Chapter 10

HOMOGENIZED MATERIAL PROPERTIES

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In this chapter we discuss the fundamental concepts of multiscale material modeling, with focus on two-scales (subscale and macroscale).

10.1 Introduction

10.1.1 Motivation

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 (or at least presumed to be) 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.

10.1.2 Literature

10.2 Basics of homogenization

10.2.1 Concept of Representative Volume Element (RVE)

The effective properties of the material are obtained upon volume averaging (or homogenization) on a "computational cell" with typical diameter $L_\square$. Although the shape of the computational cell is irrelevant in principle, it is often taken as a cube in 3D (square in 2D) for computational simplicity, as sketched in Figure 10.1. For a random microstructure the true effective properties are obtained as the converged values when $L_\square$ becomes sufficiently large. However, in practice it is always necessary (and possible) to choose a cell of finite size, the Representative Volume Element (RVE) with typical diameter L_{RVE}. The RVE is defined as a statistically representative sample of the material on the subscale.

In the case of complete scale separation, in order to qualify as an RVE its size L_{RVE} must be

- sufficiently small compared to the typical macroscale dimension of the structural component, $L_{\text{RVE}} << L^{\text{MAC}}$.
- sufficiently large compared to the typical subscale dimension of microconstituents, e.g. grains, $L^{\text{sub}} << L_{\text{RVE}}$.

That the RVE is *sufficiently small* means that the averaged field variables, e.g. stresses and strains, vary at most linearly within the RVE, a condition known as *scale separation* (or 1st order homogenization). That the RVE is *sufficiently large* means that the averaged field variables for a given macroscopic "point" do not change significantly at further increase of the RVE size, which is illustrated in Figure 10.1. It practice it may be difficult to satisfy these two requirements simultaneously.

Henceforth, we shall assume that the conditions for an RVE are satisfied by the computational cell, i.e. $L_\square \approx L_{\text{RVE}}$.

10.2.2 The average strain and stress theorems

Upon the introduction of volume averages on the RVE, defined as

$$\langle \bullet \rangle_\square \stackrel{\text{def}}{=} \frac{1}{|\Omega_\square|} \int_{\Omega_\square} \bullet \, \mathrm{d}\Omega \tag{10.1}$$

we may introduce the effective strain and stress tensors, $\bar{\boldsymbol{\epsilon}}$ and $\bar{\boldsymbol{\sigma}}$, respectively as the averages

$$\bar{\boldsymbol{\epsilon}} \stackrel{\text{def}}{=} \langle \boldsymbol{\epsilon} \rangle_\square, \quad \bar{\boldsymbol{\sigma}} \stackrel{\text{def}}{=} \langle \boldsymbol{\sigma} \rangle_\square \tag{10.2}$$

It is possible to transform the volume integrals in (10.2) for the strain and stress averages to surface integrals on the RVE. The boundary of $\Omega_\square$ is denoted $\Gamma_\square$.

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

$$\int_{\Omega_\square} \boldsymbol{u} \otimes \boldsymbol{\nabla} \, \mathrm{d}\Omega = \int_{\Gamma_\square} \boldsymbol{u} \otimes \boldsymbol{n} \, \mathrm{d}\Gamma \tag{10.3}$$

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

$$\begin{aligned} \langle \boldsymbol{\epsilon} \rangle_\square &= \frac{1}{|\Omega_\square|} \int_{\Omega_\square} \boldsymbol{\epsilon} \, \mathrm{d}\Omega = \frac{1}{2|\Omega_\square|} \int_{\Omega_\square} [\boldsymbol{u} \otimes \boldsymbol{\nabla} + [\boldsymbol{u} \otimes \boldsymbol{\nabla}]^{\mathrm{T}}] \, \mathrm{d}\Omega \\ &= \frac{1}{2|\Omega_\square|} \int_{\Gamma_\square} [\boldsymbol{u} \otimes \boldsymbol{n} + [\boldsymbol{u} \otimes \boldsymbol{n}]^{\mathrm{T}}] \, \mathrm{d}\Gamma \end{aligned} \tag{10.4}$$

For the stress average, we first consider the identity

$$\vec{\boldsymbol{\nabla}} \cdot [\boldsymbol{\sigma}^{\mathrm{T}} \otimes \boldsymbol{x}] = \boldsymbol{\sigma} \cdot \boldsymbol{I} + [\boldsymbol{\sigma} \cdot \boldsymbol{\nabla}] \otimes \boldsymbol{x} = \boldsymbol{\sigma} - \boldsymbol{f} \otimes \boldsymbol{x} \tag{10.5}$$

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

$$-\boldsymbol{\sigma} \cdot \boldsymbol{\nabla} = \boldsymbol{f} \ \text{ in } \ \Omega_\square \tag{10.6}$$

Hence, we obtain with Gauss' theorem

$$\begin{aligned}\langle\boldsymbol{\sigma}\rangle_\square &= \frac{1}{|\Omega_\square|}\int_{\Omega_\square}\boldsymbol{\sigma}\,\mathrm{d}\Omega = \frac{1}{|\Omega_\square|}\int_{\Omega_\square}\vec{\boldsymbol{\nabla}}\cdot[\boldsymbol{\sigma}^{\mathrm{T}}\otimes\boldsymbol{x}]\,\mathrm{d}\Omega + \frac{1}{|\Omega_\square|}\int_{\Omega_\square}\boldsymbol{f}\otimes\boldsymbol{x}\,\mathrm{d}\Omega \\ &= \frac{1}{|\Omega_\square|}\int_{\Gamma_\square}\underbrace{\boldsymbol{n}\cdot\boldsymbol{\sigma}^{\mathrm{T}}}_{=\boldsymbol{t}}\otimes\boldsymbol{x}\,\mathrm{d}\Gamma + \frac{1}{|\Omega_\square|}\int_{\Omega_\square}\boldsymbol{f}\otimes\boldsymbol{x}\,\mathrm{d}\Omega \end{aligned} \tag{10.7}$$

In the special case of vanishing volume load, $\boldsymbol{f}=\boldsymbol{0}$, we obtain

$$\langle\boldsymbol{\sigma}\rangle_\square = \frac{1}{|\Omega_\square|}\int_{\Gamma_\square}\boldsymbol{t}\otimes\boldsymbol{x}\,\mathrm{d}\Gamma \tag{10.8}$$

Henceforth in this Chapter, we make the significant assumption that $\boldsymbol{f}=\boldsymbol{0}$, which has a profound importance for classical homogenization results.

10.2.3 The Hill-Mandel macrohomogeneity condition

Let us introduce $\mathbb{U}_\square$, which is the space of admissible displacements $\boldsymbol{u}$ *restricted* to a given RVE occupying the domain $\Omega_\square$ with boundary $\Gamma_\square$. Hence, $\boldsymbol{u}\in\mathbb{U}_\square$ do not satisfy any a priori given values on $\Gamma_\square$ in general. In order for the macroscale variables $\bar{\boldsymbol{\sigma}}$ and $\bar{\boldsymbol{\epsilon}}$ to be admissible variables in the macroscale constitutive relation, the so-called Hill-Mandel macrohomogeneity condition must be satisfied:

$$\bar{\boldsymbol{\sigma}}:\delta\bar{\boldsymbol{\epsilon}} = \langle\boldsymbol{\sigma}:\delta\boldsymbol{\epsilon}\rangle_\square \quad \forall\delta\boldsymbol{u}\in\mathbb{U}_\square \tag{10.9}$$

where $\delta\boldsymbol{\epsilon}$ is the strain corresponding to $\delta\boldsymbol{u}$. This condition is equivalent to the statement that the virtual 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 useful relation

$$\begin{aligned}\langle\boldsymbol{\sigma}:\delta\boldsymbol{\epsilon}\rangle_\square &= \frac{1}{|\Omega_\square|}\int_{\Omega_\square}\boldsymbol{\sigma}:\delta\boldsymbol{\epsilon}\,\mathrm{d}\Omega = \frac{1}{\Omega_\square}\left[\int_{\Omega_\square}\boldsymbol{f}\cdot\delta\boldsymbol{u}\,\mathrm{d}\Omega + \int_{\Gamma_\square}\boldsymbol{t}\cdot\delta\boldsymbol{u}\,\mathrm{d}\Gamma\right] \\ &= \frac{1}{|\Omega_\square|}\int_{\Gamma_\square}\boldsymbol{t}\cdot\delta\boldsymbol{u}\,\mathrm{d}\Gamma \end{aligned} \tag{10.10}$$

where the last identity follows due to the assumption $\boldsymbol{f}=\boldsymbol{0}$. In the subsequent Section, we shall consider classical boundary conditions on $\Gamma_\square$ that make certain that the condition (10.9) is satisfied *a priori*, i.e. for any choice of boundary conditions on the RVE.

10.2.4 Effective properties

We shall, for simplicity, assume linear elastic response on the subscale, i.e. $\boldsymbol{\sigma} = \mathbf{E} : \boldsymbol{\epsilon}$, where $\mathbf{E}$ represents the most general anisotropic characteristics of the microstructure, e.g. pearlitic phase structure within a grain in steel. The effective constitutive relationship is defined as

$$\bar{\boldsymbol{\sigma}} = \bar{\mathbf{E}} : \bar{\boldsymbol{\epsilon}} \tag{10.11}$$

where the effective stiffness tensor is defined (in some fashion) via the heterogeneous subscale properties represented by $\mathbf{E}$. It is the fashion in which $\bar{\mathbf{E}}$ is computed that is the key issue in the classical homogenization theory. Subsequently we discuss two basic assumptions:

Voigt (Taylor) assumption: The subscale strain field $\boldsymbol{\epsilon}$ is uniform, i.e. $\boldsymbol{\epsilon} = \bar{\boldsymbol{\epsilon}}$ in $\Omega_\square$. Inserting this assumption in (10.11), we obtain

$$\bar{\boldsymbol{\sigma}} = \langle \boldsymbol{\sigma} \rangle_\square = \langle \mathbf{E} \rangle_\square : \bar{\boldsymbol{\epsilon}} \quad \Rightarrow \quad \bar{\mathbf{E}} = \bar{\mathbf{E}}^{\mathrm{V}} = \langle \mathbf{E} \rangle_\square \tag{10.12}$$

where superscript (V) stands for Voigt.

Reuss (Hill) assumption: The subscale stress field $\boldsymbol{\sigma}$ is uniform, i.e. $\boldsymbol{\sigma} = \bar{\boldsymbol{\sigma}}$ in $\Omega_\square$. Inserting this assumption in (10.11), we obtain[1]

$$\bar{\boldsymbol{\epsilon}} = \langle \boldsymbol{\epsilon} \rangle_\square = \langle \mathbf{E}^{-1} \rangle_\square : \bar{\boldsymbol{\sigma}} \quad \Rightarrow \quad \bar{\mathbf{E}} = \bar{\mathbf{E}}^{\mathrm{R}} = \langle \mathbf{E}^{-1} \rangle_\square^{-1} \tag{10.13}$$

The two situations associated with the Voigt and Reuss assumption, respectively, are illustrated in Figure 10.2.

We note that the approximations $\bar{\mathbf{E}}^{\mathrm{V}}$ and $\bar{\mathbf{E}}^{\mathrm{R}}$ of the true value of $\bar{\mathbf{E}}$ were computed without any specific choice of boundary conditions on the RVE. Below we show that $\bar{\mathbf{E}}^{\mathrm{V}}$ and $\bar{\mathbf{E}}^{\mathrm{R}}$ represent extremes of $\bar{\mathbf{E}}$ (or of any other possible approximation of $\bar{\mathbf{E}}$).

Remark: In the case of nonlinear (or inelastic) response, $\bar{\mathbf{E}}$ plays the role of tangent stiffness and cannot be computed a priori since it depends on the macroscale solution $\bar{\boldsymbol{\epsilon}}$. □

We conclude this preliminary discussion by noting that it is, in practice, not possible to compute $\bar{\mathbf{E}}$ exactly, since this would require the *exact* solution of the subscale fields $\boldsymbol{\epsilon}$

[1] $\mathbf{E}^{-1}$ 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 tangent 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 $\underline{\bar{\mathbf{E}}}^{\mathrm{R}} = \langle \underline{\mathbf{E}}^{-1} \rangle_\square^{-1}$.

and $\boldsymbol{\sigma}$ within the RVE. Obviously, this would require the true resolution of the subscale properties within the whole macroscopic component under consideration. Rather, it is common to opt for techniques to obtain

- sharp bounds on (the eigenvalues) of $\bar{\mathbf{E}}$, or
- a good approximation of $\bar{\mathbf{E}}$ via a suitable choice of boundary conditions on the RVE and/or "clever" approximations of the strain and stress fields within the RVE for the given boundary conditions

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). However, it is necessary to use FE-discretization of the subscale in practice, which motivates the notion of computational homogenization.

Hashin and Shtrikman **?** provided the tightest possible bounds for isotropic subscale material response in the absence of information on the actual substructural toplogy; hence, volume fractions and phase properties are the only data. For dilute concentration of hard particles (which are assumed to have ellipsoidal shape) in a soft matrix, the method of Mori and Tanaka **?** gives a good estimate of $\bar{\mathbf{E}}$ (but no bounds). A recent overview of different techniques, with emphasis on computational homogenization, can be found in Zohdi and Wriggers **?**.

10.2.5 The Hill-Reuss-Voigt bounds

In the previous Subsection, we derived the effective stiffness tensors due to Voigt and Reuss, denoted $\bar{\mathbf{E}}^{\mathrm{V}}$ and $\bar{\mathbf{E}}^{\mathrm{R}}$, respectively. Here, we shall establish that $\bar{\mathbf{E}}^{\mathrm{V}}$ and $\bar{\mathbf{E}}^{\mathrm{R}}$ are, in fact, upper and lower bounds on the exact value of $\bar{\mathbf{E}}$ or any approximate value stemming from a choice of $\boldsymbol{\epsilon}$ and $\boldsymbol{\sigma}$ within $\Omega_{\square}$ and on $\Gamma_{\square}$ such that the macrohomogeneity condition is satisfied.

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 $\boldsymbol{\epsilon}^{\mathrm{s}}(\boldsymbol{x})$:

$$\boldsymbol{\epsilon}(\boldsymbol{x}) = \bar{\boldsymbol{\epsilon}} + \boldsymbol{\epsilon}^{\mathrm{s}}(\boldsymbol{x}), \quad \boldsymbol{x} \in \Omega_{\square} \tag{10.14}$$

where we have, by definition, the condition

$$\langle \boldsymbol{\epsilon} \rangle_\square = \bar{\boldsymbol{\epsilon}} + \langle \boldsymbol{\epsilon}^{\mathrm{s}} \rangle_\square = \bar{\boldsymbol{\epsilon}} \quad \Rightarrow \quad \langle \boldsymbol{\epsilon}^{\mathrm{s}} \rangle_\square = \mathbf{0} \tag{10.15}$$

Since $\mathbf{E}$ is positive definite, we derive

$$\begin{aligned} 0 \;&\leq\; \int_{\Omega_\square} \boldsymbol{\epsilon}^{\mathrm{s}} : \mathbf{E} : \boldsymbol{\epsilon}^{\mathrm{s}} \, \mathrm{d}\Omega = \int_{\Omega_\square} [\boldsymbol{\epsilon} - \bar{\boldsymbol{\epsilon}}] : \mathbf{E} : [\boldsymbol{\epsilon} - \bar{\boldsymbol{\epsilon}}] \, \mathrm{d}\Omega \\ &=\; \int_{\Omega_\square} \boldsymbol{\epsilon} : \underbrace{\mathbf{E} : \boldsymbol{\epsilon}}_{=\boldsymbol{\sigma}} \, \mathrm{d}\Omega - 2 \int_{\Omega} \bar{\boldsymbol{\epsilon}} : \underbrace{\mathbf{E} : \boldsymbol{\epsilon}}_{=\boldsymbol{\sigma}} \mathrm{d}\Omega + \int_{\Omega} \bar{\boldsymbol{\epsilon}} : \mathbf{E} : \bar{\boldsymbol{\epsilon}} \, \mathrm{d}\Omega \\ &=\; \int_{\Omega_\square} \boldsymbol{\sigma} : \boldsymbol{\epsilon} \, \mathrm{d}\Omega - 2[\int_{\Omega} \boldsymbol{\sigma} \, \mathrm{d}\Omega] : \bar{\boldsymbol{\epsilon}} + \bar{\boldsymbol{\epsilon}} : [\int_{\Omega} \mathbf{E} \, \mathrm{d}\Omega] : \bar{\boldsymbol{\epsilon}} \, \mathrm{d}\Omega \end{aligned} \tag{10.16}$$

Using the Hill-Mandel condition (10.9), we now obtain

$$\begin{aligned} 0 \;&\leq\; \underbrace{\langle \boldsymbol{\sigma} : \boldsymbol{\epsilon} \rangle_\square}_{\bar{\boldsymbol{\sigma}} : \bar{\boldsymbol{\epsilon}}} - 2 \underbrace{\langle \boldsymbol{\sigma} \rangle_\square}_{\bar{\boldsymbol{\sigma}}} : \bar{\boldsymbol{\epsilon}} + \bar{\boldsymbol{\epsilon}} : \underbrace{\langle \mathbf{E} \rangle_\square}_{\bar{\mathbf{E}}^{\mathrm{V}}} : \bar{\boldsymbol{\epsilon}} \\ &=\; -\bar{\boldsymbol{\sigma}} : \bar{\boldsymbol{\epsilon}} + \bar{\boldsymbol{\epsilon}} : \bar{\mathbf{E}}^{\mathrm{V}} : \bar{\boldsymbol{\epsilon}} = \bar{\boldsymbol{\epsilon}} : [\bar{\mathbf{E}}^{\mathrm{V}} - \bar{\mathbf{E}}] : \bar{\boldsymbol{\epsilon}} \end{aligned} \tag{10.17}$$

where we also used that $\bar{\boldsymbol{\sigma}} = \bar{\mathbf{E}} : \bar{\boldsymbol{\epsilon}}$. Since (10.17) must hold for *any* possible field $\boldsymbol{\epsilon}$ in $\Omega_\square$, i.e. for any value of $\bar{\boldsymbol{\epsilon}}$, we conclude that the eigenvalues of $\bar{\mathbf{E}}^{\mathrm{V}}$ are *larger* than (or equal to) those of $\bar{\mathbf{E}}$. We may write this condition symbolically as

$$\bar{\mathbf{E}} \leq \bar{\mathbf{E}}^{\mathrm{V}} \tag{10.18}$$

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 $\boldsymbol{\sigma}^{\mathrm{s}}(\boldsymbol{x})$ in a fashion that is completely analogous to $\boldsymbol{\epsilon}(\boldsymbol{x})$:

$$\boldsymbol{\sigma}(\boldsymbol{x}) = \bar{\boldsymbol{\sigma}} + \boldsymbol{\sigma}^{\mathrm{s}}(\boldsymbol{x}), \quad \boldsymbol{x} \in \Omega_\square \tag{10.19}$$

where we have, by definition, that

$$\langle \boldsymbol{\sigma} \rangle_\square = \bar{\boldsymbol{\sigma}} + \langle \boldsymbol{\sigma}^{\mathrm{s}} \rangle_\square = \bar{\boldsymbol{\sigma}} \quad \Rightarrow \quad \langle \boldsymbol{\sigma}^{\mathrm{s}} \rangle_\square = \mathbf{0} \tag{10.20}$$

We now derive

$$\begin{aligned} 0 \;&\leq\; \int_{\Omega_\square} \boldsymbol{\sigma}^{\mathrm{s}} : \mathbf{E}^{-1} : \boldsymbol{\sigma}^{\mathrm{s}} \, \mathrm{d}\Omega \\ &=\; \int_{\Omega_\square} \boldsymbol{\epsilon} : \boldsymbol{\sigma} \, \mathrm{d}\Omega - 2 \left[\int_{\Omega_\square} \boldsymbol{\epsilon} \, \mathrm{d}\Omega \right] : \bar{\boldsymbol{\sigma}} + \bar{\boldsymbol{\sigma}} : \left[\int_{\Omega_\square} \mathbf{E}^{-1} \, \mathrm{d}\Omega \right] : \bar{\boldsymbol{\sigma}} \, \mathrm{d}\Omega \end{aligned} \tag{10.21}$$

Again, using the Hill-Mandel condition (10.9), we obtain

$$\begin{aligned} 0 &\leq \langle \boldsymbol{\epsilon} : \boldsymbol{\sigma} \rangle_\square - 2\langle \boldsymbol{\epsilon} \rangle_\square : \bar{\boldsymbol{\sigma}} + \bar{\boldsymbol{\sigma}} : \langle \mathbf{E}^{-1} \rangle_\square : \bar{\boldsymbol{\sigma}} \\ &= -\bar{\boldsymbol{\epsilon}} : \bar{\boldsymbol{\sigma}} + \bar{\boldsymbol{\sigma}} : [\bar{\mathbf{E}}^{\mathrm{R}}]^{-1} : \bar{\boldsymbol{\sigma}} = \bar{\boldsymbol{\sigma}} : [[\bar{\mathbf{E}}^{\mathrm{R}}]^{-1} - \bar{\mathbf{E}}^{-1}] : \bar{\boldsymbol{\sigma}} \end{aligned} \tag{10.22}$$

Since (10.22) must hold for *any* possible field $\boldsymbol{\sigma}$ in $\Omega_\square$, we conclude that the eigenvalues of $[\bar{\mathbf{E}}^{\mathrm{R}}]^{-1}$ are *larger* than (or equal to) those of $\bar{\mathbf{E}}^{-1}$. Hence, the eigenvalues of $\bar{\mathbf{E}}^{\mathrm{R}}$ are *smaller* than (or equal to) those of $\bar{\mathbf{E}}$, which can be written symbolically as

$$\bar{\mathbf{E}}^{\mathrm{R}} \leq \bar{\mathbf{E}} \tag{10.23}$$

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

Finally, we may summarize (10.18) and (10.23) as the "Hill-Reuss-Voigt" bounds

$$\bar{\mathbf{E}}^{\mathrm{R}} \leq \bar{\mathbf{E}} \leq \bar{\mathbf{E}}^{\mathrm{V}} \tag{10.24}$$

10.3 Boundary conditions on the RVE

10.3.1 Preliminaries

A 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 $\bar{\mathbf{E}}$. It must be noted that in theory this value always depends on the *actual* fine-scale (fully resolved) solution for a given boundary value problem. However, if certain assumptions are introduced, it is possible to compute a *good approximation* of $\bar{\mathbf{E}}$ *a priori* uniquely, i.e. independent on the actual solution.

As a preliminary, we introduce the macroscale coordinate $\bar{\boldsymbol{x}}$ as the "centroid" of the RVE, i.e. $\bar{\boldsymbol{x}}$ satisfies $\langle \boldsymbol{x} - \bar{\boldsymbol{x}} \rangle_\square = \mathbf{0}$ or $\bar{\boldsymbol{x}} = \langle \boldsymbol{x} \rangle_\square$.

10.3.2 Displacement boundary conditions (DBC)

Introduce displacement boundary conditions via the *ansatz*

$$\boldsymbol{u}(\boldsymbol{x}) = \bar{\boldsymbol{u}} + \boldsymbol{\epsilon}^* \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}], \quad \boldsymbol{x} \in \Gamma_\square \tag{10.25}$$

where $\boldsymbol{\epsilon}^*$ is a *constant* symmetrical tensor. We first obtain

$$\begin{aligned}\int_{\Gamma_\square} \boldsymbol{u} \otimes \boldsymbol{n} \, \mathrm{d}\Gamma &= \int_{\Gamma_\square} [\bar{\boldsymbol{u}} + \boldsymbol{\epsilon}^* \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}]] \otimes \boldsymbol{n} \, \mathrm{d}\Gamma = \int_{\Omega_\square} [\boldsymbol{\epsilon}^* \cdot \boldsymbol{x}] \otimes \boldsymbol{\nabla} \, \mathrm{d}\Omega \\ &= \int_{\Omega_\square} \boldsymbol{\epsilon}^* \cdot \boldsymbol{I} \, \mathrm{d}\Omega = \boldsymbol{\epsilon}^* |\Omega_\square| \end{aligned} \tag{10.26}$$

where it was used that $\bar{\boldsymbol{u}}$ and $\bar{\boldsymbol{x}}$ are constants w.r.t. operations with $\boldsymbol{\nabla}$.

Upon using this result in (10.4), we obtain directly

$$\bar{\boldsymbol{\epsilon}} \overset{\text{def}}{=} \langle \boldsymbol{\epsilon} \rangle_\square = \frac{1}{2|\Omega_\square|} [\boldsymbol{\epsilon}^* + [\boldsymbol{\epsilon}^*]^{\mathrm{T}}] |\Omega_\square| = \boldsymbol{\epsilon}^* \tag{10.27}$$

where we used the symmetry of $\boldsymbol{\epsilon}^*$. Hence, we may replace $\boldsymbol{\epsilon}^*$ with $\bar{\boldsymbol{\epsilon}}$ in (10.25), i.e.[2]

$$\boldsymbol{u}(\boldsymbol{x}) = \bar{\boldsymbol{u}} + \bar{\boldsymbol{\epsilon}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}], \quad \boldsymbol{x} \in \Gamma_\square \tag{10.28}$$

Figure 10.3 shows the deformed shape of a square RVE in 2D, representing a particle-reinforced matrix, for the two cases of pure normal strain and pure shear strain.

Next, we show that the choice in (10.28) is sufficient to ensure that the corresponding fine-scale fields $\boldsymbol{\epsilon}$ and $\boldsymbol{\sigma}$ do, indeed, satisfy the Hill-Mandel condition (10.9). In order to do so, we use (10.10) together with (10.28) and (10.8) to obtain

$$\begin{aligned}\langle \boldsymbol{\sigma} : \delta\boldsymbol{\epsilon} \rangle_\square &= \frac{1}{|\Omega_\square|} \int_{\Gamma_\square} \boldsymbol{t} \cdot [\delta\bar{\boldsymbol{u}} + \delta\bar{\boldsymbol{\epsilon}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}]] \, \mathrm{d}\Gamma \\ &= \frac{1}{|\Omega_\square|} \underbrace{\left[\int_{\Gamma_\square} \boldsymbol{t} \, \mathrm{d}\Gamma\right]}_{=\mathbf{0}\,\text{equilibrium}} \cdot [\delta\bar{\boldsymbol{u}} - \delta\bar{\boldsymbol{\epsilon}} \cdot \bar{\boldsymbol{x}}] + \frac{1}{|\Omega_\square|} \left[\int_{\Gamma_\square} \boldsymbol{t} \otimes \boldsymbol{x} \, \mathrm{d}\Gamma\right] : \delta\bar{\boldsymbol{\epsilon}} = \langle \boldsymbol{\sigma} \rangle_\square : \delta\bar{\boldsymbol{\epsilon}} \\ &= \bar{\boldsymbol{\sigma}} : \delta\bar{\boldsymbol{\epsilon}} \end{aligned} \tag{10.29}$$

where we, once again, used that volume load vanishes, i.e. $\boldsymbol{f} = \mathbf{0}$.

Remark: The assumption (10.25) on the how displacements vary along the boundary means that they are linear along any boundary that is straight. Since this is the case in practice it is common to speak about *linear displacement boundary conditions*. □

10.3.3 Traction boundary condition (TBC)

Introduce traction boundary conditions via the ansatz

$$\boldsymbol{t}(\boldsymbol{x}) = \boldsymbol{\sigma}^* \cdot \boldsymbol{n}, \quad \boldsymbol{x} \in \Gamma_\square \tag{10.30}$$

[2]To indicate the two-scale dependence, we may write (10.28) as $\boldsymbol{u}(\boldsymbol{x}, \bar{\boldsymbol{x}}) = \bar{\boldsymbol{u}}(\bar{\boldsymbol{x}}) + \bar{\boldsymbol{\epsilon}}(\bar{\boldsymbol{x}}) \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}]$, where $\bar{\boldsymbol{x}}$ is now considered as the macroscale independent spatial coordinate.

where $\boldsymbol{\sigma}^*$ is a *constant* symmetrical tensor. We first obtain

$$\begin{aligned}\int_{\Gamma_\square} \boldsymbol{t}\otimes\boldsymbol{x}\ \mathrm{d}\Gamma &= \int_{\Gamma_\square} \boldsymbol{n}\cdot[\boldsymbol{\sigma}^*]^{\mathrm{T}}\otimes\boldsymbol{x}\ \mathrm{d}\Gamma = \int_{\Omega_\square} \vec{\boldsymbol{\nabla}}\cdot[[\boldsymbol{\sigma}^*]^{\mathrm{T}}\otimes\boldsymbol{x}]\ \mathrm{d}\Omega \\ &= \int_{\Omega_\square} \boldsymbol{\sigma}^*\cdot\boldsymbol{I}\ \mathrm{d}\Omega = \boldsymbol{\sigma}^*|\Omega_\square| \end{aligned} \tag{10.31}$$

Upon using this result in (10.8), we obtain

$$\bar{\boldsymbol{\sigma}} \overset{\text{def}}{=} \langle\boldsymbol{\sigma}\rangle_\square = \boldsymbol{\sigma}^* \tag{10.32}$$

Hence, we may replace $\boldsymbol{\sigma}^*$ with $\bar{\boldsymbol{\sigma}}$ in (10.30), i.e.

$$\boldsymbol{t}(\boldsymbol{x}) = \bar{\boldsymbol{\sigma}}\cdot\boldsymbol{n}, \quad \boldsymbol{x}\in\Gamma_\square \tag{10.33}$$

Figure 10.4 shows the deformed shape of a square RVE in 2D, representing a particle-reinforced matrix, for the two cases of pure normal strain and pure shear strain.

Next, we show that this condition is sufficient to ensure that the Hill-Mandel condition (10.9) holds. We then use (10.10) together with (10.33) and (10.4) to obtain

$$\begin{aligned}\langle\boldsymbol{\sigma}:\delta\boldsymbol{\epsilon}\rangle_\square &= \frac{1}{|\Omega_\square|}\int_{\Gamma_\square}\boldsymbol{n}\cdot\bar{\boldsymbol{\sigma}}^{\mathrm{T}}\cdot\delta\boldsymbol{u}\ \mathrm{d}\Gamma = \frac{1}{|\Omega_\square|}\bar{\boldsymbol{\sigma}}:\int_{\Gamma_\square}\delta\boldsymbol{u}\otimes\boldsymbol{n}\ \mathrm{d}\Gamma \\ &= \frac{1}{2|\Omega_\square|}\bar{\boldsymbol{\sigma}}:\int_{\Omega_\square}\left[\delta\boldsymbol{u}\otimes\boldsymbol{n}+[\delta\boldsymbol{u}\otimes\boldsymbol{n}]^{\mathrm{T}}\right]\ \mathrm{d}\Omega = \bar{\boldsymbol{\sigma}}:\langle\delta\boldsymbol{\epsilon}\rangle_\square \\ &= \bar{\boldsymbol{\sigma}}:\delta\bar{\boldsymbol{\epsilon}} \end{aligned} \tag{10.34}$$

where we used the symmetry of $\bar{\boldsymbol{\sigma}}$.

Remark: The assumption (10.30) on the how tractions vary along the boundary means that they are constant along any boundary that is straight. Since this is the case in practice it is common to speak about *constant traction boundary conditions.* □

10.3.4 Periodic displacement and traction boundary conditions (PBC)

To be completed.

Figure 10.5 shows the deformed shape of a square RVE in 2D, representing a particle-reinforced matrix, for the two cases of pure normal strain and pure shear strain.

10.3.5 Discussion - Evaluation

To assign the "right" boundary conditions is crucial in order to obtain a good approximation of $\bar{\mathbf{E}}$[3]. In fact, it is not possible to define a general hierarchy for arbitrary heterogeneity on the subscale.

To be completed.

10.4 Computational homogenization based on DBC

10.4.1 Effective properties

Our aim is to establish the most general expression for the effective stiffness tensor $\bar{\mathbf{E}}$ while assuming the DBC-condition for the RVE. To this end, we first introduce the representation

$$\boldsymbol{u}(\boldsymbol{x}) = \boldsymbol{u}^{\mathrm{M}}(\boldsymbol{x}) + \boldsymbol{u}^{\mathrm{s}}(\boldsymbol{x}), \quad \boldsymbol{x} \in \Omega_{\square} \tag{10.35}$$

where $\boldsymbol{u}^{\mathrm{M}}(\bar{\boldsymbol{x}})$ represents the macroscale displacement field within the RVE. Adopting the classical first order homogenization approximation, we *assume* that $\boldsymbol{u}^{\mathrm{M}}$ varies *linearly* within the RVE according to the representation

$$\boldsymbol{u}^{\mathrm{M}}(\boldsymbol{x}) = \sum_{i,j} \hat{\boldsymbol{u}}^{\mathrm{M}(ij)}(\boldsymbol{x})\bar{\epsilon}_{ij} = \bar{\boldsymbol{\epsilon}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}] \tag{10.36}$$

where the displacement fields $\hat{\boldsymbol{u}}^{\mathrm{M}(ij)}$ are denoted the "unit displacement fields" that represent the value of $\boldsymbol{u}^{\mathrm{M}}$ for unit values of $\bar{\epsilon}_{ij}$. We may obtain the explicit expression for $\hat{\boldsymbol{u}}^{\mathrm{M}(ij)}$ upon comparing the two expressions in (10.36):

$$\sum_{i,j} \hat{\boldsymbol{u}}^{\mathrm{M}(ij)}\bar{\epsilon}_{ij} = \sum_{i,j} [\boldsymbol{e}_i \otimes \boldsymbol{e}_j] \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}]\bar{\epsilon}_{ij} \quad \Rightarrow \quad \hat{\boldsymbol{u}}^{\mathrm{M}(ij)} = \frac{1}{2}[\boldsymbol{e}_i \otimes \boldsymbol{e}_j + \boldsymbol{e}_j \otimes \boldsymbol{e}_i] \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}] \tag{10.37}$$

Remark: Since $\bar{\epsilon}_{ij} = \bar{\epsilon}_{ji}$ for any i, j, we have chosen here to formulate the unit displacement field corresponding to shear strains to be "symmetrical" in the sense that $\hat{\boldsymbol{u}}^{\mathrm{M}(ij)} = \hat{\boldsymbol{u}}^{\mathrm{M}(ji)}$. This is no restriction since it is always the sum $\hat{\boldsymbol{u}}^{\mathrm{M}(ij)} + \hat{\boldsymbol{u}}^{\mathrm{M}(ji)}$ that will occur in the representation of $\boldsymbol{u}^{\mathrm{M}}$ [4]. □

[3] The true value of $\bar{\mathbf{E}}$ requires the exact subscale solution except in 1D when it is possible to satisfy the condition $u^{\mathrm{s}} = 0$ at the two boundary points for the right choice of $\bar{u}$ and $\bar{\epsilon}$.

[4] For the general case of finite deformations (not treated here), it is more suitable to use the "natural" definition $\hat{\boldsymbol{u}}^{\mathrm{M}(ij)} = [\boldsymbol{e}_i \otimes \boldsymbol{e}_j] \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}]$, which would be valid here as well.

The strain corresponding to $\boldsymbol{u}^{\mathrm{M}}$ can now be written, using (10.36), as

$$\boldsymbol{\epsilon}^{\mathrm{M}} = \frac{1}{2}[\boldsymbol{u}^{\mathrm{M}} \otimes \boldsymbol{\nabla} + [\boldsymbol{u}^{\mathrm{M}} \otimes \boldsymbol{\nabla}]^{\mathrm{T}}] = \sum_{i,j} \hat{\boldsymbol{\epsilon}}^{\mathrm{M}(ij)} \bar{\epsilon}_{ij} = \bar{\boldsymbol{\epsilon}} \tag{10.38}$$

whereby the strain corresponding to $\hat{\boldsymbol{u}}^{\mathrm{M}(ij)}$, denoted $\hat{\boldsymbol{\epsilon}}^{\mathrm{M}(ij)}$, is trivially computed as

$$\hat{\boldsymbol{\epsilon}}^{\mathrm{M}(ij)} = \frac{1}{2}[\hat{\boldsymbol{u}}^{\mathrm{M}(ij)} \otimes \boldsymbol{\nabla} + [\hat{\boldsymbol{u}}^{\mathrm{M}(ij)} \otimes \boldsymbol{\nabla}]^{\mathrm{T}}] = \frac{1}{2}[\boldsymbol{e}_i \otimes \boldsymbol{e}_j + \boldsymbol{e}_j \otimes \boldsymbol{e}_i] \tag{10.39}$$

Clearly, the last identity in (10.38) is just another way of expressing the conventional expansion of $\bar{\boldsymbol{\epsilon}}$ w.r.t. the base dyads $\boldsymbol{e}_i \otimes \boldsymbol{e}_j$. We also obtain the representation

$$\bar{\epsilon}_{ij} = \hat{\boldsymbol{\epsilon}}^{\mathrm{M}(ij)} : \bar{\boldsymbol{\epsilon}} \tag{10.40}$$

Show this as homework!

Next, we aim at expressing $\boldsymbol{u}^{\mathrm{s}}(\boldsymbol{x})$ as a linear function of $\bar{\boldsymbol{\epsilon}}$ via the *ansatz*:

$$\boldsymbol{u}^{\mathrm{s}}(\boldsymbol{x}) = \sum_{i,j} \hat{\boldsymbol{u}}^{\mathrm{s}(ij)}(\boldsymbol{x}) \bar{\epsilon}_{ij} \tag{10.41}$$

in complete analogy with (10.36). How to compute $\hat{\boldsymbol{u}}^{\mathrm{s}(ij)}$ is discussed below in Subsection 10.4.2. Here, we merely note that $\hat{\boldsymbol{u}}^{\mathrm{s}(ij)}$ can be computed uniquely from the RVE-problem. The strain corresponding to $\hat{\boldsymbol{u}}^{\mathrm{s}(ij)}$ is denoted $\hat{\boldsymbol{\epsilon}}^{\mathrm{s}(ij)}$.

Now, the fine-scale displacement $\boldsymbol{u}(\boldsymbol{x})$ is completely defined within $\Omega_{\square}$ via the values $\bar{\boldsymbol{u}}$ and $\bar{\boldsymbol{\epsilon}}$, although the relation is implicit via the field $\hat{\boldsymbol{u}}^{\mathrm{s}(ij)}$. Hence, the strain corresponding to $\boldsymbol{u}^{\mathrm{s}}$ can be written using (10.41) with (10.40), as

$$\boldsymbol{\epsilon}^{\mathrm{s}} = \sum_{i,j} \hat{\boldsymbol{\epsilon}}^{\mathrm{s}(ij)} \bar{\epsilon}_{ij} = \left[\sum_{i,j} \hat{\boldsymbol{\epsilon}}^{\mathrm{s}(ij)} \otimes \hat{\boldsymbol{\epsilon}}^{\mathrm{M}(ij)} \right] : \bar{\boldsymbol{\epsilon}} \tag{10.42}$$

Finally, we may summarize to obtain the total fine-scale strain $\boldsymbol{\epsilon}$ using (10.38) with (10.42)

$$\boldsymbol{\epsilon} = \boldsymbol{\epsilon}^{\mathrm{M}} + \boldsymbol{\epsilon}^{\mathrm{s}} = \left[\mathbf{I}^{\mathrm{sym}} + \sum_{i,j} \hat{\boldsymbol{\epsilon}}^{\mathrm{s}(ij)} \otimes \hat{\boldsymbol{\epsilon}}^{\mathrm{M}(ij)} \right] : \bar{\boldsymbol{\epsilon}} = \mathbf{B}_{\epsilon} : \bar{\boldsymbol{\epsilon}} \tag{10.43}$$

where the (non-symmetric) 4th order tensor, defined as

$$\mathbf{B}_{\epsilon} \overset{\mathrm{def}}{=} \mathbf{I}^{\mathrm{sym}} + \sum_{i,j} \hat{\boldsymbol{\epsilon}}^{\mathrm{s}(ij)} \otimes \hat{\boldsymbol{\epsilon}}^{\mathrm{M}(ij)} = \sum_{i,j} \hat{\boldsymbol{\epsilon}}^{(ij)} \otimes \hat{\boldsymbol{\epsilon}}^{\mathrm{M}(ij)} \tag{10.44}$$

is often denoted the "strain concentration tensor" in the literature on homogenization.

For known $\mathbf{B}_\epsilon$, it is possible to compute the effective stiffness $\bar{\mathbf{E}}$ via the definition

$$\bar{\boldsymbol{\sigma}} = \langle \mathbf{E} : \boldsymbol{\epsilon} \rangle_\square = \underbrace{\langle \mathbf{E} : \mathbf{B}_\epsilon \rangle_\square}_{=\bar{\mathbf{E}}} : \bar{\boldsymbol{\epsilon}} \tag{10.45}$$

Hence,

$$\bar{\mathbf{E}} = \langle \mathbf{E} : \mathbf{B}_\epsilon \rangle_\square = \underbrace{\langle \mathbf{E} \rangle_\square}_{=\bar{\mathbf{E}}^{\mathrm{V}}} + \sum_{i,j} \langle \mathbf{E} : \hat{\boldsymbol{\epsilon}}^{\mathrm{s}(ij)} \rangle_\square \otimes \hat{\boldsymbol{\epsilon}}^{\mathrm{M}(ij)} = \sum_{i,j} \langle \mathbf{E} : \hat{\boldsymbol{\epsilon}}^{(ij)} \rangle_\square \otimes \hat{\boldsymbol{\epsilon}}^{\mathrm{M}(ij)} \tag{10.46}$$

The components of $\bar{\mathbf{E}}$ can be computed as

$$\begin{aligned} (\bar{\mathbf{E}})_{ijkl} &= \hat{\boldsymbol{\epsilon}}^{\mathrm{M}(ij)} : \bar{\mathbf{E}} : \hat{\boldsymbol{\epsilon}}^{\mathrm{M}(kl)} = \sum_{p,q} \langle \hat{\boldsymbol{\epsilon}}^{\mathrm{M}(ij)} : \mathbf{E} : \hat{\boldsymbol{\epsilon}}^{(pq)} \rangle_\square \otimes \underbrace{\hat{\boldsymbol{\epsilon}}^{\mathrm{M}(pq)} : \hat{\boldsymbol{\epsilon}}^{\mathrm{M}(kl)}}_{\begin{array}{l} = 1 \quad \text{if} \quad pq = kl \\ = 0 \quad \text{if} \quad pq \neq kl \end{array}} \\ &= \langle \hat{\boldsymbol{\epsilon}}^{\mathrm{M}(ij)} : \mathbf{E} : \hat{\boldsymbol{\epsilon}}^{(kl)} \rangle_\square \quad i,j,k,l = 1,2,...,3 \end{aligned} \tag{10.47}$$

When the fluctuation field (strain) is ignored, i.e. $\hat{\boldsymbol{\epsilon}}^{\mathrm{s}(ij)} = \mathbf{0}$, then we retrieve from (10.46) the stiffness pertinent to the Voigt, or Taylor, assumption. We note that the expression (10.46) is completely general w.r.t. anisotropy; the only constitutive assumption on the fine scale is linear elasticity.

Remark: From (10.46) it is not immediately clear that $\bar{\mathbf{E}}$ does, indeed, possess major symmetry (even though it is given a priori that $\mathbf{E}$ is symmetrical). Such major symmetry can, however, be shown using the Hill-Mandel condition as follows:

$$\bar{\boldsymbol{\epsilon}} : \bar{\mathbf{E}} : \delta\bar{\boldsymbol{\epsilon}} = \langle \boldsymbol{\epsilon} : \mathbf{E} : \delta\boldsymbol{\epsilon} \rangle_\square \overset{(10.46)}{=} \bar{\boldsymbol{\epsilon}} : \langle \mathbf{B}_\epsilon^{\mathrm{T}} : \mathbf{E} : \mathbf{B}_\epsilon \rangle_\square : \delta\bar{\boldsymbol{\epsilon}} \tag{10.48}$$

which must hold for all possible $\delta\bar{\boldsymbol{\epsilon}}$ consistent with the boundary conditions on $\Gamma_\square$. This means that

$$\bar{\boldsymbol{\epsilon}} : [\bar{\mathbf{E}} - \langle \mathbf{B}_\epsilon^{\mathrm{T}} : \mathbf{E} : \mathbf{B}_\epsilon \rangle_\square] = \mathbf{0} \tag{10.49}$$

and it follows that, indeed, $\bar{\mathbf{E}}$ can be expressed as

$$\bar{\mathbf{E}} = \langle \mathbf{B}_\epsilon^{\mathrm{T}} : \mathbf{E} : \mathbf{B}_\epsilon \rangle_\square \tag{10.50}$$

which is clearly symmetrical since $\mathbf{E}$ is symmetrical. □

10.4.2 RVE-problem for DBC - Computational format

The "unit fluctuation displacement" fields $\hat{\boldsymbol{u}}^{\mathrm{s}(ij)}$ are computed as follows: Introduce the space of admissible (fine scale) displacements

$$\mathbb{U}_\square = \{\boldsymbol{u} |\, \boldsymbol{u} = \bar{\boldsymbol{\epsilon}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}] \quad \text{on} \quad \Gamma_\square\} \tag{10.51}$$

The corresponding space of test functions is

$$\mathbb{U}_\square^0 = \{\boldsymbol{u} |\, \boldsymbol{u} = \boldsymbol{0} \quad \text{on} \quad \Gamma_\square\} \tag{10.52}$$

In the absence of volume forces the weak format of the RVE-problem reads: Find $\boldsymbol{u} \in \mathbb{U}_\square$ such that

$$\langle \delta\boldsymbol{\epsilon} : \boldsymbol{\sigma} \rangle_\square = 0 \quad \forall \delta\boldsymbol{u} \in \mathbb{U}_\square^0 \tag{10.53}$$

Upon expanding $\boldsymbol{\sigma}$ as

$$\begin{aligned} \boldsymbol{\sigma} &= \mathbf{E} : \boldsymbol{\epsilon} = \mathbf{E} : \bar{\boldsymbol{\epsilon}} + \mathbf{E} : \boldsymbol{\epsilon}^{\mathrm{s}} \\ &= \sum_{i,j} \left[\mathbf{E} : \hat{\boldsymbol{\epsilon}}^{\mathrm{M}(ij)} + \mathbf{E} : \hat{\boldsymbol{\epsilon}}^{\mathrm{s}(ij)} \right] \bar{\epsilon}_{ij} \end{aligned} \tag{10.54}$$

and inserting into (10.53), while noting that this relation must hold for any given values $\bar{\epsilon}_{ij}$, we obtain the RVE-problems: Find $\hat{\boldsymbol{u}}^{\mathrm{s}(ij)} \in \mathbb{U}_\square^0$ for $i, j = 1, 2, 3$ as the solution of

$$\langle \delta\boldsymbol{\epsilon} : \mathbf{E} : \hat{\boldsymbol{\epsilon}}^{\mathrm{s}(ij)} \rangle_\square = -\langle \delta\boldsymbol{\epsilon} : \mathbf{E} : \hat{\boldsymbol{\epsilon}}^{\mathrm{M}(ij)} \rangle_\square \quad \forall \delta\boldsymbol{u} \in \mathbb{U}_\square^0 \tag{10.55}$$

where the "macroscale strain" fields $\hat{\boldsymbol{\epsilon}}^{\mathrm{M}(ij)}$ were defined in (10.39). When $\hat{\boldsymbol{u}}^{\mathrm{s}(ij)}$ have been computed, it is possible to compute the corresponding strains $\hat{\boldsymbol{\epsilon}}^{\mathrm{s}(ij)}$ and, finally, insert into (10.46) to compute $\bar{\mathbf{E}}$ in the macroscale constitutive relation.

10.5 Multiscale computation

10.5.1 Preliminaries

In the case of linear elasticity and static loading it was shown above that the effective stiffness tensor $\bar{\mathbf{E}}$ can be computed *a priori* (once and for all) and then used in a linear elastic analysis of a macroscopic component subjected to external loading and prescribed boundary conditions in the usual way. In practice, of course, this solution may only be

obtainable via FE-discretization. In the more general case when the subscale constitutive properties are nonlinear, say hyperelastic or elastic-plastic, 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.

10.5.2 Concurrent hierarchical approach

The two-scale iterative approach, known as the "concurrent hierarchial approach", and in terms of finite element analysis often denoted the "nested FE-solution" or "FE^2-algorithm", may be described as follows, c.f. Figure 10.6.

1. Assume that a (nonequilibrium) macroscale stress field $\bar{\boldsymbol{\sigma}}$ is given, corresponding to $\bar{\boldsymbol{u}}$ (and $\bar{\boldsymbol{\epsilon}}$).
2. For given $\bar{\boldsymbol{\epsilon}} \stackrel{\text{def}}{=} \bar{\boldsymbol{\epsilon}}(\bar{\boldsymbol{x}}_i), i = 1, 2, ..., NQP$, in a macroscale quadrature point, typically Gauss-points in the macroscale FE-mesh, solve the nonlinear RVE-problem for $\boldsymbol{u}(\boldsymbol{x})$. The operation $\bar{\boldsymbol{\epsilon}} \rightarrow \boldsymbol{\epsilon}(\boldsymbol{x})$ is known as "prolongation", "dehomogenization" or "concentration".
3. For given $\boldsymbol{\sigma}(x)$, compute $\bar{\boldsymbol{\sigma}} \stackrel{\text{def}}{=} \bar{\boldsymbol{\sigma}}(\bar{\boldsymbol{x}}_i)$ via averaging. The operation $\boldsymbol{\sigma}(x) \rightarrow \bar{\boldsymbol{\sigma}}$ is known as "homogenization".
4. Check the macroscale residual. If convergence, then stop, else compute a new (updated) value of $\bar{\boldsymbol{u}} \rightarrow \bar{\boldsymbol{\sigma}}$ and return to 1.

A key issue is the computation of the macroscale (algorithmic) tangent stiffness tensor $\bar{\mathbf{E}}$, which is needed at the macroscale iterative solution in point 4. It turns out that the computational strategy is virtually the same as for the linear counterpart (as discussed in Section 10.4). However, the difference is that $\hat{\boldsymbol{u}}^{\mathrm{s}(ij)}$ now represent tangent properties, or *sensitivities*. This topic is the subject of the next Subsection.

10.5.3 Macroscale ATS-tensor for DBC

The strategy for computing the macroscale ATS-tensor $\bar{\mathbf{E}}$ is shown schematically in Figure 10.7. The macroscale ATS-tensor is defined via the relation

$$\mathrm{d}\bar{\boldsymbol{\sigma}} = \bar{\mathbf{E}} : \mathrm{d}\bar{\boldsymbol{\epsilon}} \tag{10.56}$$

for differential changes $\mathrm{d}\bar{\boldsymbol{\epsilon}}$. Such differential changes give rise, via the actual prolongation condition, to the full-scale differential strain changes $\mathrm{d}\boldsymbol{\epsilon}$ given as

$$\begin{aligned} \mathrm{d}\boldsymbol{\epsilon} = \mathrm{d}\boldsymbol{\epsilon}^{\mathrm{M}} + \mathrm{d}\boldsymbol{\epsilon}^{\mathrm{s}} &= \sum_{i,j} [\hat{\boldsymbol{\epsilon}}^{\mathrm{M}(ij)} + \hat{\boldsymbol{\epsilon}}^{\mathrm{s}(ij)}] \, \mathrm{d}\bar{\epsilon}_{ij} \\ &= \left[\mathbf{I}^{\mathrm{sym}} + \sum_{i,j} \hat{\boldsymbol{\epsilon}}^{\mathrm{s}(\mathrm{ij})} \otimes \hat{\boldsymbol{\epsilon}}^{\mathrm{M}(ij)} \right] : \mathrm{d}\bar{\boldsymbol{\epsilon}} = \mathbf{B}_{\epsilon} : \mathrm{d}\bar{\boldsymbol{\epsilon}} \end{aligned} \tag{10.57}$$

upon using identical arguments to those in 10.4.1 for the linear problem. Hence, we obtain the effective ATS-tensor via the relation

$$\mathrm{d}\bar{\boldsymbol{\sigma}} = \langle \mathbf{E} : \mathrm{d}\boldsymbol{\epsilon} \rangle_{\square} = \langle \mathbf{E} : \mathbf{B}_{\epsilon} \rangle : \mathrm{d}\bar{\boldsymbol{\epsilon}} \tag{10.58}$$

such that

$$\bar{\mathbf{E}} = \langle \mathbf{E} \rangle_{\square} + \sum_{i,j} \langle \mathbf{E} : \hat{\boldsymbol{\epsilon}}^{\mathrm{s}(ij)} \rangle_{\square} \otimes \hat{\boldsymbol{\epsilon}}^{\mathrm{M}(ij)} \tag{10.59}$$

It remains to compute the sensitivity fields $\hat{\boldsymbol{\epsilon}}^{\mathrm{s}(ij)}$ from the appropriate *tangent problem*. To this end we recall the weak format of the RVE-problem: Find $\boldsymbol{u} \in \mathbb{U}_{\square}$ that satisfies

$$\langle \delta\boldsymbol{\epsilon} : \boldsymbol{\sigma}(\boldsymbol{\epsilon}) \rangle_{\square} = 0 \quad \forall \delta\boldsymbol{u} \in \mathbb{U}^0_{\square} \tag{10.60}$$

However, this state equation must hold also for a varied state $\bar{\boldsymbol{\epsilon}} + \mathrm{d}\bar{\boldsymbol{\epsilon}}$ and the corresponding subscale strains $\boldsymbol{\epsilon} + \mathrm{d}\boldsymbol{\epsilon}$. In other words: We look for $\mathrm{d}\boldsymbol{u}$ such that $\boldsymbol{u} + \mathrm{d}\boldsymbol{u} \in \mathbb{U}_{\square}$ solves

$$\langle \delta\boldsymbol{\epsilon} : \boldsymbol{\sigma}(\boldsymbol{\epsilon} + \mathrm{d}\boldsymbol{\epsilon}) \rangle_{\square} = 0 \quad \forall \delta\boldsymbol{u} \in \mathbb{U}^0_{\square} \tag{10.61}$$

We may first linearize in (10.61) to obtain

$$\langle \delta\boldsymbol{\epsilon} : \boldsymbol{\sigma} + \mathbf{E} : \mathrm{d}\boldsymbol{\epsilon} \rangle_{\square} = 0 \quad \forall \delta\boldsymbol{u} \in \mathbb{U}^0_{\square} \tag{10.62}$$

and subtract (10.60) to obtain

$$\langle \delta\boldsymbol{\epsilon} : \underbrace{\mathbf{E} : \mathrm{d}\boldsymbol{\epsilon}}_{\mathrm{d}\boldsymbol{\sigma}} \rangle_{\square} = 0 \quad \forall \delta\boldsymbol{u} \in \mathbb{U}^0_{\square} \tag{10.63}$$

Upon introducing (10.57) into (10.63), and noting that the resulting expression must hold for any given values $\mathrm{d}\bar{\epsilon}_{ij}$, we obtain the problem: Find $\hat{\boldsymbol{u}}^{\mathrm{s}(ij)} \in \mathbb{U}^0_{\square}$, for $i, j = 1, 2, 3$, that solve

$$\langle \delta\boldsymbol{\epsilon} : \mathbf{E} : \hat{\boldsymbol{\epsilon}}^{\mathrm{s}(ij)} \rangle_{\square} = -\langle \delta\boldsymbol{\epsilon} : \mathbf{E} : \hat{\boldsymbol{\epsilon}}^{\mathrm{M}(ij)} \rangle_{\square} \quad \forall \delta\boldsymbol{u} \in \mathbb{U}^0_{\square} \tag{10.64}$$

Once again, when $\hat{\boldsymbol{u}}^{\mathrm{s}(ij)}$ have been computed, it is possible to compute $\hat{\boldsymbol{\epsilon}}^{\mathrm{s}(ij)}$ and, finally, compute the macroscale ATS-tensor $\bar{\mathbf{E}}$ from (10.59).

Remark: The outlined strategy for computing $\bar{\mathbf{E}}$ is known in the literature as the *primal* approach. The *dual* approach, described by LARSSON & RUNESSON **?**, is not discussed here. □

10.6 Appendix: Matrix format of macroscale stiffness tensor

10.6.1 Preliminaries

The spatial FE-discretization on $\Omega_\square$ is defined by basis functions $\{\boldsymbol{N}_i^f\}_{i=1}^{\mathrm{NVAR_f}}$ and $\{\boldsymbol{N}_j^p\}_{j=1}^{\mathrm{NVAR_p}}$, corresponding to $\mathrm{NVAR_f}$ free (internal) nodal variables and $\mathrm{NVAR_p}$ prescribed (boundary) nodal variables, respectively. These basis functions are collected as $\{\boldsymbol{N}_k\}_{k=1}^{\mathrm{NVAR}}$, where $\mathrm{NVAR} = \mathrm{NVAR_f} + \mathrm{NVAR_p}$. Hence, any displacement field $\boldsymbol{u}(\boldsymbol{X})$, for $\boldsymbol{X} \in \Omega_\square$, can be represented as

$$\boldsymbol{u} = \sum_{k=1}^{\mathrm{NVAR}} \boldsymbol{N}_k(\underline{\boldsymbol{u}})_k = \sum_{k=1}^{\mathrm{NVAR_f}} \boldsymbol{N}_k^{\mathrm{f}}(\underline{\boldsymbol{u}}^{\mathrm{f}})_k + \sum_{k=1}^{\mathrm{NVAR_p}} \boldsymbol{N}_k^{\mathrm{p}}(\underline{\boldsymbol{u}}^{\mathrm{p}})_k \tag{10.65}$$

in standard fashion, where $\underline{\boldsymbol{u}}^{\mathrm{f}}$ and $\underline{\boldsymbol{u}}^{\mathrm{p}}$ are column vectors containing all free (internal) and prescribed (boundary) variables, respectively.

Next, we introduce nodal variables $\underline{\hat{\boldsymbol{u}}}^{(ij)}$ corresponding to the 3 in-plane "unit deformation" fields $\hat{\boldsymbol{u}}^{ij}$, which are collectively denoted

$$\underline{\hat{\boldsymbol{u}}}^{\mathrm{M}} = \left[\ \underline{\hat{\boldsymbol{u}}}^{\mathrm{M}(11)},\ \ \underline{\hat{\boldsymbol{u}}}^{\mathrm{M}(22)},\ \ \underline{\hat{\boldsymbol{u}}}^{\mathrm{M}(12)}\ \right] \tag{10.66}$$

with the subdivision

$$\underline{\hat{\boldsymbol{u}}}^{\mathrm{M}} = \begin{bmatrix} \underline{\hat{\boldsymbol{u}}}^{\mathrm{M,f}} \\ \underline{\hat{\boldsymbol{u}}}^{\mathrm{M,p}} \end{bmatrix} = \begin{bmatrix} \underline{\hat{\boldsymbol{u}}}^{\mathrm{M,f}(11)}, & \underline{\hat{\boldsymbol{u}}}^{\mathrm{M,f}(22)}, & \underline{\hat{\boldsymbol{u}}}^{\mathrm{M,f}(12)} \\ \underline{\hat{\boldsymbol{u}}}^{\mathrm{M,p}(11)}, & \underline{\hat{\boldsymbol{u}}}^{\mathrm{M,p}(22)}, & \underline{\hat{\boldsymbol{u}}}^{\mathrm{M,p}(12)} \end{bmatrix} \tag{10.67}$$

It must be noted that *a*ll components in $\underline{\hat{\boldsymbol{u}}}^{\mathrm{M}}$ are *prescribed*; it is only for convenience of notation that the subdivision in (10.67) into internal and boundary variables is introduced.

Next, we introduce, in analogy with (10.66), the corresponding total displacement fields

$$\underline{\hat{\boldsymbol{u}}} = \left[\ \underline{\hat{\boldsymbol{u}}}^{(11)},\ \ \underline{\hat{\boldsymbol{u}}}^{(22)},\ \ \underline{\hat{\boldsymbol{u}}}^{(12)}\ \right] \tag{10.68}$$

In particular, it is noted that

$$\left[\begin{array}{c} \hat{\underline{\boldsymbol{u}}}^{\mathrm{f}} \\ \hat{\underline{\boldsymbol{u}}}^{\mathrm{p}} \end{array}\right] = \left[\begin{array}{c} \hat{\underline{\boldsymbol{u}}}^{\mathrm{M,f}} \\ \hat{\underline{\boldsymbol{u}}}^{\mathrm{M,p}} \end{array}\right] + \left[\begin{array}{c} \hat{\underline{\boldsymbol{u}}}^{\mathrm{s,f}} \\ \hat{\underline{\boldsymbol{u}}}^{\mathrm{s,p}} \end{array}\right] = \left[\begin{array}{c} \hat{\underline{\boldsymbol{u}}}^{\mathrm{M,f}} \\ \hat{\underline{\boldsymbol{u}}}^{\mathrm{M,p}} \end{array}\right] + \left[\begin{array}{c} \hat{\underline{\boldsymbol{u}}}^{\mathrm{s,f}} \\ \underline{\mathbf{0}} \end{array}\right] \tag{10.69}$$

We note that a macroscopic (in-plane) strain on the form $\bar{\boldsymbol{\epsilon}} = \sum_{i=1,2,\, j=1,2} \bar{\epsilon}_{ij} \boldsymbol{e}_i \otimes \boldsymbol{e}_j$ can be characterized by its matrix notation

$$\underline{\bar{\boldsymbol{\epsilon}}} = \left[\begin{array}{c} \bar{\epsilon}_{11} \\ \bar{\epsilon}_{22} \\ 2\bar{\epsilon}_{12} \end{array}\right] = \left[\begin{array}{c} \bar{\epsilon}_{11} \\ \bar{\epsilon}_{22} \\ \bar{\gamma}_{12} \end{array}\right] \tag{10.70}$$

where $\bar{\gamma}_{12}$ is the engineering shear strain that accounts for the symmetry of $\bar{\boldsymbol{\epsilon}}$. For a given set of macroscale strain components, the subscale displacement field (inside the RVE) can thus be superposed as

$$\underline{\boldsymbol{u}} = \hat{\underline{\boldsymbol{u}}}^{(11)}\bar{\epsilon}_{11} + \hat{\underline{\boldsymbol{u}}}^{(22)}\bar{\epsilon}_{22} + 2\hat{\underline{\boldsymbol{u}}}^{(12)}\bar{\epsilon}_{12} = \left[\begin{array}{ccc} \hat{\underline{\boldsymbol{u}}}^{(11)}, & \hat{\underline{\boldsymbol{u}}}^{(22)}, & \hat{\underline{\boldsymbol{u}}}^{(12)} \end{array}\right] \underline{\bar{\boldsymbol{\epsilon}}} \tag{10.71}$$

Finally, we note that the work-conjugated stresses are given in matrix notation as

$$\underline{\bar{\boldsymbol{\sigma}}} = \left[\begin{array}{c} \bar{\sigma}_{11} \\ \bar{\sigma}_{22} \\ \bar{\sigma}_{12} \end{array}\right] \tag{10.72}$$

10.6.2 Computing the effective stiffness

In order to define the subscale tangent stiffness $\underline{\boldsymbol{K}}$ for the subscale FE-problem on the RVE, we introduce the FE-representation of strain as

$$\boldsymbol{\epsilon} = \sum_{k=1}^{\mathrm{NVAR}} (\boldsymbol{N}_k \otimes \boldsymbol{\nabla})^{\mathrm{sym}} (\underline{\boldsymbol{u}})_k = \sum_{k=1}^{\mathrm{NVAR}} \boldsymbol{B}_k (\underline{\boldsymbol{u}})_k \quad \text{with } \boldsymbol{B}_k \overset{\mathrm{def}}{=} (\boldsymbol{N}_k \otimes \boldsymbol{\nabla})^{\mathrm{sym}} \tag{10.73}$$

We may then obtain

$$\begin{aligned} \langle \delta\boldsymbol{\epsilon} : \mathsf{E} : \boldsymbol{\epsilon} \rangle_{\square} &= \sum_{i,j=1}^{\mathrm{NVAR}} (\delta\underline{\boldsymbol{u}})_i \langle \boldsymbol{B}_i : \mathsf{E} : \boldsymbol{B}_j \rangle_{\square} (\underline{\boldsymbol{u}})_j = \sum_{i,j=1}^{\mathrm{NVAR}} (\delta\underline{\boldsymbol{u}})_i (\underline{\boldsymbol{K}})_{ij} (\underline{\boldsymbol{u}})_j \\ &= [\delta\underline{\boldsymbol{u}}]^{\mathrm{T}} \underline{\boldsymbol{K}}\underline{\boldsymbol{u}} \end{aligned} \tag{10.74}$$

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

$$(\underline{\boldsymbol{K}})_{ij} = \langle \boldsymbol{B}_i : \mathsf{E} : \boldsymbol{B}_j \rangle_{\square} \quad i,j = 1,2,...,\mathrm{NVAR} \tag{10.75}$$

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

$$\underline{\boldsymbol{K}} = \begin{bmatrix} \underline{\boldsymbol{K}}^{\mathrm{f,f}} & \underline{\boldsymbol{K}}^{\mathrm{f,p}} \\ \underline{\boldsymbol{K}}^{\mathrm{p,f}} & \underline{\boldsymbol{K}}^{\mathrm{p,p}} \end{bmatrix}, \quad \underline{\boldsymbol{K}}^{\mathrm{p,f}} = [\underline{\boldsymbol{K}}^{\mathrm{f,p}}]^{\mathrm{T}} \tag{10.76}$$

We are now in the position to formulate the RVE-problem in (10.55) in matrix format

$$\begin{bmatrix} \underline{\boldsymbol{K}}^{\mathrm{f,f}} & \underline{\boldsymbol{K}}^{\mathrm{f,p}} \end{bmatrix} \begin{bmatrix} \hat{\underline{\boldsymbol{u}}}^{\mathrm{f}} \\ \hat{\underline{\boldsymbol{u}}}^{\mathrm{M,p}} \end{bmatrix} = \underline{\mathbf{0}} \tag{10.77}$$

or

$$\begin{bmatrix} \underline{\boldsymbol{K}}^{\mathrm{f,f}} & \underline{\boldsymbol{K}}^{\mathrm{f,p}} \end{bmatrix} \begin{bmatrix} \hat{\underline{\boldsymbol{u}}}^{\mathrm{s,f}} \\ \underline{\mathbf{0}} \end{bmatrix} = - \begin{bmatrix} \underline{\boldsymbol{K}}^{\mathrm{f,f}} & \underline{\boldsymbol{K}}^{\mathrm{f,p}} \end{bmatrix} \begin{bmatrix} \hat{\underline{\boldsymbol{u}}}^{\mathrm{M,f}} \\ \hat{\underline{\boldsymbol{u}}}^{\mathrm{M,p}} \end{bmatrix} \tag{10.78}$$

Upon rewriting (10.77) in terms of the unknown (total) displacement vector $\hat{\underline{\boldsymbol{u}}}^{\mathrm{f}}$, we obtain the matrix equation

$$\underline{\boldsymbol{K}}^{\mathrm{f,f}} \hat{\underline{\boldsymbol{u}}}^{\mathrm{f}} = -\underline{\boldsymbol{K}}^{\mathrm{f,p}} \hat{\underline{\boldsymbol{u}}}^{\mathrm{M,p}} \tag{10.79}$$

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 $-\underline{\boldsymbol{K}}^{\mathrm{f,p}}$. Formally, the solution of (10.79) can be written as

$$\hat{\underline{\boldsymbol{u}}}^{\mathrm{f}} = - \left[\underline{\boldsymbol{K}}^{\mathrm{f,f}}\right]^{-1} \underline{\boldsymbol{K}}^{\mathrm{f,p}} \hat{\underline{\boldsymbol{u}}}^{\mathrm{M,p}} \tag{10.80}$$

From a computational point of view, it is quite obvious that computing the inverse of $\underline{\boldsymbol{K}}^{\mathrm{f,f}}$ is far more expensive than solving the system of FE-equations in (10.79).

Next, we establish the macroscale stiffness matrix from the component expression in (10.47) pertinent to the Voigt matrix relation $\underline{\bar{\boldsymbol{\sigma}}} = \underline{\bar{\mathbf{E}}}\, \underline{\bar{\boldsymbol{\epsilon}}}$:

$$(\bar{\mathbf{E}})_{ijkl} = \langle \hat{\boldsymbol{\epsilon}}^{\mathrm{M}(ij)} : \mathbf{E} : \hat{\boldsymbol{\epsilon}}^{(kl)} \rangle_{\square} = \left[\hat{\underline{\boldsymbol{u}}}^{\mathrm{M}(ij)}\right]^{\mathrm{T}} \underline{\boldsymbol{K}} \hat{\underline{\boldsymbol{u}}}^{(kl)} \tag{10.81}$$

Hence, we obtain

$$\underline{\bar{\mathbf{E}}} = \left[\hat{\underline{\boldsymbol{u}}}^{\mathrm{M}}\right]^{\mathrm{T}} \underline{\boldsymbol{K}} \hat{\underline{\boldsymbol{u}}} = \begin{bmatrix} \left[\hat{\underline{\boldsymbol{u}}}^{\mathrm{M,f}}\right]^{\mathrm{T}}, & \left[\hat{\underline{\boldsymbol{u}}}^{\mathrm{M,p}}\right]^{\mathrm{T}} \end{bmatrix} \begin{bmatrix} \underline{\boldsymbol{K}}^{\mathrm{f,f}} & \underline{\boldsymbol{K}}^{\mathrm{f,p}} \\ \underline{\boldsymbol{K}}^{\mathrm{p,f}} & \underline{\boldsymbol{K}}^{\mathrm{p,p}} \end{bmatrix} \begin{bmatrix} \hat{\underline{\boldsymbol{u}}}^{\mathrm{f}} \\ \hat{\underline{\boldsymbol{u}}}^{\mathrm{M,p}} \end{bmatrix} \tag{10.82}$$

Upon using the identity in (10.77), we may simplify (10.82) as follows:

$$\underline{\bar{\mathbf{E}}} = \left[\hat{\underline{\boldsymbol{u}}}^{\mathrm{M,p}}\right]^{\mathrm{T}} \begin{bmatrix} \underline{\boldsymbol{K}}^{\mathrm{p,f}} & \underline{\boldsymbol{K}}^{\mathrm{p,p}} \end{bmatrix} \begin{bmatrix} \hat{\underline{\boldsymbol{u}}}^{\mathrm{f}} \\ \hat{\underline{\boldsymbol{u}}}^{\mathrm{M,p}} \end{bmatrix} = \left[\hat{\underline{\boldsymbol{u}}}^{\mathrm{M,p}}\right]^{\mathrm{T}} \left[\underline{\boldsymbol{K}}^{\mathrm{p,p}} \hat{\underline{\boldsymbol{u}}}^{\mathrm{M,p}} + \underline{\boldsymbol{K}}^{\mathrm{p,f}} \hat{\underline{\boldsymbol{u}}}^{\mathrm{f}}\right] \tag{10.83}$$

This is the operational format of $\underline{\bar{\mathbf{E}}}$ in practice when $\underline{\hat{\boldsymbol{u}}}^{\mathrm{f}}$ is solved for from (10.79). Formally, however, we may introduce (10.80) into (10.83) to obtain

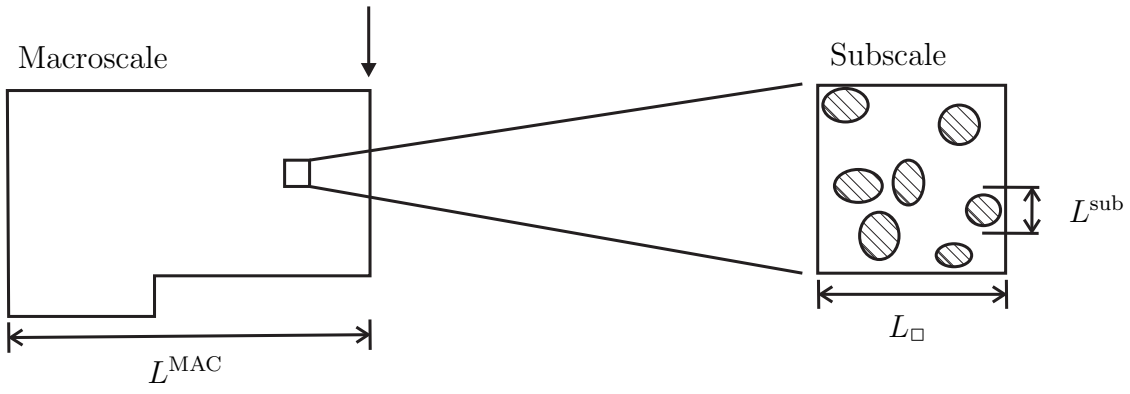
$$\underline{\bar{\mathbf{E}}} = \left[\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,p}}\right]^{\mathrm{T}} \underline{\tilde{\boldsymbol{K}}}^{\mathrm{p,p}} \underline{\hat{\boldsymbol{u}}}^{\mathrm{M,p}} \tag{10.84}$$

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

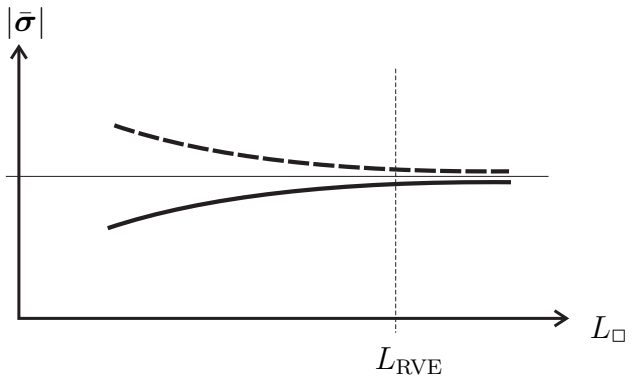
$$\underline{\tilde{\boldsymbol{K}}}^{\mathrm{p,p}} = \underline{\boldsymbol{K}}^{\mathrm{p,p}} - \underline{\boldsymbol{K}}^{\mathrm{p,f}} \left[\underline{\boldsymbol{K}}^{\mathrm{f,f}}\right]^{-1} \underline{\boldsymbol{K}}^{\mathrm{f,p}} \tag{10.85}$$

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

$$\begin{aligned}
dim(\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,p}}) &= 2\mathrm{NVAR_p} \times 3 \\
dim(\underline{\hat{\boldsymbol{u}}}^{\mathrm{M,f}}) &= 2\mathrm{NVAR_f} \times 3 \\
dim(\underline{\boldsymbol{K}}^{\mathrm{p,p}}) &= 2\mathrm{NVAR_p} \times 2\mathrm{NVAR_p} = dim(\underline{\tilde{\boldsymbol{K}}}^{\mathrm{p,p}}) \\
dim(\underline{\boldsymbol{K}}^{\mathrm{f,f}}) &= 2\mathrm{NVAR_f} \times 2\mathrm{NVAR_f} \\
dim(\underline{\boldsymbol{K}}^{\mathrm{f,p}}) &= 2\mathrm{NVAR_f} \times 2\mathrm{NVAR_p} = dim(\left[\underline{\boldsymbol{K}}^{\mathrm{p,f}}\right]^{\mathrm{T}}) \\
dim(\underline{\bar{\mathbf{E}}}) &= 3 \times 3
\end{aligned} \tag{10.86}$$



(a)



(b)

Figure 10.1: *Characteristics of "computational cell" in the case of complete scale separation. (a) Characteristic dimensions. (b) Convergence of averaged (macroscopic) stress with increasing size of the computational cell.*

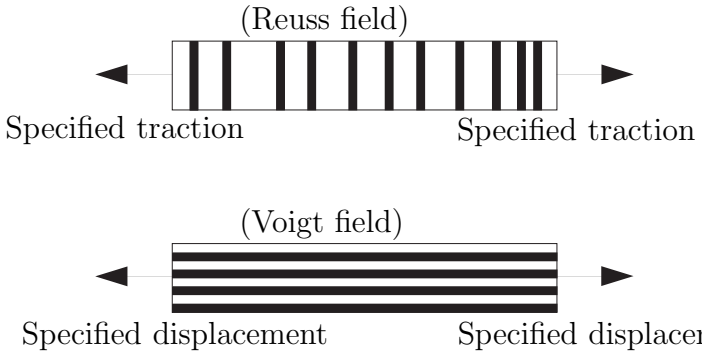


Figure 10.2: *One-dimensional representation of the Voigt and Reuss assumptions.*

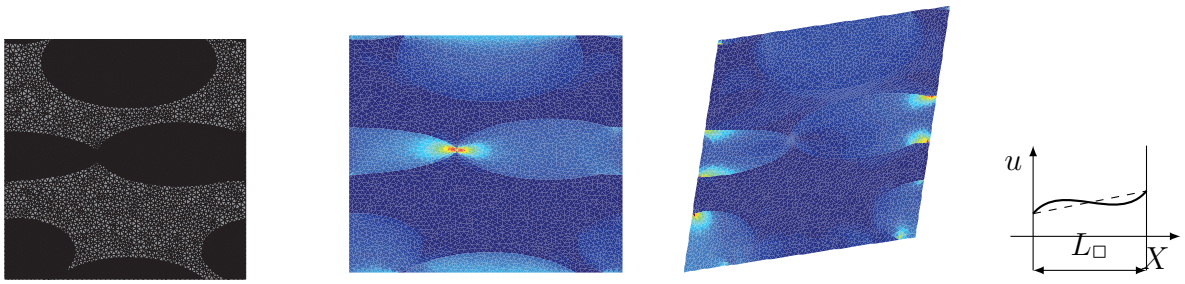


Figure 10.3: *Examples of deformed shapes of square RVE with particles in matrix subjected to DBC. Left: Undeformed RVE. Middle: Normal strain: Only* $\bar{\epsilon}_{11}$ *is non-zero. Right: Shear strain: Only* $\bar{\epsilon}_{12} = \bar{\epsilon}_{21}$ *is non-zero.*

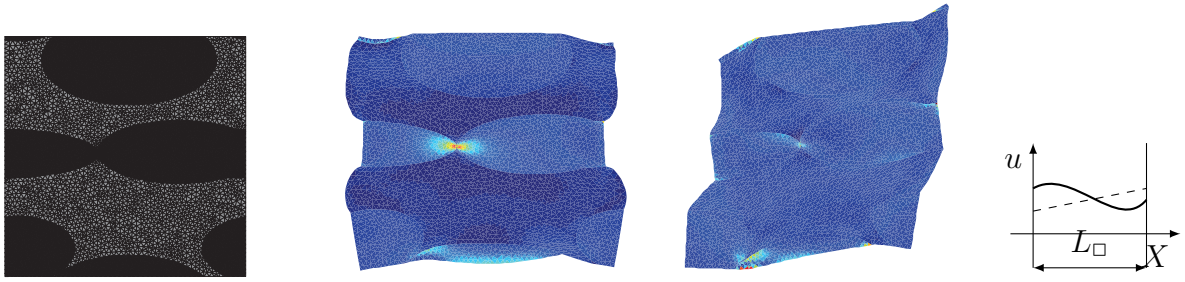


Figure 10.4: *Examples of deformed shapes of square RVE with particles in matrix subjected to TBC. Left: Undeformed RVE. Middle: Normal strain: Only* $\bar{\epsilon}_{11}$ *is non-zero. Right: Shear strain: Only* $\bar{\epsilon}_{12} = \bar{\epsilon}_{21}$ *is non-zero.*

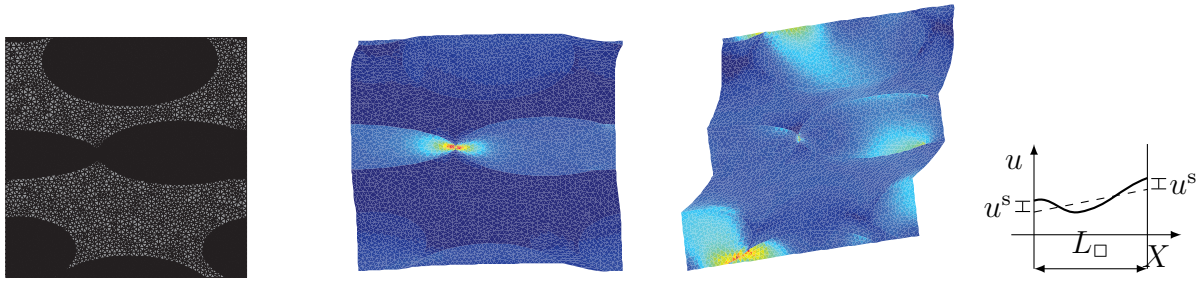


Figure 10.5: *Examples of deformed shapes of square RVE with particles in matrix subjected to SPBC. Left: Undeformed RVE. Middle: Normal strain: Only* $\bar{\epsilon}_{11}$ *is non-zero. Right: Shear strain: Only* $\bar{\epsilon}_{12} = \bar{\epsilon}_{21}$ *is non-zero.*

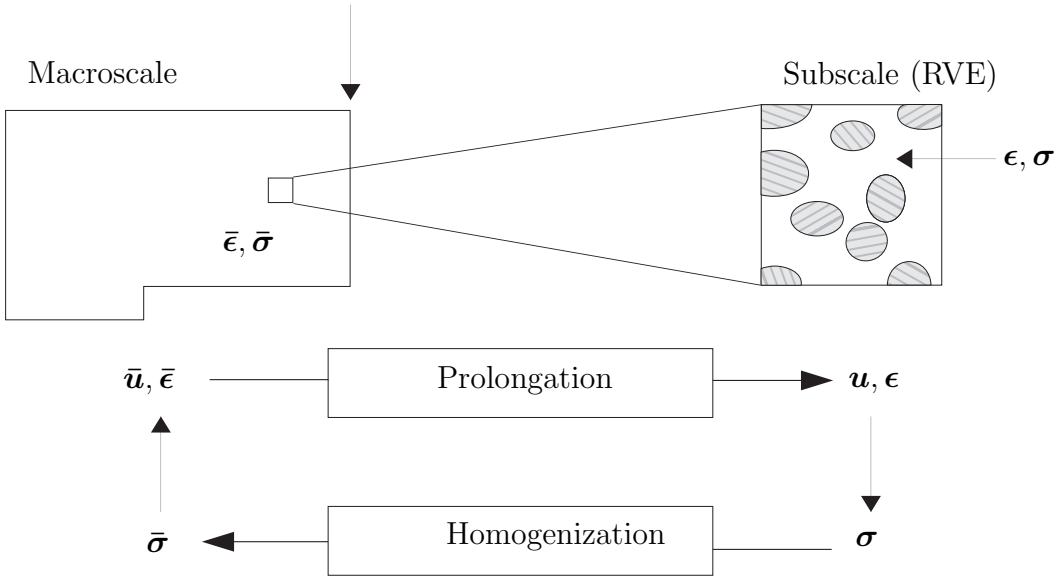


Figure 10.6: *Concurrent hierarchical strategy characterizing computational homogenization for stress problems.*

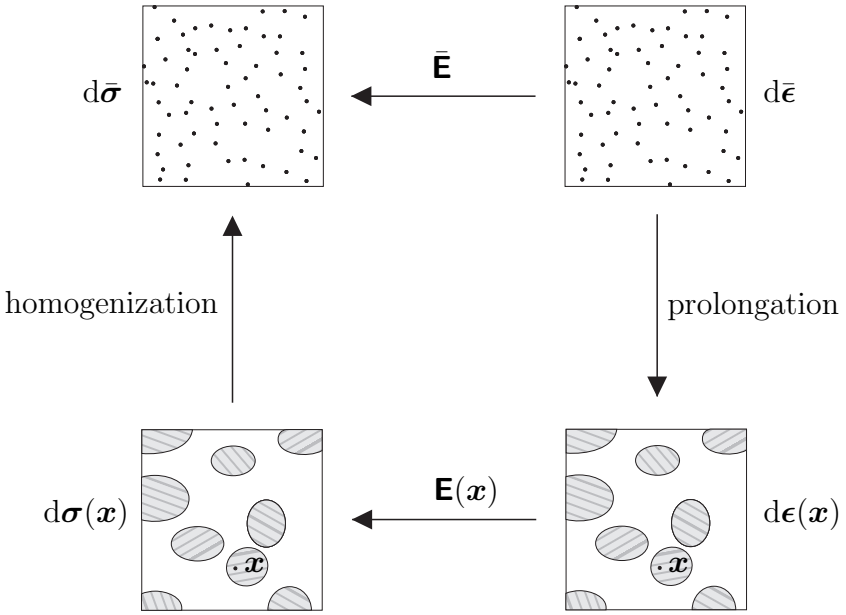


Figure 10.7: *Sketch of the computation of* $\bar{\mathbf{E}}$.

10.7 Questions and problems

1. Consider the 1D-situation of uniaxial stress for a composite of two linear elastic phases with volume fractions n_1 and n_2 ($n_1 + n_2 = 1$). The corresponding elastic moduli are E_1 and E_2.

   (a) Show that the Voigt and Reuss bounds for the effective modulus $\bar{E}$ is given as

   $$\bar{E}^{\mathrm{V}} = n_1 E_1 + n_2 E_2, \quad \bar{E}^{\mathrm{R}} = \frac{E_1 E_2}{n_2 E_1 + n_1 E_2}$$

   (b) Show, by direct comparison, that $\bar{E}^{\mathrm{V}} \geq \bar{E}^{\mathrm{R}}$. Give an analytical expression for the value of n_1 for which this difference is maximum.

2. Consider the situation of multiaxial stress and strain for a composite of two isotropic linear elastic phases with volume fractions n_1 and n_2 ($n_1 + n_2 = 1$). The corresponding elastic moduli are G_1, K_1 and G_2, K_2.

   (a) Show that the Voigt and Reuss bounds for the effective moduli $\bar{G}, \bar{K}$ are given as in the uniaxial case, e.g.

   $$\bar{G}^{\mathrm{V}} = n_1 G_1 + n_2 G_2, \quad \bar{G}^{\mathrm{R}} = \frac{G_1 G_2}{n_2 G_1 + n_1 G_2}$$

   (b) Use the Voigt and Reuss bounds to obtain upper and lower bounds on the effective Poisson's ratio.

3. Consider the situation of multiaxial stress and strain for a composite with isotropic linear elastic subscale properties that may vary arbitrarily. Using the strategy for proving the Hill-Reuss-Voigt bounds, show that

   $$\bar{G}^{\mathrm{R}} \leq \bar{G} \leq \bar{G}^{\mathrm{V}}, \quad \bar{K}^{\mathrm{R}} \leq \bar{K} \leq \bar{K}^{\mathrm{V}}$$

4. Consider a square(cubic) RVE in 2D(3D) with side length l_{rve}.

   (a) Show that the displacements vary linearly along all boundaries when the RVE is subjected to Dirichlet boundary conditions.

   (b) Show that the tractions are piecewise constant along all boundaries when the RVE is subjected to Neumann boundary conditions.

5. Consider an elastic composite consisting of a homogeneous matrix (stiffness $\mathbf{E}_{\mathrm{m}}$, volume fraction n_{m}) containing N homogeneous inclusions (stiffness $\mathbf{E}_i$, volume fraction n_i, $i = 1, 2, ..., N$).

   (a) Show that the effective stiffness tensor $\bar{\mathbf{E}}$ can be expressed as

$$\bar{\mathbf{E}} = n_{\mathrm{m}}\mathbf{E}_{\mathrm{m}} : \langle \mathbf{B}_\epsilon \rangle_{\square,\mathrm{m}} + \sum_{i=1}^{N} n_i \mathbf{E}_i : \langle \mathbf{B}_\epsilon \rangle_{\square,i}$$

   where

$$\langle [\bullet] \rangle_{\square,\mathrm{m}} = \frac{1}{|\Omega_{\square,\mathrm{m}}|} \int_{\Omega_{\square,\mathrm{m}}} [\bullet] \, \mathrm{d}\Omega \,, \quad \langle [\bullet] \rangle_{\square,i} = \frac{1}{|\Omega_{\square,i}|} \int_{\Omega_{\square,i}} [\bullet] \, \mathrm{d}\Omega$$

   (b) For the Voigt assumption, verify that

$$\langle \mathbf{B}_\epsilon \rangle_{\square,\mathrm{m}} = \langle \mathbf{B}_\epsilon \rangle_{\square,i} = \mathbf{I}^{\mathrm{sym}}$$

   In addition, simplify $\bar{\mathbf{E}}$ accordingly and compare with the result in Q1(a).