colon \langle \boldsymbol{\epsilon}[\boldsymbol{u}] \rangle_\square = -\delta \bar{\boldsymbol{\sigma}} \colon \bar{\boldsymbol{\epsilon}} \qquad \forall \delta \bar{\boldsymbol{\sigma}} \in \mathbb{R}^{3\times3}_{\mathrm{sym}} \tag{4.50b}$$

Now, an approximation for $\bar{\boldsymbol{\sigma}}^{\mathrm{opt}}$ is

{eq:4-35}
$$\bar{\boldsymbol{\sigma}}^{\mathrm{opt}} \approx E\left[\bar{\boldsymbol{\sigma}}^{\mathrm{N}}\{\bar{\boldsymbol{\epsilon}}, \tilde{\omega}\}\right] \tag{4.51}$$

Remark: It is possible to reduce the computational effort by choosing the solution $\bar{\boldsymbol{\sigma}}^{\mathrm{N}}\{\bar{\boldsymbol{\epsilon}}, \omega_K\}$ for *any* given realization ω_K or to select only a few realizations. □

Approximate lower bound

It is possible to avoid solving the stress-controlled Neumann problems associated with (4.43) by simply accepting the solution (6.5) as an approximation. In other words, for each realization we compute

{eq:4-41}
$$\mathring{\psi}^{\mathrm{N}}_\square\{\bar{\boldsymbol{\epsilon}}, \omega_i\} := \max_{\hat{\bar{\boldsymbol{\sigma}}} \in \mathbb{R}^{3\times3}_{\mathrm{sym}}} \min_{\hat{\boldsymbol{u}} \in \mathbb{U}_\square} \left[\Psi_\square(\hat{\boldsymbol{u}}) - \hat{\bar{\boldsymbol{\sigma}}} : \langle \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}] \rangle_{\square,i} + \hat{\bar{\boldsymbol{\sigma}}} : \bar{\boldsymbol{\epsilon}} \right] \tag{4.52}$$

[4] We have here dropped the subscript i on the function spaces, for brevity.

which corresponds to the approximate lower bound

{eq:4-42}
$$\bar{\psi}\{\bar{\boldsymbol{\epsilon}}\} \gtrsim E[\mathring{\bar{\psi}}^{\mathrm{N}}_{\square}\{\bar{\boldsymbol{\epsilon}},\tilde{\omega}\}] =: \mathring{\bar{\psi}}^{\mathrm{lb}}\{\bar{\boldsymbol{\epsilon}}\}. \tag{4.53}$$

Once again, it is emphasized that $\mathring{\bar{\psi}}^{\mathrm{lb}}\{\bar{\boldsymbol{\epsilon}}\}$ does not provide a guaranteed lower bound on $\bar{\psi}\{\bar{\boldsymbol{\epsilon}}\}$. In particular, as the SVE size becomes smaller, $\mathring{\bar{\psi}}^{\mathrm{lb}}$ degenerates to $\bar{\psi}^{\mathrm{D}}$ (defined below), which does not bound $\bar{\psi}$.

Remark: Since the stationarity condition gives the identity

$$\bar{\boldsymbol{\sigma}} : [\bar{\boldsymbol{\epsilon}} - \langle \boldsymbol{\epsilon}[\boldsymbol{u}\{\bar{\boldsymbol{\epsilon}}\}]\rangle_{\square}] = 0 \tag{4.54}$$

at the stationary point, we conclude that $\mathring{\bar{\psi}}^{\mathrm{N}}_{\square}\{\bar{\boldsymbol{\epsilon}},\tilde{\omega}\}$ can be computed as

$$\mathring{\bar{\psi}}^{\mathrm{N}}_{\square}\{\bar{\boldsymbol{\epsilon}},\tilde{\omega}\} = \Psi_{\square}(\boldsymbol{u}\{\bar{\boldsymbol{\epsilon}},\tilde{\omega}\}). \tag{4.55}$$

for $i = 1, 2, \dots, K$. $\square$

4.5 Bounds on the effective strain energy – A summary

$$\max_{\hat{\boldsymbol{\sigma}}\in\mathbb{R}^{3\times 3}_{\mathrm{sym}}} \left[\hat{\boldsymbol{\sigma}} : \bar{\boldsymbol{\epsilon}} - E\left[\bar{\psi}^{*\mathrm{N}}_{\square}\{\hat{\boldsymbol{\sigma}},\tilde{\omega}\}\right]\right] \le \bar{\psi}\{\bar{\boldsymbol{\epsilon}}\} \qquad \le E\left[\bar{\psi}^{\mathrm{D}}_{\square}\{\bar{\boldsymbol{\epsilon}},\tilde{\omega}\}\right] \tag{4.56a}$$ {eq:4-711a}

4.6 Linear elasticity – Bounds on effective elastic stiffness tensor

4.6.1 Preliminaries

$$\bar{\psi}\{\bar{\boldsymbol{\epsilon}}\} = \lim_{|\Omega_{\square}|\to\infty} \bar{\psi}_{\square}\{\bar{\boldsymbol{\epsilon}},\omega\} = \frac{1}{2}\bar{\boldsymbol{\epsilon}} : \bar{\mathbf{E}} : \bar{\boldsymbol{\epsilon}} \tag{4.57}$$ {eq:4-16}

4.6.2 Upper bound on effective elastic stiffness

In the case of linear elasticity, we may obtain the upper bound explicitly. Firstly, we note the identity

$$\Psi_{\square,i}(\boldsymbol{u}\{\bar{\boldsymbol{\epsilon}}\}) = \frac{1}{2}\langle \boldsymbol{\epsilon}[\boldsymbol{u}\{\bar{\boldsymbol{\epsilon}}\}] : \mathbf{E} : \boldsymbol{\epsilon}[\boldsymbol{u}\{\bar{\boldsymbol{\epsilon}}\}]\rangle_{\square} = \frac{1}{2}\bar{\boldsymbol{\epsilon}} : \bar{\mathbf{E}}^{\mathrm{D}}_{\square,i} : \bar{\boldsymbol{\epsilon}} \tag{4.58}$$ {eq:4-19c}

where $\bar{\mathbf{E}}^{\mathrm{D}}_{\square,i}$ is the apparent stiffness tensor for the DBC-problem. We thus obtain the explicit expression in (4.35)

$$\begin{aligned} \bar{\psi}^{\mathrm{ub}}\{\bar{\boldsymbol{\epsilon}}\} &= E\left[\frac{1}{2}\bar{\boldsymbol{\epsilon}} : \bar{\mathbf{E}}^{\mathrm{D}}_{\square}(\tilde{\omega})\bar{\boldsymbol{\epsilon}}\right] \\ &= \frac{1}{2}\bar{\boldsymbol{\epsilon}} : \underbrace{E[\bar{\mathbf{E}}^{\mathrm{D}}_{\square}(\tilde{\omega})]}_{=\bar{\mathbf{E}}^{\mathrm{D}}} : \bar{\boldsymbol{\epsilon}} = \frac{1}{2}\bar{\boldsymbol{\epsilon}} : \bar{\mathbf{E}}^{\mathrm{D}} : \bar{\boldsymbol{\epsilon}} \end{aligned} \tag{4.59}$$ {eq:4-20a}

Operational format

The precise formulation of the operational format of a DBC-problem was outlined in Chapter 3; however, for completeness it is recalled here. Firstly, it is convenient to introduce the displacement space that is pertinent to the Dirichlet condition:

$$\mathbb{U}_{\square}^{\mathrm{D},0} = \{\hat{\boldsymbol{u}} \in \mathbb{U}_{\square} \,|\, \hat{\boldsymbol{u}} = \boldsymbol{0} \text{ on } \Gamma_{\square}\} \tag{4.60}$$ {eq:4-21}

The operational format (suitable for implementation) for computing $\bar{\mathbf{E}}_{\square}^{\mathrm{D}}(\tilde{\omega}_i)$ for any given ω_i (SVE-realization) is then formulated as follows[5]: For prescribed value of $\bar{\boldsymbol{\epsilon}}$, find $\boldsymbol{u}^{\mu} \in \mathbb{U}_{\square}^{\mathrm{D},0}$ that solves

$$\langle [\bar{\boldsymbol{\epsilon}} + \boldsymbol{\epsilon}[\boldsymbol{u}^{\mu}]] : \mathbf{E} : \boldsymbol{\epsilon}[\delta \boldsymbol{u}]\rangle_{\square} = 0 \quad \forall \delta \boldsymbol{u} \in \mathbb{U}_{\square}^{\mathrm{D},0}. \tag{4.61}$$

4.6.3 Lower bound on effective elastic stiffness

In the case of linear elasticity, we may obtain the lower bound explicitly. Firstly, we note the identity

{eq:4-119c}
$$\Psi_{\square,i}(\boldsymbol{u}\{\hat{\boldsymbol{\sigma}}\}) = \frac{1}{2}\langle \boldsymbol{\epsilon}[\boldsymbol{u}\{\hat{\boldsymbol{\sigma}}\}] : \mathbf{E} : \boldsymbol{\epsilon}[\boldsymbol{u}\{\hat{\boldsymbol{\sigma}}\}]\rangle_{\square} = \frac{1}{2}\hat{\boldsymbol{\sigma}} : \bar{\mathbf{C}}_{\square,i}^{\mathrm{N}} : \hat{\boldsymbol{\sigma}} \tag{4.62}$$

{eq:4-119d}
$$\langle \boldsymbol{\epsilon}[\boldsymbol{u}\{\hat{\boldsymbol{\sigma}}\}]\rangle_{\square} := \hat{\bar{\boldsymbol{\epsilon}}}_i^{\mathrm{N}} = \bar{\mathbf{C}}_{\square,i}^{\mathrm{N}} : \hat{\boldsymbol{\sigma}} \tag{4.63}$$

where $\bar{\mathbf{C}}_{\square,i}^{\mathrm{N}}$ is the apparent compliance tensor for the NBC-problem. We thus obtain the explicit expression in (4.35)

{eq:4-119c}
$$\psi_{\square,i}^{*}(\boldsymbol{u}\{\hat{\boldsymbol{\sigma}}\}) = \frac{1}{2}\hat{\boldsymbol{\sigma}} : \bar{\mathbf{C}}_{\square,i}^{\mathrm{N}} : \hat{\boldsymbol{\sigma}} \tag{4.64}$$

From eq:4-711a then follows that

{eq:4-20a}
$$\begin{aligned}
\bar{\psi}^{\mathrm{lb}}\{\bar{\boldsymbol{\epsilon}}\} &= \max_{\hat{\boldsymbol{\sigma}} \in \mathbb{R}^{3\times 3}_{\mathrm{sym}}} \left[\hat{\boldsymbol{\sigma}} : \bar{\boldsymbol{\epsilon}} - E\left[\frac{1}{2}\hat{\boldsymbol{\sigma}} : \bar{\mathbf{C}}_{\square}^{\mathrm{N}}(\tilde{\omega}) : \hat{\boldsymbol{\sigma}}\right]\right] \\
&= \max_{\hat{\boldsymbol{\sigma}} \in \mathbb{R}^{3\times 3}_{\mathrm{sym}}} \left[\hat{\boldsymbol{\sigma}} : \bar{\boldsymbol{\epsilon}} - \frac{1}{2}\hat{\boldsymbol{\sigma}} : \underbrace{E\left[\bar{\mathbf{C}}_{\square}^{\mathrm{N}}(\tilde{\omega})\right]}_{=\bar{\mathbf{C}}^{\mathrm{N}}} : \hat{\boldsymbol{\sigma}}\right] \\
&= \frac{1}{2}\bar{\boldsymbol{\epsilon}} : [\bar{\mathbf{C}}^{\mathrm{N}}]^{-1} : \bar{\boldsymbol{\epsilon}}
\end{aligned} \tag{4.65}$$

where we used the stationarity condition to obtain the relation

{eq:4-20b}
$$\bar{\boldsymbol{\epsilon}} = \bar{\mathbf{C}}^{\mathrm{N}} : \bar{\boldsymbol{\sigma}}^{\mathrm{N}} \quad \Rightarrow \quad \bar{\boldsymbol{\sigma}}^{\mathrm{N}} = [\bar{\mathbf{C}}^{\mathrm{N}}]^{-1} : \bar{\boldsymbol{\epsilon}} \tag{4.66}$$

Operational format

The precise formulation of the operational format of a NBC-problem was outlined in Chapter 3; however, for completeness it is recalled here. The operational format (suitable for implementation) for computing $\bar{\mathbf{C}}_{\square}^{\mathrm{N}}(\tilde{\omega})$ for any given ω_i (SVE-realization) is then formulated as follows[6]: For given value of $\bar{\boldsymbol{\sigma}}$, find $\boldsymbol{u} \in \mathbb{U}_{\square}$ that solves

{eq:4-30a}
$$\langle \boldsymbol{\epsilon}[\boldsymbol{u}] : \mathbf{E} : \boldsymbol{\epsilon}[\delta \boldsymbol{u}]\rangle_{\square} = \bar{\boldsymbol{\sigma}} : \langle \boldsymbol{\epsilon}[\delta \boldsymbol{u}]\rangle_{\square} \quad \forall \delta \boldsymbol{u} \in \mathbb{U}_{\square} \tag{4.67}$$

[5] We have here dropped the subscript i on the function spaces, for brevity.

[6] We have here dropped the subscript i on the function spaces, for brevity.

4.7 Bounds on linear elastic stiffness and compliance tensors – A summary

{eq:4-712a}

$$[\bar{\mathbf{C}}^{\mathrm{N}}]^{-1} \quad \leq \quad \bar{\mathbf{E}} \quad \leq \quad \bar{\mathbf{E}}^{\mathrm{D}} \tag{4.68}$$

Chapter 5

FE^2 FOR NONLINEAR MATERIAL MODELING – NONLINEAR ELASTICITY

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5.1 Subscale modeling - nonlinear elasticity

5.1.1 Generic algorithmic constitutive stress-strain relation

In this Chapter we shall assume the existence of a stress-strain relation $\boldsymbol{\sigma}_{\mathrm{A}}\{\boldsymbol{\epsilon}\}$, which is generally of algorithmic character. Its origin can be different. Two major subclasses of material models can be envisioned:

- Nonlinear (hyper)elasticity: $\boldsymbol{\sigma}(\boldsymbol{\epsilon})$ is an explicit function expressing elastic, i.e. non-dissipative, response, and represents a straightforward extension of linear elasticity to the nonlinear regime.

- Standard Dissipative Material constitutive model: $\boldsymbol{\sigma}(\boldsymbol{\epsilon}, \underline{\boldsymbol{k}})$ is an explicit function of a set of internal variables $\underline{\boldsymbol{k}}$, in addition to strain. After time integration of the evolution equations for $\underline{\boldsymbol{k}}$ subject to data in the form of given strain history, we obtain the algorithmic relation $\underline{\boldsymbol{k}} = \underline{\boldsymbol{k}}_{\mathrm{A}}\{\boldsymbol{\epsilon}\}$. We then obtain $\boldsymbol{\sigma}_{\mathrm{A}}\{\boldsymbol{\epsilon}\} := \boldsymbol{\sigma}(\boldsymbol{\epsilon}, \underline{\boldsymbol{k}}_{\mathrm{A}}\{\boldsymbol{\epsilon}\})$.

In either of the above-mentioned situations, we shall assume that it is possible to construct an algorithmic free energy density $\psi_{\mathrm{A}}\{\boldsymbol{\epsilon}\}$ such that it serves as a potential for $\boldsymbol{\sigma}_{\mathrm{A}}\{\boldsymbol{\epsilon}\}$. As a consequence, the exact linearization of $\boldsymbol{\sigma}_{\mathrm{A}}\{\boldsymbol{\epsilon}\}$ gives

$$\mathsf{E}_{\mathrm{AT}}\{\boldsymbol{\epsilon}\} = \frac{\partial \boldsymbol{\sigma}_{\mathrm{A}}\{\boldsymbol{\epsilon}\}}{\partial \boldsymbol{\epsilon}} = \frac{\partial^2 \psi_{\mathrm{A}}\{\boldsymbol{\epsilon}\}}{\partial \boldsymbol{\epsilon} \otimes \partial \boldsymbol{\epsilon}} \tag{5.1}$$ {eq:4-102}

where $\mathsf{E}_{\mathrm{AT}}\{\boldsymbol{\epsilon}\}$ is the Algorithmic Tangent stiffness tensor that possesses major as well as minor symmetry.

Henceforth, we ignore the "algorithmic" character and use the simpler notation $\boldsymbol{\sigma}(\boldsymbol{\epsilon})$ and $\mathsf{E}_{\mathrm{T}}(\boldsymbol{\epsilon})$ for brevity of notation.

5.1.2 Displacement-based variational formulations

The weak format of the equilibrium equation is: Find $\boldsymbol{u} \in \mathbb{U}$ that solves

$$a(\boldsymbol{u}; \delta\boldsymbol{u}) = l(\delta\boldsymbol{u}) \quad \forall \delta\boldsymbol{u} \in \mathbb{U}^0 \tag{5.2}$$ {eq:4-1}

This is the same formulation as for linear elasticity with the generalization that $a(\boldsymbol{u}; \delta\boldsymbol{u})$ is now the semi-linear form

{eq:4-3a}
$$a(\boldsymbol{u}; \delta\boldsymbol{u}) \overset{\text{def}}{=} \int_\Omega \boldsymbol{\sigma}(\boldsymbol{\epsilon}[\boldsymbol{u}]) : \boldsymbol{\epsilon}[\delta\boldsymbol{u}]\,\mathrm{dV} \tag{5.3}$$

{eq:4-3b}
$$l(\delta\boldsymbol{u}) \overset{\text{def}}{=} \int_\Omega \boldsymbol{f} \cdot \delta\boldsymbol{u}\,\mathrm{dV} + \int_{\partial\Omega_\mathrm{N}} \boldsymbol{t}_\mathrm{P} \cdot \delta\boldsymbol{u}\,\mathrm{dS} \tag{5.4}$$

Extending the MPE-principle from linear elasticity is also straightforward. We introduce the potential energy $\Pi(\hat{\boldsymbol{u}})$ of any $\hat{\boldsymbol{u}} \in \mathbb{U}$ as

{eq:4-34}
$$\Pi(\hat{\boldsymbol{u}}) = \Psi(\hat{\boldsymbol{u}}) - l(\hat{\boldsymbol{u}}), \tag{5.5}$$

where we define the stored elastic strain energy as

{eq:4-34a}
$$\Psi(\boldsymbol{v}) \overset{\text{def}}{=} \int_\Omega \psi(\boldsymbol{\epsilon}[\boldsymbol{v}])\,\mathrm{d}\Omega. \tag{5.6}$$

The directional derivative of Π at any point $\hat{\boldsymbol{u}} \in \mathbb{U}$ in the direction $\delta\boldsymbol{u} \in \mathbb{U}^0$ is given as

{eq:4-35}
$$\Pi'_u(\hat{\boldsymbol{u}}; \delta\boldsymbol{u}) \frac{\mathrm{d}}{\mathrm{d}\gamma} \Pi(\hat{\boldsymbol{u}} + \gamma\delta\boldsymbol{u})|_{\gamma=0} = \int_\Omega \boldsymbol{\sigma}(\boldsymbol{\epsilon}[\hat{\boldsymbol{u}}]) : \boldsymbol{\epsilon}[\delta\hat{\boldsymbol{u}}]\,\mathrm{d}\Omega - l(\delta\boldsymbol{u}) = a(\hat{\boldsymbol{u}}; \delta\boldsymbol{u}) - l(\delta\boldsymbol{u}) \tag{5.7}$$

5.1.3 Solution of nonlinear problem - Linearization

The continuous (weak) problem format (6.2) is nonlinear in $\boldsymbol{u}$, and its solution thus requires some sort of iteration strategy. As a prototype of solution procedure, we consider Newton iterations, which are based on (exact) linearization of the nonlinear form $a(\boldsymbol{u}; \delta\boldsymbol{u})$. As the starting point, consider (6.2) for any given field $\boldsymbol{u}^{(k)} \neq \boldsymbol{u}$ in the iteration k, whereby the residual is defined as

{eq:4-48}
$$R(\boldsymbol{u}^{(k)}; \delta\boldsymbol{u}) = a(\boldsymbol{u}^{(k)}; \delta\boldsymbol{u}) - l(\delta\boldsymbol{u}) \quad \forall \delta\boldsymbol{u} \in \mathbb{U}^0 \tag{5.8}$$

and it is noted that $R(\boldsymbol{u}^{(k)}; \delta\boldsymbol{u}) \neq 0$ if $\boldsymbol{u}^{(k)} \neq \boldsymbol{u}$.

{grp} Newton's method is to compute the improved field $\boldsymbol{u}^{(k+1)}$ from the algorithm

{eq:4-49a}
$$\boldsymbol{u}^{(k+1)} = \boldsymbol{u}^{(k)} + \Delta\boldsymbol{u} \tag{5.9a}$$

{eq:4-49b}
$$R'_u(\boldsymbol{u}^{(k)}; \delta\boldsymbol{u}, \Delta\boldsymbol{u}) = -R(\boldsymbol{u}^{(k)}; \delta\boldsymbol{u}) \quad \forall \delta\boldsymbol{u} \in \mathbb{U}^0 \tag{5.9b}$$

Hence, we exploit the linearization of $R(\boldsymbol{u}; \delta\boldsymbol{u})$

{eq:4-50}
$$\begin{aligned} R'_u(\boldsymbol{u}; \delta\boldsymbol{u}_1, \delta\boldsymbol{u}_2) &= \frac{\mathrm{d}}{\mathrm{d}\gamma} R(\boldsymbol{u} + \gamma\delta\boldsymbol{u}_2, \delta\boldsymbol{u}_1)|_{\gamma=0} = \Pi''_{uu}(\boldsymbol{u}; \delta\boldsymbol{u}_1, \delta\boldsymbol{u}_2) = a'(\boldsymbol{u}; \delta\boldsymbol{u}_1, \delta\boldsymbol{u}_2) \\ &= \int_\Omega \boldsymbol{\epsilon}[\delta\boldsymbol{u}_1] : \mathbf{E}_\mathrm{T} : \boldsymbol{\epsilon}[\delta\boldsymbol{u}_2]\,\mathrm{d}V = \int_\Omega [\delta\boldsymbol{u}_1 \otimes \boldsymbol{\nabla}] : \mathbf{E}_\mathrm{T} : [\delta\boldsymbol{u}_2 \otimes \boldsymbol{\nabla}]\,\mathrm{d}V \end{aligned} \tag{5.10}$$

where it was used that $\mathbf{E}_\mathrm{T}$ is the tangent stiffness tensor that represents the (exact) linearization of $\boldsymbol{\sigma}(\boldsymbol{\epsilon})$

{eq:4-51}
$$\mathrm{d}\boldsymbol{\sigma}(\boldsymbol{\epsilon}) = \mathbf{E}_\mathrm{T}(\boldsymbol{\epsilon}) :\, \mathrm{d}\boldsymbol{\epsilon} \tag{5.11}$$

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5.2 FE^2

5.2.1 Preliminaries

Let us recall the standard variational format of the fine-scale representation of the pertinent nonlinear material model: Find $\boldsymbol{u} \in \mathbb{U}$ that solves

{eq:4-101}
$$a(\boldsymbol{u}; \delta\boldsymbol{u}) = l(\delta\boldsymbol{u}) \quad \forall \delta\boldsymbol{u} \in \mathbb{U}^0. \tag{5.12}$$

The purpose of homogenization is to replace this problem with a macroscale problem, whose unknown displacement field is a globally defined macroscale field $\bar{\boldsymbol{u}} \neq \boldsymbol{u}$ that is significantly smoother than $\boldsymbol{u}$. Note that there is no hope to retrofit the finescale solution from $\bar{\boldsymbol{u}}$ as a postprocessing step. The local field is thus replaced (as a smoothing approximation) by the spatially homogenized field on a suitably chosen RVE in any given macroscale point $\bar{\boldsymbol{x}} \in \Omega$. A consequence of this fact is that the RVE:s for two sufficiently close macroscale points are "overlapping"; however, this fact does not incur any conceptual difficulty or anomally since the concept of homogenization is a model assumption. Moreover, at the algorithmic implementation numerical quadrature is employed at the evaluation of integrals in the spatial domain. Hence, homogenization on the RVE's is carried out (only) in these macroscale quadrature points in practice.

With the introduced homogenization, the original problem formulation remains formally unchanged *if integrands are replaced by the homogenized quantities* in all space-variational forms. Hence, (6.3) and (6.4) are replaced by

$$a(\boldsymbol{u}; \delta\boldsymbol{u}) \overset{\text{def}}{=} \int_\Omega \langle \boldsymbol{\sigma}(\boldsymbol{\epsilon}[\boldsymbol{u}]) : \boldsymbol{\epsilon}[\delta\boldsymbol{u}] \rangle_\square \, \mathrm{d}V, \tag{5.13}$$ {eq:4-102}

$$l(\delta\boldsymbol{u}) \overset{\text{def}}{=} \int_\Omega \langle \boldsymbol{f} \cdot \delta\boldsymbol{u} \rangle_\square \, \mathrm{d}V + \int_{\Gamma_\mathrm{N}} \langle\langle \boldsymbol{t}_\mathrm{p} \cdot \delta\boldsymbol{u} \rangle\rangle_\square \, \mathrm{d}S \tag{5.14}$$ {eq:4-103}

Inside each RVE, the subscale solution[1] is split additively into the smooth part, $\boldsymbol{u}^\mathrm{M}$, and the non-smooth (fluctuation) part, $\boldsymbol{u}^\mu$ in accordance with the assumption of 1st order homogenization:

$$\boldsymbol{u}(\bar{\boldsymbol{x}}; \boldsymbol{x}) = \boldsymbol{u}^\mathrm{M}(\bar{\boldsymbol{x}}; \boldsymbol{x}) + \boldsymbol{u}^\mu(\boldsymbol{x}), \quad \boldsymbol{u}^\mathrm{M}(\bar{\boldsymbol{x}}; \boldsymbol{x}) = \bar{\boldsymbol{u}}(\bar{\boldsymbol{x}}) + \boldsymbol{h}[\bar{\boldsymbol{u}}](\bar{\boldsymbol{x}}) \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}] \tag{5.15}$$ {eq:4-104}

whereby it is noted that the macroscale displacement gradient $\bar{\boldsymbol{h}}$ is connected kinematically to the macroscale displacement field $\bar{\boldsymbol{u}}$ as $\bar{\boldsymbol{h}} = \boldsymbol{h}[\bar{\boldsymbol{u}}] = \bar{\boldsymbol{u}} \otimes \boldsymbol{\nabla}$. We shall therefore henceforth use the operator notation $\boldsymbol{u}^\mathrm{M} = \boldsymbol{u}^\mathrm{M}[\bar{\boldsymbol{u}}]$.

5.2.2 Macroscale problem

By merely introducing volume averages on RVE's and introducing the kinematic decomposition in (6.18), the "dimension" on the problem is not reduced, i.e. it is still as complex as the original fine-scale problem. The reduction is obtained upon introducing the following assumptions/steps:

- Define $\boldsymbol{u}^\mu$ as an implicit operator[2] of $\bar{\boldsymbol{u}}$, which is henceforth expressed as $\boldsymbol{u}^\mu \overset{\text{def}}{=} \boldsymbol{u}^\mu\{\bar{\boldsymbol{u}}\}$. Hence, $\boldsymbol{u} = \boldsymbol{u}\{\bar{\boldsymbol{u}}\} = \boldsymbol{u}^\mathrm{M}[\bar{\boldsymbol{u}}] + \boldsymbol{u}^\mu\{\bar{\boldsymbol{u}}\}$.

[1] Double arguments, e.g. $\boldsymbol{u}(\bar{\boldsymbol{x}}, \boldsymbol{x})$, are used to explicitly point out the underlying scale separation.
[2] Curly brackets $\{(\bullet)\}$ indicate implicit functional dependence on $(\bullet)$.

- Assume that $\boldsymbol{u}^\mu\{\bar{\boldsymbol{u}}\}$ is the solution of a (local) problem on each RVE, whereby it is noted that it is sufficient to "feed" the RVE-problem only with the gradient in terms of its symmetric part, i.e. the value $\bar{\boldsymbol{\epsilon}} = \bar{\boldsymbol{h}}^{\mathrm{sym}} = \boldsymbol{\epsilon}[\bar{\boldsymbol{u}}]$ (and not the value of $\bar{\boldsymbol{u}}$ itself, nor the skew-symmetric part $\bar{\boldsymbol{h}}^{\mathrm{skw}}$).
- Replace the test function $\delta\boldsymbol{u}$ with $\boldsymbol{u}^{\mathrm{M}}[\delta\bar{\boldsymbol{u}}] = \delta\bar{\boldsymbol{u}} + \boldsymbol{h}[\delta\bar{\boldsymbol{u}}] \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}]$, which will act as the "homogenizer" on each RVE.

Remark: The rationale behind the suggested strategy to arrive at the macroscle problem is not elaborated here; rather, it is postponed to Chapter 6. □

Next, we introduce the macroscale $\bar{\mathbb{U}}$ such that $\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}$. We are now in the position to replace the problem (6.15) by the *homogenized* problem: Find $\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}$ that is the solution of

{eq:4-106}
$$a(\boldsymbol{u}\{\bar{\boldsymbol{u}}\}; \boldsymbol{u}^{\mathrm{M}}[\delta\bar{\boldsymbol{u}}]) = l(\boldsymbol{u}^{\mathrm{M}}[\delta\bar{\boldsymbol{u}}]) \quad \forall \delta\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}^0. \tag{5.16}$$

In order to establish the appropriate (space-)variational format of the continuous macroscale problem, we first simplify by henceforth assuming that $\boldsymbol{u}$ is sufficiently smooth on Γ to allow the approximation $\boldsymbol{u}^\mu = \boldsymbol{0}$ (and $\delta\boldsymbol{u}^\mu = \boldsymbol{0}$) on Γ. Moreover, we restrict to the situation that the boundary values $\boldsymbol{u}_{\mathrm{p}}$ and $\boldsymbol{t}_{\mathrm{p}}$ vary sufficiently slowly to represent the macroscopic (homogenized) values in the sense that

{eq:4-107}
$$\langle \boldsymbol{u} \rangle_\square = \bar{\boldsymbol{u}}_{\mathrm{p}} \text{ on } \Gamma_{\mathrm{D}} \quad \text{and} \quad \langle\langle \boldsymbol{t}_{\mathrm{p}} \cdot \delta\boldsymbol{u} \rangle\rangle_\square = \bar{\boldsymbol{t}}_{\mathrm{p}} \cdot \delta\bar{\boldsymbol{u}} \text{ on } \Gamma_{\mathrm{N}} \tag{5.17}$$

where $\bar{\boldsymbol{u}}_{\mathrm{p}}$ and $\bar{\boldsymbol{t}}_{\mathrm{p}}$ are prescribed boundary values. In particular, the condition $(6.21)_2$ infers that
face average $\langle\langle \boldsymbol{t}_{\mathrm{p}} \rangle\rangle_\square = \bar{\boldsymbol{t}}_{\mathrm{p}}$ and $\langle\langle \boldsymbol{t}_{\mathrm{p}} \otimes [\boldsymbol{x} - \bar{\boldsymbol{x}}] \rangle\rangle_\square = \boldsymbol{0}$. In this way certain technical difficulties associated with the homogenization on the boundary are avoided. We shall also assume that the volume-specific load $\boldsymbol{f}$ is smooth such that $\langle \boldsymbol{f} \cdot \delta\boldsymbol{u} \rangle_\square = \bar{\boldsymbol{f}} \cdot \delta\bar{\boldsymbol{u}}$, whereby $\bar{\boldsymbol{f}} \overset{\mathrm{def}}{=} \langle \boldsymbol{f} \rangle_\square$ and $\langle \boldsymbol{f} \otimes [\boldsymbol{x} - \bar{\boldsymbol{x}}] \rangle_\square = \boldsymbol{0}$.

We may now evaluate the forms that occur in (6.20) as follows:

{eq:4-108a}
$$\begin{aligned} a(\boldsymbol{u}\{\bar{\boldsymbol{u}}\}; \boldsymbol{u}^{\mathrm{M}}[\delta\bar{\boldsymbol{u}}]) &= \int_\Omega \langle \boldsymbol{\sigma}(\boldsymbol{\epsilon}[\boldsymbol{u}\{\bar{\boldsymbol{u}}\}]) : \boldsymbol{\epsilon}[\boldsymbol{u}^{\mathrm{M}}[\delta\bar{\boldsymbol{u}}]] \rangle_\square \,\mathrm{d}\bar{\Omega} \\ &= \int_\Omega \langle \boldsymbol{\sigma}(\boldsymbol{\epsilon}[\boldsymbol{u}\{\bar{\boldsymbol{u}}\}]) \rangle_\square : \boldsymbol{\epsilon}[\delta\bar{\boldsymbol{u}}] \,\mathrm{d}\bar{\Omega} \\ &= \int_\Omega \bar{\boldsymbol{\sigma}}\{\bar{\boldsymbol{\epsilon}}\} : \boldsymbol{\epsilon}[\delta\bar{\boldsymbol{u}}] \,\mathrm{d}\bar{\Omega} \end{aligned} \tag{5.18}$$

{eq:4-108b}
$$\begin{aligned} l(\boldsymbol{u}^{\mathrm{M}}(\delta\bar{\boldsymbol{\epsilon}})) &= \int_\Omega \langle \boldsymbol{f} \cdot \boldsymbol{u}^{\mathrm{M}}[\delta\bar{\boldsymbol{u}}] \rangle_\square \,\mathrm{d}\bar{\Omega} + \int_{\Gamma_{\mathrm{N}}} \langle\langle \boldsymbol{t}_{\mathrm{p}} \cdot \boldsymbol{u}^{\mathrm{M}}[\delta\bar{\boldsymbol{u}}] \rangle\rangle_\square \,\mathrm{d}\bar{\Gamma} \\ &= \int_\Omega \bar{\boldsymbol{f}} \cdot \delta\bar{\boldsymbol{u}} \,\mathrm{d}\bar{\Omega} + \int_{\Gamma_{\mathrm{N}}} \bar{\boldsymbol{t}}_{\mathrm{p}} \cdot \delta\bar{\boldsymbol{u}} \,\mathrm{d}\bar{\Gamma} \end{aligned} \tag{5.19}$$

Remark: Since $\bar{\boldsymbol{\sigma}}$ is invariant to the values $\bar{\boldsymbol{u}}$ and $\bar{\boldsymbol{h}}^{\mathrm{skw}} := (\bar{\boldsymbol{u}} \otimes \boldsymbol{\nabla})^{\mathrm{skw}}$, we use the notion $\bar{\boldsymbol{\sigma}}\{\bar{\boldsymbol{\epsilon}}\}$. □

The macroscale problem can now be formulated as follows: Find $\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}$ such that the macroscale residual vanishes,

{eq:4-110}
$$\bar{R}\{\bar{\boldsymbol{u}}; \delta\bar{\boldsymbol{u}}\} \overset{\mathrm{def}}{=} \bar{l}\{\delta\bar{\boldsymbol{u}}\} - \bar{a}\{\bar{\boldsymbol{u}}; \delta\bar{\boldsymbol{u}}\} = 0 \quad \forall \delta\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}^0. \tag{5.20}$$

where we introduced the macroscale space-variational forms

{eq:4-111}
$$\bar{a}\{\bar{\boldsymbol{u}}; \delta\bar{\boldsymbol{u}}\} \overset{\mathrm{def}}{=} \int_\Omega \bar{\boldsymbol{\sigma}}\{\bar{\boldsymbol{\epsilon}}\} : \boldsymbol{\epsilon}[\delta\bar{\boldsymbol{u}}] \,\mathrm{d}\bar{\Omega} \tag{5.21}$$

{eq:4-112} $$\bar{l}\{\delta\bar{\boldsymbol{u}}\} \overset{\text{def}}{=} \int_{\Omega} \bar{\boldsymbol{f}} \cdot \delta\bar{\boldsymbol{u}} \, \mathrm{d}\bar{\Omega} + \int_{\Gamma_{\mathrm{N}}} \bar{\boldsymbol{t}}_{\mathrm{p}} \cdot \delta\bar{\boldsymbol{u}} \, \mathrm{d}\bar{\Gamma} \tag{5.22}$$

The nonlinear (and implicit) equation (6.25) can be solved, for example, via Newton iterations, whereby the tangent form $\bar{a}'$ is utilized:

$$\bar{a}'\{\bar{\boldsymbol{u}}; \delta\bar{\boldsymbol{u}}, \Delta\bar{\boldsymbol{u}}\} \quad \overset{\text{def}}{=} \quad \int_{\Omega} \boldsymbol{\epsilon}[\delta\bar{\boldsymbol{u}}] : \bar{\mathbf{E}}_{\mathrm{T}} : \boldsymbol{\epsilon}[\Delta\bar{\boldsymbol{u}}] \, \mathrm{d}\bar{\Omega} \tag{5.23}$$ {eq:4-113}

The appropriate macroscale (algorithmic) tangent stiffness tensor, $\bar{\mathbf{E}}_{\mathrm{T}}$, is obtained upon linearizing the relation $\bar{\boldsymbol{\sigma}}\{\bar{\boldsymbol{\epsilon}}\}$ as follows:

$$\mathrm{d}\bar{\boldsymbol{\sigma}}\{\bar{\boldsymbol{\epsilon}}\} = \bar{\mathbf{E}}_{\mathrm{T}}\{\bar{\boldsymbol{\epsilon}}\} : \mathrm{d}\bar{\boldsymbol{\epsilon}} = \bar{\mathbf{E}}_{\mathrm{T}}\{\bar{\boldsymbol{\epsilon}}\} : \boldsymbol{\epsilon}[\,\mathrm{d}\bar{\boldsymbol{u}}] \tag{5.24}$$ {eq:4-114}

and it is computed by *linearization* of the RVE-problem, which leads to a *sensitivity* or *tangent* problem. How to formulate and solve this sensitivity problem in practice depends strongly on the actual choice of prolongation condition (as will be discussed below). In particular, the specific variational setting for every type of prolongation condition is different.

5.2.3 Summary of (nested) FE^2-algorithm

The two-scale problem must be solved in a *nested* fashion, involving iterations on the macroscale (structural component) as well as the subscale (RVE) level: As a consequence the concept of "effective properties" has no obvious relevance any longer, which is a major difference/disadvantage as compared to the linear static problem. In terms of finite element analysis, the two-scale "nested FE-algorithm" or "FE^2-algorithm", may be described as follows, c.f. Figure 6.1.

1. Assume that a (nonequilibrium) macroscale displacement field $\bar{\boldsymbol{u}}$ (and $\bar{\boldsymbol{\epsilon}} = [\bar{\boldsymbol{u}} \otimes \boldsymbol{\nabla}]$) is given in the macroscale iteration procedure.

2. **Prolongation-homogenization**: For given $\bar{\boldsymbol{\epsilon}} = \bar{\boldsymbol{\epsilon}}(\bar{\boldsymbol{x}}_i)$ in each macroscale quadrature point with centroid $\bar{\boldsymbol{x}}_i$, typically Gauss-points in the macroscale FE-mesh, solve the nonlinear RVE-problem (with chosen prolongation conditions) for the subscale field $\boldsymbol{u}(\bar{\boldsymbol{x}}_i, \boldsymbol{x})$ and the homogenized (macroscale) stress $\bar{\boldsymbol{\sigma}}(\bar{\boldsymbol{x}}_i)$.

3. Check the macroscale residual. If convergence defined by $|\bar{R}| < TOL$ has been achieved, then stop, else compute a new (updated) value of the macroscale displacement $\bar{\boldsymbol{u}}$ (while using the macroscale ATS-tensor $\bar{\mathbf{E}}_{\mathrm{T}}$) and then return to 1.

Remark: The operation $\bar{\boldsymbol{\epsilon}} \to \boldsymbol{\epsilon}(\boldsymbol{x})$ is known as "prolongation", "dehomogenization" or "concentration". The operation $\boldsymbol{\sigma}(\boldsymbol{x}) \to \bar{\boldsymbol{\sigma}}$ is known as "homogenization". □

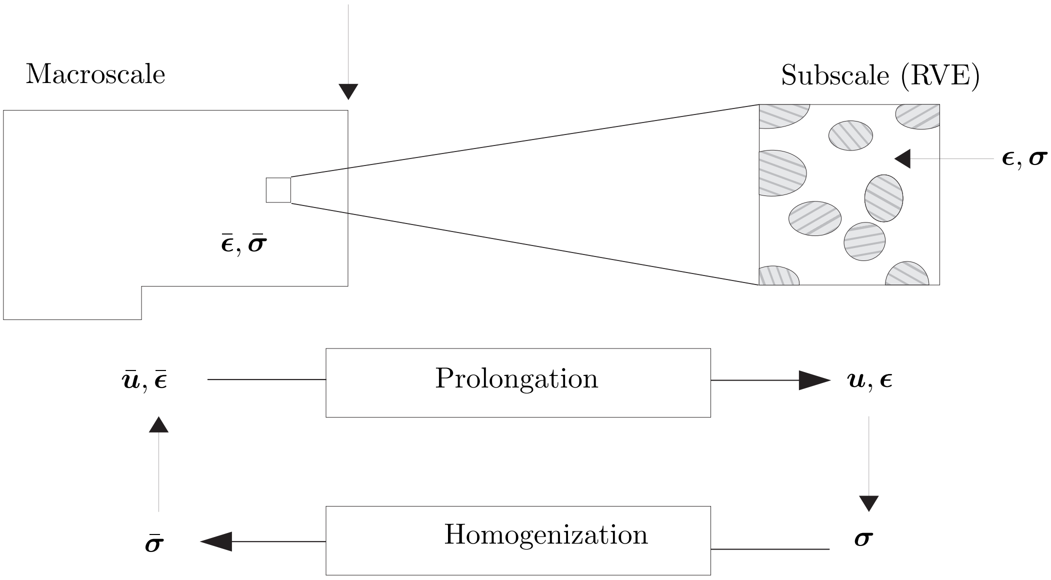


Figure 5.1: *Nested macro-micro iteration strategy characterizing computational homogenization for static stress problems.* {fig:ch4_fig1

As a preliminary to the subsequent presentations of different formulations of the RVE-problem, we introduce the following variational forms:

{eq:4-116a}
$$a_\square(\boldsymbol{u}; \delta\boldsymbol{u}) \overset{\text{def}}{=} \langle \boldsymbol{\sigma}(\boldsymbol{\epsilon}[\boldsymbol{u}]) : \boldsymbol{\epsilon}[\delta\boldsymbol{u}] \rangle_\square \tag{5.25}$$

{eq:4-116b}
$$c_\square(\boldsymbol{u}; \bar{\boldsymbol{\sigma}}) \overset{\text{def}}{=} \langle \boldsymbol{\epsilon}[\boldsymbol{u}] \rangle_\square : \bar{\boldsymbol{\sigma}} \tag{5.26}$$

Remark: In the context of the RVE-problem it is sufficient to set $\boldsymbol{u}^{\mathrm{M}} = \bar{\boldsymbol{\epsilon}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}]$. We may thus replace the operator format $\boldsymbol{u}^{\mathrm{M}}[\bar{\boldsymbol{u}}]$ with the simpler functional relation $\boldsymbol{u}^{\mathrm{M}}(\bar{\boldsymbol{\epsilon}})$ in what follows. $\square$

5.3 Dirichlet boundary conditions (DBC-problem)

5.3.1 DBC-problem

The subscale space-variational problem on the SVE associated with a typical macroscopic point $\bar{\boldsymbol{x}} \in \Omega$ can be phrased as follows: For given value of the macroscale strain $\bar{\boldsymbol{\epsilon}} \in \mathbb{R}^{3\times 3}_{\mathrm{sym}}$, find $\boldsymbol{u}^\mu \in \mathbb{U}_\square^{\mathrm{D},0}$ that solves

{eq:4-117}
$$a_\square(\boldsymbol{u}^{\mathrm{M}}(\bar{\boldsymbol{\epsilon}}) + \boldsymbol{u}^\mu; \delta\boldsymbol{u}) = 0 \quad \forall \delta\boldsymbol{u} \in \mathbb{U}_\square^{\mathrm{D},0}. \tag{5.27}$$

where the space $\mathbb{U}_\square^{\mathrm{D},0}$ was defined already in Chapter 3. When the solution has been found it is possible to compute $\bar{\boldsymbol{\sigma}}$ in a "post-processing step": $\bar{\boldsymbol{\sigma}} = \langle \boldsymbol{\sigma} \rangle_\square$.

The nonlinear problem (6.33) must be solved iteratively. Newton's iteration method for finding $\boldsymbol{u}^\mu$ then becomes: For $k = 1, 2, \ldots,$ compute

{eq:4-118}
$$\boldsymbol{u}^{\mu(k+1)} = \boldsymbol{u}^{\mu(k)} + \Delta\boldsymbol{u}^\mu \tag{5.28}$$

where the iterative updates $\Delta \boldsymbol{u}^{\mu} \in \mathbb{U}_{\square}^{\mathrm{D},0}$ are solved from the tangent equations

{eq:4-119} $$(a_{\square})'(\bullet^{(k)}; \delta \boldsymbol{u}, \Delta \boldsymbol{u}^{\mu}) = R_{\square}(\bullet^{(k)}; \delta \boldsymbol{u}) \quad \forall \delta \boldsymbol{u} \in \mathbb{U}_{\square}^{\mathrm{D},0} \tag{5.29}$$

until the residual $R_{\square}(\bullet^{(k)}; \delta \boldsymbol{u}) \stackrel{\mathrm{def}}{=} -a_{\square}(\bullet^{(k)}; \delta \boldsymbol{u})$ is sufficiently small. The tangent form $(a_{\square})'$ is given explicitly as[3]

$$(a_{\square})'(\bullet; \delta \boldsymbol{u}, \Delta \boldsymbol{u}) = \langle \boldsymbol{\epsilon}[\delta \boldsymbol{u}] : \mathbf{E}_{\mathrm{T}} : \boldsymbol{\epsilon}[\Delta \boldsymbol{u}^{\mu}] \rangle_{\square} \tag{5.30}$$ {eq:4-120}

5.3.2 Macroscale TS-tensor - Primal and dual formats

The macroscale TS-tensor, $\bar{\mathbf{E}}_{\mathrm{T}}$, is obtained for perturbations of the macroscale solution (expressed in terms of $\bar{\boldsymbol{\epsilon}}$). Like in the case of linear elasticity, as discussed in Chapter 3, we shall then need to compute "unit fluctuation fields" or, rather, *sensitivity fields*, corresponding to a unit variation of $\bar{\boldsymbol{\epsilon}}$. Hence, we shall need to compute the differential $\mathrm{d}\boldsymbol{u} = \boldsymbol{u}^{\mathrm{M}}(\mathrm{d}\bar{\boldsymbol{\epsilon}}) + \mathrm{d}\boldsymbol{u}^{\mu} = \boldsymbol{u}^{\mathrm{M}}(\mathrm{d}\bar{\boldsymbol{\epsilon}}) + (\boldsymbol{u}^{\mu})'\{\bar{\boldsymbol{\epsilon}}; \mathrm{d}\bar{\boldsymbol{\epsilon}}\}$ in terms of $\mathrm{d}\bar{\boldsymbol{\epsilon}}$. From the first order representation of $\boldsymbol{u}^{\mathrm{M}}$, we obtain

$$\boldsymbol{u}^{\mathrm{M}}(\mathrm{d}\bar{\boldsymbol{\epsilon}}) = \mathrm{d}\bar{\boldsymbol{\epsilon}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}] = \sum_{i,j=1}^{NDIM} \hat{\boldsymbol{u}}^{\mathrm{M}(ij)} \, \mathrm{d}\bar{\epsilon}_{ij} \tag{5.31}$$ {eq:4-122}

where the "unit displacement fields" $\hat{\boldsymbol{u}}^{\mathrm{M}(ij)}$ are given as

$$\hat{\boldsymbol{u}}^{\mathrm{M}(ij)} \stackrel{\mathrm{def}}{=} \boldsymbol{e}_i \otimes \boldsymbol{e}_j \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}] \tag{5.32}$$ {eq:4-123}

Upon using the identity $\bar{\boldsymbol{\sigma}} = \langle \boldsymbol{\sigma} \rangle_{\square}$ together with the relation (6.30), we obtain the representation of $\mathrm{d}\bar{\sigma}_{ij}$ as

$$\mathrm{d}\bar{\sigma}_{ij} = \mathrm{d}\left[\langle \boldsymbol{\sigma} : [\boldsymbol{e}_i \otimes \boldsymbol{e}_j] \rangle_{\square}\right] = \mathrm{d}\left[a_{\square}(\bullet; \hat{\boldsymbol{u}}^{\mathrm{M}(ij)})\right] = (a_{\square})'(\bullet; \hat{\boldsymbol{u}}^{\mathrm{M}(ij)}, \mathrm{d}\boldsymbol{u}) \tag{5.33}$$ {eq:4-124}

Next, we conclude that the state equation (6.33) must hold for $\bar{\boldsymbol{\epsilon}}$ as well as for a perturbed state $\bar{\boldsymbol{\epsilon}} + \mathrm{d}\bar{\boldsymbol{\epsilon}}$. However, a given change $\mathrm{d}\bar{\boldsymbol{\epsilon}}$ gives rise to changes $\mathrm{d}\boldsymbol{u}^{\mu} \in \mathbb{U}_{\square}^{\mathrm{D},0}$, whereby we obtain the relation

$$a_{\square}(\boldsymbol{u}^{\mathrm{M}}(\bar{\boldsymbol{\epsilon}}) + \boldsymbol{u}^{\mu} + \boldsymbol{u}^{\mathrm{M}}(\mathrm{d}\bar{\boldsymbol{\epsilon}}) + \mathrm{d}\boldsymbol{u}^{\mu}; \delta \boldsymbol{u}) = 0 \quad \forall \delta \boldsymbol{u} \in \mathbb{U}_{\square}^{\mathrm{D},0}. \tag{5.34}$$ {eq:4-125}

where it is emphasized that $\boldsymbol{u}^{\mu}$ depends on $\bar{\boldsymbol{\epsilon}}$ in an implicit fashion; $\boldsymbol{u}^{\mu} = \boldsymbol{u}^{\mu}\{\bar{\boldsymbol{\epsilon}}\}$.

Now, upon linearizing in (6.42) and subtracting (6.33) from the resulting expression, we obtain the appropriate tangent problem:

$$(a_{\square})'(\bullet; \delta \boldsymbol{u}, \boldsymbol{u}^{\mathrm{M}}(\mathrm{d}\bar{\boldsymbol{\epsilon}}) + \mathrm{d}\boldsymbol{u}^{\mu}) = 0 \quad \forall \delta \boldsymbol{u} \in \mathbb{U}_{\square}^{\mathrm{D},0}. \tag{5.35}$$ {eq:4-126}

from which $\mathrm{d}\boldsymbol{u}^{\mu}$ can be solved for any given $\mathrm{d}\bar{\boldsymbol{\epsilon}}$. In analogy with the definition of $\hat{\boldsymbol{u}}^{\mathrm{M}(ij)}$ in (6.39), we then introduce the "unit fields", or sensitivities, $\hat{\boldsymbol{u}}^{\mu(ij)}$, due to a unit value of the components $\mathrm{d}\bar{\epsilon}_{ij}$, via the *ansatz*

$$\mathrm{d}\boldsymbol{u}^{\mu} = \sum_{i,j} \hat{\boldsymbol{u}}^{\mu(ij)} \, \mathrm{d}\bar{\epsilon}_{ij} \tag{5.36}$$ {eq:4-127}

which may be inserted into (6.43), together with (6.39), to give the equations that must hold for $k, l = 1, 2, ..., NDIM$:

$$(a_{\square})'(\bullet; \delta \boldsymbol{u}, \hat{\boldsymbol{u}}^{\mu(kl)}) = -(a_{\square})'(\bullet; \delta \boldsymbol{u}, \hat{\boldsymbol{u}}^{\mathrm{M}(kl)}) \quad \forall \delta \boldsymbol{u} \in \mathbb{U}_{\square}^{\mathrm{D},0} \tag{5.37}$$ {eq:4-128}

[3] $\mathbf{E}_{\mathrm{T}}$ or $\mathbf{E}_{\square,\mathrm{T}}$?

Two different options are available in practice for computing the components of $\bar{\mathbf{E}}_{\rm T}$: (i) The "primal approach" was originally proposed in a discrete format in the context of the full (unrestricted) space of deformations pertinent to 3D modeling and plane strain, cf. Miehe and Koch , Temizer and Wriggers . This approach was then formulated in a continuous variational setting by Larsson and Runesson , Lillbacka et al. . (ii) The "dual approach" was proposed by Larsson and Runesson in the very same continuous variational setting. It is particularly attractive in conjunction with adaptive computations aiming for control of the subscale discretization error and for the computation of the dual load.

Primal approach for computing the ATS tensor

In the primal approach, the "unit fields" $\hat{\boldsymbol{u}}^{\mu(ij)}$ are solved from (6.44) and inserted into (6.41) to give the expression

{eq:4-130}
$$\begin{aligned} \mathrm{d}\bar{\sigma}_{ij} &= \sum_{k,l=1}^{NDIM} \left[(a_\square)'(\bullet; \hat{\boldsymbol{u}}^{\mathrm{M}(ij)}, \hat{\boldsymbol{u}}^{\mathrm{M}(kl)}) + (a_\square)'(\bullet; \hat{\boldsymbol{u}}^{\mathrm{M}(ij)}, \hat{\boldsymbol{u}}^{\mu(kl)}) \right] \mathrm{d}\bar{\epsilon}_{kl} \\ &= \sum_{k,l=1}^{NDIM} (a_\square)'(\bullet; \hat{\boldsymbol{u}}^{\mathrm{M}(ij)}, \hat{\boldsymbol{u}}^{(kl)}) \mathrm{d}\bar{\epsilon}_{kl} \end{aligned} \tag{5.38}$$

where we introduced $\hat{\boldsymbol{u}}^{(ij)} \overset{\rm def}{=} \hat{\boldsymbol{u}}^{\mathrm{M}(ij)} + \hat{\boldsymbol{u}}^{\mu(kl)}$.

Hence, with known values of $\hat{\boldsymbol{u}}^{\mu(ij)}$, for $i, j = 1, 2, ..., NDIM$, we are in the position to compute the components of $\bar{\mathbf{E}}_{\rm T}$ explicitly from (6.47) as

{eq:4-131}
$$\begin{aligned} (\bar{\mathbf{E}}_{\rm T})_{ijkl} &= (a_\square)'(\bullet; \hat{\boldsymbol{u}}^{\mathrm{M}(ij)}, \hat{\boldsymbol{u}}^{\mathrm{M}(kl)}) + (a_\square)'(\bullet; \hat{\boldsymbol{u}}^{\mathrm{M}(ij)}, \hat{\boldsymbol{u}}^{\mu(kl)}) \\ &= \langle (\mathbf{E}_{\rm T})_{ijkl} \rangle_\square + \left\langle \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{\mathrm{M}(ij)}] : \mathbf{E}_{\rm T} : \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{\mu(kl)}] \right\rangle_\square \\ &= \left\langle \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{\mathrm{M}(ij)}] : \mathbf{E}_{\rm T} : \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{(kl)}] \right\rangle_\square \end{aligned} \tag{5.39}$$

where the following identities were used:

{eq:42a}
$$(a_\square)'(\bullet; \hat{\boldsymbol{u}}^{\mathrm{M}(ij)}, \hat{\boldsymbol{u}}^{\mathrm{M}(kl)}) = \langle (\mathbf{E}_{\rm T})_{ijkl} \rangle_\square , \tag{5.40}$$

{eq:4-132}
$$(a_\square)'(\bullet; \hat{\boldsymbol{u}}^{\mathrm{M}(ij)}, \hat{\boldsymbol{u}}^{\mu(kl)}) = \left\langle \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{\mathrm{M}(ij)}] : \mathbf{E}_{\rm T} : \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{\mu(kl)}] \right\rangle_\square \tag{5.41}$$

Dual approach for computing the ATS tensor

In the dual approach, we compute the dual solutions $\hat{\boldsymbol{u}}^{*(ij)} \in \mathbb{U}_\square$, for $i, j = 1, 2, ..., NDIM$ from the pertinent dual equations

{eq:4-134}
$$(a_\square)'(\bullet; \hat{\boldsymbol{u}}^{*(ij)}, \delta\boldsymbol{u}) = (a_\square)'(\bullet; \hat{\boldsymbol{u}}^{\mathrm{M}(ij)}, \delta\boldsymbol{u}) \quad \forall \delta\boldsymbol{u} \in \mathbb{U}_\square \tag{5.42}$$

With the choice $\delta\boldsymbol{u} = \hat{\boldsymbol{u}}^{\mu(kl)}$ in (6.51), and with $\delta\boldsymbol{u} = \hat{\boldsymbol{u}}^{*(ij)}$ in (6.44), we may combine these results to obtain the identity

{eq:4-134a}
$$(a_\square)'(\bullet; \hat{\boldsymbol{u}}^{\mathrm{M}(ij)}, \hat{\boldsymbol{u}}^{\mu(kl)}) = -(a_\square)'(\bullet; \hat{\boldsymbol{u}}^{*(ij)}, \hat{\boldsymbol{u}}^{\mathrm{M}(kl)}) \tag{5.43}$$

whereby it is possible to replace the 2nd term of the 1st row in (6.47) obtain

{eq:4-135}
$$\mathrm{d}\bar{\sigma}_{ij} = \sum_{k,l} [(a_\square)'(\bullet; \hat{\boldsymbol{u}}^{\mathrm{M}(ij)}, \hat{\boldsymbol{u}}^{\mathrm{M}(kl)}) - (a_\square)'(\bullet; \hat{\boldsymbol{u}}^{*(ij)}, \hat{\boldsymbol{u}}^{\mathrm{M}(kl)})] \mathrm{d}\bar{\epsilon}_{kl} \tag{5.44}$$

Finally, we may express the components of $\bar{\mathsf{E}}_{\mathrm{T}}$ explicitly from (6.53) as

{eq:4-136}

$$(\bar{\mathsf{E}}_{\mathrm{T}})_{ijkl} = (a_{\Box})'(\bullet;\hat{\boldsymbol{u}}^{\mathrm{M}(ij)},\hat{\boldsymbol{u}}^{\mathrm{M}(kl)}) - (a_{\Box})'(\bullet;\hat{\boldsymbol{u}}^{*(ij)},\hat{\boldsymbol{u}}^{\mathrm{M}(kl)}) = \langle(\mathsf{E}_{\mathrm{T}})_{ijkl}\rangle_{\Box} - \left\langle \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{*(ij)}] : \mathsf{E}_{\mathrm{T}} : \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{\mathrm{M}(kl)}]\right\rangle_{\Box} \tag{5.45}$$

In comparison with the "primal approach", the advantage is that there is no need to solve for $\hat{\boldsymbol{u}}^{\mu(ij)}$ from (6.44), which in practice is done using the current FE-discretization on $\Omega_{\Box}$. Computing the dual fields $\hat{\boldsymbol{u}}^{*(ij)}$ is of the same computational effort as solving for $\hat{\boldsymbol{u}}^{\mu(ij)}$. However, the essential feature is that the same dual solutions can be used both for error control and the ATS-tensor computation. This shows the power of duality!

Remark: In the special case that E_{T} possesses major symmetry, i.e. $(\mathsf{E}_{\mathrm{T}})_{ijkl} = (\mathsf{E}_{\mathrm{T}})_{klij}$, then we obtain the identity $\hat{\boldsymbol{u}}^{*(ij)} = -\hat{\boldsymbol{u}}^{\mu(ij)}$. Clearly, in this case we may use the primal perturbation (or the dual fields) for both error estimation and ATS-tensor computation. It is sufficient to utilize *one* set of solution fields for both purposes. □

5.3.3 FE-approximation – Matrix format (in 2D)

Preliminaries

Using the notation introduced in Chapter 3, we recall the nodal expansion of the FE-approximation $\boldsymbol{u}_h$:

$$\boldsymbol{u}_h = \sum_{k=1}^{\mathrm{NVAR}} \boldsymbol{N}_k(\underline{\boldsymbol{u}})_k = \sum_{k=1}^{\mathrm{NVAR_i}} \boldsymbol{N}^{\mathrm{i}}_k(\underline{\boldsymbol{u}}^{\mathrm{i}})_k + \sum_{k=1}^{\mathrm{NVAR_b}} \boldsymbol{N}^{\mathrm{b}}_k(\underline{\boldsymbol{u}}^{\mathrm{b}})_k \tag{5.46}$$ {eqa1}

in standard fashion, where $\underline{\boldsymbol{u}}^{\mathrm{i}}$ and $\underline{\boldsymbol{u}}^{\mathrm{b}}$ are column vectors containing all *internal* and *boundary* variables, respectively, such that the complete set of nodal variables are thus

$$\underline{\boldsymbol{u}} = \begin{bmatrix} \underline{\boldsymbol{u}}^{\mathrm{i}} \\ \underline{\boldsymbol{u}}^{\mathrm{b}} \end{bmatrix}. \tag{5.47}$$ {eq:appB_1_

The macroscale strain $\bar{\boldsymbol{\epsilon}}$ and stress $\bar{\boldsymbol{\sigma}}$ are given in matrix notation as

$$\underline{\bar{\boldsymbol{\epsilon}}} = \begin{bmatrix} \bar{\epsilon}_{11} \\ \bar{\epsilon}_{22} \\ \bar{\gamma}_{12} \end{bmatrix}, \quad \underline{\bar{\boldsymbol{\sigma}}} = \begin{bmatrix} \bar{\sigma}_{11} \\ \bar{\sigma}_{22} \\ \bar{\sigma}_{12} \end{bmatrix} \tag{5.48}$$ {eq:appB_1_

We split the nodal variables into "macroscale" and "fluctuation" parts as follows:

$$\underline{\boldsymbol{u}} = \begin{bmatrix} \underline{\boldsymbol{u}}^{\mathrm{i}} \\ \underline{\boldsymbol{u}}^{\mathrm{b}} \end{bmatrix} = \begin{bmatrix} \underline{\boldsymbol{u}}^{\mathrm{M,i}} + \underline{\boldsymbol{u}}^{\mu,\mathrm{i}} \\ \underline{\boldsymbol{u}}^{\mathrm{M,b}} + \underbrace{\underline{\boldsymbol{u}}^{\mu,\mathrm{b}}}_{=\underline{\mathbf{0}}} \end{bmatrix} = \begin{bmatrix} \hat{\underline{\boldsymbol{u}}}^{\mathrm{M,i}} \\ \hat{\underline{\boldsymbol{u}}}^{\mathrm{M,b}} \end{bmatrix} \underline{\bar{\boldsymbol{\epsilon}}} + \begin{bmatrix} \underline{\boldsymbol{u}}^{\mu,\mathrm{i}} \\ \underline{\mathbf{0}} \end{bmatrix} \tag{5.49}$$ {eq:appB_6a

In (5.49), we introduced nodal variables $\hat{\underline{\boldsymbol{u}}}^{\mathrm{M,i}(ij)}$ and $\hat{\underline{\boldsymbol{u}}}^{\mathrm{M,b}(ij)}$ that correspond to "unit macroscale deformations", i. e. nodal displacements that correspond to $\bar{\epsilon}_{ij} = 1$ for $i, j = 1, 2, ..., NDIM$. In the 2D-case, we have

$$\underline{\boldsymbol{u}}^{\mathrm{M,i}} = \hat{\underline{\boldsymbol{u}}}^{\mathrm{M,i}}\underline{\bar{\boldsymbol{\epsilon}}} = \left[\ \hat{\underline{\boldsymbol{u}}}^{\mathrm{M,i}(11)}, \hat{\underline{\boldsymbol{u}}}^{\mathrm{M,i}(22)}, \hat{\underline{\boldsymbol{u}}}^{\mathrm{M,i}(12)}\ \right] \begin{bmatrix} \bar{\epsilon}_{11} \\ \bar{\epsilon}_{22} \\ \bar{\gamma}_{12} \end{bmatrix} \tag{5.50}$$ {eq:appB_2a

$$\underline{\boldsymbol{u}}^{\mathrm{M,b}} = \underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}} \underline{\bar{\boldsymbol{\epsilon}}} = \left[\ \underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b(11)}}, \underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b(22)}}, \underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b(12)}}\ \right] \begin{bmatrix} \bar{\epsilon}_{11} \\ \bar{\epsilon}_{22} \\ \bar{\gamma}_{12} \end{bmatrix} \tag{5.51}$$

{eq:appB_2b}

as elaborated on in Chapter 3.

In order to establish variationally consistent nodal forces, the test function $\delta \boldsymbol{u}$ is given as

q:appB_7_1}

$$\delta \boldsymbol{u}_h = \sum_{k=1}^{\mathrm{NVAR}} \boldsymbol{N}_k (\delta \underline{\boldsymbol{u}})_k = \sum_{k=1}^{\mathrm{NVAR_i}} \boldsymbol{N}_k^{\mathrm{i}} (\delta \underline{\boldsymbol{u}}^{\mathrm{i}})_k + \sum_{k=1}^{\mathrm{NVAR_b}} \boldsymbol{N}_k^{\mathrm{b}} (\delta \underline{\boldsymbol{u}}^{\mathrm{b}})_k \tag{5.52}$$

and the corresponding nodal values are decomposed as

q:appB_7_2}

$$\delta \underline{\boldsymbol{u}} = \begin{bmatrix} \delta \underline{\boldsymbol{u}}^{\mathrm{i}} \\ \delta \underline{\boldsymbol{u}}^{\mathrm{b}} \end{bmatrix} \tag{5.53}$$

We then obtain

{eq:appB_8}

$$\begin{aligned} a_{\square}(\boldsymbol{u}_h; \delta \boldsymbol{u}_h) = \langle \boldsymbol{\epsilon}[\delta \boldsymbol{u}_h] : \boldsymbol{\sigma} \rangle_{\square} &= \sum_{i=1}^{\mathrm{NVAR_u}} (\delta \underline{\boldsymbol{u}})_i \langle \boldsymbol{B}_i : \boldsymbol{\sigma} \rangle_{\square} = \sum_{i=1}^{\mathrm{NVAR_u}} (\delta \underline{\boldsymbol{u}})_i (\underline{\boldsymbol{f}})_i \\ &= [\delta \underline{\boldsymbol{u}}]^{\mathrm{T}} \underline{\boldsymbol{f}} = [\delta \underline{\boldsymbol{u}}^{\mathrm{i}}]^{\mathrm{T}} \underline{\boldsymbol{f}}^{\mathrm{i}} + [\delta \underline{\boldsymbol{u}}^{\mathrm{b}}]^{\mathrm{T}} \underline{\boldsymbol{f}}^{\mathrm{b}} \end{aligned} \tag{5.54}$$

whereby it follows that the (internal) nodal forces $(\underline{\boldsymbol{f}})_i$ are given as

{eq:appB_9}

$$(\underline{\boldsymbol{f}})_i = \langle \boldsymbol{B}_i : \boldsymbol{\sigma} \rangle_{\square} \quad i, j = 1, 2, ..., \mathrm{NVAR} \tag{5.55}$$

Moreover, the nodal force column matrix (column vector) is partitioned corresponding to the internal and boundary variables:

eq:appB_10}

$$\underline{\boldsymbol{f}}(\underline{\boldsymbol{u}}^{\mathrm{i}}, \underline{\boldsymbol{u}}^{\mathrm{b}}) = \begin{bmatrix} \underline{\boldsymbol{f}}^{\mathrm{i}}(\underline{\boldsymbol{u}}^{\mathrm{i}}, \underline{\boldsymbol{u}}^{\mathrm{b}}) \\ \underline{\boldsymbol{f}}^{\mathrm{b}}(\underline{\boldsymbol{u}}^{\mathrm{i}}, \underline{\boldsymbol{u}}^{\mathrm{b}}) \end{bmatrix} \tag{5.56}$$

Linearizing (5.56), we obtain the AT-stiffness relation

eq:appB_12}

$$\begin{bmatrix} \mathrm{d}\underline{\boldsymbol{f}}^{\mathrm{i}} \\ \mathrm{d}\underline{\boldsymbol{f}}^{\mathrm{b}} \end{bmatrix} = \begin{bmatrix} \underline{\boldsymbol{K}}_{\mathrm{T}}^{\mathrm{ii}} & \underline{\boldsymbol{K}}_{\mathrm{T}}^{\mathrm{ib}} \\ \underline{\boldsymbol{K}}_{\mathrm{T}}^{\mathrm{bi}} & \underline{\boldsymbol{K}}_{\mathrm{T}}^{\mathrm{bb}} \end{bmatrix} \begin{bmatrix} \mathrm{d}\underline{\boldsymbol{u}}^{\mathrm{i}} \\ \mathrm{d}\underline{\boldsymbol{u}}^{\mathrm{b}} \end{bmatrix} \tag{5.57}$$

The total stiffness matrix $\underline{\boldsymbol{K}}_{\mathrm{T}}$ is defined in terms of its matrix elements $(\underline{\boldsymbol{K}}_{\mathrm{T}})_{ij}$ as

eq:appB_13}

$$(\underline{\boldsymbol{K}}_{\mathrm{T}})_{ij} = \langle \boldsymbol{B}_i : \mathsf{E}_{\mathrm{T}} : \boldsymbol{B}_j \rangle_{\square} \quad i, j = 1, 2, ..., \mathrm{NVAR} \tag{5.58}$$

Remark: In the case the underlying algorithmic stiffness tensor E_{T} has major symmetry, then the tangent stiffness matrix $\underline{\boldsymbol{K}}_{\mathrm{T}}$ is symmetrical, i e. $\underline{\boldsymbol{K}}_{\mathrm{T}}^{\mathrm{bi}} = [\underline{\boldsymbol{K}}_{\mathrm{T}}^{\mathrm{ib}}]^{\mathrm{T}}$. $\square$

SVE-problem – Formulation and solution

We are now in the position to formulate the FE-problem in (6.33) in matrix format. First, introduce the actual boundary conditions

appB_11_1}

$$\underline{\boldsymbol{u}}^{\mathrm{b}} = \underline{\boldsymbol{u}}^{\mathrm{M,b}} \quad [\underline{\boldsymbol{u}}^{\mu,\mathrm{b}} = \underline{\boldsymbol{0}}], \quad \delta \underline{\boldsymbol{u}}^{\mathrm{b}} = \underline{\boldsymbol{0}} \tag{5.59}$$

Hence, the SVE-problem reduces to vanishing (internal) forces on the internal nodes:

eq:appB_11}

$$\underline{\boldsymbol{f}}^{\mathrm{i}}(\underline{\boldsymbol{u}}^{\mathrm{i}}, \underline{\boldsymbol{u}}^{\mathrm{b}}) = \underline{\boldsymbol{0}} \tag{5.60}$$

This set of nonlinear algebraic equations can be solved for the unknown variables $\underline{\boldsymbol{u}}^{\mathrm{i}}$ (or, rather $\underline{\boldsymbol{u}}^{\mu,\mathrm{i}}$), for given value of the macrostrain $\bar{\boldsymbol{\epsilon}}$, using Newton iterations. Each iterative increment has the properties

{eq:appB_14a}
$$\Delta\underline{\boldsymbol{u}}^{\mathrm{i}} = \underbrace{\Delta\underline{\boldsymbol{u}}^{\mathrm{M,i}}}_{=\underline{\mathbf{0}}} + \Delta\underline{\boldsymbol{u}}^{\mu,\mathrm{i}} = \Delta\underline{\boldsymbol{u}}^{\mu,\mathrm{i}} \tag{5.61}$$

{eq:appB_14b}
$$\Delta\underline{\boldsymbol{u}}^{\mathrm{b}} = \underbrace{\Delta\underline{\boldsymbol{u}}^{\mathrm{M,b}}}_{=\underline{\mathbf{0}}} = \underline{\mathbf{0}} \tag{5.62}$$

Newton's iteration method for finding $\underline{\boldsymbol{u}}^{\mu,\mathrm{i}}$ then becomes: For $k = 1, 2, \ldots,$ compute

$$\underline{\boldsymbol{u}}^{\mu,\mathrm{i}(k+1)} = \underline{\boldsymbol{u}}^{\mu,\mathrm{i}(k)} + \Delta\underline{\boldsymbol{u}}^{\mu,\mathrm{i}} \tag{5.63}$$ {eq:appB_15

where the iterative updates $\Delta\underline{\boldsymbol{u}}^{\mu,\mathrm{i}}$ are solved from the tangent equations

$$\underline{\boldsymbol{K}}_{\mathrm{T}}^{\mathrm{ii}(k)}\Delta\underline{\boldsymbol{u}}^{\mu,\mathrm{i}} = -\underline{\boldsymbol{f}}^{\mathrm{i}(k)}, \quad \underline{\boldsymbol{f}}^{\mathrm{i}(k)} = \underline{\boldsymbol{f}}^{\mathrm{i}}(\underline{\boldsymbol{u}}^{\mathrm{i}(k)}, \underline{\boldsymbol{u}}^{\mathrm{b}}) \tag{5.64}$$ {eq:appB_16

When $\underline{\boldsymbol{u}}^{\mu,\mathrm{i}}$ is known, it is possible to to compute the macroscale stress $\bar{\boldsymbol{\sigma}}$ in a post-processing step. Firstly, from (5.54), we have the general relation for any given choice of $\delta\boldsymbol{u}_h$ (and $\boldsymbol{\epsilon}[\delta\boldsymbol{u}_h]$):

$$\langle\boldsymbol{\epsilon}[\delta\boldsymbol{u}_h] : \boldsymbol{\sigma}\rangle_{\square} = [\delta\underline{\boldsymbol{u}}]^{\mathrm{T}}\underline{\boldsymbol{f}} \tag{5.65}$$ {eq:appB_16

Setting $\delta\boldsymbol{u}_h = \hat{\boldsymbol{u}}^{\mathrm{M}(ij)}$ with nodal values $\underline{\hat{\boldsymbol{u}}}^{\mathrm{M}(ij)}$, which gives $\boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{\mathrm{M}(ij)}] = (\boldsymbol{e}_i \otimes \boldsymbol{e}_j)^{\mathrm{sym}}$, we obtain

$$\bar{\sigma}_{ij} = \langle[\boldsymbol{e}_i \otimes \boldsymbol{e}_j] : \boldsymbol{\sigma}\rangle_{\square} = \left[\underline{\hat{\boldsymbol{u}}}^{\mathrm{M}(ij)}\right]^{\mathrm{T}}\underline{\boldsymbol{f}} \tag{5.66}$$ {eq:appB_17

Hence

$$\begin{aligned} \underline{\bar{\boldsymbol{\sigma}}} = &= \left[\underline{\hat{\boldsymbol{u}}}^{\mathrm{M}}\right]^{\mathrm{T}}\underline{\boldsymbol{f}} \\ &= \left[\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,i}}\right]^{\mathrm{T}}\underbrace{\underline{\boldsymbol{f}}^{\mathrm{i}}}_{=\mathbf{0}} + \left[\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}}\right]^{\mathrm{T}}\underline{\boldsymbol{f}}^{\mathrm{b}} = \left[\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}}\right]^{\mathrm{T}}\underline{\boldsymbol{f}}^{\mathrm{b}} \end{aligned} \tag{5.67}$$ {eq:appB_18

where the matrix $\underline{\hat{\boldsymbol{u}}}^{\mathrm{M}}$ is given as

$$\underline{\hat{\boldsymbol{u}}}^{\mathrm{M}} = \left[\ \underline{\hat{\boldsymbol{u}}}^{\mathrm{M}(11)}, \quad \underline{\hat{\boldsymbol{u}}}^{\mathrm{M}(12)}, \quad \underline{\hat{\boldsymbol{u}}}^{\mathrm{M}(22)}\ \right] \tag{5.68}$$ {eq:appB_18

Remark: The result in Eq. (5.67) pertains to a discrete form of the stress identity in Eq. (2.53), in the sence that it only evaluates reaction forces on the boundary of the SVE. Note, however, that the terms in $\underline{\boldsymbol{f}}^{\mathrm{b}}$ are evaluated using *volume* integrals. Approximating $\boldsymbol{t}$ in (2.53) on the boundary from a finite element approximation yields poor numerical accuracy, and is thus not suitable. □

Computing the macroscale tangent stiffness in practice

Next, we establish the macroscale tangent stiffness matrix from the component expression in (6.47) pertinent to the Voigt matrix relation

$$\mathrm{d}\underline{\bar{\boldsymbol{\sigma}}} = \underline{\bar{\mathbf{E}}}_{\square,\mathrm{T}}\,\mathrm{d}\underline{\bar{\boldsymbol{\epsilon}}} \tag{5.69}$$ {eq:appB_19

In order to establish $\bar{\underline{\mathbf{E}}}_{\square,\mathrm{T}}$, we first need to introduce the sensitivities of the nodal vectors $\underline{\boldsymbol{u}}^{\mathrm{i}}$ and $\underline{\boldsymbol{u}}^{\mathrm{b}}$ for a change in the "control variable" $\bar{\underline{\boldsymbol{\epsilon}}}$. To this end we introduce the sensitivity relation

$$\mathrm{d}\underline{\boldsymbol{u}}^{\mu,\mathrm{i}} = \hat{\underline{\boldsymbol{u}}}^{\mu,\mathrm{i}}\,\mathrm{d}\bar{\underline{\boldsymbol{\epsilon}}} \tag{5.70}$$ {eq:appB_20}

in addition to the already established

$$\mathrm{d}\underline{\boldsymbol{u}}^{\mathrm{M,i}} = \hat{\underline{\boldsymbol{u}}}^{\mathrm{M,i}}\,\mathrm{d}\bar{\underline{\boldsymbol{\epsilon}}}, \quad \mathrm{d}\underline{\boldsymbol{u}}^{\mathrm{M,b}} = \hat{\underline{\boldsymbol{u}}}^{\mathrm{M,b}}\,\mathrm{d}\bar{\underline{\boldsymbol{\epsilon}}} \tag{5.71}$$ {eq:appB_21}

where $\hat{\underline{\boldsymbol{u}}}^{\mathrm{M},\bullet}$ was given in (**??**). With the expressions in (5.70), we obtain from (5.49)

$$\mathrm{d}\underline{\boldsymbol{u}}^{\mathrm{i}} = \underbrace{\left[\hat{\underline{\boldsymbol{u}}}^{\mathrm{M,i}} + \hat{\underline{\boldsymbol{u}}}^{\mu,\mathrm{i}}\right]}_{\hat{\underline{\boldsymbol{u}}}^{\mathrm{i}}}\mathrm{d}\bar{\underline{\boldsymbol{\epsilon}}}, \quad \mathrm{d}\underline{\boldsymbol{u}}^{\mathrm{b}} = \hat{\underline{\boldsymbol{u}}}^{\mathrm{M,b}}\,\mathrm{d}\bar{\underline{\boldsymbol{\epsilon}}} \tag{5.72}$$ {eq:appB_22}

Equilibrium for sensitivities gives, corresponding to the first row in (5.57), the equation for $\hat{\underline{\boldsymbol{u}}}^{\mathrm{i}}$ as

q:appB_23} $$\mathrm{d}\underline{\boldsymbol{f}}^{\mathrm{i}} = \underline{\mathbf{0}} \quad \Rightarrow \quad \underline{\boldsymbol{K}}_{\mathrm{T}}^{\mathrm{ii}}\hat{\underline{\boldsymbol{u}}}^{\mathrm{i}} + \underline{\boldsymbol{K}}_{\mathrm{T}}^{\mathrm{ib}}\hat{\underline{\boldsymbol{u}}}^{\mathrm{M,b}} = \underline{\mathbf{0}} \quad \Rightarrow \quad \underline{\boldsymbol{K}}_{\mathrm{T}}^{\mathrm{ii}}\hat{\underline{\boldsymbol{u}}}^{\mathrm{i}} = -\underline{\boldsymbol{K}}_{\mathrm{T}}^{\mathrm{ib}}\hat{\underline{\boldsymbol{u}}}^{\mathrm{M,b}} \tag{5.73}$$

This equation is readily seen to correspond exactly to that of solving a few FE-problems on the SVE with different prescribed boundary displacements corresponding to the unit deformation fields. Formally, the solution of (5.73) can be written as

q:appB_24} $$\hat{\underline{\boldsymbol{u}}}^{\mathrm{i}} = -\left[\underline{\boldsymbol{K}}_{\mathrm{T}}^{\mathrm{ii}}\right]^{-1}\underline{\boldsymbol{K}}_{\mathrm{T}}^{\mathrm{ib}}\hat{\underline{\boldsymbol{u}}}^{\mathrm{M,b}} \tag{5.74}$$

From a computational point of view, it is quite obvious that computing the inverse of $\underline{\boldsymbol{K}}_{\mathrm{T}}^{\mathrm{ii}}$ is far more expensive than solving the system of FE-equations in (5.73).

We next use the relation for $\bar{\underline{\boldsymbol{\sigma}}}$ in (5.67) to obtain

q:appB_25} $$\mathrm{d}\bar{\underline{\boldsymbol{\sigma}}} = \left[\hat{\underline{\boldsymbol{u}}}^{\mathrm{M,b}}\right]^{\mathrm{T}}\mathrm{d}\underline{\boldsymbol{f}}^{\mathrm{b}} = \underbrace{\left[\hat{\underline{\boldsymbol{u}}}^{\mathrm{M,b}}\right]^{\mathrm{T}}\left[\underline{\boldsymbol{K}}_{\mathrm{T}}^{\mathrm{bi}}\hat{\underline{\boldsymbol{u}}}^{\mathrm{i}} + \underline{\boldsymbol{K}}_{\mathrm{T}}^{\mathrm{bb}}\hat{\underline{\boldsymbol{u}}}^{\mathrm{M,b}}\right]}_{\bar{\underline{\mathbf{E}}}_{\square,\mathrm{T}}}\mathrm{d}\bar{\underline{\boldsymbol{\epsilon}}} \tag{5.75}$$

whereby the macroscale tangent stiffness matrix is computed as

q:appB_26} $$\bar{\underline{\mathbf{E}}}_{\square,\mathrm{T}} = \left[\hat{\underline{\boldsymbol{u}}}^{\mathrm{M,b}}\right]^{\mathrm{T}}\left[\underline{\boldsymbol{K}}_{\mathrm{T}}^{\mathrm{bb}}\hat{\underline{\boldsymbol{u}}}^{\mathrm{M,b}} + \underline{\boldsymbol{K}}_{\mathrm{T}}^{\mathrm{bi}}\hat{\underline{\boldsymbol{u}}}^{\mathrm{i}}\right] \tag{5.76}$$

This is the operational format of $\bar{\underline{\mathbf{E}}}_{\square,\mathrm{T}}$ in practice when $\hat{\underline{\boldsymbol{u}}}^{\mathrm{i}}$ is solved from $(5.73)_2$.

Remark 1 *Formally, we may introduce (5.74) into (5.76) to obtain*

q:appB_27} $$\bar{\underline{\mathbf{E}}}_{\square,T} = \left[\hat{\underline{\boldsymbol{u}}}^{\mathrm{M,b}}\right]^{\mathrm{T}}\tilde{\underline{\boldsymbol{K}}}_{T}^{\mathrm{bb}}\hat{\underline{\boldsymbol{u}}}^{\mathrm{M,b}} \tag{5.77}$$

where $\tilde{\underline{\boldsymbol{K}}}^{\mathrm{bb}}$ is the part-inverted matrix defined as follows

q:appB_28} $$\tilde{\underline{\boldsymbol{K}}}_{T}^{\mathrm{bb}} = \underline{\boldsymbol{K}}_{T}^{\mathrm{bb}} - \underline{\boldsymbol{K}}_{T}^{\mathrm{bi}}\left[\underline{\boldsymbol{K}}_{T}^{\mathrm{ii}}\right]^{-1}\underline{\boldsymbol{K}}_{T}^{\mathrm{ib}} \tag{5.78}$$

□

As to the dimensions of the matrices involved, we have in the 2D-case:

$$
\begin{aligned}
dim(\underline{\hat{\boldsymbol{u}}}^{\mathrm{i}}) &= \mathrm{NVAR}_{\mathrm{i}} \times 3 \\
dim(\underline{\hat{\boldsymbol{u}}}^{\mathrm{b}}) &= \mathrm{NVAR}_{\mathrm{b}} \times 3 \\
dim(\underline{\boldsymbol{K}}_{\mathrm{T}}^{\mathrm{ii}}) &= \mathrm{NVAR}_{\mathrm{i}} \times \mathrm{NVAR}_{\mathrm{i}} \\
dim(\underline{\boldsymbol{K}}_{\mathrm{T}}^{\mathrm{ib}}) &= \mathrm{NVAR}_{\mathrm{i}} \times \mathrm{NVAR}_{\mathrm{b}} = dim(\left[\underline{\boldsymbol{K}}_{\mathrm{T}}^{\mathrm{bi}}\right]^{\mathrm{T}}) \\
dim(\underline{\boldsymbol{K}}_{\mathrm{T}}^{\mathrm{bb}}) &= \mathrm{NVAR}_{\mathrm{b}} \times \mathrm{NVAR}_{\mathrm{b}} = dim(\underline{\tilde{\boldsymbol{K}}}_{\mathrm{T}}^{\mathrm{bb}}) \\
dim(\underline{\bar{\mathbf{E}}}_{\square,\mathrm{T}}) &= 3 \times 3
\end{aligned} \tag{5.79}
$$
{eq:appB_29}

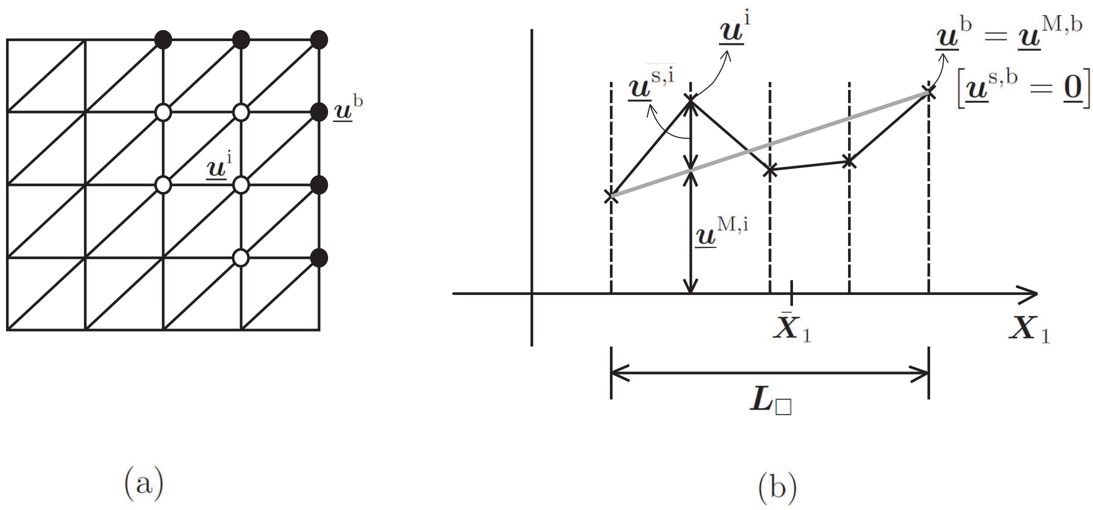


Figure 5.2: *(a) FE-mesh in SVE with internal nodes (open rings) and boundary nodes (filled rings). (b) Split of nodal values* $\underline{\mathbf{u}}$ *into* $\underline{\mathbf{u}}^{\mathrm{M}}$ *and* $\underline{\mathbf{u}}^{\mu}$ *for internal and boundary nodes. For the boundary nodes,* $\underline{\mathbf{u}}^{\mu,\mathrm{b}} = \underline{\mathbf{0}}$ *in the DBC-problem.* {fig:appB_f

5.4 Strongly periodic boundary conditions (SPBC-problem)

5.4.1 FE-approximation – Matrix format (in 2D)

Preliminaries

The starting point for the operational formulation is the following set of equilibrium equations {eq:appB_100}

$$\underline{\boldsymbol{f}}^{\mathrm{i}}(\underline{\boldsymbol{u}}^{\mathrm{i}}, \underline{\boldsymbol{u}}^{\mathrm{b}}) = \underline{\mathbf{0}} \tag{5.80a}$$ {eq:appB_100a

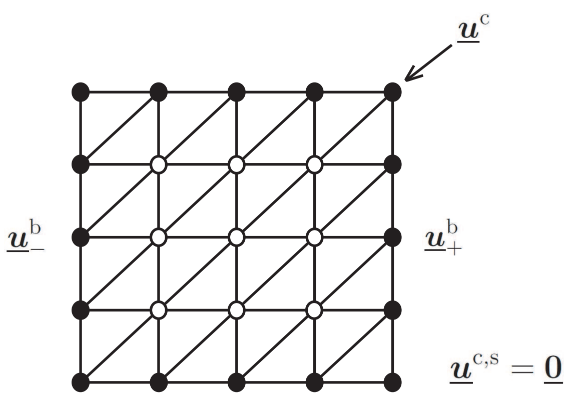
$$\underline{\boldsymbol{f}}^{\mathrm{b}}(\underline{\boldsymbol{u}}^{\mathrm{i}}, \underline{\boldsymbol{u}}^{\mathrm{b}}) - \underline{\boldsymbol{g}}^{\mathrm{b}} = \underline{\mathbf{0}} \tag{5.80b}$$ {eq:appB_100b

where the nodal column matrix $\underline{\boldsymbol{g}}^{\mathrm{b}}$ represents loading from the tractions on $\Gamma_\square$ (that may be considered as "reaction forces" at the outset). In order to formulate the periodicity condition and account for removed RBM, the column matrices pertinent to the boundary are split as follows:

:appB_101}

$$\underline{\boldsymbol{u}}^{\mathrm{b}} = \begin{bmatrix} \underline{\boldsymbol{u}}_+^{\mathrm{b}} \\ \underline{\boldsymbol{u}}_-^{\mathrm{b}} \\ \underline{\boldsymbol{u}}^{\mathrm{c}} \end{bmatrix}, \quad \underline{\boldsymbol{f}}^{\mathrm{b}} = \begin{bmatrix} \underline{\boldsymbol{f}}_+^{\mathrm{b}}(\underline{\boldsymbol{u}}^{\mathrm{i}}, \underline{\boldsymbol{u}}_+^{\mathrm{b}}, \underline{\boldsymbol{u}}_-^{\mathrm{b}}, \underline{\boldsymbol{u}}^{\mathrm{c}}) \\ \underline{\boldsymbol{f}}_-^{\mathrm{b}}(\underline{\boldsymbol{u}}^{\mathrm{i}}, \underline{\boldsymbol{u}}_+^{\mathrm{b}}, \underline{\boldsymbol{u}}_-^{\mathrm{b}}, \underline{\boldsymbol{u}}^{\mathrm{c}}) \\ \underline{\boldsymbol{f}}^{\mathrm{c}}(\underline{\boldsymbol{u}}^{\mathrm{i}}, \underline{\boldsymbol{u}}_+^{\mathrm{b}}, \underline{\boldsymbol{u}}_-^{\mathrm{b}}, \underline{\boldsymbol{u}}^{\mathrm{c}}) \end{bmatrix}, \quad \underline{\boldsymbol{g}}^{\mathrm{b}} = \begin{bmatrix} \underline{\boldsymbol{g}}_+^{\mathrm{b}} \\ \underline{\boldsymbol{g}}_-^{\mathrm{b}} \\ \underline{\boldsymbol{g}}^{\mathrm{c}} \end{bmatrix} \tag{5.81}$$

The displacements on the image and mirror boundary parts are denoted $\underline{\boldsymbol{u}}_+^{\mathrm{b}}$ and $\underline{\boldsymbol{u}}_-^{\mathrm{b}}$, respectively (as shown in Figure 5.3). The exception is the corner variables (4 corners in 2D) that are collected separately in $\underline{\boldsymbol{u}}^{\mathrm{c}}$ in order to provide for removed RBM.



appB_fig4}

Figure 5.3: *Strongly periodic FE-mesh in SVE with internal nodes (open rings) and boundary nodes (filled rings). Decomposition of boundary nodal values* $\underline{\boldsymbol{u}}^{\mathrm{b}}$ *into (i)* $\underline{\boldsymbol{u}}_+^{\mathrm{b}}$ *on image boundary* $\Gamma_\square^+$, *(ii)* $\underline{\boldsymbol{u}}_-^{\mathrm{b}}$ *on mirror boundary* $\Gamma_\square^-$ *and (iii)* $\underline{\boldsymbol{u}}^{\mathrm{c}}$ *in the corners.*

Linearizing the nodal forces, with the parametrization in (5.81_2), we obtain the tangent stiffness relation

$$\begin{bmatrix} \mathrm{d}\underline{\boldsymbol{f}}^{\mathrm{i}} \\ \mathrm{d}\underline{\boldsymbol{f}}^{\mathrm{b}}_{+} \\ \mathrm{d}\underline{\boldsymbol{f}}^{\mathrm{b}}_{-} \\ \mathrm{d}\underline{\boldsymbol{f}}^{\mathrm{c}} \end{bmatrix} = \begin{bmatrix} \underline{\boldsymbol{K}}^{\mathrm{ii}} & \underline{\boldsymbol{K}}^{\mathrm{ib}}_{+} & \underline{\boldsymbol{K}}^{\mathrm{ib}}_{-} & \underline{\boldsymbol{K}}^{\mathrm{ic}} \\ \underline{\boldsymbol{K}}^{\mathrm{bi}}_{+} & \underline{\boldsymbol{K}}^{\mathrm{bb}}_{++} & \underline{\boldsymbol{K}}^{\mathrm{bb}}_{+-} & \underline{\boldsymbol{K}}^{\mathrm{bc}}_{+} \\ \underline{\boldsymbol{K}}^{\mathrm{bi}}_{-} & \underline{\boldsymbol{K}}^{\mathrm{bb}}_{-+} & \underline{\boldsymbol{K}}^{\mathrm{bb}}_{--} & \underline{\boldsymbol{K}}^{\mathrm{bc}}_{-} \\ \underline{\boldsymbol{K}}^{\mathrm{ci}} & \underline{\boldsymbol{K}}^{\mathrm{cb}}_{+} & \underline{\boldsymbol{K}}^{\mathrm{cb}}_{-} & \underline{\boldsymbol{K}}^{\mathrm{cc}} \end{bmatrix} \begin{bmatrix} \mathrm{d}\underline{\boldsymbol{u}}^{\mathrm{i}} \\ \mathrm{d}\underline{\boldsymbol{u}}^{\mathrm{b}}_{+} \\ \mathrm{d}\underline{\boldsymbol{u}}^{\mathrm{b}}_{-} \\ \mathrm{d}\underline{\boldsymbol{u}}^{\mathrm{c}} \end{bmatrix} \tag{5.82}$$ {eq:appB_10

which can be abbreviated as

$$\begin{bmatrix} \mathrm{d}\underline{\boldsymbol{f}}^{\mathrm{i}} \\ \mathrm{d}\underline{\boldsymbol{f}}^{\mathrm{b}} \end{bmatrix} = \begin{bmatrix} \underline{\boldsymbol{K}}^{\mathrm{ii}} & \underline{\boldsymbol{K}}^{\mathrm{ib}} \\ \underline{\boldsymbol{K}}^{\mathrm{bi}} & \underline{\boldsymbol{K}}^{\mathrm{bb}} \end{bmatrix} \begin{bmatrix} \mathrm{d}\underline{\boldsymbol{u}}^{\mathrm{i}} \\ \mathrm{d}\underline{\boldsymbol{u}}^{\mathrm{b}} \end{bmatrix} \tag{5.83}$$ {eq:appB_10

where

$$\underline{\boldsymbol{K}}^{\mathrm{ib}} = \begin{bmatrix} \underline{\boldsymbol{K}}^{\mathrm{ib}}_{+} & \underline{\boldsymbol{K}}^{\mathrm{ib}}_{-} & \underline{\boldsymbol{K}}^{\mathrm{ic}} \end{bmatrix}, \quad \underline{\boldsymbol{K}}^{\mathrm{bi}} = \begin{bmatrix} \underline{\boldsymbol{K}}^{\mathrm{bi}}_{+} \\ \underline{\boldsymbol{K}}^{\mathrm{bi}}_{-} \\ \underline{\boldsymbol{K}}^{\mathrm{ci}} \end{bmatrix}, \quad \underline{\boldsymbol{K}}^{\mathrm{bb}} = \begin{bmatrix} \underline{\boldsymbol{K}}^{\mathrm{bb}}_{++} & \underline{\boldsymbol{K}}^{\mathrm{bb}}_{+-} & \underline{\boldsymbol{K}}^{\mathrm{bc}}_{+} \\ \underline{\boldsymbol{K}}^{\mathrm{bb}}_{-+} & \underline{\boldsymbol{K}}^{\mathrm{bb}}_{--} & \underline{\boldsymbol{K}}^{\mathrm{bc}}_{-} \\ \underline{\boldsymbol{K}}^{\mathrm{cb}}_{+} & \underline{\boldsymbol{K}}^{\mathrm{cb}}_{-} & \underline{\boldsymbol{K}}^{\mathrm{cc}} \end{bmatrix}, \tag{5.84}$$ {eq:appB_10

SVE-problem – Formulation and solution

Periodicity of the nodal displacement fluctuations on $\Gamma_\square$ can be expressed as the constraints

$$\underline{\boldsymbol{u}}^{\mu,\mathrm{b}}_{+} = \underline{\boldsymbol{u}}^{\mu,\mathrm{b}}_{-} \overset{\mathrm{def}}{=} \underline{\boldsymbol{u}}^{\mu,\mathrm{b}} \quad \Rightarrow \quad \underline{\boldsymbol{u}}^{\mathrm{b}}_{+} = \underline{\boldsymbol{u}}^{\mathrm{M,b}}_{+} + \underline{\boldsymbol{u}}^{\mu,\mathrm{b}}, \quad \underline{\boldsymbol{u}}^{\mathrm{b}}_{-} = \underline{\boldsymbol{u}}^{\mathrm{M,b}}_{-} + \underline{\boldsymbol{u}}^{\mu,\mathrm{b}} \tag{5.85}$$ {eq:appB_10

Moreover, antiperiodicity of the nodal traction forces on $\Gamma_\square$ can be expressed as the constraints

$$\underline{\boldsymbol{g}}^{\mathrm{b}}_{+} + \underline{\boldsymbol{g}}^{\mathrm{b}}_{-} = \underline{\boldsymbol{0}} \quad \Rightarrow \quad \underline{\boldsymbol{f}}^{\mathrm{b}}_{+} + \underline{\boldsymbol{f}}^{\mathrm{b}}_{-} = \underline{\boldsymbol{0}} \tag{5.86}$$ {eq:appB_10

We choose to set the displacement fluctuation in all coordinate directions to zero at any (arbitrarily chosen) corner node. However, due to periodicity this means that the fluctuation in all corner nodes will vanish, i.e.

$$\underline{\boldsymbol{u}}^{\mu,\mathrm{c}} = \underline{\boldsymbol{0}} \quad \Rightarrow \quad \underline{\boldsymbol{u}}^{\mathrm{c}} = \underline{\boldsymbol{u}}^{\mathrm{M,c}} \tag{5.87}$$ {eq:appB_10

Observing (5.85) and (5.87), we note that $\mathrm{d}\underline{\boldsymbol{u}}^{\mathrm{b}}$ can be expanded as

$$\mathrm{d}\underline{\boldsymbol{u}}^{\mathrm{b}} = \begin{bmatrix} \mathrm{d}\underline{\boldsymbol{u}}^{\mathrm{b}}_{+} \\ \mathrm{d}\underline{\boldsymbol{u}}^{\mathrm{b}}_{-} \\ \mathrm{d}\underline{\boldsymbol{u}}^{\mathrm{c}} \end{bmatrix} = \begin{bmatrix} \mathrm{d}\underline{\boldsymbol{u}}^{\mathrm{M,b}}_{+} \\ \mathrm{d}\underline{\boldsymbol{u}}^{\mathrm{M,b}}_{-} \\ \mathrm{d}\underline{\boldsymbol{u}}^{\mathrm{M,c}} \end{bmatrix} + \begin{bmatrix} \mathrm{d}\underline{\boldsymbol{u}}^{\mu,\mathrm{b}}_{+} \\ \mathrm{d}\underline{\boldsymbol{u}}^{\mu,\mathrm{b}}_{-} \\ \underline{\boldsymbol{0}} \end{bmatrix} \tag{5.88}$$ {eq:appB_10

The SVE-problem is then formulated in matrix format as the reduced version of (5.80a,5.80b): {eq:appB_10

$$\underline{\boldsymbol{f}}^{\mathrm{i}}(\underline{\boldsymbol{u}}^{\mu,\mathrm{i}}, \underline{\boldsymbol{u}}^{\mu,\mathrm{b}}) = \underline{\boldsymbol{0}} \tag{5.89a}$$ {eq:appB_10

$$\underline{\boldsymbol{f}}^{\mathrm{b}}_{\pm}(\underline{\boldsymbol{u}}^{\mu,\mathrm{i}}, \underline{\boldsymbol{u}}^{\mu,\mathrm{b}}) = \underline{\boldsymbol{0}} \quad \text{with} \quad \underline{\boldsymbol{f}}^{\mathrm{b}}_{\pm} \overset{\mathrm{def}}{=} \underline{\boldsymbol{f}}^{\mathrm{b}}_{+} + \underline{\boldsymbol{f}}^{\mathrm{b}}_{-} \tag{5.89b}$$ {eq:appB_10

Newton's iteration method for finding $\underline{\boldsymbol{u}}^{\mu,\mathrm{i}}$ and $\underline{\boldsymbol{u}}^{\mu,\mathrm{b}}$ then becomes: For $k = 1, 2, \ldots$, compute

$$\underline{\boldsymbol{u}}^{\mu,\mathrm{i}(k+1)} = \underline{\boldsymbol{u}}^{\mu,\mathrm{i}(k)} + \Delta\underline{\boldsymbol{u}}^{\mu,\mathrm{i}}, \quad \underline{\boldsymbol{u}}^{\mu,\mathrm{b}(k+1)} = \underline{\boldsymbol{u}}^{\mu,\mathrm{b}(k)} + \Delta\underline{\boldsymbol{u}}^{\mu,\mathrm{b}} \tag{5.90}$$ {eq:appB_10

where the iterative updates $\Delta\underline{\boldsymbol{u}}^{\mu,\mathrm{i}}$ and $\Delta\underline{\boldsymbol{u}}^{\mu,\mathrm{b}}$ are solved from the tangent equations

$$\begin{bmatrix} \underline{\boldsymbol{K}}^{\mathrm{ii}(k)} & \underline{\boldsymbol{K}}^{\mathrm{ib}(k)}_{\pm} \\ \underline{\boldsymbol{K}}^{\mathrm{bi}(k)}_{\pm} & \underline{\boldsymbol{K}}^{\mathrm{bb}(k)}_{\pm} \end{bmatrix} \begin{bmatrix} \Delta\underline{\boldsymbol{u}}^{\mu,\mathrm{i}} \\ \Delta\underline{\boldsymbol{u}}^{\mu,\mathrm{b}} \end{bmatrix} = \begin{bmatrix} -\underline{\boldsymbol{f}}^{\mathrm{i}(k)} \\ -\underline{\boldsymbol{f}}^{\mathrm{b}(k)}_{\pm} \end{bmatrix} \overset{\mathrm{def}}{=} \begin{bmatrix} \underline{\boldsymbol{r}}^{\mathrm{i}(k)} \\ \underline{\boldsymbol{r}}^{\mathrm{b}(k)} \end{bmatrix} \tag{5.91}$$ {eq:appB_10

where we introduced the notation {eq:appB_109

$$\underline{\boldsymbol{K}}^{\mathrm{ib}}_{\substack{+\\-}} = \underline{\boldsymbol{K}}^{\mathrm{ib}}_{+} + \underline{\boldsymbol{K}}^{\mathrm{ib}}_{-} \tag{5.92a}$$ {eq:appB_109

$$\underline{\boldsymbol{K}}^{\mathrm{bi}}_{\substack{+\\-}} = \underline{\boldsymbol{K}}^{\mathrm{bi}}_{+} + \underline{\boldsymbol{K}}^{\mathrm{bi}}_{-} \tag{5.92b}$$ {eq:appB_109

$$\underline{\boldsymbol{K}}^{\mathrm{bb}}_{\substack{+\\-}} = \underline{\boldsymbol{K}}^{\mathrm{bb}}_{++} + \underline{\boldsymbol{K}}^{\mathrm{bb}}_{+-} + \underline{\boldsymbol{K}}^{\mathrm{bb}}_{-+} + \underline{\boldsymbol{K}}^{\mathrm{bb}}_{--} \tag{5.92c}$$ {eq:appB_109

Remark: In order to obtain the pertinent form of the tangent relation in (5.91), we first used (5.82) subjected to the condition of fixed value of $\underline{\boldsymbol{\epsilon}}$, i.e.

ppB_110_2}
$$\mathrm{d}\underline{\boldsymbol{u}}^{\mathrm{i}} = \mathrm{d}\underline{\boldsymbol{u}}^{\mu,\mathrm{i}}, \quad \mathrm{d}\underline{\boldsymbol{u}}^{\mathrm{b}}_{+} = \mathrm{d}\underline{\boldsymbol{u}}^{\mathrm{b}}_{-} = \mathrm{d}\underline{\boldsymbol{u}}^{\mu,\mathrm{b}}, \quad \mathrm{d}\underline{\boldsymbol{u}}^{\mathrm{c}} = \underline{\mathbf{0}} \tag{5.93}$$

to obtain

ppB_110_1}
$$\begin{bmatrix} \mathrm{d}\underline{\boldsymbol{f}}^{\mathrm{i}} \\ \mathrm{d}\underline{\boldsymbol{f}}^{\mathrm{b}}_{\substack{+\\-}} \end{bmatrix} = \begin{bmatrix} \underline{\boldsymbol{K}}^{\mathrm{ii}} & \underline{\boldsymbol{K}}^{\mathrm{ib}}_{\substack{+\\-}} \\ \underline{\boldsymbol{K}}^{\mathrm{bi}}_{\substack{+\\-}} & \underline{\boldsymbol{K}}^{\mathrm{bb}}_{\substack{+\\-}} \end{bmatrix} \begin{bmatrix} \mathrm{d}\underline{\boldsymbol{u}}^{\mu,\mathrm{i}} \\ \mathrm{d}\underline{\boldsymbol{u}}^{\mu,\mathrm{b}} \end{bmatrix} \tag{5.94}$$

□

When $\underline{\boldsymbol{u}}^{\mu,\mathrm{i}}$ and $\underline{\boldsymbol{u}}^{\mu,\mathrm{b}}$ are known, it is possible to to compute the macroscale stress $\underline{\bar{\boldsymbol{\sigma}}}$ in a post-processing step:

q:appB_110}
$$\begin{aligned} \underline{\bar{\boldsymbol{\sigma}}} &= \left[\underline{\hat{\boldsymbol{u}}}^{\mathrm{M}}\right]^{\mathrm{T}} \underline{\boldsymbol{f}} \\ &= \left[\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,i}}\right]^{\mathrm{T}} \underbrace{\underline{\boldsymbol{f}}^{\mathrm{i}}}_{=\mathbf{0}} + \left[\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}}_{+}\right]^{\mathrm{T}} \underline{\boldsymbol{f}}^{\mathrm{b}}_{+} + \left[\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}}_{-}\right]^{\mathrm{T}} \underline{\boldsymbol{f}}^{\mathrm{b}}_{-} + \left[\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,c}}\right]^{\mathrm{T}} \underline{\boldsymbol{f}}^{\mathrm{c}} \\ &= \left[\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}}_{+}\right]^{\mathrm{T}} \underline{\boldsymbol{f}}^{\mathrm{b}}_{+} + \left[\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}}_{-}\right]^{\mathrm{T}} \underline{\boldsymbol{f}}^{\mathrm{b}}_{-} + \left[\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,c}}\right]^{\mathrm{T}} \underline{\boldsymbol{f}}^{\mathrm{c}} \\ &= \left[\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}}\right]^{\mathrm{T}} \underline{\boldsymbol{f}}^{\mathrm{b}} \end{aligned} \tag{5.95}$$

where we introduced the notation

ppB_110_1}
$$\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}} = \begin{bmatrix} \underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}}_{+} \\ \underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}}_{+} \\ \underline{\hat{\boldsymbol{u}}}^{\mathrm{M,c}} \end{bmatrix} \tag{5.96}$$

Computing the macroscale tangent stiffness in practice

Linearizing (5.95) w.r.t. $\underline{\bar{\boldsymbol{\epsilon}}}$ gives

q:appB_111}
$$\begin{aligned} \mathrm{d}\underline{\bar{\boldsymbol{\sigma}}} &= \left[\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}}_{+}\right]^{\mathrm{T}} \mathrm{d}\underline{\boldsymbol{f}}^{\mathrm{b}}_{+} + \left[\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}}_{-}\right]^{\mathrm{T}} \mathrm{d}\underline{\boldsymbol{f}}^{\mathrm{b}}_{-} + \left[\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,c}}\right]^{\mathrm{T}} \mathrm{d}\underline{\boldsymbol{f}}^{\mathrm{c}} \\ &= \left[\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}}\right]^{\mathrm{T}} \mathrm{d}\underline{\boldsymbol{f}}^{\mathrm{b}} \end{aligned} \tag{5.97}$$

Again, we use the general tangent stiffness relation (5.82) to express the differential changes $\mathrm{d}\underline{\boldsymbol{f}}^{\mathrm{b}}_{+}$, $\mathrm{d}\underline{\boldsymbol{f}}^{\mathrm{b}}_{-}$, $\mathrm{d}\underline{\boldsymbol{f}}^{\mathrm{c}}$ in terms of the differential changes $(\mathrm{d}\underline{\boldsymbol{u}}^{\mathrm{i}}, \mathrm{d}\underline{\boldsymbol{u}}^{\mu,\mathrm{b}})$ and $(\mathrm{d}\underline{\boldsymbol{u}}^{\mathrm{M,b}}_{+}, \mathrm{d}\underline{\boldsymbol{u}}^{\mathrm{M,b}}_{-}, \mathrm{d}\underline{\boldsymbol{u}}^{\mathrm{M,c}})$, whereby these differential changes are considered as sensitivities for a given change of $\underline{\bar{\boldsymbol{\epsilon}}}$. Equilibrium of the "perturbed state" then requires

ppB_112_1}
$$\begin{bmatrix} \mathrm{d}\underline{\boldsymbol{f}}^{\mathrm{i}} \\ \mathrm{d}\underline{\boldsymbol{f}}^{\mathrm{b}}_{\substack{+\\-}} \end{bmatrix} = \underline{\mathbf{0}} \tag{5.98}$$

which gives the set of equations

$$\begin{bmatrix} \underline{\boldsymbol{K}}^{\mathrm{ii}} & \underline{\boldsymbol{K}}^{\mathrm{ib}}_{\substack{+\\-}} \\ \underline{\boldsymbol{K}}^{\mathrm{bi}}_{\substack{+\\-}} & \underline{\boldsymbol{K}}^{\mathrm{bb}}_{\substack{+\\-}} \end{bmatrix} \begin{bmatrix} \mathrm{d}\underline{\boldsymbol{u}}^{\mathrm{i}} \\ \mathrm{d}\underline{\boldsymbol{u}}^{\mu,\mathrm{b}} \end{bmatrix} + \begin{bmatrix} \underline{\boldsymbol{K}}^{\mathrm{ib}}_{+} & \underline{\boldsymbol{K}}^{\mathrm{ib}}_{-} & \underline{\boldsymbol{K}}^{\mathrm{ic}} \\ \underline{\boldsymbol{K}}^{\mathrm{bi}}_{++} + \underline{\boldsymbol{K}}^{\mathrm{bb}}_{-+} & \underline{\boldsymbol{K}}^{\mathrm{bi}}_{+-} + \underline{\boldsymbol{K}}^{\mathrm{bb}}_{--} & \underline{\boldsymbol{K}}^{\mathrm{bc}}_{+} + \underline{\boldsymbol{K}}^{\mathrm{bc}}_{-} \end{bmatrix} \begin{bmatrix} \mathrm{d}\underline{\boldsymbol{u}}^{\mathrm{M,b}}_{+} \\ \mathrm{d}\underline{\boldsymbol{u}}^{\mathrm{M,b}}_{-} \\ \mathrm{d}\underline{\boldsymbol{u}}^{\mathrm{M,c}} \end{bmatrix} = \begin{bmatrix} \underline{\boldsymbol{0}} \\ \underline{\boldsymbol{0}} \end{bmatrix} \tag{5.99}$$

{eq:appB_112}

To solve this system, we introduce sensitivities w.r.t. to a perturbation of $\bar{\underline{\boldsymbol{\epsilon}}}$:

$$\mathrm{d}\underline{\boldsymbol{u}}^{\mathrm{i}} = \hat{\underline{\boldsymbol{u}}}^{\mathrm{i}}\,\mathrm{d}\bar{\underline{\boldsymbol{\epsilon}}}, \quad \mathrm{d}\underline{\boldsymbol{u}}^{\mu,\mathrm{b}} = \hat{\underline{\boldsymbol{u}}}^{\mu,\mathrm{b}}\,\mathrm{d}\bar{\underline{\boldsymbol{\epsilon}}} \tag{5.100}$$

{eq:appB_11

whereby (5.99) is rephrased as

$$\begin{bmatrix} \underline{\boldsymbol{K}}^{\mathrm{ii}} & \underline{\boldsymbol{K}}^{\mathrm{ib}}_{\substack{+\\-}} \\ \underline{\boldsymbol{K}}^{\mathrm{bi}}_{\substack{+\\-}} & \underline{\boldsymbol{K}}^{\mathrm{bb}}_{\substack{+\\-}} \end{bmatrix} \begin{bmatrix} \hat{\underline{\boldsymbol{u}}}^{\mathrm{i}} \\ \hat{\underline{\boldsymbol{u}}}^{\mu,\mathrm{b}} \end{bmatrix} = - \begin{bmatrix} \underline{\boldsymbol{K}}^{\mathrm{ib}}_{+} & \underline{\boldsymbol{K}}^{\mathrm{ib}}_{-} & \underline{\boldsymbol{K}}^{\mathrm{ic}} \\ \underline{\boldsymbol{K}}^{\mathrm{bi}}_{++} + \underline{\boldsymbol{K}}^{\mathrm{bb}}_{-+} & \underline{\boldsymbol{K}}^{\mathrm{bi}}_{+-} + \underline{\boldsymbol{K}}^{\mathrm{bb}}_{--} & \underline{\boldsymbol{K}}^{\mathrm{bc}}_{+} + \underline{\boldsymbol{K}}^{\mathrm{bc}}_{-} \end{bmatrix} \begin{bmatrix} \hat{\underline{\boldsymbol{u}}}^{\mathrm{M,b}}_{+} \\ \hat{\underline{\boldsymbol{u}}}^{\mathrm{M,b}}_{-} \\ \hat{\underline{\boldsymbol{u}}}^{\mathrm{M,c}} \end{bmatrix} \tag{5.101}$$

{eq:appB_11

This is the same system already solved as part of the Newton iterations (with another RHS). Given the solution of (5.101), we use (5.82) to obtain

$$\mathrm{d}\underline{\boldsymbol{f}}^{\mathrm{b}} = \left[\underline{\boldsymbol{K}}^{\mathrm{bi}}\hat{\underline{\boldsymbol{u}}}^{\mathrm{i}} + \underline{\boldsymbol{K}}^{\mathrm{bb}}\hat{\underline{\boldsymbol{u}}}^{\mathrm{b}}\right]\mathrm{d}\bar{\underline{\boldsymbol{\epsilon}}} \tag{5.102}$$

{eq:appB_11

where

$$\hat{\underline{\boldsymbol{u}}}^{\mathrm{b}} = \begin{bmatrix} \hat{\underline{\boldsymbol{u}}}^{\mathrm{M,b}}_{+} \\ \hat{\underline{\boldsymbol{u}}}^{\mathrm{M,b}}_{-} \\ \hat{\underline{\boldsymbol{u}}}^{\mathrm{M,c}} \end{bmatrix} + \begin{bmatrix} \hat{\underline{\boldsymbol{u}}}^{\mu,\mathrm{b}}_{+} \\ \hat{\underline{\boldsymbol{u}}}^{\mu,\mathrm{b}}_{-} \\ \underline{\boldsymbol{0}} \end{bmatrix} \tag{5.103}$$

{eq:appB_10

Combining (5.102) with (5.97), we finally obtain

$$\mathrm{d}\bar{\underline{\boldsymbol{\sigma}}} = \left[\hat{\underline{\boldsymbol{u}}}^{\mathrm{M,b}}\right]^{\mathrm{T}}\mathrm{d}\underline{\boldsymbol{f}}^{\mathrm{b}} = \underbrace{\left[\hat{\underline{\boldsymbol{u}}}^{\mathrm{M,b}}\right]^{\mathrm{T}}\left[\underline{\boldsymbol{K}}^{\mathrm{bi}}\hat{\underline{\boldsymbol{u}}}^{\mathrm{i}} + \underline{\boldsymbol{K}}^{\mathrm{bb}}\hat{\underline{\boldsymbol{u}}}^{\mathrm{b}}\right]}_{\bar{\underline{\mathsf{E}}}_{\Box,\mathrm{T}}}\mathrm{d}\bar{\underline{\boldsymbol{\epsilon}}} \tag{5.104}$$

{eq:appB_11

whereby the macroscale tangent stiffness is computed (in the operational format) as

$$\bar{\underline{\mathsf{E}}}_{\Box,\mathrm{T}} = \left[\hat{\underline{\boldsymbol{u}}}^{\mathrm{M,b}}\right]^{\mathrm{T}}\left[\underline{\boldsymbol{K}}^{\mathrm{bi}}\hat{\underline{\boldsymbol{u}}}^{\mathrm{i}} + \underline{\boldsymbol{K}}^{\mathrm{bb}}\hat{\underline{\boldsymbol{u}}}^{\mathrm{b}}\right] \tag{5.105}$$

{eq:appB_12

As to the dimensions of the matrices involved, we have in the 2D-case:

$$\begin{aligned} dim(\hat{\underline{\boldsymbol{u}}}^{\mathrm{i}}) &= \mathrm{NVAR_i} \times 3 \\ dim(\hat{\underline{\boldsymbol{u}}}^{\mathrm{b}}) &= \mathrm{NVAR_b} \times 3 \\ dim(\underline{\boldsymbol{K}}^{\mathrm{bi}}) &= \mathrm{NVAR_b} \times \mathrm{NVAR_i} \\ dim(\underline{\boldsymbol{K}}^{\mathrm{bb}}) &= \mathrm{NVAR_b} \times \mathrm{NVAR_b} \\ dim(\bar{\underline{\mathsf{E}}}_{\Box,\mathrm{T}}) &= 3 \times 3 \end{aligned} \tag{5.106}$$

{eq:appB_12

5.5 Neumann boundary conditions (NBC-problem)

5.5.1 NBC-problem

We shall now consider the case where the prolongation is defined by the "weak" assumption on RVE-boundary tractions generated from the constant stress tensor $\bar{\boldsymbol{\sigma}}$. The corresponding subscale space-variational problem on the RVE associated with a typical macroscopic point $\bar{\boldsymbol{x}} \in \Omega$ can be phrased as follows: For given value of the macroscale displacement gradient $\bar{\boldsymbol{\epsilon}} \in \mathbb{R}^{3\times 3}_{\text{sym}}$, find $\boldsymbol{u} \in \mathbb{U}^{\text{N}}_{\square}$ and $\bar{\boldsymbol{\sigma}} \in \mathbb{R}^{3\times 3}_{\text{sym}}$ that solve {eq:4-143}

$$a_{\square}(\boldsymbol{u}; \delta\boldsymbol{u}) - c_{\square}(\delta\boldsymbol{u}; \bar{\boldsymbol{\sigma}}) = 0 \qquad \forall \delta\boldsymbol{u} \in \mathbb{U}^{\text{N}}_{\square} \tag{5.107a}$$
{eq:4-143a}

$$-c_{\square}(\boldsymbol{u}; \delta\bar{\boldsymbol{\sigma}}) = -\delta\bar{\boldsymbol{\sigma}} : \bar{\boldsymbol{\epsilon}} \qquad \forall \delta\bar{\boldsymbol{\sigma}} \in \mathbb{R}^{3\times 3}_{\text{sym}} \tag{5.107b}$$
{eq:4-143b}

As to the iterative solution of the system given in (6.55), Newton's method for finding $\boldsymbol{u}$ and $\bar{\boldsymbol{\sigma}}$ becomes: For $k = 1, 2, \ldots,$ compute

{eq:4-144}
$$\boldsymbol{u}^{(k+1)} = \boldsymbol{u}^{(k)} + \Delta\boldsymbol{u}, \quad \bar{\boldsymbol{\sigma}}^{(k+1)} = \bar{\boldsymbol{\sigma}}^{(k)} + \Delta\bar{\boldsymbol{\sigma}} \tag{5.108}$$

{eq:4-145} where the iterative updates $\Delta\boldsymbol{u} \in \mathbb{U}^{\text{N}}_{\square}$ and $\Delta\bar{\boldsymbol{\epsilon}} \in \mathbb{R}^{3\times 3}_{\text{sym}}$ are solved from the tangent equations

{eq:4-145a}
$$(a_{\square})'_u(\bullet^{(k)}; \delta\boldsymbol{u}, \Delta\boldsymbol{u}) - c_{\square}(\delta\boldsymbol{u}, \Delta\bar{\boldsymbol{\sigma}}) = R^{(\text{u})}_{\square}(\bullet^{(k)}; \delta\boldsymbol{u}) \qquad \forall \delta\boldsymbol{u} \in \mathbb{U}^{\text{N}}_{\square} \tag{5.109a}$$

{eq:4-145b}
$$-c_{\square}(\Delta\boldsymbol{u}, \delta\bar{\boldsymbol{\sigma}}) = R^{(\text{P})}_{\square}(\bullet^{(k)}; \delta\bar{\boldsymbol{\sigma}}) \qquad \forall \delta\bar{\boldsymbol{\sigma}} \in \mathbb{R}^{3\times 3}_{\text{sym}} \tag{5.109b}$$

{eq:4-146} where the residuals are

{eq:4-146a}
$$R^{(\text{u})}_{\square}(\bullet^{(k)}; \delta\boldsymbol{u}) \overset{\text{def}}{=} -a_{\square}(\bullet^{(k)}; \delta\boldsymbol{u}) + c_{\square}(\delta\boldsymbol{u}, \bar{\boldsymbol{\sigma}}^{(k)}) \tag{5.110a}$$

{eq:4-146b}
$$R^{(\text{P})}_{\square}(\bullet^{(k)}; \delta\bar{\boldsymbol{\sigma}}) \overset{\text{def}}{=} -\delta\bar{\boldsymbol{\sigma}} : \bar{\boldsymbol{\epsilon}} + c_{\square}(\boldsymbol{u}^{(k)}; \delta\bar{\boldsymbol{\sigma}}) \tag{5.110b}$$

The appropriate tangent (stiffness) forms were given above, however, the explicit results are
{eq:4-147} reiterated here for completeness:

{eq:4-147a}
$$(a_{\square})'(\bullet; \delta\boldsymbol{u}, \Delta\boldsymbol{u}) = \langle \boldsymbol{\epsilon}[\delta\boldsymbol{u}] : \mathbf{E}_{\text{T}} : \boldsymbol{\epsilon}[\Delta\boldsymbol{u}] \rangle_{\square} \tag{5.111a}$$

{eq:4-147c}
$$c_{\square}(\delta\boldsymbol{u}, \Delta\bar{\boldsymbol{\sigma}}) = \langle \boldsymbol{\epsilon}[\delta\boldsymbol{u}] \rangle_{\square} : \Delta\bar{\boldsymbol{\sigma}} \tag{5.111b}$$

{eq:4-147d}
$$c_{\square}(\Delta\boldsymbol{u}, \delta\bar{\boldsymbol{\sigma}}) = \delta\bar{\boldsymbol{\sigma}} : \langle \boldsymbol{\epsilon}[\Delta\boldsymbol{u}] \rangle_{\square} \tag{5.111c}$$

5.5.2 Macroscale ATS-tensor

The state equations (6.55) must hold for $\bar{\boldsymbol{\epsilon}}$ as well as for a perturbed state $\bar{\boldsymbol{\epsilon}} + \mathrm{d}\bar{\boldsymbol{\epsilon}}$. However, a
{eq:4-151} given change $\mathrm{d}\bar{\boldsymbol{\epsilon}}$ gives rise to changes $\mathrm{d}\boldsymbol{u} \in \mathbb{U}^{\text{N}}_{\square}$ and $\mathrm{d}\bar{\boldsymbol{\sigma}} \in \mathbb{R}^{3\times 3}_{\text{sym}}$, whereby we obtain the relations

{eq:4-151a}
$$a_{\square}(\boldsymbol{u} + \mathrm{d}\boldsymbol{u}; \delta\boldsymbol{u}) - c_{\square}(\delta\boldsymbol{u}, \bar{\boldsymbol{\sigma}} + \mathrm{d}\bar{\boldsymbol{\sigma}}) = 0 \qquad \forall \delta\boldsymbol{u} \in \mathbb{U}^{\text{N}}_{\square} \tag{5.112a}$$

{eq:4-151b}
$$-c_{\square}(\boldsymbol{u} + \mathrm{d}\boldsymbol{u}, \delta\bar{\boldsymbol{\sigma}}) = -\delta\bar{\boldsymbol{\sigma}} : [\bar{\boldsymbol{\epsilon}} + \mathrm{d}\bar{\boldsymbol{\epsilon}}] \qquad \forall \delta\bar{\boldsymbol{\sigma}} \in \mathbb{R}^{3\times 3}_{\text{sym}} \tag{5.112b}$$

Now, upon linearizing in (6.64) and subtracting (6.55) from the resulting expressions, we obtain
{eq:4-152} the appropriate tangent problem:

{eq:4-152a}
$$(a_{\square})'(\bullet; \delta\boldsymbol{u}, \mathrm{d}\boldsymbol{u}) - c_{\square}(\delta\boldsymbol{u}, \mathrm{d}\bar{\boldsymbol{\sigma}}) = 0 \qquad \forall \delta\boldsymbol{u} \in \mathbb{U}^{\text{N}}_{\square} \tag{5.113a}$$

{eq:4-152c}
$$-c_{\square}(\mathrm{d}\boldsymbol{u}, \delta\bar{\boldsymbol{\sigma}}) = -\delta\bar{\boldsymbol{\sigma}} : \mathrm{d}\bar{\boldsymbol{\epsilon}} \qquad \forall \delta\bar{\boldsymbol{\sigma}} \in \mathbb{R}^{3\times 3}_{\text{sym}} \tag{5.113b}$$

from which, in principle, $\mathrm{d}\boldsymbol{u}$ and $\mathrm{d}\bar{\boldsymbol{\sigma}}$ can be solved for any given $\mathrm{d}\bar{\boldsymbol{\epsilon}}$. Again, we use the "unit fields", or sensitivities, $\hat{\boldsymbol{u}}^{(ij)}$, due to a unit value of the components $\mathrm{d}\bar{\epsilon}_{ij}$, and an analogous *ansatz* for $\mathrm{d}\bar{\boldsymbol{\sigma}}$

{eq:4-153}
$$\mathrm{d}\boldsymbol{u} = \sum_{i,j} \hat{\boldsymbol{u}}^{(ij)}\, \mathrm{d}\bar{\epsilon}_{ij}, \quad \mathrm{d}\bar{\boldsymbol{\sigma}} = \sum_{i,j} \hat{\bar{\boldsymbol{\sigma}}}^{(ij)}\, \mathrm{d}\bar{\epsilon}_{ij} \tag{5.114}$$

{eq:4-154} into (6.65) to obtain the set of equations that must hold for $k, l = 1, 2, ..., NDIM$:

{eq:4-154a}

$$(a_\square)'(\bullet; \delta\boldsymbol{u}, \hat{\boldsymbol{u}}^{(kl)}) - c_\square(\delta\boldsymbol{u}, \hat{\bar{\boldsymbol{\sigma}}}^{(kl)}) = 0 \qquad \forall \delta\boldsymbol{u} \in \mathbb{U}_\square^{\mathrm{N}} \tag{5.115a}$$

$$-c_\square(\hat{\boldsymbol{u}}^{(kl)}, \delta\bar{\boldsymbol{\sigma}}) = -(\delta\bar{\sigma})_{kl} \qquad \forall \delta\bar{\boldsymbol{\sigma}} \in \mathbb{R}^{3\times3}_{\mathrm{sym}} \tag{5.115b}$$

where we used the identity $\delta\bar{\boldsymbol{\sigma}} : [\boldsymbol{e}_k \otimes \boldsymbol{e}_l] = \boldsymbol{e}_k \cdot \delta\bar{\boldsymbol{\sigma}} \cdot \boldsymbol{e}_l = (\delta\bar{\sigma})_{kl}$.

Obviously, the unit fields $\hat{\bar{\boldsymbol{\sigma}}}^{(ij)}$ are obtained as part of the solution of the system (6.67), whereafter they are inserted into $(6.66)_2$ to give the explicit expression

$$\bar{\mathsf{E}}_{\mathrm{T}} = \sum_{k,l=1}^{NDIM} \hat{\bar{\boldsymbol{\sigma}}}^{(kl)} \otimes \boldsymbol{e}_k \otimes \boldsymbol{e}_l \tag{5.116}$$ {eq:4-155}

5.5.3 FE-approximation – Matrix format (in 2D)

Preliminaries

We recall the expressions in Section 3.4.4 to express the form $c_\square(\boldsymbol{u}_h; \bar{\boldsymbol{\sigma}}_h)$ in matrix format as {eq:appB_3

$$c_\square(\delta\boldsymbol{u}_h; \bar{\boldsymbol{\sigma}}) \stackrel{\mathrm{def}}{=} \langle \boldsymbol{\epsilon}[\delta\boldsymbol{u}_h] \rangle_\square : \bar{\boldsymbol{\sigma}} = \sum_{k=1}^{\mathrm{NVAR_b}} (\delta\underline{\boldsymbol{u}}^{\mathrm{b}})_k \underline{\boldsymbol{C}}_k \underline{\bar{\boldsymbol{\sigma}}} = [\delta\underline{\boldsymbol{u}}^{\mathrm{b}}]^{\mathrm{T}} \underline{\boldsymbol{C}} \underline{\bar{\boldsymbol{\sigma}}} \tag{5.117a}$$ {eq:appB_3

$$c_\square(\boldsymbol{u}_h; \delta\bar{\boldsymbol{\sigma}}) = [\delta\underline{\bar{\boldsymbol{\sigma}}}]^{\mathrm{T}} \underline{\boldsymbol{C}}^{\mathrm{T}} \underline{\boldsymbol{u}}^{\mathrm{b}} \tag{5.117b}$$ {eq:appB_3

where we introduced the row matrices

$$\underline{\boldsymbol{C}}_k = \left[\ (\boldsymbol{C}_k)_{11} \quad (\boldsymbol{C}_k)_{12} \quad (\boldsymbol{C}_k)_{22}\ \right] \tag{5.118}$$ {eq:appB_3

to represent the tensors

$$\boldsymbol{C}_k \stackrel{\mathrm{def}}{=} \frac{1}{|\Omega_\square|} \int_{\Gamma_\square} \boldsymbol{N}_k^{\mathrm{b}} \otimes \boldsymbol{n} \, \mathrm{d}\Gamma \tag{5.119}$$ {eq:appB_3

Moreover, the matrix $\underline{\boldsymbol{C}}$ is defined as

$$\underline{\boldsymbol{C}} = \begin{bmatrix} (\boldsymbol{C}_1)_{11} & (\boldsymbol{C}_1)_{12} & (\boldsymbol{C}_1)_{22} \\ (\boldsymbol{C}_2)_{11} & (\boldsymbol{C}_2)_{12} & (\boldsymbol{C}_2)_{22} \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ (\boldsymbol{C}_{\mathrm{NVAR_{u,b}}})_{11} & (\boldsymbol{C}_{\mathrm{NVAR_{u,b}}})_{12} & (\boldsymbol{C}_{\mathrm{NVAR_{u,b}}})_{22} \end{bmatrix} \tag{5.120}$$ {eq:appB_3

Each of the 3 columns in $\underline{\boldsymbol{C}}$ can be assembled elementwise like a "load vector" from line loading along element edges.

SVE-problem – Formulation and solution

All nodal displacement variables are free variables that are determined as part of the solution. The SVE-problem is then formulated in matrix format as: {eq:appB_3

$$\underline{\boldsymbol{f}}^{\mathrm{i}}(\underline{\boldsymbol{u}}^{\mathrm{i}}, \underline{\boldsymbol{u}}^{\mathrm{b}}) = \underline{\boldsymbol{0}} \tag{5.121a}$$ {eq:appB_3

$$\underline{\boldsymbol{f}}^{\mathrm{b}}(\underline{\boldsymbol{u}}^{\mathrm{i}}, \underline{\boldsymbol{u}}^{\mathrm{b}}) - \underline{\boldsymbol{C}} \underline{\bar{\boldsymbol{\sigma}}} = \underline{\boldsymbol{0}} \tag{5.121b}$$ {eq:appB_3

$$\underline{\boldsymbol{C}}^{\mathrm{T}} \underline{\boldsymbol{u}}^{\mathrm{b}} = \underline{\bar{\boldsymbol{\epsilon}}} \tag{5.121c}$$ {eq:appB_3

Newton's iteration method for finding $\underline{\boldsymbol{u}}^{\mathrm{i}}, \underline{\boldsymbol{u}}^{\mathrm{b}}$ and $\underline{\bar{\boldsymbol{\sigma}}}$ then becomes: For $k = 1, 2, \ldots,$ compute

$$\underline{\boldsymbol{u}}^{\mathrm{i}(k+1)} = \underline{\boldsymbol{u}}^{\mathrm{i}(k)} + \Delta\underline{\boldsymbol{u}}^{\mathrm{i}}, \quad \underline{\boldsymbol{u}}^{\mathrm{b}(k+1)} = \underline{\boldsymbol{u}}^{\mathrm{b}(k)} + \Delta\underline{\boldsymbol{u}}^{\mathrm{b}}, \quad \underline{\bar{\boldsymbol{\sigma}}}^{(k+1)} = \underline{\bar{\boldsymbol{\sigma}}}^{(k)} + \Delta\underline{\bar{\boldsymbol{\sigma}}} \tag{5.122}$$ {eq:appB_34}

where the iterative updates $\Delta\underline{\boldsymbol{u}}^{\mathrm{i}}, \Delta\underline{\boldsymbol{u}}^{\mathrm{b}}$ and $\Delta\underline{\bar{\boldsymbol{\sigma}}}$ are solved from the tangent equations

eq:appB_35}
$$\begin{bmatrix} \underline{\boldsymbol{K}}^{\mathrm{ii}(k)} & \underline{\boldsymbol{K}}^{\mathrm{ib}(k)} & \underline{\boldsymbol{0}} \\ \underline{\boldsymbol{K}}^{\mathrm{bi}(k)} & \underline{\boldsymbol{K}}^{\mathrm{bb}(k)} & -\underline{\boldsymbol{C}} \\ \underline{\boldsymbol{0}} & -\underline{\boldsymbol{C}}^{\mathrm{T}} & \underline{\boldsymbol{0}} \end{bmatrix} \begin{bmatrix} \Delta\underline{\boldsymbol{u}}^{\mathrm{i}} \\ \Delta\underline{\boldsymbol{u}}^{\mathrm{b}} \\ \Delta\underline{\bar{\boldsymbol{\sigma}}} \end{bmatrix} = \begin{bmatrix} -\underline{\boldsymbol{f}}^{\mathrm{i}(k)} \\ \underline{\boldsymbol{C}}\underline{\bar{\boldsymbol{\sigma}}}^{(k)} - \underline{\boldsymbol{f}}^{\mathrm{b}(k)} \\ \underline{\boldsymbol{C}}^{\mathrm{T}}\underline{\boldsymbol{u}}^{\mathrm{b}(k)} - \underline{\bar{\boldsymbol{\epsilon}}} \end{bmatrix} = \begin{bmatrix} \underline{\boldsymbol{r}}^{\mathrm{i}(k)} \\ \underline{\boldsymbol{r}}^{\mathrm{b}(k)} \\ \underline{\boldsymbol{R}}^{(k)} \end{bmatrix} \tag{5.123}$$

To solve (5.123), while preserving the the "FE-structure" of the tangent stiffness matrix $\underline{\boldsymbol{K}}$, introduce the decomposition via sensitivities w.r.t. to a perturbation of $\underline{\bar{\boldsymbol{\sigma}}}$:

eq:appB_36}
$$\Delta\underline{\boldsymbol{u}}^{\mathrm{i}} = \underline{\hat{\boldsymbol{u}}}^{\mathrm{i}}_{\mathrm{P}}\Delta\underline{\bar{\boldsymbol{\sigma}}} + \Delta\underline{\boldsymbol{u}}^{\mathrm{i}}_{\mathrm{R}}, \quad \Delta\underline{\boldsymbol{u}}^{\mathrm{b}} = \underline{\hat{\boldsymbol{u}}}^{\mathrm{b}}_{\mathrm{P}}\Delta\underline{\bar{\boldsymbol{\sigma}}} + \Delta\underline{\boldsymbol{u}}^{\mathrm{b}}_{\mathrm{R}} \tag{5.124}$$

Upon inserting into (5.123), we obtain the two sets of FE-equations

eq:appB_37}
$$\begin{bmatrix} \underline{\boldsymbol{K}}^{\mathrm{ii}(k)} & \underline{\boldsymbol{K}}^{\mathrm{ib}(k)} \\ \underline{\boldsymbol{K}}^{\mathrm{bi}(k)} & \underline{\boldsymbol{K}}^{\mathrm{bb}(k)} \end{bmatrix} \begin{bmatrix} \Delta\underline{\boldsymbol{u}}^{\mathrm{i}}_{\mathrm{R}} \\ \Delta\underline{\boldsymbol{u}}^{\mathrm{b}}_{\mathrm{R}} \end{bmatrix} = \begin{bmatrix} \underline{\boldsymbol{r}}^{\mathrm{i}(k)} \\ \underline{\boldsymbol{r}}^{\mathrm{b}(k)} \end{bmatrix} \tag{5.125}$$

eq:appB_38}
$$\begin{bmatrix} \underline{\boldsymbol{K}}^{\mathrm{ii}(k)} & \underline{\boldsymbol{K}}^{\mathrm{ib}(k)} \\ \underline{\boldsymbol{K}}^{\mathrm{bi}(k)} & \underline{\boldsymbol{K}}^{\mathrm{bb}(k)} \end{bmatrix} \begin{bmatrix} \underline{\hat{\boldsymbol{u}}}^{\mathrm{i}}_{\mathrm{P}} \\ \underline{\hat{\boldsymbol{u}}}^{\mathrm{b}}_{\mathrm{P}} \end{bmatrix} = \begin{bmatrix} \underline{\boldsymbol{0}} \\ \underline{\boldsymbol{C}} \end{bmatrix} \tag{5.126}$$

Note: Special requirement on b.c. to remove RBM and obtain a non-singular tangent stiffness matrix. □

Given the solution $(\underline{\hat{\boldsymbol{u}}}^{\mathrm{i}}_{\mathrm{P}}, \underline{\hat{\boldsymbol{u}}}^{\mathrm{i}}_{\mathrm{P}})$, and $(\Delta\underline{\boldsymbol{u}}^{\mathrm{i}}_{\mathrm{R}}, \Delta\underline{\boldsymbol{u}}^{\mathrm{i}}_{\mathrm{R}})$, we obtain from the last equation in (5.123) the final equation from which $\Delta\underline{\bar{\boldsymbol{\sigma}}}$ is solved:

eq:appB_39}
$$\Delta\underline{\bar{\boldsymbol{\sigma}}} = -\underbrace{\left[\underline{\boldsymbol{C}}^{\mathrm{T}}\underline{\hat{\boldsymbol{u}}}^{\mathrm{b}}_{\mathrm{P}}\right]^{-1}}_{\underline{\bar{\mathsf{E}}}_{\square,\mathrm{T}}}\left[\underline{\boldsymbol{R}}^{(k)} + \underline{\boldsymbol{C}}^{\mathrm{T}}\Delta\underline{\hat{\boldsymbol{u}}}^{\mathrm{b}}_{\mathrm{R}}\right] \tag{5.127}$$

That the matrix $\left[\underline{\boldsymbol{C}}^{\mathrm{T}}\underline{\hat{\boldsymbol{u}}}^{\mathrm{b}}_{\mathrm{P}}\right]^{-1}$ is, indeed, identical to the tangent stiffness matrix $\underline{\bar{\mathsf{E}}}_{\square,\mathrm{T}}$ is shown below.

Note: Requirement on b.c. to remove RBM and obtaining a non-singular tangent stiffness matrix.

Computing the macroscale tangent stiffness in practice

Linearizing the SVE-problem (**??**)-(**??**) w.r.t. $\underline{\bar{\boldsymbol{\epsilon}}}$ gives the "perturbed" system

eq:appB_40}
$$\begin{bmatrix} \underline{\boldsymbol{K}}^{\mathrm{ii}} & \underline{\boldsymbol{K}}^{\mathrm{ib}} & \underline{\boldsymbol{0}} \\ \underline{\boldsymbol{K}}^{\mathrm{bi}} & \underline{\boldsymbol{K}}^{\mathrm{bb}} & -\underline{\boldsymbol{C}} \\ \underline{\boldsymbol{0}} & -\underline{\boldsymbol{C}}^{\mathrm{T}} & \underline{\boldsymbol{0}} \end{bmatrix} \begin{bmatrix} \mathrm{d}\underline{\boldsymbol{u}}^{\mathrm{i}} \\ \mathrm{d}\underline{\boldsymbol{u}}^{\mathrm{b}} \\ \mathrm{d}\underline{\bar{\boldsymbol{\sigma}}} \end{bmatrix} = \begin{bmatrix} \underline{\boldsymbol{0}} \\ \underline{\boldsymbol{0}} \\ -\mathrm{d}\underline{\bar{\boldsymbol{\epsilon}}} \end{bmatrix} \tag{5.128}$$

To solve (5.128) for given $\mathrm{d}\underline{\bar{\boldsymbol{\epsilon}}}$, while preserving the the "FE-structure" of the tangent stiffness matrix $\underline{\boldsymbol{K}}$, introduce the decomposition via sensitivities w.r.t. to a perturbation of $\underline{\bar{\boldsymbol{\sigma}}}$:

eq:appB_41}
$$\mathrm{d}\underline{\boldsymbol{u}}^{\mathrm{i}} = \underline{\hat{\boldsymbol{u}}}^{\mathrm{i}}_{\mathrm{P}}\,\mathrm{d}\underline{\bar{\boldsymbol{\sigma}}}, \quad \mathrm{d}\underline{\boldsymbol{u}}^{\mathrm{b}} = \underline{\hat{\boldsymbol{u}}}^{\mathrm{b}}_{\mathrm{P}}\,\mathrm{d}\underline{\bar{\boldsymbol{\sigma}}} \tag{5.129}$$

Upon inserting into (5.128), we obtain the set of FE-equations

{eq:appB_42}
$$\begin{bmatrix} \underline{\boldsymbol{K}}^{\mathrm{ii}} & \underline{\boldsymbol{K}}^{\mathrm{ib}} \\ \underline{\boldsymbol{K}}^{\mathrm{bi}} & \underline{\boldsymbol{K}}^{\mathrm{bb}} \end{bmatrix} \begin{bmatrix} \underline{\hat{\boldsymbol{u}}}^{\mathrm{i}}_{\bar{\mathrm{P}}} \\ \underline{\hat{\boldsymbol{u}}}^{\mathrm{b}}_{\bar{\mathrm{P}}} \end{bmatrix} = \begin{bmatrix} \underline{\boldsymbol{0}} \\ \underline{\boldsymbol{C}} \end{bmatrix} \tag{5.130}$$

which is exactly the same system already solved as part of the Newton iterations. Given the sensitivities $\underline{\hat{\boldsymbol{u}}}^{\mathrm{i}}_{\bar{\mathrm{P}}}, \underline{\hat{\boldsymbol{u}}}^{\mathrm{i}}_{\bar{\mathrm{P}}}$ and the sensitivity $\underline{\hat{\boldsymbol{\sigma}}}$ w.r.t. $\underline{\bar{\boldsymbol{\epsilon}}}$, we obtain

eq:appB_42_1}
$$\mathrm{d}\underline{\boldsymbol{u}}^{\mathrm{i}} = \underline{\hat{\boldsymbol{u}}}^{\mathrm{i}}_{\bar{\mathrm{P}}} \underline{\hat{\boldsymbol{\sigma}}}\, \mathrm{d}\underline{\bar{\boldsymbol{\epsilon}}}, \quad \mathrm{d}\underline{\boldsymbol{u}}^{\mathrm{b}} = \underline{\hat{\boldsymbol{u}}}^{\mathrm{b}}_{\bar{\mathrm{P}}} \underline{\hat{\boldsymbol{\sigma}}}\, \mathrm{d}\underline{\bar{\boldsymbol{\epsilon}}} \tag{5.131}$$

Upon inserting into the last equation in (5.128), we obtain:

$$\underline{\boldsymbol{C}}^{\mathrm{T}} \underline{\hat{\boldsymbol{u}}}^{\mathrm{b}}_{\bar{\mathrm{P}}} \underline{\hat{\boldsymbol{\sigma}}} = \underline{\mathbf{I}} \quad \rightarrow \quad \underline{\hat{\boldsymbol{\sigma}}} = \left[\underline{\boldsymbol{C}}^{\mathrm{T}} \underline{\hat{\boldsymbol{u}}}^{\mathrm{b}}_{\bar{\mathrm{P}}} \right]^{-1} \tag{5.132}$$
{eq:appB_43

Finally, we obtain:

$$\underline{\bar{\boldsymbol{\sigma}}} = \underbrace{\left[\underline{\boldsymbol{C}}^{\mathrm{T}} \underline{\hat{\boldsymbol{u}}}^{\mathrm{b}}_{\bar{\mathrm{P}}} \right]^{-1}}_{\underline{\bar{\mathsf{\mathbf{E}}}}_{\Box,\mathrm{T}}} \underline{\bar{\boldsymbol{\epsilon}}} \tag{5.133}$$
{eq:appB_39

i.e. we have deduced the operational expression for $\underline{\bar{\mathsf{\mathbf{E}}}}_{\Box,\mathrm{T}}$

$$\underline{\bar{\mathsf{\mathbf{E}}}}_{\Box,\mathrm{T}} = \left[\underline{\boldsymbol{C}}^{\mathrm{T}} \underline{\hat{\boldsymbol{u}}}^{\mathrm{b}}_{\bar{\mathrm{P}}} \right]^{-1} \tag{5.134}$$
{eq:appB_39

As to the dimensions of the matrices involved, we have in the 2D-case:

$$\begin{aligned} dim(\underline{\hat{\boldsymbol{u}}}^{\mathrm{i}}) &= \mathrm{NVAR}_{\mathrm{i}} \times 3 \\ dim(\underline{\hat{\boldsymbol{u}}}^{\mathrm{b}}) &= \mathrm{NVAR}_{\mathrm{b}} \times 3 \\ dim(\underline{\boldsymbol{C}}) &= \mathrm{NVAR}_{\mathrm{b}} \times 3 \\ dim(\underline{\bar{\mathsf{\mathbf{E}}}}_{\Box,\mathrm{T}}) &= 3 \times 3 \end{aligned} \tag{5.135}$$
{eq:appB_47

5.6 Weakly periodic boundary conditions (WPBC-problem)

5.6.1 WPBC-problem

Based on the developments in the previous Subsection, the variational form of the subscale problem for weakly imposed microperiodicity in the displacements can now be formulated for the case of macrostrain control as follows: Find $\boldsymbol{u} \in \mathbb{U}_\Box$, and $\boldsymbol{\lambda} \in \mathbb{T}^+_\Box$ that, for given value of the macroscale displacement gradient $\bar{\boldsymbol{\epsilon}}$, solve the system

$$\begin{aligned} a_\Box(\boldsymbol{u}; \delta\boldsymbol{u}) - d_\Box(\boldsymbol{t}, \delta\boldsymbol{u}) &= 0 & \forall \delta\boldsymbol{u} \in \mathbb{U}_\Box \\ -d_\Box(\delta\boldsymbol{\lambda}, \boldsymbol{u}) &= -d_\Box(\delta\boldsymbol{\lambda}, \bar{\boldsymbol{\epsilon}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}]) & \forall \delta\boldsymbol{\lambda} \in \mathbb{T}^+_\Box \end{aligned} \tag{5.136}$$
{eq521b}

It is noted that $(5.136)_2$ represents a trivial reformulation of the variational micro-periodicity condition in (**??**) when the assumed linear variation of $\boldsymbol{u}^{\mathrm{M}}$ within the SVE is used.

As to the iterative solution of the system (5.136), Newton's method for finding $\boldsymbol{u}$ and $\boldsymbol{\lambda}$ becomes: For $k = 1, 2, \ldots,$ compute

$$\boldsymbol{u}^{(k+1)} = \boldsymbol{u}^{(k)} + \Delta\boldsymbol{u}, \quad \boldsymbol{\lambda}^{(k+1)} = \boldsymbol{\lambda}^{(k)} + \Delta\boldsymbol{\lambda} \tag{5.137}$$
{eq522}

where the iterative updates $\Delta \boldsymbol{u} \in \mathbb{U}_\square$ and $\Delta \boldsymbol{\lambda} \in \mathbb{T}_\square^+$ are solved from the tangent equations

$$\begin{aligned}(a_\square)'_u(\bullet^{(k)}; \delta \boldsymbol{u}, \Delta \boldsymbol{u}) - d_\square(\Delta \boldsymbol{\lambda}, \delta \boldsymbol{u}) &= R_\square^{(\mathrm{u})}(\bullet^{(k)}; \delta \boldsymbol{u}) \qquad \forall \delta \boldsymbol{u} \in \mathbb{U}_\square \\ -d_\square(\delta \boldsymbol{\lambda}, \Delta \boldsymbol{u}) &= R_\square^{(\mathrm{t})}(\bullet^{(k)}; \delta \boldsymbol{\lambda}) \qquad \forall \delta \boldsymbol{\lambda} \in \mathbb{T}_\square^+\end{aligned} \tag{5.138}$$ {eq523b}

where the residuals are

$$R_\square^{(\mathrm{u})}(\bullet^{(k)}; \delta \boldsymbol{u}) \stackrel{\text{def}}{=} d_\square(\boldsymbol{\lambda}^{(k)}, \delta \boldsymbol{u}) - a(\boldsymbol{u}^{(k)}; \delta \boldsymbol{u}) \tag{5.139}$$ {eq524a}

$$R_\square^{(\mathrm{t})}(\bullet^{(k)}; \delta \boldsymbol{\lambda}) \stackrel{\text{def}}{=} -d_\square(\delta \boldsymbol{\lambda}; \bar{\boldsymbol{\epsilon}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}]) + d_\square(\delta \boldsymbol{\lambda}; \boldsymbol{u}^{(k)}) \tag{5.140}$$ {eq524b}

The appropriate algorithmic tangent (stiffness) forms are given here for completeness:

{eq525a} $$(a_\square)'(\bullet; \delta \boldsymbol{u}_1, \delta \boldsymbol{u}_2) = \langle \boldsymbol{\epsilon}[\delta \boldsymbol{u}_1] : \mathbf{E}_{\mathrm{T}} : \boldsymbol{\epsilon}[\delta \boldsymbol{u}_2] \rangle_\square \tag{5.141}$$

Remark: It is necessary to ensure that the space $\mathbb{T}_\square^+$ contains tractions that can be generated by the constant generally non-symmetric tensor $\delta \bar{\boldsymbol{\sigma}}$, i.e. $\delta \boldsymbol{\lambda} = \delta \bar{\boldsymbol{\sigma}} \cdot \boldsymbol{n} \in \mathbb{T}_\square^+$. In such a case, it follows from the "constraint" equation $(5.136)_2$ that

$$\delta \bar{\boldsymbol{\sigma}} : \langle \boldsymbol{u} \otimes \boldsymbol{\nabla} \rangle_\square = \delta \bar{\boldsymbol{\sigma}} : \bar{\boldsymbol{\epsilon}} \quad \forall \delta \bar{\boldsymbol{\sigma}} \in \mathbb{R}^{3 \times 3} \Rightarrow \begin{cases} \langle \boldsymbol{u} \otimes \boldsymbol{\nabla} \rangle^{\mathrm{sym}} = \langle \boldsymbol{\epsilon}[\boldsymbol{u}] \rangle = \bar{\boldsymbol{\epsilon}} \\ \langle \boldsymbol{u} \otimes \boldsymbol{\nabla} \rangle^{\mathrm{skw}} = \mathbf{0} \end{cases}$$

{eq526}
(5.142)

which are precisely the conditions of average strain in (**??**) and the removal of rigid body rotation in (**??**), respectively. ☐

5.6.2 Macroscale ATS-tensor for WPBC

How to compute $\bar{\mathbf{E}}_{\mathrm{T}}$ is briefly reviewed as what follows: We shall need to compute "unit fluctuation fields" or, rather, *sensitivity fields*, corresponding to a unit variation of $\bar{\boldsymbol{\epsilon}}$. Hence, we shall need to compute differentials in terms of $\mathrm{d}\bar{\boldsymbol{\epsilon}}$. From the first order representation of $\boldsymbol{u}^{\mathrm{M}}$, we obtain

{eq:4-122} $$\mathrm{d}\boldsymbol{u}^{\mathrm{M}} = \mathrm{d}\bar{\boldsymbol{\epsilon}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}] = \sum_{i,j=1}^{NDIM} \hat{\boldsymbol{u}}^{\mathrm{M}(ij)} \, \mathrm{d}\bar{\epsilon}_{ij} \tag{5.143}$$

where the "unit displacement fields" $\hat{\boldsymbol{u}}^{\mathrm{M}(ij)}$ and their gradients $\hat{\boldsymbol{\epsilon}}^{\mathrm{M}(ij)}$ are given as

{eq:4-123} $$\hat{\boldsymbol{u}}^{\mathrm{M}(ij)} \stackrel{\text{def}}{=} \boldsymbol{e}_i \otimes \boldsymbol{e}_j \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}] = \boldsymbol{e}_i \, [x_j - \bar{x}_j] \,, \quad \hat{\boldsymbol{\epsilon}}^{\mathrm{M}(ij)} \stackrel{\text{def}}{=} \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{\mathrm{M}(ij)}] = (\boldsymbol{e}_i \otimes \boldsymbol{e}_j)^{\mathrm{sym}} \tag{5.144}$$

Upon using the identity $\bar{\boldsymbol{\sigma}} = \langle \boldsymbol{\sigma} \rangle_\square$ together with the relation (6.40), we first obtain the representation of $\mathrm{d}\bar{\sigma}_{ij}$ as

{eq:4-124} $$\mathrm{d}\bar{\sigma}_{ij} = \mathrm{d}\left[\langle \boldsymbol{\sigma} \colon [\boldsymbol{e}_i \otimes \boldsymbol{e}_j] \rangle_\square\right] = \mathrm{d}\left[a_\square(\bullet; \hat{\boldsymbol{u}}^{\mathrm{M}(ij)})\right] = (a_\square)'(\bullet; \hat{\boldsymbol{u}}^{\mathrm{M}(ij)}, \mathrm{d}\boldsymbol{u}) \tag{5.145}$$

Next, we conclude that the state equations (5.136) must hold for $\bar{\boldsymbol{\epsilon}}$ as well as for a perturbed state $\bar{\boldsymbol{\epsilon}} + \mathrm{d}\bar{\boldsymbol{\epsilon}}$. However, a given change $\mathrm{d}\bar{\boldsymbol{\epsilon}}$ gives rise to changes $\mathrm{d}\boldsymbol{u} \in \mathbb{U}_\square$ and $\mathrm{d}\boldsymbol{t} \in \mathbb{T}_\square^+$. Upon linearizing the state equations (5.136), we obtain

{eq523b} $$\begin{aligned}(a_\square)'(\boldsymbol{u}; \delta \boldsymbol{u}, \mathrm{d}\boldsymbol{u}) - d_\square(\mathrm{d}\boldsymbol{\lambda}, \delta \boldsymbol{u}) &= 0 \qquad \forall \delta \boldsymbol{u} \in \mathbb{U}_\square \\ -d_\square(\delta \boldsymbol{\lambda}, \mathrm{d}\boldsymbol{u}) &= -d_\square(\delta \boldsymbol{\lambda}, \mathrm{d}\bar{\boldsymbol{\epsilon}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}]) \qquad \forall \delta \boldsymbol{\lambda} \in \mathbb{T}_\square^+\end{aligned} \tag{5.146}$$

from which $\mathrm{d}\boldsymbol{u}$ and $\mathrm{d}\boldsymbol{\lambda}$ can be solved for any given $\mathrm{d}\bar{\boldsymbol{\epsilon}}$.

In analogy with the definition of $\hat{\boldsymbol{u}}^{\mathrm{M}(ij)}$ in Eq. (6.39), we then introduce the "unit fields", or sensitivities, $\hat{\boldsymbol{u}}^{(ij)}$ and $\hat{\boldsymbol{\lambda}}^{(ij)}$, due to a unit value of the components $\mathrm{d}\bar{\epsilon}_{ij}$, via the *ansatz*

{eq39b}
$$\mathrm{d}\boldsymbol{u} = \sum_{i,j} \hat{\boldsymbol{u}}^{(ij)}\,\mathrm{d}\bar{\epsilon}_{ij}, \quad \mathrm{d}\boldsymbol{t} = \sum_{i,j} \hat{\boldsymbol{\lambda}}^{(ij)}\,\mathrm{d}\bar{\epsilon}_{ij} \tag{5.147}$$

which may be inserted into Eq. (5.146) together with Eq. (6.39) to give the equations that must hold for $k, l = 1, 2, ..., NDIM$:

$$\begin{array}{rcll} (a_\square)'(\boldsymbol{u}; \delta\boldsymbol{u}, \hat{\boldsymbol{u}}^{(kl)}) - d_\square(\hat{\boldsymbol{\lambda}}^{(kl)}, \delta\boldsymbol{u}) & = & 0 & \forall \delta\boldsymbol{u} \in \mathbb{U}_\square \\ -d_\square(\delta\boldsymbol{\lambda}, \hat{\boldsymbol{u}}^{(kl)}) & = & -d_\square(\delta\boldsymbol{\lambda}, \hat{\boldsymbol{\epsilon}}^{\mathrm{M}(kl)} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}]) & \forall \delta\boldsymbol{\lambda} \in \mathbb{T}_\square^+ \end{array} \tag{5.148}$$
{eq524b}

whereby it is noted that $\hat{\boldsymbol{\epsilon}}^{\mathrm{M}(kl)} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}] = \boldsymbol{e}_k [X_l - \bar{X}_l]$.

The "unit fields" $\hat{\boldsymbol{u}}^{(ij)}$, which are obtained as part of the solution of from Eq. (5.148), are inserted into Eq. (6.41) to give the explicit expression for $\bar{\mathsf{E}}_\lambda$:

$$\bar{\mathsf{E}}_{\mathrm{T}} = \sum_{k,l=1}^{NDIM} (a_\square)'(\bullet; \hat{\boldsymbol{u}}^{\mathrm{M}(ij)}, \hat{\boldsymbol{u}}^{(kl)}) \boldsymbol{e}_i \otimes \boldsymbol{e}_j \otimes \boldsymbol{e}_k \otimes \boldsymbol{e}_l = \sum_{k,l=1}^{NDIM} \left\langle \mathsf{E}_{\mathrm{T}} : \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{(kl)}] \right\rangle_\square \boldsymbol{e}_k \otimes \boldsymbol{e}_l \tag{5.149}$$
{eq:4-133}

Remark: The Neumann condition represents the weakest possible way of enforcing the micro-periodicity condition. Here it is considered as a *model assumption*; however, it is also possible to view this choice as a (crude) FE-approximation of the traction field, cf. discussion below. □

5.6.3 Mixed FE-approximation – Matrix format (in 2D)

Preliminaries

From Subsection 3.5.6 we recall the result

$$d_\square(\boldsymbol{\lambda}_h, \delta\boldsymbol{u}_h) = [\delta\underline{\boldsymbol{u}}_+^{\mathrm{b}}]^{\mathrm{T}} \underline{\boldsymbol{D}}_+ \underline{\boldsymbol{\lambda}} - [\delta\underline{\boldsymbol{u}}_-^{\mathrm{b}}]^{\mathrm{T}} \underline{\boldsymbol{D}}_- \underline{\boldsymbol{\lambda}} \tag{5.150}$$
{eq:appB_50

where $\underline{\boldsymbol{D}}_+$ and $\underline{\boldsymbol{D}}_-$ are defined as

$$(\underline{\boldsymbol{D}}_+)_{kl} = \frac{1}{|\Omega_\square|} \int_{\Gamma_\square^+} \boldsymbol{N}_k^{\mathrm{u,b+}} \cdot \boldsymbol{N}_l^\lambda \,\mathrm{d}\Gamma \tag{5.151}$$
{eq:appB_51

$$(\underline{\boldsymbol{D}}_-)_{kl} = \frac{1}{|\Omega_\square|} \int_{\Gamma_\square^+} \boldsymbol{N}_k^{\mathrm{u,b-}} \cdot \boldsymbol{N}_l^\lambda \,\mathrm{d}\Gamma \tag{5.152}$$
{eq:appB_51

We introduce

$$\underline{\boldsymbol{u}}^{\mathrm{b}} = \begin{bmatrix} \underline{\boldsymbol{u}}_+^{\mathrm{b}} \\ \underline{\boldsymbol{u}}_-^{\mathrm{b}} \end{bmatrix}, \quad \underline{\boldsymbol{f}}^{\mathrm{b}} = \begin{bmatrix} \underline{\boldsymbol{f}}_+^{\mathrm{b}}(\underline{\boldsymbol{u}}^{\mathrm{i}}, \underline{\boldsymbol{u}}_+^{\mathrm{b}}, \underline{\boldsymbol{u}}_-^{\mathrm{b}}) \\ \underline{\boldsymbol{f}}_-^{\mathrm{b}}(\underline{\boldsymbol{u}}^{\mathrm{i}}, \underline{\boldsymbol{u}}_+^{\mathrm{b}}, \underline{\boldsymbol{u}}_-^{\mathrm{b}}) \end{bmatrix}, \quad \underline{\boldsymbol{D}} = \begin{bmatrix} \underline{\boldsymbol{D}}_+ \\ -\underline{\boldsymbol{D}}_- \end{bmatrix} \tag{5.153}$$
{eq:appB_51

whereby {eq:appB_51

$$\begin{aligned} d_\square(\boldsymbol{\lambda}_h, \delta\boldsymbol{u}_h) &= [\delta\underline{\boldsymbol{u}}_+^{\mathrm{b}}]^{\mathrm{T}} \underline{\boldsymbol{D}}_+ \underline{\boldsymbol{\lambda}} - [\delta\underline{\boldsymbol{u}}_-^{\mathrm{b}}]^{\mathrm{T}} \underline{\boldsymbol{D}}_- \underline{\boldsymbol{\lambda}} \\ &= [\delta\underline{\boldsymbol{u}}^{\mathrm{b}}]^{\mathrm{T}} \underline{\boldsymbol{D}} \underline{\boldsymbol{\lambda}} \end{aligned} \tag{5.154a}$$
{eq:appB_51

$$\begin{aligned} d_\square(\delta\boldsymbol{\lambda}_h, \boldsymbol{u}_h) &= [\delta\underline{\boldsymbol{\lambda}}]^{\mathrm{T}} \underline{\boldsymbol{D}}_+^{\mathrm{T}} \underline{\boldsymbol{u}}_+^{\mathrm{b}} - [\delta\underline{\boldsymbol{\lambda}}]^{\mathrm{T}} \underline{\boldsymbol{D}}_-^{\mathrm{T}} \underline{\boldsymbol{u}}_-^{\mathrm{b}} \\ &= [\delta\underline{\boldsymbol{\lambda}}]^{\mathrm{T}} \underline{\boldsymbol{D}}^{\mathrm{T}} \underline{\boldsymbol{u}}^{\mathrm{b}} \end{aligned} \tag{5.154b}$$
{eq:appB_51

We also obtain

$$d_\square(\delta\boldsymbol{\lambda}_h, \bar{\boldsymbol{\epsilon}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}]) = [\delta\underline{\boldsymbol{\lambda}}]^{\mathrm{T}} \underline{\boldsymbol{D}}^{\mathrm{T}} \underline{\boldsymbol{u}}^{\mathrm{M,b}} = [\delta\underline{\boldsymbol{\lambda}}]^{\mathrm{T}} \underline{\boldsymbol{D}}^{\mathrm{T}} \underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}} \underline{\bar{\boldsymbol{\epsilon}}} \tag{5.155}$$
{eq:appB_52

SVE-problem – Formulation and solution

All nodal displacement variables are free variables that are determined as part of the solution. The SVE-problem is then formulated in matrix format as: {eq:appB_54}

$$\underline{\boldsymbol{f}}^{\mathrm{i}}(\underline{\boldsymbol{u}}^{\mathrm{i}},\underline{\boldsymbol{u}}^{\mathrm{b}}) = \underline{\boldsymbol{0}} \tag{5.156a}$$
{eq:appB_54a}

$$\underline{\boldsymbol{f}}^{\mathrm{b}}(\underline{\boldsymbol{u}}^{\mathrm{i}},\underline{\boldsymbol{u}}^{\mathrm{b}}) - \underline{\boldsymbol{D}}\underline{\boldsymbol{\lambda}} = \underline{\boldsymbol{0}} \tag{5.156b}$$
{eq:appB_54b}

$$\underline{\boldsymbol{D}}^{\mathrm{T}}\underline{\boldsymbol{u}}^{\mathrm{b}} = \underline{\boldsymbol{D}}^{\mathrm{T}}\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}}\underline{\bar{\boldsymbol{\epsilon}}} \tag{5.156c}$$
{eq:appB_54c}

Newton's iteration method for finding $\underline{\boldsymbol{u}}^{\mathrm{i}},\underline{\boldsymbol{u}}^{\mathrm{b}}$ and $\underline{\boldsymbol{\lambda}}$ then becomes: For $k = 1, 2, \ldots,$ compute

{eq:appB_55}
$$\underline{\boldsymbol{u}}^{\mathrm{i}(k+1)} = \underline{\boldsymbol{u}}^{\mathrm{i}(k)} + \Delta\underline{\boldsymbol{u}}^{\mathrm{i}}, \quad \underline{\boldsymbol{u}}^{\mathrm{b}(k+1)} = \underline{\boldsymbol{u}}^{\mathrm{b}(k)} + \Delta\underline{\boldsymbol{u}}^{\mathrm{b}}, \quad \underline{\boldsymbol{\lambda}}^{(k+1)} = \underline{\boldsymbol{\lambda}}^{(k)} + \Delta\underline{\boldsymbol{\lambda}} \tag{5.157}$$

where the iterative updates $\Delta\underline{\boldsymbol{u}}^{\mathrm{i}}, \Delta\underline{\boldsymbol{u}}^{\mathrm{b}}$ and $\Delta\underline{\boldsymbol{\lambda}}$ are solved from the tangent equations

{eq:appB_56}
$$\begin{bmatrix} \underline{\boldsymbol{K}}^{\mathrm{ii}(k)} & \underline{\boldsymbol{K}}^{\mathrm{ib}(k)} & \underline{\boldsymbol{0}} \\ \underline{\boldsymbol{K}}^{\mathrm{bi}(k)} & \underline{\boldsymbol{K}}^{\mathrm{bb}(k)} & -\underline{\boldsymbol{D}} \\ \underline{\boldsymbol{0}} & -\underline{\boldsymbol{D}}^{\mathrm{T}} & \underline{\boldsymbol{0}} \end{bmatrix} \begin{bmatrix} \Delta\underline{\boldsymbol{u}}^{\mathrm{i}} \\ \Delta\underline{\boldsymbol{u}}^{\mathrm{b}} \\ \Delta\underline{\boldsymbol{\lambda}} \end{bmatrix} = \begin{bmatrix} -\underline{\boldsymbol{f}}^{\mathrm{i}(k)} \\ \underline{\boldsymbol{D}}\underline{\boldsymbol{\lambda}}^{(k)} - \underline{\boldsymbol{f}}^{\mathrm{b}(k)} \\ \underline{\boldsymbol{D}}^{\mathrm{T}}\left[\underline{\boldsymbol{u}}^{\mathrm{b}(k)} - \underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}}\underline{\bar{\boldsymbol{\epsilon}}}\right] \end{bmatrix} \stackrel{\mathrm{def}}{=} \begin{bmatrix} \underline{\boldsymbol{r}}^{\mathrm{i}(k)} \\ \underline{\boldsymbol{r}}^{\mathrm{b}(k)} \\ \underline{\boldsymbol{R}}^{(k)} \end{bmatrix} \tag{5.158}$$

To solve (5.158), while preserving the the "FE-structure" of the tangent stiffness matrix $\underline{\boldsymbol{K}}$, introduce the decomposition via sensitivities w.r.t. to a perturbation of $\underline{\boldsymbol{\lambda}}$:

{eq:appB_57}
$$\Delta\underline{\boldsymbol{u}}^{\mathrm{i}} = \underline{\hat{\boldsymbol{u}}}^{\mathrm{i}}_{\lambda}\Delta\underline{\boldsymbol{\lambda}} + \Delta\underline{\boldsymbol{u}}^{\mathrm{i}}_{\mathrm{R}}, \quad \Delta\underline{\boldsymbol{u}}^{\mathrm{b}} = \underline{\hat{\boldsymbol{u}}}^{\mathrm{b}}_{\lambda}\Delta\underline{\boldsymbol{\lambda}} + \Delta\underline{\boldsymbol{u}}^{\mathrm{b}}_{\mathrm{R}} \tag{5.159}$$

Upon inserting into (5.158), we obtain the two sets of FE-equations

{eq:appB_58}
$$\begin{bmatrix} \underline{\boldsymbol{K}}^{\mathrm{ii}(k)} & \underline{\boldsymbol{K}}^{\mathrm{ib}(k)} \\ \underline{\boldsymbol{K}}^{\mathrm{bi}(k)} & \underline{\boldsymbol{K}}^{\mathrm{bb}(k)} \end{bmatrix} \begin{bmatrix} \Delta\underline{\boldsymbol{u}}^{\mathrm{i}}_{\mathrm{R}} \\ \Delta\underline{\boldsymbol{u}}^{\mathrm{b}}_{\mathrm{R}} \end{bmatrix} = \begin{bmatrix} \underline{\boldsymbol{r}}^{\mathrm{i}(k)} \\ \underline{\boldsymbol{r}}^{\mathrm{b}(k)} \end{bmatrix} \tag{5.160}$$

{eq:appB_59}
$$\begin{bmatrix} \underline{\boldsymbol{K}}^{\mathrm{ii}(k)} & \underline{\boldsymbol{K}}^{\mathrm{ib}(k)} \\ \underline{\boldsymbol{K}}^{\mathrm{bi}(k)} & \underline{\boldsymbol{K}}^{\mathrm{bb}(k)} \end{bmatrix} \begin{bmatrix} \underline{\hat{\boldsymbol{u}}}^{\mathrm{i}}_{\lambda} \\ \underline{\hat{\boldsymbol{u}}}^{\mathrm{b}}_{\lambda} \end{bmatrix} = \begin{bmatrix} \underline{\boldsymbol{0}} \\ \underline{\boldsymbol{D}} \end{bmatrix} \tag{5.161}$$

Given the solution $(\underline{\hat{\boldsymbol{u}}}^{\mathrm{i}}_{\lambda}, \underline{\hat{\boldsymbol{u}}}^{\mathrm{i}}_{\lambda})$, and $(\Delta\underline{\boldsymbol{u}}^{\mathrm{i}}_{\mathrm{R}}, \Delta\underline{\boldsymbol{u}}^{\mathrm{i}}_{\mathrm{R}})$, we obtain from the last equation in (5.158) the equation from which $\Delta\underline{\boldsymbol{\lambda}}$ is solved:

{eq:appB_60}
$$\Delta\underline{\boldsymbol{\lambda}} = -\left[\underline{\boldsymbol{D}}^{\mathrm{T}}\underline{\hat{\boldsymbol{u}}}^{\mathrm{b}}_{\lambda}\right]^{-1}\left[\underline{\boldsymbol{R}}^{(k)} + \underline{\boldsymbol{D}}^{\mathrm{T}}\Delta\underline{\hat{\boldsymbol{u}}}^{\mathrm{b}}_{\mathrm{R}}\right] \tag{5.162}$$

As a postprocessing step, compute

appB_60_1}
$$\underline{\bar{\boldsymbol{\sigma}}} = \left[\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}}\right]^{\mathrm{T}}\underline{\boldsymbol{f}}^{\mathrm{b}} = \left[\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}}\right]^{\mathrm{T}}\underline{\boldsymbol{D}}\underline{\boldsymbol{\lambda}} \tag{5.163}$$

where the last identity follows from (5.156b).

Computing the macroscale tangent stiffness in practice

Linearizing the SVE-problem (5.156a)-(5.156c) w.r.t. $\underline{\bar{\boldsymbol{\epsilon}}}$ gives the "perturbed" system

{eq:appB_61}
$$\begin{bmatrix} \underline{\boldsymbol{K}}^{\mathrm{ii}} & \underline{\boldsymbol{K}}^{\mathrm{ib}} & \underline{\boldsymbol{0}} \\ \underline{\boldsymbol{K}}^{\mathrm{bi}} & \underline{\boldsymbol{K}}^{\mathrm{bb}} & -\underline{\boldsymbol{D}} \\ \underline{\boldsymbol{0}} & -\underline{\boldsymbol{D}}^{\mathrm{T}} & \underline{\boldsymbol{0}} \end{bmatrix} \begin{bmatrix} \mathrm{d}\underline{\boldsymbol{u}}^{\mathrm{i}} \\ \mathrm{d}\underline{\boldsymbol{u}}^{\mathrm{b}} \\ \mathrm{d}\underline{\boldsymbol{\lambda}} \end{bmatrix} = \begin{bmatrix} \underline{\boldsymbol{0}} \\ \underline{\boldsymbol{0}} \\ -\underline{\boldsymbol{D}}^{\mathrm{T}}\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}}\,\mathrm{d}\underline{\bar{\boldsymbol{\epsilon}}} \end{bmatrix} \tag{5.164}$$

To solve (5.164) for given $\mathrm{d}\underline{\bar{\boldsymbol{\epsilon}}}$, while preserving the the "FE-structure" of the tangent stiffness matrix $\underline{\boldsymbol{K}}$, introduce the decomposition via sensitivities w.r.t. to a perturbation of $\underline{\boldsymbol{\lambda}}$:

{eq:appB_62}
$$\mathrm{d}\underline{\boldsymbol{u}}^{\mathrm{i}} = \underline{\hat{\boldsymbol{u}}}_{\lambda}^{\mathrm{i}}\,\mathrm{d}\underline{\boldsymbol{\lambda}}, \quad \mathrm{d}\underline{\boldsymbol{u}}^{\mathrm{b}} = \underline{\hat{\boldsymbol{u}}}_{\lambda}^{\mathrm{b}}\,\mathrm{d}\underline{\boldsymbol{\lambda}} \tag{5.165}$$

Upon inserting into (5.164), we obtain the set of FE-equations

{eq:appB_63}
$$\begin{bmatrix} \underline{\boldsymbol{K}}^{\mathrm{ii}} & \underline{\boldsymbol{K}}^{\mathrm{ib}} \\ \underline{\boldsymbol{K}}^{\mathrm{bi}} & \underline{\boldsymbol{K}}^{\mathrm{bb}} \end{bmatrix} \begin{bmatrix} \underline{\hat{\boldsymbol{u}}}_{\lambda}^{\mathrm{i}} \\ \underline{\hat{\boldsymbol{u}}}_{\lambda}^{\mathrm{b}} \end{bmatrix} = \begin{bmatrix} \underline{\mathbf{0}} \\ \underline{\boldsymbol{D}} \end{bmatrix} \tag{5.166}$$

which is exactly the same system already solved as part of the Newton iterations.
Given the sensitivities $\underline{\hat{\boldsymbol{u}}}_{\lambda}^{\mathrm{i}}, \underline{\hat{\boldsymbol{u}}}_{\lambda}^{\mathrm{b}}$, and defining the sensitivity $\underline{\hat{\boldsymbol{\lambda}}}$ w.r.t $\underline{\bar{\boldsymbol{\epsilon}}}$ in (**??**)$_3$, we obtain

$$\mathrm{d}\underline{\boldsymbol{u}}^{\mathrm{i}} = \underline{\hat{\boldsymbol{u}}}_{\lambda}^{\mathrm{i}}\underline{\hat{\boldsymbol{\lambda}}}\,\mathrm{d}\underline{\bar{\boldsymbol{\epsilon}}}, \quad \mathrm{d}\underline{\boldsymbol{u}}^{\mathrm{b}} = \underline{\hat{\boldsymbol{u}}}_{\lambda}^{\mathrm{b}}\underline{\hat{\boldsymbol{\lambda}}}\,\mathrm{d}\underline{\bar{\boldsymbol{\epsilon}}} \tag{5.167}$$ {eq:appB_63

Upon inserting into the last equation in (5.164), we obtain the equation from which $\underline{\hat{\boldsymbol{\lambda}}}$ is solved:

$$\underline{\boldsymbol{D}}^{\mathrm{T}}\underline{\hat{\boldsymbol{u}}}_{\lambda}^{\mathrm{b}}\underline{\hat{\boldsymbol{\lambda}}} = \underline{\boldsymbol{D}}^{\mathrm{T}}\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}} \quad \rightarrow \quad \underline{\hat{\boldsymbol{\lambda}}} = \left[\underline{\boldsymbol{D}}^{\mathrm{T}}\underline{\hat{\boldsymbol{u}}}_{\lambda}^{\mathrm{b}}\right]^{-1}\underline{\boldsymbol{D}}^{\mathrm{T}}\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}} \tag{5.168}$$ {eq:appB_64

Finally, we obtain from (5.163)

$$\mathrm{d}\underline{\bar{\boldsymbol{\sigma}}} = \underbrace{\left[\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}}\right]^{\mathrm{T}}\underline{\boldsymbol{D}}\underline{\hat{\boldsymbol{\lambda}}}}_{\underline{\bar{\mathsf{E}}}_{\square,\mathrm{T}}}\,\mathrm{d}\underline{\bar{\boldsymbol{\epsilon}}} \tag{5.169}$$ {eq:appB_64

We have thus derived the tangent stiffness in the operational format

$$\underline{\bar{\mathsf{E}}}_{\square,\mathrm{T}} = \left[\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,b}}\right]^{\mathrm{T}}\underline{\boldsymbol{D}}\underline{\hat{\boldsymbol{\lambda}}} \tag{5.170}$$ {eq:appB_64

As to the dimensions of the matrices involved, we have in the 2D-case:

$$\begin{aligned} dim(\underline{\boldsymbol{D}}_{+}) &= \mathrm{NVAR}_{\mathrm{u,b+}} \times \mathrm{NVAR}_{\lambda} \\ dim(\underline{\boldsymbol{D}}_{-}) &= \mathrm{NVAR}_{\mathrm{u,b-}} \times \mathrm{NVAR}_{\lambda} \\ dim(\underline{\boldsymbol{D}}) &= \mathrm{NVAR}_{\mathrm{u,b}} \times \mathrm{NVAR}_{\lambda} \\ dim(\underline{\bar{\mathsf{E}}}_{\square,\mathrm{T}}) &= 3 \times 3_{\square,\mathrm{T}} \end{aligned} \tag{5.171}$$ {eq:appB_71

□

Chapter 6

FE^2 FOR FINITE DEFORMATION – HYPERELASTICITY

6.1 Subscale nonlinear elasticity

6.1.1 Strain and stress energy densities for subscale modeling

We assume the existence of a volume-specific strain energy density $\psi(\boldsymbol{\epsilon})$ with the following properties:

- It serves a a potential for $\boldsymbol{\sigma}$, i.e. $\boldsymbol{\sigma}(\boldsymbol{\epsilon}) = \frac{\partial \psi}{\partial \boldsymbol{\epsilon}}(\boldsymbol{\epsilon})$
- It is strictly convex[1], i.e. $\psi(\boldsymbol{\epsilon}_2) - \psi(\boldsymbol{\epsilon}_1) \geq \frac{\partial \psi}{\partial \boldsymbol{\epsilon}}(\boldsymbol{\epsilon}_1) : [\boldsymbol{\epsilon}_2 - \boldsymbol{\epsilon}_1] = \boldsymbol{\sigma}(\boldsymbol{\epsilon}_1) : [\boldsymbol{\epsilon}_2 - \boldsymbol{\epsilon}_1]$ for any two $\boldsymbol{\epsilon}_1$ and $\boldsymbol{\epsilon}_2$.

We also introduce the stress energy density $\psi^*(\boldsymbol{\sigma})$, often denoted the complementary strain energy, via the Legendre transformation

$$\psi^*(\boldsymbol{\sigma}) = \max_{\hat{\boldsymbol{\epsilon}}} \left[\boldsymbol{\sigma} : \hat{\boldsymbol{\epsilon}} - \psi(\hat{\boldsymbol{\epsilon}})\right] \qquad (6.1) \quad \{\texttt{eq:4-2b}\}$$

It then turns out that $\psi^*(\boldsymbol{\sigma})$ has the following properties:

- It serves as a potential for $\boldsymbol{\epsilon}$, i.e. $\boldsymbol{\epsilon}(\boldsymbol{\sigma}) = \frac{\partial \psi^*}{\partial \boldsymbol{\sigma}}(\boldsymbol{\sigma})$
- It is strictly convex, i.e. $\psi^*(\boldsymbol{\sigma}_2) - \psi(\boldsymbol{\sigma}_1) \geq \frac{\partial \psi^*}{\partial \boldsymbol{\sigma}}(\boldsymbol{\sigma}_1) : [\boldsymbol{\sigma}_2 - \boldsymbol{\sigma}_1] = \boldsymbol{\epsilon}(\boldsymbol{\sigma}_1) : [\boldsymbol{\sigma}_2 - \boldsymbol{\sigma}_1]$ for any two $\boldsymbol{\sigma}_1$ and $\boldsymbol{\sigma}_2$.

Proof: Homework!

6.1.2 Principle of Minimum of Potential Energy (MPE-principle)

The weak format of the equilibrium equation is: Find $\boldsymbol{u} \in \mathbb{U}$ that solves

$$a(\boldsymbol{u}; \delta\boldsymbol{u}) = l(\delta\boldsymbol{u}) \quad \forall \delta\boldsymbol{u} \in \mathbb{U}^0 \qquad (6.2) \quad \{\texttt{eq:4-1}\}$$

[1] Convexity is a necessary condition for uniqueness of boundary value problems.

This is the same formulation as for linear elasticity with the generalization that $a(\boldsymbol{u};\delta\boldsymbol{u})$ is now the semi-linear form

$$\begin{aligned} a(\boldsymbol{u};\delta\boldsymbol{u}) &\stackrel{\text{def}}{=} \int_\Omega \boldsymbol{\sigma}(\boldsymbol{\epsilon}[\boldsymbol{u}]) : \boldsymbol{\epsilon}[\delta\boldsymbol{u}]\,\mathrm{dV} && (6.3) \quad \texttt{\{eq:4-3a\}} \\ l(\delta\boldsymbol{u}) &\stackrel{\text{def}}{=} \int_\Omega \boldsymbol{f}\cdot\delta\boldsymbol{u}\,\mathrm{dV} + \int_{\partial\Omega_\mathrm{N}} \boldsymbol{t}_\mathrm{P}\cdot\delta\boldsymbol{u}\,\mathrm{dS} && (6.4) \quad \texttt{\{eq:4-3b\}} \end{aligned}$$

Extending the MPE-principle from linear elasticity is also straightforward. We introduce the potential energy $\Pi(\hat{\boldsymbol{u}})$ of any $\hat{\boldsymbol{u}} \in \mathbb{U}$ as

{eq:4-34}
$$\Pi(\hat{\boldsymbol{u}}) = \Psi(\hat{\boldsymbol{u}}) - l(\hat{\boldsymbol{u}}), \tag{6.5}$$

where we define the stored elastic strain energy as

{eq:4-34a}
$$\Psi(\boldsymbol{v}) \stackrel{\text{def}}{=} \int_\Omega \psi(\boldsymbol{\epsilon}[\boldsymbol{v}])\,\mathrm{d}\Omega. \tag{6.6}$$

The directional derivative of Π at any point $\hat{\boldsymbol{u}} \in \mathbb{U}$ in the direction $\delta\boldsymbol{u} \in \mathbb{U}^0$ is given as

{eq:4-35}
$$\Pi'_u(\hat{\boldsymbol{u}};\delta\boldsymbol{u})\frac{\mathrm{d}}{\mathrm{d}\gamma}\Pi(\hat{\boldsymbol{u}}+\gamma\delta\boldsymbol{u})|_{\gamma=0} = \int_\Omega \boldsymbol{\sigma}(\boldsymbol{\epsilon}[\hat{\boldsymbol{u}}]) : \boldsymbol{\epsilon}[\delta\hat{\boldsymbol{u}}]\,\mathrm{d}\Omega - l(\delta\boldsymbol{u}) = a(\hat{\boldsymbol{u}};\delta\boldsymbol{u}) - l(\delta\boldsymbol{u}) \tag{6.7}$$

From the convexity of ψ, we conclude that Π is convex in the sense that, for any given pair $\boldsymbol{u}_1 \in \mathbb{U}$ and $\boldsymbol{u}_2 \in \mathbb{U}$, we have the inequality

{eq:4-36}
$$\begin{aligned} \Pi(\boldsymbol{u}_2) - \Pi(\boldsymbol{u}_1) &= \int_\Omega [\psi(\boldsymbol{\epsilon}_2) - \psi(\boldsymbol{\epsilon}_1)]\,\mathrm{d}\Omega - l(\boldsymbol{u}_2 - \boldsymbol{u}_1) \\ &\geq \int_\Omega \boldsymbol{\sigma}(\boldsymbol{\epsilon}_1) : [\boldsymbol{\epsilon}_2 - \boldsymbol{\epsilon}_1]\,\mathrm{d}\Omega - l(\boldsymbol{u}_2 - \boldsymbol{u}_1) = \Pi'_u(\boldsymbol{u}_1;\boldsymbol{u}_2 - \boldsymbol{u}_1) \end{aligned} \tag{6.8}$$

The solution $\boldsymbol{u} \in \mathbb{U}$ of the weak problem (6.2) is also the minimizer of $\Pi(\hat{\boldsymbol{u}})$, i.e.

{eq:4-37}
$$\boldsymbol{u} = \arg\left[\min_{\hat{\boldsymbol{u}}\in\mathbb{U}} \Pi(\hat{\boldsymbol{u}})\right] \tag{6.9}$$

In other words,

{eq:4-38}
$$\Pi(\boldsymbol{u}) \leq \Pi(\hat{\boldsymbol{u}}) \quad \forall\hat{\boldsymbol{u}} \in \mathbb{U} \quad \text{or} \quad \Pi(\boldsymbol{u}) = \min_{\hat{\boldsymbol{u}}\in\mathbb{U}} \Pi(\hat{\boldsymbol{u}}) \tag{6.10}$$

Proof: The proof follows closely that of linear elasticity in Chapter 2. □

6.1.3 Solution of nonlinear problem - Linearization

The continuous (weak) problem format (6.2) is nonlinear in $\boldsymbol{u}$, and its solution thus requires some sort of iteration strategy. As a prototype of solution procedure, we consider Newton iterations, which are based on (exact) linearization of the nonlinear form $a(\boldsymbol{u};\delta\boldsymbol{u})$. As the starting point, consider (6.2) for any given field $\boldsymbol{u}^{(k)} \neq \boldsymbol{u}$ in the iteration k, whereby the residual is defined as

{eq:4-48}
$$R(\boldsymbol{u}^{(k)};\delta\boldsymbol{u}) = \Pi'_u(\boldsymbol{u}^{(k)};\delta\boldsymbol{u}) = a(\boldsymbol{u}^{(k)};\delta\boldsymbol{u}) - l(\delta\boldsymbol{u}) \quad \forall\delta\boldsymbol{u} \in \mathbb{U}^0 \tag{6.11}$$

and it is noted that $R(\boldsymbol{u}^{(k)};\delta\boldsymbol{u}) \neq 0$ if $\boldsymbol{u}^{(k)} \neq \boldsymbol{u}$.

{grp} Newton's method is to compute the improved field $\boldsymbol{u}^{(k+1)}$ from the algorithm

{eq:4-49a}
$$\boldsymbol{u}^{(k+1)} = \boldsymbol{u}^{(k)} + \Delta\boldsymbol{u} \tag{6.12a}$$

{eq:4-49b}
$$R'_u(\boldsymbol{u}^{(k)}; \delta\boldsymbol{u}, \Delta\boldsymbol{u}) = -R(\boldsymbol{u}^{(k)}; \delta\boldsymbol{u}) \quad \forall \delta\boldsymbol{u} \in \mathbb{U}^0 \tag{6.12b}$$

Hence, we exploit the linearization of $R(\boldsymbol{u}; \delta\boldsymbol{u})$

{eq:4-50}
$$\begin{aligned} R'_u(\boldsymbol{u}; \delta\boldsymbol{u}_1, \delta\boldsymbol{u}_2) &= \frac{\mathrm{d}}{\mathrm{d}\gamma} R(\boldsymbol{u} + \gamma\delta\boldsymbol{u}_2, \delta\boldsymbol{u}_1)|_{\gamma=0} = \Pi''_{uu}(\boldsymbol{u}; \delta\boldsymbol{u}_1, \delta\boldsymbol{u}_2) = a'(\boldsymbol{u}; \delta\boldsymbol{u}_1, \delta\boldsymbol{u}_2) \\ &= \int_\Omega \boldsymbol{\epsilon}[\delta\boldsymbol{u}_1] : \mathbf{E}_\mathrm{t} : \boldsymbol{\epsilon}[\delta\boldsymbol{u}_2] \, \mathrm{d}V = \int_\Omega [\delta\boldsymbol{u}_1 \otimes \boldsymbol{\nabla}] : \mathbf{E}_\mathrm{t} : [\delta\boldsymbol{u}_2 \otimes \boldsymbol{\nabla}] \, \mathrm{d}V \end{aligned} \tag{6.13}$$

where it was used that $\mathbf{E}_\mathrm{t}$ is the tangent stiffness tensor that represents the (exact) linearization of $\boldsymbol{\sigma}(\boldsymbol{\epsilon})$

$$\mathrm{d}\boldsymbol{\sigma}(\boldsymbol{\epsilon}) = \mathbf{E}_\mathrm{t}(\boldsymbol{\epsilon}) : \mathrm{d}\boldsymbol{\epsilon} \tag{6.14}$$ {eq:4-51}

6.2 Macroscale problem obtained from homogenization

6.2.1 Preliminaries

Let us recall the standard variational format of the fine-scale representation of of nonlinear elasticity in (6.2): Find $\boldsymbol{u} \in \mathbb{U}$ that solves

$$a(\boldsymbol{u}; \delta\boldsymbol{u}) = l(\delta\boldsymbol{u}) \quad \forall \delta\boldsymbol{u} \in \mathbb{U}^0. \tag{6.15}$$ {eq:4-101}

The purpose of homogenization is to replace this problem with a macroscale problem, whose unknown displacement field is a globally defined macroscale field $\bar{\boldsymbol{u}} \neq \boldsymbol{u}$ that is significantly smoother than $\boldsymbol{u}$. Note that there is no hope to retrofit the finescale solution from $\bar{\boldsymbol{u}}$ as a postprocessing step. The local field is thus replaced (as a smoothing approximation) by the spatially homogenized field on a suitably chosen RVE in any given macroscale point $\bar{\boldsymbol{x}} \in \Omega$. A consequence of this fact is that the RVE:s for two sufficiently close macroscale points are "overlapping"; however, this fact does not incur any conceptual difficulty or anomally since the concept of homogenization is a model assumption. Moreover, at the algorithmic implementation numerical quadrature is employed at the evaluation of integrals in the spatial domain. Hence, homogenization on the RVE's is carried out (only) in these macroscale quadrature points in practice.

With the introduced homogenization, the original problem formulation remains formally unchanged *if integrands are replaced by the homogenized quantities* in all space-variational forms. Hence, (6.3) and (6.4) are replaced by

$$a(\boldsymbol{u}; \delta\boldsymbol{u}) \stackrel{\mathrm{def}}{=} \int_\Omega \langle \boldsymbol{\sigma}(\boldsymbol{\epsilon}[\boldsymbol{u}]) : \boldsymbol{\epsilon}[\delta\boldsymbol{u}] \rangle_\square \, \mathrm{d}V, \tag{6.16}$$ {eq:4-102}

$$l(\delta\boldsymbol{u}) \stackrel{\mathrm{def}}{=} \int_\Omega \langle \boldsymbol{f} \cdot \delta\boldsymbol{u} \rangle_\square \, \mathrm{d}V + \int_{\Gamma_\mathrm{N}} \langle\langle \boldsymbol{t}_\mathrm{p} \cdot \delta\boldsymbol{u} \rangle\rangle_\square \, \mathrm{d}S \tag{6.17}$$ {eq:4-103}

Inside each RVE, the subscale solution[2] is split additively into the smooth part, $\boldsymbol{u}^\mathrm{M}$, and the nonsmooth (fluctuation) part, $\boldsymbol{u}^\mu$ in accordance with the assumption of 1st order homogenization:

$$\boldsymbol{u}(\bar{\boldsymbol{x}}; \boldsymbol{x}) = \boldsymbol{u}^\mathrm{M}(\bar{\boldsymbol{x}}; \boldsymbol{x}) + \boldsymbol{u}^\mu(\boldsymbol{x}), \quad \boldsymbol{u}^\mathrm{M}(\bar{\boldsymbol{x}}; \boldsymbol{x}) = \bar{\boldsymbol{u}}(\bar{\boldsymbol{x}}) + \bar{\boldsymbol{\epsilon}}(\bar{\boldsymbol{x}})[\boldsymbol{x} - \bar{\boldsymbol{x}}] \tag{6.18}$$ {eq:4-104}

where $\bar{\boldsymbol{\epsilon}}$ is connected kinematically to the macroscale displacement field $\bar{\boldsymbol{u}}$ as $\bar{\boldsymbol{\epsilon}} = (\bar{\boldsymbol{u}} \otimes \boldsymbol{\nabla})^\mathrm{sym}$.

[2] Double arguments, e.g. $\boldsymbol{u}(\bar{\boldsymbol{x}}, \boldsymbol{x})$, are used to explicitly point out the underlying scale separation.

6.2.2 Variationally consistent homogenization??? UPDATE!

Update without explicit reference to "variationally consistent"? This concept in separate Chapter?

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By merely introducing volume averages on RVE's and introducing the kinematic decomposition in (6.18), the "dimension" on the problem is not reduced, i.e. it is still as complex as the original fine-scale problem. The reduction is obtained upon introducing the following assumptions/steps:

- Define $\boldsymbol{u}^\mu$ as an implicit function[3] of $\boldsymbol{u}^{\mathrm{M}}$, which is henceforth expressed as $\boldsymbol{u}^\mu \stackrel{\text{def}}{=} \boldsymbol{u}^\mu\{\boldsymbol{u}^{\mathrm{M}}\}$ for given $\boldsymbol{u}^{\mathrm{M}}$. Hence, $\boldsymbol{u} = \boldsymbol{u}\{\boldsymbol{u}^{\mathrm{M}}\} = \boldsymbol{u}^{\mathrm{M}} + \boldsymbol{u}^\mu\{\boldsymbol{u}^{\mathrm{M}}\}$.
- Assume that $\boldsymbol{u}^\mu\{\boldsymbol{u}^{\mathrm{M}}\}$ is the solution of a (local) problem on each RVE, whereby $\boldsymbol{u}^{\mathrm{M}}$ represents "prolongation" of the macroscale solution $\bar{\boldsymbol{u}}$ to the RVE.
- Replace the test function $\delta\boldsymbol{u}$ with $\delta\boldsymbol{u}^{\mathrm{M}}$ which will act as the "homogenizer" on each RVE.

Remark: It is noted that the task of finding $\boldsymbol{u}^{\mathrm{M}} \in \mathbb{U}^{\mathrm{M}}$ is equivalent to that of finding $\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}$. □

Next, we introduce the appropriate "two-scale" space $\mathbb{U}^{\mathrm{M}}$ as follows:

{eq:4-105}
$$\mathbb{U}^{\mathrm{M}} = \{\boldsymbol{u}^{\mathrm{M}}|_{\Omega_\square(\bar{\boldsymbol{x}})} : \boldsymbol{u}^{\mathrm{M}}[\bar{\boldsymbol{u}}](\boldsymbol{x};\bar{\boldsymbol{x}}) = \bar{\boldsymbol{u}}(\bar{\boldsymbol{x}}) + \bar{\boldsymbol{\epsilon}}(\bar{\boldsymbol{x}}) \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}], \quad \bar{\boldsymbol{u}} \in \bar{\mathbb{U}}\} \tag{6.19}$$

where $\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}$ is the (global) macroscale displacement field, and where $\bar{\boldsymbol{\epsilon}} \stackrel{\text{def}}{=} (\bar{\boldsymbol{u}} \otimes \boldsymbol{\nabla})^{\mathrm{sym}}$ is the macroscale strain. We are now in the position to replace the problem (6.15) by the *homogenized* problem: Find $\boldsymbol{u}^{\mathrm{M}} \in \mathbb{U}^{\mathrm{M}}$ that is the solution of

{eq:4-106}
$$a(\boldsymbol{u}\{\boldsymbol{u}^{\mathrm{M}}\}; \delta\boldsymbol{u}^{\mathrm{M}}) = l(\delta\boldsymbol{u}^{\mathrm{M}}) \quad \forall \delta\boldsymbol{u}^{\mathrm{M}} \in \mathbb{U}^{\mathrm{M},0}. \tag{6.20}$$

In order to establish the appropriate (space-)variational format of the continuous macroscale problem, we first simplify by henceforth assuming that $\boldsymbol{u}$ is sufficiently smooth on Γ to allow the approximation $\boldsymbol{u}^\mu = \boldsymbol{0}$ (and $\delta\boldsymbol{u}^\mu = \boldsymbol{0}$) on Γ. Moreover, we restrict to the situation that the boundary values $\boldsymbol{u}_{\mathrm{p}}$ and $\boldsymbol{t}_{\mathrm{p}}$ vary sufficiently slowly to represent the macroscopic (homogenized) values in the sense that

{eq:4-107}
$$\langle \boldsymbol{u} \rangle_\square = \bar{\boldsymbol{u}}_{\mathrm{p}} \text{ on } \Gamma_{\mathrm{D}} \quad \text{and} \quad \langle\langle \boldsymbol{t}_{\mathrm{p}} \cdot \delta\boldsymbol{u} \rangle\rangle_\square = \bar{\boldsymbol{t}}_{\mathrm{p}} \cdot \delta\bar{\boldsymbol{u}} \text{ on } \Gamma_{\mathrm{N}} \tag{6.21}$$

where $\bar{\boldsymbol{u}}_{\mathrm{p}}$ and $\bar{\boldsymbol{t}}_{\mathrm{p}}$ are prescribed boundary values. In particular, the condition $(6.21)_2$ infers that
face average $\langle\langle \boldsymbol{t}_{\mathrm{p}} \rangle\rangle_\square = \bar{\boldsymbol{t}}_{\mathrm{p}}$ and $\langle\langle \boldsymbol{t}_{\mathrm{p}} \otimes [\boldsymbol{x} - \bar{\boldsymbol{x}}] \rangle\rangle_\square = \boldsymbol{0}$. In this way certain technical difficulties associated with the homogenization on the boundary are avoided. We shall also assume that the volume-specific load $\boldsymbol{f}$ is smooth such that $\langle \boldsymbol{f} \cdot \delta\boldsymbol{u} \rangle_\square = \bar{\boldsymbol{f}} \cdot \delta\bar{\boldsymbol{u}}$, whereby $\bar{\boldsymbol{f}} \stackrel{\text{def}}{=} \langle \boldsymbol{f} \rangle_\square$ and $\langle \boldsymbol{f} \otimes [\boldsymbol{x} - \bar{\boldsymbol{x}}] \rangle_\square = \boldsymbol{0}$.

[3] Curly brackets $\{(\bullet)\}$ indicate implicit functional dependence on $(\bullet)$.

We may now evaluate the forms that occur in (6.20) as follows:

$$
\begin{aligned}
a(\boldsymbol{u}\{\boldsymbol{u}^{\mathrm{M}}\};\delta\boldsymbol{u}^{\mathrm{M}}) &= \int_\Omega \langle \boldsymbol{\sigma}(\boldsymbol{\epsilon}[\boldsymbol{u}\{\boldsymbol{u}^{\mathrm{M}}\}]) : \boldsymbol{\epsilon}[\delta\boldsymbol{u}^{\mathrm{M}}]\rangle_\square \,\mathrm{d}\bar{V} \\
&= \int_\Omega \langle \boldsymbol{\sigma}(\boldsymbol{\epsilon}[\boldsymbol{u}\{\boldsymbol{u}^{\mathrm{M}}\}]) : \delta\bar{\boldsymbol{\epsilon}}\rangle_\square \,\mathrm{d}\bar{V} = \int_\Omega \langle \boldsymbol{\sigma}(\boldsymbol{\epsilon}[\boldsymbol{u}\{\boldsymbol{u}^{\mathrm{M}}\}])\rangle_\square \,\mathrm{d}\bar{V} : \delta\bar{\boldsymbol{\epsilon}} \\
&= \bar{\boldsymbol{\sigma}} : \delta\bar{\boldsymbol{\epsilon}} && (6.22)\\
l(\delta\boldsymbol{u}^{\mathrm{M}}) &= \int_\Omega \langle \boldsymbol{f}\cdot\delta\boldsymbol{u}^{\mathrm{M}}\rangle_\square \,\mathrm{d}\bar{V} + \int_{\Gamma_{\mathrm{N}}} \langle\langle \boldsymbol{t}_{\mathrm{p}}\cdot\delta\boldsymbol{u}^{\mathrm{M}}\rangle\rangle_\square \,\mathrm{d}\bar{S} \\
&= \int_\Omega \bar{\boldsymbol{f}}\cdot\delta\bar{\boldsymbol{u}}\,\mathrm{d}\bar{V} + \int_{\Gamma_{\mathrm{N}}} \bar{\boldsymbol{t}}_{\mathrm{p}}\cdot\delta\bar{\boldsymbol{u}}\,\mathrm{d}\bar{S} && (6.23)
\end{aligned}
$$

{eq:4-108a} {eq:4-108b}

It is concluded from the underlying assumptions that the RVE-averages take the explicit forms

$$\langle \boldsymbol{\sigma} : \delta\boldsymbol{\epsilon}\rangle_\square = \bar{\boldsymbol{\sigma}} : \delta\bar{\boldsymbol{\epsilon}}, \quad \langle \boldsymbol{f}\cdot\delta\boldsymbol{u}^{\mathrm{M}}\rangle_\square = \bar{\boldsymbol{f}}\cdot\delta\bar{\boldsymbol{u}}, \quad \langle\langle \boldsymbol{t}_{\mathrm{p}}\cdot\delta\boldsymbol{u}^{\mathrm{M}}\rangle\rangle_\square = \bar{\boldsymbol{t}}_{\mathrm{p}}\cdot\delta\bar{\boldsymbol{u}} \qquad (6.24)$$ {eq:4-109}

Remark: The virtual work identity in $(6.24)_1$ satisfies the classical form of the Hill-Mandel condition. □

The macroscale problem can now be formulated as follows: Find $\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}$ such that the macroscale residual vanishes,

$$\bar{R}\{\bar{\boldsymbol{u}};\delta\bar{\boldsymbol{u}}\} \overset{\mathrm{def}}{=} \bar{l}\{\delta\bar{\boldsymbol{u}}\} - \bar{a}\{\bar{\boldsymbol{u}};\delta\bar{\boldsymbol{u}}\} = 0 \quad \forall \delta\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}^0. \qquad (6.25)$$ {eq:4-110}

where we introduced the macroscale space-variational forms

$$\bar{a}\{\bar{\boldsymbol{u}};\delta\bar{\boldsymbol{u}}\} \overset{\mathrm{def}}{=} \int_\Omega \bar{\boldsymbol{\sigma}}\{\bar{\boldsymbol{\epsilon}}\} : \boldsymbol{\epsilon}[\delta\bar{\boldsymbol{u}}]\,\mathrm{d}\bar{V} \qquad (6.26)$$ {eq:4-111}

$$\bar{l}\{\delta\bar{\boldsymbol{u}}\} \overset{\mathrm{def}}{=} \int_\Omega \bar{\boldsymbol{f}}\cdot\delta\bar{\boldsymbol{u}}\,\mathrm{d}\bar{V} + \int_{\Gamma_{\mathrm{N}}} \bar{\boldsymbol{t}}_{\mathrm{p}}\cdot\delta\bar{\boldsymbol{u}}\,\mathrm{d}\bar{S} \qquad (6.27)$$ {eq:4-112}

The nonlinear (and implicit) equation (6.25) can be solved, for example, via Newton iterations, whereby the tangent form $\bar{a}'$ is given as

$$
\begin{aligned}
\bar{a}'\{\bar{\boldsymbol{u}};\delta\bar{\boldsymbol{u}},\Delta\bar{\boldsymbol{u}}\} &\overset{\mathrm{def}}{=} \int_\Omega a'_\square(\boldsymbol{u}\{\boldsymbol{u}^{\mathrm{M}}\};\delta\boldsymbol{u}^{\mathrm{M}},\Delta\boldsymbol{u}^{\mathrm{M}} + (\boldsymbol{u}^\mu)'\{\boldsymbol{u}^{\mathrm{M}};\Delta\boldsymbol{u}^{\mathrm{M}}\})\,\mathrm{d}\,\bar{V} \\
&= \int_\Omega \boldsymbol{\epsilon}[\delta\bar{\boldsymbol{u}}] : \bar{\mathsf{E}}_{\mathrm{t}} : \boldsymbol{\epsilon}[\Delta\bar{\boldsymbol{u}}]\,\mathrm{d}\,\bar{V} && (6.28)
\end{aligned}
$$ {eq:4-113}

is utilized. The appropriate macroscale (algorithmic) tangent stiffness tensor, $\bar{\mathsf{E}}_{\mathrm{T}}$, is obtained upon linearizing the relation $\bar{\boldsymbol{\sigma}}\{\bar{\boldsymbol{\epsilon}}\}$ as follows:

$$\mathrm{d}\bar{\boldsymbol{\sigma}}\{\bar{\boldsymbol{\epsilon}}\} = \bar{\mathsf{E}}_{\mathrm{T}}\{\bar{\boldsymbol{\epsilon}}\} : \mathrm{d}\bar{\boldsymbol{\epsilon}} \qquad (6.29)$$ {eq:4-114}

and it is computed by *linearization* of the RVE-problem, which leads to a *sensitivity* or *tangent* problem. How to formulate and solve this sensitivity problem in practice depends strongly on the actual choice of prolongation condition (as will be discussed below). In particular, the specific variational setting for every type of prolongation condition is different.

Remark: It is possible to establish the sensitivity problem in the *primal* or the *dual* format. Both are described subsequently. □

6.2.3 Summary of (nested) FE^2-algorithm

The two-scale problem must be solved in a *nested* fashion, involving iterations on the macroscale (structural component) as well as the subscale (RVE) level: As a consequence the concept of "effective properties" has no obvious relevance any longer, which is a major difference/disadvantage as compared to the linear static problem. In terms of finite element analysis, the two-scale "nested FE-algorithm" or "FE^2-algorithm", may be described as follows, c.f. Figure 6.1.

1. Assume that a (nonequilibrium) macroscale stress field $\bar{\boldsymbol{\sigma}}$ is given in the macroscale iteration procedure, corresponding to given $\bar{\boldsymbol{u}}$ (and $\bar{\boldsymbol{\epsilon}}$).

2. **Prolongation-homogenization**: For given $\bar{\boldsymbol{\epsilon}} = \bar{\boldsymbol{\epsilon}}(\bar{\boldsymbol{x}}_i)$ in each macroscale quadrature point with centroid $\bar{\boldsymbol{x}}_i$, typically Gauss-points in the macroscale FE-mesh, solve the nonlinear RVE-problem (with chosen prolongation conditions) for the subscale field $\boldsymbol{u}(\bar{\boldsymbol{x}}_i, \boldsymbol{x})$ and the homogenized (macroscale) stress $\bar{\boldsymbol{\sigma}}(\bar{\boldsymbol{x}}_i)$.

3. Check the macroscale residual. If convergence defined by $|\bar{R}| < TOL$ has been achieved, then stop, else compute a new (updated) value of the macroscale displacement $\bar{\boldsymbol{u}}$ (while using the macroscale ATS-tensor $\bar{\mathsf{E}}_{\mathrm{T}}$) and then return to 1.

Remark: The operation $\bar{\boldsymbol{\epsilon}} \rightarrow \boldsymbol{\epsilon}(\boldsymbol{x})$ is known as "prolongation", "dehomogenization" or "concentration". The operation $\boldsymbol{\sigma}(\boldsymbol{x}) \rightarrow \bar{\boldsymbol{\sigma}}$ is known as "homogenization". □

Figure 6.1: *Nested macro-micro iteration strategy characterizing computational homogenization for static stress problems.*
g:ch4_fig1}

As a preliminary to the subsequent presentations of different formulations of the RVE-problem, we introduce the following variational forms:

eq:4-116a}
$$a_{\Box}(\boldsymbol{u};\delta\boldsymbol{u}) \overset{\text{def}}{=} \langle \boldsymbol{\sigma}(\boldsymbol{\epsilon}[\boldsymbol{u}]) : \boldsymbol{\epsilon}[\delta\boldsymbol{u}]\rangle_{\Box} \tag{6.30}$$
eq:4-116b}
$$c_{\Box}^{(\mathrm{H})}(\boldsymbol{u};\bar{\boldsymbol{\sigma}}) \overset{\text{def}}{=} \langle \boldsymbol{\epsilon}[\boldsymbol{u}]\rangle_{\Box} : \bar{\boldsymbol{\sigma}} \tag{6.31}$$
eq:4-116c}
$$c_{\Box}^{(\mathrm{P})}(\boldsymbol{u};\bar{\boldsymbol{\epsilon}}) \overset{\text{def}}{=} \langle \boldsymbol{\sigma}(\boldsymbol{\epsilon}[\boldsymbol{u}])\rangle_{\Box} : \bar{\boldsymbol{\epsilon}} \tag{6.32}$$

Below, we introduce two different variational formulations for each choice of control variables, denoted the "standard" and "nonstandard" format, respectively. Only the standard format will be further investigated in some detail, e.g. by numerical comparisons. The nonstandard format is included for completeness only.

6.3 Dirichlet boundary conditions (DBC-problem)

6.3.1 DBC-problem

The subscale space-variational problem on the RVE ??? or SVE ??? associated with a typical macroscopic point $\bar{\boldsymbol{x}} \in \Omega$ can be phrased as follows: For given value of the macroscale displacement gradient $\bar{\boldsymbol{\epsilon}} \in \mathbb{R}^{3\times3}$, find $\boldsymbol{u}^\mu \in \mathbb{U}_\square^{\mathrm{D},0}$ that solves

$$a_\square(\boldsymbol{u}^{\mathrm{M}}(\bar{\boldsymbol{\epsilon}}) + \boldsymbol{u}^\mu; \delta\boldsymbol{u}) = 0 \quad \forall \delta\boldsymbol{u} \in \mathbb{U}_\square^{\mathrm{D},0}. \tag{6.33}$$ {eq:4-117}

where the space $\mathbb{U}_\square^{\mathrm{D},0}$ was defined already in Chapter 3.

When the solution has been found it is possible to compute $\bar{\boldsymbol{\sigma}}$ in a "post-processing step": $\bar{\boldsymbol{\sigma}} = \langle \boldsymbol{\sigma} \rangle_\square$.

The nonlinear problem (6.33) must be solved iteratively. Newton's iteration method for finding $\boldsymbol{u}^\mu$ then becomes: For $k = 1, 2, \ldots$, compute

$$\boldsymbol{u}^{\mu(k+1)} = \boldsymbol{u}^{\mu(k)} + \Delta\boldsymbol{u}^\mu \tag{6.34}$$ {eq:4-118}

where the iterative updates $\Delta\boldsymbol{u}^\mu \in \mathbb{U}_\square^{\mathrm{D},0}$ are solved from the tangent equations

$$(a_\square)'(\bullet^{(k)}; \delta\boldsymbol{u}, \Delta\boldsymbol{u}^\mu) = R_\square(\bullet^{(k)}; \delta\boldsymbol{u}) \quad \forall \delta\boldsymbol{u} \in \mathbb{U}_\square^{\mathrm{D},0} \tag{6.35}$$ {eq:4-119}

until the residual $R_\square(\bullet^{(k)}; \delta\boldsymbol{u}) \overset{\mathrm{def}}{=} -a_\square(\bullet^{(k)}; \delta\boldsymbol{u})$ is sufficiently small. The tangent form $(a_\square)'$ is given explicitly as

$$(a_\square)'(\bullet; \delta\boldsymbol{u}, \Delta\boldsymbol{u}) = \langle \boldsymbol{\epsilon}[\delta\boldsymbol{u}] : \mathbf{E}_{\mathrm{T}} : \boldsymbol{\epsilon}[\Delta\boldsymbol{u}^\mu] \rangle_\square \tag{6.36}$$ {eq:4-120}

where the subscale tangent stiffness tensor, $\mathbf{E}_{\mathrm{T}}$[4], is defined in standard fashion via the relation

$$\mathrm{d}\boldsymbol{\sigma} = \mathbf{E}_{\mathrm{T}} : \mathrm{d}\boldsymbol{\epsilon} \tag{6.37}$$ {eq:4-121}

Non-standard format

As an alternative, it is possible to use the (nonstandard) space $\mathbb{U}_\square^{\mathrm{D}}$ to formulate the subscale space-variational RVE-problem in terms of the total displacement field $\boldsymbol{u}$ as follows: For given value of the macroscale displacement gradient $\bar{\boldsymbol{\epsilon}} \in \mathbb{R}^{3\times3}$, find $\boldsymbol{u} \in \mathbb{U}_\square^{\mathrm{D}}$ and $\bar{\boldsymbol{\sigma}} \in \mathbb{R}^{3\times3}$ that solve {eq:4-121}

$$a_\square(\boldsymbol{u}; \delta\boldsymbol{u}) - c_\square^{(\mathrm{H})}(\delta\boldsymbol{u}; \bar{\boldsymbol{\sigma}}) = 0 \qquad \forall \delta\boldsymbol{u} \in \mathbb{U}_\square^{\mathrm{D}} \tag{6.38a}$$ {eq:4-121a}

$$c_\square^{(\mathrm{H})}(\boldsymbol{u}; \delta\bar{\boldsymbol{\sigma}}) = \delta\bar{\boldsymbol{\sigma}} : \bar{\boldsymbol{\epsilon}} \qquad \forall \delta\bar{\boldsymbol{\sigma}} \in \mathbb{R}^{3\times3} \tag{6.38b}$$ {eq:4-121b}

As to the interpretation of $\bar{\boldsymbol{\sigma}}$ in this case, we may choose $\delta\boldsymbol{u} = \boldsymbol{u}^{\mathrm{M}}(\delta\boldsymbol{\epsilon})$ in (6.38a) whereby it follows that $\boldsymbol{\epsilon}[\delta\boldsymbol{u}] = \delta\bar{\boldsymbol{\epsilon}}$ is constant and the relation $\bar{\boldsymbol{\sigma}} = \langle \boldsymbol{\sigma} \rangle_\square$ is obtained. We note that (6.38b) can be interpreted as an auxiliary constraint equation.

[4] For brevity of notation, we consider $\mathbf{E}_{\mathrm{T}}$ as the effective Tangent Stiffness (TS) tensor that is relevant to the respone of an RVE (sufficiently large SVE).

6.3.2 Macroscale TS-tensor - Primal and dual formats

The macroscale TS-tensor, $\bar{\mathsf{E}}_{\mathrm{T}}$, is obtained for perturbations of the macroscale solution (expressed in terms of $\bar{\boldsymbol{\epsilon}}$). Like in the case of linear elasticity, as discussed in Chapter 3 **?????**, we shall then need to compute "unit fluctuation fields" or, rather, *sensitivity fields*, corresponding to a unit variation of $\bar{\boldsymbol{\epsilon}}$[1]. Hence, we shall need to compute the differential $\mathrm{d}\boldsymbol{u} = \boldsymbol{u}^{\mathrm{M}}(\mathrm{d}\bar{\boldsymbol{\epsilon}}) + \mathrm{d}\boldsymbol{u}^{\mu} = \boldsymbol{u}^{\mathrm{M}}(\mathrm{d}\bar{\boldsymbol{\epsilon}}) + (\boldsymbol{u}^{\mu})'\{\bar{\boldsymbol{\epsilon}}; \mathrm{d}\bar{\boldsymbol{\epsilon}}\}$ in terms of $\mathrm{d}\bar{\boldsymbol{\epsilon}}$. From the first order representation of $\boldsymbol{u}^{\mathrm{M}}$, we obtain

{eq:4-122}
$$\boldsymbol{u}^{\mathrm{M}}(\mathrm{d}\bar{\boldsymbol{\epsilon}}) = \mathrm{d}\bar{\boldsymbol{\epsilon}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}] = \sum_{i,j=1}^{NDIM} \hat{\boldsymbol{u}}^{\mathrm{M}(ij)} \, \mathrm{d}\bar{\epsilon}_{ij} \tag{6.39}$$

where the "unit displacement fields" $\hat{\boldsymbol{u}}^{\mathrm{M}(ij)}$ are given as

{eq:4-123}
$$\hat{\boldsymbol{u}}^{\mathrm{M}(ij)} \stackrel{\mathrm{def}}{=} \boldsymbol{e}_i \otimes \boldsymbol{e}_j \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}] \tag{6.40}$$

Upon using the identity $\bar{\boldsymbol{\sigma}} = \langle \boldsymbol{\sigma} \rangle_{\square}$ together with the relation (6.30), we obtain the representation of $\mathrm{d}\bar{\sigma}_{ij}$ as

{eq:4-124}
$$\mathrm{d}\bar{\sigma}_{ij} = \mathrm{d}\left[\langle \boldsymbol{\sigma} : [\boldsymbol{e}_i \otimes \boldsymbol{e}_j] \rangle_{\square}\right] = \mathrm{d}\left[a_{\square}(\bullet; \hat{\boldsymbol{u}}^{\mathrm{M}(ij)})\right] = (a_{\square})'(\bullet; \hat{\boldsymbol{u}}^{\mathrm{M}(ij)}, \mathrm{d}\boldsymbol{u}) \tag{6.41}$$

Next, we conclude that the state equation (6.33) must hold for $\bar{\boldsymbol{\epsilon}}$ as well as for a perturbed state $\bar{\boldsymbol{\epsilon}} + \mathrm{d}\bar{\boldsymbol{\epsilon}}$. However, a given change $\mathrm{d}\bar{\boldsymbol{\epsilon}}$ gives rise to changes $\mathrm{d}\boldsymbol{u}^{\mu} \in \mathbb{U}_{\square}^{\mathrm{D},0}$, whereby we obtain the relation

{eq:4-125}
$$a_{\square}(\boldsymbol{u}^{\mathrm{M}}(\bar{\boldsymbol{\epsilon}}) + \boldsymbol{u}^{\mu} + \boldsymbol{u}^{\mathrm{M}}(\mathrm{d}\bar{\boldsymbol{\epsilon}}) + \mathrm{d}\boldsymbol{u}^{\mu}; \delta\boldsymbol{u}) = 0 \quad \forall \delta\boldsymbol{u} \in \mathbb{U}_{\square}^{\mathrm{D},0}. \tag{6.42}$$

where it is emphasized that $\boldsymbol{u}^{\mu}$ depends on $\bar{\boldsymbol{\epsilon}}$ in an implicit fashion; $\boldsymbol{u}^{\mu} = \boldsymbol{u}^{\mu}\{\bar{\boldsymbol{\epsilon}}\}$.

Now, upon linearizing in (6.42) and subtracting (6.33) from the resulting expression, we obtain the appropriate tangent problem:

{eq:4-126}
$$(a_{\square})'(\bullet; \delta\boldsymbol{u}, \boldsymbol{u}^{\mathrm{M}}(\mathrm{d}\bar{\boldsymbol{\epsilon}}) + \mathrm{d}\boldsymbol{u}^{\mu}) = 0 \quad \forall \delta\boldsymbol{u} \in \mathbb{U}_{\square}^{\mathrm{D},0}. \tag{6.43}$$

from which $\mathrm{d}\boldsymbol{u}^{\mu}$ can be solved for any given $\mathrm{d}\bar{\boldsymbol{\epsilon}}$. In analogy with the definition of $\hat{\boldsymbol{u}}^{\mathrm{M}(ij)}$ in (6.39), we then introduce the "unit fields", or sensitivities, $\hat{\boldsymbol{u}}^{\mu(ij)}$, due to a unit value of the components $\mathrm{d}\bar{\epsilon}_{ij}$, via the *ansatz*

{eq:4-127}
$$\mathrm{d}\boldsymbol{u}^{\mu} = \sum_{i,j} \hat{\boldsymbol{u}}^{\mu(ij)} \, \mathrm{d}\bar{\epsilon}_{ij} \tag{6.44}$$

which may be inserted into (6.43), together with (6.39), to give the equations that must hold for $k, l = 1, 2, ..., NDIM$:

{eq:4-128}
$$(a_{\square})'(\bullet; \delta\boldsymbol{u}, \hat{\boldsymbol{u}}^{\mu(kl)}) = -(a_{\square})'(\bullet; \delta\boldsymbol{u}, \hat{\boldsymbol{u}}^{\mathrm{M}(kl)}) \quad \forall \delta\boldsymbol{u} \in \mathbb{U}_{\square}^{\mathrm{D},0} \tag{6.45}$$

Remark: We may define "algorithmic strain concentration tensor" A_{T} in the differential (tangent) relation $\mathrm{d}\boldsymbol{\epsilon} = \mathsf{A}_{\mathrm{T}} : \mathrm{d}\bar{\boldsymbol{\epsilon}}$ as follows: Combining (6.39) and (6.44), we obtain

{eq:4-129}
$$\begin{aligned} \boldsymbol{\epsilon}[\mathrm{d}\boldsymbol{u}] &= \sum_{i,j=1}^{NDIM} \left[\epsilon[\hat{\boldsymbol{u}}^{\mathrm{M}(ij)}] + \epsilon[\hat{\boldsymbol{u}}^{\mu(ij)}]\right] \mathrm{d}\bar{\epsilon}_{ij} = \left[\mathsf{I} + \sum_{i,j} \epsilon[\hat{\boldsymbol{u}}^{\mu(ij)}] \otimes \epsilon[\hat{\boldsymbol{u}}^{\mathrm{M}(ij)}]\right] : \mathrm{d}\bar{\boldsymbol{\epsilon}} \\ &= \mathsf{A}_{\mathrm{T}} : \mathrm{d}\bar{\boldsymbol{\epsilon}} \end{aligned} \tag{6.46}$$

[1] For a more general problem than the considered quasistatic one, it would be necessary to consider unit fluctuation fields for unit variation of $\bar{\boldsymbol{u}}$ as well.

It thus appears that $\mathbf{A}_{\mathrm{T}}$ takes the same expression as for linear elasticity; however, it now depends on the macroscale solution $\bar{\boldsymbol{\epsilon}}$ since $\hat{\boldsymbol{u}}^{\mu(ij)}$ are sensitivities for a given state. $\square$

Two different options are available in practice for computing the components of $\bar{\mathbf{E}}_{\mathrm{T}}$: (i) The "primal approach" was originally proposed in a discrete format in the context of the full (unrestricted) space of deformations pertinent to 3D modeling and plane strain, cf. Miehe and Koch ?, Temizer and Wriggers ?. This approach was then formulated in a continuous variational setting by Larsson and Runesson ?, Lillbacka et al. ?. (ii) The "dual approach" was proposed by Larsson and Runesson ? in the very same continuous variational setting. It is particularly attractive in conjunction with adaptive computations aiming for control of the subscale discretization error and for the computation of the dual load.

Primal approach for computing the ATS tensor

In the primal approach, the "unit fields" $\hat{\boldsymbol{u}}^{\mu(ij)}$ are solved from (6.44) and inserted into (6.41) to give the expression

$$\begin{aligned} \mathrm{d}\bar{\sigma}_{ij} &= \sum_{k,l=1}^{NDIM}\Big[(a_\square)'(\bullet;\hat{\boldsymbol{u}}^{\mathrm{M}(ij)},\hat{\boldsymbol{u}}^{\mathrm{M}(kl)}) + (a_\square)'(\bullet;\hat{\boldsymbol{u}}^{\mathrm{M}(ij)},\hat{\boldsymbol{u}}^{\mu(kl)})\Big]\,\mathrm{d}\bar{\epsilon}_{kl} \\ &= \sum_{k,l=1}^{NDIM}(a_\square)'(\bullet;\hat{\boldsymbol{u}}^{\mathrm{M}(ij)},\hat{\boldsymbol{u}}^{(kl)})\mathrm{d}\bar{\epsilon}_{kl} \end{aligned} \qquad (6.47) \quad \{eq:4-130\}$$

where we introduced $\hat{\boldsymbol{u}}^{(ij)} \stackrel{\mathrm{def}}{=} \hat{\boldsymbol{u}}^{\mathrm{M}(ij)} + \hat{\boldsymbol{u}}^{\mu(kl)}$.

Hence, with known values of $\hat{\boldsymbol{u}}^{\mu(ij)}$, for $i,j = 1,2,...,NDIM$, we are in the position to compute the components of $\bar{\mathbf{E}}_{\mathrm{T}}$ explicitly from (6.47) as

$$\begin{aligned} (\bar{\mathbf{E}}_{\mathrm{T}})_{ijkl} &= (a_\square)'(\bullet;\hat{\boldsymbol{u}}^{\mathrm{M}(ij)},\hat{\boldsymbol{u}}^{\mathrm{M}(kl)}) + (a_\square)'(\bullet;\hat{\boldsymbol{u}}^{\mathrm{M}(ij)},\hat{\boldsymbol{u}}^{\mu(kl)}) \\ &= \langle(\mathbf{E}_{\mathrm{T}})_{ijkl}\rangle_\square + \Big\langle\boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{\mathrm{M}(ij)}]:\mathbf{E}_{\mathrm{T}}:\boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{\mu(kl)}]\Big\rangle_\square \\ &= \Big\langle\boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{\mathrm{M}(ij)}]:\mathbf{E}_{\mathrm{T}}:\boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{(kl)}]\Big\rangle_\square \end{aligned} \qquad (6.48) \quad \{eq:4-131\}$$

where the following identities were used:

$$(a_\square)'(\bullet;\hat{\boldsymbol{u}}^{\mathrm{M}(ij)},\hat{\boldsymbol{u}}^{\mathrm{M}(kl)}) = \langle(\mathbf{E}_{\mathrm{t}})_{ijkl}\rangle_\square\,, \qquad (6.49) \quad \{eq:42a\}$$

$$(a_\square)'(\bullet;\hat{\boldsymbol{u}}^{\mathrm{M}(ij)},\hat{\boldsymbol{u}}^{\mu(kl)}) = \Big\langle\boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{\mathrm{M}(ij)}]:\mathbf{E}_{\mathrm{T}}:\boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{\mu(kl)}]\Big\rangle_\square \qquad (6.50) \quad \{eq:4-132\}$$

Dual approach for computing the ATS tensor

In the dual approach, we compute the dual solutions $\hat{\boldsymbol{u}}^{*(ij)} \in \mathbb{U}_\square$, for $i,j = 1,2,...,NDIM$ from the pertinent dual equations (ref to error computation, Larsson and Runesson?????

$$(a_\square)'(\bullet;\hat{\boldsymbol{u}}^{*(ij)},\delta\boldsymbol{u}) = (a_\square)'(\bullet;\hat{\boldsymbol{u}}^{\mathrm{M}(ij)},\delta\boldsymbol{u}) \quad \forall\delta\boldsymbol{u}\in\mathbb{U}_\square \qquad (6.51) \quad \{eq:4-134\}$$

With the choice $\delta\boldsymbol{u} = \hat{\boldsymbol{u}}^{\mu(kl)}$ in (6.51), and with $\delta\boldsymbol{u} = \hat{\boldsymbol{u}}^{*(ij)}$ in (6.44), we may combine these results to obtain the identity

$$(a_\square)'(\bullet;\hat{\boldsymbol{u}}^{\mathrm{M}(ij)},\hat{\boldsymbol{u}}^{\mu(kl)}) = -(a_\square)'(\bullet;\hat{\boldsymbol{u}}^{*(ij)},\hat{\boldsymbol{u}}^{\mathrm{M}(kl)}) \qquad (6.52) \quad \{eq:4-134a\}$$

whereby it is possible to replace the 2nd term of the 1st row in (6.47) obtain

$$\mathrm{d}\bar{\sigma}_{ij} = \sum_{k,l} [(a_\Box)'(\bullet; \hat{\boldsymbol{u}}^{\mathrm{M}(ij)}, \hat{\boldsymbol{u}}^{\mathrm{M}(kl)}) - (a_\Box)'(\bullet; \hat{\boldsymbol{u}}^{*(ij)}, \hat{\boldsymbol{u}}^{\mathrm{M}(kl)})]\mathrm{d}\bar{\epsilon}_{kl} \tag{6.53}$$ {eq:4-135}

Finally, we may express the components of $\bar{\mathbf{E}}_{\mathrm{T}}$ explicitly from (6.53) as

{eq:4-136}
$$\begin{aligned}(\bar{\mathbf{E}}_{\mathrm{T}})_{ijkl} &= (a_\Box)'(\bullet; \hat{\boldsymbol{u}}^{\mathrm{M}(ij)}, \hat{\boldsymbol{u}}^{\mathrm{M}(kl)}) - (a_\Box)'(\bullet; \hat{\boldsymbol{u}}^{*(ij)}, \hat{\boldsymbol{u}}^{\mathrm{M}(kl)}) \\ &= \langle (\mathbf{E}_{\mathrm{t}})_{ijkl} \rangle_\Box - \left\langle \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{*(ij)}] : \mathbf{E}_{\mathrm{T}} : \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}^{\mathrm{M}(kl)}] \right\rangle_\Box \end{aligned} \tag{6.54}$$

In comparison with the "primal approach", the advantage is that there is no need to solve for $\hat{\boldsymbol{u}}^{\mu(ij)}$ from (6.44), which in practice is done using the current FE-discretization on $\Omega_\Box$. Computing the dual fields $\hat{\boldsymbol{u}}^{*(ij)}$ is of the same computational effort as solving for $\hat{\boldsymbol{u}}^{\mu(ij)}$. However, the essential feature is that the same dual solutions can be used both for error control and the ATS-tensor computation. This shows the power of duality! ?????????

Remark: In the special case that $\mathbf{E}_{\mathrm{T}}$ possesses major symmetry, i.e. $(\mathbf{E}_{\mathrm{T}})_{ijkl} = (\mathbf{E}_{\mathrm{T}})_{klij}$, then we obtain the identity $\hat{\boldsymbol{u}}^{*(ij)} = -\hat{\boldsymbol{u}}^{\mu(ij)}$. Clearly, in this case we may use the primal perturbation (or the dual fields) for both error estimation and ATS-tensor computation. It is sufficient to utilize *one* set of solution fields for both purposes. □

6.3.3 FE-approximation – Matrix format (in 2D)

COMPLETE

6.4 Neumann boundary conditions (NBC-problem)

6.4.1 NBC-problem

We shall now consider the case where the prolongation is defined by the "weak" assumption on RVE-boundary tractions generated from the constant stress tensor $\bar{\boldsymbol{\sigma}}$. The corresponding subscale space-variational problem on the RVE associated with a typical macroscopic point $\bar{\boldsymbol{x}} \in \Omega$ can be phrased as follows: For given value of the macroscale displacement gradient
{eq:4-143} $\bar{\boldsymbol{\epsilon}} \in \mathbb{R}^{3\times3}_{\mathrm{sym}}$, find $\boldsymbol{u} \in \mathbb{U}^{\mathrm{N}}_\Box$ and $\bar{\boldsymbol{\sigma}} \in \mathbb{R}^{3\times3}_{\mathrm{sym}}$ that solve

{eq:4-143a}
$$a_\Box(\boldsymbol{u}; \delta\boldsymbol{u}) - c^{(\mathrm{H})}_\Box(\delta\boldsymbol{u}; \bar{\boldsymbol{\sigma}}) = 0 \qquad \forall \delta\boldsymbol{u} \in \mathbb{U}^{\mathrm{N}}_\Box \tag{6.55a}$$
{eq:4-143b}
$$-c^{(\mathrm{H})}_\Box(\boldsymbol{u}; \delta\bar{\boldsymbol{\sigma}}) = -\delta\bar{\boldsymbol{\sigma}} : \bar{\boldsymbol{\epsilon}} \qquad \forall \delta\bar{\boldsymbol{\sigma}} \in \mathbb{R}^{3\times3}_{\mathrm{sym}} \tag{6.55b}$$

Remark: With the only difference that $\mathbb{U}^{\mathrm{D}}_\Box$ has been replaced by $\mathbb{U}^{\mathrm{N}}_\Box$, this is the "non-standard format" for the Dirichlet boundary conditions in (6.38). □

As to the iterative solution of the system given in (6.55), Newton's method for finding $\boldsymbol{u}$ and $\bar{\boldsymbol{\sigma}}$ becomes: For $k = 1, 2, \dots$, compute

{eq:4-144}
$$\boldsymbol{u}^{(k+1)} = \boldsymbol{u}^{(k)} + \Delta\boldsymbol{u}, \quad \bar{\boldsymbol{\sigma}}^{(k+1)} = \bar{\boldsymbol{\sigma}}^{(k)} + \Delta\bar{\boldsymbol{\sigma}} \tag{6.56}$$

{eq:4-145} where the iterative updates $\Delta\boldsymbol{u} \in \mathbb{U}^{\mathrm{N}}_\Box$ and $\Delta\bar{\boldsymbol{\epsilon}} \in \mathbb{R}^{3\times3}_{\mathrm{sym}}$ are solved from the tangent equations

{eq:4-145a}
$$(a_\Box)'_u(\bullet^{(k)}; \delta\boldsymbol{u}, \Delta\boldsymbol{u}) - c^{(\mathrm{H})}_\Box(\delta\boldsymbol{u}, \Delta\bar{\boldsymbol{\sigma}}) = R^{(\mathrm{u})}_\Box(\bullet^{(k)}; \delta\boldsymbol{u}) \qquad \forall \delta\boldsymbol{u} \in \mathbb{U}^{\mathrm{N}}_\Box \tag{6.57a}$$
{eq:4-145b}
$$-c^{(\mathrm{H})}_\Box(\Delta\boldsymbol{u}, \delta\bar{\boldsymbol{\sigma}}) = R^{(\mathrm{P})}_\Box(\bullet^{(k)}; \delta\bar{\boldsymbol{\sigma}}) \qquad \forall \delta\bar{\boldsymbol{\sigma}} \in \mathbb{R}^{3\times3}_{\mathrm{sym}} \tag{6.57b}$$

{eq:4-146} where the residuals are

{eq:4-146a}
$$R_{\Box}^{(\mathrm{u})}(\bullet^{(k)};\delta\boldsymbol{u}) \overset{\text{def}}{=} -a_{\Box}(\bullet^{(k)};\delta\boldsymbol{u}) + c_{\Box}^{(\mathrm{H})}(\delta\boldsymbol{u},\bar{\boldsymbol{\sigma}}^{(k)}) \tag{6.58a}$$

{eq:4-146b}
$$R_{\Box}^{(\mathrm{P})}(\bullet^{(k)};\delta\bar{\boldsymbol{\sigma}}) \overset{\text{def}}{=} -\delta\bar{\boldsymbol{\sigma}} : \bar{\boldsymbol{\epsilon}} + c_{\Box}^{(\mathrm{H})}(\boldsymbol{u}^{(k)};\delta\bar{\boldsymbol{\sigma}}) \tag{6.58b}$$

The appropriate tangent (stiffness) forms were given above, however, the explicit results are reiterated here for completeness:

$$(a_{\Box})'_u(\bullet;\delta\boldsymbol{u},\Delta\boldsymbol{u}) = \langle \delta\boldsymbol{\epsilon} : \mathbf{E}_{\mathrm{T}} : \Delta\boldsymbol{\epsilon}\rangle_{\Box} \tag{6.59}$$
{eq:4-147a}

$$c_{\Box}^{(\mathrm{H})}(\delta\boldsymbol{u},\Delta\bar{\boldsymbol{\sigma}}) = \langle \delta\boldsymbol{\epsilon}\rangle_{\Box} : \Delta\bar{\boldsymbol{\sigma}} \tag{6.60}$$
{eq:4-147c}

$$c_{\Box}^{(\mathrm{H})}(\Delta\boldsymbol{u},\delta\bar{\boldsymbol{\sigma}}) = \delta\bar{\boldsymbol{\sigma}} : \langle \Delta\boldsymbol{\epsilon}\rangle_{\Box} \tag{6.61}$$
{eq:4-147d}

Non-standard format

As an alternative, we may consider the (non-standard) formulation of solving for the fluctuation field $\boldsymbol{u}^{\mu} \in \mathbb{U}_{\Box}^{\mathrm{N},0}$ explicitly, where we introduced the new space $\mathbb{U}_{\Box}^{\mathrm{N},0}$ that is non-standard in terms of the construction of FE-subspaces:

$$\mathbb{U}_{\Box}^{\mathrm{N},0} = \{\boldsymbol{u} \in \mathbb{U}_{\Box} : \langle \boldsymbol{\epsilon}[\boldsymbol{u}]\rangle_{\Box} = \boldsymbol{0}\} \tag{6.62}$$
{eq:4-141b}

The subscale space-variational problem on the RVE associated with each macroscopic point $\bar{\boldsymbol{x}} \in \Omega$ can then be phrased as follows: For given value of the macroscale displacement gradient $\bar{\boldsymbol{\epsilon}} \in \mathbb{R}^{3\times 3}$, find $\boldsymbol{u}^{\mu} \in \mathbb{U}_{\Box}^{\mathrm{N},0}$ that solves

$$a_{\Box}(\boldsymbol{u}^{\mathrm{M}}(\bar{\boldsymbol{\epsilon}}) + \boldsymbol{u}^{\mu};\delta\boldsymbol{u}^{\mu}) = 0 \quad \forall \delta\boldsymbol{u}^{\mu} \in \mathbb{U}_{\Box}^{\mathrm{N},0}. \tag{6.63}$$
{eq:4-148}

When the solution has been found it is possible to compute $\bar{\boldsymbol{\sigma}}$ in a "post-processing step": $\bar{\boldsymbol{\sigma}} = \langle \boldsymbol{\sigma}\rangle_{\Box}$. With the only difference that $\mathbb{U}_{\Box}^{\mathrm{D},0}$ has been replaced by $\mathbb{U}_{\Box}^{\mathrm{N},0}$, this the "standard format" for the Dirichlet boundary conditions given in Eq. (6.33).

6.4.2 Macroscale ATS-tensor

The state equations (6.55) must hold for $\bar{\boldsymbol{\epsilon}}$ as well as for a perturbed state $\bar{\boldsymbol{\epsilon}} + \mathrm{d}\bar{\boldsymbol{\epsilon}}$. However, a given change $\mathrm{d}\bar{\boldsymbol{\epsilon}}$ gives rise to changes $\mathrm{d}\boldsymbol{u} \in \mathbb{U}_{\Box}^{\mathrm{N}}$ and $\mathrm{d}\bar{\boldsymbol{\sigma}} \in \mathbb{R}_{\mathrm{sym}}^{3\times 3}$, whereby we obtain the relations {eq:4-151}

$$a_{\Box}(\boldsymbol{u} + \mathrm{d}\boldsymbol{u};\delta\boldsymbol{u}) - c_{\Box}^{(\mathrm{H})}(\delta\boldsymbol{u},\bar{\boldsymbol{\sigma}} + \mathrm{d}\bar{\boldsymbol{\sigma}}) = 0 \qquad \forall \delta\boldsymbol{u} \in \mathbb{U}_{\Box}^{\mathrm{N}} \tag{6.64a}$$
{eq:4-151a}

$$-c_{\Box}^{(\mathrm{H})}(\boldsymbol{u} + \mathrm{d}\boldsymbol{u},\delta\bar{\boldsymbol{\sigma}}) = -\delta\bar{\boldsymbol{\sigma}} : [\bar{\boldsymbol{\epsilon}} + \mathrm{d}\bar{\boldsymbol{\epsilon}}] \qquad \forall \delta\bar{\boldsymbol{\sigma}} \in \mathbb{R}_{\mathrm{sym}}^{3\times 3} \tag{6.64b}$$
{eq:4-151b}

Now, upon linearizing in (6.64) and subtracting (6.55) from the resulting expressions, we obtain the appropriate tangent problem: {eq:4-152}

$$(a_{\Box})'(\bullet;\delta\boldsymbol{u},\,\mathrm{d}\boldsymbol{u}) - c_{\Box}^{(\mathrm{H})}(\delta\boldsymbol{u},\,\mathrm{d}\bar{\boldsymbol{\sigma}}) = 0 \qquad \forall \delta\boldsymbol{u} \in \mathbb{U}_{\Box}^{\mathrm{N}} \tag{6.65a}$$
{eq:4-152a}

$$-c_{\Box}^{(\mathrm{H})}(\,\mathrm{d}\boldsymbol{u},\delta\bar{\boldsymbol{\sigma}}) = -\delta\bar{\boldsymbol{\sigma}} :\, \mathrm{d}\bar{\boldsymbol{\epsilon}} \qquad \forall \delta\bar{\boldsymbol{\sigma}} \in \mathbb{R}_{\mathrm{sym}}^{3\times 3} \tag{6.65b}$$
{eq:4-152c}

from which, in principle, $\mathrm{d}\boldsymbol{u}$ and $\mathrm{d}\bar{\boldsymbol{\sigma}}$ can be solved for any given $\mathrm{d}\bar{\boldsymbol{\epsilon}}$. Again, we use the "unit fields", or sensitivities, $\hat{\boldsymbol{u}}^{(ij)}$, due to a unit value of the components $\mathrm{d}\bar{\epsilon}_{ij}$, and an analogous *ansatz* for $\mathrm{d}\bar{\boldsymbol{\sigma}}$

$$\mathrm{d}\boldsymbol{u} = \sum_{i,j} \hat{\boldsymbol{u}}^{(ij)}\,\mathrm{d}\bar{\epsilon}_{ij}, \qquad \mathrm{d}\bar{\boldsymbol{\sigma}} = \sum_{i,j} \hat{\bar{\boldsymbol{\sigma}}}^{(ij)}\,\mathrm{d}\bar{\epsilon}_{ij} \tag{6.66}$$
{eq:4-153}

into (6.65) to obtain the set of equations that must hold for $k, l = 1, 2, ..., NDIM$: {eq:4-154}

$$(a_\square)'(\bullet; \delta\boldsymbol{u}, \hat{\boldsymbol{u}}^{(kl)}) - c_\square^{(\mathrm{H})}(\delta\boldsymbol{u}, \hat{\bar{\boldsymbol{\sigma}}}^{(kl)}) = 0 \qquad \forall \delta\boldsymbol{u} \in \mathbb{U}_\square^{\mathrm{N}} \tag{6.67a}$$ {eq:4-154a}

$$-c_\square^{(\mathrm{H})}(\hat{\boldsymbol{u}}^{(kl)}, \delta\bar{\boldsymbol{\sigma}}) = -(\delta\bar{\sigma})_{kl} \qquad \forall \delta\bar{\boldsymbol{\sigma}} \in \mathbb{R}_{\mathrm{sym}}^{3\times 3} \tag{6.67b}$$

where we used the identity $\delta\bar{\boldsymbol{\sigma}} : [\boldsymbol{e}_k \otimes \boldsymbol{e}_l] = \boldsymbol{e}_k \cdot \delta\bar{\boldsymbol{\sigma}} \cdot \boldsymbol{e}_l = (\delta\bar{\sigma})_{kl}$.

Obviously, the unit fields $\hat{\bar{\boldsymbol{\sigma}}}^{(ij)}$ are obtained as part of the solution of the system (6.67), whereafter they are inserted into $(6.66)_2$ to give the explicit expression

{eq:4-155}

$$\bar{\mathsf{E}}_{\mathrm{T}} = \sum_{k,l=1}^{NDIM} \hat{\bar{\boldsymbol{\sigma}}}^{(kl)} \otimes \boldsymbol{e}_k \otimes \boldsymbol{e}_l \tag{6.68}$$

6.4.3 FE-approximation – Matrix format (in 2D)

COMPLETE

Part II

VARIATIONALLY CONSISTENT HOMOGENIZATION (VCH)

Chapter 7

VCH – THE ABSTRACT FORMAT – APPLICATION TO LINEAR ELASTICITY

Linear elasticity (prototype model)
Magnetoelasticity (coupled problem)

Use manuscript in progress

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7.1 Introduction

7.2 VMS for a linear elliptic problem – The abstract format

7.2.1 Preliminaries

Consider a random micro-heterogenous material structure within a (solid) body occupying the domain Ω with boundary $\Gamma = \Gamma_\mathrm{D} \cup \Gamma_\mathrm{N}$, where Γ_D and Γ_N are associated with Dirichlet and Neumann boundary conditions (for simplicity), respectively. Here, we consider an abstract format; however, we may think of stationary heat conduction, in which case prescribed temperature represents a Dirichlet condition, whereas prescribed in/outflow represents a Neumann condition[1]. Further, we envision the existing of a volume-specific source in Ω that represents data on the fine scale. For simplicity, it is assumed that the topology is contiguous, i. e. the density is non-zero (no holes) everywhere in Ω.

In order to establish the variational format, we introduce the standard solution space $\mathbb{U}$ and test space $\mathbb{U}^0$, respectively, as follows[2]:

$$\mathbb{U}(= \mathbb{U}^0) = \{u \text{ suff. regular} |\ u = 0 \text{ on } \Gamma_\mathrm{D}\} \tag{7.1}$$ {eq:6-1}

[1] To avoid unnecessary technical difficulty, we assume (in this Section) that all boundary conditions are homogeneous.

[2] For the particular case of homogeneous Dirichlet conditions, these spaces are identical.

{figure:6-1} Figure 7.1: Domain decomposition **NEW FIGURE**

The fine-scale variational problem then reads: Find $u \in \mathbb{U}$ such that

$$a(u, \delta u) = l(\delta u), \quad \forall \delta u \in \mathbb{U}^0 \tag{7.2}$$ {eq:6-2}

where $a(u, v)$ is a bilinear form for $u, v \in \mathbb{U}$, whereas $l(u)$ is a linear functional for $u \in \mathbb{U}$. In {eq:6-3} terms of the heat conduction problem, u is the temperature, and

{eq:6-3a}
$$a(u, v) \stackrel{\text{def}}{=} \int_\Omega \boldsymbol{\nabla} u \cdot \boldsymbol{K} \cdot \boldsymbol{\nabla} v \, \mathrm{d}\Omega \tag{7.3a}$$

{eq:6-3b}
$$l(u) \stackrel{\text{def}}{=} \int_\Omega f u \, \mathrm{d}\Omega \tag{7.3b}$$

Next, we introduce the associated potential energy for $\hat{u} \in \mathbb{U}$

{eq:6-4}
$$\Pi(\hat{u}) = \frac{1}{2} a(\hat{u}, \hat{u}) - l(\hat{u}) \tag{7.4}$$

The sought fine-scale solution $u \in \mathbb{U}$ is the minimizer of $\Pi(\hat{u})$ on $\mathbb{U}$, i. e.

{eq:6-5}
$$u = \arg \left[\inf_{u \in \mathbb{U}} \Pi(u) \right] \tag{7.5}$$

and the corresponding stationarity condition becomes

{eq:6-5}
$$\Pi'(u; \delta u) = a(u, \delta u) - l(\delta u) = 0 \quad \forall \delta u \in \mathbb{U}^0, \tag{7.6}$$

where Π' denotes the directional derivative of Π. Clearly, (8.6) is identical to (8.3).

7.2.2 VMS – Single-scale setting

As a preliminary to the subsequent discussion of homogenization, we assume that each $u \in \mathbb{U}$ can be decomposed into macroscale (smooth) and subscale (fluctuating) parts via the unique hierarchical decomposition $\mathbb{U}^{\mathrm{M}} \oplus \mathbb{U}^{\mu}$ in the spirit of VMS = Variational MultiScale method, Hughes (1995), Målqvist & Larson (2003-): More precisely, each $u \in \mathbb{U}$ can be additively split *uniquely* into

{eq:6-11}
$$u = u^{\mathrm{M}} + u^{\mu}, \quad (u^{\mathrm{M}}, u^{\mu}) \in \mathbb{U}^{\mathrm{M}} \oplus \mathbb{U}^{\mu} \tag{7.7}$$

We remark that $u^{\mu} \in \mathbb{U}^{\mu} \subseteq \mathbb{U}$ means that $u^{\mu} = 0$ on Γ_{D} (the Dirichlet boundary). In addition, we henceforth assume ???? (to avoid unnecessary technicalities) that $u^{\mu} = 0$ on Γ_{N} as well.

Application of classical (single-scale) VMS-strategy

Mälqvist et al. Fredrik, kan du skriva nagot om traditionell och nyare resultat?

7.2.3 Two-scale setting – Homogenization as a smoothing procedure

In the previous Subsection no special reference was made to homogenization; hence, only one single scale was considered. In order to set the stage for (model-based) homogenization, we

Figure 7.2: Homogenization of integral??? {figure:6-2

introduce the domain decomposition $\Omega = \cup_i \Omega_{\Box,i}$, as shown in Figure 8.2. As a consequence, any volume integral can be rephrased as

{eq:6-12}
$$\int_\Omega f \,\mathrm{d}\Omega = \sum_i \int_{\Omega_{\Box,i}} f \,\mathrm{d}\Omega = \sum_i |\Omega_{\Box,i}| \underbrace{\frac{1}{|\Omega_{\Box,i}|} \int_{\Omega_{\Box,i}} f \,\mathrm{d}\Omega}_{\stackrel{\mathrm{def}}{=} f_{\Box,i}} \tag{7.8}$$

Introducing the averaging operator[3]

$$\langle f \rangle_\Box(\boldsymbol{x}) \stackrel{\mathrm{def}}{=} \frac{1}{|\Omega_\Box(\boldsymbol{x})|} \int_{\Omega_\Box(\boldsymbol{x})} f \,\mathrm{d}\Omega \tag{7.9}$$ {eq:6-12}

and setting $\Omega_\Box(\boldsymbol{x}) = \Omega_{\Box,i}$ when $\boldsymbol{x} \in \Omega_{\Box,i}$ implies that $\langle f \rangle_\Box(\boldsymbol{x}) = f_{\Box,i}$ when $\boldsymbol{x} \in \Omega_{\Box,i}$ p.w. constant, c.f. Figure **??**. Hence, we have the trivial identity $\int_\Omega f \,\mathrm{d}\Omega = \int_\Omega \langle f \rangle_\Box \,\mathrm{d}\Omega$, which holds also when $|\Omega_{\Box,i}| \to 0$. However, the approach taken in classical model-based homogenization is to introduce finite-sized "RVE:s" that occupy *overlapping subdomains* $\Omega_\Box(\boldsymbol{x})$, with $diam(\Omega_\Box) = L_\Box$, for each $\boldsymbol{x} \in \Omega$. Hence, we introduce the *approximation*

$$\int_\Omega f \,\mathrm{d}\Omega \approx \int_\Omega \langle f \rangle_\Box \,\mathrm{d}\Omega \tag{7.10}$$ {eq:6-13}

where $\langle f \rangle_\Box$ is the "running average" that is defined by (8.10) with the choice that $\Omega_\Box(\boldsymbol{x})$ is centered[4] at $\boldsymbol{x}$. It is noted that $\langle f \rangle_\Box$ is smoother than f, and the smoothness increases with $L_\Box$. Moreover, since the homogenized integral approximates the fine-scale integral, the introduced model error is expected to increase with $L_\Box$.

We are now in the position to replace the fine-scale potential in (8.5) with the homogenized potential[5]

$$\Pi(\hat{u}^{\mathrm{M}}, \hat{u}^\mu) = \int_\Omega \left[\frac{1}{2} a_\Box(\hat{u}^{\mathrm{M}} + \hat{u}^\mu, \hat{u}^{\mathrm{M}} + \hat{u}^\mu) - l_\Box(\hat{\boldsymbol{u}}^{\mathrm{M}} + \hat{\boldsymbol{u}}^\mu) \right] \mathrm{d}\Omega \tag{7.11}$$ {eq:6-14}

where we introduced the RVE-functionals $a_\Box(u, v)$ and $l_\Box(u)$ for $u, v \in \mathbb{U}$. Once again, in terms of the heat conduction problem, we have the identities {eq:6-15}

$$a_\Box(u, v) \stackrel{\mathrm{def}}{=} \langle \boldsymbol{\nabla} u \cdot \boldsymbol{K} \cdot \boldsymbol{\nabla} v \rangle_\Box, \tag{7.12a}$$ {eq:6-15a}

$$l_\Box(\hat{u}) \stackrel{\mathrm{def}}{=} \langle f u \rangle_\Box \tag{7.12b}$$ {eq:6-15b}

The minimization problem (8.5) is replaced by

$$\inf_{u^{\mathrm{M}} \in \mathbb{U}^{\mathrm{M}}} \inf_{\hat{u}^\mu \in \mathbb{U}^\mu} \Pi(u^{\mathrm{M}}, \hat{u}^\mu) \tag{7.13}$$ {eq:6-16}

[3]Subsequently, we use the concept of a "running average" in the classical fashion for homogenization; however, this far it is merely a matter of convenient notation.

[4]The precise definition of the "center" will be given later.

[5]For brevity, the same notation Π is used.

whose stationary condition is the two independent (global) problems of finding $u^{\mathrm{M}} \in \mathbb{U}^{\mathrm{M}}$ and $u^{\mu} \in \mathbb{U}^{\mu}$ that satisfy {eq:6-16}

$$\Pi'_{u^{\mathrm{M}}}(u^{\mathrm{M}}, u^{\mu}; \delta u^{\mathrm{M}}) = \int_{\Omega} \left[a_{\square}(u^{\mathrm{M}} + u^{\mu}; \delta u^{\mathrm{M}}) - l_{\square}(\delta u^{\mathrm{M}}) \right] \, \mathrm{d}\Omega = 0 \quad \forall \delta u^{\mathrm{M}} \in \mathbb{U}^{\mathrm{M},0}, \tag{7.14a}$$ {eq:6-16a}

$$\Pi'_{u^{\mu}}(u^{\mathrm{M}}, u^{\mu}; \delta u^{\mu}) = \int_{\Omega} \left[a_{\square}(u^{\mathrm{M}} + u^{\mu}; \delta u^{\mu}) - l_{\square}(\delta u^{\mu}) \right] \, \mathrm{d}\Omega = 0 \quad \forall \delta u^{\mu} \in \mathbb{U}^{\mu} \tag{7.14b}$$ {eq:6-16b}

7.2.4 Homogenization and prolongation operators – Uniqueness of decomposition

We introduce homogenization ??? and prolongation operators with the purpose to ensure a unique hierarchical additive decomposition of u into slowly varying (macroscale) and rapidly varying (fluctuation) components. A key feature of model-based homogenization (Note: not in discretization-based homogenization) is the possibility to ensure such uniqueness by "way of construction" upon introducing a "generating macrofield" $\bar{u} \in \bar{\mathbb{U}}$ and the pertinent surjective (onto) map defined by the *homogenization operator ????* $\mathcal{A}^*$

{eq:6-21}
$$\mathcal{A}^* : \; \mathbb{U} \to \bar{\mathbb{U}} \text{ (surjective)} \tag{7.15}$$

Remark 2 *It is clear that the regularity requirements on $\bar{\mathbb{U}}$ may be entirely different than those of $\mathbb{U}$, and that the pertinent requirements depend on the properties of $\mathcal{A}^*$.*

We also define, in an implicit fashion, the set $\mathbb{U}^{\mathrm{M}} \subset \mathbb{U}$ via the choice of a bijective map defined by the *prolongation operator* $\mathcal{A}$

{eq:6-22}
$$\mathcal{A} : \; \bar{\mathbb{U}} \to \mathbb{U}^{\mathrm{M}} \text{ (bijective)} \tag{7.16}$$

and we require that the operators satisfy the condition $\mathcal{A}^*\mathcal{A} = \mathcal{I}$ (while $\mathcal{A}\mathcal{A}^* \neq \mathcal{I}$), where $\mathcal{I}$ denotes the identity operator on $\bar{\mathbb{U}}$. Finally, the set of microscale (or fluctuation) functions is defined as

{eq:6-23}
$$\mathbb{U}^{\mu} := \{ \boldsymbol{v} \in \mathbb{U} : \; \mathcal{A}^* \boldsymbol{v} = \boldsymbol{0} \} \tag{7.17}$$

{eq:6-24} **Lemma 1**: Any function $u \in \mathbb{U}$ can be decomposed additively as $u = u^{\mathrm{M}} + u^{\mu}$ with

{eq:6-24a}
$$\mathbb{U}^{\mathrm{M}} \ni \boldsymbol{u}^{\mathrm{M}} \stackrel{\mathrm{def}}{=} \mathcal{A}\mathcal{A}^* \boldsymbol{u} \tag{7.18a}$$

{eq:6-24b}
$$\mathbb{U}^{\mu} \ni \boldsymbol{u}^{\mu} \stackrel{\mathrm{def}}{=} [\mathcal{I} - \mathcal{A}\mathcal{A}^*] \boldsymbol{u} \tag{7.18b}$$

where $\mathcal{I}$ is (here) the identity operator on $\mathbb{U}$.

Proof: Since range$\{\mathcal{A}\} = \mathbb{U}$, range$\{\mathcal{A}^*\} = \bar{\mathbb{U}}$, $\mathcal{A}$ is defined on range$\{\mathcal{A}^*\}$ and $\mathcal{A}^*$ is defined on $\mathbb{U}$, we note that the operator $\mathcal{A}\mathcal{A}^*$ maps from $\mathbb{U} \to \mathbb{U}$. Hence, the operators trivially satisfy the identity **????** Next, we consider u^{M} and u^{μ} constructed in (8.20a) and (8.20b), respectively. We first conclude that $u^{\mathrm{M}} \in \mathbb{U}^{\mathrm{M}}$ since range$\{\mathcal{A}\} = \mathbb{U}^{\mathrm{M}}$. Finally, we may show that $u^{\mu} \in \mathbb{U}^{\mu}$ with $\mathbb{U}^{\mu}$ defined in (8.19). Indeed, since $u^{\mu} \in \mathbb{U}$, we have

$$\mathcal{A}^* u^{\mu} = \mathcal{A}^* \left[\mathcal{I} - \mathcal{A}\mathcal{A}^* \right] u = \left[\mathcal{A}^* - \underbrace{\mathcal{A}^*\mathcal{A}}_{=\mathcal{I}} \mathcal{A}^* \right] u = 0$$

where it was used that $\mathcal{A}^*\mathcal{A} = \mathcal{I}$. □

Lemma 2: The homogenization operator $\mathcal{A}^*$ is a bijective map on $\mathbb{U}^{\mathrm{M}}$, i.e.

$$\mathcal{A}^*|_{\mathbb{U}^{\mathrm{M}}} : \; \mathbb{U}^{\mathrm{M}} \rightarrow \bar{\mathbb{U}} \text{ (bijective)} \tag{7.19}$$ {eq:6-25}

Proof: Since range$\{\mathcal{A}\} = \mathbb{U}^{\mathrm{M}}$, we obtain $\mathcal{I} = \mathcal{A}^*\mathcal{A} = \mathcal{A}^*|_{\mathbb{U}^{\mathrm{M}}}\mathcal{A}$, and using the fact that $\mathcal{A}$ is bijective, we conclude that, indeed, $\mathcal{A}^*|_{\mathbb{U}^{\mathrm{M}}} = \mathcal{A}^{-1}$ is a bijective operator. □

Theorem 1: The set $\mathbb{U}^{\mu}$ defined in (**??**) is the hierarchical complement to $\mathbb{U}^{\mathrm{M}}$, i.e. $\mathbb{U} = \mathbb{U}^{\mathrm{M}} \oplus \mathbb{U}^{\mu}$. In other words, it holds that

$$\mathbb{U} = \mathbb{U}^{\mathrm{M}} \oplus \mathbb{U}^{\mu} \text{ and } \mathbb{U}^{\mathrm{M}} \cap \mathbb{U}^{\mu} = \{\mathbf{0}\} \tag{7.20}$$ {eq:6-26}

Proof: From Lemma 1 follows that any function in $\mathbb{U}$ can be written as the sum of two functions, one in $\mathbb{U}^{\mathrm{M}}$ and the other in $\mathbb{U}^{\mu}$. Furthermore, since $\mathbb{U}^{\mathrm{M}} \subset \mathbb{U}$ and $\mathbb{U}^{\mu} \subset \mathbb{U}$, the sum must be in $\mathbb{U}$. Hence, we conclude that $\mathbb{U}^{\mathrm{M}} \cup \mathbb{U}^{\mu} = \mathbb{U}$. Next we consider the issue of uniqueness: To this end, consider any function $u^{\mathrm{M}} \in \mathbb{U}^{\mathrm{M}}$. Since $\mathcal{A}^*|_{\mathbb{U}^{\mathrm{M}}}$ is linear and bijective, cf. Lemma 2, the condition that must be fullfilled for u^{M} being an element of $\mathbb{U}^{\mu}$ as well can be expressed as

$$\mathcal{A}^* u^{\mathrm{M}} = \mathcal{A}^*|_{\mathbb{U}^{\mathrm{M}}} u^{\mathrm{M}} = 0 \;\Leftrightarrow\; u^{\mathrm{M}} = 0$$

Hence, if $u^{\mathrm{M}} \in \mathbb{U}^{\mathrm{M}} \cap \mathbb{U}^{\mu}$ then $u^{\mathrm{M}} = \mathbf{0}$, which completes the proof. □

7.2.5 The generating macro-field – Separation of scales

The assumption of *separation of scales* is implicitly introduced via the particular definition of the prolongation operator $\mathcal{A}$ within each subdomain $\Omega_\square$. More specifically, the two-scale function $u^{\mathrm{M}}(\bar{\boldsymbol{x}}, \boldsymbol{x})$ for $(\bar{\boldsymbol{x}}, \boldsymbol{x}) \in \Omega \times \Omega_\square(\bar{\boldsymbol{x}})$, is constructed via the prolongation of a generating macrofield $\bar{u}$ via a Taylor series expansion of $\bar{u}$ within $\Omega_\square$ to a suitable order (of homogenization). *The standard situation of 1st order homogenization is discussed in detail below.* More formally, the operators $\mathcal{A}$ and $\mathcal{A}^*$ are defined as the maps {eq:6-31}

$$\mathcal{A}(\bar{\boldsymbol{x}}) : \bar{\mathbb{U}} \rightarrow \mathbb{U}^{\mathrm{M}}_\square(\bar{\boldsymbol{x}}) \tag{7.21a}$$ {eq:6-31a}

$$\mathcal{A}^*(\bar{\boldsymbol{x}}) : \mathbb{U}^{\mathrm{M}}_\square(\bar{\boldsymbol{x}}) \rightarrow \bar{\mathbb{U}} \tag{7.21b}$$ {eq:6-31b}

where $\mathbb{U}^{\mathrm{M}}_\square(\bar{\boldsymbol{x}}) = \mathbb{U}^{\mathrm{M}}|_{\Omega_\square}$ is a local vector space (on the SVE).

Next, we interpret the functional dependence $u^{\mu}\{\bar{u}\}$[6] on each $\Omega_\square$ in such a fashion that u^{μ} depends implicitly on $\bar{u}(\bar{\boldsymbol{x}}), [\bar{u} \otimes \boldsymbol{\nabla}](\bar{\boldsymbol{x}})$ and, possibly, on higher order gradients of the field $\bar{u} \in \bar{\mathbb{U}}$ to the desired degree. In particular, this means that we may rephrase (8.15) as follows: Find the two independent (global) fields $\bar{u}$ and u^{μ} that satisfy {eq:6-32}

$$\int_\Omega [a_\square(\mathcal{A}\bar{u} + u^{\mu}; \mathcal{A}\delta\bar{u}) - l_\square(\mathcal{A}\delta\bar{u})] \,\mathrm{d}\Omega = 0 \quad \forall \delta\bar{u} \in \bar{\mathbb{U}}^0 \tag{7.22a}$$ {eq:6-32a}

$$\int_\Omega [a_\square(\mathcal{A}\bar{u} + u^{\mu}; \delta\boldsymbol{u}^{\mu}) - l_\square(\delta u^{\mu})] \,\mathrm{d}\Omega = 0 \quad \forall \delta u^{\mu} \in \mathbb{U}^{\mu} \tag{7.22b}$$ {eq:6-32b}

In particular, the "homogenized" relation (8.24a), exploiting $\delta u^{\mathrm{M}} = \mathcal{A}\delta\bar{u}$ as the homogenizer, defines *Variationally Consistent Homogenization* (VCH), and its solution $\bar{u} \in \bar{\mathbb{U}}$ represents a smoother field that does $u \in \mathbb{U}$.

To construct $u^{\mu} \in \mathbb{U}^{\mu}_\square \overset{\text{def}}{=} \mathbb{U}^{\mu}|_{\Omega_\square}$ that inherently satisfies the constraint relations $\mathcal{A}^* u^{\mu} = 0$ may turn out as a quite difficult task in practice. A possible strategy would then be to

[6] Brackets indicate implicit function.

$$
\begin{tikzcd}
\min\limits_{\boldsymbol{u}} \Pi(\boldsymbol{u}) \arrow[r, "\text{(I)}", "\text{stat}"'] \arrow[d, "\text{VCMH}"', "\text{(II)}"] & \Pi'(\boldsymbol{u}; \delta\boldsymbol{u}) = 0 \quad \forall \delta\boldsymbol{u} \arrow[d, "\text{VCMH}"', "\text{(I)}"] \\
\min\limits_{\bar{\boldsymbol{u}}} \bar{\Pi}\{\bar{\boldsymbol{u}}\} \arrow[r, "\text{(II)}", "\text{stat+VCMH}"'] & \bar{\Pi}'\{\bar{\boldsymbol{u}}; \delta\bar{\boldsymbol{u}}\} = \bar{R}\{\bar{\boldsymbol{u}}; \delta\bar{\boldsymbol{u}}\} = 0 \quad \forall \delta\bar{\boldsymbol{u}}
\end{tikzcd}
$$

{figure:6-4} Figure 7.3: The role of VCMH-condition in computational homogenization

- (i) opt for a larger space by relaxing the requirements on $\mathbb{U}^{\mu}_{\square}$ in terms of the conditions $\mathcal{A}^* u^{\mu} = 0$ (or at least a subset of them) and to
- (ii) satisfy the said conditions $\mathcal{A}^* u^{\mu} = 0$ (or at least a subset of them) in a weak sense as additional constraint conditions using Lagrangian multipliers.

The strategy (ii) is used henceforth, cf. **Subsection ????** , where it is shown that the assumption of (weakly) periodic fluctuations u^{μ} on each RVE serves precisely this purpose. In fact, such weak periodicity has been exploited extensively (in the context of 1st order homogenization) by the authors, cf. LARSSON ET AL. **?**, and it will be introduced as a "workhouse" subsequently in order to formulate a "closed", i.e. solvable, RVE-problem on each domain $\Omega_{\square}$.

In conclusion, the pertinent "localized" RVE-problems replace the global weak form (8.24b). Obviously, it is convenient in practice to establish these local RVE-problems only in the macroscale quadrature points in the FE^2-setting. This means that the equations in (8.24) represent a (nested) two-scale problem that must be solved by some type of iteration method.

7.2.6 The role of a Variationally Consistent Macrohomogeneity Condition (VCMH-condition)

As shown in Figure 8.3, it is possible to take the fine-scale minimization problem as the point of departure and eventually end up with the macroscale equation (8.24a). However, this result can be achieved in two different ways, corresponding to path (I) or path (II) in Figure 8.3.

Path I: *Evaluate the stationarity condition associated with the fine-scale problem and apply the VCH-strategy.* Start from (8.12) and derive the stationarity condition (8.15) for the fine-scale problem. Then, apply the VCH-strategy that gives (8.24a), i.e.

{eq:6-35}
$$
\begin{aligned}
\bar{R}\{\bar{u}; \delta\bar{u}\} &\overset{\text{def}}{=} \Pi'_{u^{\mathrm{M}}}(\mathcal{A}\bar{u}, u^{\mu}\{\bar{u}\}; \mathcal{A}\delta\bar{u}) \\
&= \int_{\Omega} \left[a_{\square}(\mathcal{A}\bar{u} + u^{\mu}\{\bar{u}\}; \mathcal{A}\delta\bar{u}) - l_{\square}(\mathcal{A}\delta\bar{u})\right] \,\mathrm{d}\Omega \\
&= 0 \quad \forall \delta\bar{u} \in \bar{\mathbb{U}}^0
\end{aligned}
\tag{7.23}
$$

Path II. *Apply the VCH-strategy to the fine-scale potential and evaluate the stationarity condition.* Start from (8.12), apply the VCH-strategy to arrive at the macroscale potential

{eq:6-36}
$$
\bar{\Pi}\{\hat{\bar{u}}\} \overset{\text{def}}{=} \Pi(\mathcal{A}\hat{\bar{u}}, u^{\mu}\{\hat{\bar{u}}\}) \tag{7.24}
$$

and consider the problem

{eq:6-37} $$\inf_{\hat{\bar{u}}\in\bar{\mathbb{U}}} \bar{\Pi}\{\hat{\bar{u}}\}. \tag{7.25}$$

The corresponding stationarity condition is

{eq:6-38} $$\bar{\Pi}'\{\bar{u};\delta\bar{u}\} = 0 \quad \forall \delta\bar{u} \in \bar{\mathbb{U}}^0 \tag{7.26}$$

Now, the key question is whether this condition is satisfied by the same solution $\bar{u}$ as that of (8.25). To establish the condition that must be satisfied for such an identity to hold true, we first note that $\bar{\Pi}'$ can be expanded as

$$\begin{aligned}\bar{\Pi}'\{\bar{u};\delta\bar{u}\} &= \underbrace{\Pi'_{u^{\mathrm{M}}}(\mathcal{A}\bar{u}, u^\mu\{\bar{u}\}; \mathcal{A}\delta\bar{u})}_{=0 \text{ from } (8.25)} \\ &\quad + \Pi'_{u^\mu}(\mathcal{A}\bar{u}, u^\mu\{\bar{u}\}; \underbrace{(u^\mu)'\{\bar{u},\delta\bar{u}\}}_{=\mathcal{S}\delta\bar{u}})\end{aligned} \tag{7.27}$$ {eq:6-39}

where a sensitivity (linear operator) $\mathcal{S}$ is defined as a directional derivative, i. e. $\mathcal{S}\delta\bar{u} = (u^\mu)'\{\bar{u};\delta\bar{u}\} \stackrel{\text{def}}{=} \frac{\mathrm{d}}{\mathrm{d}\epsilon} u^\mu\{\bar{u} + \epsilon\delta\bar{u}\}|_{\epsilon=0}$. In order that $\bar{\Pi}$ is stationary at the global solution $\bar{u}$, we must obviously require that

$$\Pi'_{u^\mu}(\mathcal{A}\bar{u}, u^\mu\{\bar{u}\}; \mathcal{S}\delta\bar{u}) = 0 \quad \forall \delta\bar{u} \in \bar{\mathbb{U}}^0 \tag{7.28}$$ {eq:6-41}

Upon localizing (8.30) to each RVE, we obtain the sufficient (localized or stronger) condition

$$a_\square(\mathcal{A}\bar{u} + u^\mu\{\bar{u}\}; \mathcal{S}\delta\bar{u}) - l_\square(\mathcal{S}\delta\bar{u}) = 0 \quad \forall \delta\bar{u} \in \bar{\mathbb{U}}^0 \tag{7.29}$$ {eq:6-42}

or, equivalently,

$$\begin{aligned}&a_\square(\mathcal{A}\bar{u} + u^\mu\{\bar{u}\}; \mathcal{A}\delta\bar{u} + \mathcal{S}\delta\bar{u}) - a_\square(\mathcal{A}\bar{u} + u^\mu\{\bar{u}\}; \mathcal{A}\delta\bar{u}) \\ &= l_\square(\mathcal{A}\delta\bar{u} + \mathcal{S}\delta\bar{u}) - l_\square(\mathcal{A}\delta\bar{u}) \quad \forall \delta\bar{u} \in \bar{\mathbb{U}}^0\end{aligned} \tag{7.30}$$ {eq:6-43}

The identity in (8.31) or (8.32) is coined the (local version of the) *Variationally Consistent Macrohomogeneity Condition* (abbreviated VCMH-condition henceforth). It is commonly known as the Hill-Mandel condition in the context of stress problems[7]; however, it can readily be generalized to other classes of problems, cf. examples below.

When/if the VCMH-condition is satisfied, it is also guaranteed that the global tangent stiffness operator is symmetrical. In other words,

$$\bar{\Pi}''_{\bar{u}\bar{u}}\{\bar{u};\delta\bar{u}_1,\delta\bar{u}_2\} = \bar{\Pi}''_{\bar{u}\bar{u}}\{\bar{u};\delta\bar{u}_2,\delta\bar{u}_1\} \quad \forall \delta\bar{u}_1,\delta\bar{u}_2 \in \bar{\mathbb{U}}^0 \tag{7.31}$$ {eq:6-44}

which is shown as follows: From the expansion of $\bar{\Pi}'_{\bar{u}}\{\bar{u};\delta\bar{u}_1\}$ in (**??**), we may carry out the second variation to obtain

$$\begin{aligned}\bar{\Pi}''_{\bar{u}\bar{u}}\{\bar{u};\delta\bar{u}_1,\delta\bar{u}_2\} &\stackrel{\text{def}}{=} \Pi''_{u^{\mathrm{M}}u^{\mathrm{M}}}(\mathcal{A}\bar{u}, u^\mu\{\bar{u}\}; \mathcal{A}\delta\bar{u}_1, \mathcal{A}\delta\bar{u}_2) \\ &\quad + \Pi''_{u^{\mathrm{M}}u^\mu}(\mathcal{A}\bar{u}, u^\mu\{\bar{u}\}; \mathcal{A}\delta\bar{u}_1, \mathcal{S}\delta\bar{u}_2) + \Pi''_{u^\mu u^{\mathrm{M}}}(\mathcal{A}\bar{u}, u^\mu\{\bar{u}\}; \mathcal{S}\delta\bar{u}_1, \mathcal{A}\delta\bar{u}_2) \\ &\quad + \Pi''_{u^\mu u^\mu}(\mathcal{A}\bar{u}, u^\mu\{\bar{u}\}; \mathcal{S}\delta\bar{u}_1, \mathcal{S}\delta\bar{u}_2) \\ &= \int_\Omega a_\square(\mathcal{S}^{\mathrm{tot}}\delta\bar{u}_1, \mathcal{S}^{\mathrm{tot}}\delta\bar{u}_2)\,\mathrm{d}\Omega \quad \forall \delta\bar{u}_1,\delta\bar{u}_2 \in \bar{\mathbb{U}}^0\end{aligned} \tag{7.32}$$ {eq:6-45}

where we introduced the "total sensitivity operator" $\mathcal{S}^{\mathrm{tot}} \stackrel{\text{def}}{=} \mathcal{A} + \mathcal{S}$, and where it was used that

$$(a_\square)'_u(u;\delta u_1,\delta u_2) = a_\square(\delta u_1,\delta u_2) \tag{7.33}$$ {eq:6-46}

and that $a_\square$ is biolinear and symmetrical.

This symmetry property corresponds to the classical notion of "symmetric VMS", cf. LARSON Check!!

[7]The classical assumption is $l_\square(\mathcal{S}\delta\bar{u}) = 0$.

?, and can be interpreted as a "Galerkin property". Indeed, whenever the fine-scale problem is self-adjoint (like the present model problem of nonlinear elasticity), it is reasonable to expect that the resulting homogenized problem is self-adjoint as well.

Remark 3 *There is no need to compute the sensitivity $\mathcal{S}$ explicitly for the single purpose of showing that MH-condition is valid; it is rather sufficient to merely note that it exists (which is shown subsequently in the context of weakly periodic boundary conditions). However, in order to compute the macroscale tangent operator defined implicitly in (??), we do indeed require the computation of $\mathcal{S}$. This is conveniently done only after specifying the operator $\mathcal{A}$ that defines the "order of homogenization".*

7.3 A model problem – Nonlinear elasticity revisited

7.3.1 Fine-scale problem formulation

Consider a random micro-heterogenous material structure within a solid body occupying the domain Ω with boundary $\Gamma = \Gamma_\mathrm{D} \cup \Gamma_\mathrm{N}$. The body is subjected to distributed body load $\boldsymbol{b}$ in Ω and prescribed tractions on Γ_N. Displacements are prescribed on Γ_D. For simplicity, it is assumed that the topology is contiguous, i. e. the density is non-zero (no holes) everywhere in Ω.

Restricting to quasistatics, we seek the displacement field $\boldsymbol{u}(\boldsymbol{x}) : \Omega \to \mathbb{R}^3$ that solves the system

{eq:6-101}

eq:6-101a}

$$-\boldsymbol{\sigma}(\boldsymbol{\epsilon}[\boldsymbol{u}]) \cdot \boldsymbol{\nabla} = \boldsymbol{b} \quad \text{in } \Omega \tag{7.34a}$$

eq:6-101c}

$$\boldsymbol{u} = \boldsymbol{u}_\mathrm{p} \quad \text{on } \Gamma_\mathrm{D} \tag{7.34b}$$

eq:6-101d}

$$\boldsymbol{t} \overset{\text{def}}{=} \boldsymbol{\sigma} \cdot \boldsymbol{n} = \boldsymbol{t}_\mathrm{p} \quad \text{on } \Gamma_\mathrm{N} \tag{7.34c}$$

where $\boldsymbol{\epsilon}[\hat{\boldsymbol{u}}] \overset{\text{def}}{=} (\hat{\boldsymbol{u}} \otimes \boldsymbol{\nabla})^{\text{sym}}$ is the "small strain operator". It is assumed that the subscale material is described by nonlinear elasticity, whereby the convex volume-specific strain energy density $\psi(\boldsymbol{\epsilon})$ serves as the potential for the stress $\boldsymbol{\sigma}(\boldsymbol{\epsilon})$, i.e.

{eq:6-102}

$$\boldsymbol{\sigma}(\boldsymbol{\epsilon}) = \frac{\partial \psi(\boldsymbol{\epsilon})}{\partial \boldsymbol{\epsilon}} \tag{7.35}$$

In order to establish the variational format for the fine-scale problem, we introduce the potential energy

{eq:6-103}

$$\Pi(\hat{\boldsymbol{u}}) = \Psi(\hat{\boldsymbol{u}}) - l(\hat{\boldsymbol{u}}) \tag{7.36}$$

{eq:6-104} where

eq:6-104a}

$$\Psi(\hat{\boldsymbol{u}}) \overset{\text{def}}{=} \int_\Omega \psi(\boldsymbol{\epsilon}[\hat{\boldsymbol{u}}]) \, \mathrm{d}\Omega \tag{7.37a}$$

eq:6-104b}

$$l(\hat{\boldsymbol{u}}) \overset{\text{def}}{=} \int_\Omega \boldsymbol{b} \cdot \hat{\boldsymbol{u}} \, \mathrm{d}\Omega + \int_{\Gamma_\mathrm{N}} \boldsymbol{t}_\mathrm{p} \cdot \hat{\boldsymbol{u}} \, \mathrm{d}\Gamma \tag{7.37b}$$

The sought fine-scale solution $\boldsymbol{u} \in \mathbb{U}$ is the minimizer of $\Pi(\hat{\boldsymbol{u}})$ on $\mathbb{U}$, i. e.

{eq:6-105}

$$\boldsymbol{u} = \arg \left[\inf_{\hat{\boldsymbol{u}} \in \mathbb{U}} \Pi(\hat{\boldsymbol{u}}) \right] \tag{7.38}$$

and the corresponding stationarity condition becomes

{eq:6-106}
$$\Pi'(\boldsymbol{u};\delta\boldsymbol{u}) = \int_\Omega \boldsymbol{\sigma}(\boldsymbol{\epsilon}[\boldsymbol{u}])\colon \boldsymbol{\epsilon}[\delta\boldsymbol{u}]\,\mathrm{d}\Omega - l(\delta\boldsymbol{u}) = 0 \quad \forall\delta\boldsymbol{u}\in\mathbb{U}^0, \tag{7.39}$$

{eq:6-107} where the standard solution space $\mathbb{U}$ and test space $\mathbb{U}^0$ are defined as, respectively,

{eq:6-107a}
$$\mathbb{U} = \{\boldsymbol{u} \text{ suff. regular}|\ \boldsymbol{u} = \bar{\boldsymbol{u}}_{\mathrm{p}} \text{ on } \Gamma_{\mathrm{D}}\} \tag{7.40a}$$

{eq:6-107b}
$$\mathbb{U}^0 = \{\boldsymbol{u} \text{ suff. regular}|\ \boldsymbol{u} = \boldsymbol{0} \text{ on } \Gamma_{\mathrm{D}}\} \tag{7.40b}$$

7.3.2 Two-scale setting – Homogenization as a smoothing procedure

We assume that each $\boldsymbol{u}\in\mathbb{U}$ can be decomposed into macroscale (smooth) and subscale (fluctuating) parts via the unique hierarchical decomposition $\mathbb{U}^{\mathrm{M}}\oplus\mathbb{U}^{\mu}$. More precisely, each $\boldsymbol{u}\in\mathbb{U}$ can be additively split *uniquely* into

$$\boldsymbol{u} = \boldsymbol{u}^{\mathrm{M}} + \boldsymbol{u}^{\mu}, \quad (\boldsymbol{u}^{\mathrm{M}},\boldsymbol{u}^{\mu})\in\mathbb{U}^{\mathrm{M}}\oplus\mathbb{U}^{\mu} \tag{7.41}$$
{eq:6-108}

UPDATE We remark that $\boldsymbol{u}^{\mu}\in\mathbb{U}^{\mu}\subseteq\mathbb{U}^0$ means that $\boldsymbol{u}^{\mu}=\boldsymbol{0}$ on Γ_{D} (the Dirichlet boundary). In addition, we henceforth assume (to avoid unnecessary technicalities) that $\boldsymbol{u}^{\mu}=0$ on Γ_{N} as well. We thus obtain $\int_{\Gamma_{\mathrm{N}}}\boldsymbol{t}_{\mathrm{p}}\cdot\hat{\boldsymbol{u}}^{\mu}\,\mathrm{d}\Gamma=0$ for $\hat{\boldsymbol{u}}^{\mu}\in\mathbb{U}^{\mu}$ and, as a consequence, $l(\hat{\boldsymbol{u}}^{\mu})=\int_\Omega\boldsymbol{b}\cdot\hat{\boldsymbol{u}}^{\mu}\,\mathrm{d}\Omega$ for $\hat{\boldsymbol{u}}^{\mu}\in\mathbb{U}^{\mu}$. Surface subscaling is thus outside the scope of this text.

The fine-scale potential in (8.3) is replaced with the homogenized potential[8]

$$\Pi(\hat{\boldsymbol{u}}^{\mathrm{M}},\hat{\boldsymbol{u}}^{\mu}) = \int_\Omega\left[\psi_\Box(\hat{\boldsymbol{u}}^{\mathrm{M}}+\hat{\boldsymbol{u}}^{\mu}) - l_\Box(\hat{\boldsymbol{u}}^{\mathrm{M}}+\hat{\boldsymbol{u}}^{\mu})\right]\mathrm{d}\Omega - \int_{\Gamma_{\mathrm{N}}}\boldsymbol{t}_{\mathrm{p}}\cdot\hat{\boldsymbol{u}}^{\mathrm{M}}\,\mathrm{d}\Gamma \tag{7.42}$$
{eq:6-109}

where we introduced the RVE-functionals {eq:6-110}

$$\psi_\Box(\hat{\boldsymbol{u}}) \overset{\mathrm{def}}{=} \langle\psi(\boldsymbol{\epsilon}[\hat{\boldsymbol{u}}])\rangle_\Box, \tag{7.43a}$$
{eq:6-110a}

$$l_\Box(\hat{\boldsymbol{u}}) \overset{\mathrm{def}}{=} \langle\boldsymbol{b}\cdot\hat{\boldsymbol{u}}\rangle_\Box \tag{7.43b}$$
{eq:6-110b}

The minimization problem (8.5) is replaced by

$$\inf_{\hat{\boldsymbol{u}}^{\mathrm{M}}\in\mathbb{U}^{\mathrm{M}}}\ \inf_{\hat{\boldsymbol{u}}^{\mu}\in\mathbb{U}^{\mu}}\Pi(\hat{\boldsymbol{u}}^{\mathrm{M}},\hat{\boldsymbol{u}}^{\mu}) \tag{7.44}$$
{eq:6-111}

whose stationary condition is the two independent (global) problems of finding $\boldsymbol{u}^{\mathrm{M}}\in\mathbb{U}^{\mathrm{M}}$ and $\boldsymbol{u}^{\mu}\in\mathbb{U}^{\mu}$ that satisfy {eq:6-112}

$$\begin{aligned}\Pi'_{u^{\mathrm{M}}}(\boldsymbol{u}^{\mathrm{M}},\boldsymbol{u}^{\mu};\delta\boldsymbol{u}^{\mathrm{M}}) &= \int_\Omega\left[a_\Box(\boldsymbol{u}^{\mathrm{M}}+\boldsymbol{u}^{\mu};\delta\boldsymbol{u}^{\mathrm{M}}) - l_\Box(\delta\boldsymbol{u}^{\mathrm{M}})\right]\mathrm{d}\Omega - \int_{\Gamma_{\mathrm{N}}}\boldsymbol{t}_{\mathrm{p}}\cdot\delta\boldsymbol{u}^{\mathrm{M}}\,\mathrm{d}\Gamma\\ &= 0 \quad \forall\delta\boldsymbol{u}^{\mathrm{M}}\in\mathbb{U}^{\mathrm{M},0},\end{aligned} \tag{7.45a}$$
{eq:6-112a}

$$\begin{aligned}\Pi'_{u^{\mu}}(\boldsymbol{u}^{\mathrm{M}},\boldsymbol{u}^{\mu};\delta\boldsymbol{u}^{\mu}) &= \int_\Omega\left[a_\Box(\boldsymbol{u}^{\mathrm{M}}+\boldsymbol{u}^{\mu};\delta\boldsymbol{u}^{\mu}) - l_\Box(\delta\boldsymbol{u}^{\mu})\right]\mathrm{d}\Omega\\ &= 0 \quad \forall\delta\boldsymbol{u}^{\mu}\in\mathbb{U}^{\mu}\end{aligned} \tag{7.45b}$$
{eq:6-112b}

where

$$a_\Box(\boldsymbol{u};\delta\boldsymbol{u}) \overset{\mathrm{def}}{=} (\psi_\Box)'_u(\boldsymbol{u};\delta\boldsymbol{u}) = \langle\boldsymbol{\sigma}(\boldsymbol{\epsilon}[\boldsymbol{u}])\colon\boldsymbol{\epsilon}[\delta\boldsymbol{u}]\rangle_\Box \tag{7.46}$$
{eq:6-113}

[8] For brevity, the same notation Π is used.

We note that the form $a_\Box$ is nonlinear in its first argument, whereas it is linear in the second argument.

Next, we introduce a unique hierarchical additive decomposition of $\boldsymbol{u}$ into slowly varying (macroscale) and rapidly varying (fluctuation) components. Thereby, we introduce the linear prolongation operator $\boldsymbol{\mathcal{A}}\bar{\boldsymbol{u}}$ such that

$$\boldsymbol{u} = \boldsymbol{\mathcal{A}}\bar{\boldsymbol{u}} + \boldsymbol{u}^\mu \tag{7.47}$$ {eq:6-114}

where $\bar{\boldsymbol{u}}(\bullet, t) \in \bar{\mathbb{U}}$ is the macroscale displacement field.

7.3.3 A remark on the VCMH-condition

In view of the generic expression of the local VCMH-condition in ???, we conclude this condition reads

{eq:6-115}
$$a_\Box(\mathcal{A}\bar{\boldsymbol{u}} + \boldsymbol{u}^\mu\{\bar{\boldsymbol{u}}\}; \boldsymbol{\mathcal{S}}\delta\bar{\boldsymbol{u}}) - l_\Box(\boldsymbol{\mathcal{S}}\delta\bar{\boldsymbol{u}}) = 0 \quad \forall \delta\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}^0 \tag{7.48}$$

or, equivalently,

{eq:6-116}
$$\begin{aligned} &a_\Box(\boldsymbol{\mathcal{A}}\bar{\boldsymbol{u}} + \boldsymbol{u}^\mu\{\bar{\boldsymbol{u}}\}; \boldsymbol{\mathcal{A}}\delta\bar{\boldsymbol{u}} + \boldsymbol{\mathcal{S}}\delta\bar{\boldsymbol{u}}) - a_\Box(\boldsymbol{\mathcal{A}}\bar{\boldsymbol{u}} + \boldsymbol{u}^\mu\{\bar{\boldsymbol{u}}\}; \boldsymbol{\mathcal{A}}\delta\bar{\boldsymbol{u}}) \\ &= l_\Box(\boldsymbol{\mathcal{A}}\delta\bar{\boldsymbol{u}} + \boldsymbol{\mathcal{S}}\delta\bar{\boldsymbol{u}}) - l_\Box(\boldsymbol{\mathcal{A}}\delta\bar{\boldsymbol{u}}) \quad \forall \delta\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}^0 \end{aligned} \tag{7.49}$$

Remark 4 *Upon introducing the identity (by way of notation)* $\mathrm{d}\boldsymbol{u} = \boldsymbol{\mathcal{A}}\,\mathrm{d}\bar{\boldsymbol{u}} + \boldsymbol{\mathcal{S}}\,\mathrm{d}\bar{\boldsymbol{u}}$ *for given* $\mathrm{d}\bar{\boldsymbol{u}}$*, we may rewrite (8.109) in the more explicit fashion as follows:*

{eq:6-117}
$$\langle \boldsymbol{\sigma} : \boldsymbol{\epsilon}[\boldsymbol{\mathcal{S}}\,\mathrm{d}\bar{\boldsymbol{u}}]\rangle_\Box - \langle \boldsymbol{b} \cdot \boldsymbol{\mathcal{S}}\,\mathrm{d}\bar{\boldsymbol{u}}\rangle_\Box = 0 \quad \forall \delta\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}^0 \tag{7.50}$$

where it is recalled that $\boldsymbol{\sigma} = \boldsymbol{\sigma}(\boldsymbol{\epsilon}[\mathcal{A}\bar{\boldsymbol{u}} + \boldsymbol{u}^\mu\{\bar{\boldsymbol{u}}\}])$*. Moreover, upon using the weak form of equilibrium, we first note the trivial relation*

{eq:6-118}
$$\int_{\Omega_\Box} \boldsymbol{\sigma} : \boldsymbol{\epsilon}[\boldsymbol{\mathcal{S}}\,\mathrm{d}\bar{\boldsymbol{u}}]\,\mathrm{d}\Omega - \int_{\Omega_\Box} \boldsymbol{b} \cdot \mathcal{S}\,\mathrm{d}\bar{\boldsymbol{u}}\,\mathrm{d}\Omega - \int_{\Gamma_\Box} \boldsymbol{t} \cdot \boldsymbol{\mathcal{S}}\,\mathrm{d}\bar{\boldsymbol{u}}\,\mathrm{d}\Gamma = 0 \quad \forall \delta\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}^0 \tag{7.51}$$

which can be combined with (8.33) to yield the relation

{eq:6-119}
$$\frac{1}{|\Omega_\Box|} \int_{\Gamma_\Box} \boldsymbol{t} \cdot \boldsymbol{\mathcal{S}}\,\mathrm{d}\bar{\boldsymbol{u}}\,\mathrm{d}\Gamma = 0 \quad \forall \delta\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}^0 \tag{7.52}$$

However, we have the closure condition

{eq:6-120}
$$\langle \boldsymbol{\epsilon}[\boldsymbol{\mathcal{S}}\,\mathrm{d}\bar{\boldsymbol{u}}]\rangle_\Box = 0 \quad \Rightarrow \quad \bar{\boldsymbol{\sigma}} : \langle \boldsymbol{\epsilon}[\boldsymbol{\mathcal{S}}\,\mathrm{d}\bar{\boldsymbol{u}}]\rangle_\Box = 0 \tag{7.53}$$

for any $\bar{\boldsymbol{\sigma}} \in \mathbb{R}^{3\times 3}_{sym}$*, and we may use Gauss' theorem to obtain*

{eq:6-121}
$$\frac{1}{|\Omega_\Box|} \int_{\Gamma_\Box} [\bar{\boldsymbol{\sigma}} \cdot \boldsymbol{n}] \cdot [\boldsymbol{\mathcal{S}}\,\mathrm{d}\bar{\boldsymbol{u}}]\,\mathrm{d}\Gamma = 0 \tag{7.54}$$

Combining the results in (8.35) *and* (8.37)*, we finally obtain the alternative formulation of the VCMH-condition*

{eq:6-122}
$$\frac{1}{|\Omega_\Box|} \int_{\Gamma_\Box} [\boldsymbol{t} - \bar{\boldsymbol{\sigma}} \cdot \boldsymbol{n}] \cdot [\,\mathrm{d}\boldsymbol{u} - \boldsymbol{\mathcal{A}}\,\mathrm{d}\bar{\boldsymbol{u}}]\,\mathrm{d}\Gamma = 0 \quad \forall \delta\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}^0, \quad \bar{\boldsymbol{\sigma}} \in \mathbb{R}^{3\times 3}_{sym} \tag{7.55}$$

□

7.3.4 1st order homogenization – Standard macroscale model

In the standard case of 1st order homogenization, $\bar{\boldsymbol{u}}$ is prolonged via assumed linear variation of $\boldsymbol{u}^{\mathrm{M}}$ within each RVE:

{eq:6-131}
$$\boldsymbol{u}^{\mathrm{M}}(\bar{\boldsymbol{x}}, \boldsymbol{x}) = (\boldsymbol{\mathcal{A}}\bar{\boldsymbol{u}})(\bar{\boldsymbol{x}}, \boldsymbol{x}) := \bar{\boldsymbol{u}}(\bar{\boldsymbol{x}}) + \bar{\boldsymbol{h}}(\bar{\boldsymbol{x}}) \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}] \text{ for } \boldsymbol{x} \in \Omega_{\square} \tag{7.56}$$

where $\bar{\boldsymbol{h}} \stackrel{\text{def}}{=} \bar{\boldsymbol{u}} \otimes \boldsymbol{\nabla}$ is the macroscale displacement gradient, and where $\bar{\boldsymbol{x}}$ is the *volume average*

$$\bar{\boldsymbol{x}} \stackrel{\text{def}}{=} \langle \boldsymbol{x} \rangle_{\square} \Leftrightarrow \quad \int_{\Omega_{\square}} [\boldsymbol{x} - \bar{\boldsymbol{x}}] \, \mathrm{d}\Omega = \boldsymbol{0} \tag{7.57}$$ {eq:6-132}

Remark 5 *As an alternative it would be possible to assume that $\bar{\boldsymbol{x}}$ represents the surface average on the RVE. The chosen definition is crucial in the sense that it pertains to the definition of the operator $\boldsymbol{\mathcal{A}}^*$ (as defined below). See also the discussion below as regards non-corrupted fine-scale problems within the RVE.*

Next, we construct the operator $\boldsymbol{\mathcal{A}}^*$ such that, for any given $\hat{\boldsymbol{u}} \in ???$, it is represented by the "RVE-prolongation functionals" $\bar{\boldsymbol{u}}_{\square}(\hat{\boldsymbol{u}})$ and $\bar{\boldsymbol{h}}_{\square}(\hat{\boldsymbol{u}})$ defined as {eq:6-133}

$$\bar{\boldsymbol{u}}_{\square}(\hat{\boldsymbol{u}}) \stackrel{\text{def}}{=} \langle \hat{\boldsymbol{u}} \rangle_{\square} \tag{7.58a}$$ {eq:6-133a}

$$\bar{\boldsymbol{h}}_{\square}(\hat{\boldsymbol{u}}) \stackrel{\text{def}}{=} \frac{1}{|\Omega_{\square}|} \int_{\Gamma_{\square}} \hat{\boldsymbol{u}} \otimes \boldsymbol{n} \, \mathrm{d}\Gamma \tag{7.58b}$$ {eq:6-133b}

and we postulate the constraint conditions for the solution of the RVE-problem

$$\bar{\boldsymbol{u}}_{\square}(\boldsymbol{u}) = \bar{\boldsymbol{u}}, \quad \bar{\boldsymbol{h}}_{\square}(\boldsymbol{u}) = \bar{\boldsymbol{h}} \tag{7.59}$$ {eq:6-134}

However, it can readily be checked that, by the definition of $\boldsymbol{u}^{\mathrm{M}}$ in (8.122), the following identities hold:

$$\bar{\boldsymbol{u}}_{\square}(\boldsymbol{u}^{\mathrm{M}}) = \bar{\boldsymbol{u}}, \quad \bar{\boldsymbol{h}}_{\square}(\boldsymbol{u}^{\mathrm{M}}) = \bar{\boldsymbol{h}} \tag{7.60}$$ {eq:6-135}

whereby we have shown that the relation $\boldsymbol{\mathcal{A}}^*\boldsymbol{\mathcal{A}} = \boldsymbol{\mathcal{I}}d$ holds. Incorporating (8.127), we may thus rephrase (8.126) as

$$\bar{\boldsymbol{u}}_{\square}(\boldsymbol{u}^{\mu}) = \boldsymbol{0}, \quad \bar{\boldsymbol{h}}_{\square}(\boldsymbol{u}^{\mu}) = \boldsymbol{0} \tag{7.61}$$ {eq:6-136}

Homogenized quantities are obtained from testing (8.42) with $\boldsymbol{\mathcal{A}}\delta\bar{\boldsymbol{u}} = \delta\bar{\boldsymbol{u}} + \delta\bar{\boldsymbol{h}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}]$, whereby the homogenized problem (weak format) in (8.42) becomes: Find $\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}$ s.t.

$$\int_{\Omega} \bar{\boldsymbol{\sigma}}\{\bar{\boldsymbol{u}}\} : [\delta\bar{\boldsymbol{u}} \otimes \boldsymbol{\nabla}] \, \mathrm{d}\Omega = \int_{\Omega} \left[\bar{\boldsymbol{b}} \cdot \delta\bar{\boldsymbol{u}} + \bar{\boldsymbol{b}}^{(2)} : [\delta\bar{\boldsymbol{u}} \otimes \boldsymbol{\nabla}]\right] \mathrm{d}\Omega + \int_{\Gamma_{\mathrm{N}}} \boldsymbol{t}_{\mathrm{p}} \cdot \delta\bar{\boldsymbol{u}} \, \mathrm{d}\Gamma \quad \forall \delta\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}^0 \tag{7.62}$$ {eq:6-137}

where it was used that $[[\boldsymbol{\mathcal{A}}\delta\bar{\boldsymbol{u}}] \otimes \boldsymbol{\nabla}](\bar{\boldsymbol{x}}) = \delta\bar{\boldsymbol{h}}(\bar{\boldsymbol{x}}) = [\delta\bar{\boldsymbol{u}} \otimes \boldsymbol{\nabla}](\bar{\boldsymbol{x}})$, and where we derived the macroscale variables: {eq:6-138}

$$\bar{\boldsymbol{\sigma}}\{\bar{\boldsymbol{u}}\} \stackrel{\text{def}}{=} \langle \boldsymbol{\sigma}(\bar{\boldsymbol{\epsilon}} + \boldsymbol{\epsilon}[\boldsymbol{u}^{\mu}\{\bar{\boldsymbol{u}}\}]) \rangle_{\square}, \tag{7.63a}$$ {eq:6-138a}

$$\bar{\boldsymbol{b}} \stackrel{\text{def}}{=} \langle \boldsymbol{b} \rangle_{\square}, \tag{7.63b}$$ {eq:6-138b}

$$\bar{\boldsymbol{b}}^{(2)} \stackrel{\text{def}}{=} \langle \boldsymbol{b} \otimes [\boldsymbol{x} - \bar{\boldsymbol{x}}] \rangle_{\square} \tag{7.63c}$$ {eq:6-138c}

where $\bar{\boldsymbol{\epsilon}} \stackrel{\text{def}}{=} \bar{\boldsymbol{h}}^{\mathrm{sym}}$. In particular, $\bar{\boldsymbol{\sigma}}$ is the macroscale (homogenized) stress. As to the external boundary, we tacitly assume that boundary conditions can be imposed in terms of prescribed displacement $\bar{\boldsymbol{u}}_{\mathrm{p}}$ and (possibly) in terms of prescribed traction $\bar{\boldsymbol{t}}_{\mathrm{p}}$. In fact the boundary term in (8.49) becomes this simple only if the traction is sufficiently smooth, thereby avoiding homogenization on the exterior boundary (in this text).

{figure:6-5} Figure 7.4: Local problem for RVE based on microperiodicity. (a) Image and mirror boundaries $\Gamma_{\square}^{+}$ and $\Gamma_{\square}^{-}$. (b) Lagrange multiplier field on $\Gamma_{\square}^{+}$.

7.3.5 RVE-problem for weak periodicity

The global problem (8.24b)???? is replaced with "local" RVE-problems on each $\Omega_{\square}$. The most general form of the equilibrium equation for a "cut-out" RVE reads: Find fluctuation displacements $\boldsymbol{u}^{\mu}$ and tractions $\boldsymbol{t}$ that solve

{eq:6-201}
$$a_{\square}(\boldsymbol{u}^{\mathrm{M}}+\boldsymbol{u}^{\mu},\delta\boldsymbol{u}^{\mu}) = l_{\square}(\delta\boldsymbol{u}^{\mu}) + \frac{1}{|\Omega_{\square}|}\int_{\Gamma_{\square}} \boldsymbol{t}\cdot\delta\boldsymbol{u}^{\mu}\,\mathrm{d}\Gamma \tag{7.64}$$

where the properties of test functions $\delta\boldsymbol{u}^{\mu}$ need to be specified. Moreover, a model assumption for $\boldsymbol{t}$ is needed.

A viable possibility is to introduce the assumption of micro-periodicity, illustrated in Figure **??**, which leads to the WPBC-problem that was discussed extensively in the context of linear elasticity in Chapter 3. The assumption of (weak) periodicity is natural since it can be cast in a variational format that admits the Dirichlet (displacement) and Neumann (traction) boundary conditions to be obtained as special cases. Recall the bilinear form $d_{\square}(\boldsymbol{\lambda}',\boldsymbol{u}')$ introduced in (**??**):

{eq:6-139}
$$d_{\square}(\boldsymbol{\lambda}',\boldsymbol{u}') \stackrel{\text{def}}{=} \frac{1}{|\Omega_{\square}|}\int_{\Gamma_{\square}^{+}} \boldsymbol{\lambda}'\cdot[\![\boldsymbol{u}']\!]_{\square}\,\mathrm{d}\Gamma \tag{7.65}$$

We note the following:

- Introducing the model assumption for tractions

{eq:6-202}
$$\boldsymbol{t}=\boldsymbol{\lambda} \text{ on } \Gamma_{\square}^{+}, \quad \boldsymbol{t}=-\boldsymbol{\lambda} \text{ on } \Gamma_{\square}^{-} \tag{7.66}$$

  i.e. $\boldsymbol{t}$ is anti-periodic across the RVE, we may rewrite the boundary term in (8.143)

{eq:6-203}
$$\frac{1}{|\Omega_{\square}|}\int_{\Gamma_{\square}} \boldsymbol{t}\cdot\delta\boldsymbol{u}^{\mu}\,\mathrm{d}\Gamma = \frac{1}{|\Omega_{\square}|}\int_{\Gamma_{\square}^{+}} \boldsymbol{\lambda}\cdot[\![\delta\boldsymbol{u}^{\mu}]\!]_{\square}\,\mathrm{d}\Gamma = d_{\square}(\boldsymbol{\lambda},\delta\boldsymbol{u}^{\mu}) \tag{7.67}$$

- The condition of (weakly) periodic fluctuations $\boldsymbol{u}^{\mu}$ is expressed as

{eq:6-140}
$$d_{\square}(\delta\boldsymbol{\lambda},\boldsymbol{u}^{\mu}) = 0, \quad \forall\delta\boldsymbol{\lambda}\in\mathbb{T}_{\square}^{+} \tag{7.68}$$

  where $\mathbb{T}_{\square} = \mathbb{L}_2^{+}(\Gamma_{\square}^{+})$. In conclusion, $\boldsymbol{\lambda}$ are Lagrangian multipliers (that play the role of tractions on $\Gamma_{\square}^{+}$).

{eq:6-141} Next, we introduce solution and test spaces

{eq:6-141a}
$$\mathbb{U}_{\square} = \{\boldsymbol{u}' \text{ sufficiently regular}\} \tag{7.69a}$$

{eq:6-141b}
$$\mathbb{U}_{\square}^{\mu} = \{\boldsymbol{u}'\in\mathbb{U}_{\square}:\ \bar{\boldsymbol{u}}_{\square}(\boldsymbol{u}')=\boldsymbol{0},\ \bar{\boldsymbol{h}}_{\square}(\boldsymbol{u}')=\boldsymbol{0}\} \tag{7.69b}$$

It is clear that the solution $\boldsymbol{u}^{\mu}\in\mathbb{U}_{\square}^{\mu}$ in view of the conditions (8.128). We are now in the position to state the complete (solvable) RVE-problem: For any given macroscale field values $\bar{\boldsymbol{u}}$

and $\bar{\boldsymbol{h}}$ (which define the prolongation $\boldsymbol{u}^{\mathrm{M}}$ from the macroscale), find $\boldsymbol{u}^{\mu} \in \mathbb{U}^{\mu}_{\square}$ and $\boldsymbol{\lambda} \in \mathbb{T}^{+}_{\square}$ that
{eq:6-144} solve

{eq:6-144a}
{eq:6-144b}
$$a_{\square}(\mathcal{A}\bar{\boldsymbol{u}} + \boldsymbol{u}^{\mu}; \delta\boldsymbol{u}^{\mu}) - d_{\square}(\boldsymbol{\lambda}, \delta\boldsymbol{u}^{\mu}) = l_{\square}(\delta\boldsymbol{u}^{\mu}) \quad \forall \delta\boldsymbol{u}^{\mu} \in \mathbb{U}^{\mu}_{\square}, \tag{7.70a}$$
$$-d_{\square}(\delta\boldsymbol{\lambda}, \boldsymbol{u}^{\mu}) = 0 \quad \forall \delta\boldsymbol{\lambda} \in \mathbb{T}^{+}_{\square}. \tag{7.70b}$$

Once again, this problem represents localization in the sense that the local approximations $\boldsymbol{u}^{\mu}$ and $\boldsymbol{\lambda}$ are computed on each RVE independently for given macrofield $\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}$.

For computational purposes it is suitable to rephrase (8.136). To this end, we first make the following observations:

- Since $\delta\boldsymbol{u}^{\mu} \in \mathbb{U}^{\mu}_{\square}$, i.e. $\bar{\boldsymbol{u}}_{\square}(\delta\boldsymbol{u}^{\mu}) = \boldsymbol{0}$, $\bar{\boldsymbol{h}}_{\square}(\delta\boldsymbol{u}^{\mu}) = \boldsymbol{0}$, it holds that
$$l_{\square}(\delta\boldsymbol{u}^{\mu}) = l_{\square}(\delta\boldsymbol{u}^{\mu} - \bar{\boldsymbol{u}}_{\square}(\delta\boldsymbol{u}^{\mu}) - \bar{\boldsymbol{h}}_{\square}(\delta\boldsymbol{u}^{\mu}) \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}]) =: l^{\mu}_{\square}(\delta\boldsymbol{u}^{\mu}) \tag{7.71}$$ {eq:6-205}

- The condition $\bar{\boldsymbol{u}}_{\square}(\boldsymbol{u}') = \boldsymbol{0}$ is automatically satisfied for any $\boldsymbol{u}'$ that satisfies the condition
$$d_{\square}(\delta\boldsymbol{\lambda}, \boldsymbol{u}') = 0, \quad \forall \delta\boldsymbol{\lambda} \in \mathbb{T}^{+}_{\square} \tag{7.72}$$ {eq:6-206}

  which is shown as follows: Choose $\delta\boldsymbol{\lambda} = \delta\bar{\boldsymbol{\sigma}} \cdot \boldsymbol{n}$ for arbitrary constant 2nd order tensor $\delta\bar{\boldsymbol{\sigma}}$ (need not be symmetrical).

As a result, it appears to be possible to restate the RVE-problem (8.136) as follows: For any given values $\bar{\boldsymbol{u}}$ and $\bar{\boldsymbol{h}}$, find $\boldsymbol{u}^{\mu} \in \mathbb{U}_{\square}$, $\boldsymbol{\lambda} \in \mathbb{T}^{+}_{\square}$ and $\bar{\boldsymbol{\lambda}} \in \mathbb{R}^3$ that solve {eq:6-144}

$$a_{\square}(\mathcal{A}\bar{\boldsymbol{u}} + \boldsymbol{u}^{\mu}; \delta\boldsymbol{u}) - d_{\square}(\boldsymbol{\lambda}, \delta\boldsymbol{u}) - \bar{\boldsymbol{\lambda}} \cdot \langle \delta\boldsymbol{u} \rangle_{\square} = l^{\mu}_{\square}(\delta\boldsymbol{u}) \quad \forall \delta\boldsymbol{u} \in \mathbb{U}_{\square}, \tag{7.73a}$$ {eq:6-144a}
$$-d_{\square}(\delta\boldsymbol{\lambda}, \boldsymbol{u}^{\mu}) = 0 \quad \forall \delta\boldsymbol{\lambda} \in \mathbb{T}^{+}_{\square}. \tag{7.73b}$$ {eq:6-144b}
$$-\delta\bar{\boldsymbol{\lambda}} \cdot \langle \boldsymbol{u}^{\mu} \rangle_{\square} = 0 \quad \forall \delta\bar{\boldsymbol{\lambda}} \in \mathbb{R}^3. \tag{7.73c}$$ {eq:6-144c}

However, for computational purposes it turns out to be convenient to choose $\boldsymbol{u}$ (rather than $\boldsymbol{u}^{\mu}$) as the unknown field in a canonical format of the RVE-problem. We then note that the RVE-problem is reformulated as follows: For any given macroscale field values $\bar{\boldsymbol{u}}$ and $\bar{\boldsymbol{h}}$, find $\boldsymbol{u} \in \mathbb{U}_{\square}$, $\boldsymbol{\lambda} \in \mathbb{T}^{+}_{\square}$ and $\bar{\boldsymbol{\lambda}} \in \mathbb{R}^3$ that solve {eq:6-145}

$$a_{\square}(\boldsymbol{u}; \delta\boldsymbol{u}) - d_{\square}(\boldsymbol{\lambda}, \delta\boldsymbol{u}) - \bar{\boldsymbol{\lambda}} \cdot \langle \delta\boldsymbol{u} \rangle_{\square} = l^{\mu}_{\square}(\delta\boldsymbol{u}) \quad \forall \delta\boldsymbol{u} \in \mathbb{U}_{\square}, \tag{7.74a}$$ {eq:6-145a}
$$-d_{\square}(\delta\boldsymbol{\lambda}, \boldsymbol{u}) = -d_{\square}(\delta\boldsymbol{\lambda}, \bar{\boldsymbol{h}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}]) \quad \forall \delta\boldsymbol{\lambda} \in \mathbb{T}^{+}_{\square}. \tag{7.74b}$$ {eq:6-145b}
$$-\delta\bar{\boldsymbol{\lambda}} \cdot \langle \boldsymbol{u} \rangle_{\square} = -\delta\bar{\boldsymbol{\lambda}} \cdot \bar{\boldsymbol{u}} \quad \forall \delta\bar{\boldsymbol{\lambda}} \in \mathbb{R}^3. \tag{7.74c}$$ {eq:6-145c}

Solvability - Invariance for macroscale RBM

Consider the RVE-problem as formulated in (8.136): We note that $a_{\square}(\boldsymbol{\mathcal{A}}\bar{\boldsymbol{u}} + \boldsymbol{u}^{\mu}, \delta\boldsymbol{u}) = a_{\square}(\bar{\boldsymbol{\epsilon}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}] + \boldsymbol{u}^{\mu}, \delta\boldsymbol{u})$. Only $\bar{\boldsymbol{\epsilon}} := h^{\mathrm{sym}}$ (and not $\bar{\boldsymbol{u}}$ and $\bar{\boldsymbol{h}}^{\mathrm{skw}}$) appear as data in the problem; hence, $\boldsymbol{u}^{\mu} = \boldsymbol{u}^{\mu}\{\bar{\boldsymbol{\epsilon}}\}$. In other words, the solution $\boldsymbol{u}^{\mu}$ is invariant to any chosen (or superimposed) values of $\bar{\boldsymbol{u}}$ and $\bar{\boldsymbol{h}}^{\mathrm{skw}}$, which represent the RBM. For example, we may choose $\bar{\boldsymbol{u}} = \boldsymbol{0}$ and $\bar{\boldsymbol{h}}^{\mathrm{skw}} = \boldsymbol{0}$.

This conclusion on invariance obviously holds also for the macroscale stress $\bar{\boldsymbol{\sigma}}$, which is the single dynamic variable that is fed to the macroscale from the RVE-computation:

$$\bar{\boldsymbol{\sigma}} = \langle \boldsymbol{\sigma}(\boldsymbol{\epsilon}[\boldsymbol{\mathcal{A}}\bar{\boldsymbol{u}} + \boldsymbol{u}^{\mu}\{\boldsymbol{\mathcal{A}}\bar{\boldsymbol{u}}\}]) \rangle_{\square} = \langle \boldsymbol{\sigma}(\bar{\boldsymbol{\epsilon}} + \boldsymbol{\epsilon}[\boldsymbol{u}^{\mu}\{\bar{\boldsymbol{\epsilon}}\}]) \rangle_{\square} \tag{7.75}$$ {eq:6-148}

However, the RBM-variables/fields $\bar{\boldsymbol{u}}(\bar{\boldsymbol{x}})$ and $\bar{\boldsymbol{h}}^{\text{skw}}(\bar{\boldsymbol{x}})$ are certainly relevant in solving the macroscale boundary value problem.

In summary, we formulate the "reduced" RVE-problem format: For any given value $\bar{\boldsymbol{\epsilon}} = \bar{\boldsymbol{h}}^{\text{sym}}$, find $\boldsymbol{u} \in \mathbb{U}_\square$, $\boldsymbol{\lambda} \in \mathbb{T}_\square^+$ and $\bar{\boldsymbol{\lambda}} \in \mathbb{R}^3$ that solve {eq:6-149}

$$a_\square(\boldsymbol{u};\delta\boldsymbol{u}) - d_\square(\boldsymbol{\lambda},\delta\boldsymbol{u}) - \bar{\boldsymbol{\lambda}}\cdot\langle\delta\boldsymbol{u}\rangle_\square = l_\square^\mu(\delta\boldsymbol{u}) \qquad \forall\delta\boldsymbol{u}\in\mathbb{U}_\square, \tag{7.76a}$$ {eq:6-149a}

$$-d_\square(\delta\boldsymbol{\lambda},\boldsymbol{u}) = -d_\square(\delta\boldsymbol{\lambda},\bar{\boldsymbol{\epsilon}}\cdot[\boldsymbol{x}-\bar{\boldsymbol{x}}]) \quad \forall\delta\boldsymbol{\lambda}\in\mathbb{T}_\square^+. \tag{7.76b}$$ {eq:6-149b}

$$-\delta\bar{\boldsymbol{\lambda}}\cdot\langle\boldsymbol{u}\rangle_\square = 0 \qquad \forall\delta\bar{\boldsymbol{\lambda}}\in\mathbb{R}^3. \tag{7.76c}$$ {eq:6-149c}

UPDATE An associated SVE-potential (a local Lagrangian potential) can be constructed, for any given $\bar{\boldsymbol{\epsilon}}$, as follows:

{eq:6-161}
$$\pi_\square(\bar{\boldsymbol{\epsilon}};\hat{\boldsymbol{u}},\hat{\boldsymbol{\lambda}}) \overset{\text{def}}{=} \psi_\square(\hat{\boldsymbol{u}}) - d_\square(\hat{\boldsymbol{\lambda}},\hat{\boldsymbol{u}}-\bar{\boldsymbol{\epsilon}}\cdot[\boldsymbol{x}-\bar{\boldsymbol{x}}]) - l_\square(\hat{\boldsymbol{u}}-\bar{\boldsymbol{\epsilon}}\cdot[\boldsymbol{x}-\bar{\boldsymbol{x}}]) \tag{7.77}$$

and the RVE-problem reads: For given value of $\bar{\boldsymbol{\epsilon}}$, solve for $\boldsymbol{u}$ and $\boldsymbol{\lambda}$ from the saddle-point problem

{eq:6-162}
$$(\boldsymbol{u},\boldsymbol{\lambda}) = \arg\left[\inf_{\hat{\boldsymbol{u}}\in\mathbb{U}_\square}\ \sup_{\hat{\boldsymbol{\lambda}}\in\mathbb{T}_\square^+} \pi(\bar{\boldsymbol{\epsilon}};\hat{\boldsymbol{u}},\hat{\boldsymbol{\lambda}})\right] \tag{7.78}$$

The corresponding stationarity conditions define local problems on $\Omega_\square$, which are precisely those given in (7.76).

Operational format of RVE-problem

A completely valid format was given in (8.136) or (7.76). However, it is possible to avoid the constraint (8.136a) (or (7.76c)) completely by simply constraining the translation of an arbitrary point $\boldsymbol{x}_0 \in \Omega_\square$, e.g. we may prescribe $\boldsymbol{u}(\boldsymbol{x}_0) = \boldsymbol{0}$. The argument goes as follows:

Firstly, we recall that $\boldsymbol{u}^\mu$ and $\bar{\boldsymbol{\sigma}}$ are unaffected by the value of $\bar{\boldsymbol{u}}$. Now, for given value $\bar{\boldsymbol{u}}^{(1)}$, consider the solution field $\boldsymbol{u}$ and compute (in particular) $\boldsymbol{u}(\boldsymbol{x}_0) := \bar{\boldsymbol{u}}_0^{(1)}$. Next, consider, the *translated field* $\boldsymbol{u}' := \boldsymbol{u} - \bar{\boldsymbol{u}}_0^{(1)}$, for which we note that $\boldsymbol{u}'(\boldsymbol{x}_0) = \boldsymbol{0}$. Further, we note that the condition (7.76c) is replaced by

{eq:6-162}
$$\delta\bar{\boldsymbol{\lambda}}'\cdot\langle\boldsymbol{u}'\rangle_\square = \delta\bar{\boldsymbol{\lambda}}'\cdot[\bar{\boldsymbol{u}}^{(1)} - \bar{\boldsymbol{u}}_0^{(1)}] \quad \forall\delta\bar{\boldsymbol{\lambda}}'\in\mathbb{R}^3 \tag{7.79}$$

However, due to invariance w.r.t. translation, the translated and non-translated fields will give the same value of $\boldsymbol{u}^\mu$. As a consequence, we may introduce the alternative solution (and test) space $\mathbb{U}_\square'$ as follows:

{eq:6-150}
$$\mathbb{U}_\square' = \{\boldsymbol{u}' \text{ suff. regular in } \Omega_\square,\ \boldsymbol{u}'(\boldsymbol{x}_0) = \boldsymbol{0}\} \tag{7.80}$$

and we replace (7.76) with the simpler RVE-problem: For given value of $\bar{\boldsymbol{\epsilon}}$, find $\boldsymbol{u}' \in \mathbb{U}_\square'$ and
{eq:6-151} $\boldsymbol{\lambda}' \in \mathbb{T}_\square^+$ that solve the system

{eq:6-151a}
$$a_\square(\boldsymbol{u}';\delta\boldsymbol{u}) - d_\square(\boldsymbol{\lambda}',\delta\boldsymbol{u}) = l_\square^\mu(\delta\boldsymbol{u}) \qquad \forall\delta\boldsymbol{u}\in\mathbb{U}_\square', \tag{7.81a}$$

{eq:6-151b}
$$-d_\square(\delta\boldsymbol{\lambda},\boldsymbol{u}') = -d_\square(\delta\boldsymbol{\lambda},\bar{\boldsymbol{\epsilon}}\cdot[\boldsymbol{x}-\bar{\boldsymbol{x}}]) \quad \forall\delta\boldsymbol{\lambda}\in\mathbb{T}_\square^+. \tag{7.81b}$$

Satisfaction of Hill-Mandel macrohomogeneity condition

To show that the VCMH-condition is satisfied upon adopting the (model) assumption of micro-periodic fluctuations, we argue as follows:

- Linearize (7.76b,7.76c) w.r.t. $\bar{\boldsymbol{u}}$ along $\mathrm{d}\bar{\boldsymbol{u}}$, i.e. $\boldsymbol{u} \to \mathrm{d}\boldsymbol{u}$. Choose $\delta\boldsymbol{\lambda} = \boldsymbol{\lambda}\{\bar{\boldsymbol{\epsilon}}\} \in \mathbb{T}_\square^+$ in the linearized equation (7.76b) and $\delta\bar{\boldsymbol{\lambda}} = \bar{\boldsymbol{\lambda}}\{\bar{\boldsymbol{\epsilon}}\} \in \mathbb{R}^3$ in the linearized equation (7.76c).
- For any given perturbation $\mathrm{d}\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}^0$, choose $\delta\boldsymbol{u} = \mathrm{d}\boldsymbol{u} - \mathrm{d}\bar{\boldsymbol{\epsilon}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}]$ in (7.76a) to obtain

$$\langle \boldsymbol{\sigma} : \boldsymbol{\epsilon}[\,\mathrm{d}\boldsymbol{u}] \rangle_\square - \langle \boldsymbol{b} \cdot \mathrm{d}\boldsymbol{u} \rangle_\square \;\; = \left[\bar{\boldsymbol{\sigma}} - \bar{\boldsymbol{b}}^{(2)} \right] : \mathrm{d}\bar{\boldsymbol{\epsilon}} \quad \forall \delta\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}^0 \tag{7.82}$$ {eq:6-153}

where it was used that

$$a_\square(\boldsymbol{u}, \mathrm{d}\boldsymbol{u} - \mathrm{d}\bar{\boldsymbol{\epsilon}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}]) = \langle \boldsymbol{\sigma} : \boldsymbol{\epsilon}[\,\mathrm{d}\boldsymbol{u}] \rangle_\square - \bar{\boldsymbol{\sigma}} : \mathrm{d}\bar{\boldsymbol{\epsilon}}, \quad l_\square^\mu(\boldsymbol{u}, \mathrm{d}\boldsymbol{u} - \mathrm{d}\bar{\boldsymbol{\epsilon}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}]) = \langle \boldsymbol{b} \cdot \mathrm{d}\boldsymbol{u} \rangle_\square - \bar{\boldsymbol{b}}^{(2)} : \mathrm{d}\bar{\boldsymbol{\epsilon}} \tag{7.83}$$ {eq:6-207}

Clearly, in the special case that $\boldsymbol{b} = \boldsymbol{0}$, we obtain the classical format of the Hill-Mandel condition

$$\langle \boldsymbol{\sigma} : \boldsymbol{\epsilon}[\,\mathrm{d}\boldsymbol{u}] \rangle_\square = \bar{\boldsymbol{\sigma}} : \mathrm{d}\bar{\boldsymbol{\epsilon}} \quad \forall \delta\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}^0 \tag{7.84}$$ {eq:6-154}

which was given in Subsection 2.2.6.???

Remark 6 *Note that the result in (8.64) is, in fact, independent on the order of homogenization defined by the specific choice of prolongation operator $\boldsymbol{\mathcal{A}}$. For example, it applies to the case when $\boldsymbol{\mathcal{A}}$ represents socalled 2nd order homogenization, as proposed by* KOUZNETSOVA **?**.

7.3.6 2nd order homogenization – Nonlocal continuum

SKALL VI HA MED ????

ALT: Micropolar?

$$(\mathcal{A}\bar{\boldsymbol{u}})(\bar{\boldsymbol{x}}, \boldsymbol{x}) = \bar{\boldsymbol{u}}(\bar{\boldsymbol{x}}) + \bar{\boldsymbol{\epsilon}}(\bar{\boldsymbol{x}}) \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}] + \frac{1}{2} \bar{\boldsymbol{u}} \otimes \boldsymbol{\nabla} \otimes \boldsymbol{\nabla} \colon [\boldsymbol{x} - \bar{\boldsymbol{x}}] \otimes [\boldsymbol{x} - \bar{\boldsymbol{x}}], \quad \text{for } \boldsymbol{x} \in \Omega_\square \tag{7.85}$$ {eq:6-75}

7.4 A model problem with multiphysics couplings – Magneto-elasticity

7.5 A model problem with time-dependence – Kelvin-type viscoelasticity

Chapter 8

VCH – SELECTED TRANSIENT PROBLEMS

Transient heat conduction (prototype model)
Kelvin-type viscoelasticity Standard Dissipative material (viscoplasticity), incremental format

Use manuscript in progress

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

8.1 Introduction

8.2 Variationally consistent homogenization – Application to a stationary model problem

8.2.1 Nonlinear elasticity

Consider a random micro-heterogenous material structure within a solid body occupying the domain Ω with boundary $\Gamma = \Gamma_{\rm D} \cup \Gamma_{\rm N}$. The body is subjected to distributed body load $\boldsymbol{b}$ in Ω and prescribed tractions on $\Gamma_{\rm N}$. Displacements are prescribed on $\Gamma_{\rm D}$. For simplicity, it is assumed that the topology is contiguous, i. e. the density is non-zero (no holes) everywhere in Ω.

Restricting to quasistatics, we seek the displacement field $\boldsymbol{u}(\boldsymbol{x}) : \Omega \rightarrow \mathbb{R}^3$ that solves the system

{eq:6-1}

$$-\boldsymbol{\sigma}(\boldsymbol{\epsilon}[\boldsymbol{u}]) \cdot \boldsymbol{\nabla} = \boldsymbol{b} \quad \text{in } \Omega \tag{8.1a}$$ {eq:6-1a}

$$\boldsymbol{u} = \boldsymbol{u}_{\rm p} \quad \text{on } \Gamma_{\rm D} \tag{8.1b}$$ {eq:6-1c}

$$\boldsymbol{t} \stackrel{\text{def}}{=} \boldsymbol{\sigma} \cdot \boldsymbol{n} = \boldsymbol{t}_{\rm p} \quad \text{on } \Gamma_{\rm N} \tag{8.1c}$$ {eq:6-1d}

where $\boldsymbol{\epsilon}[\hat{\boldsymbol{u}}] \stackrel{\text{def}}{=} (\hat{\boldsymbol{u}} \otimes \boldsymbol{\nabla})^{\rm sym}$ is the "small strain operator". It is assumed that the subscale material is described by nonlinear elasticity, whereby the convex volume-specific strain energy density $\psi(\boldsymbol{\epsilon})$ serves as the potential for the stress $\boldsymbol{\sigma}(\boldsymbol{\epsilon})$, i.e.

$$\boldsymbol{\sigma}(\boldsymbol{\epsilon}) = \frac{\partial \psi(\boldsymbol{\epsilon})}{\partial \boldsymbol{\epsilon}} \tag{8.2}$$ {eq:6-1a}

{figure:6-1} Figure 8.1: Domain decomposition **NEW FIGURE**

In order to establish the variational format for the fine-scale problem, we introduce the potential energy

{eq:6-2}
$$\Pi(\hat{\boldsymbol{u}}) = \Psi(\hat{\boldsymbol{u}}) - l(\hat{\boldsymbol{u}}) \tag{8.3}$$

{eq:6-3} where

{eq:6-3a}
$$\Psi(\hat{\boldsymbol{u}}) \overset{\text{def}}{=} \int_\Omega \psi(\boldsymbol{\epsilon}[\hat{\boldsymbol{u}}])\, \mathrm{d}\Omega \tag{8.4a}$$

{eq:6-3b}
$$l(\hat{\boldsymbol{u}}) \overset{\text{def}}{=} \int_\Omega \boldsymbol{b} \cdot \hat{\boldsymbol{u}}\, \mathrm{d}\Omega + \int_{\Gamma_\mathrm{N}} \boldsymbol{t}_\mathrm{p} \cdot \hat{\boldsymbol{u}}\, \mathrm{d}\Gamma \tag{8.4b}$$

The sought fine-scale solution $\boldsymbol{u} \in \mathbb{U}$ is the minimizer of $\Pi(\hat{\boldsymbol{u}})$ on $\mathbb{U}$, i. e.

{eq:6-4}
$$\boldsymbol{u} = \arg \left[\inf_{\hat{\boldsymbol{u}} \in \mathbb{U}} \Pi(\hat{\boldsymbol{u}}) \right] \tag{8.5}$$

and the corresponding stationarity condition becomes

{eq:6-5}
$$\Pi'(\boldsymbol{u}; \delta\boldsymbol{u}) = \int_\Omega \boldsymbol{\sigma}(\boldsymbol{\epsilon}[\boldsymbol{u}]) : \boldsymbol{\epsilon}[\delta\boldsymbol{u}]\, \mathrm{d}\Omega - l(\delta\boldsymbol{u}) = 0 \quad \forall \delta\boldsymbol{u} \in \mathbb{U}^0, \tag{8.6}$$

where Π' denotes the directional derivative of Π, and where the standard solution space $\mathbb{U}$ and
{eq:6-6} test space $\mathbb{U}^0$ are defined as, respectively,

{eq:6-6a}
$$\mathbb{U} = \{\boldsymbol{u} \text{ suff. regular} |\ \boldsymbol{u} = \bar{\boldsymbol{u}}_\mathrm{p} \text{ on } \Gamma_\mathrm{D}\} \tag{8.7a}$$

{eq:6-6b}
$$\mathbb{U}^0 = \{\boldsymbol{u} \text{ suff. regular} |\ \boldsymbol{u} = \boldsymbol{0} \text{ on } \Gamma_\mathrm{D}\} \tag{8.7b}$$

8.2.2 Single-scale setting – VMS

As a preliminary to the subsequent discussion of homogenization, we assume that each $\boldsymbol{u} \in \mathbb{U}$ can be decomposed into macroscale (smooth) and subscale (fluctuating) parts via the unique hierarchical decomposition $\mathbb{U}^\mathrm{M} \oplus \mathbb{U}^\mu$ in the spirit of VMS = Variational MultiScale method, Hughes (1995), Målqvist & Larson (2003-): More precisely, each $\boldsymbol{u} \in \mathbb{U}$ can be additively split *uniquely* into

{eq:6-11}
$$\boldsymbol{u} = \boldsymbol{u}^\mathrm{M} + \boldsymbol{u}^\mu, \quad (\boldsymbol{u}^\mathrm{M}, \boldsymbol{u}^\mu) \in \mathbb{U}^\mathrm{M} \oplus \mathbb{U}^\mu \tag{8.8}$$

UPDATE We remark that $\boldsymbol{u}^\mu \in \mathbb{U}^\mu \subseteq \mathbb{U}^0$ means that $\boldsymbol{u}^\mu = \boldsymbol{0}$ on Γ_D (the Dirichlet boundary). In addition, we henceforth assume (to avoid unnecessary technicalities) that $\boldsymbol{u}^\mu = 0$ on Γ_N as well. We thus obtain $\int_{\Gamma_\mathrm{N}} \boldsymbol{t}_\mathrm{p} \cdot \hat{\boldsymbol{u}}^\mu\, \mathrm{d}\Gamma = 0$ for $\hat{\boldsymbol{u}}^\mu \in \mathbb{U}^\mu$ and, as a consequence, $l(\hat{\boldsymbol{u}}^\mu) = \int_\Omega \boldsymbol{b} \cdot \hat{\boldsymbol{u}}^\mu\, \mathrm{d}\Omega$ for $\hat{\boldsymbol{u}}^\mu \in \mathbb{U}^\mu$. Surface subscaling is thus outside the scope of this text.

Application of classical (single-scale) VMS-strategy

Mälqvist et al. Fredrik, kan du skriva nagot om traditionell och nyare resultat?

Figure 8.2: Homogenization of integral??? {figure:6-2

8.2.3 Two-scale setting – Homogenization as a smoothing procedure

In the previous Subsection no special reference was made to homogenization; hence, only one single scale was considered. In order to set the stage for (model-based) homogenization, we introduce the domain decomposition $\Omega = \cup_i \Omega_{\square,i}$, as shown in Figure 8.2. As a consequence, any volume integral can be rephrased as

{eq:6-12}
$$\int_\Omega f \, \mathrm{d}\Omega = \sum_i \int_{\Omega_{\square,i}} f \, \mathrm{d}\Omega = \sum_i |\Omega_{\square,i}| \underbrace{\frac{1}{|\Omega_{\square,i}|} \int_{\Omega_{\square,i}} f \, \mathrm{d}\Omega}_{\stackrel{\text{def}}{=} f_{\square,i}} \tag{8.9}$$

Introducing the averaging operator[1]

$$\langle f \rangle_\square(\boldsymbol{x}) \stackrel{\text{def}}{=} \frac{1}{|\Omega_\square(\boldsymbol{x})|} \int_{\Omega_\square(\boldsymbol{x})} f \, \mathrm{d}\Omega \tag{8.10}$$ {eq:6-12}

and setting $\Omega_\square(\boldsymbol{x}) = \Omega_{\square,i}$ when $\boldsymbol{x} \in \Omega_{\square,i}$ implies that $\langle f \rangle_\square(\boldsymbol{x}) = f_{\square,i}$ when $\boldsymbol{x} \in \Omega_{\square,i}$ p.w. constant, c.f. Figure **??**. Hence, we have the trivial identity $\int_\Omega f \, \mathrm{d}\Omega = \int_\Omega \langle f \rangle_\square \, \mathrm{d}\Omega$, which holds also when $|\Omega_{\square,i}| \to 0$. However, the approach taken in classical model-based homogenization is to introduce finite-sized "RVE:s" that occupy *overlapping subdomains* $\Omega_\square(\boldsymbol{x})$, with $diam(\Omega_\square) = L_\square$, for each $\boldsymbol{x} \in \Omega$. Hence, we introduce the *approximation*

$$\int_\Omega f \, \mathrm{d}\Omega \approx \int_\Omega \langle f \rangle_\square \, \mathrm{d}\Omega \tag{8.11}$$ {eq:6-13}

where $\langle f \rangle_\square$ is the "running average" that is defined by (8.10) with the choice that $\Omega_\square(\boldsymbol{x})$ is centered[2] at $\boldsymbol{x}$. It is noted that $\langle f \rangle_\square$ is smoother than f, and the smoothness increases with $L_\square$. Moreover, since the homogenized integral approximates the fine-scale integral, the introduced model error is expected to increase with $L_\square$.

We are now in the position to replace the fine-scale potential in (8.3) with the homogenized potential[3]

$$\Pi(\hat{\boldsymbol{u}}^{\mathrm{M}}, \hat{\boldsymbol{u}}^\mu) = \int_\Omega \left[\psi_\square(\hat{\boldsymbol{u}}^{\mathrm{M}} + \hat{\boldsymbol{u}}^\mu) - l_\square(\hat{\boldsymbol{u}}^{\mathrm{M}} + \hat{\boldsymbol{u}}^\mu)\right] \mathrm{d}\Omega - \int_{\Gamma_{\mathrm{N}}} \boldsymbol{t}_{\mathrm{p}} \cdot \hat{\boldsymbol{u}}^{\mathrm{M}} \, \mathrm{d}\Gamma \tag{8.12}$$ {eq:6-14}

where we introduced the RVE-functionals {eq:6-15}

$$\psi_\square(\hat{\boldsymbol{u}}) \stackrel{\text{def}}{=} \langle \psi(\boldsymbol{\epsilon}[\hat{\boldsymbol{u}}]) \rangle_\square, \tag{8.13a}$$ {eq:6-15a}

$$l_\square(\hat{\boldsymbol{u}}) \stackrel{\text{def}}{=} \langle \boldsymbol{b} \cdot \hat{\boldsymbol{u}} \rangle_\square \tag{8.13b}$$ {eq:6-15b}

The minimization problem (8.5) is replaced by

$$\inf_{\hat{\boldsymbol{u}}^{\mathrm{M}} \in \mathbb{U}^{\mathrm{M}}} \inf_{\hat{\boldsymbol{u}}^\mu \in \mathbb{U}^\mu} \Pi(\hat{\boldsymbol{u}}^{\mathrm{M}}, \hat{\boldsymbol{u}}^\mu) \tag{8.14}$$ {eq:6-16}

[1]Subsequently, we use the concept of a "running average" in the classical fashion for homogenization; however, this far it is merely a matter of convenient notation.

[2]The precise definition of the "center" will be given later.

[3]For brevity, the same notation Π is used.

whose stationary condition is the two independent (global) problems of finding $\boldsymbol{u}^{\mathrm{M}} \in \mathbb{U}^{\mathrm{M}}$ and $\boldsymbol{u}^{\mu} \in \mathbb{U}^{\mu}$ that satisfy {eq:6-16}

$$\begin{aligned}\Pi'_{u^{\mathrm{M}}}(\boldsymbol{u}^{\mathrm{M}}, \boldsymbol{u}^{\mu}; \delta\boldsymbol{u}^{\mathrm{M}}) &= \int_{\Omega} \left[a_{\Box}(\boldsymbol{u}^{\mathrm{M}} + \boldsymbol{u}^{\mu}; \delta\boldsymbol{u}^{\mathrm{M}}) - l_{\Box}(\delta\boldsymbol{u}^{\mathrm{M}})\right] \,\mathrm{d}\Omega - \int_{\Gamma_{\mathrm{N}}} \boldsymbol{t}_{\mathrm{p}} \cdot \delta\boldsymbol{u}^{\mathrm{M}} \,\mathrm{d}\Gamma \\ &= 0 \quad \forall \delta\boldsymbol{u}^{\mathrm{M}} \in \mathbb{U}^{\mathrm{M},0}, \end{aligned} \tag{8.15a}$$ {eq:6-16a}

$$\begin{aligned}\Pi'_{u^{\mu}}(\boldsymbol{u}^{\mathrm{M}}, \boldsymbol{u}^{\mu}; \delta\boldsymbol{u}^{\mu}) &= \int_{\Omega} \left[a_{\Box}(\boldsymbol{u}^{\mathrm{M}} + \boldsymbol{u}^{\mu}; \delta\boldsymbol{u}^{\mu}) - l_{\Box}(\delta\boldsymbol{u}^{\mu})\right] \,\mathrm{d}\Omega \\ &= 0 \quad \forall \delta\boldsymbol{u}^{\mu} \in \mathbb{U}^{\mu} \end{aligned} \tag{8.15b}$$ {eq:6-16b}

where

{eq:6-17}
$$a_{\Box}(\boldsymbol{u}; \delta\boldsymbol{u}) \stackrel{\text{def}}{=} (\psi_{\Box})'_{u}(\boldsymbol{u}; \delta\boldsymbol{u}) = \langle \boldsymbol{\sigma}(\boldsymbol{\epsilon}[\boldsymbol{u}]) : \boldsymbol{\epsilon}[\delta\boldsymbol{u}] \rangle_{\Box} \tag{8.16}$$

8.2.4 Homogenization and prolongation operators – Uniqueness of decomposition

We introduce homogenization ??? and prolongation operators with the purpose to ensure a unique hierarchical additive decomposition of $\boldsymbol{u}$ into slowly varying (macroscale) and rapidly varying (fluctuation) components. A key feature of model-based homogenization (Note: not in discretization-based homogenization) is the possibility to ensure such uniqueness by "way of construction" upon introducing a "generating macrofield" $\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}$ and the pertinent surjective (onto) map defined by the *homogenization operator ????* $\mathcal{A}^*$

{eq:6-21}
$$\mathcal{A}^* : \ \mathbb{U} \to \bar{\mathbb{U}} \text{ (surjective)} \tag{8.17}$$

Remark 7 *It is clear that the regularity requirements on $\bar{\mathbb{U}}$ may be entirely different than those of $\mathbb{U}$, and that the pertinent requirements depend on the properties of $\mathcal{A}^*$.*

We also define, in an implicit fashion, the set $\mathbb{U}^{\mathrm{M}} \subset \mathbb{U}$ via the choice of a bijective map defined by the *prolongation operator* $\mathcal{A}$

{eq:6-22}
$$\mathcal{A} : \ \bar{\mathbb{U}} \to \mathbb{U}^{\mathrm{M}} \text{ (bijective)} \tag{8.18}$$

and we require that the operators satisfy the condition $\mathcal{A}^*\mathcal{A} = \mathcal{I}$ (while $\mathcal{A}\mathcal{A}^* \neq \mathcal{I}$), where $\mathcal{I}$ denotes the identity operator on $\bar{\mathbb{U}}$. Finally, the set of microscale (or fluctuation) functions is defined as

{eq:6-23}
$$\mathbb{U}^{\mu} := \{\boldsymbol{v} \in \mathbb{U} : \ \mathcal{A}^*\boldsymbol{v} = \boldsymbol{0}\} \tag{8.19}$$

{eq:6-24} **Lemma 1**: Any function $\boldsymbol{u} \in \mathbb{U}$ can be decomposed additively as $\boldsymbol{u} = \boldsymbol{u}^{\mathrm{M}} + \boldsymbol{u}^{\mu}$ with

{eq:6-24a}
$$\mathbb{U}^{\mathrm{M}} \ni \boldsymbol{u}^{\mathrm{M}} \stackrel{\text{def}}{=} \mathcal{A}\mathcal{A}^*\boldsymbol{u} \tag{8.20a}$$

{eq:6-24b}
$$\mathbb{U}^{\mu} \ni \boldsymbol{u}^{\mu} \stackrel{\text{def}}{=} [\mathcal{I} - \mathcal{A}\mathcal{A}^*]\boldsymbol{u} \tag{8.20b}$$

where $\mathcal{I}$ is (here) the identity operator on $\mathbb{U}$.
Proof: Since range$\{\mathcal{A}\} = \mathbb{U}$, range$\{\mathcal{A}^*\} = \bar{\mathbb{U}}$, $\mathcal{A}$ is defined on range$\{\mathcal{A}^*\}$ and $\mathcal{A}^*$ is defined on $\mathbb{U}$, we note that the operator $\mathcal{A}\mathcal{A}^*$ maps from $\mathbb{U} \to \mathbb{U}$. Hence, the operators trivially satisfy the identity **????** Next, we consider $\boldsymbol{u}^{\mathrm{M}}$ and $\boldsymbol{u}^{\mu}$ constructed in (8.20a) and (8.20b), respectively.

We first conclude that $\boldsymbol{u}^{\mathrm{M}} \in \mathbb{U}^{\mathrm{M}}$ since range$\{\mathcal{A}\} = \mathbb{U}^{\mathrm{M}}$. Finally, we may show that $\boldsymbol{u}^{\mu} \in \mathbb{U}^{\mu}$ with $\mathbb{U}^{\mu}$ defined in (8.19). Indeed, since $\boldsymbol{u}^{\mu} \in \mathbb{U}$, we have

$$\mathcal{A}^*\boldsymbol{u}^{\mu} = \mathcal{A}^*\left[\mathcal{I} - \mathcal{A}\mathcal{A}^*\right]\boldsymbol{u} = \left[\mathcal{A}^* - \underbrace{\mathcal{A}^*\mathcal{A}}_{=\mathcal{I}}\mathcal{A}^*\right]\boldsymbol{u} = \boldsymbol{0}$$

where it was used that $\mathcal{A}^*\mathcal{A} = \mathcal{I}$. □

Lemma 2: The homogenization operator $\mathcal{A}^*$ is a bijective map on $\mathbb{U}^{\mathrm{M}}$, i.e.

$$\mathcal{A}^*|_{\mathbb{U}^{\mathrm{M}}} : \ \mathbb{U}^{\mathrm{M}} \to \bar{\mathbb{U}} \text{ (bijective)} \tag{8.21}$$ {eq:6-25}

Proof: Since range$\{\mathcal{A}\} = \mathbb{U}^{\mathrm{M}}$, we obtain $\mathcal{I} = \mathcal{A}^*\mathcal{A} = \mathcal{A}^*|_{\mathbb{U}^{\mathrm{M}}}\mathcal{A}$, and using the fact that $\mathcal{A}$ is bijective, we conclude that, indeed, $\mathcal{A}^*|_{\mathbb{U}^{\mathrm{M}}} = \mathcal{A}^{-1}$ is a bijective operator. □

Theorem 1: The set $\mathbb{U}^{\mu}$ defined in (**??**) is the hierarchical complement to $\mathbb{U}^{\mathrm{M}}$, i.e. $\mathbb{U} = \mathbb{U}^{\mathrm{M}} \oplus \mathbb{U}^{\mu}$. In other words, it holds that

$$\mathbb{U} = \mathbb{U}^{\mathrm{M}} \oplus \mathbb{U}^{\mu} \text{ and } \mathbb{U}^{\mathrm{M}} \cap \mathbb{U}^{\mu} = \{\boldsymbol{0}\} \tag{8.22}$$ {eq:6-26}

Proof: From Lemma 1 follows that any function in $\mathbb{U}$ can be written as the sum of two functions, one in $\mathbb{U}^{\mathrm{M}}$ and the other in $\mathbb{U}^{\mu}$. Furthermore, since $\mathbb{U}^{\mathrm{M}} \subset \mathbb{U}$ and $\mathbb{U}^{\mu} \subset \mathbb{U}$, the sum must be in $\mathbb{U}$. Hence, we conclude that $\mathbb{U}^{\mathrm{M}} \cup \mathbb{U}^{\mu} = \mathbb{U}$. Next we consider the issue of uniqueness: To this end, consider any function $\boldsymbol{u}^{\mathrm{M}} \in \mathbb{U}^{\mathrm{M}}$. Since $\mathcal{A}^*|_{\mathbb{U}^{\mathrm{M}}}$ is linear and bijective, cf. Lemma 2, the condition that must be fullfilled for $\boldsymbol{u}^{\mathrm{M}}$ being an element of $\mathbb{U}^{\mu}$ as well can be expressed as

$$\mathcal{A}^*\boldsymbol{u}^{\mathrm{M}} = \mathcal{A}^*|_{\mathbb{U}^{\mathrm{M}}}\boldsymbol{u}^{\mathrm{M}} = \boldsymbol{0} \ \Leftrightarrow \ \boldsymbol{u}^{\mathrm{M}} = \boldsymbol{0}$$

Hence, if $\boldsymbol{u}^{\mathrm{M}} \in \mathbb{U}^{\mathrm{M}} \cap \mathbb{U}^{\mu}$ then $\boldsymbol{u}^{\mathrm{M}} = \boldsymbol{0}$, which completes the proof. □

8.2.5 The generating macrofield – Separation of scales

The assumption of *separation of scales* is implicitly introduced via the particular definition of the prolongation operator $\mathcal{A}$ within each subdomain $\Omega_\Box$. More specifically, the two-scale function $\boldsymbol{u}^{\mathrm{M}}(\bar{\boldsymbol{x}}, \boldsymbol{x})$ for $(\bar{\boldsymbol{x}}, \boldsymbol{x}) \in \Omega \times \Omega_\Box(\bar{\boldsymbol{x}})$, is constructed via the prolongation of a generating macrofield $\bar{\boldsymbol{u}}$ via a Taylor series expansion of $\bar{\boldsymbol{u}}$ within $\Omega_\Box$ to a suitable order (of homogenization). *The standard situation of 1st order homogenization is discussed in detail below.* More formally, the operators $\mathcal{A}$ and $\mathcal{A}^*$ are defined as the maps {eq:6-31}

$$\mathcal{A}(\bar{\boldsymbol{x}}) : \bar{\mathbb{U}} \to \mathbb{U}_\Box^{\mathrm{M}}(\bar{\boldsymbol{x}}) \tag{8.23a}$$ {eq:6-31a}

$$\mathcal{A}^*(\bar{\boldsymbol{x}}) : \mathbb{U}_\Box^{\mathrm{M}}(\bar{\boldsymbol{x}}) \to \bar{\mathbb{U}} \tag{8.23b}$$ {eq:6-31b}

where $\mathbb{U}_\Box^{\mathrm{M}}(\bar{\boldsymbol{x}}) = \mathbb{U}^{\mathrm{M}}|_{\Omega_\Box}$ is a local vector space (on the SVE).

Next, we interpret the functional dependence $\boldsymbol{u}^{\mu}\{\bar{\boldsymbol{u}}\}$[4] on each $\Omega_\Box$ in such a fashion that $\boldsymbol{u}^{\mu}$ depends implicitly on $\bar{\boldsymbol{u}}(\bar{\boldsymbol{x}}), [\bar{\boldsymbol{u}} \otimes \boldsymbol{\nabla}](\bar{\boldsymbol{x}})$ and, possibly, on higher order gradients of the field $\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}$ to the desired degree. In particular, this means that we may rephrase (8.15) as follows: Find the two independent (global) fields $\bar{\boldsymbol{u}}$ and $\boldsymbol{u}^{\mu}$ that satisfy {eq:6-32}

$$\int_\Omega \left[a_\Box(\mathcal{A}\bar{\boldsymbol{u}} + \boldsymbol{u}^{\mu}; \mathcal{A}\delta\bar{\boldsymbol{u}}) - l_\Box(\mathcal{A}\delta\bar{\boldsymbol{u}})\right] \mathrm{d}\Omega - \int_{\Gamma_{\mathrm{N}}} \boldsymbol{t}_{\mathrm{p}} \cdot \mathcal{A}\delta\bar{\boldsymbol{u}}\, \mathrm{d}\Gamma = 0 \quad \forall \delta\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}^0 \tag{8.24a}$$ {eq:6-32a}

$$\int_\Omega \left[a_\Box(\mathcal{A}\bar{\boldsymbol{u}} + \boldsymbol{u}^{\mu}; \delta\boldsymbol{u}^{\mu}) - l_\Box(\delta\boldsymbol{u}^{\mu})\right] \mathrm{d}\Omega = 0 \quad \forall \delta\boldsymbol{u}^{\mu} \in \mathbb{U}^{\mu} \tag{8.24b}$$ {eq:6-32b}

[4]Brackets indicate implicit function.

$$
\begin{tikzcd}
\min\limits_{\boldsymbol{u}} \Pi(\boldsymbol{u}) \arrow[r, "\text{(I)}", "\text{stat}"'] \arrow[d, "\text{VCMH}"', "\text{(II)}"] & \Pi'(\boldsymbol{u};\delta\boldsymbol{u}) = 0 \quad \forall\delta\boldsymbol{u} \arrow[d, "\text{VCMH}"', "\text{(I)}"] \\
\min\limits_{\bar{\boldsymbol{u}}} \bar{\Pi}\{\bar{\boldsymbol{u}}\} \arrow[r, "\text{(II)}", "\text{stat+VCMH}"'] & \bar{\Pi}'\{\bar{\boldsymbol{u}};\delta\bar{\boldsymbol{u}}\} = \bar{R}\{\bar{\boldsymbol{u}};\delta\bar{\boldsymbol{u}}\} = 0 \quad \forall\delta\bar{\boldsymbol{u}}
\end{tikzcd}
$$

{figure:6-4} Figure 8.3: The role of VCMH-condition in computational homogenization

In particular, the "homogenized" relation (8.24a), exploiting $\delta\boldsymbol{u}^{\mathrm{M}} = \mathcal{A}\delta\bar{\boldsymbol{u}}$ as the homogenizer, defines *Variationally Consistent Homogenization* (VCH), and its solution $\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}$ represents a smoother field that does $\boldsymbol{u} \in \mathbb{U}$.

To construct $\boldsymbol{u}^\mu \in \mathbb{U}^\mu_\square \overset{\text{def}}{=} \mathbb{U}^\mu|_{\Omega_\square}$ that inherently satisfies the constraint relations $\mathcal{A}^*\boldsymbol{u}^\mu = \mathbf{0}$ may turn out as a quite difficult task in practice. A possible strategy would then be to

- (i) opt for a larger space by relaxing the requirements on $\mathbb{U}^\mu_\square$ in terms of the conditions $\mathcal{A}^*\boldsymbol{u}^\mu = \mathbf{0}$ (or at least a subset of them) and to
- (ii) satisfy the said conditions $\mathcal{A}^*\boldsymbol{u}^\mu = \mathbf{0}$ (or at least a subset of them) in a weak sense as additional constraint conditions using Lagrangian multipliers.

This is the strategy used henceforth, cf. **Subsection ????** , where it is shown that the assumption of (weakly) periodic fluctuations $\boldsymbol{u}^\mu$ on each RVE serves precisely this purpose. In fact, such weak periodicity has been exploited extensively (in the context of 1st order homogenization) by the authors, cf. Larsson et al. **?**, and it will be introduced as a "workhouse" subsequently in order to formulate a "closed", i.e. solvable, RVE-problem on each domain $\Omega_\square$.

In conclusion, the pertinent "localized" RVE-problems replace the global weak form (8.24b). Obviously, it is convenient in practice to establish these local RVE-problems only in the macroscale quadrature points in the FE^2-setting. This means that the equations in (8.24) represent a (nested) two-scale problem that must be solved by some type of iteration method.

8.2.6 The role of a Variationally Consistent Macrohomogeneity Condition (VCMH-condition)

As shown in Figure 8.3, it is possible to take the fine-scale minimization problem as the point of departure and eventually end up with the macroscale equation (8.24a). However, this result can be achieved in two different ways, corresponding to path (I) or path (II) in Figure 8.3.

Path I: *Evaluate the stationarity condition associated with the fine-scale problem and apply the VCH-strategy.* Start from (8.12) and derive the stationarity condition (8.15) for the fine-scale problem. Then, apply the VCH-strategy that gives (8.24a), i.e.

{eq:6-35}

$$
\begin{aligned}
\bar{R}\{\bar{\boldsymbol{u}};\delta\bar{\boldsymbol{u}}\} &\overset{\text{def}}{=} \Pi'_{u^{\mathrm{M}}}(\mathcal{A}\bar{\boldsymbol{u}}, \boldsymbol{u}^\mu\{\bar{\boldsymbol{u}}\}; \mathcal{A}\delta\bar{\boldsymbol{u}}) \\
&= \int_\Omega \left[a_\square(\mathcal{A}\bar{\boldsymbol{u}} + \boldsymbol{u}^\mu\{\bar{\boldsymbol{u}}\}; \mathcal{A}\delta\bar{\boldsymbol{u}}) - l_\square(\mathcal{A}\delta\bar{\boldsymbol{u}})\right] \mathrm{d}\Omega - \int_{\Gamma_{\mathrm{N}}} \boldsymbol{t}_{\mathrm{p}} \cdot \mathcal{A}\delta\bar{\boldsymbol{u}}\, \mathrm{d}\Gamma \\
&= 0 \quad \forall\delta\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}^0
\end{aligned}
\tag{8.25}
$$

Path II. *Apply the VCH-strategy to the fine-scale potential and evaluate the stationarity condition.* Start from (8.12), apply the VCH-strategy to arrive at the macroscale potential

$$\bar{\Pi}\{\hat{\bar{\boldsymbol{u}}}\} \stackrel{\text{def}}{=} \Pi(\mathcal{A}\hat{\bar{\boldsymbol{u}}}, \boldsymbol{u}^\mu\{\hat{\bar{\boldsymbol{u}}}\}) \tag{8.26}$$ {eq:6-36}

and consider the problem

$$\inf_{\hat{\bar{\boldsymbol{u}}}\in\bar{\mathbb{U}}} \bar{\Pi}\{\hat{\bar{\boldsymbol{u}}}\}. \tag{8.27}$$ {eq:6-37}

The corresponding stationarity condition is

$$\bar{\Pi}'\{\bar{\boldsymbol{u}}; \delta\bar{\boldsymbol{u}}\} = 0 \quad \forall \delta\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}^0 \tag{8.28}$$ {eq:6-38}

Now, the key question is whether this condition is satisfied by the same solution $\bar{\boldsymbol{u}}$ as that of (8.25). To establish the condition that must be satisfied for such an identity to hold true, we first note that $\bar{\Pi}'$ can be expanded as

$$\begin{aligned}\bar{\Pi}'\{\bar{\boldsymbol{u}}; \delta\bar{\boldsymbol{u}}\} \quad = \quad & \underbrace{\Pi'_{u^{\mathrm{M}}}(\mathcal{A}\bar{\boldsymbol{u}}, \boldsymbol{u}^\mu\{\bar{\boldsymbol{u}}\}; \mathcal{A}\delta\bar{\boldsymbol{u}})}_{=0 \text{ from } (8.25)} \\ & + \Pi'_{u^\mu}(\mathcal{A}\bar{\boldsymbol{u}}, \boldsymbol{u}^\mu\{\bar{\boldsymbol{u}}\}; \underbrace{(\boldsymbol{u}^\mu)'\{\bar{\boldsymbol{u}}, \delta\bar{\boldsymbol{u}}\}}_{=\mathcal{S}\delta\bar{\boldsymbol{u}}})\end{aligned} \tag{8.29}$$ {eq:6-39}

where a sensitivity (linear operator) $\mathcal{S}$ is defined as a directional derivative, i. e. $\mathcal{S}\delta\bar{\boldsymbol{u}} = (\boldsymbol{u}^\mu)'\{\bar{\boldsymbol{u}}; \delta\bar{\boldsymbol{u}}\} \stackrel{\text{def}}{=} \frac{\mathrm{d}}{\mathrm{d}\epsilon}\boldsymbol{u}^\mu\{\bar{\boldsymbol{u}} + \epsilon\delta\bar{\boldsymbol{u}}\}|_{\epsilon=0}$. In order that $\bar{\Pi}$ is stationary at the global solution $\bar{\boldsymbol{u}}$, we must obviously require that

$$\Pi'_{u^\mu}(\mathcal{A}\bar{\boldsymbol{u}}, \boldsymbol{u}^\mu\{\bar{\boldsymbol{u}}\}; \mathcal{S}\delta\bar{\boldsymbol{u}}) = 0 \quad \forall \delta\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}^0 \tag{8.30}$$ {eq:6-41}

Upon localizing (8.30) to each RVE, we obtain the sufficient (localized or stronger) condition

$$a_\square(\mathcal{A}\bar{\boldsymbol{u}} + \boldsymbol{u}^\mu\{\bar{\boldsymbol{u}}\}; \mathcal{S}\delta\bar{\boldsymbol{u}}) - l_\square(\mathcal{S}\delta\bar{\boldsymbol{u}}) = 0 \quad \forall \delta\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}^0 \tag{8.31}$$ {eq:6-42}

or, equivalently,

$$\begin{aligned}& a_\square(\mathcal{A}\bar{\boldsymbol{u}} + \boldsymbol{u}^\mu\{\bar{\boldsymbol{u}}\}; \mathcal{A}\delta\bar{\boldsymbol{u}} + \mathcal{S}\delta\bar{\boldsymbol{u}}) - a_\square(\mathcal{A}\bar{\boldsymbol{u}} + \boldsymbol{u}^\mu\{\bar{\boldsymbol{u}}\}; \mathcal{A}\delta\bar{\boldsymbol{u}}) \\ &= l_\square(\mathcal{A}\delta\bar{\boldsymbol{u}} + \mathcal{S}\delta\bar{\boldsymbol{u}}) - l_\square(\mathcal{A}\delta\bar{\boldsymbol{u}}) \quad \forall \delta\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}^0\end{aligned} \tag{8.32}$$ {eq:6-43}

The identity in (8.31) or (8.32) is coined the (local version of the) *Variationally Consistent Macrohomogeneity Condition* (abbreviated VCMH-condition henceforth). It is commonly known as the Hill-Mandel condition in the context of stress problems[5]; however, it can readily be generalized to other classes of problems, cf. examples below.

Remark 8 *Upon introducing the identity (by way of notation)* $\mathrm{d}\boldsymbol{u} = \mathcal{A}\,\mathrm{d}\bar{\boldsymbol{u}} + \mathcal{S}\,\mathrm{d}\bar{\boldsymbol{u}}$ *for given* $\mathrm{d}\bar{\boldsymbol{u}}$*, we may rewrite (8.32) in the more explicit fashion as follows:*

$$\langle \boldsymbol{\sigma} : \boldsymbol{\epsilon}[\mathcal{S}\,\mathrm{d}\bar{\boldsymbol{u}}]\rangle_\square - \langle \boldsymbol{b} \cdot \mathcal{S}\,\mathrm{d}\bar{\boldsymbol{u}}\rangle_\square = 0 \quad \forall \delta\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}^0 \tag{8.33}$$ {eq:6-543}

where it is recalled that $\boldsymbol{\sigma} = \boldsymbol{\sigma}(\boldsymbol{\epsilon}[\mathcal{A}\bar{\boldsymbol{u}} + \boldsymbol{u}^\mu\{\bar{\boldsymbol{u}}\}])$*. Moreover, upon using the weak form of equilibrium, we first note the trivial relation*

$$\int_{\Omega_\square} \boldsymbol{\sigma} : \boldsymbol{\epsilon}[\mathcal{S}\,\mathrm{d}\bar{\boldsymbol{u}}]\,\mathrm{d}\Omega - \int_{\Omega_\square} \boldsymbol{b} \cdot \mathcal{S}\,\mathrm{d}\bar{\boldsymbol{u}}\,\mathrm{d}\Omega - \int_{\Gamma_\square} \boldsymbol{t} \cdot \mathcal{S}\,\mathrm{d}\bar{\boldsymbol{u}}\,\mathrm{d}\Gamma = 0 \quad \forall \delta\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}^0 \tag{8.34}$$ {eq:6-144}

[5] The classical assumption is $l_\square(\mathcal{S}\delta\bar{\boldsymbol{u}}) = 0$.

which can be combined with (8.33) to yield the relation

$$\frac{1}{|\Omega_\square|}\int_{\Gamma_\square} \boldsymbol{t}\cdot\mathcal{S}\,\mathrm{d}\bar{\boldsymbol{u}}\,\mathrm{d}\Gamma = 0 \quad \forall\delta\bar{\boldsymbol{u}}\in\bar{\mathbb{U}}^0 \tag{8.35}$$ {eq:6-545}

However, we have the closure condition

$$\langle\boldsymbol{\epsilon}[\mathcal{S}\,\mathrm{d}\bar{\boldsymbol{u}}]\rangle_\square = 0 \quad\Rightarrow\quad \bar{\boldsymbol{\sigma}}:\langle\boldsymbol{\epsilon}[\mathcal{S}\,\mathrm{d}\bar{\boldsymbol{u}}]\rangle_\square = 0 \tag{8.36}$$ {eq:6-146}

for any $\bar{\boldsymbol{\sigma}}\in\mathbb{R}^{3\times3}_{sym}$, and we may use Gauss' theorem to obtain

{eq:6-146}
$$\frac{1}{|\Omega_\square|}\int_{\Gamma_\square}[\bar{\boldsymbol{\sigma}}\cdot\boldsymbol{n}]\cdot[\mathcal{S}\,\mathrm{d}\bar{\boldsymbol{u}}]\,\mathrm{d}\Gamma = 0 \tag{8.37}$$

Combining the results in (8.35) *and* (8.37)*, we finally obtain the alternative formulation of the VCMH-condition*

{eq:6-147}
$$\frac{1}{|\Omega_\square|}\int_{\Gamma_\square}[\boldsymbol{t}-\bar{\boldsymbol{\sigma}}\cdot\boldsymbol{n}]\cdot[\,\mathrm{d}\boldsymbol{u}-\mathcal{A}\,\mathrm{d}\bar{\boldsymbol{u}}]\,\mathrm{d}\Gamma = 0 \quad \forall\delta\bar{\boldsymbol{u}}\in\bar{\mathbb{U}}^0,\quad \bar{\boldsymbol{\sigma}}\in\mathbb{R}^{3\times3}_{sym} \tag{8.38}$$

□

When/if the VCMH-condition is satisfied, it is also guaranteed that the global tangent stiffness operator is symmetrical. In other words,

{eq:6-44}
$$\bar{\Pi}''_{\bar{u}\bar{u}}\{\bar{\boldsymbol{u}};\delta\bar{\boldsymbol{u}}_1,\delta\bar{\boldsymbol{u}}_2\} = \bar{\Pi}''_{\bar{u}\bar{u}}\{\bar{\boldsymbol{u}};\delta\bar{\boldsymbol{u}}_2,\delta\bar{\boldsymbol{u}}_1\} \quad \forall\delta\bar{\boldsymbol{u}}_1,\delta\bar{\boldsymbol{u}}_2\in\bar{\mathbb{U}}^0 \tag{8.39}$$

which is shown as follows: From the expansion of $\bar{\Pi}'_{\bar{u}}\{\bar{\boldsymbol{u}};\delta\bar{\boldsymbol{u}}_1\}$ in (**??**), we may carry out the second variation to obtain

{eq:6-45}
$$\begin{aligned}
\bar{\Pi}''_{\bar{u}\bar{u}}\{\bar{\boldsymbol{u}};\delta\bar{\boldsymbol{u}}_1,\delta\bar{\boldsymbol{u}}_2\} &\stackrel{\text{def}}{=} \Pi''_{u^{\mathrm{M}}u^{\mathrm{M}}}(\mathcal{A}\bar{\boldsymbol{u}},\boldsymbol{u}^\mu\{\bar{\boldsymbol{u}}\};\mathcal{A}\delta\bar{\boldsymbol{u}}_1,\mathcal{A}\delta\bar{\boldsymbol{u}}_2)\\
&\quad+\Pi''_{u^{\mathrm{M}}u^{\mu}}(\mathcal{A}\bar{\boldsymbol{u}},\boldsymbol{u}^\mu\{\bar{\boldsymbol{u}}\};\mathcal{A}\delta\bar{\boldsymbol{u}}_1,\mathcal{S}\delta\bar{\boldsymbol{u}}_2)+\Pi''_{u^{\mu}u^{\mathrm{M}}}(\mathcal{A}\bar{\boldsymbol{u}},\boldsymbol{u}^\mu\{\bar{\boldsymbol{u}}\};\mathcal{S}\delta\bar{\boldsymbol{u}}_1,\mathcal{A}\delta\bar{\boldsymbol{u}}_2)\\
&\quad+\Pi''_{u^{\mu}u^{\mu}}(\mathcal{A}\bar{\boldsymbol{u}},\boldsymbol{u}^\mu\{\bar{\boldsymbol{u}}\};\mathcal{S}\delta\bar{\boldsymbol{u}}_1,\mathcal{S}\delta\bar{\boldsymbol{u}}_2)\\
&= \int_\Omega(\psi_\square)''_{uu}(\mathcal{A}\bar{\boldsymbol{u}}+\boldsymbol{u}^\mu\{\bar{\boldsymbol{u}}\};\mathcal{S}^{\mathrm{tot}}\delta\bar{\boldsymbol{u}}_1,\mathcal{S}^{\mathrm{tot}}\delta\bar{\boldsymbol{u}}_2)\,\mathrm{d}\Omega\\
&= \int_\Omega\langle\boldsymbol{\epsilon}[\mathcal{S}^{\mathrm{tot}}\delta\bar{\boldsymbol{u}}_1]:\mathbf{E}_{\mathrm{T}}:\boldsymbol{\epsilon}[\mathcal{S}^{\mathrm{tot}}\delta\bar{\boldsymbol{u}}_2]\rangle_\square\,\mathrm{d}\Omega \quad \forall\delta\bar{\boldsymbol{u}}_1,\delta\bar{\boldsymbol{u}}_2\in\bar{\mathbb{U}}^0
\end{aligned} \tag{8.40}$$

where we introduced the "total sensitivity operator" $\mathcal{S}^{\mathrm{tot}}\stackrel{\text{def}}{=}\mathcal{A}+\mathcal{S}$, and where it was used that

{eq:6-46}
$$(\psi_\square)''_{uu}(\boldsymbol{u};\delta\boldsymbol{u}_1,\delta\boldsymbol{u}_2) = (a_\square)'_u(\boldsymbol{u};\delta\boldsymbol{u}_1,\delta\boldsymbol{u}_2) = \langle\boldsymbol{\epsilon}[\delta\boldsymbol{u}_1]:\mathbf{E}_{\mathrm{T}}(\boldsymbol{\epsilon}[\boldsymbol{u}]):\boldsymbol{\epsilon}[\delta\boldsymbol{u}_2]\rangle_\square \tag{8.41}$$

and $\mathbf{E}_{\mathrm{T}}$, defined via the relation $\mathrm{d}\boldsymbol{\sigma}=\mathbf{E}_{\mathrm{T}}:\,\mathrm{d}\boldsymbol{\epsilon}$, is the local tangent stiffness tensor that possesses major (as well as minor) symmetry in standard fashion.

This symmetry property corresponds to the classical notion of "symmetric VMS", cf. Larson **?**, and can be interpreted as a "Galerkin property". Indeed, whenever the fine-scale problem is self-adjoint (like the present model problem of nonlinear elasticity), it is reasonable to expect that the resulting homogenized problem is self-adjoint as well.

Remark 9 *There is no need to compute the sensitivity $\mathcal{S}$ explicitly for the single purpose of showing that MH-condition is valid; it is rather sufficient to merely note that it exists (which is shown subsequently in the context of weakly periodic boundary conditions). However, in order to compute the macroscale tangent operator defined implicitly in (??), we do indeed require the computation of $\mathcal{S}$. This is conveniently done only after specifying the operator $\mathcal{A}$ that defines the "order of homogenization".*

Remark 10 *The more general situation is that no potential Π can be constructed. In such a case the basic homogenization problem format is still that given in (??):*

{eq:6-47} $$\bar{R}(\bar{\boldsymbol{u}};\delta\bar{\boldsymbol{u}}) \overset{\text{def}}{=} \int_{\Omega} [a_{\square}(\mathcal{A}\bar{\boldsymbol{u}} + \boldsymbol{u}^{\mu}\{\bar{\boldsymbol{u}}\}; \mathcal{A}\delta\bar{\boldsymbol{u}}) - l_{\square}(\mathcal{A}\delta\bar{\boldsymbol{u}})]\, \mathrm{d}\Omega - \int_{\Gamma_N} \boldsymbol{t}_p \cdot \mathcal{A}\delta\bar{\boldsymbol{u}}\, \mathrm{d}\Gamma = 0 \quad \forall \delta\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}^0 \quad (8.42)$$

where $\boldsymbol{u}^{\mu}\{\bar{\boldsymbol{u}}\}$ is the solution of the RVE-problem. Since no energy density $\psi_{\square}$ exists, (??) is replaced by

$$a_{\square}(\boldsymbol{u};\delta\boldsymbol{u}) \overset{\text{def}}{=} \langle \boldsymbol{\sigma}(\boldsymbol{\epsilon}[\boldsymbol{u}]) : \boldsymbol{\epsilon}[\delta\boldsymbol{u}]\rangle_{\square} \quad (8.43)$$ {eq:6-48}

In this more general case, the VCMH-condition in (??) obviously does not follow from "symmetry arguments"; however, it may still be adopted for convenience although the theoretical justification is much weaker than in the restricted case when a potential does exist. Obviously, even if the VCMH-condition is satisfied, symmetry of the macroscale tangent operator can not be expected due to (possible) lack of major symmetry of the local tangent $\mathbf{E}_{\mathrm{T}}$.

8.2.7 1st order homogenization – Standard macroscale model

In the standard case of 1st order homogenization, $\bar{\boldsymbol{u}}$ is prolonged via assumed linear variation of $\boldsymbol{u}^{\mathrm{M}}$ within each RVE:

$$\boldsymbol{u}^{\mathrm{M}}(\bar{\boldsymbol{x}},\boldsymbol{x}) = (\mathcal{A}\bar{\boldsymbol{u}})(\bar{\boldsymbol{x}},\boldsymbol{x}) := \bar{\boldsymbol{u}}(\bar{\boldsymbol{x}}) + \bar{\boldsymbol{h}}(\bar{\boldsymbol{x}}) \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}] \text{ for } \boldsymbol{x} \in \Omega_{\square} \quad (8.44)$$ {eq:6-51}

where $\bar{\boldsymbol{h}} \overset{\text{def}}{=} \bar{\boldsymbol{u}} \otimes \boldsymbol{\nabla}$ is the macroscale displacement gradient, and where $\bar{\boldsymbol{x}}$ is the *volume average*

$$\bar{\boldsymbol{x}} \overset{\text{def}}{=} \langle \boldsymbol{x}\rangle_{\square} \Leftrightarrow \quad \int_{\Omega_{\square}} [\boldsymbol{x} - \bar{\boldsymbol{x}}]\, \mathrm{d}\Omega = \boldsymbol{0} \quad (8.45)$$ {eq:6-52}

Remark 11 *As an alternative it would be possible to assume that $\bar{\boldsymbol{x}}$ represents the surface average on the RVE. The chosen definition is crucial in the sense that it pertains to the definition of the operator $\mathcal{A}^*$ (as defined below). See also the discussion below as regards non-corrupted fine-scale problems within the RVE.*

Next, we construct the operator $\mathcal{A}^*$ such that, for any given $\hat{\boldsymbol{u}} \in$???, it is represented by the functionals $\bar{\boldsymbol{\mathcal{U}}}_{\square}(\hat{\boldsymbol{u}})$ and $\bar{\boldsymbol{\mathcal{H}}}_{\square}(\hat{\boldsymbol{u}})$ defined as {eq:6-53}

$$\bar{\boldsymbol{\mathcal{U}}}_{\square}(\hat{\boldsymbol{u}}) \overset{\text{def}}{=} \langle \hat{\boldsymbol{u}}\rangle_{\square} \quad (8.46a)$$ {eq:6-53a}

$$\bar{\boldsymbol{\mathcal{H}}}_{\square}(\hat{\boldsymbol{u}}) \overset{\text{def}}{=} \frac{1}{|\Omega_{\square}|} \int_{\Gamma_{\square}} \hat{\boldsymbol{u}} \otimes \boldsymbol{n}\, \mathrm{d}\Gamma \quad (8.46b)$$ {eq:6-53b}

It can readily be checked that, upon choosing $\hat{\boldsymbol{u}} = \boldsymbol{u}^{\mathrm{M}}$ as defined in (8.44), the "RVE-prolongation functionals" take the values

$$\bar{\boldsymbol{\mathcal{U}}}_{\square}(\boldsymbol{u}^{\mathrm{M}}\} = \bar{\boldsymbol{u}}, \quad \bar{\boldsymbol{\mathcal{H}}}_{\square}(\boldsymbol{u}^{\mathrm{M}}) = \bar{\boldsymbol{h}} \quad (8.47)$$ {eq:6-54}

Figure 8.4: Local problem for RVE based on microperiodicity. (a) Image and mirror boundaries $\Gamma_\square^+$ and $\Gamma_\square^-$. (b) Lagrange multiplier field on $\Gamma_\square^+$. {figure:6-5}

whereby we have shown that the relation $\mathcal{A}^*\mathcal{A} = \mathcal{I}d$ holds. Finally, we are in the position to define the subscale function space

$$\mathbb{U}_\square^\mu = \{\boldsymbol{u}' \text{ sufficiently regular} : \; \bar{\boldsymbol{\mathcal{U}}}_\square(\boldsymbol{u}') = \boldsymbol{0}, \; \bar{\boldsymbol{\mathcal{H}}}_\square(\boldsymbol{u}') = \boldsymbol{0}\} \tag{8.48}$$ {eq:6-55}

Homogenized quantities are obtained from testing (8.42) with $\mathcal{A}\delta\bar{\boldsymbol{u}} = \delta\bar{\boldsymbol{u}} + \delta\bar{\boldsymbol{h}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}]$, whereby the homogenized problem (weak format) in (8.42) becomes: Find $\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}$ s.t.

{eq:6-56}
$$\int_\Omega \bar{\boldsymbol{\sigma}}\{\bar{\boldsymbol{u}}\} : [\delta\bar{\boldsymbol{u}} \otimes \boldsymbol{\nabla}] \, \mathrm{d}\Omega = \int_\Omega \left[\bar{\boldsymbol{b}} \cdot \delta\bar{\boldsymbol{u}} + \bar{\boldsymbol{b}}^{(2)} : [\delta\bar{\boldsymbol{u}} \otimes \boldsymbol{\nabla}]\right] \, \mathrm{d}\Omega + \int_{\Gamma_\mathrm{N}} \boldsymbol{t}_\mathrm{p} \cdot \delta\bar{\boldsymbol{u}} \, \mathrm{d}\Gamma \quad \forall \delta\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}^0 \tag{8.49}$$

where it was used that $[[\mathcal{A}\delta\bar{\boldsymbol{u}}] \otimes \boldsymbol{\nabla}](\bar{\boldsymbol{x}}) = \delta\bar{\boldsymbol{h}}(\bar{\boldsymbol{x}}) = [\delta\bar{\boldsymbol{u}} \otimes \boldsymbol{\nabla}](\bar{\boldsymbol{x}})$, and where we derived the
{eq:6-57} macroscale variables:

{eq:6-57a}
$$\bar{\boldsymbol{\sigma}}\{\bar{\boldsymbol{u}}\} \overset{\text{def}}{=} \langle \boldsymbol{\sigma}(\bar{\boldsymbol{\epsilon}} + \boldsymbol{\epsilon}[\boldsymbol{u}^\mu\{\bar{\boldsymbol{u}}\}]) \rangle_\square, \tag{8.50a}$$

{eq:6-57b}
$$\bar{\boldsymbol{b}} \overset{\text{def}}{=} \langle \boldsymbol{b} \rangle_\square, \tag{8.50b}$$

{eq:6-57c}
$$\bar{\boldsymbol{b}}^{(2)} \overset{\text{def}}{=} \langle \boldsymbol{b} \otimes [\boldsymbol{x} - \bar{\boldsymbol{x}}] \rangle_\square \tag{8.50c}$$

where $\bar{\boldsymbol{\epsilon}} \overset{\text{def}}{=} \bar{\boldsymbol{h}}^{\text{sym}}$. In particular, $\bar{\boldsymbol{\sigma}}$ is the macroscale (homogenized) stress. As to the external boundary, we tacitly assume that boundary conditions can be imposed in terms of prescribed displacement $\bar{\boldsymbol{u}}_\mathrm{p}$ and (possibly) in terms of prescribed traction $\bar{\boldsymbol{t}}_\mathrm{p}$. In fact the boundary term in (8.49) becomes this simple only if the traction is sufficiently smooth, thereby avoiding homogenization on the exterior boundary (in this text).

8.2.8 RVE-problem for weak periodicity

The global problem (8.24b) is replaced with "local" RVE-problems on each $\Omega_\square$, whose solution is $\boldsymbol{u}^\mu\{\bar{\boldsymbol{u}}\} \in \mathbb{U}_\square^\mu$. A viable possibility is to introduce the "model assumption" of micro-periodicity, illustrated in Figure **??**, which leads to the WPBC-problem that was discussed in the context of linear elasticity in Chapter and in the context of nonlinear material response in Chapter 4. The assumption of (weak) peridicity is natural since (i) it is standard choice for mathematical homogenization theory and (ii) this condition can be cast in a variational format that admits the Dirichlet (displacement) and Neumann (traction) boundary conditions to be obtained as special cases. Recall the bilinear form expressing weak periodicity: $d_\square(\boldsymbol{\lambda}, \boldsymbol{u})$

{eq:6-58}
$$d_\square(\boldsymbol{\lambda}, \boldsymbol{u}) \overset{\text{def}}{=} \frac{1}{|\Omega_\square|} \int_{\Gamma_\square^+} \boldsymbol{\lambda} \cdot [\![\boldsymbol{u}]\!]_\square \, \mathrm{d}\Gamma \tag{8.51}$$

where $\boldsymbol{\lambda}$ are Lagrangian multipliers (that play the role of tractions). The condition of (weakly) periodic fluctuations $\boldsymbol{u}^\mu$ can then be expressed as

{eq:6-59}
$$d_\square(\delta\boldsymbol{\lambda}, \boldsymbol{u}^\mu) = 0, \quad \forall \delta\boldsymbol{\lambda} \in \mathbb{T}_\square^+ \tag{8.52}$$

where $\mathbb{T}_\square = \mathbb{L}_2^+(\Gamma_\square^+)$. From micro-periodicity it follows immediately that $\bar{\boldsymbol{\mathcal{H}}}_\square(\boldsymbol{u}^\mu) = \boldsymbol{0}$, which can be shown by the choice $\delta\boldsymbol{\lambda} = \delta\bar{\boldsymbol{\sigma}} \cdot \boldsymbol{n}$ for arbitrary constant 2nd order tensor $\delta\bar{\boldsymbol{\sigma}}$ (need not be symmetrical). As a consequence, it is possible (and indeed convenient) to expand the trial space for the fluctuations as follows:

{eq:6-61}
$$\mathbb{U}^{\mu}_{\square} = \{\boldsymbol{u}' \text{ sufficiently regular} : \ \bar{\boldsymbol{\mathcal{U}}}_{\square}(\boldsymbol{u}') = \boldsymbol{0}\} \tag{8.53}$$

and include (8.52) in the explicit formulation of the pertinent weak form. The "sufficient" regularity properties are inherited from $\mathbb{U}^0$.

Remark 12 *It would be possible to satisfy* $\bar{\boldsymbol{\mathcal{U}}}_{\square}(\boldsymbol{u}^{\mu}) = \boldsymbol{0}$ *weakly, i.e.*

$$\delta\bar{\boldsymbol{\lambda}} \cdot \langle \boldsymbol{u}^{\mu} \rangle_{\square} = 0 \quad \forall \delta\bar{\boldsymbol{\lambda}} \in \mathbb{R}^3 \tag{8.54}$$ {eq:6-62}

whereby $\mathbb{U}^{\mu}_{\square}$ *would be further enlarged to*

$$\mathbb{U}^{\mu}_{\square} = \{\boldsymbol{u}' \textit{ sufficiently regular}\} \tag{8.55}$$ {eq:6-63}

However, this option is not used henceforth. $\square$

We are now in the position to state the RVE-problem as follows: For any given macroscale field $\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}$, compute $\boldsymbol{u}^{\mu}\{\bar{\boldsymbol{u}}\} \in \mathbb{U}^{\mu}_{\square}$ and $\boldsymbol{\lambda}\{\bar{\boldsymbol{u}}\} \in \mathbb{T}^{+}_{\square}$ that solve {eq:6-64}

$$a_{\square}(\mathcal{A}\bar{\boldsymbol{u}} + \boldsymbol{u}^{\mu}; \delta\boldsymbol{u}^{\mu}) - d_{\square}(\boldsymbol{\lambda}, \delta\boldsymbol{u}^{\mu}) = l_{\square}(\delta\boldsymbol{u}^{\mu}) \quad \forall \delta\boldsymbol{u}^{\mu} \in \mathbb{U}^{\mu}_{\square}, \tag{8.56a}$$ {eq:6-64a}

$$-d_{\square}(\delta\boldsymbol{\lambda}, \boldsymbol{u}^{\mu}) = 0 \qquad \forall \delta\boldsymbol{\lambda} \in \mathbb{T}^{+}_{\square}. \tag{8.56b}$$ {eq:6-64b}

Once again, this problem represents localization in the sense that the local approximations $\boldsymbol{u}^{\mu} \approx \boldsymbol{u}^{\mu}\{\bar{\boldsymbol{u}}\}$ and $\boldsymbol{\lambda} \approx \boldsymbol{\lambda}\{\bar{\boldsymbol{u}}\}$ are computed on each RVE independently for given $\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}$.

Solvability

In order to ensure that the system (8.56) is solvable, we observe the following:

- The kernel of $a_{\square}(\boldsymbol{u}; \delta\boldsymbol{u})$ consists only of rigid body motion, which is prevented by the definition of $\mathbb{U}^{\mu}_{\square}$ and by the auxiliary condition of micro-periodicity as expressed by $d_{\square}(\delta\boldsymbol{\lambda}, \boldsymbol{u}^{\mu}) = 0 \ \forall \delta\boldsymbol{\lambda} \in \mathbb{T}^{+}_{\square}$. We remark that, in particular, rigid body *rotation* is prevented by this auxiliary condition, since we enforce the total displacement gradient $\bar{\boldsymbol{h}}$ and not only its symmetric part $\bar{\boldsymbol{\epsilon}}$.
- Reaction forces will occur only on $\Gamma_{\square}$, whereby the fine-scale problem is "uncorrupted" in the interior of $\Omega_{\square}$. We remark that the commonly adopted choice $\bar{\boldsymbol{\mathcal{U}}}_{\square}(\boldsymbol{v}) \overset{\text{def}}{=} \langle \boldsymbol{v} \rangle_{\square}$ would result in reactions that can be characterized as "spurious body forces" (Lagrange multipliers) within $\Omega_{\square}$, since these are not present in the original fine-scale problem.

As to the practical implementation of the constraint represented by $\bar{\boldsymbol{\mathcal{U}}}_{\square}(\boldsymbol{v}) = \boldsymbol{0}$ for $\boldsymbol{v} \in \mathbb{U}^{\mu}_{\square}$, we may argue as follows: It is possible to restate the SVE-problem (8.56) as {eq:6-65}

$$a_{\square}(\mathcal{A}\bar{\boldsymbol{u}} + \boldsymbol{u}^{\mu}; \delta\boldsymbol{u}^{\mu}) - d_{\square}(\boldsymbol{\lambda}, \delta\boldsymbol{u}^{\mu}) = \tilde{l}_{\square}(\delta\boldsymbol{u}^{\mu}) \quad \forall \delta\boldsymbol{u}^{\mu} \in \mathbb{U}^{\mu}_{\square}, \tag{8.57a}$$ {eq:6-65a}

$$-d_{\square}(\delta\boldsymbol{\lambda}, \boldsymbol{u}^{\mu}) = 0 \qquad \forall \delta\boldsymbol{\lambda} \in \mathbb{T}^{+}_{\square}. \tag{8.57b}$$ {eq:6-65b}

where $\tilde{l}_{\square}(\delta\boldsymbol{u}^{\mu}) \overset{\text{def}}{=} l_{\square}(\delta\boldsymbol{u}^{\mu} - \bar{\boldsymbol{\mathcal{U}}}_{\square}(\delta\boldsymbol{u}^{\mu}))$ represents the *self-equilibrated load.* Clearly, for any constant $\boldsymbol{V}$ we have the identity $\tilde{l}_{\square}(\boldsymbol{V}) = l_{\square}(\boldsymbol{V})$, which means that (8.57) is equivalent to

(8.56). However, since $\tilde{l}_\square$ represents self-equilibrated loading, it is obvious that no reaction forces occur due to the restriction in $\mathbb{U}_\square^\mu$. In conclusion, it is possible to circumvent the issue of a complicated implementation of $\bar{\boldsymbol{\mathcal{U}}}_\square(\boldsymbol{v}) = \boldsymbol{0}$ by simply constraining the translation of an arbitrary point $\tilde{\boldsymbol{x}}$, i.e. by redefining $\mathbb{U}_\square^\mu$ as

$$\mathbb{U}_\square^\mu = \{\boldsymbol{u}' \text{ sufficiently regular}: \ \boldsymbol{u}'(\tilde{\boldsymbol{x}}) = \boldsymbol{0}\} \tag{8.58}$$ {eq:6-66}

Invariance

Firstly, since $\boldsymbol{\epsilon}[\mathcal{A}\bar{\boldsymbol{u}}] = \bar{\boldsymbol{\epsilon}} \overset{\text{def}}{=} \bar{\boldsymbol{h}}^{\text{sym}}$, it is only the macroscale strain $\bar{\boldsymbol{\epsilon}}$ that "drives" the RVE-problems; hence, we may express $\boldsymbol{u}^\mu = \boldsymbol{u}^\mu\{\bar{\boldsymbol{\epsilon}}\}$, $\boldsymbol{\lambda} = \boldsymbol{\lambda}\{\bar{\boldsymbol{\epsilon}}\}$. Secondly, the macroscale stress is parameterized as

{eq:6-67}
$$\bar{\boldsymbol{\sigma}} = \langle \boldsymbol{\sigma}(\boldsymbol{\epsilon}[\mathcal{A}\bar{\boldsymbol{u}} + \boldsymbol{u}^\mu\{\bar{\boldsymbol{\epsilon}}\}]) \rangle_\square = \langle \boldsymbol{\sigma}(\bar{\boldsymbol{\epsilon}} + \boldsymbol{u}^\mu\{\bar{\boldsymbol{\epsilon}}\}) \rangle_\square = \bar{\boldsymbol{\sigma}}\{\bar{\boldsymbol{\epsilon}}\} \tag{8.59}$$

In conclusion, the response is invariant to $\bar{\boldsymbol{u}}(\bar{\boldsymbol{x}})$ and $\bar{\boldsymbol{h}}^{\text{skw}}(\bar{\boldsymbol{x}})$, although these variables/fields are certainly relevant in solving the macroscale boundary value problem.

Operational format of RVE-problem

A completely valid format was given in (8.56). However, for computational purposes it turns out to be convenient to choose $\boldsymbol{u}$ (rather than $\boldsymbol{u}^\mu$) as the unknown field in a canonical format of the RVE-problem. To this end, we introduce the solution and test spaces $\mathbb{U}_\square$ and $\mathbb{L}_\square$ as follows:

{eq:6-68}

{eq:6-68a}
$$\mathbb{U}_\square = \{\boldsymbol{u}' \text{ suff. regular in } \Omega_\square, \ \boldsymbol{u}'(\tilde{\boldsymbol{x}}) = \boldsymbol{0}\} \tag{8.60a}$$
{eq:6-68b}
$$\mathbb{T}_\square^+ = \mathbb{L}_2(\Gamma_\square^+) \tag{8.60b}$$

and we propose the following format of the RVE-problem: For given value of $\bar{\boldsymbol{\epsilon}}$, find $\boldsymbol{u} \in \mathbb{U}_\square$ and
{eq:6-71} $\boldsymbol{\lambda} \in \mathbb{L}_\square$ that solve the system

{eq:6-71a}
$$a_\square(\boldsymbol{u}; \delta\boldsymbol{u}) - d_\square(\boldsymbol{\lambda}, \delta\boldsymbol{u}) = l_\square(\delta\boldsymbol{u}) \qquad \forall \delta\boldsymbol{u} \in \mathbb{U}_\square, \tag{8.61a}$$
{eq:6-71b}
$$-d_\square(\delta\boldsymbol{\lambda}, \boldsymbol{u}) = -d_\square(\delta\boldsymbol{\lambda}, \bar{\boldsymbol{\epsilon}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}]) \quad \forall \delta\boldsymbol{\lambda} \in \mathbb{T}_\square^+. \tag{8.61b}$$

Since the rigid body rotation is implicitly prescribed in the weak format by the constraint condition (8.61b), it is sufficient to remove the (rigid body) translation. Indeed, this is achieved by the particular choice of $\mathbb{U}_\square$ in (8.60a).

An associated SVE-potential (a local Lagrangian potential) can be constructed, for any given $\bar{\boldsymbol{\epsilon}}$, as follows:

{eq:6-72}
$$\pi_\square(\bar{\boldsymbol{\epsilon}}; \hat{\boldsymbol{u}}, \hat{\boldsymbol{\lambda}}) \overset{\text{def}}{=} \psi_\square(\hat{\boldsymbol{u}}) - d_\square(\hat{\boldsymbol{\lambda}}, \hat{\boldsymbol{u}} - \bar{\boldsymbol{\epsilon}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}]) - l_\square(\hat{\boldsymbol{u}} - \bar{\boldsymbol{\epsilon}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}]) \tag{8.62}$$

and the RVE-problem reads: For given value of $\bar{\boldsymbol{\epsilon}}$, solve for $\boldsymbol{u}$ and $\boldsymbol{\lambda}$ from the saddle-point problem

{eq:6-73}
$$(\boldsymbol{u}, \boldsymbol{\lambda}) = \arg \left[\inf_{\hat{\boldsymbol{u}} \in \mathbb{U}_\square} \sup_{\hat{\boldsymbol{\lambda}} \in \mathbb{T}_\square^+} \pi(\bar{\boldsymbol{\epsilon}}; \hat{\boldsymbol{u}}, \hat{\boldsymbol{\lambda}}) \right] \tag{8.63}$$

The corresponding stationarity conditions define local problems on $\Omega_\square$, which are precisely those given in (8.61).

Satisfaction of Hill-Mandel macrohomogeneity condition

Finally in this Subsubsection, we show that the VCMH-condition is satisfied upon adopting the (model) assumption of micro-periodic fluctuations. We argue as follows:

- For any given perturbation $\mathrm{d}\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}^0$, choose $\delta \boldsymbol{u}^\mu = \mathcal{S}\,\mathrm{d}\bar{\boldsymbol{u}} \subseteq \mathbb{U}^\mu_\square$ in (8.56a)
- Linearize (8.56b) w.r.t. $\bar{\boldsymbol{u}}$ along $\mathrm{d}\bar{\boldsymbol{u}}$, i.e. $\mathrm{d}\boldsymbol{u}^\mu = \mathcal{S}\,\mathrm{d}\bar{\boldsymbol{u}}$. Finally, choose $\delta\boldsymbol{\lambda} = \boldsymbol{\lambda}\{\bar{\boldsymbol{u}}\} \in \mathbb{T}^+_\square$ in the linearized equation

Subtracting the resulting equations, we obtain

$$a_\square(\mathcal{A}\bar{\boldsymbol{u}} + \boldsymbol{u}^\mu\{\bar{\boldsymbol{u}}\}; \mathcal{S}\,\mathrm{d}\bar{\boldsymbol{u}}) - l_\square(\mathcal{S}\,\mathrm{d}\bar{\boldsymbol{u}}) = 0 \quad \forall\,\mathrm{d}\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}^0 \tag{8.64}$$ {eq:6-74}

which is precisely (8.31). It is possible to rephrase (8.64) in the more explicit form

$$\langle \boldsymbol{\sigma} : \boldsymbol{\epsilon}[\,\mathrm{d}\boldsymbol{u}]\rangle_\square - \bar{\boldsymbol{\sigma}} : \mathrm{d}\bar{\boldsymbol{\epsilon}} \;\; = \langle \boldsymbol{b} \cdot \mathrm{d}\boldsymbol{u}\rangle_\square - \bar{\boldsymbol{b}} \cdot \mathrm{d}\bar{\boldsymbol{u}} - \bar{\boldsymbol{b}}^{(2)} : \mathrm{d}\bar{\boldsymbol{\epsilon}} \quad \forall \delta\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}^0 \tag{8.65}$$ {eq:6-77}

where it was used that $\mathcal{A}\,\mathrm{d}\bar{\boldsymbol{u}}(\boldsymbol{x}, \bar{\boldsymbol{x}}) = \mathrm{d}\bar{\boldsymbol{u}}(\bar{\boldsymbol{x}}) + \mathrm{d}\bar{\boldsymbol{\epsilon}}(\bar{\boldsymbol{x}}) \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}]$ and, hence, $\boldsymbol{\epsilon}[\mathcal{A}\,\mathrm{d}\bar{\boldsymbol{u}}](\boldsymbol{x}, \bar{\boldsymbol{x}}) = \mathrm{d}\bar{\boldsymbol{\epsilon}}(\bar{\boldsymbol{x}})$ with $\mathrm{d}\bar{\boldsymbol{\epsilon}}(\boldsymbol{x}) \stackrel{\text{def}}{=} \boldsymbol{\epsilon}[\,\mathrm{d}\bar{\boldsymbol{u}}(\boldsymbol{x})]$. Moreover, we used that $\langle \boldsymbol{\sigma}\rangle_\square = \bar{\boldsymbol{\sigma}}$. Clearly, in the special case that $\boldsymbol{b} = \boldsymbol{0}$, we obtain the classical format of the Hill-Mandel condition (for macroscale strain control)

$$\langle \boldsymbol{\sigma} : \boldsymbol{\epsilon}[\,\mathrm{d}\boldsymbol{u}]\rangle_\square = \bar{\boldsymbol{\sigma}} : \mathrm{d}\bar{\boldsymbol{\epsilon}} \quad \forall \delta\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}^0 \tag{8.66}$$ {eq:6-78}

which was given in Subsection 2.2.6.???

Remark 13 *Note that the result in (8.64) is, in fact, independent on the order of homogenization defined by the specific choice of prolongation operator $\mathcal{A}$. For example, it applies to the case when $\mathcal{A}$ represents socalled 2nd order homogenization, as proposed by* Kouznetsova **?** *and discussed below.*

8.2.9 2nd order homogenization – Nonlocal continuum

SKALL VI HA MED ????

ALT: Micropolar?

$$(\mathcal{A}\bar{\boldsymbol{u}})(\bar{\boldsymbol{x}}, \boldsymbol{x}) = \bar{\boldsymbol{u}}(\bar{\boldsymbol{x}}) + \bar{\boldsymbol{\epsilon}}(\bar{\boldsymbol{x}}) \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}] + \frac{1}{2}\bar{\boldsymbol{u}} \otimes \boldsymbol{\nabla} \otimes \boldsymbol{\nabla} \colon [\boldsymbol{x} - \bar{\boldsymbol{x}}] \otimes [\boldsymbol{x} - \bar{\boldsymbol{x}}], \quad \text{for } \boldsymbol{x} \in \Omega_\square \tag{8.67}$$ {eq:6-75}

8.3 Variationally consistent homogenization – Application to a model problem with time-dependence

8.3.1 Preliminaries

8.3.2 Kelvin-type viscoelasticity

We extend the model in Section 6.2 by introducing rate-dependence, which leads to a transient (quasistatic) problem. To this end, we introduce a specific subclass of Standard Dissipative

Materials that is defined by the volume-specific strain energy (free energy) density $\psi(\boldsymbol{\epsilon})$ and, in addition, the volume-specific dissipation potential $\phi(\dot{\boldsymbol{\epsilon}})$. It then appears that $\psi(\boldsymbol{\epsilon})$ represents (in general nonlinear) elasticity, whereas $\phi(\dot{\boldsymbol{\epsilon}})$ represents linear viscoelasticity (the Kelvin model). The corresponding rheological model is shown in Figure ???. For simplicity, we shall here choose isotropic viscous response via

$$\phi(\dot{\boldsymbol{\epsilon}}) = \frac{1}{2}\mu|\dot{\boldsymbol{\epsilon}}|^2 \tag{8.68}$$ {eq:6-81}

whereby the equilibrium stress $\boldsymbol{\sigma}$ becomes

{eq:6-82}
$$\boldsymbol{\sigma}(\boldsymbol{\epsilon}, \dot{\boldsymbol{\epsilon}}) = \boldsymbol{\sigma}^{\mathrm{en}}(\boldsymbol{\epsilon}) + \boldsymbol{\sigma}^{\mathrm{di}}(\dot{\boldsymbol{\epsilon}}) \tag{8.69}$$

{eq:6-83} where the "energetic" and "dissipative" parts are given as

{eq:6-83a}
$$\boldsymbol{\sigma}^{\mathrm{en}}(\boldsymbol{\epsilon}) = \frac{\partial \psi}{\partial \boldsymbol{\epsilon}} \tag{8.70a}$$

{eq:6-83b}
$$\boldsymbol{\sigma}^{\mathrm{di}}(\dot{\boldsymbol{\epsilon}}) = \frac{\partial \phi}{\partial \dot{\boldsymbol{\epsilon}}} = \mu\,\dot{\boldsymbol{\epsilon}} \tag{8.70b}$$

The loading and boundary conditions are the same as for nonlinear elasticity, whereby the quasistatic fine-scale problem can be formulated as follows: Restricting to quasistatics, we seek
{eq:6-84} the displacement $\boldsymbol{u}(\boldsymbol{x}, t) : \Omega \times \mathbb{R}^+ \to \mathbb{R}^3$ that solves the system

$$-\boldsymbol{\sigma}(\boldsymbol{\epsilon}[\boldsymbol{u}], \boldsymbol{\epsilon}[\dot{\boldsymbol{u}}]) \cdot \boldsymbol{\nabla} = \boldsymbol{b} \qquad \text{in } \Omega \times (0, T] \tag{8.71a}$$

$$\boldsymbol{u} = \boldsymbol{u}_{\mathrm{p}}(t) \qquad \text{on } \Gamma_{\mathrm{D}} \times (0, T] \tag{8.71b}$$

$$\boldsymbol{t} \overset{\mathrm{def}}{=} \boldsymbol{\sigma} \cdot \boldsymbol{n} = \boldsymbol{t}_{\mathrm{p}}(t) \qquad \text{on } \Gamma_{\mathrm{N}} \times (0, T] \tag{8.71c}$$

together with the constitutive relations in (8.69), (8.70) and the initial condition

{eq:6-85}
$$\boldsymbol{\epsilon}[\boldsymbol{u}](\bullet, 0) = \boldsymbol{\epsilon}[\boldsymbol{u}_0](= \boldsymbol{0}) \quad \text{in } \Omega \tag{8.72}$$

As to the spatial variation of the material parameters $\mathbf{E}$ (elasticity modulus tensor) ??? and μ (viscosity parameter), they may be strongly heterogeneous on the fine scale.

The weak form of the problem in (8.71) reads: Find $\boldsymbol{u}$ in the appropriate space $\mathbb{U}$ that solves

{eq:6-86}
$$\int_\Omega \mu \boldsymbol{\epsilon}[\dot{\boldsymbol{u}}] : \boldsymbol{\epsilon}[\delta \boldsymbol{u}]\,\mathrm{d}\Omega + \int_\Omega \boldsymbol{\sigma}^{\mathrm{en}}(\boldsymbol{\epsilon}[\boldsymbol{u}]) : \boldsymbol{\epsilon}[\delta \boldsymbol{u}]\,\mathrm{d}\Omega - l(\delta \boldsymbol{u}) = 0 \quad \forall \delta \boldsymbol{u} \in \mathbb{U}^0, \tag{8.73}$$

where $\boldsymbol{\sigma}^{\mathrm{en}}(\boldsymbol{\epsilon})$ was defined in (8.70a) and $l(\delta \boldsymbol{u})$ was defined in (8.4b). Due to the presence of the dissipative part of the equilibrium stress, it is not possible to identify (8.73) as the stationarity condition of any functional in the spatial domain.

8.3.3 Two-scale setting – Homogenization

Like for the model problem of (nonlinear) elasticity discussed above, we exploit the VMS-idea that each $\boldsymbol{u} \in \mathbb{U}$ can be decomposed into macroscale (smooth) and subscale (fluctuating) parts via the unique hierarchical decomposition $\mathbb{U}^{\mathrm{M}} \oplus \mathbb{U}^{\mu}$. Hence, the weak form (8.73) is replaced by
{eq:6-87} the problem of finding $\boldsymbol{u}^{\mathrm{M}} \in \mathbb{U}^{\mathrm{M}}$ and $\boldsymbol{u}^{\mu} \in \mathbb{U}^{\mu}$ that satisfy

{eq:6-87a}
$$\begin{aligned}&\int_\Omega \left[m_\square(\dot{\boldsymbol{u}}^{\mathrm{M}} + \dot{\boldsymbol{u}}^{\mu}; \delta \boldsymbol{u}^{\mathrm{M}}) + a_\square(\boldsymbol{u}^{\mathrm{M}} + \boldsymbol{u}^{\mu}; \delta \boldsymbol{u}^{\mathrm{M}}) - l_\square(\delta \boldsymbol{u}^{\mathrm{M}}) \right] \mathrm{d}\Omega - \int_{\Gamma_{\mathrm{N}}} \boldsymbol{t}_{\mathrm{p}} \cdot \delta \boldsymbol{u}^{\mathrm{M}}\,\mathrm{d}\Gamma \\ &= 0 \quad \forall \delta \boldsymbol{u}^{\mathrm{M}} \in \mathbb{U}^{\mathrm{M},0},\end{aligned} \tag{8.74a}$$

{eq:6-87b}
$$\begin{aligned}&\int_\Omega \left[m_\square(\dot{\boldsymbol{u}}^{\mathrm{M}} + \dot{\boldsymbol{u}}^{\mu}; \delta \boldsymbol{u}^{\mu}) + a_\square(\boldsymbol{u}^{\mathrm{M}} + \boldsymbol{u}^{\mu}; \delta \boldsymbol{u}^{\mu}) - l_\square(\delta \boldsymbol{u}^{\mu}) \right] \mathrm{d}\Omega \\ &= 0 \quad \forall \delta \boldsymbol{u}^{\mu} \in \mathbb{U}^{\mu}\end{aligned} \tag{8.74b}$$

{eq:6-88} where we used the forms

{eq:6-88a}
$$a_\square(\boldsymbol{u};\delta\boldsymbol{u}) = \langle \boldsymbol{\sigma}^{\mathrm{en}}(\boldsymbol{\epsilon}[\boldsymbol{u}])\colon \boldsymbol{\epsilon}[\delta\boldsymbol{u}]\rangle_\square \tag{8.75a}$$
{eq:6-88b}
$$m_\square(\boldsymbol{u};\delta\boldsymbol{u}) = \langle \mu\boldsymbol{\epsilon}[\boldsymbol{u}]\colon \boldsymbol{\epsilon}[\delta\boldsymbol{u}]\rangle_\square \tag{8.75b}$$
{eq:6-88b}
$$l_\square(\delta\boldsymbol{u}) = \langle \boldsymbol{b}\cdot\delta\boldsymbol{u}\rangle_\square \tag{8.75c}$$

Next, we introduce the linear prolongation operator $\mathcal{A}\bar{\boldsymbol{u}}$ such that

$$\boldsymbol{u} = \mathcal{A}\bar{\boldsymbol{u}} + \boldsymbol{u}^\mu \tag{8.76}$$ {eq:6-89}

where $\bar{\boldsymbol{u}}(\bullet,t)\in\bar{\mathbb{U}}$ is the macroscale displacement field. The purpose of localization to RVE-problems is to obtain the solution $\boldsymbol{u}^\mu\{\bar{\boldsymbol{u}}\}$ for any given value of $\bar{\boldsymbol{u}}$. However, the appropriate field $\bar{\boldsymbol{u}}(\bullet,t)\in\bar{\mathbb{U}}$ is the solution of the homogenization problem

$$\int_\Omega \left[m_\square(\dot{\bar{\boldsymbol{u}}}+\dot{\boldsymbol{u}}^\mu\{\bar{\boldsymbol{u}}\};\mathcal{A}\delta\bar{\boldsymbol{u}}) + a_\square(\mathcal{A}\bar{\boldsymbol{u}}+\boldsymbol{u}^\mu\{\bar{\boldsymbol{u}}\};\mathcal{A}\delta\bar{\boldsymbol{u}}) - l_\square(\mathcal{A}\delta\bar{\boldsymbol{u}})\right]\,\mathrm{d}\Omega - \int_{\Gamma_\mathrm{N}} \boldsymbol{t}_\mathrm{p}\cdot\mathcal{A}\delta\bar{\boldsymbol{u}}\,\mathrm{d}\Gamma$$
$$= 0 \quad \forall\delta\bar{\boldsymbol{u}}\in\bar{\mathbb{U}}^0 \tag{8.77}$$ {eq:6-91}

The local version of the VCMH-condition reads:

$$m_\square(\mathcal{A}\dot{\bar{\boldsymbol{u}}}+\dot{\boldsymbol{u}}^\mu\{\bar{\boldsymbol{u}}\};\mathcal{S}\delta\bar{\boldsymbol{u}}) + a_\square(\mathcal{A}\bar{\boldsymbol{u}}+\boldsymbol{u}^\mu\{\bar{\boldsymbol{u}}\};\mathcal{S}\delta\bar{\boldsymbol{u}}) - l_\square(\mathcal{S}\delta\bar{\boldsymbol{u}}) = 0 \quad \forall\delta\bar{\boldsymbol{u}}\in\bar{\mathbb{U}}^0 \tag{8.78}$$ {eq:6-92}

which represents a straightforward extension of (**??**).

8.3.4 1st order homogenization

In the standard case of 1st order homogenization, $\bar{\boldsymbol{u}}$ is prolonged via assumed linear variation of $\boldsymbol{u}^\mathrm{M}$ within each RVE:

$$\boldsymbol{u}^\mathrm{M}(\bar{\boldsymbol{x}},\boldsymbol{x}) = (\mathcal{A}\bar{\boldsymbol{u}})(\bar{\boldsymbol{x}},\boldsymbol{x}) := \bar{\boldsymbol{u}}(\bar{\boldsymbol{x}}) + \bar{\boldsymbol{h}}(\bar{\boldsymbol{x}})\cdot[\boldsymbol{x}-\bar{\boldsymbol{x}}] \text{ for } \boldsymbol{x}\in\Omega_\square \tag{8.79}$$ {eq:6-93}

Homogenized quantities are obtained from testing with $\mathcal{A}\delta\bar{\boldsymbol{u}} = \delta\bar{\boldsymbol{u}}+\delta\bar{\boldsymbol{h}}\cdot[\boldsymbol{x}-\bar{\boldsymbol{x}}]$ in (8.77), whereby the homogenized problem (weak format) becomes: Find $\bar{\boldsymbol{u}}(\bullet,t)\in\bar{\mathbb{U}}$ s.t.

$$\begin{aligned}&\int_\Omega \bar{\boldsymbol{\sigma}}\{\bar{\boldsymbol{u}},\dot{\bar{\boldsymbol{u}}}\} : [\delta\bar{\boldsymbol{u}}\otimes\boldsymbol{\nabla}]\,\mathrm{d}\Omega\\ &= \int_\Omega \left[\bar{\boldsymbol{b}}\cdot\delta\bar{\boldsymbol{u}} + \bar{\boldsymbol{b}}^{(2)} : [\delta\bar{\boldsymbol{u}}\otimes\boldsymbol{\nabla}]\right]\,\mathrm{d}\Omega + \int_{\Gamma_\mathrm{N}} \boldsymbol{t}_\mathrm{p}\cdot\delta\bar{\boldsymbol{u}}\,\mathrm{d}\Gamma \quad \forall\delta\bar{\boldsymbol{u}}\in\bar{\mathbb{U}}^0\end{aligned} \tag{8.80}$$ {eq:6-94}

where

$$\bar{\boldsymbol{\sigma}} = \bar{\boldsymbol{\sigma}}^\mathrm{en} + \bar{\boldsymbol{\sigma}}^\mathrm{di} \tag{8.81}$$ {eq:6-98}

and we derived the macroscale variables: {eq:6-95}

$$\bar{\boldsymbol{\sigma}}^\mathrm{en} \overset{\mathrm{def}}{=} \langle \boldsymbol{\sigma}^\mathrm{en}(\bar{\boldsymbol{\epsilon}}+\boldsymbol{\epsilon}[\boldsymbol{u}^\mu])\rangle_\square, \tag{8.82a}$$ {eq:6-95a}
$$\bar{\boldsymbol{\sigma}}^\mathrm{di} \overset{\mathrm{def}}{=} \langle \mu[\dot{\bar{\boldsymbol{\epsilon}}}+\boldsymbol{\epsilon}[\dot{\boldsymbol{u}}^\mu])\rangle_\square, \tag{8.82b}$$ {eq:6-95d}
$$\bar{\boldsymbol{b}} \overset{\mathrm{def}}{=} \langle \boldsymbol{b}\rangle_\square, \tag{8.82c}$$ {eq:6-95b}
$$\bar{\boldsymbol{b}}^{(2)} \overset{\mathrm{def}}{=} \langle \boldsymbol{b}\otimes[\boldsymbol{x}-\bar{\boldsymbol{x}}]\rangle_\square \tag{8.82d}$$ {eq:6-95c}

where $\bar{\boldsymbol{\epsilon}} \overset{\mathrm{def}}{=} \bar{\boldsymbol{h}}^\mathrm{sym}$. As to the external boundary, we tacitly assume (like for the prototype model of nonlinear elasticity) that boundary conditions can be imposed in terms of prescribed displacement $\bar{\boldsymbol{u}}_\mathrm{p}$ and (possibly) in terms of prescribed traction $\bar{\boldsymbol{t}}_\mathrm{p}$.

8.3.5 RVE-problem based on weak periodicity

for computational purposes it turns out to be convenient to choose $\boldsymbol{u}$ (rather than $\boldsymbol{u}^{\mu}$) as the unknown field in a canonical format of the RVE-problem. To this end, we introduce the solution and test spaces $\mathbb{U}_{\square}$ and $\mathbb{T}_{\square}^{+}$ as follows: {eq:6-96}

{eq:6-96a}
$$\mathbb{U}_{\square} = \{\boldsymbol{u}'(\bullet, t) \text{ suff. regular in } \Omega_{\square}\} \tag{8.83a}$$

{eq:6-96b}
$$\mathbb{T}_{\square}^{+} = \mathbb{L}_2(\Gamma_{\square}^{+}) \tag{8.83b}$$

and we propose the following format of the RVE-problem: For given history of $\bar{\boldsymbol{\epsilon}}(t)$, find $\boldsymbol{u}(\bullet, t) \in$ {eq:6-97} $\mathbb{U}_{\square}$ and $\boldsymbol{\lambda}(\bullet, t) \in \mathbb{T}_{\square}^{+}$ that solve the system

{eq:6-97a}
$$m_{\square}(\dot{\boldsymbol{u}}; \delta\boldsymbol{u}) + a_{\square}(\boldsymbol{u}; \delta\boldsymbol{u}) - d_{\square}(\boldsymbol{\lambda}, \delta\boldsymbol{u}) = l_{\square}(\delta\boldsymbol{u}) \quad \forall \delta\boldsymbol{u} \in \mathbb{U}_{\square}, \tag{8.84a}$$

{eq:6-97b}
$$-d_{\square}(\delta\boldsymbol{\lambda}, \boldsymbol{u}) = -d_{\square}(\delta\boldsymbol{\lambda}, \bar{\boldsymbol{\epsilon}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}]) \quad \forall \delta\boldsymbol{\lambda} \in \mathbb{T}_{\square}^{+}. \tag{8.84b}$$

UPDATE! Since the rigid body rotation is implicitly prescribed in the weak format by the constraint condition (8.84b), it is sufficient to remove the (rigid body) translation. Indeed, this is achieved by the particular choice of $\mathbb{U}_{\square}$ in (8.60a).

Satisfaction of VCMH-condition

Finally in this Subsection, we show that the VCMH-condition is satisfied upon adopting the {eq:6-99} (model) assumption of micro-periodic fluctuations. Firstly, we recall

{eq:6-99a}
$$m_{\square}(\dot{\boldsymbol{u}}, \delta\boldsymbol{u}^{\mu}) + a_{\square}(\boldsymbol{u}; \delta\boldsymbol{u}^{\mu}) - d_{\square}(\boldsymbol{\lambda}, \delta\boldsymbol{u}^{\mu}) = l_{\square}(\delta\boldsymbol{u}^{\mu}) \quad \forall \delta\boldsymbol{u}^{\mu} \in \mathbb{U}_{\square}, \tag{8.85a}$$

{eq:6-99b}
$$-d_{\square}(\delta\boldsymbol{\lambda}, \boldsymbol{u}^{\mu}) = 0 \quad \forall \delta\boldsymbol{\lambda} \in \mathbb{T}_{\square}^{+}. \tag{8.85b}$$

We then argue as follows:

- For any given perturbation $\mathrm{d}\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}^0$, choose $\delta\boldsymbol{u}^{\mu} = \mathcal{S}\,\mathrm{d}\bar{\boldsymbol{u}} \subseteq \mathbb{U}_{\square}^{\mu}$ in (8.85a).
- Linearize (8.85b) w.r.t. $\bar{\boldsymbol{u}}$ along $\mathrm{d}\bar{\boldsymbol{u}}$, i.e. $\mathrm{d}\boldsymbol{u}^{\mu} = \mathcal{S}\,\mathrm{d}\bar{\boldsymbol{u}}$. Finally, choose $\delta\boldsymbol{\lambda} = \boldsymbol{\lambda}\{\bar{\boldsymbol{u}}\} \in \mathbb{L}_{\square}$ in the linearized equation.

Subtracting the resulting equations, we obtain

{eq:6-101}
$$m_{\square}(\mathcal{A}\dot{\bar{\boldsymbol{u}}} + \dot{\boldsymbol{u}}^{\mu}\{\bar{\boldsymbol{u}}\}; \mathcal{S}\,\mathrm{d}\bar{\boldsymbol{u}}) + a_{\square}(\mathcal{A}\bar{\boldsymbol{u}} + \boldsymbol{u}^{\mu}\{\bar{\boldsymbol{u}}\}; \mathcal{S}\,\mathrm{d}\bar{\boldsymbol{u}}) - l_{\square}(\mathcal{S}\,\mathrm{d}\bar{\boldsymbol{u}}) = 0 \quad \forall\, \mathrm{d}\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}^0 \tag{8.86}$$

which is precisely (8.92). Once again, we note that it is possible to rephrase (8.86) in the more explicit form

{eq:6-102}
$$\langle \boldsymbol{\sigma} : \boldsymbol{\epsilon}[\,\mathrm{d}\boldsymbol{u}] \rangle_{\square} - \bar{\boldsymbol{\sigma}} : \mathrm{d}\bar{\boldsymbol{\epsilon}} = \langle \boldsymbol{b} \cdot \mathrm{d}\boldsymbol{u} \rangle_{\square} - \bar{\boldsymbol{b}} \cdot \mathrm{d}\bar{\boldsymbol{u}} - \bar{\boldsymbol{b}}^{(2)} : \mathrm{d}\bar{\boldsymbol{\epsilon}} \quad \forall \delta\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}^0 \tag{8.87}$$

We note that (8.87) is identical to (8.65) that is pertinent to (rate-independent) nonlinear elasticity.

xxxxxxxxxxxxxxxxxxxxxxxxxx

Reprase in boundary-format, independent of transient term!

8.4 Variationally consistent homogenization – Application to a parabolic model problem

8.4.1 Preliminaries

We consider the fine-scale problem of transient heat flow (conduction) in a solid medium with strongly heterogeneous microstructure. This problem serves as the prototype problem for a class of problem that has parabolic character.

8.4.2 Heat conduction in a solid material

We thus seek the temperature $u(\boldsymbol{x}, t) : \Omega \times \mathbb{R}^+ \to \mathbb{R}$ that solves the (uncoupled) energy balance equation with boundary conditions {eq:11-21}

$$\dot{\Phi}(u) + \boldsymbol{q}(\boldsymbol{\zeta}[u]) \cdot \boldsymbol{\nabla} = f \quad \text{in } \Omega \times (0, T] \tag{8.88a}$$ {eq:11-21b}

$$u = u_\mathrm{p} \quad \text{on } \Gamma_\mathrm{D} \times (0, T] \tag{8.88b}$$ {eq:11-21e}

$$z \stackrel{\text{def}}{=} \boldsymbol{q} \cdot \boldsymbol{n} = z_\mathrm{p} \quad \text{on } \Gamma_\mathrm{N} \times (0, T] \tag{8.88c}$$ {eq:11-21f}

together with the initial condition

$$\Phi(\bullet, 0) = c\, u(\bullet, 0) = 0 \quad \text{in } \Omega \tag{8.89}$$ {eq:11-22}

where we used that $u(\bullet, 0) = u_0(\bullet) = 0$.

Here, $\Phi = \Phi(u)$ is the stored volume-specific internal energy (which is a conservation quantity and taken as a function of the absolute temperature, u, in the simplest modeling approach), whereas $\boldsymbol{q} = \boldsymbol{q}(\boldsymbol{\zeta})$ is the heat flux (which is taken as a function of the temperature gradient, $\boldsymbol{\zeta} \stackrel{\text{def}}{=} \boldsymbol{\nabla} u$, in the simplest modeling approach). Moreover, f is a (bulk)volume-specific heat source (supply of energy) within Ω.

We choose the simplest possible constitutive equations for Φ and $\boldsymbol{q}$ of the form {eq:11-23}

$$\Phi(u) = c\, u, \tag{8.90a}$$ {eq:11-23a}

$$\boldsymbol{q}(\boldsymbol{\zeta}) = -\boldsymbol{K} \cdot \boldsymbol{\zeta} \tag{8.90b}$$ {eq:11-23b}

where we introduced the constant, but strongly micro-heterogenous, coefficient of thermal capacity, denoted c, and thermal conductivity tensor, denoted $\boldsymbol{K}$, respectively. The resulting model problem is, thus, completely linear.

The standard space-variational format corresponding to (8.88) reads: Find $u(\bullet, t)$ in the appropriately defined space $\mathbb{U}$ that solves

$$\int_\Omega [c\, u\, \delta u + \boldsymbol{\zeta}[u] \cdot \boldsymbol{K} \cdot \boldsymbol{\zeta}[\delta u]]\, \mathrm{d}\Omega = \int_\Omega f\, \delta u\, \mathrm{d}\Omega + \int_{\Gamma_\mathrm{N}} z_\mathrm{p}\, \delta u\, \mathrm{d}\Gamma \quad \forall \delta u \in \mathbb{U}^0 \tag{8.91}$$ {eq:11-24}

??

8.4.3 Two-scale setting – Homogenization

Like for the model problem of (nonlinear) elasticity discussed above,

???

The local version of the VCMH-condition reads:

$$m_\square(\dot{\bar{u}} + \dot{u}^\mu\{\bar{u}\}; \delta\bar{u}) + a_\square(\bar{u} + u^\mu\{\bar{u}\}; \delta\bar{u}) - l_\square(\delta\bar{u}) = 0 \quad \forall \delta\bar{u} \in \bar{\mathbb{U}}^0 \qquad (8.92)$$ {eq:6-92}

which represents a straightforward extension of (8.30).

8.4.4 1st order homogenization

In the standard case of 1st order homogenization, $\bar{u}$ is prolonged via assumed linear variation of u^M within each RVE:

{eq:6-93} $$u^\mathrm{M}(\bar{\boldsymbol{x}}, \boldsymbol{x}) = (\bar{u})(\bar{\boldsymbol{x}}, \boldsymbol{x}) := \bar{u}(\bar{\boldsymbol{x}}) + \bar{\boldsymbol{\zeta}}(\bar{\boldsymbol{x}}) \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}] \text{ for } \boldsymbol{x} \in \Omega_\square \qquad (8.93)$$

Homogenized quantities are obtained from testing with $\delta\bar{u} = \delta\bar{u} + \delta\bar{\boldsymbol{\zeta}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}]$ in (8.77), whereby the homogenized problem (weak format) becomes: Find $\bar{u}(\bullet, t) \in \bar{\mathbb{U}}$ s.t.

{eq:6-94} $$\begin{aligned} &\int_\Omega \left[\dot{\bar{\Phi}}\delta\bar{u} + \dot{\bar{\boldsymbol{\Phi}}}^{(2)} \cdot \boldsymbol{\nabla}\delta u + \bar{\boldsymbol{q}} \cdot \boldsymbol{\nabla}\delta u\right] \mathrm{d}\Omega \\ &= \int_\Omega \left[\bar{f}\delta\bar{u} + \bar{\boldsymbol{f}}^{(2)} \cdot \boldsymbol{\nabla}\delta\bar{u}\right] \mathrm{d}\Omega + \int_{\Gamma_\mathrm{N}} z_\mathrm{p}\delta\bar{u}\,\mathrm{d}\Gamma \quad \forall \delta\bar{u} \in \bar{\mathbb{U}}^0 \end{aligned} \qquad (8.94)$$

{eq:6-95} where we derived the macroscale variables:

{eq:6-95a} $$\bar{\Phi} \overset{\text{def}}{=} \langle \Phi \rangle_\square = \langle c\, u \rangle_\square, \qquad (8.95a)$$

{eq:6-95b} $$\bar{\boldsymbol{\Phi}}^{(2)} \overset{\text{def}}{=} \langle \Phi\, [\boldsymbol{x} - \bar{\boldsymbol{x}}] \rangle_\square = \langle c\, u\, [\boldsymbol{x} - \bar{\boldsymbol{x}}] \rangle_\square, \qquad (8.95b)$$

{eq:6-95c} $$\bar{\boldsymbol{q}} \overset{\text{def}}{=} \langle \boldsymbol{q} \rangle_\square = -\langle \boldsymbol{K} \cdot \boldsymbol{\zeta}[u] \rangle_\square, \qquad (8.95c)$$

{eq:6-95d} $$\bar{f} \overset{\text{def}}{=} \langle f \rangle_\square, \qquad (8.95d)$$

{eq:6-95e} $$\bar{\boldsymbol{f}}^{(2)} \overset{\text{def}}{=} \langle f\, [\boldsymbol{x} - \bar{\boldsymbol{x}}] \rangle_\square \qquad (8.95e)$$

8.4.5 RVE-problem based on weak periodicity

For computational purposes it turns out to be convenient to choose u (rather than u^μ) as the unknown field in a canonical format of the RVE-problem. To this end, we introduce the solution and test spaces $\mathbb{U}_\square$ and $\mathbb{L}_\square$ as follows:

{eq:6-96a} $$\mathbb{U}_\square = \{u'(\bullet, t) \text{ suff. regular in } \Omega_\square\} \qquad (8.96)$$

{eq:6-96b} $$\mathbb{Q}_\square^+ = \mathbb{L}_2(\Gamma_\square^+) \qquad (8.97)$$

and we propose the following format of the RVE-problem: The space-variational RVE-problem[6] can now be stated as follows: For given history of $\bar{u}(t)$, $\bar{\boldsymbol{\zeta}}(t)$, find $u(\bullet, t) \in \mathbb{U}_\square$, $\mu(\bullet, t) \in \mathbb{Q}_\square^+$,
{eq:11-554} $\bar{\mu}(t) \in \mathbb{R}$ that solve

{eq:11-554b} $$m_\square(\dot{u}; \delta u) + a_\square(u; \delta u) + d_\square(\mu; \delta u) + \bar{\mu}\,\langle\langle \delta u \rangle\rangle_\square = \langle f\, \delta u \rangle_\square \qquad \forall \delta u \in \mathbb{U}_\square, \qquad (8.98a)$$

{eq:11-554d} $$d_\square(\delta\mu; u) = d_\square(\delta\mu; \bar{\boldsymbol{\zeta}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}]) \qquad \forall \delta\mu \in \mathbb{Q}_\square^+, \qquad (8.98b)$$

{eq:11-554f} $$\delta\bar{\mu}\,\langle\langle u \rangle\rangle_\square = \delta\bar{\mu}\,\bar{u} \qquad \forall \delta\bar{\mu} \in \mathbb{R}. \qquad (8.98c)$$

[6] To simplify notation, without losing generality, we assume henceforth that the natural boundary conditions are sufficiently smooth to effect only the macroscale problem.

Satisfaction of VCMH condition

Finally in this Subsection, we show that the VCMH-condition is satisfied upon adopting the
{eq:11-555} (model) assumption of micro-periodic fluctuations. Firstly, we recall (8.98) rewritten as

{eq:11-555b} {eq:11-555d} {eq:11-555f}
$$\begin{aligned} m_\square(\dot{u};\delta u^\mu) + a_\square(u;\delta u^\mu) + d_\square(\mu;\delta u^\mu) + \bar{\mu}\,\langle\langle \delta u^\mu\rangle\rangle_\square &= \langle f\,\delta u^\mu\rangle_\square \qquad && \forall \delta u^\mu \in \mathbb{U}_\square, && (8.99a)\\ d_\square(\delta\mu;u^\mu) &= 0 && \forall \delta\mu \in \mathbb{Q}_\square^+, && (8.99b)\\ \delta\bar{\mu}\,\langle\langle u^\mu\rangle\rangle_\square &= 0 && \forall \delta\bar{\mu} \in \mathbb{R}. && (8.99c) \end{aligned}$$

We then argue as follows:

- For a given perturbation $\mathrm{d}\bar{u} \in \bar{\mathbb{U}}^0$, choose $\delta u = \mathrm{d}\bar{u} \subseteq \mathbb{U}_\square$ in (8.99a) to obtain

$$m_\square(\dot{\bar{u}} + \dot{u}^\mu;\,\mathrm{d}\bar{u}) + a_\square(\bar{u} + u^\mu;\,\mathrm{d}\bar{u}) + d_\square(\mu,\,\mathrm{d}\bar{u}) + \bar{\mu}\langle\langle\,\mathrm{d}\bar{u}\rangle\rangle_\square = \langle f\ \mathrm{d}\bar{u}\rangle_\square \qquad (8.100)$$ {eq:11-558}

- Linearize (8.99b) and (8.99c) w.r.t. $\bar{u}$. Introduce $\mathrm{d}u^\mu = \mathrm{d}\bar{u}$. Choose $\delta\mu = \mu\{\bar{u}\} \in \mathbb{Q}_\square^+$ and $\delta\bar{\mu} = \bar{\mu}\{\bar{u}\} \in \mathbb{R}$ in the linearized versions of (8.99b) and (8.99c), respectively. We then obtain {eq:11-559}

$$\begin{aligned} d_\square(\mu,\,\mathrm{d}\bar{u}) &= 0 \qquad (8.101a)\\ \bar{\mu}\langle\langle\,\mathrm{d}\bar{u}\rangle\rangle_\square &= 0 \qquad (8.101b) \end{aligned}$$ {eq:11-559a} {eq:11-559b}

Now, combining (8.100) and (8.101), we obtain the identity

$$m_\square(\dot{\bar{u}} + \dot{u}^\mu;\,\mathrm{d}\bar{u}) + a_\square(\bar{u} + u^\mu;\,\mathrm{d}\bar{u}) = \langle f\ \mathrm{d}\bar{u}\rangle_\square \qquad (8.102)$$ {eq:11-61}

which is precisely (8.92). Once again, we note that it is possible to rephrase (8.86) in the more explicit form

$$\langle\dot{\Phi}\,\mathrm{d}u\rangle_\square - \langle \boldsymbol{q}\cdot\boldsymbol{\zeta}[\,\mathrm{d}q]\rangle_\square - \langle f\,\mathrm{d}u\rangle_\square = \dot{\bar{\Phi}}\,\mathrm{d}\bar{q} + \dot{\bar{\boldsymbol{\Phi}}}^{(2)}\cdot\,\mathrm{d}\bar{\boldsymbol{\zeta}} - \bar{\boldsymbol{q}}\cdot\,\mathrm{d}\bar{\boldsymbol{\zeta}} - \bar{f}\,\mathrm{d}\bar{u} - \bar{\boldsymbol{f}}^{(2)}\cdot\,\mathrm{d}\bar{\boldsymbol{\zeta}} \qquad (8.103)$$ {eq:11-62}

We note that (8.87)??? is identical to (8.65)??? that is pertinent to (rate-independent) nonlinear elasticity.

8.5 Variationally consistent selective homogenization – Application to a model problem with multi-physical couplings

8.5.1 Preliminaries

8.5.2 Coupled magneto-elasticity

Next, consider a random micro-heterogenous material structure (a composite), whose constituents are magneto-elastic in the sense that they express a (strong) coupling between the elastic deformation and a magnetic field. In order to focus the discussion, we restrict to the situation of quasistatic condition and small strain kinematics. For simplicity, body forces and the volume-specific magnetization source are ignored.

The boundary Γ is decomposed in two different ways: $\Gamma = \Gamma_{\mathrm{D}}^{(u)} \cup \Gamma_{\mathrm{N}}^{(u)} = \Gamma_{\mathrm{D}}^{(y)} \cup \Gamma_{\mathrm{N}}^{(y)}$. On the one hand, boundary conditions of the Dirichlet type are imposed in terms of prescribed displacements, $\boldsymbol{u} = \bar{\boldsymbol{u}}_\text{p}$ on $\Gamma_\text{D}^{(u)}$, and prescribed magnetic potential, $y = \bar{y}_\text{p}$ on $\Gamma_\text{D}^{(y)}$. On the other hand, boundary conditions of the Neumann type are imposed in terms of prescribed mechanical tractions $\boldsymbol{t} \overset{\text{def}}{=} \boldsymbol{\sigma}\cdot\boldsymbol{n} = \boldsymbol{t}_\text{p}$ on the boundary part $\Gamma_\text{N}^{(u)}$, and prescribed magnetic flux, $q \overset{\text{def}}{=} \boldsymbol{b}\cdot\boldsymbol{n} = \bar{q}_\text{p}$[7] on the boundary part $\Gamma_\text{N}^{(y)}$. Here, $\boldsymbol{\sigma}$ is the total stress and $\boldsymbol{b}$ is the magnetic induction. We thus seek the displacement $\boldsymbol{u}(\boldsymbol{x}) : \Omega \to \mathbb{R}^3$ and the magnetic potential $y(\boldsymbol{x}) : \Omega \to \mathbb{R}$ that solve the system {eq:6-111}

{eq:6-111a} $$-\boldsymbol{\sigma}(\boldsymbol{\epsilon}[\boldsymbol{u}], \boldsymbol{\zeta}[y]) \cdot \boldsymbol{\nabla} = \boldsymbol{0} \quad \text{in } \Omega \tag{8.104a}$$

{eq:6-111b} $$-\boldsymbol{b}(\boldsymbol{\epsilon}[\boldsymbol{u}], \boldsymbol{\zeta}[y]) \cdot \boldsymbol{\nabla} = \boldsymbol{0} \quad \text{in } \Omega \tag{8.104b}$$

{eq:6-111c} $$\boldsymbol{u} = \boldsymbol{u}_\text{p} \quad \text{on } \Gamma_\text{D}^{(u)} \tag{8.104c}$$

{eq:6-111d} $$\boldsymbol{t} \overset{\text{def}}{=} \boldsymbol{\sigma} \cdot \boldsymbol{n} = \boldsymbol{t}_\text{p} \quad \text{on } \Gamma_\text{N}^{(u)} \tag{8.104d}$$

{eq:6-111e} $$y = y_\text{p} \quad \text{on } \Gamma_\text{D}^{(y)} \tag{8.104e}$$

{eq:6-111f} $$q \overset{\text{def}}{=} \boldsymbol{b} \cdot \boldsymbol{n} = q_\text{p} \quad \text{on } \Gamma_\text{N}^{(y)} \tag{8.104f}$$

As to the relevant constitutive models, we assume the existence of a volume-specific free energy $\psi(\boldsymbol{\epsilon}, \boldsymbol{\zeta})$, where $\boldsymbol{\epsilon} = \boldsymbol{\epsilon}[\boldsymbol{u}] \overset{\text{def}}{=} (\boldsymbol{u} \otimes \boldsymbol{\nabla})^\text{sym}$ is the strain tensor and $\boldsymbol{\zeta} = \boldsymbol{\zeta}[y] \overset{\text{def}}{=} \boldsymbol{\nabla} y$ is the magnetic
{eq:6-112} field. We thus propose the constitutive relations

{eq:6-112a} $$\boldsymbol{\sigma}(\boldsymbol{\epsilon}, \boldsymbol{\zeta}) = \frac{\partial \psi(\boldsymbol{\epsilon}, \boldsymbol{\zeta})}{\partial \boldsymbol{\epsilon}}, \tag{8.105a}$$

{eq:6-112b} $$\boldsymbol{b}(\boldsymbol{\epsilon}, \boldsymbol{\zeta}) = -\frac{\partial \psi(\boldsymbol{\epsilon}, \boldsymbol{\zeta})}{\partial \boldsymbol{\zeta}} \tag{8.105b}$$

The variational format for the fine-scale problem can be established from the potential energy

{eq:6-113} $$\Pi(\hat{\boldsymbol{u}}, \hat{y}) = \Psi(\hat{\boldsymbol{u}}, \hat{y}) - l^{(u)}(\hat{\boldsymbol{u}}) - l^{(y)}(\hat{y}) \tag{8.106}$$

{eq:6-114} where

{eq:6-114a} $$\Psi(\hat{\boldsymbol{u}}, \hat{y}) \overset{\text{def}}{=} \int_\Omega \psi(\boldsymbol{\epsilon}[\hat{\boldsymbol{u}}], \boldsymbol{\zeta}[\hat{y}]) \, \mathrm{d}\Omega, \tag{8.107a}$$

{eq:6-114b} $$l^{(u)}(\hat{\boldsymbol{u}}) \overset{\text{def}}{=} \int_{\Gamma_\text{N}^{(u)}} \boldsymbol{t}_\text{p} \cdot \hat{\boldsymbol{u}} \, \mathrm{d}\Gamma, \tag{8.107b}$$

{eq:6-114c} $$l^{(y)}(\hat{y}) \overset{\text{def}}{=} -\int_{\Gamma_\text{N}^{(y)}} \bar{q}_\text{p} \, \hat{y} \, \mathrm{d}\Gamma. \tag{8.107c}$$

In order to establish the appropriate variational format, we first assume that $\psi(\boldsymbol{\epsilon}, \boldsymbol{\zeta})$ is convex in the first argument, whereas it is concave in the second argument. [Indeed, this property is verified for the specific choice of constitutive model discussed below.] As a result, it is possible to show that $\Pi(\hat{\boldsymbol{u}}, \hat{y})$ is convex/concave in $\mathbb{U} \times \mathbb{Y}$ such that the stationary point is, indeed, a unique saddle-point in the sense that

{eq:6-115} $$(\boldsymbol{u}, y) = \arg\left[\inf_{\hat{\boldsymbol{u}} \in \mathbb{U}} \sup_{\hat{y} \in \mathbb{Y}} \Pi(\hat{\boldsymbol{u}}, \hat{y})\right] = \arg\left[\sup_{\hat{y} \in \mathbb{Y}} \inf_{\hat{\boldsymbol{u}} \in \mathbb{U}} \Pi(\hat{\boldsymbol{u}}, \hat{y})\right] \tag{8.108}$$

[7] $\boldsymbol{n}$ is the outward unit normal to Γ.

{eq:6-116} The stationarity conditions of $\Pi(\boldsymbol{u}, y)$ are

{eq:6-116a}
$$\Pi'_u(\boldsymbol{u}, y; \delta\boldsymbol{u}) = \int_\Omega \boldsymbol{\sigma}(\boldsymbol{\epsilon}[\boldsymbol{u}], \boldsymbol{\zeta}[y]) \colon \boldsymbol{\epsilon}[\delta\boldsymbol{u}]\,\mathrm{d}\Omega - l^{(u)}(\delta\boldsymbol{u}) = 0 \quad \forall \delta\boldsymbol{u} \in \mathbb{U}^0 \tag{8.109a}$$

{eq:6-116b}
$$\Pi'_y(\boldsymbol{u}, y; \delta y) = -\int_\Omega \boldsymbol{b}(\boldsymbol{\epsilon}[\boldsymbol{u}], \boldsymbol{\zeta}[y]) \cdot \boldsymbol{\zeta}[\delta y]\,\mathrm{d}\Omega - l^{(y)}(\delta y) = 0 \quad \forall \delta y \in \mathbb{Y}^0 \tag{8.109b}$$

Finally, in order to show that the stationary point does indeed define a saddle-point, i. e. to verify that $\Pi(\hat{\boldsymbol{u}}, \hat{y})$ is convex/concave, we introduce the tangent tensors {eq:6-117}

$$\mathsf{E}_\mathrm{T} = \frac{\partial^2 \psi}{\partial\boldsymbol{\epsilon} \otimes \partial\boldsymbol{\epsilon}}, \tag{8.110a}$$ {eq:6-117a}

$$\boldsymbol{D}_\mathrm{T} = \frac{\partial^2 \psi}{\partial\boldsymbol{\zeta} \otimes \partial\boldsymbol{\zeta}} \tag{8.110b}$$ {eq:6-117b}

and we note the following properties of the 2nd variation of Π {eq:6-118}

$$\Pi''_{uu}(\boldsymbol{u}, y; \delta\boldsymbol{u}, \delta\boldsymbol{u}) = \int_\Omega \boldsymbol{\epsilon}[\delta\boldsymbol{u}] \colon \mathsf{E}_\mathrm{T}(\boldsymbol{\epsilon}[\boldsymbol{u}], \boldsymbol{\zeta}[y]) \colon \boldsymbol{\epsilon}[\delta\boldsymbol{u}]\,\mathrm{d}\Omega > 0 \quad \forall \delta\boldsymbol{u} \in \mathbb{U}^0, \delta\boldsymbol{u} \neq \boldsymbol{0} \tag{8.111a}$$ {eq:6-118a}

$$\Pi''_{yy}(\boldsymbol{u}, y; \delta y, \delta y) = \int_\Omega \boldsymbol{\zeta}[\delta y] \cdot \boldsymbol{D}_\mathrm{T}(\boldsymbol{\epsilon}[\boldsymbol{u}], \boldsymbol{\zeta}[y]) \cdot \boldsymbol{\zeta}[\delta y]\,\mathrm{d}\Omega < 0 \quad \forall \delta y \in \mathbb{Y}^0, \delta y \neq 0 \tag{8.111b}$$ {eq:6-118b}

That these are sufficient conditions for the existence of a saddle-point is proved in Appendix A.1.

Example of constitutive model: A simple prototype model is defined by isotropic elasticity and isotropic magnetic permeability, and the free energy is chosen as[8]

$$\psi(\boldsymbol{\epsilon}, \boldsymbol{\zeta}) = \frac{1}{2}\boldsymbol{\epsilon} \colon \mathsf{E} \colon \boldsymbol{\epsilon} - \frac{1}{2}\mu\boldsymbol{\zeta} \cdot [\boldsymbol{I} - \boldsymbol{\epsilon}] \cdot \boldsymbol{\zeta} \tag{8.112}$$ {eq:6-119}

with the standard isotropic stiffness tensor of elastic moduli is given as $\mathsf{E} = 2G\mathsf{I}^\mathrm{sym}_\mathrm{dev} + K\boldsymbol{I} \otimes \boldsymbol{I}$. The material parameters are G, K, μ. It is straightforward to show that ψ is convex in the first argument ($\boldsymbol{\epsilon}$), while it is concave in the second argument ($\boldsymbol{\zeta}$); hence, the proof is omitted here. We then obtain {eq:6-121}

$$\boldsymbol{\sigma} = \frac{\partial\psi}{\partial\boldsymbol{\epsilon}} = \mathsf{E} \colon \boldsymbol{\epsilon} + \frac{1}{2}\mu\boldsymbol{\zeta} \otimes \boldsymbol{\zeta}, \tag{8.113a}$$ {eq:6-121a}

$$\boldsymbol{b} = -\frac{\partial\psi}{\partial\boldsymbol{\zeta}} = \mu[\boldsymbol{I} - \boldsymbol{\epsilon}] \cdot \boldsymbol{\zeta} \tag{8.113b}$$ {eq:6-121b}

and {eq:6-122}

$$\mathsf{E}_\mathrm{T} = \mathsf{E}, \tag{8.114a}$$ {eq:6-122a}

$$\boldsymbol{D}_\mathrm{T} = -\mu[\boldsymbol{I} - \boldsymbol{\epsilon}] \tag{8.114b}$$ {eq:6-122b}

The magneto-mechanical coupling disappears when $\boldsymbol{\epsilon}$ becomes small, in which situation $\boldsymbol{b} = \mu\boldsymbol{\zeta}$. As a result, a "one-way coupling" is obtained, i.e. the uncoupled magnetic problem can first be solved, whereafter the mechanical problem is solved with known field $\boldsymbol{\zeta}$ (that affects the stress). $\square$

[8] Compared with finite strain modeling, we introduced the linearization $\boldsymbol{\zeta} \cdot \boldsymbol{C}^{-1} \cdot \boldsymbol{\zeta} \approx \boldsymbol{\zeta} \cdot [\boldsymbol{I} - \boldsymbol{\epsilon}] \cdot \boldsymbol{\zeta}$, where $\boldsymbol{C}$ is Cauchy's deformation tensor.

8.5.3 Two-scale setting – Selective homogenization

Like for the model problem of micro-heterogeneous elasticity, we exploit the VMS-idea that each $\boldsymbol{u} \in \mathbb{U}$ can be decomposed into macroscale (smooth) and subscale (fluctuating) parts via the unique hierarchical decomposition $\mathbb{U}^{\mathrm{M}} \oplus \mathbb{U}^{\mu}$. However, it is important to note that no such decomposition is proposed for y, and we may set $\mathbb{Y} = \mathbb{Y}^{\mu}$.

Moreover, we introduce homogenization upon replacing integrands by running averages on the RVE:s; hence, the fine-scale potential in (8.113)??? is replaced by the homogenized potential

{eq:6-123}
$$\Pi(\hat{\boldsymbol{u}}^{\mathrm{M}}, \hat{\boldsymbol{u}}^{\mu}, \hat{y}) = \int_{\Omega} \psi_{\square}(\hat{\boldsymbol{u}}^{\mathrm{M}} + \hat{\boldsymbol{u}}^{\mu}, \hat{y})\, \mathrm{d}\Omega - l^{(u)}(\hat{\boldsymbol{u}}^{\mathrm{M}} + ??) - l^{(y)}(\hat{y}) \tag{8.115}$$

where we introduced the RVE-functional

{eq:6-124}
$$\psi_{\square}(\hat{\boldsymbol{u}}, \hat{y}) \stackrel{\text{def}}{=} \langle \psi(\boldsymbol{\epsilon}[\hat{\boldsymbol{u}}], \boldsymbol{\zeta}[\hat{y}]) \rangle_{\square} \tag{8.116}$$

{eq:6-125} and the external potentials $\mathrm{l}^{(u)}(\hat{\boldsymbol{u}}) \stackrel{\text{def}}{=} \int_{\Gamma_{\mathrm{N}}^{(u)}} \boldsymbol{t}_{\mathrm{p}} \cdot \hat{\boldsymbol{u}}\, \mathrm{d}\Gamma$,
$l^{(y)}(\hat{y}) \stackrel{\text{def}}{=} \int_{\Gamma_{\mathrm{N}}^{(y)}} q_{\mathrm{p}} \hat{y}\, \mathrm{d}\Gamma$,

The saddle-point problem (8.108) is replaced by

{eq:6-126}
$$\inf_{\hat{\boldsymbol{u}}^{\mathrm{M}} \in \mathbb{U}^{\mathrm{M}}} \inf_{\hat{\boldsymbol{u}}^{\mu} \in \mathbb{U}^{\mu}} \sup_{\hat{y} \in \mathbb{Y}} \Pi(\hat{\boldsymbol{u}}^{\mathrm{M}}, \hat{\boldsymbol{u}}^{\mu}, \hat{y}) \tag{8.118}$$

{eq:6-127} whose corresponding stationarity conditions are given as

$$\begin{aligned} \Pi'_{u^{\mathrm{M}}}(\boldsymbol{u}^{\mathrm{M}}, \boldsymbol{u}^{\mu}, y; \delta\boldsymbol{u}^{\mathrm{M}}) &= \int_{\Omega} a_{\square}^{(u)}(\boldsymbol{u}^{\mathrm{M}} + \boldsymbol{u}^{\mu}, y; \delta\boldsymbol{u}^{\mathrm{M}})\, \mathrm{d}\Omega - l^{(u)}(\delta\boldsymbol{u}^{\mathrm{M}}) \\ &= 0 \quad \forall \delta\boldsymbol{u}^{\mathrm{M}} \in \mathbb{U}^{\mathrm{M},0}, \end{aligned} \tag{8.119a}$$
{eq:6-127a}

$$\begin{aligned} \Pi'_{u^{\mu}}(\boldsymbol{u}^{\mathrm{M}}, \boldsymbol{u}^{\mu}, y; \delta\boldsymbol{u}^{\mu}) &= \int_{\Omega} a_{\square}^{(u)}(\boldsymbol{u}^{\mathrm{M}} + \boldsymbol{u}^{\mu}, y; \delta\boldsymbol{u}^{\mu})\, \mathrm{d}\Omega \\ &= 0 \quad \forall \delta\boldsymbol{u}^{\mu} \in \mathbb{U}^{\mu} \end{aligned} \tag{8.119b}$$
{eq:6-127b}

$$\begin{aligned} \Pi'_{y}(\boldsymbol{u}^{\mathrm{M}}, \boldsymbol{u}^{\mu}, y; \delta y) &= \int_{\Omega} a_{\square}^{(y)}(\boldsymbol{u}^{\mathrm{M}} + \boldsymbol{u}^{\mu}, y; \delta y)\, \mathrm{d}\Omega - l^{(y)}(\delta y) \\ &= 0 \quad \forall \delta y \in \mathbb{Y}^{0} \end{aligned} \tag{8.119c}$$
{eq:6-127c}

{eq:6-128} where the following RVE-forms are introduced:

{eq:6-128a}
$$a_{\square}^{(u)}(\boldsymbol{u}, y; \delta\boldsymbol{u}) = (\psi_{\square})'_{u}(\boldsymbol{u}, y; \delta\boldsymbol{u}) \stackrel{\text{def}}{=} \langle \boldsymbol{\sigma}(\boldsymbol{\epsilon}[\boldsymbol{u}], \boldsymbol{\zeta}[y]) : \boldsymbol{\epsilon}[\delta\boldsymbol{u}] \rangle_{\square} \tag{8.120a}$$
{eq:6-128b}
$$a_{\square}^{(y)}((\boldsymbol{u}, y; \delta y) = (\psi_{\square})'_{y}((\boldsymbol{u}, y; \delta y) \stackrel{\text{def}}{=} \langle -\boldsymbol{b}(\boldsymbol{\epsilon}[\boldsymbol{u}], \boldsymbol{\zeta}[y]) \cdot \boldsymbol{\zeta}[\delta y] \rangle_{\square} \tag{8.120b}$$

Next, we introduce the linear prolongation operator $\mathcal{A}^{(u)}$ such that

{eq:6-129}
$$\boldsymbol{u} = \mathcal{A}^{(u)} \bar{\boldsymbol{u}} + \boldsymbol{u}^{\mu}, \tag{8.121}$$

where $\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}$ is the macroscale displacement field.

For any given $\hat{\boldsymbol{u}}$, the purpose of localization to RVE-problems is to obtain solutions $\boldsymbol{u}^{\mu}\{\hat{\boldsymbol{u}}\}$ and $y\{\hat{\boldsymbol{u}}\}$. The macroscale solution $\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}$ then satisfies the homogenized problem

{eq:6-131}
$$\begin{aligned} R^{(u)}\{\bar{\boldsymbol{u}};\delta\bar{\boldsymbol{u}}\} &= \Pi'_{u^{\mathrm{M}}}(\mathcal{A}^{(u)}\bar{\boldsymbol{u}}, \boldsymbol{u}^{\mu}\{\bar{\boldsymbol{u}}\}, y\{\bar{\boldsymbol{u}}\}; \mathcal{A}^{(u)}\delta\bar{\boldsymbol{u}}) \\ &= \int_{\Omega} \left[a_{\square}^{(u)}(\mathcal{A}^{(u)}\bar{\boldsymbol{u}} + \boldsymbol{u}^{\mu}\{\bar{\boldsymbol{u}}\}, y\{\bar{\boldsymbol{u}}\}; \mathcal{A}^{(u)}\delta\bar{\boldsymbol{u}})\,\mathrm{d}\Omega - l_{\square}^{(u)}(\mathcal{A}^{(u)}\delta\bar{\boldsymbol{u}}) \right] \mathrm{d}\Omega \\ &= 0 \quad \forall \delta\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}^0 \end{aligned} \tag{8.122}$$

Next, we define the macroscale potential

$$\bar{\Pi}\{\hat{\boldsymbol{u}}\} \stackrel{\text{def}}{=} \Pi(\mathcal{A}^{(u)}\hat{\boldsymbol{u}}, \boldsymbol{u}^{\mu}\{\hat{\boldsymbol{u}}\}, y\{\hat{\boldsymbol{u}}\}) \tag{8.123}$$ {eq:6-132}

which is assumed to have its minimum at the homogenized solution $\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}$, i.e.

$$\bar{\boldsymbol{u}} = \arg\left[\inf_{\hat{\boldsymbol{u}} \in \hat{\mathbb{U}}} \bar{\Pi}\{\hat{\boldsymbol{u}}\} \right] \tag{8.124}$$ {eq:6-133}

provided that the appropriate VCMH-condition is satisfied by the local fields $\boldsymbol{u}^{\mu}\{\bar{\boldsymbol{u}}\}$ and $y\{\bar{\boldsymbol{u}}\}$. The corresponding VCMH-condition is

$$\begin{aligned} \Pi'_{\bar{u}}\{\bar{\boldsymbol{u}};\delta\bar{\boldsymbol{u}}\} = & \underbrace{\Pi'_{u^{\mathrm{M}}}(\mathcal{A}^{(u)}\bar{\boldsymbol{u}}, \boldsymbol{u}^{\mu}\{\bar{\boldsymbol{u}}\}, y\{\bar{\boldsymbol{u}}\}; \mathcal{A}^{(u)}\delta\bar{\boldsymbol{u}})}_{=0 \text{ from } (\mathbf{??})} \\ & + \Pi'_{u^{\mu}}(\mathcal{A}^{(u)}\bar{\boldsymbol{u}}, \boldsymbol{u}^{\mu}\{\bar{\boldsymbol{u}}\}, y\{\bar{\boldsymbol{u}}\}; \mathcal{S}_u^{(u)}\delta\bar{\boldsymbol{u}}) \\ & + \Pi'_{y}(\mathcal{A}^{(u)}\bar{\boldsymbol{u}}, \boldsymbol{u}^{\mu}\{\bar{\boldsymbol{u}}\}, y\{\bar{\boldsymbol{u}}\}; \mathcal{S}_u^{(y)}\delta\bar{\boldsymbol{u}}) \\ = & 0 \quad \forall \delta\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}^0 \end{aligned} \tag{8.125}$$ {eq:6-133}

where we introduced the sensitivities $\mathcal{S}_u^{(u)}\delta\bar{\boldsymbol{u}} \stackrel{\text{def}}{=} (\boldsymbol{u}^{\mu})'_u\{\bar{\boldsymbol{u}},\delta\bar{\boldsymbol{u}}\}$ and $\mathcal{S}_u^{(y)}\delta\bar{\boldsymbol{u}} \stackrel{\text{def}}{=} (y)'_u\{\bar{\boldsymbol{u}};\delta\bar{\boldsymbol{u}}\}$. Utilizing the explicit expressions for $\Pi'_{u^{\mu}}$ and Π'_{y}, we conclude that the local version of the VCMH-condition reads as follows:

$$a_{\square}^{(u)}(\mathcal{A}^{(u)}\bar{\boldsymbol{u}}+\boldsymbol{u}^{\mu}\{\bar{\boldsymbol{u}}\}, y\{\bar{\boldsymbol{u}}\}; \mathcal{S}_u^{(u)}\delta\bar{\boldsymbol{u}}) + a_{\square}^{(y)}(\mathcal{A}^{(u)}\bar{\boldsymbol{u}}+\boldsymbol{u}^{\mu}\{\bar{\boldsymbol{u}}\}, y\{\bar{\boldsymbol{u}}\}; \mathcal{S}_u^{(y)}\delta\bar{\boldsymbol{u}}) = 0 \quad \forall \delta\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}^0 \tag{8.126}$$ {eq:6-134}

We may directly proceed to establish the pertinent relations for the standard 1st order homogenization applied to the displacement field.

8.5.4 1st order homogenization

In the standard case of 1st order homogenization, $\bar{\boldsymbol{u}}$ is prolonged via assumed linear variation within each RVE:

$$(\mathcal{A}^{(u)}\bar{\boldsymbol{u}})(\bar{\boldsymbol{x}},\boldsymbol{x}) = \bar{\boldsymbol{u}}(\bar{\boldsymbol{x}}) + \bar{\boldsymbol{h}}(\bar{\boldsymbol{x}}) \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}], \quad \bar{\boldsymbol{h}} \stackrel{\text{def}}{=} \bar{\boldsymbol{u}} \otimes \boldsymbol{\nabla}, \quad \boldsymbol{x} \in \Omega_{\square} \tag{8.127}$$ {eq:6-135}

It is a straightforward task to show that the prolongation $\mathcal{A}^{(u)}\bar{\boldsymbol{u}}$ to the total local strain only involves the macroscale strain $\bar{\boldsymbol{\epsilon}}$. We thus conclude that it is only $\bar{\boldsymbol{\epsilon}}$ that "drives" the RVE-problems; hence, we may express $\boldsymbol{u}^{\mu} = \boldsymbol{u}^{\mu}\{\bar{\boldsymbol{\epsilon}}\}$, $y = y\{\bar{\boldsymbol{\epsilon}}\}$, $\boldsymbol{\lambda}_{\mathrm{t}} = \boldsymbol{\lambda}_{\mathrm{t}}\{\bar{\boldsymbol{\epsilon}}\}$, $\lambda_{\mathrm{q}} = \lambda_{\mathrm{q}}\{\bar{\boldsymbol{\epsilon}}\}$. As a result, the homogenized problem (weak format) becomes: Find $\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}$ s.t.

$$\int_{\Omega} \bar{\boldsymbol{\sigma}}\{\bar{\boldsymbol{\epsilon}}\} : [\delta\bar{\boldsymbol{u}} \otimes \boldsymbol{\nabla}]\,\mathrm{d}\Omega = \int_{\Gamma_{\mathrm{N}}^{(u)}} \bar{\boldsymbol{t}}_{\mathrm{p}} \cdot \delta\bar{\boldsymbol{u}}\,\mathrm{d}\Gamma \quad \forall \delta\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}^0 \tag{8.128}$$ {eq:6-136}

where we derived the macroscale variables:

$$\bar{\boldsymbol{\sigma}}\{\bar{\boldsymbol{\epsilon}}\} = \langle \boldsymbol{\sigma} \rangle_{\square}, \tag{8.129}$$ {eq:6-137}

We recall the constitutive relation for $\boldsymbol{\sigma}$ in (8.113a).

8.5.5 RVE-problem based on weak periodicity

Like for the model problem of nonlinear elasticity, it turns out to be convenient to choose $\boldsymbol{u}$ and y (rather than $\boldsymbol{u}^\mu$ and y^μ) as the unknown fields in a canonical format of the RVE-problem. To this end, we introduce the solution and test spaces as follows:

$$\mathbb{U}_\square = \{\boldsymbol{u}' \text{ suff. regular in } \Omega_\square,\ \boldsymbol{u}'(\tilde{\boldsymbol{x}}) = \boldsymbol{0}\} \tag{8.130a}$$

$$\mathbb{Y}_\square = \{y' \text{ suff. regular in } \Omega_\square,\ y'(\tilde{\boldsymbol{x}}) = 0\} \tag{8.130b}$$

$$\mathbb{L}_{\mathrm{t},\square} = \mathbb{L}_2(\Gamma_\square^+) \tag{8.130c}$$

$$\mathbb{L}_{\mathrm{q},\square} = \mathbb{L}_2(\Gamma_\square^+) \tag{8.130d}$$

{eq:6-138} Further, we introduce the bilinear forms expressing weak periodicity:

{eq:6-138a}
$$d_\square^{(u)}(\boldsymbol{\lambda}_\mathrm{t}, \boldsymbol{u}) \stackrel{\mathrm{def}}{=} \frac{1}{|\Omega_\square|} \int_{\Gamma_\square^+} \boldsymbol{\lambda}_\mathrm{t} \cdot [\![\boldsymbol{u}]\!] \,\mathrm{d}\Gamma \tag{8.131a}$$

{eq:6-138b}
$$d_\square^{(y)}(\lambda_\mathrm{q}, y) \stackrel{\mathrm{def}}{=} \frac{1}{|\Omega_\square|} \int_{\Gamma_\square^+} \lambda_\mathrm{q} [\![y]\!] \,\mathrm{d}\Gamma \tag{8.131b}$$

and we propose a canonical format of the RVE-problem: For given value of $\bar{\boldsymbol{\epsilon}}$, find $\boldsymbol{u} \in \mathbb{U}_\square$, $y \in \mathbb{Y}_\square$
{eq:6-139} and $\boldsymbol{\lambda}_\mathrm{t} \in \mathbb{L}_{\mathrm{t},\square}$, $\lambda_\mathrm{q} \in \mathbb{L}_{\mathrm{q},\square}$ that solve the system

{eq:6-139a}
$$a_\square^{(u)}(\boldsymbol{u}, y; \delta\boldsymbol{u}) - d_\square^{(u)}(\boldsymbol{\lambda}_\mathrm{t}, \delta\boldsymbol{u}) = 0 \qquad \forall \delta\boldsymbol{u} \in \mathbb{U}_\square \tag{8.132a}$$

{eq:6-139b}
$$a_\square^{(y)}(\boldsymbol{u}, y; \delta y) - d_\square^{(y)}(\lambda_\mathrm{q}, \delta y) = 0 \qquad \forall \delta y \in \mathbb{Y}_\square \tag{8.132b}$$

{eq:6-139c}
$$-d_\square^{(u)}(\delta\boldsymbol{\lambda}_\mathrm{t}, \boldsymbol{u}) = -d_\square^{(u)}(\delta\boldsymbol{\lambda}_\mathrm{t}, \bar{\boldsymbol{\epsilon}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}]) \qquad \forall \delta\boldsymbol{\lambda}_\mathrm{t} \in \mathbb{L}_{\mathrm{t},\square} \tag{8.132c}$$

{eq:6-139d}
$$-d_\square^{(y)}(\delta\lambda_\mathrm{q}, y) = 0 \qquad \forall \delta\lambda_\mathrm{q} \in \mathbb{L}_{\mathrm{q},\square} \tag{8.132d}$$

The pertinent RVE-potential is[9], for any given $\bar{\boldsymbol{\epsilon}}$,

{eq:6-141}
$$\pi_\square(\bar{\boldsymbol{\epsilon}}; \hat{\boldsymbol{u}}, \hat{y}, \hat{\boldsymbol{\lambda}}_\mathrm{t}, \hat{\lambda}_\mathrm{q}) = \psi_\square(\hat{\boldsymbol{u}}, \hat{y}) - d_\square^{(u)}(\hat{\boldsymbol{\lambda}}_\mathrm{t}, \hat{\boldsymbol{u}} - \bar{\boldsymbol{\epsilon}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}]) - d_\square^{(\mathrm{q})}(\hat{\lambda}_\mathrm{q}, \hat{y}) \tag{8.133}$$

whose stationarity conditions are those given in (8.132).

Satisfaction of VCMH-condition

Finally in this Subsection, we show that the VCMH-condition is satisfied upon adopting the model assumption of micro-periodic fluctuations. Firstly, rewrite (8.132) as follows: For any given macroscale fields $\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}$, compute $\boldsymbol{u}^\mu \in \mathbb{U}_\square$, $y \in \mathbb{Y}_\square$ and $\boldsymbol{\lambda}_\mathrm{t} \in \mathbb{L}_{\mathrm{t},\square}$, $\lambda_\mathrm{q} \in \mathbb{L}_{\mathrm{q},\square}$ that solve
{eq:6-142} the system

{eq:6-142a}
$$a_\square^{(u)}(\mathcal{A}^{(u)}\bar{\boldsymbol{u}} + \boldsymbol{u}^\mu, y; \delta\boldsymbol{u}^\mu) - d_\square^{(u)}(\boldsymbol{\lambda}_\mathrm{t}, \delta\boldsymbol{u}^\mu) = 0 \quad \forall \delta\boldsymbol{u}^\mu \in \mathbb{U}_\square \tag{8.134a}$$

{eq:6-142b}
$$a_\square^{(y)}(\mathcal{A}^{(u)}\bar{\boldsymbol{u}} + \boldsymbol{u}^\mu, y; \delta y) - d_\square^{(y)}(\lambda_\mathrm{q}, \delta y) = 0 \quad \forall \delta y \in \mathbb{Y}_\square \tag{8.134b}$$

{eq:6-142c}
$$-d_\square^{(u)}(\delta\boldsymbol{\lambda}_\mathrm{t}, \boldsymbol{u}^\mu) = 0 \quad \forall \delta\boldsymbol{\lambda}_\mathrm{t} \in \mathbb{L}_{\mathrm{t},\square} \tag{8.134c}$$

{eq:6-142d}
$$-d_\square^{(y)}(\delta\lambda_\mathrm{q}, y) = 0 \quad \forall \delta\lambda_\mathrm{q} \in \mathbb{L}_{\mathrm{q},\square} \tag{8.134d}$$

We then argue as follows:

[9] The source $l_\square$ is ignored for brevity of notation.

Figure 8.5: Fine-scale features of seepage through a porous rigid medium **NEW FIGURE** {figure5}

- For a given perturbation $\mathrm{d}\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}^0$, choose $\delta \boldsymbol{u}^\mu = \mathcal{S}_u^{(u)}\,\mathrm{d}\bar{\boldsymbol{u}} \subseteq \mathbb{U}_\Box$ in (8.134a) and $\delta y = \mathcal{S}_u^{(y)}\,\mathrm{d}\bar{\boldsymbol{u}} \subseteq \mathbb{Y}_\Box$ in (8.134b) to obtain {eq:6-143}

{eq:6-143a}
{eq:6-143b}
$$a_\Box^{(u)}(\mathcal{A}^{(u)}\bar{\boldsymbol{u}} + \boldsymbol{u}^\mu, y; \mathcal{S}_u^{(u)}\,\mathrm{d}\bar{\boldsymbol{u}}) - d_\Box^{(u)}(\boldsymbol{\lambda}_\mathrm{t}, \mathcal{S}_u^{(u)}\,\mathrm{d}\bar{\boldsymbol{u}}) = 0 \tag{8.135a}$$
$$a_\Box^{(y)}(\mathcal{A}^{(u)}\bar{\boldsymbol{u}} + \boldsymbol{u}^\mu, y; \mathcal{S}_u^{(y)}\,\mathrm{d}\bar{\boldsymbol{u}}) - d_\Box^{(y)}(\lambda_\mathrm{q}, \mathcal{S}_u^{(y)}\,\mathrm{d}\bar{\boldsymbol{u}}) = 0 \tag{8.135b}$$

- Linearize (8.134c) and (8.134d), respectively, w.r.t. $\bar{\boldsymbol{u}}$. Introduce $\mathrm{d}\boldsymbol{u}^\mu = \mathcal{S}_u^{(u)}\,\mathrm{d}\bar{\boldsymbol{u}}$ and $\mathrm{d}y = \mathcal{S}_u^{(y)}\,\mathrm{d}\bar{\boldsymbol{u}}$, respectively. Choose $\delta\boldsymbol{\lambda}_\mathrm{t} = \boldsymbol{\lambda}_\mathrm{t}\{\bar{\boldsymbol{u}}\} \in \mathbb{L}_{\mathrm{t},\Box}$ and $\delta\lambda_\mathrm{q} = \lambda_\mathrm{q}\{\bar{\boldsymbol{u}}\} \in \mathbb{L}_{\mathrm{q},\Box}$ in the linearized (8.134c) and (8.134d), respectively. We then obtain {eq:6-144}

$$-d_\Box^{(u)}(\boldsymbol{\lambda}_\mathrm{t}, \mathcal{S}_u^{(u)}\,\mathrm{d}\bar{\boldsymbol{u}}) = 0 \tag{8.136a}$$ {eq:6-144c}
$$-d_\Box^{(y)}(\lambda_\mathrm{q}, \mathcal{S}_u^{(y)}\,\mathrm{d}\bar{\boldsymbol{u}}) = 0 \tag{8.136b}$$ {eq:6-144d}

Now, combining (8.135) and (8.136), we obtain the two identities {eq:6-145}

$$a_\Box^{(u)}(\mathcal{A}^{(u)}\bar{\boldsymbol{u}} + \boldsymbol{u}^\mu, y; \mathcal{S}_u^{(u)}\,\mathrm{d}\bar{\boldsymbol{u}}) = 0 \tag{8.137a}$$ {eq:6-145a}
$$a_\Box^{(y)}(\mathcal{A}^{(u)}\bar{\boldsymbol{u}} + \boldsymbol{u}^\mu, y; \mathcal{S}_u^{(y)}\,\mathrm{d}\bar{\boldsymbol{u}}) = 0 \tag{8.137b}$$ {eq:6-145b}

which represent *sufficient* conditions for satisfying the VCMH-conditions (8.126).

8.6 Variationally consistent selective homogenization and equation switching – Application to a model problem of seepage in a rigid medium

8.6.1 Preliminaries

8.6.2 Stokes' flow in rigid medium

We consider the classical problem of a fluid that seeps through the open pore system of a rgid porous medium, typically a granular material. On the fine scale, the fluid flow is assumed here to be goverened by incompressible Stokes' flow (as a model), whereas the corresponding macroscale representation is Darcy-type seepage. This model, which is obtained from homogenization, is characterized by the macroscale permeability, and it is driven by the macroscale pressure gradient. Since only the continuity equation is homogenized and, thus, the momentum equation remains completely local, cf. SandstrÃ¶m et al. **?**, we encounter a situation of "selective homogenization".

The fine-scale problem is defined as follows: The fluid flow takes place within the connected flow domain Ω^f with exterior boundary Γ^f, as shown in Figure 8.5. The internal boundary of the obstacles (rigid medium) is denoted Γ^obs. In standard fashion, we have $\Gamma^\mathrm{f} = \Gamma^\mathrm{f}_\mathrm{D} \cup \Gamma^\mathrm{f}_\mathrm{N}$ with prescribed tractions $\boldsymbol{t} = \boldsymbol{t}_\mathrm{p}$ on $\Gamma^\mathrm{f}_\mathrm{N}$ and prescribed velocity $\boldsymbol{v} = \bar{\boldsymbol{v}}_\mathrm{p}$ on $\Gamma^\mathrm{f}_\mathrm{N}$. For simplicity, we also choose the condition $\boldsymbol{v} = \boldsymbol{0}$ on Γ^obs. We thus seek the velocity $\boldsymbol{v}(\boldsymbol{x}) : \Omega^\mathrm{f} \to \mathbb{R}^3$ and the pressure

$p(\boldsymbol{x}) : \Omega^{\mathrm{f}} \to \mathbb{R}$ that solve the system {eq4-03}

$$-\boldsymbol{\sigma}(\boldsymbol{d}[\boldsymbol{v}], p) \cdot \boldsymbol{\nabla} = \boldsymbol{0} \quad \text{in } \Omega^{\mathrm{f}} \tag{8.138a}$$ {eq4-03a}

$$\boldsymbol{v} \cdot \boldsymbol{\nabla} = 0 \quad \text{in } \Omega^{\mathrm{f}} \tag{8.138b}$$ {eq4-03b}

$$\boldsymbol{u} = \boldsymbol{u}_{\mathrm{p}} \quad \text{on } \Gamma_{\mathrm{D}}^{\mathrm{f}} \text{ and } \boldsymbol{u} = \boldsymbol{0} \quad \text{on } \Gamma^{\mathrm{obs}} \tag{8.138c}$$ {eq4-03c}

$$\boldsymbol{t} \stackrel{\text{def}}{=} \boldsymbol{\sigma} \cdot \boldsymbol{n} = \boldsymbol{t}_{\mathrm{p}} \quad \text{on } \Gamma_{\mathrm{N}}^{\mathrm{f}} \tag{8.138d}$$ {eq4-03d}

Clearly, (8.138a) represents equilibrium, whereas (8.138b) expresses incompressibility of the fluid.

As to the definition of constitutive relations, we assume the existence of a volume-specific potential

{eq4-1}

$$\phi(\boldsymbol{d}, p) \stackrel{\text{def}}{=} \phi_{\mathrm{v}}(\boldsymbol{d}) - p\boldsymbol{I} : \boldsymbol{d}, \quad \boldsymbol{d} = \boldsymbol{d}[\boldsymbol{v}] \stackrel{\text{def}}{=} (\boldsymbol{v} \otimes \boldsymbol{\nabla})^{\mathrm{sym}}, \tag{8.139}$$

i. e. $\boldsymbol{I} : \boldsymbol{d} = \boldsymbol{v} \cdot \boldsymbol{\nabla}$, whereby the total stress $\boldsymbol{\sigma}(\boldsymbol{d}, p)$ can be computed as

{eq4-2}

$$\boldsymbol{\sigma}(\boldsymbol{d}, p) = \frac{\partial \phi(\boldsymbol{d}, p)}{\partial \boldsymbol{d}} = \frac{\partial \phi_{\mathrm{v}}(\boldsymbol{d})}{\partial \boldsymbol{d}} - p\boldsymbol{I} = \boldsymbol{\sigma}^{\mathrm{v}}(\boldsymbol{d}) - p\boldsymbol{I}, \quad \boldsymbol{\sigma}^{\mathrm{v}}(\boldsymbol{d}) = \frac{\partial \phi_{\mathrm{v}}(\boldsymbol{d})}{\partial \boldsymbol{d}} \tag{8.140}$$

We assume that $\phi_{\mathrm{v}}(\boldsymbol{d})$ is convex, whereby we conclude that $\phi(\boldsymbol{d}[\boldsymbol{v}], p)$ is convex in $\boldsymbol{d}$ and linear in p. Obviously, the simplest model is a Newtonian fluid defined by $\phi_{\mathrm{v}}(\boldsymbol{d}) = \mu|\boldsymbol{d}|^2$ which infers $\boldsymbol{\sigma}^{\mathrm{v}}(\boldsymbol{d}) = 2\mu\boldsymbol{d}$.

Next, we introduce the Hellinger-Reissner type potential

{eq4-3}

$$\Pi(\hat{\boldsymbol{v}}, \hat{p}) = \Phi(\hat{\boldsymbol{v}}, \hat{p}) - l(\hat{\boldsymbol{v}}) \tag{8.141}$$

where

{eq4-4}

$$\Phi(\hat{\boldsymbol{v}}, \hat{p}) \stackrel{\text{def}}{=} \int_{\Omega^{\mathrm{f}}} \phi(\boldsymbol{d}[\hat{\boldsymbol{v}}], \hat{p}) \, \mathrm{d}\Omega, \quad l(\hat{\boldsymbol{v}}) \stackrel{\text{def}}{=} \int_{\Gamma_{\mathrm{N}}^{\mathrm{f}}} \boldsymbol{t}_{\mathrm{p}} \cdot \hat{\boldsymbol{v}} \, \mathrm{d}\Gamma, \tag{8.142}$$

{eq:6-201} and we define the appropriate spaces

eq:6-201a}

$$\mathbb{V} = \{\boldsymbol{v}' \text{ suff. regular} |\ \boldsymbol{v}' = \boldsymbol{v}_{\mathrm{p}} \text{ on } \Gamma_{\mathrm{D}}^{\mathrm{f}}\} \tag{8.143a}$$

eq:6-201b}

$$\mathbb{V}^0 = \{\boldsymbol{v}' \text{ suff. regular} |\ \boldsymbol{v}' = \boldsymbol{0} \text{ on } \Gamma_{\mathrm{D}}^{\mathrm{f}}\} \tag{8.143b}$$

eq:6-201c}

$$\mathbb{P} = \{p' \text{ suff. regular}\}. \tag{8.143c}$$

It is possible to show that $\Phi(\hat{\boldsymbol{v}}, \hat{p})$ is convex/linear in $\mathbb{V} \times \mathbb{P}$, i.e. we are in the position to pose the
remal prop fine-scale problem as the constrained minimization problem (degenerated saddle-point problem)

{eq4-6}

$$(\boldsymbol{v}, p) = \arg\left[\inf_{\hat{\boldsymbol{v}} \in \mathbb{V}} \sup_{\hat{p} \in \mathbb{P}} \Pi(\hat{\boldsymbol{v}}, \hat{p})\right] = \arg\left[\sup_{\hat{p} \in \mathbb{P}} \inf_{\hat{\boldsymbol{v}} \in \mathbb{V}} \Pi(\hat{\boldsymbol{v}}, \hat{p})\right] \tag{8.144}$$

{eq4-7} The stationarity conditions of $\Pi(\boldsymbol{v}, p)$ are given as

{eq4-7a}

$$\begin{aligned}\Pi'_v(\boldsymbol{v}, p; \delta\boldsymbol{v}) &= \int_{\Omega^{\mathrm{f}}} \boldsymbol{\sigma}^{\mathrm{v}}(\boldsymbol{d}[\boldsymbol{v}]) : \boldsymbol{d}[\delta\boldsymbol{v}] \, \mathrm{d}\Omega - \int_{\Omega^{\mathrm{f}}} p \, [\delta\boldsymbol{v} \cdot \boldsymbol{\nabla}] \, \mathrm{d}\Omega - l(\delta\boldsymbol{v}) \\ &= 0 \quad \forall \delta\boldsymbol{v} \in \mathbb{V}^0\end{aligned} \tag{8.145a}$$

{eq4-7b}

$$\begin{aligned}\Pi'_p(\boldsymbol{v}, p; \delta p) &= -\int_{\Omega^{\mathrm{f}}} \delta p \, [\boldsymbol{v} \cdot \boldsymbol{\nabla}] \, \mathrm{d}\Omega \\ &= 0 \quad \forall \delta p \in \mathbb{P}\end{aligned} \tag{8.145b}$$

8.6.3 Two-scale setting – Preliminaries

Next, we pave the way for "selective homogenization" by introducing the VMS-split of the pressure

{eq4-10}
$$p = p^{\mathrm{M}} + p^{\mu}, \quad (p^{\mathrm{M}}, p^{\mu}) \in \mathbb{P}^{\mathrm{M}} \oplus \mathbb{P}^{\mu} \tag{8.146}$$

whereas the velocity $\boldsymbol{v}$ does not possess any macroscale component, i.e. $\boldsymbol{v} = \boldsymbol{v}^{\mu}$. As a consequence, (8.145) is rephrased as the three equations {eq4-322}

$$\int_{\Omega^{\mathrm{f}}} \boldsymbol{\sigma}^{\mathrm{v}}(\boldsymbol{d}[\boldsymbol{v}])\colon \boldsymbol{d}[\delta\boldsymbol{v}]\,\mathrm{d}\Omega - \int_{\Omega^{\mathrm{f}}} [p^{\mathrm{M}} + p^{\mu}]\,[\delta\boldsymbol{v}\cdot\boldsymbol{\nabla}]\,\mathrm{d}\Omega - l(\delta\boldsymbol{v}) = 0 \quad \forall\delta\boldsymbol{v} \in \mathbb{V}^0 \tag{8.147a}$$ {eq4-322a}

$$-\int_{\Omega^{\mathrm{f}}} \delta p^{\mathrm{M}}\,[\boldsymbol{v}\cdot\boldsymbol{\nabla}]\,\mathrm{d}\Omega = 0 \quad \forall\delta p^{\mathrm{M}} \in \mathbb{P}^{\mathrm{M},0} \tag{8.147b}$$ {eq4-322b}

$$-\int_{\Omega^{\mathrm{f}}} \delta p^{\mu}\,[\boldsymbol{v}\cdot\boldsymbol{\nabla}]\,\mathrm{d}\Omega = 0 \quad \forall\delta p^{\mu} \in \mathbb{P}^{\mu} \tag{8.147c}$$ {eq4-322c}

The definition of $\mathbb{P}^{\mathrm{M}}$, $\mathbb{P}^{\mathrm{M},0}$ requires some further clarification. To this end, we make the specific assumption that the prescribed traction on $\Gamma_{\mathrm{N}}^{\mathrm{f}}$ can be represented as $\boldsymbol{t}_{\mathrm{p}} = -\boldsymbol{n}\bar{p}_{\mathrm{p}}$, where the pressure $\bar{p}_{\mathrm{p}}$ is a prescribed value on the boundary part $\Gamma_{\mathrm{N}}^{\mathrm{f}}$. As a consequence, pressures in the space $\mathbb{P}^{\mathrm{M}}$ will satisfy the condition $p^{\mathrm{M}} = \bar{p}_{\mathrm{p}}$ on $\Gamma_{\mathrm{N}}^{\mathrm{f}}$ and, hence, $\delta p^{\mathrm{M}} \in \mathbb{P}^{\mathrm{M},0}$ will satisfy the condition $\delta p^{\mathrm{M}} = 0$ on $\Gamma_{\mathrm{N}}^{\mathrm{f}}$. Moreover, the boundary term $l(\delta\boldsymbol{v})$ in (8.147a) becomes

$$l(\delta\boldsymbol{v}) = -\int_{\Gamma_{\mathrm{N}}^{\mathrm{f}}} \bar{p}_{\mathrm{p}}\,[\delta\boldsymbol{v}\cdot\boldsymbol{n}]\,\mathrm{d}\Gamma \tag{8.148}$$ {eq4-10a}

Next, we integrate the volume integrals containing p^{M} in (8.147a) and δp^{M} in (8.147b) by parts, which is followed by rearranging the order of the resulting equations, whereby we obtain {eq4-323}

$$\int_{\Omega^{\mathrm{f}}} \boldsymbol{v}\cdot\boldsymbol{\nabla}\delta p^{\mathrm{M}}\,\mathrm{d}\Omega - \int_{\Gamma_{\mathrm{D}}^{\mathrm{f}}} q\,\delta p^{\mathrm{M}}\,\mathrm{d}\Gamma = 0 \qquad \forall\delta p^{\mathrm{M}} \in \mathbb{P}^{\mathrm{M},0} \tag{8.149a}$$ {eq4-323a}

$$\int_{\Omega^{\mathrm{f}}} \boldsymbol{\sigma}^{\mathrm{v}}(\boldsymbol{d}[\boldsymbol{v}])\colon \boldsymbol{d}[\delta\boldsymbol{v}]\,\mathrm{d}\Omega - \int_{\Omega^{\mathrm{f}}} p^{\mu}\,[\delta\boldsymbol{v}\cdot\boldsymbol{\nabla}]\,\mathrm{d}\Omega = -\int_{\Omega^{\mathrm{f}}} \boldsymbol{\nabla}p^{\mathrm{M}}\cdot\delta\boldsymbol{v}\,\mathrm{d}\Omega \quad \forall\delta\boldsymbol{v} \in \mathbb{V}^0 \tag{8.149b}$$ {eq4-323b}

$$-\int_{\Omega^{\mathrm{f}}} \delta p^{\mu}\,[\boldsymbol{v}\cdot\boldsymbol{\nabla}]\,\mathrm{d}\Omega = 0 \qquad \forall\delta p^{\mu} \in \mathbb{P}^{\mu} \tag{8.149c}$$ {eq4-323c}

where $q \overset{\mathrm{def}}{=} \boldsymbol{v}\cdot\boldsymbol{n}$ is the outflow velocity on the boundary Γ^{f}. In order to obtain (8.149a) we used that $\delta p^{\mathrm{M}} = 0$ on $\Gamma_{\mathrm{N}}^{\mathrm{f}}$ for $\delta p^{\mathrm{M}} \in \mathbb{P}^{\mathrm{M},0}$. Moreover, in order to obtain (8.149b) we used that $\delta\boldsymbol{v} = \boldsymbol{0}$ on $\Gamma_{\mathrm{D}}^{\mathrm{f}}$ for $\delta\boldsymbol{v} \in \mathbb{V}^0$, with the result that all boundary terms disappear in this equation.

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$\langle\langle q\rangle\rangle_{\square} = \bar{q}_{\mathrm{p}}$ when $q = \boldsymbol{v}_{\mathrm{p}}\cdot\boldsymbol{n}$, prescribed velocÃty ???

8.6.4 Two-scale setting – Homogenization

Homogenization is introduced as volume averaging on the bulk domain $\Omega_{\square}$ that is occupied by the porous RVE and which contains the flow domain, $\Omega_{\square}^{\mathrm{f}} \subset \Omega_{\square}$, cf. Figure **??**. We thus introduce the following notation for the running bulk volume averages

$$\langle f\rangle_{\square}(\boldsymbol{x}) \overset{\mathrm{def}}{=} \frac{1}{|\Omega_{\square}(\boldsymbol{x})|}\int_{\Omega_{\square}^{\mathrm{f}}(\boldsymbol{x})} f\,\mathrm{d}\Omega, \quad \langle\langle g\rangle\rangle_{\square}(\boldsymbol{x}) \overset{\mathrm{def}}{=} \frac{1}{|\Omega_{\square}(\boldsymbol{x})|}\int_{\Omega_{\square}^{\mathrm{f}}(\boldsymbol{x})} g\,\mathrm{d}\Omega????? \tag{8.150}$$ {eq4-21}

We also introduce the change of notation $\Gamma_{\mathrm{D}}^{\mathrm{f}} \leftrightarrow \Gamma_{\mathrm{N}}$, $\Gamma_{\mathrm{N}}^{\mathrm{f}} \leftrightarrow \Gamma_{\mathrm{D}}$, whereby the boundary parts $\Gamma_{\mathrm{D}}, \Gamma_{\mathrm{N}}$ refer to Dirichlet and Neumann boundary conditions on the macroscale pressure $\bar{p}$. The
o satisfy fine-scale equations in (8.149) are then replaced by {eq4-522}
51c?

{eq4-522a} $$\int_{\Omega} \langle \boldsymbol{v} \cdot \boldsymbol{\nabla} \delta p^{\mathrm{M}} \rangle_{\Box} \, \mathrm{d}\Omega - \int_{\Gamma_{\mathrm{N}}} \langle\langle q \, \delta p^{\mathrm{M}} \rangle\rangle_{\Box} \, \mathrm{d}\Gamma = 0 \qquad \forall \delta p^{\mathrm{M}} \in \mathbb{P}^{\mathrm{M},0} \tag{8.151a}$$

{eq4-522b} $$\int_{\Omega} a_{\Box}(\boldsymbol{v}; \delta \boldsymbol{v}) \, \mathrm{d}\Omega - \int_{\Omega} b_{\Box}(p^{\mu}, \delta \boldsymbol{v}) \, \mathrm{d}\Omega = - \int_{\Omega} \langle \boldsymbol{\nabla} p^{\mathrm{M}} \cdot \delta \boldsymbol{v} \rangle_{\Box} \, \mathrm{d}\Omega \quad \forall \delta \boldsymbol{v} \in \mathbb{V}^0 \tag{8.151b}$$

{eq4-522c} $$- \int_{\Omega} b_{\Box}(\delta p^{\mu}, \boldsymbol{v}) \, \mathrm{d}\Omega = 0 \qquad \forall \delta p^{\mu} \in \mathbb{P}^{\mu} \tag{8.151c}$$

{eq4-523} where we introduced the RVE-forms

{eq4-523a} $$a_{\Box}(\boldsymbol{v}; \delta \boldsymbol{v}) = (\phi_{\Box})'_{v}(\boldsymbol{v}, p; \delta \boldsymbol{v}) \stackrel{\text{def}}{=} \langle \boldsymbol{\sigma}^{\mathrm{v}}(\boldsymbol{d}[\boldsymbol{v}]) : \boldsymbol{d}[\delta \boldsymbol{v}] \rangle_{\Box} \tag{8.152a}$$

{eq4-523b} $$b_{\Box}(\delta p, \boldsymbol{v}) = (\phi_{\Box})'_{p}(\boldsymbol{v}, p; \delta p) \stackrel{\text{def}}{=} \langle \delta p \, [\boldsymbol{v} \cdot \boldsymbol{\nabla}] \rangle_{\Box} \tag{8.152b}$$

{eq4-523c} $$\phi_{\Box}(\boldsymbol{v}, p) \stackrel{\text{def}}{=} \langle \phi(\boldsymbol{d}[\boldsymbol{v}], p) \rangle_{\Box} \tag{8.152c}$$

It appears that (8.151) can be identified as the stationarity condition of the problem

{eq4-524} $$\inf_{\hat{\boldsymbol{v}} \in \mathbb{V}} \sup_{\hat{p}^{\mathrm{M}} \in \mathbb{P}^{\mathrm{M}}} \sup_{\hat{p}^{\mu} \in \mathbb{P}^{\mu}} \Pi(\hat{\boldsymbol{v}}, \hat{p}^{\mathrm{M}}, \hat{p}^{\mu}) = \sup_{\hat{p}^{\mathrm{M}} \in \mathbb{P}^{\mathrm{M}}} \inf_{\hat{\boldsymbol{v}} \in \mathbb{V}} \sup_{\hat{p}^{\mu} \in \mathbb{P}^{\mu}} \Pi(\hat{\boldsymbol{v}}, \hat{p}^{\mathrm{M}}, \hat{p}^{\mu}) \tag{8.153}$$

where the potential Π is defined as

{eq4-524} $$\Pi(\hat{\boldsymbol{v}}, \hat{p}^{\mathrm{M}}, \hat{p}^{\mu}) = \int_{\Omega} \phi_{\Box}(\hat{\boldsymbol{v}}, \hat{p}^{\mu})_{\Box} \, \mathrm{d}\Omega + \int_{\Omega} \langle \hat{\boldsymbol{v}} \cdot \boldsymbol{\nabla} \hat{p}^{\mathrm{M}} \rangle_{\Box} \, \mathrm{d}\Omega - \int_{\Gamma_{\mathrm{N}}} \langle\langle q \, \hat{p}^{\mathrm{M}} \rangle\rangle_{\Box} \, \mathrm{d}\Gamma \tag{8.154}$$

{eq4-601} Hence, (8.151) can be written as

{eq4-601a} $$\Pi'_{p^{\mathrm{M}}}(\boldsymbol{v}, p^{\mathrm{M}}, p^{\mu}; \delta p^{\mathrm{M}}) = 0 \quad \forall \delta p^{\mathrm{M}} \in \mathbb{P}^{\mathrm{M},0} \tag{8.155a}$$

{eq4-601b} $$\Pi'_{v}(\boldsymbol{v}, p^{\mathrm{M}}, p^{\mu}; \delta \boldsymbol{v}) = 0 \qquad \forall \delta \boldsymbol{v} \in \mathbb{V}^0 \tag{8.155b}$$

{eq4-601c} $$\Pi'_{p^{\mu}}(\boldsymbol{v}, p^{\mathrm{M}}, p^{\mu}; \delta p^{\mu}) = 0 \qquad \forall \delta p^{\mu} \in \mathbb{P}^{\mu} \tag{8.155c}$$

Remark 14 *Since $\phi_{\Box}(\hat{\boldsymbol{v}}, \hat{p}^{\mu})_{\Box} = \langle \phi_v(\boldsymbol{d}[\hat{\boldsymbol{v}}]) \rangle_{\Box} - \langle \hat{p}^{\mu}[\hat{\boldsymbol{v}} \cdot \boldsymbol{\nabla}] \rangle_{\Box}$, ...we may interprete $\hat{p}^M, \hat{p}^{\mu}$ as Lagrange multipliers.*

Next, we construct $\mathbb{P}^{\mathrm{M}}$ formally via the prolongation operator $\mathcal{A}^{(p)}$ s. t.

{eq4-525} $$p = \mathcal{A}^{(p)} \bar{p} + p^{\mu}, \quad \boldsymbol{v} = \boldsymbol{v}^{\mu} \; [\boldsymbol{v}^{\mathrm{M}} = \boldsymbol{0}] \tag{8.156}$$

where $\bar{p} \in \mathbb{P}$ is the macroscale pressure field. The (homogenized) macroscale problem is then defined by (8.151a): Find $\bar{p} \in \mathbb{P}$ from

{eq4-526} $$\int_{\Omega} \langle \boldsymbol{v} \cdot \boldsymbol{\nabla}(\mathcal{A}^{(p)} \delta \bar{p}) \rangle_{\Box} \, \mathrm{d}\Omega - \int_{\Gamma_{\mathrm{N}}} \langle\langle q \, \mathcal{A}^{(p)} \delta \bar{p} \rangle\rangle_{\Box} \, \mathrm{d}\Gamma = 0 \quad \forall \delta \bar{p} \in \bar{\mathbb{P}}^0 \tag{8.157}$$

Remark 15 *It is noted that the "diffusion form" characterizing the macroscale problem does not occur as part of the original fine-scale problem formulation. This is an example of "equation switching" that is brought about via the manipulation on the VMS-split.*

Next, we introduce the macroscale potential

{eq4-527} $$\bar{\Pi}\{\hat{\bar{p}}\} \stackrel{\text{def}}{=} \Pi(\boldsymbol{v}\{\hat{\bar{p}}\}, \mathcal{A}^{(p)}\hat{\bar{p}}, p^\mu\{\hat{\bar{p}}\}) \tag{8.158}$$

which has a minimum-point at the homogenized solution $\bar{p} \in \bar{\mathbb{P}}$ satisfying (8.157), i.e.

{eq4-528} $$\bar{p} = \arg\left[\inf_{\hat{\bar{p}}\in\mathbb{P}} \bar{\Pi}\{\hat{\bar{p}}\}\right], \tag{8.159}$$

provided that the appropriate VCMH-condition condition is satisfied by the local fields $\boldsymbol{v}\{\bar{p}\}, p^\mu\{\bar{p}\}$. From the stationarity condition corresponding to (8.159), the VCMH-condition condition is expressed as

$$\begin{aligned}
\bar{\Pi}'\{\bar{p};\delta\bar{p}\} &= \underbrace{\Pi'_{p^{\mathrm{M}}}(\boldsymbol{v}\{\bar{p}\}, \mathcal{A}^{(p)}\bar{p}, p^\mu\{\bar{p}\}; \mathcal{A}^{(p)}\delta\bar{p})}_{=0 \text{ from } (8.157)} \\
&\quad + \Pi'_v(\boldsymbol{v}\{\bar{p}\}, \mathcal{A}^{(p)}\bar{p}, p^\mu\{\bar{p}\}; \mathcal{S}_p^{(v)}\delta\bar{p}) + \Pi'_{p^\mu}(\boldsymbol{v}\{\bar{p}\}, \mathcal{A}^{(p)}\bar{p}, p^\mu\{\bar{p}\}; \mathcal{S}_p^{(p)}\delta\bar{p}) \\
&= 0 \quad \forall\delta\bar{p} \in \bar{\mathbb{P}}^0
\end{aligned} \tag{8.160}$$ {eq4-529}

where we introduced the sensitivities $\mathcal{S}_p^{(v)}\delta\bar{p} \stackrel{\text{def}}{=} (\boldsymbol{v})'_p\{\bar{p},\delta\bar{p}\}$ and $\mathcal{S}_p^{(p)}\delta\bar{p} \stackrel{\text{def}}{=} (p^\mu)'_p\{\bar{p},\delta\bar{p}\}$. Utilizing the explicit expressions for Π'_v and Π'_{p^μ}, we conclude that the local version of the VCMH-condition reads as follows:

$$a_\square(\boldsymbol{v}\{\bar{p}\}; \mathcal{S}_p^{(v)}\delta\bar{p}) - b_\square(p^\mu\{\bar{p}\}, \mathcal{S}_p^{(v)}\delta\bar{p}) - b_\square(\mathcal{S}_p^{(p)}\delta\bar{p}, \boldsymbol{v}\{\bar{p}\}) + \langle \boldsymbol{\nabla}\mathcal{A}^{(p)}\bar{p} \cdot \mathcal{S}_p^{(v)}\delta\bar{p}\rangle_\square = 0 \quad \forall\delta\bar{p} \in \bar{\mathbb{P}}^0 \tag{8.161}$$ {eq4-530}

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RVE-problem: Comment on the computation of $\boldsymbol{v}\{\bar{p}\}, p^\mu\{\bar{p}\}$ for given $\mathcal{A}^{(p)}\bar{p}$.

8.6.5 1st order homogenization

In the standard case of 1st order homogenization, $\bar{p}$ is prolonged via assumed linear variation within each RVE:

$$p^{\mathrm{M}}(\bar{\boldsymbol{x}}, \boldsymbol{x}) = (\mathcal{A}^{(p)}\bar{p})(\bar{\boldsymbol{x}}, \boldsymbol{x}) = \bar{p}(\bar{\boldsymbol{x}}) + \bar{\boldsymbol{\zeta}}(\bar{\boldsymbol{x}}) \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}], \quad \bar{\boldsymbol{\zeta}} \stackrel{\text{def}}{=} \boldsymbol{\nabla}\bar{p}, \quad \boldsymbol{x} \in \Omega_\square \tag{8.162}$$ {eq4-31}

whereby we obtain the identities $\boldsymbol{\nabla}p^{\mathrm{M}} = \bar{\boldsymbol{\zeta}}$, $\boldsymbol{\nabla}\delta p^{\mathrm{M}} = \delta\bar{\boldsymbol{\zeta}} \stackrel{\text{def}}{=} \boldsymbol{\nabla}\delta\bar{p}$. Upon inserting (8.162) into (8.157), we obtain the macroscale problem

$$\int_\Omega \bar{\boldsymbol{w}}\{\bar{\boldsymbol{\zeta}}\} \cdot \boldsymbol{\zeta}[\delta\bar{p}]\,\mathrm{d}\Omega = \int_{\Gamma_{\mathrm{N}}} q_{\mathrm{p}}\delta\bar{p}\,\mathrm{d}\Gamma \quad \forall\delta\bar{p} \in \bar{\mathbb{P}}^0 \tag{8.163}$$ {eq4-32}

where we derived the (macroscale) seepage velocity and the **????**

$$\bar{\boldsymbol{w}}\{\bar{\boldsymbol{\zeta}}\} = \langle \boldsymbol{v}\rangle_\square, \quad \bar{q} = \langle\langle q\rangle\rangle_\square \tag{8.164}$$ {eq4-32}

8.6.6 RVE-problem based on weak periodicity

To establish the canonical format of the RVE-problem, we introduce the solution and test spaces as follows:

$$\mathbb{V}_\square = \{\boldsymbol{v}' \text{ suff. regular in } \Omega_\square,\ \boldsymbol{v}' = \boldsymbol{0} \text{ on } \Gamma_\square^{\text{obs}}\}\boldsymbol{???} \tag{8.165}$$

$$\mathbb{P}_\square^\mu = \{p' \text{ suff. regular in } \Omega_\square,\ \int_{\Gamma_\square^+} p' \, \mathrm{d}\Gamma = 0\}\boldsymbol{???} \tag{8.166}$$

$$\mathbb{L}_{\mathrm{t},\square} = \{\boldsymbol{\lambda}_\mathrm{t}' \text{ suff. regular in } \Omega_\square\} \tag{8.167}$$

$$\mathbb{L}_{\mathrm{q},\square} = \{\lambda_\mathrm{q}' \text{ suff. regular in } \Omega_\square\} \tag{8.168}$$

{eq4-509} Further, we introduce the bilinear forms expressing weak periodicity:

{eq4-509a}
$$d_\square^{(v)}(\boldsymbol{\lambda}_\mathrm{t}, \boldsymbol{v}) \overset{\text{def}}{=} \frac{1}{|\Omega_\square|} \int_{\Gamma_\square^{\mathrm{f},+}} \boldsymbol{\lambda}_\mathrm{t} \cdot [\![\boldsymbol{v}]\!] \, \mathrm{d}\Gamma \tag{8.169a}$$

{eq4-509b}
$$d_\square^{(p)}(\lambda_\mathrm{q}, p^\mu) \overset{\text{def}}{=} \frac{1}{|\Omega_\square|} \int_{\Gamma_\square^{\mathrm{f},+}} \lambda_\mathrm{q} [\![p^\mu]\!] \, \mathrm{d}\Gamma \tag{8.169b}$$

The canonical format of the RVE-problem then reads: For given value of $\bar{\boldsymbol{\zeta}}$, find $\boldsymbol{v} \in \mathbb{V}_\square$, $p^\mu \in \mathbb{P}_\square^\mu$,
{eq4-511} $\boldsymbol{\lambda}_\mathrm{t} \in \mathbb{L}_{\mathrm{t},\square}$, and $\lambda_\mathrm{q} \in \mathbb{L}_{\mathrm{q},\square}$ that solve the system

{eq4-511a}
$$a_\square(\boldsymbol{v}; \delta\boldsymbol{v}) - b_\square(p^\mu, \delta\boldsymbol{v}) - d_\square^{(v)}(\boldsymbol{\lambda}_\mathrm{t}, \delta\boldsymbol{v}) = -\bar{\boldsymbol{\zeta}} \cdot \langle \delta\boldsymbol{v} \rangle_\square \quad \forall \delta\boldsymbol{v} \in \mathbb{V}_\square \tag{8.170a}$$

{eq4-511b}
$$-b_\square(\delta p^\mu, \boldsymbol{v}) - d_\square^{(p)}(\lambda_\mathrm{q}, \delta p^\mu) = 0 \quad \forall \delta p^\mu \in \mathbb{P}_\square^\mu \tag{8.170b}$$

{eq4-511c}
$$-d_\square^{(v)}(\delta\boldsymbol{\lambda}_\mathrm{t}, \boldsymbol{v}) = 0 \quad \forall \delta\boldsymbol{\lambda}_\mathrm{t} \in \mathbb{L}_{\mathrm{t},\square} \tag{8.170c}$$

{eq4-511d}
$$-d_\square^{(p)}(\delta\lambda_\mathrm{q}, p^\mu) = 0 \quad \forall \delta\lambda_\mathrm{q} \in \mathbb{L}_{\mathrm{q},\square} \tag{8.170d}$$

The pertinent RVE-potential is, for any given $\bar{\boldsymbol{\zeta}}$,

{eq4-3221}
$$\pi_\square(\bar{\boldsymbol{\zeta}}; \hat{\boldsymbol{v}}, \hat{p}^\mu, \hat{\boldsymbol{\lambda}}_\mathrm{t}, \hat{\lambda}_\mathrm{q}) = \phi_\square(\hat{\boldsymbol{v}}, \hat{p}^\mu) + \bar{\boldsymbol{\zeta}} \cdot \langle \hat{\boldsymbol{v}} \rangle_\square - d_\square^{(v)}(\hat{\boldsymbol{\lambda}}_\mathrm{t}, \hat{\boldsymbol{v}}) - d_\square^{(\mathrm{q})}(\hat{\lambda}_\mathrm{q}, \hat{p}^\mu) \tag{8.171}$$

whose stationarity conditions are (8.170).

Satisfaction of macrohomogeneity condition

That the MH-condition is satisfied is shown as follows:

- For given perturbation $\delta\bar{p} \in \bar{\mathbb{P}}^0$, choose $\delta\boldsymbol{v} = \mathcal{S}^{(v)}\delta\bar{p} \in \mathbb{V}_\square^0$ in (8.170a) and $\delta p^\mu = \mathcal{S}^{(p)}\delta\bar{p} \in \mathbb{P}_\square^\mu$ in (8.170b).
- Linearize (8.170c) and (8.170d) w.r.t. $\bar{p}$ along $\delta\bar{p}$ and choose $\delta\boldsymbol{\lambda}_\mathrm{t} = \boldsymbol{\lambda}_\mathrm{t}\{\bar{p}\} \in \mathbb{L}_{\mathrm{t},\square}$ and $\delta\lambda_\mathrm{q} = \lambda_\mathrm{q}\{\bar{p}\} \in \mathbb{L}_{\mathrm{q},\square}$, respectively.

Upon eliminating among the resulting equations, we obtain

{eq4-512}
$$a_\square(\boldsymbol{v}\{\bar{p}\}; \mathcal{S}_p^{(v)}\delta\bar{p}) - b_\square(p^\mu\{\bar{p}\}, \mathcal{S}_p^{(v)}\delta\bar{p}) - b_\square(\mathcal{S}_p^{(p)}\delta\bar{p}, \boldsymbol{v}\{\bar{p}\}) + \bar{\boldsymbol{\zeta}} \cdot \langle \mathcal{S}_p^{(v)}\delta\bar{p} \rangle_\square = 0 \quad \forall \delta\bar{p} \in \bar{\mathbb{P}}^0 \tag{8.172}$$

which is precisely (8.161) when we used the identity $\boldsymbol{\nabla}\mathcal{A}^{(p)}\bar{p} = \bar{\boldsymbol{\zeta}}$.

Part III

EFFICIENT FINITE ELEMENT PROCEDURES

Chapter 9

NUMERICAL MODEL REDUCTION

9.1 Preliminaries

9.2 A prototype model: Viscoplasticity without hardening

9.2.1 Strong format

Considering a micro-heterogeneous porous microstructure, we assume that the fine-scale features of the solid skeleton are sufficiently well described by a elastic-viscoplastic model (for the sake of simplicity) with the following characteristics: The volume-specific free energy density $\psi(\boldsymbol{\epsilon})$ is chosen as

$$\psi(\boldsymbol{\epsilon}, \boldsymbol{\epsilon}^{\mathrm{p}}) = \frac{1}{2} \left[\boldsymbol{\epsilon} - \boldsymbol{\epsilon}^{\mathrm{p}}\right] : \mathbf{E} \colon \left[\boldsymbol{\epsilon} - \boldsymbol{\epsilon}^{\mathrm{p}}\right] \tag{9.1}$$ {eq:12-1}

which gives the energetic (equilibrium) stress $\boldsymbol{\sigma}$ and the energetic stress $\boldsymbol{\sigma}^{\mathrm{p,en}}$ that are energy-conjugated to $\boldsymbol{\epsilon}$ and $\boldsymbol{\epsilon}^{\mathrm{p}}$, respectively: {eq:12-2}

$$\boldsymbol{\sigma}(\boldsymbol{\epsilon}, \boldsymbol{\epsilon}^{\mathrm{p}}) = \boldsymbol{\sigma}^{\mathrm{en}}(\boldsymbol{\epsilon}, \boldsymbol{\epsilon}^{\mathrm{p}}) \stackrel{\mathrm{def}}{=} \frac{\partial \psi}{\partial \boldsymbol{\epsilon}}(\boldsymbol{\epsilon}, \boldsymbol{\epsilon}^{\mathrm{p}}) = \mathbf{E} \colon \left[\boldsymbol{\epsilon} - \boldsymbol{\epsilon}^{\mathrm{p}}\right], \tag{9.2a}$$ {eq:12-2a}

$$\boldsymbol{\sigma}^{\mathrm{p,en}}(\boldsymbol{\epsilon}, \boldsymbol{\epsilon}^{\mathrm{p}}) \stackrel{\mathrm{def}}{=} \frac{\partial \psi}{\partial \boldsymbol{\epsilon}^{\mathrm{p}}}(\boldsymbol{\epsilon}, \boldsymbol{\epsilon}^{\mathrm{p}}) = -\boldsymbol{\sigma}(\boldsymbol{\epsilon}, \boldsymbol{\epsilon}^{\mathrm{p}}) = -\mathbf{E} \colon \left[\boldsymbol{\epsilon} - \boldsymbol{\epsilon}^{\mathrm{p}}\right] \tag{9.2b}$$ {eq:12-2b}

We also introduce the dual dissipation potential $\phi^*(\boldsymbol{\sigma}^{\mathrm{p,di}})$, whose argument is the (dissipative) inelastic stress, such that the evolution rule for $\boldsymbol{\epsilon}^{\mathrm{p}}$ becomes

$$\dot{\boldsymbol{\epsilon}}^{\mathrm{p}} = \frac{\partial \phi^*}{\partial \boldsymbol{\sigma}^{\mathrm{p,di}}}(\boldsymbol{\sigma}^{\mathrm{p,di}}) := \boldsymbol{\varphi}^*(\boldsymbol{\sigma}^{\mathrm{p,di}}) \tag{9.3}$$ {eq:12-3}

Moreover, we note the relation (constraint)

$$\boldsymbol{\sigma}^{\mathrm{p,di}} + \boldsymbol{\sigma}^{\mathrm{p,en}}(\boldsymbol{\epsilon}, \boldsymbol{\epsilon}^{\mathrm{p}}) = \mathbf{0} \tag{9.4}$$ {eq:12-3a}

Restricting to quasistatics, we thus seek the displacement $\boldsymbol{u}(\boldsymbol{x}, t) : \Omega \times \mathbb{R}^+ \to \mathbb{R}^3$, the dissipative stress $\boldsymbol{\sigma}^{\mathrm{p,di}}(\boldsymbol{x}, t) : \Omega \times \mathbb{R}^+ \to \mathbb{R}^{3\times3}_{\mathrm{sym}}$ and the inelastic strain $\boldsymbol{\epsilon}^{\mathrm{p}}(\boldsymbol{x}, t) : \Omega \times \mathbb{R}^+ \to \mathbb{R}^{3\times3}_{\mathrm{sym}}$ that solve the system {eq:12-4}

$$-\boldsymbol{\sigma}(\boldsymbol{\epsilon}[\boldsymbol{u}], \boldsymbol{\epsilon}^{\mathrm{p}}) \cdot \boldsymbol{\nabla} = \mathbf{0} \quad \text{in } \Omega \times (0, T] \tag{9.5a}$$ {eq:12-4a}

$$\boldsymbol{\sigma}^{\mathrm{p,di}} + \boldsymbol{\sigma}^{\mathrm{p,en}}(\boldsymbol{\epsilon}[\boldsymbol{u}], \boldsymbol{\epsilon}^{\mathrm{p}}) = \mathbf{0} \quad \text{in } \Omega \times (0, T] \tag{9.5b}$$ {eq:12-4b}

$$\dot{\boldsymbol{\epsilon}}^{\mathrm{p}} - \boldsymbol{\varphi}^{*}(\boldsymbol{\epsilon}[\boldsymbol{u}], \boldsymbol{\epsilon}^{\mathrm{p}}) = \mathbf{0} \quad \text{in } \Omega \times (0, T] \tag{9.5c}$$ {eq:12-4c}

$$\boldsymbol{u} = \boldsymbol{u}_{\mathrm{p}} \quad \text{on } \Gamma_{\mathrm{D}}^{(u)} \times (0, T] \tag{9.5d}$$ {eq:12-4d}

$$\boldsymbol{t} \stackrel{\text{def}}{=} \boldsymbol{\sigma} \cdot \boldsymbol{n} = \boldsymbol{t}_{\mathrm{p}} \quad \text{on } \Gamma_{\mathrm{N}}^{(u)} \times (0, T] \tag{9.5e}$$ {eq:12-4e}

together with the constitutive relations for $\boldsymbol{\sigma}$ in (9.2a) and for $\boldsymbol{\sigma}^{\mathrm{p,en}}$ in (9.2b). The initial condition is chosen as

{eq:12-5}
$$\boldsymbol{\epsilon}^{\mathrm{p}}(\bullet, 0) = \mathbf{0} \quad \text{in } \Omega \tag{9.6}$$

9.2.2 Space-variational formulation

Introduce the solution space

{eq:12-105}
$$\mathbb{U} = \{\boldsymbol{u} \text{ suff. regular} \mid \boldsymbol{u} = \boldsymbol{u}_{\mathrm{p}} \text{ on } \Gamma_{\mathrm{D}}^{(u)}\} \tag{9.7}$$

The standard space-variational format corresponding to (9.5) reads: Find $\boldsymbol{u}(\bullet, t) \in \mathbb{U}$, $\boldsymbol{\epsilon}^{\mathrm{p}}(\bullet, t) \in$
{eq:12-6} $\mathbb{L}_2(\Omega)$, and $\boldsymbol{\sigma}^{\mathrm{p,di}}(\bullet, t) \in \mathbb{L}_2(\Omega)$ that solve

{eq:12-6a}
$$\int_{\Omega} [[\boldsymbol{\epsilon}[\boldsymbol{u}] - \boldsymbol{\epsilon}^{\mathrm{p}}] : \mathsf{E} : \boldsymbol{\epsilon}[\delta \boldsymbol{u}]] \, \mathrm{d}\Omega = \int_{\Gamma_{\mathrm{N}}^{(u)}} \boldsymbol{t}_{\mathrm{p}} \cdot \delta \boldsymbol{u} \, \mathrm{d}\Gamma \qquad \forall \delta \boldsymbol{u} \in \mathbb{U}^0 \tag{9.8a}$$

{eq:12-6b}
$$\int_{\Omega} \left[\boldsymbol{\sigma}^{\mathrm{p,di}} : \delta \boldsymbol{\epsilon}^{\mathrm{p}} - [\boldsymbol{\epsilon}[\boldsymbol{u}] - \boldsymbol{\epsilon}^{\mathrm{p}}] : \mathsf{E} : \delta \boldsymbol{\epsilon}^{\mathrm{p}}\right] \mathrm{d}\Omega = 0 \qquad \forall \delta \boldsymbol{\epsilon}^{\mathrm{p}} \in \mathbb{L}_2(\Omega) \tag{9.8b}$$

{eq:12-6c}
$$\int_{\Omega} \left[\dot{\boldsymbol{\epsilon}}^{\mathrm{p}} : \delta \boldsymbol{\sigma}^{\mathrm{p,di}} - \boldsymbol{\varphi}^{*}(\boldsymbol{\sigma}^{\mathrm{p,di}}) : \delta \boldsymbol{\sigma}^{\mathrm{p,di}}\right] \mathrm{d}\Omega = 0 \qquad \forall \delta \boldsymbol{\sigma}^{\mathrm{p,di}} \in \mathbb{L}_2(\Omega) \tag{9.8c}$$

where $\mathbb{U}^0$ is the appropriately defined test space.

Remark 16 *The standard strategy is to eliminate* $\boldsymbol{\sigma}^{p,di}$ *from* (9.8b) *in terms of* $\boldsymbol{\epsilon}$ *and* $\boldsymbol{\epsilon}^p$ *by retaining the strong format of the equations given in* (9.5b) *and* (9.5c). *However, as will also be evident below, it is beneficial to keep the general weak formulation of the evolution equation in* (9.8c) *for the purpose of exploiting NMR (to be discussed below).* □

9.2.3 Paving the way for model reduction

Let us consider the single-phase problem in (9.5) and/or (9.8). We introduce the additive decomposition of $\boldsymbol{u}$:

{eq:12-7}
$$\boldsymbol{u} = \boldsymbol{u}_0 + \tilde{\boldsymbol{u}} \tag{9.9}$$

{eq:12-8} where it is assumed that $\boldsymbol{u}_0 \in \mathbb{U}^0$ solves the elasticity problem

{eq:12-8a}
$$-\boldsymbol{\sigma}_0 \cdot \boldsymbol{\nabla} = \mathbf{0} \qquad \text{in } \Omega \tag{9.10a}$$

{eq:12-8b}
$$\boldsymbol{u}_0 = \boldsymbol{u}_{\mathrm{p}} \qquad \text{on } \Gamma_{D}^{(u)} \tag{9.10b}$$

{eq:12-8c}
$$\boldsymbol{t}_0 \stackrel{\text{def}}{=} \boldsymbol{\sigma}_0 \cdot \boldsymbol{n} = \boldsymbol{t}_{\mathrm{p}} \qquad \text{on } \Gamma_{N}^{(u)} \tag{9.10c}$$

with

{eq:12-9}
$$\boldsymbol{\sigma}_0 = \boldsymbol{\sigma}(\boldsymbol{\epsilon}[\boldsymbol{u}_0], \mathbf{0}) = \mathsf{E} : \boldsymbol{\epsilon}[\boldsymbol{u}_0]. \tag{9.11}$$

{eq:12-10} Subtracting (9.10) from (9.5), we obtain the eigenstrain problem

{eq:12-10a} {eq:12-10b} {eq:12-10c} {eq:12-10d}
$$\begin{aligned}
-\tilde{\boldsymbol{\sigma}}(\boldsymbol{\epsilon}[\tilde{\boldsymbol{u}}], \boldsymbol{\epsilon}^{\mathrm{p}}) \cdot \boldsymbol{\nabla} &= \mathbf{0} && \text{in } \Omega && (9.12\mathrm{a})\\
\tilde{\boldsymbol{\sigma}}^{\mathrm{p,di}} + \boldsymbol{\sigma}^{\mathrm{p,en}}(\boldsymbol{\epsilon}[\tilde{\boldsymbol{u}}], \boldsymbol{\epsilon}^{\mathrm{p}}) &= \mathbf{0} && \text{in } \Omega && (9.12\mathrm{b})\\
\dot{\boldsymbol{\epsilon}}^{\mathrm{p}} - \boldsymbol{\varphi}^*(\boldsymbol{\sigma}_0 + \tilde{\boldsymbol{\sigma}}^{\mathrm{p,di}}) &= \mathbf{0} && \text{in } \Omega && (9.12\mathrm{c})\\
\tilde{\boldsymbol{u}} &= \mathbf{0} && \text{on } \Gamma_{\mathrm{D}}^{(u)} && (9.12\mathrm{d})\\
\tilde{\boldsymbol{t}} \overset{\mathrm{def}}{=} \tilde{\boldsymbol{\sigma}} \cdot \boldsymbol{n} &= \mathbf{0} && \text{on } \Gamma_{\mathrm{N}}^{(u)} && (9.12\mathrm{e})
\end{aligned}$$

where

$$\tilde{\boldsymbol{\sigma}} = \boldsymbol{\sigma} - \boldsymbol{\sigma}_0 = \mathsf{E} : [\boldsymbol{\epsilon}[\tilde{\boldsymbol{u}}] - \boldsymbol{\epsilon}^{\mathrm{p}}] \tag{9.13}$$ {eq:12-13}

$$\tilde{\boldsymbol{\sigma}}^{\mathrm{p,di}} = \boldsymbol{\sigma}^{\mathrm{p,di}} - \boldsymbol{\sigma}_0 = \boldsymbol{\sigma}^{\mathrm{p,di}} - \mathsf{E} : \boldsymbol{\epsilon}[\boldsymbol{u}_0] \tag{9.14}$$ {eq:12-13-1

The corresponding space-variational formulation reads: Find $\tilde{\boldsymbol{u}}(\bullet, t) \in \mathbb{U}^0$, $\boldsymbol{\epsilon}^{\mathrm{p}}(\bullet, t) \in \mathbb{L}_2(\Omega)$, and $\tilde{\boldsymbol{\sigma}}^{\mathrm{p,di}}(\bullet, t) \in \mathbb{L}_2(\Omega)$ that solve {eq:12-14}

$$\int_\Omega [\boldsymbol{\epsilon}[\tilde{\boldsymbol{u}}] - \boldsymbol{\epsilon}^{\mathrm{p}}] : \mathsf{E} : \boldsymbol{\epsilon}[\delta \boldsymbol{u}] \, \mathrm{d}\Omega = 0 \qquad \forall\, \delta \boldsymbol{u} \in \mathbb{U}^0 \tag{9.15a}$$ {eq:12-14a}

$$\int_\Omega \left[\tilde{\boldsymbol{\sigma}}^{\mathrm{p,di}} : \delta\boldsymbol{\epsilon}^{\mathrm{p}} - [\boldsymbol{\epsilon}[\tilde{\boldsymbol{u}}] - \boldsymbol{\epsilon}^{\mathrm{p}}] : \mathsf{E} : \delta\boldsymbol{\epsilon}^{\mathrm{p}}\right] \, \mathrm{d}\Omega = 0 \qquad \forall\, \delta\boldsymbol{\epsilon}^{\mathrm{p}} \in \mathbb{L}_2(\Omega). \tag{9.15b}$$ {eq:12-14b}

$$\int_\Omega \left[\dot{\boldsymbol{\epsilon}}^{\mathrm{p}} : \delta\boldsymbol{\sigma}^{\mathrm{p,di}} - \boldsymbol{\varphi}^*(\boldsymbol{\sigma}_0 + \tilde{\boldsymbol{\sigma}}^{\mathrm{p,di}}) : \delta\boldsymbol{\sigma}^{\mathrm{p,di}}\right] \, \mathrm{d}\Omega = 0 \qquad \forall\, \delta\boldsymbol{\sigma}^{\mathrm{p,di}} \in \mathbb{L}_2(\Omega) \tag{9.15c}$$ {eq:12-14c}

9.3 Numerical model reduction (NMR)

9.3.1 Preliminaries

REWRITE!! HERE???

NMR to represent the fields in a more efficient way with much fewer basis functions (global) than FE, leading to small systems of algebraic equations

XXXXXXXXXXXXXXXXXXXXXXXXXXX

In order to reduce the computational effort in solving the RVE-problem (**??**), we exploit Numerical Model Reduction (NMR) for one or more fields in the spatial domain. A few alternative approaches (or strategies) can then be envisioned and which one is the most efficient is not entirely obvious ??.

1. The straightforward approach (which will be adopted subsequently in this paper) is to introduce $\mathbb{U}^0_{\square,\mathrm{R}} \subset \mathbb{U}^0_\square$ (rather $\mathbb{U}^0_{\mathrm{R}} \subset \mathbb{U}^0$!!!!!), that is spanned by a set of linearly independent global displacement basis functions. As to the choice of $\mathbb{K}^0_\square$, it is chosen as infinite-dimensional, i.e. the constitutive relation (**??**) is forced to be satisfied strongly in $\Omega_\square$ at every instant in time. Thereby it is possible to solve for $\boldsymbol{k}_{\mathrm{R}}$ as a (linear) function of $\boldsymbol{u}^\mu_{\mathrm{R}}$ in each spatial point $\boldsymbol{x} \in \Omega$. **Extension to nonlinear problem: Nested iterations!!!**

2. The classical approach is NTFA (Nonuniform Field Transformation Analysis), whereby $\mathbb{K}^0_\square$ is kept "global" and the reduced space $\mathbb{K}^0_{\square,\mathrm{R}} \subset \mathbb{K}^0_\square$ is introduced a priori. However, this approach is feasible only if it is possible to derive the corresponding basis functions that span the reduced space $\mathbb{U}^0_{\square,\mathrm{R}}$ in a simple fashion via a sensitivity analysis based on the equilibrium equation (**??**).

3. **Remark:** A third option would (at least in theory) be to introduce completely independent basis functions spanning $\mathbb{U}^0_{\square,\mathrm{R}}$ and $\mathbb{K}^0_{\square,\mathrm{R}}$, whereby both spaces contain global functions. This is the natural approach when gradient effects are accounted for, whereby the constitutive equation will have an additional term with divergence of ????. **REPHRASE**

9.3.2 Proper Orthogonal Decomposition (POD)

Fredrik's notes from meeting 190417

9.3.3 The idea of Nonuniform Transformation Field Analysis (NTFA)

UPDATE!

The idea of NTFA is now to assume that the set of basis modes $\{\hat{\boldsymbol{\epsilon}}^{\mathrm{p}}_a(\boldsymbol{x})\}_{a=1}^{N_R}$ are available "offline" such that each field $\boldsymbol{\epsilon}^{\mathrm{p}}(\boldsymbol{x},t)$ can be expressed as ....

9.3.4 NMR – Version I based on NTFA

We first note that (9.15a), (9.15b) are linear and homogeneous equations , i.e. if $(\tilde{\boldsymbol{u}}_1, \boldsymbol{\epsilon}^{\mathrm{p}}_1, \tilde{\boldsymbol{\sigma}}^{\mathrm{p,di}}_1)$ solve (9.15a), (9.15b), then so does $(\tilde{\boldsymbol{u}}_2, \boldsymbol{\epsilon}^{\mathrm{p}}_2, \tilde{\boldsymbol{\sigma}}^{\mathrm{p,di}}_2) = \alpha(\tilde{\boldsymbol{u}}_1, \boldsymbol{\epsilon}^{\mathrm{p}}_1, \tilde{\boldsymbol{\sigma}}^{\mathrm{p,di}}_1)$, where α is an arbitrary scalar. This property is used in NTFA. One possibility is to assume that a set of basis modes $\left\{\hat{\boldsymbol{\sigma}}^{\mathrm{p,di}}_a(\boldsymbol{x})\right\}_{a=1}^{N_R}$ are available "offline" such that each field $\tilde{\boldsymbol{\sigma}}^{\mathrm{p,di}}(\boldsymbol{x},t)$ can be expressed via the expansion

{eq:12-115}
$$\tilde{\boldsymbol{\sigma}}^{\mathrm{p,di}}(\boldsymbol{x},t) \simeq \tilde{\boldsymbol{\sigma}}^{\mathrm{p,di}}_{\mathrm{R}}(\boldsymbol{x},t) := \sum_{a=1}^{N_R} \hat{\boldsymbol{\sigma}}^{\mathrm{p,di}}_a(\boldsymbol{x})\,\xi_a(t) \tag{9.16}$$

where the set of mode activity coefficients $\{\xi_a(t)\}_{a=1}^{N_R}$ are to be found.

We now make the fundamental assumption that $\tilde{\boldsymbol{u}}(\boldsymbol{x},t)$ and $\boldsymbol{\epsilon}^{\mathrm{p}}(\boldsymbol{x},t)$ can be expressed in the basis modes $\{\hat{\boldsymbol{u}}_a(\boldsymbol{x})\}_{a=1}^{N_R}$ and $\{\hat{\boldsymbol{\epsilon}}^{\mathrm{p}}_a(\boldsymbol{x})\}_{a=1}^{N_R}$, respectively, with the same set of mode activity coefficients
{eq:12-116} as for $\tilde{\boldsymbol{\sigma}}^{\mathrm{p,di}}$, i.e. we make the ansatz

eq:12-116a}
$$\tilde{\boldsymbol{u}}(\boldsymbol{x},t) \simeq \tilde{\boldsymbol{u}}_{\mathrm{R}}(\boldsymbol{x},t) := \sum_{a=1}^{N_R} \hat{\boldsymbol{u}}_a(\boldsymbol{x})\,\xi_a(t), \tag{9.17a}$$

eq:12-116b}
$$\boldsymbol{\epsilon}^{\mathrm{p}}(\boldsymbol{x},t) \simeq \boldsymbol{\epsilon}^{\mathrm{p}}_{\mathrm{R}}(\boldsymbol{x},t) := \sum_{a=1}^{N_R} \hat{\boldsymbol{\epsilon}}^{\mathrm{p}}_a(\boldsymbol{x})\,\xi_a(t), \tag{9.17b}$$

Due to the linearity and homogeneity of (9.15a), (9.15b), it then follows that $\hat{\boldsymbol{u}}_a \in \mathbb{U}^0$, $\hat{\boldsymbol{\epsilon}}^{\mathrm{p}}_a \in \mathbb{L}_2(\Omega)$

{eq:12-117} and $\hat{\boldsymbol{\sigma}}_a^{\mathrm{p,di}} \in \mathbb{L}_2(\Omega)$ must satisfy the equations

{eq:12-117a}
$$\int_\Omega [\boldsymbol{\epsilon}[\hat{\boldsymbol{u}}_a] - \hat{\boldsymbol{\epsilon}}_a^{\mathrm{p}}] : \mathbf{E} : \boldsymbol{\epsilon}[\delta \boldsymbol{u}] \, \mathrm{d}\Omega = 0 \qquad \forall\, \delta \boldsymbol{u} \in \mathbb{U}^0 \tag{9.18a}$$

{eq:12-117b}
$$-\int_\Omega [\boldsymbol{\epsilon}[\hat{\boldsymbol{u}}_a] - \hat{\boldsymbol{\epsilon}}_a^{\mathrm{p}}] : \mathbf{E} : \delta \boldsymbol{\epsilon}^{\mathrm{p}} \, \mathrm{d}\Omega = -\int_\Omega \hat{\boldsymbol{\sigma}}_a^{\mathrm{p,di}} : \delta \boldsymbol{\epsilon}^{\mathrm{p}} \qquad \forall\, \delta \boldsymbol{\epsilon}^{\mathrm{p}} \in \mathbb{L}_2(\Omega). \tag{9.18b}$$

Now, for given $\hat{\boldsymbol{\sigma}}_a^{\mathrm{p,di}}$, we seek the solution $\hat{\boldsymbol{u}}_a$, $\hat{\boldsymbol{\epsilon}}_a^{\mathrm{p}}$. However, it is clear that such a solution is not unique: If $\hat{\boldsymbol{u}}_a^{(1)}$, $\hat{\boldsymbol{\epsilon}}_a^{\mathrm{p}(1)}$ solve (9.18) so does $\hat{\boldsymbol{u}}_a^{(2)}$, $\hat{\boldsymbol{\epsilon}}_a^{\mathrm{p}(2)} := \hat{\boldsymbol{\epsilon}}_a^{\mathrm{p}(1)} + \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}_a^{(2)}] - \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}_a^{(1)}]$ for any choice $\hat{\boldsymbol{u}}_a^{(2)} \in \mathbb{U}^0$.

9.3.5 NMR – Version II based on NTFA

As an alternative, it is possible to assume that the set of basis modes $\{\hat{\boldsymbol{\epsilon}}_a^{\mathrm{p}}(\boldsymbol{x})\}_{a=1}^{N_R}$ is available "offline" such that each field $\boldsymbol{\epsilon}^{\mathrm{p}}(\boldsymbol{x},t)$ can be expressed as

$$\boldsymbol{\epsilon}^{\mathrm{p}}(\boldsymbol{x},t) \simeq \boldsymbol{\epsilon}_{\mathrm{R}}^{\mathrm{p}}(\boldsymbol{x},t) := \sum_{a=1}^{N_R} \hat{\boldsymbol{\epsilon}}_a^{\mathrm{p}}(\boldsymbol{x})\, \xi_a(t) \tag{9.19}$$ {eq:12-15}

where the set of mode activity coefficients $\{\xi_a(t)\}_{a=1}^{N_R}$ are to be found.

We now make the fundamental assumption that $\tilde{\boldsymbol{u}}(\boldsymbol{x},t)$ can be expressed in the basis modes $\{\hat{\boldsymbol{u}}_a(\boldsymbol{x})\}_{a=1}^{N_R}$ with the same set of mode activity coefficients as for $\boldsymbol{\epsilon}^{\mathrm{p}}$, i.e. we make the ansatz

$$\tilde{\boldsymbol{u}}(\boldsymbol{x},t) \simeq \tilde{\boldsymbol{u}}_R(\boldsymbol{x},t) := \sum_{a=1}^{N_R} \hat{\boldsymbol{u}}_a(\boldsymbol{x})\, \xi_a(t). \tag{9.20}$$ {eq:12-16}

It is then possible to solve for $\hat{\boldsymbol{u}}_a$ in terms of $\hat{\boldsymbol{\epsilon}}_a^{\mathrm{p}}$, $a = 1, 2, \ldots, N_R$, from (9.15a). Upon inserting the expansions in (9.19) and (9.20) into (9.15a), we obtain the following problem: Find $\hat{\boldsymbol{u}}_a \in \mathbb{U}^0$ that, for $a = 1, 2, \ldots, N_R$, solves

$$\int_\Omega \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}_a] : \mathbf{E} : \boldsymbol{\epsilon}[\delta \boldsymbol{u}] \, \mathrm{d}\Omega = \int_\Omega \hat{\boldsymbol{\epsilon}}_a^{\mathrm{p}} : \mathbf{E} : \boldsymbol{\epsilon}[\delta \boldsymbol{u}] \, \mathrm{d}\Omega = 0 \quad \forall\, \delta \boldsymbol{u} \in \mathbb{U}^0. \tag{9.21}$$ {eq:12-19}

Clearly, these linear elasticity problems with different "loads" for $a = 1, 2, \ldots, N_R$ represent the "offline" stage. For known basis modes $\hat{\boldsymbol{u}}_a$ and $\hat{\boldsymbol{\epsilon}}_a^{\mathrm{p}}$, we may thus obtain from (9.15b),(9.15c) the following problem: Find the mode activity coefficients ξ_a, $a = 1, 2, ..., N_R$ and $\tilde{\boldsymbol{\sigma}}^{\mathrm{p,di}}$ that solve[1].

{eq:12-119}

$$\int_\Omega \hat{\boldsymbol{\epsilon}}_a^{\mathrm{p}} : \tilde{\boldsymbol{\sigma}}^{\mathrm{p,di}}\{\underline{\boldsymbol{\xi}}\} \, \mathrm{d}\Omega - \sum_{b=1}^{N_R} \left[\int_\Omega \hat{\boldsymbol{\epsilon}}_a^{\mathrm{p}} : \mathbf{E} : [\boldsymbol{\epsilon}[\hat{\boldsymbol{u}}_b] - \hat{\boldsymbol{\epsilon}}_b^{\mathrm{p}}] \, \mathrm{d}\Omega \right] \xi_b = 0 \qquad a = 1, 2, ..., N_R \tag{9.22a}$$ {eq:12-119b}

$$\int_\Omega \delta \boldsymbol{\sigma}^{\mathrm{p,di}} : \left[\sum_{a=1}^{N_R} \hat{\boldsymbol{\epsilon}}_a^{\mathrm{p}}\, \dot{\xi}_a - \boldsymbol{\varphi}^*(\boldsymbol{\sigma}_0 + \tilde{\boldsymbol{\sigma}}^{\mathrm{p,di}}\{\underline{\boldsymbol{\xi}}\}) \right] \, \mathrm{d}\Omega = 0 \qquad \forall\, \delta \boldsymbol{\sigma}^{\mathrm{p,di}} \in \mathbb{L}_2(\Omega) \tag{9.22b}$$ {eq:12-119c}

[1] Curly brackets, e.g. in $\tilde{\boldsymbol{\sigma}}^{\mathrm{p,di}}\{\underline{\boldsymbol{\xi}}\}$, denotes implicit dependence.

It should be noted that (9.22b) is, indeed, local such that it can be replaced by the strong format, whereby the system (9.22) can be replaced by {eq:12-120}

$$\int_\Omega \hat{\boldsymbol{\epsilon}}^{\mathrm{p}}_a : \tilde{\boldsymbol{\sigma}}^{\mathrm{p,di}}\{\underline{\boldsymbol{\xi}}\}\,\mathrm{d}\Omega + \underline{\boldsymbol{S}}\,\underline{\boldsymbol{\xi}} = 0 \qquad a = 1, 2, ..., N_R \tag{9.23a}$$ {eq:12-120b}

$$\sum_{a=1}^{N_R} \hat{\boldsymbol{\epsilon}}^{\mathrm{p}}_a\,\dot{\xi}_a - \boldsymbol{\varphi}^*(\boldsymbol{\sigma}_0 + \tilde{\boldsymbol{\sigma}}^{\mathrm{p,di}}\{\underline{\boldsymbol{\xi}}\}) = 0 \qquad \boldsymbol{x} \in \Omega \tag{9.23b}$$ {eq:12-120c}

{eq:12-200} where

{eq:12-201a}
$$(\underline{\boldsymbol{S}})_{ab} = -\int_\Omega \hat{\boldsymbol{\epsilon}}^{\mathrm{p}}_a : \mathbf{E} : [\boldsymbol{\epsilon}[\hat{\boldsymbol{u}}_b] - \hat{\boldsymbol{\epsilon}}^{\mathrm{p}}_b]\,\mathrm{d}\Omega \tag{9.24a}$$

{eq:12-201b}
$$(\underline{\boldsymbol{f}}(\underline{\boldsymbol{\xi}}))_a = \int_\Omega \hat{\boldsymbol{\epsilon}}^{\mathrm{e}}_a : \mathbf{E} : \boldsymbol{\varphi}^*(\boldsymbol{\sigma}^{\mathrm{p,di}}(\underline{\boldsymbol{\xi}}))\,\mathrm{d}\Omega????? \tag{9.24b}$$

The system (9.23) can be solved by suitable quadrature to obtain sufficient accuracy of the first integral of (9.23a).

In order to show that $\underline{\boldsymbol{S}}$ is, indeed, symmetrical and positive definite, we proceed as follows: Setting $\delta\boldsymbol{u} = \hat{\boldsymbol{u}}_b$ in (9.30), we obtain

{eq:12-202}
$$\int_\Omega \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}_a] : \mathbf{E} : \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}_b]\,\mathrm{d}\Omega = \int_\Omega \hat{\boldsymbol{\epsilon}}^{\mathrm{p}}_a : \mathbf{E} : \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}_b]\,\mathrm{d}\Omega = \int_\Omega \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}_a] : \mathbf{E} : \hat{\boldsymbol{\epsilon}}^{\mathrm{p}}_b\,\mathrm{d}\Omega \tag{9.25}$$

or

{eq:12-203}
$$\int_\Omega \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}_a] : \mathbf{E} : \left[\boldsymbol{\epsilon}[\hat{\boldsymbol{u}}_b] - \hat{\boldsymbol{\epsilon}}^{\mathrm{p}}_b\right]\,\mathrm{d}\Omega = 0 \tag{9.26}$$

which can be added to the expression in (9.33a) to give

{eq:12-204}
$$(\underline{\boldsymbol{S}})_{ab} = \int_\Omega [\boldsymbol{\epsilon}[\hat{\boldsymbol{u}}_a] - \hat{\boldsymbol{\epsilon}}^{\mathrm{p}}_a] : \mathbf{E} : \left[\boldsymbol{\epsilon}[\hat{\boldsymbol{u}}_b] - \hat{\boldsymbol{\epsilon}}^{\mathrm{p}}_b\right]\,\mathrm{d}\Omega. \tag{9.27}$$

It is clear that $(\underline{\boldsymbol{S}})_{ab}$ is symmetrical.

9.3.6 NMR – Version III based on NTFA

{eq:12-121} A third option is to adopt a priori independent expansions of $\boldsymbol{\epsilon}^{\mathrm{p}}$ and $\tilde{\boldsymbol{\sigma}}^{\mathrm{p,di}}$ as follows

{eq:12-121a}
$$\boldsymbol{\epsilon}^{\mathrm{p}}(\boldsymbol{x}, t) \simeq \boldsymbol{\epsilon}^{\mathrm{p}}_{\mathrm{R}}(\boldsymbol{x}, t) := \sum_{a=1}^{N_R^{(\epsilon)}} \hat{\boldsymbol{\epsilon}}^{\mathrm{p}}_a(\boldsymbol{x})\,\xi_a(t), \tag{9.28a}$$

{eq:12-121b}
$$\tilde{\boldsymbol{\sigma}}^{\mathrm{p,di}}(\boldsymbol{x}, t) \simeq \tilde{\boldsymbol{\sigma}}^{\mathrm{p,di}}_{\mathrm{R}}(\boldsymbol{x}, t) := \sum_{a=1}^{N_R^{(\epsilon)}} \hat{\boldsymbol{\sigma}}^{\mathrm{p,di}}_a(\boldsymbol{x})\,\eta_a(t) \tag{9.28b}$$

Like in the previous case, we can express $\tilde{\boldsymbol{u}}(\boldsymbol{x}, t)$ in the basis modes $\{\hat{\boldsymbol{u}}_a(\boldsymbol{x})\}_{a=1}^{N_R^{(\epsilon)}}$ with the activity coefficients ξ_a, i.e.

{eq:12-122}
$$\tilde{\boldsymbol{u}}(\boldsymbol{x}, t) \simeq \tilde{\boldsymbol{u}}_{\mathrm{R}}(\boldsymbol{x}, t) := \sum_{a=1}^{N_R^{(\epsilon)}} \hat{\boldsymbol{u}}_a(\boldsymbol{x})\,\xi_a(t). \tag{9.29}$$

whereby $\hat{\boldsymbol{u}}_a$, $a = 1, 2, \ldots, N_R^{(\epsilon)}$, can be solved in terms of $\hat{\boldsymbol{\epsilon}}_a^{\mathrm{p}}$ from

{eq:12-123}
$$\int_\Omega \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}_a] : \mathbf{E} : \boldsymbol{\epsilon}[\delta \boldsymbol{u}] \,\mathrm{d}\Omega = \int_\Omega \hat{\boldsymbol{\epsilon}}_a^{\mathrm{p}} : \mathbf{E} : \boldsymbol{\epsilon}[\delta \boldsymbol{u}] \,\mathrm{d}\Omega = 0 \quad \forall\, \delta \boldsymbol{u} \in \mathbb{U}^0. \tag{9.30}$$

Upon inserting all expansions into (9.15b), (9.15c), we now obtain the following problem: Find
{eq:12-124} ξ_a, $a = 1, 2, \ldots, N_R^{(\epsilon)}$ and η_a, $a = 1, 2, \ldots, N_R^{(\sigma)}$ that solve

$$\sum_{b=1}^{N_R^{(\sigma)}} \left[\int_\Omega \hat{\boldsymbol{\epsilon}}_a^{\mathrm{p}} : \hat{\boldsymbol{\sigma}}_b^{\mathrm{p,di}} \,\mathrm{d}\Omega \right] \eta_b - \sum_{b=1}^{N_R^{(\epsilon)}} \left[\int_\Omega \hat{\boldsymbol{\epsilon}}_a^{\mathrm{p}} : \mathbf{E} : [\boldsymbol{\epsilon}[\hat{\boldsymbol{u}}_b] - \hat{\boldsymbol{\epsilon}}_b^{\mathrm{p}}] \,\mathrm{d}\Omega \right] \xi_b = 0 \qquad a = 1, 2, ..., N_R^{(\epsilon)} \tag{9.31a}$$
{eq:12-124b}

$$\sum_{b=1}^{N_R^{(\epsilon)}} \left[\int_\Omega \hat{\boldsymbol{\sigma}}_a^{\mathrm{p,di}} : \hat{\boldsymbol{\epsilon}}_b^{\mathrm{p}} \,\mathrm{d}\Omega \right] \dot{\xi}_b - \int_\Omega \hat{\boldsymbol{\sigma}}_a^{\mathrm{p,di}} : \boldsymbol{\varphi}^*(\boldsymbol{\sigma}_0 + \tilde{\boldsymbol{\sigma}}^{\mathrm{p,di}}\{\underline{\boldsymbol{\eta}}\}) \,\mathrm{d}\Omega = 0 \qquad a = 1, 2, ..., N_R^{(\sigma)} \tag{9.31b}$$
{eq:12-124c}

We may express (9.31) in matrix form as the nonlinear evolution problem {eq:12-125}

$$\underline{\boldsymbol{S}}\,\underline{\boldsymbol{\xi}} + \underline{\boldsymbol{G}}\,\underline{\boldsymbol{\eta}} = \underline{\boldsymbol{0}}, \tag{9.32a}$$
{eq:12-125a}
$$\underline{\boldsymbol{G}}^{\mathrm{T}}\,\dot{\underline{\boldsymbol{\xi}}} - \underline{\boldsymbol{f}}(\underline{\boldsymbol{\eta}}) = \underline{\boldsymbol{0}}. \tag{9.32b}$$
{eq:12-125b}

where {eq:12-126}

$$(\underline{\boldsymbol{S}})_{ab} = -\int_\Omega \hat{\boldsymbol{\epsilon}}_a^{\mathrm{p}} : \mathbf{E} : \left[\boldsymbol{\epsilon}[\hat{\boldsymbol{u}}_b] - \hat{\boldsymbol{\epsilon}}_b^{\mathrm{p}}\right] \,\mathrm{d}\Omega = \int_\Omega [\boldsymbol{\epsilon}[\hat{\boldsymbol{u}}_a] - \hat{\boldsymbol{\epsilon}}_a^{\mathrm{p}}] : \mathbf{E} : \left[\boldsymbol{\epsilon}[\hat{\boldsymbol{u}}_b] - \hat{\boldsymbol{\epsilon}}_b^{\mathrm{p}}\right] \,\mathrm{d}\Omega. \tag{9.33a}$$
{eq:12-126a}
$$(\underline{\boldsymbol{G}})_{ab} = \int_\Omega \hat{\boldsymbol{\epsilon}}_a^{\mathrm{p}} : \hat{\boldsymbol{\sigma}}_b^{\mathrm{p,di}} \,\mathrm{d}\Omega \tag{9.33b}$$
{eq:12-126b}
$$(\underline{\boldsymbol{f}}(\underline{\boldsymbol{\eta}}))_a = \int_\Omega \hat{\boldsymbol{\sigma}}_a^{\mathrm{p,di}} : \boldsymbol{\varphi}^*(\boldsymbol{\sigma}_0 + \tilde{\boldsymbol{\sigma}}^{\mathrm{p,di}}(\underline{\boldsymbol{\eta}})) \,\mathrm{d}\Omega \tag{9.33c}$$
{eq:12-126c}

with $(\underline{\boldsymbol{\xi}})_a = \xi_a$ and $(\underline{\boldsymbol{\eta}})_a = \eta_a$. The initial condition is

$$\underline{\boldsymbol{\xi}}(0) = \underline{\boldsymbol{0}} \quad \text{and} \quad \underline{\boldsymbol{\eta}}(0) = \underline{\boldsymbol{0}} \tag{9.34}$$
{eq:12-127}

It is possible to eliminate $\underline{\boldsymbol{\xi}}$ from (9.32a):

$$\underline{\boldsymbol{\xi}} = -\underline{\boldsymbol{S}}^{-1}\underline{\boldsymbol{G}}\underline{\boldsymbol{\eta}} \tag{9.35}$$
{eq:12-134}

and insert the result into (9.32b) to obtain the reduced problem

$$\underline{\boldsymbol{G}}^{\mathrm{T}}\underline{\boldsymbol{S}}^{-1}\underline{\boldsymbol{G}}\dot{\underline{\boldsymbol{\eta}}} + \underline{\boldsymbol{f}}(\underline{\boldsymbol{\eta}}) = \underline{\boldsymbol{0}} \tag{9.36}$$
{eq:12-135}

9.3.7 NMR – Version IV obtained via approximation of Version III

Let us introduced the approximate relation

$$\underline{\boldsymbol{G}}^{\mathrm{T}}\underline{\boldsymbol{S}}^{-1}\underline{\boldsymbol{G}}\dot{\underline{\boldsymbol{\eta}}} + \underline{\boldsymbol{f}}(\underline{\boldsymbol{\eta}}) = \underline{\boldsymbol{0}} \tag{9.37}$$
{eq:12-136}

instead of the independent choice in (9.15b). From (9.15b) we then obtain the identity $\xi_a = \eta_a$ and $N_R^{(\epsilon)} = N_R^{(\sigma)} := N_R$. Inserting this simplification into (9.15b), we obtain the following system of NMR equations for $a = 1, 2, \ldots, N_R$:

$$\sum_{b=1}^{N_R} \left[\int_\Omega \hat{\boldsymbol{\epsilon}}_b^{\mathrm{p}} : \mathbf{E} : [\boldsymbol{\epsilon}[\hat{\boldsymbol{u}}]_a - \hat{\boldsymbol{\epsilon}}_a^{\mathrm{p}}] \ \mathrm{d}\Omega \right] \dot{\xi}_b - \int_\Omega [\boldsymbol{\epsilon}[\hat{\boldsymbol{u}}]_a - \hat{\boldsymbol{\epsilon}}_a^{\mathrm{p}}] : \mathbf{E} : \boldsymbol{\varphi}^* \left(\boldsymbol{\sigma}_0 + \tilde{\boldsymbol{\sigma}}^{\mathrm{p,di}}(\underline{\boldsymbol{\xi}}) \right) \ \mathrm{d}\Omega = 0, \quad (9.38)$$ {eq:12-27}

We may express (9.38) in matrix form as the nonlinear problem

$$\underline{\boldsymbol{S}}\, \dot{\underline{\boldsymbol{\xi}}} + \underline{\boldsymbol{f}}'(\underline{\boldsymbol{\xi}}) = \underline{\boldsymbol{0}}, \quad (9.39)$$ {eq:12-37}

{eq:12-38} where

{eq:12-38a} $$(\underline{\boldsymbol{S}})_{ab} = \int_\Omega [\boldsymbol{\epsilon}[\hat{\boldsymbol{u}}_a] - \hat{\boldsymbol{\epsilon}}_a^{\mathrm{p}}] : \mathbf{E} : \left[\boldsymbol{\epsilon}[\hat{\boldsymbol{u}}_b] - \hat{\boldsymbol{\epsilon}}_b^{\mathrm{p}} \right] \ \mathrm{d}\Omega. \quad (9.40a)$$

{eq:12-38b} $$(\underline{\boldsymbol{f}}'(\underline{\boldsymbol{\xi}}))_a = \int_\Omega [\boldsymbol{\epsilon}[\hat{\boldsymbol{u}}_a] - \hat{\boldsymbol{\epsilon}}_a^{\mathrm{p}}] : \mathbf{E} : \boldsymbol{\varphi}^* \left(\boldsymbol{\sigma}_0 + \tilde{\boldsymbol{\sigma}}^{\mathrm{p,di}}(\underline{\boldsymbol{\xi}} \right) \ \mathrm{d}\Omega \quad (9.40b)$$

with $(\underline{\boldsymbol{\xi}})_a = \xi_a$. The initial condition is

{eq:12-39} $$\underline{\boldsymbol{\xi}}(0) = \underline{\boldsymbol{0}} \quad (9.41)$$

The next step is to discretize in time. Using the BE rule for integration of (**??**), we obtain the problem: For given ${}^{n-1}\underline{\boldsymbol{\xi}}$, compute the updated $\underline{\boldsymbol{\xi}} := {}^{n}\underline{\boldsymbol{\xi}}$ from

{eq:12-30} $$\underline{\boldsymbol{S}}\,\underline{\boldsymbol{\xi}} + \Delta t\, \underline{\boldsymbol{f}}(\underline{\boldsymbol{\xi}}) = \underline{\boldsymbol{S}}\, {}^{n-1}\underline{\boldsymbol{\xi}}, \quad (9.42)$$

which can be expressed as the residual equation

{eq:12-31} $$\underline{\boldsymbol{R}}(\underline{\boldsymbol{\xi}}) := \underline{\boldsymbol{S}} \left[\underline{\boldsymbol{\xi}} -{}^{n-1} \underline{\boldsymbol{\xi}} \right] + \Delta t\, \underline{\boldsymbol{f}}(\underline{\boldsymbol{\xi}}) = \underline{\boldsymbol{0}}. \quad (9.43)$$

The nonlinear system (9.43) can be solved in straightforward fashion using Newton iterations, whereby we have the algorithm

{eq:12-32} $$\underline{\boldsymbol{\xi}}^{(k+1)} = \underline{\boldsymbol{\xi}}^{(k)} + \Delta \underline{\boldsymbol{\xi}}, \quad (9.44)$$

where $\Delta\underline{\boldsymbol{\xi}}$ is solved from the linear set of equations

{eq:12-33} $$\underline{\boldsymbol{J}}^{(k)}\, \Delta\underline{\boldsymbol{\xi}} = -\underline{\boldsymbol{R}}(\underline{\boldsymbol{\xi}}^{(k)}), \quad \underline{\boldsymbol{J}} := \frac{\mathrm{d}\underline{\boldsymbol{R}}}{\mathrm{d}\underline{\boldsymbol{\xi}}}. \quad (9.45)$$

In order to compute $\underline{\boldsymbol{J}}$, we first consider the linearization of $\underline{\boldsymbol{f}}$, i.e.

{eq:12-34} $$\frac{\partial (\underline{\boldsymbol{f}})_a}{\partial \xi_b} = \int_\Omega [\boldsymbol{\epsilon}[\hat{\boldsymbol{u}}]_a - \hat{\boldsymbol{\epsilon}}_a^{\mathrm{p}}] : \mathbf{E} : \underbrace{\frac{\partial^2 \phi^*(\boldsymbol{\sigma})}{\partial \boldsymbol{\sigma}^{\mathrm{p,di}} \otimes \partial \boldsymbol{\sigma}^{\mathrm{p,di}}}}_{:=\mathbf{G}} : \mathbf{E} : \left[\boldsymbol{\epsilon}[\hat{\boldsymbol{u}}]_b - \hat{\boldsymbol{\epsilon}}_b^{\mathrm{p}} \right] \quad (9.46)$$

where it was used that

{eq:12-35} $$\frac{\partial \boldsymbol{\sigma}}{\partial \xi_b} = \mathbf{E} : \left[\boldsymbol{\epsilon}[\hat{\boldsymbol{u}}]_b - \hat{\boldsymbol{\epsilon}}_b^{\mathrm{p}} \right] \quad (9.47)$$

We thus obtain

{eq:12-36} $$(\underline{\boldsymbol{J}})_{ab} = (\underline{\boldsymbol{S}})_{ab} + \Delta t \int_\Omega [\boldsymbol{\epsilon}[\hat{\boldsymbol{u}}]_a - \hat{\boldsymbol{\epsilon}}_a^{\mathrm{p}}] : \mathbf{E} : \mathbf{G} : \mathbf{E} : \left[\boldsymbol{\epsilon}[\hat{\boldsymbol{u}}]_b - \hat{\boldsymbol{\epsilon}}_b^{\mathrm{p}} \right] \ \mathrm{d}\Omega. \quad (9.48)$$

Since the 4th order tensor $\mathbf{G}$ possesses major (and minor) symmetry, it is clear that $\underline{\boldsymbol{J}}$ is a symmetric (and positive definite???) matrix.

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9.3.8 Special case: Maxwell's model of linear viscoelasticity

Maxwell's model of linear viscoelasticity is the simplest possible choice that fits to the framework of viscoplasticity discussed above. It is defined via the evolution rule

{eq:12-43} $$\dot{\boldsymbol{\epsilon}}^{\mathrm{p}} = \frac{1}{\mu}\boldsymbol{\sigma}^{\mathrm{p,di}}, \quad \text{i.e. } \boldsymbol{\varphi}^*(\boldsymbol{\sigma}^{\mathrm{p,di}}) = \frac{1}{\mu}\boldsymbol{\sigma}^{\mathrm{p,di}} \tag{9.49}$$

with the viscosity μ. it then follows that

$$f_a := \int_\Omega \hat{\boldsymbol{\epsilon}}^{\mathrm{e}}_a : \mathbf{E} : \boldsymbol{\sigma}^{\mathrm{p,di}} \,\mathrm{d}\Omega = \underbrace{\int_\Omega \frac{1}{\mu}\hat{\boldsymbol{\epsilon}}^{\mathrm{e}}_a : \mathbf{E} : \boldsymbol{\sigma}_0 \,\mathrm{d}\Omega}_{:=f_{0,a}} + \sum_{b=1}^{N_R} \underbrace{\left[\frac{1}{\mu}\hat{\boldsymbol{\epsilon}}^{\mathrm{e}}_a : \mathbf{E}^2 : \hat{\boldsymbol{\epsilon}}^{\mathrm{e}}_b \,\mathrm{d}\Omega\right]}_{:=B_{ab}} \xi_b, \tag{9.50}$$ {eq:12-44}

or, in matrix notation {eq:12-45}

$$\underline{\boldsymbol{f}} = \underline{\boldsymbol{f}}_0 + \underline{\boldsymbol{B}}\,\underline{\boldsymbol{\xi}}, \qquad \text{where} \tag{9.51a}$$ {eq:12-45a}

$$\left(\underline{\boldsymbol{f}}_0\right)_a = f_{0,a} = \int_\Omega \frac{1}{\mu}\hat{\boldsymbol{\epsilon}}^{\mathrm{e}}_a : \mathbf{E} : \boldsymbol{\sigma}_0 \,\mathrm{d}\Omega \tag{9.51b}$$ {eq:12-45b}

$$(\underline{\boldsymbol{B}})_{ab} = B_{ab} = \int_\Omega \frac{1}{\mu}\hat{\boldsymbol{\epsilon}}^{\mathrm{e}}_a : \mathbf{E}^2 : \hat{\boldsymbol{\epsilon}}^{\mathrm{e}}_b \,\mathrm{d}\Omega \tag{9.51c}$$

Remark 17 *The 4th rank tensor* $\mathbf{G}$ *computes in this case as*

$$\mathbf{G} = \frac{\partial^2\phi^*}{\partial\boldsymbol{\sigma}^{p,di}\otimes\partial\boldsymbol{\sigma}^{p,di}} = \frac{1}{\mu}\mathbf{I}^{sym} \tag{9.52}$$ {eq:12-46}

with the 4th order identity tensor $\mathbf{I}^{sym}$ *for symmetric tensors.* □

Eq. (**??**) thus takes the explicit form

$$\underline{\boldsymbol{S}}\,\dot{\underline{\boldsymbol{\xi}}} + \underline{\boldsymbol{B}}\,\underline{\boldsymbol{\xi}} = -\underline{\boldsymbol{f}}_0(t), \quad \underline{\boldsymbol{\xi}}(0) = \underline{\boldsymbol{0}}. \tag{9.53}$$ {eq:12-47}

Remark 18 *The time-dependent loadings* $\boldsymbol{u}_{\mathrm{p}}$ *and* $\boldsymbol{t}_{\mathrm{p}}$ *are reflected by* $\underline{\boldsymbol{f}}_0(t)$. □

9.4 RVE-problem

9.4.1 Canonical format for strain control

In the (standard) case of complete *macroscale strain control*, $\bar{\boldsymbol{\epsilon}}$ is a known quantity at the solution of the RVE-problem: Find $\boldsymbol{u} \in \mathbb{U}_\square$, $\boldsymbol{t} \in \mathbb{T}_\square$ and $\boldsymbol{\epsilon}^{\mathrm{p}} \in \mathbb{L}_2(\Omega_\square)$ that solve the system: {eq:12-11}

$$\langle[\boldsymbol{\epsilon}[\boldsymbol{u}] - \boldsymbol{\epsilon}^{\mathrm{p}}] : \mathbf{E} : \boldsymbol{\epsilon}[\delta\boldsymbol{u}]\rangle_\square - \langle\langle \boldsymbol{t}\cdot\delta\boldsymbol{u}\rangle\rangle_\square = 0 \qquad \forall\delta\boldsymbol{u}\in\mathbb{U}^0 \tag{9.54a}$$ {eq:12-11a}

$$-\langle\langle\delta\boldsymbol{t}\cdot\boldsymbol{u}\rangle\rangle_\square = -\bar{\boldsymbol{\epsilon}} : \langle\langle\delta\boldsymbol{t}\otimes[\boldsymbol{x}-\bar{\boldsymbol{x}}]\rangle\rangle_\square \qquad \forall\delta\boldsymbol{t}\in\mathbb{T} \tag{9.54b}$$ {eq:12-11b}

$$\langle\dot{\boldsymbol{\epsilon}}^{\mathrm{p}} : \delta\boldsymbol{\sigma}^{\mathrm{p,di}}\rangle_\square - \langle\boldsymbol{\varphi}^*(\boldsymbol{\sigma}^{\mathrm{p,di}}) : \delta\boldsymbol{\sigma}^{\mathrm{p,di}}\rangle_\square = 0 \qquad \forall\,\delta\boldsymbol{\sigma}^{\mathrm{p,di}}\in\mathbb{L}_2(\Omega) \tag{9.54c}$$ {eq:12-11c}

$$\langle\boldsymbol{\sigma}^{\mathrm{p,di}} : \delta\boldsymbol{\epsilon}^{\mathrm{p}}\rangle_\square - \langle[\boldsymbol{\epsilon}[\boldsymbol{u}] - \boldsymbol{\epsilon}^{\mathrm{p}}] : \mathbf{E} : \delta\boldsymbol{\epsilon}^{\mathrm{p}}\rangle_\square = 0 \qquad \forall\delta\boldsymbol{\epsilon}^{\mathrm{p}}\in\mathbb{L}_2(\Omega) \tag{9.54d}$$ {eq:12-11d}

where we recall the boundary form

$$\langle\langle\bullet\rangle\rangle_\square := \frac{1}{|\Omega_\square|}\int_{\Gamma_\square}\bullet\,\mathrm{d}\Gamma \tag{9.55}$$ {eq:12-11d}

9.4.2 Dirichlet boundary conditions (DBC)

For given value of the macroscale strain $\bar{\boldsymbol{\epsilon}}$, find the fluctuation displacement field $\boldsymbol{u}^{\mu} \in \mathbb{U}_{\square}^{\mathrm{D},0}$ and $\boldsymbol{\epsilon}^{\mathrm{p}} \in \mathbb{L}_2(\Omega_{\square})$ which solve {eq:12-12}

$$a_{\square}(\boldsymbol{u}^{\mu}, \delta\boldsymbol{u}) - \langle \boldsymbol{\epsilon}^{\mathrm{p}} : \mathbf{E} : \boldsymbol{\epsilon}[\delta\boldsymbol{u}] \rangle_{\square} = -a_{\square}(\bar{\boldsymbol{\epsilon}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}], \delta\boldsymbol{u}) \qquad \forall \delta\boldsymbol{u} \in \mathbb{U}_{\square}^{\mathrm{D},0} \tag{9.56a}$$ {eq:12-12a}

$$\langle \dot{\boldsymbol{\epsilon}}^{\mathrm{p}} : \delta\boldsymbol{\sigma}^{\mathrm{p,di}} \rangle_{\square} - \langle \boldsymbol{\varphi}^{*}(\boldsymbol{\sigma}^{\mathrm{p,di}}) : \delta\boldsymbol{\sigma}^{\mathrm{p,di}} \rangle_{\square} = 0 \qquad \forall\, \delta\boldsymbol{\sigma}^{\mathrm{p,di}} \in \mathbb{L}_2(\Omega) \tag{9.56b}$$ {eq:12-12b}

$$\langle \boldsymbol{\sigma}^{\mathrm{p,di}} : \delta\boldsymbol{\epsilon}^{\mathrm{p}} \rangle_{\square} - \langle [\boldsymbol{\epsilon}[\boldsymbol{u}] - \boldsymbol{\epsilon}^{\mathrm{p}}] : \mathbf{E} : \delta\boldsymbol{\epsilon}^{\mathrm{p}} \rangle_{\square} = 0 \qquad \forall \delta\boldsymbol{\epsilon}^{\mathrm{p}} \in \mathbb{L}_2(\Omega) \tag{9.56c}$$ {eq:12-12c}

9.4.3 NTFA applied to the RVE-problem (DBC)

Following the recepy given above, we introduce the additive decomposition

{eq:12-48}
$$\boldsymbol{u} = \boldsymbol{u}^{M} + \boldsymbol{u}^{\mu} = \boldsymbol{u}^{M} + \boldsymbol{u}_0^{\mu} + \tilde{\boldsymbol{u}}^{\mu} \tag{9.57}$$

where it is assumed that $\boldsymbol{u}_0^{\mu} \in \mathbb{U}_{\square}^{D,0}$ solve the elasticity problem

{eq:12-49}
$$a_{\square}(\boldsymbol{u}_0^{\mu}, \delta\boldsymbol{u}) = -a_{\square}(\bar{\boldsymbol{\epsilon}} : [\boldsymbol{x} - \bar{\boldsymbol{x}}], \delta\boldsymbol{u}) = 0 \quad \forall\, \delta\boldsymbol{u} \in \mathbb{U}_{\square}^{D,0}. \tag{9.58}$$

{eq:12-50} Subtracting (9.58) from (9.56a), we obtain the eigenstrain problem

{eq:12-50a}
$$a_{\square}(\tilde{\boldsymbol{u}}^{\mu}, \delta\boldsymbol{u}) - \langle \boldsymbol{\epsilon}^{\mathrm{p}} : \mathbf{E} : \boldsymbol{\epsilon}[\delta\boldsymbol{u}] \rangle_{\square} = 0 \qquad \forall \delta\boldsymbol{u} \in \mathbb{U}_{\square}^{D,0} \tag{9.59a}$$

{eq:12-50b}
$$\langle \dot{\boldsymbol{\epsilon}}^{\mathrm{p}} : \delta\boldsymbol{\sigma}^{\mathrm{p,di}} \rangle_{\square} - \langle \boldsymbol{\varphi}^{*}(\boldsymbol{\sigma}^{p,di}) : \delta\boldsymbol{\sigma}^{\mathrm{p,di}} \rangle_{\square} = 0 \qquad \forall \delta\boldsymbol{\sigma}^{\mathrm{p,di}} \in \mathbb{L}_2(\Omega) \tag{9.59b}$$

where

{eq:12-51}
$$\boldsymbol{\sigma}^{\mathrm{p,di}} = \mathbf{E} : \left[\boldsymbol{\epsilon}[\boldsymbol{u}^{M} + \boldsymbol{u}_0^{\mu} + \tilde{\boldsymbol{u}}^{\mu}] - \boldsymbol{\epsilon}^{\mathrm{p}}\right] = \underbrace{\mathbf{E} : \left[\boldsymbol{\epsilon}[\boldsymbol{u}^{M} + \boldsymbol{u}_0^{\mu}]\right]}_{:=\boldsymbol{\sigma}_0} + \underbrace{\mathbf{E} : \left[\boldsymbol{\epsilon}[\tilde{\boldsymbol{u}}^{\mu}] - \boldsymbol{\epsilon}^{\mathrm{p}}\right]}_{:=\tilde{\boldsymbol{\sigma}}} \tag{9.60}$$

{eq:12-52} Adopting NTFA, we introduce the ansatz

{eq:12-52a}
$$\boldsymbol{\epsilon}^{\mathrm{p}}(\boldsymbol{x}, t) \simeq \boldsymbol{\epsilon}_R^{\mathrm{p}}(\boldsymbol{x}, t) := \sum_{a=1}^{N_R} \hat{\boldsymbol{\epsilon}}_a^{\mathrm{p}}\, \xi_a(t) \tag{9.61a}$$

{eq:12-52b}
$$\tilde{\boldsymbol{u}}^{\mu}(\boldsymbol{x}, t) \simeq \tilde{\boldsymbol{u}}_R^{\mu}(\boldsymbol{x}, t) := \sum_{a=1}^{N_R} \hat{\boldsymbol{u}}_a(\boldsymbol{x})\, \xi_a(t), \tag{9.61b}$$

whereby

{eq:12-53}
$$\tilde{\boldsymbol{\sigma}}(\boldsymbol{x}, t) \simeq \tilde{\boldsymbol{\sigma}}_R(\boldsymbol{x}, t) := \sum_{a=1}^{N_R} \hat{\boldsymbol{\epsilon}}_a^{\mathrm{e}}(\boldsymbol{x})\, \xi_a(t) \quad \text{with } \hat{\boldsymbol{\epsilon}}_a^{\mathrm{e}} := \boldsymbol{\epsilon}[\hat{\boldsymbol{u}}_a] - \hat{\boldsymbol{\epsilon}}_{\boldsymbol{a}}^{\mathrm{p}}. \tag{9.62}$$

For the "offline" stage, we may solve for $\hat{\boldsymbol{u}}_a$ in terms of $\hat{\boldsymbol{\epsilon}}_a$, $a = 1, 2, \ldots, N_R$, from (9.59a) as follows

{eq:12-54}
$$a_{\square}(\hat{\boldsymbol{u}}_a, \delta\boldsymbol{u}) = \langle \hat{\boldsymbol{\epsilon}}_a^{\mathrm{p}} : \mathbf{E} : \boldsymbol{\epsilon}[\delta\boldsymbol{u}] \rangle_{\square} \quad \forall\, \delta\boldsymbol{u} \in \mathbb{U}_{\square}^{D,0} \tag{9.63}$$

which, once again, constitute linear plasticity problems for $a = 1, 2, \ldots, N_R$.

Upon introducing the expansion for $\boldsymbol{\epsilon}^{\mathrm{p}}$ in (9.61a) and using the test functions

{eq:12-55}
$$\delta\boldsymbol{\sigma}^{\mathrm{p,di}} = \delta\tilde{\boldsymbol{\sigma}}_R = \mathbf{E} : \sum_{b=1}^{N_R} \hat{\boldsymbol{\epsilon}}\, \delta\xi_b \tag{9.64}$$

we obtain from (9.59b) the following system of NMR equations

{eq:12-56}
$$\sum_{b=1}^{N_R} \langle \hat{\boldsymbol{\epsilon}}_a^{\mathrm{e}} : \mathbf{E} : \hat{\boldsymbol{\epsilon}}_b^{\mathrm{p}} \rangle_{\square}\, \dot{\xi}_b - \langle \hat{\boldsymbol{\epsilon}}^{\mathrm{e}} : \mathbf{E} : \boldsymbol{\varphi}^{*}(\boldsymbol{\sigma}_R^{\mathrm{p,di}}(\underline{\boldsymbol{\xi}})) \rangle_{\square} = 0, \quad a = 1, 2, \ldots, N_R. \tag{9.65}$$

9.5 A general problem class: Standard dissipative material

NFTA is not applicable

Chapter 10

FE^2 WITH ERROR CONTROL AND ADAPTIVITY – NONLINEAR ELASTICITY

Scale separation, assumed linear variation of macroscale displacement within RVE (FL,KR,FS:Part I), FE^2, error computation for nonlinear problem

Material model: Nonlinear elasticity

COMPLETE Chapter with FE-format

Paper: "Fine-scale accuracy"

Chapter 11

DISCRETIZATION-BASED HOMOGENIZATION AND SEAMLESS SCALE-BRIDGING

Basic formulation: Dirichlet b.c. consistent with FE displacement method
Updated (KR:s VR-project): Neumann b.c. based on mixed FE method $\bar{\boldsymbol{u}}, \bar{\boldsymbol{\sigma}}$.