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Plasticity and Beyond

Microstructures, Crystal-Plasticity and Phase Transitions

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Editors

Plasticity and Beyond:
Microstructures, Crystal-Plasticity and Phase Transitions

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PREFACE

Many applications in mechanics, material science and technology require a comprehensive understanding and reliable representation of the elastoplastic behavior observed in a large class of engineering materials. In the last few decades several phenomenological theories have been developed on the macroscopic level. Extensions of these classic models taking into account the formation of microstructures and the microheterogeneity of multiphase materials have attracted a more pronounced scientific interest rather recently. The role of microstructures becomes more and more important with a decreasing size of the considered material specimen because then scale-effects play a dominant role. Microstructure is indeed crucial, since plastic behavior typically results from the interaction of complex substructures on several length scales. The macroscopic behavior is then determined by appropriate averages over the (evolving) microstructure.

The CISM course on "Plasticity and Beyond: Microstructures, Crystal-Plasticity and Phase Transitions", held in Udine from June 27 to July 1, 2011, was addressed to master students, doctoral students, post docs and experienced researchers in engineering, applied mathematics and material science who wished to broaden their knowledge in classical and extended continuum thermodynamics, incremental variational formulations, phase-field modeling, higher-order models like gradient plasticity or numerical multiscale approaches at finite deformations.

It is our pleasure to thank the lecturers of the CISM course Samuel Forest (Paris, France), Jan Kratochvil (Prague, Czech Republic), Mitsutoshi Kuroda (Yamagata, Japan), Valery Levitas (Ames, USA), as well as the additional contributors to these CISM lecture notes Kais Ammar (Paris, France), Benoît Appolaire (Châtillon, France), Daniel Balzani (Essen, Germany), Dominik Brands (Essen, Germany), Nicolas Cordero (Paris, France), Anaïs Gaubert (Châtillon, France), Ulrich Hoppe (Bochum, Germany), and Dennis Kochmann (Pasadena, USA). We furthermore thank the 47 participants from 9 countries who made the course a success. Finally, we extend our thanks to the Rectors, the Board, and the staff of CISM for the excellent support and kind help.

Jörg Schröder and Klaus Hackl

CONTENTS

A numerical two-scale homogenization scheme: the FE^2-method

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Abstract A wide class of micro-heterogeneous materials is designed to satisfy the advanced challenges of modern materials occurring in a variety of technical applications. The effective macroscopic properties of such materials are governed by the complex interaction of the individual constituents of the associated microstructure. A *sufficient* macroscopic phenomenological description of these materials up to a certain order of accuracy can be very complicated or even impossible. On the contrary, a whole resolution of the fine scale for the macroscopic boundary value problem by means of a classical discretization technique seems to be too elaborate.

Instead of developing a macroscopic phenomenological constitutive law, it is possible to attach a representative volume element ($\mathcal{RVE}$) of the microstructure at each point of the macrostructure; this results in a two-scale modeling scheme. A discrete version of this scheme performing finite element (FE) discretizations of the boundary value problems on both scales, the macro- and the micro-scale, is denoted as the FE^2-method or as the multilevel finite element method. The main advantage of this procedure is based on the fact that we do not have to define a macroscopic phenomenological constitutive law; this is replaced by suitable averages of stress measures and deformation tensors over the microstructure.

Details concerning the definition of the macroscopic quantities in terms of their microscopic counterparts, the definition/construction of boundary conditions on the $\mathcal{RVE}$ as well as the consistent linearization of the macroscopic constitutive equations are discussed in this contribution.

Furthermore, remarks concerning stability problems on both scales as well as their interactions are given and representative numerical examples for elasto-plastic microstructures are discussed.

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1 Introduction

For the analysis of micro-heterogeneous materials, we define two different scales, the macroscopic scale (coarse scale) and the microscopic scale (fine scale). The fine scale is assumed to be the scale of the heterogeneities of characteristic length l, whereas the characteristic length of the coarse scale is denoted by L. If we assume that the domain size at the fine scale is sufficient for homogenization requirements, then the *separation of scales* expressed by

$$l \ll L \tag{1}$$

has to hold. A homogenized – that means effective macroscopic – description of the micro-heterogeneous material requires the definition of a representative volume element ($\mathcal{RVE}$) or a *statistically homogeneous volume element*, which is here assumed to be possible. In classical works, effective quantities of micro-heterogeneous media, such as stiffness or compliance tensors, have been discussed by Voigt (1910) and Reuss (1929). The arithmetical mean value of Voigt and the harmonic mean value of Reuss were shown later to be upper and lower bounds of effective parameters, see Hill (1965b, 1964a,b, 1963). However, the gap between these approximations can be quite wide, see e.g. Babuska (1976). General procedures for the derivation of inequalities between various moduli of mixtures have been discussed by Hill (1963) and Kröner (1971). A variety of methods for the computation of overall properties of micro-heterogeneous materials are documented in the monograph Nemat-Nasser and Hori (1999).
A fundamental assumption for the scale-transition is the *macro-homogeneity condition*, also denoted as *Hill condition* or *Hill-Mandel condition*, which asserts the equality of the virtual work between both scales, see Hill (1965a, 1963), Mandel and Dantu (1963), Mandel (1972). There are several "additive" mechanical quantities which could be averaged over the representative volume element when transferred to the macro-scale, e.g. the mass, internal energy, entropy and dissipation. Furthermore, macroscopic measures of plastic work for micro-heterogeneous materials have been analyzed in Hill (1971).

A suitable framework for the solution of two-scale problems is the mathematical homogenization theory. There, it is usually assumed that the microstructure is locally built by the spatial repetition of a suitable, very small part of the whole microstructure, a unit cell. Thus, it is assumed that the morphology and the distribution of the material properties are periodic functions of the microscopic spatial parametrization y. As an introductionary example we consider a simple one-dimensional bar. For this purpose, let

the periodic function $EA(y)$ denote the axial stiffness of a bar, $u(\overline{x}, y)$ the axial displacement, $\overline{x}$ the parametrization of the coarse scale, and $n(\overline{x})$ the distributed axial load, then the axial displacements of the bar are described by the differential equation

$$\frac{d}{d\overline{x}} N(\overline{x}, y) + n(\overline{x}) = 0 \quad \text{with} \quad N(\overline{x}, y) := EA(y) \, \frac{du(\overline{x}, y)}{d\overline{x}} \, . \tag{2}$$

The mathematical homogenization theory is based on the double scale asymptotic expansion of the yet unknown y-periodic field variable $u(\overline{x}, y)$, i.e.,

$$u(\overline{x}, y) = u^{(0)}(\overline{x}, y) + \epsilon \, u^{(1)}(\overline{x}, y) + \epsilon^2 \, u^{(2)}(\overline{x}, y) + \cdots \, , \tag{3}$$

where ϵ, defined as the microscopic to macroscopic dimension ratio (l/L), is a very small number. The asymptotic expansion (3) has to be substituted into the underlying partial differential equation with oscillating coefficients. Applying the chain rule, i.e.,

$$\frac{d}{d\overline{x}} N(\overline{x}, y) = \frac{\partial N(\overline{x}, y)}{\partial \overline{x}} + \epsilon^{-1} \frac{\partial N(\overline{x}, y)}{\partial y} \, , \tag{4}$$

yields a set of equations with factors in powers of ϵ. Equating the terms of the different orders of ϵ with zero yields the set of differential equations, which have to be solved. Fundamentals of this framework can be found in Bensoussan et al. (1978), Sanchez-Palencia and Zaoui (1986) and Bakhvalov and Panasenko (1984). Based on this approach, a computational homogenization framework in the field of linear elasticity as well as the application of adaptive finite element methods has been proposed in Guedes and Kikuchi (1990). Extensions of this method to locally non-periodic microheterogeneous media are given by Fish and Wagiman (1993). A framework of a two-scale homogenization technique using a Voronoi cell finite element formulation has been proposed by Ghosh et al. (1995). Generalized convergence arguments for the interpretation of the homogenized variational equations have been used by Terada and Kikuchi (2001). An extension of the latter simultaneous two-scale method to geometrical nonlinear formulations of the associated two-scale boundary value problems in a material and a spatial setting has been developed in Terada et al. (2003). Several mathematical aspects of homogenization theory are discussed in Tartar (2000). For the treatment of finite thermoelasticity in this scheme, we refer to Temizer (2012).

A homogenization technique without recourse to the two-scale asymptotic expansion is governed by the above mentioned *Hill-Mandel condition*.

Here, the boundary value problems on the macro- and on the micro-scale are prescribed by the balance of linear and angular momentum and suitable boundary conditions on both scales, where the micro-scale is approximated by means of a representative volume element. A summary of recent developments in this field of applied computational mechanics of the overall description of micro-heterogeneous materials up to the mid 1980's is given in Suquet (1987). In this context we also refer to Michel et al. (1999) where the boundary value problem on the micro-scale is solved using the Finite-Element-Method (FEM) and, alternatively, using a Fast Fourier Transformation. The authors also discuss the constraints on discrete unknown displacements arising when periodic boundary conditions are used.
A multilevel finite element method (FE^2-method) for nonlinear heterogeneous systems has been discussed by Smit et al. (1998), where the authors implemented their algorithms in an Updated Lagrange environment. Another FE^2-method for the analysis of the elasto-viscoplastic behavior of fiber-reinforced composite materials was presented by Feyel and Chaboche (2000), where the tangent matrix has been approximated by a perturbation method. A framework for geometrically and/or physically linear/nonlinear homogenization techniques in the sense of the FE^2-method has been developed by Miehe et al. (1999a,b), including a closed-form representation of the macroscopic (homogenized) tangent moduli. In order to design "deformation-driven" microstructures, Miehe and Koch (2002) proposed a Lagrangian multiplier method for the computational treatment of the constraints arising from the different boundary conditions: i) linear displacements, ii) constant tractions, and iii) periodic displacements in combination with antiperiodic tractions; for the discussion of the distinct boundary conditions, see also van der Sluis et al. (2000), Terada et al. (2000), Kouznetsova et al. (2001), Miehe and Bayreuther (2007) and Perić et al. (2011). A family of algorithms and matrix representations of overall stresses and tangent moduli of discretized micro-heterogeneous materials at finite strains is descriped in Miehe (2003). Different methods for the computation of the macroscopic tangent, e.g. the penalty method, have been investigated in Temizer and Wriggers (2008).

The nature of finite deformation continuum mechanics is the non-uniqueness of solutions at specific thermodynamic states. As an example, this can be associated to stability problems like buckling of columns under compressive loadings. Although in micro-heterogeneous materials, like aligned fiber-reinforced composites, cellular solids or in general arbitrary arrangements of inhomogeneities, buckling phenomena may occur on the micro-scale. A challenging issue in homogenization schemes at finite strains is the ana-

lysis of instabilities at the macro- and micro-scale and their interactions. In general, we distinguish between structural instabilities and material instabilities: structural instabilities are associated to the non-uniqueness of the underlying boundary value problem, whereas material instabilities are understood as the violation of the Legendre-Hadamard-condition (loss of rank-one convexity) of the free-energy. Nevertheless, there exits a relation between material instabilities on the macro-scale and specific structural instabilities on the micro-scale. Abeyaratne and Triantafyllidis (1984) studied the macroscopic material instability occuring in nonlinear elastic composites with periodically arranged voids. It was shown that a homogenized material instability occurs although the matrix material was polyconvex in the sense of Ball (1977b). Bifurcation modes of fiber-reinforced composites as well as possible macroscopic material instabilities have been analyzed in Triantafyllidis and Maker (1985). Structural instability problems on the micro-scale are associated to the homogenization of a nonconvex boundary value problem on the micro-scale, see Müller (1987). The main challenge here is the a priori unknown size of the $\mathcal{RVE}$. A systematic investigation of the problems pointed out in Abeyaratne and Triantafyllidis (1984) and Triantafyllidis and Maker (1985) is given in Geymonat et al. (1993). Applying a Bloch-wave ansatz to a fiber-reinforced composite, the authors showed that the onset of a bifurcation on the micro-scale corresponding to the long-wavelength limit (infinite wavelength) leads to a macroscopic material instability. A detailed computational homogenization analysis of structural instabilities on the micro-scale and possible material instabilities on the macro-scale as well as their interactions is performed in Miehe et al. (2002), in this context see also Agoras et al. (2009) and Aubert et al. (2008). A microscopic bifurcation condition of cellular solids, like elastic cellular honeycombs, have been presented in Ohno et al. (2002). A procedure, based on a block-diagonalization method for periodic microstructures, for the estimation of the number of unit cells necessary for the definition of a $\mathcal{RVE}$ of cellular solids in microscopic bifurcation problems has been proposed in Saiki et al. (2002). In the context of homogenization of non-convex integral functionals and especially for the relation between linearization and homogenization in finite elasticity, we refer to Müller and Neukamm (2011). For the treatment of localized failure with softening in this multi-scale approach see Hautefeuille et al. (2012).

If the classical assumption of scale separation does not hold or if it is necessary to capture size dependency, then in general higher-order homogenization techniques can be applied. A second-order homogenization scheme, implying a second gradient continuum on the macro-scale and a remaining classical continuum on the micro-scale, has been proposed by Geers et al.

(2001, 2003) and Kouznetsova et al. (2004). A multilevel finite element method coupling a classical continuum, a Cauchy continuum, on the fine scale with a Cosserat continuum at the coarse scale has been proposed by Feyel (2003). A critical analysis of the two-scale homogenization of macroscopic second gradient and micromorphic models based on a Cauchy continuum on the fine scale with emphasis on non-homogeneous boundary conditions is given by Forest and Trinh (2011), in this context see also Forest (2002) and Jänicke et al. (2009). An application of the computational homogenization scheme for structured thin sheets has been proposed by Geers et al. (2007) and Gruttmann and Wagner (2013). Here, the $\mathcal{RVE}$ resolves the full thickness of the thin sheet and the nature of the coupling of deformation between the shell-type macro-scale and the microstructure is of second-order.
Another non-classical approach, denoted as a multi-scale strategy for *strongly coupled scales*, has been proposed by Ibrahimbegović and Markovič (2003). Here, the authors attach a part of the microstructure at each finite element of the macro-scale, for details see Markovic et al. (2005) and Niekamp et al. (2009). This is in contrast to the *weakly coupled scales*, where we attach an $\mathcal{RVE}$ of the microstructure at each point of the macrostructure, i.e., at each Gauss point in the discrete version obtained from the FE^2-method.

Recent developments are concerned with direct two-scale homogenization techniques for thermo-mechanically coupled problems, Özdemir et al. (2008), and for electro-mechanically coupled problems concerning the general localization and homogenization scheme, Schröder (2009), as well as the numerical treatment Schröder and Keip (2011, 2012).
Another important topic is the characterization of random microstructures, Ohser and Mücklich (2000), and the identification of statistically representative volume elements, see e.g. Kanit et al. (2003), Stroeven and Askes (2004), Temizer and Zohdi (2007). From the computational point of view, the application of statistically similar representative volume elements, which have less complexity than the original random microstructure, could lead to a significant reduction in computation time. Basic considerations for the definition and optimization procedures based on suitable statistical measure are discussed in Povirk (1995), Ostoja-Starzewski (2006), Balzani et al. (2009, 2010), Schröder et al. (2010), Ambrozinski et al. (2012), in this context see also Swaminathan et al. (2006) and Zohdi and Wriggers (2005). Details on the construction of statistically similar representative volume elements are presented in the contribution by Balzani et al. in this book.

2 Direct Micro-Macro Transition Approach

For the analysis of micro-heterogeneous materials, where we want to take into account the microstructure directly, the transition between the macro- and the micro scale has to be defined, cf. Fig. 1. The direct micro-macro homogenization scheme, based on the finite element discretization of both scales, allows for the computation of macroscopic boundary value problems in consideration of $\mathcal{RVE}s$, which should represent the main characteristics of the associated micro-continuum.

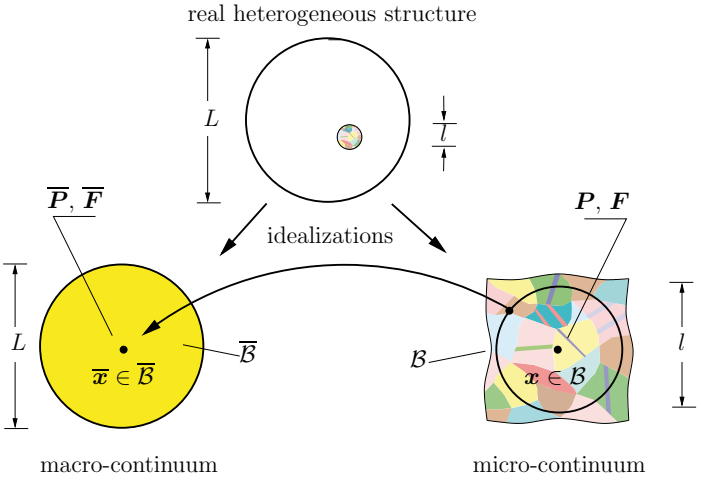

Figure 1. Schematic illustration of the direct homogenization procedure. Notation: macroscopic first Piola-Kirchhoff stresses $\overline{\boldsymbol{P}}$ and deformation gradient $\overline{\boldsymbol{F}}$; their microscopic counterparts are denoted by $\boldsymbol{P}$ and $\boldsymbol{F}$, taken from Schröder et al. (2010)

Since the definition of the individual scales, like macro-, meso- and micro-scale, is somewhat arbitrary, we denote the coarse and fine scale as the macro- and micro-scale, respectively. The main technical ingredients for the two-scale homogenization procedure for mechanical problems are:

- Definition of a $\mathcal{RVE}$ and choosing suitable boundary conditions: The boundary conditions for the microscopic boundary value problem are in general not given a priori. Suitable boundary conditions can be derived by the Hill-Mandel condition, which equates the virtual macroscopic work with the averaged virtual work performed within the $\mathcal{RVE}$.
- Discretization of the microscopic boundary value problem.
- Discretization of the macroscopic boundary value problem.

The main advantage of a direct two-scale homogenization scheme is that we do not have to define a macroscopic phenomenological constitutive law; this is replaced by suitable averages over the $\mathcal{RVE}$. Nevertheless, we have to set up constitutive models for the individual phases on the fine scale. If the local distributions of the deformation and stress measures within the $\mathcal{RVE}$ are computed, we can calculate their macroscopic counterparts by suitable surface or volume integrals over the representative volume element, which are attached at each macroscopic point. Therefore, the numerical micro-to-macro procedure is based on the following consecutive steps:

a) *Localization step, boundary value problem on the micro-scale*: computation of the local distribution of the deformation and stress measures within the $\mathcal{RVE}$ by solving the weak form of the balance of linear momentum.

b) *Homogenization step*: computation of the macroscopic quantities, e.g. the first Piola-Kirchhoff stresses, by means of suitable averages.

c) *Boundary value problem on the macro-scale*: solving the weak form of balance of linear momentum on the coarse scale.

These steps have to be repeated until convergence on both scales is obtained.

2.1 Boundary value problem on the macro-scale

Let the reference configuration of the body of interest on the macroscopic scale $\overline{\mathcal{B}}_0 \subset R^3$ be parameterized in $\overline{\boldsymbol{X}}$. The macroscopic nonlinear deformation map is denoted as $\overline{\boldsymbol{\varphi}}_t(\overline{\boldsymbol{X}})$; it maps points $\overline{\boldsymbol{X}}$ of the reference configuration onto points $\overline{\boldsymbol{x}}$ of the actual configuration $\overline{B}_t$, see Figure 2. The fundamental deformation measure is the macroscopic deformation gradient, defined by

$$\overline{\boldsymbol{F}}(\overline{\boldsymbol{X}}) := \mathrm{Grad}_{\overline{X}}[\overline{\boldsymbol{\varphi}}_t(\overline{\boldsymbol{X}})] \quad \text{with} \quad \overline{F}^a{}_A := \frac{\partial \overline{x}^a}{\partial \overline{X}^A}\,, \tag{5}$$

which maps macroscopic infinitesimal line elements $d\overline{\boldsymbol{X}}$ from the reference configuration to the current configuration, i.e.,

$$d\overline{\boldsymbol{x}} = \overline{\boldsymbol{F}}\, d\overline{\boldsymbol{X}}\,. \tag{6}$$

Let $d\overline{\boldsymbol{A}} = \overline{\boldsymbol{N}}\, d\overline{A}$ and $d\overline{\boldsymbol{a}} = \overline{\boldsymbol{n}}\, d\overline{a}$ denote the infinitesimal vectorial area elements with respect to the reference and current configuration, repectively. The transformation between the quantities is

$$d\overline{\boldsymbol{a}} = [\mathrm{Cof}\, \overline{\boldsymbol{F}}]\, d\overline{\boldsymbol{A}} \quad \text{with} \quad \mathrm{Cof}\, \overline{\boldsymbol{F}} = \overline{J}\, \overline{\boldsymbol{F}}^{-T}\,, \tag{7}$$

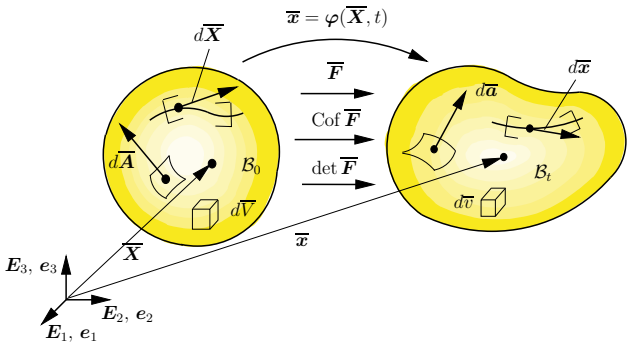

Figure 2. Mapping of infinitesimal line-, vectorial area- and volume-elements from the reference to the actual configuration at the macro-scale.

using Nanson's formula and the abbreviation $\overline{J} = \det \overline{\boldsymbol{F}}$ for their Jacobian determinant. The relation between the macroscopic infinitesimal volume elements $d\overline{V}$ of the reference and $d\overline{v}$ of the current configuration reads

$$d\overline{v} = \overline{J}\, d\overline{V}\,. \tag{8}$$

As a suitable deformation measure, we introduce the macroscopic right Cauchy-Green tensor

$$\overline{\boldsymbol{C}} := \overline{\boldsymbol{F}}^T \overline{\boldsymbol{F}}\,. \tag{9}$$

With the first Piola-Kirchhoff stress tensor $\overline{\boldsymbol{P}}$ the Kirchhoff stresses, the Cauchy stresses and the second Piola-Kirchhoff stresses can be computed by

$$\overline{\boldsymbol{\tau}} = \overline{\boldsymbol{P}}\,\overline{\boldsymbol{F}}^T\,, \quad \overline{\boldsymbol{\sigma}} = \frac{1}{\overline{J}}\,\overline{\boldsymbol{P}}\,\overline{\boldsymbol{F}}^T \quad \text{and} \quad \overline{\boldsymbol{S}} = \overline{\boldsymbol{F}}^{-1}\,\overline{\boldsymbol{P}}\,, \tag{10}$$

respectively. The balance of linear momentum at the macroscopic scale, neglecting acceleration terms, requires

$$\mathrm{Div}_{\overline{X}}\overline{\boldsymbol{P}} + \overline{\boldsymbol{f}} = \boldsymbol{0}\,. \tag{11}$$

Furthermore, the macroscopic balance of moment of momentum, i.e.,

$$\overline{\boldsymbol{P}}\,\overline{\boldsymbol{F}}^T = \overline{\boldsymbol{F}}\,\overline{\boldsymbol{P}}^T \tag{12}$$

is assumed to be satisfied a priori by symmetry requirements of the macroscopic Kirchhoff stress tensor.

2.2 Boundary value problem on the micro-scale

In analogy to the description of the mechanical quantities on the macro-scale, we parametrize the reference placement of the $\mathcal{RVE}$ on the micro-scale $\mathcal{B}_0 \subset \mathbb{R}^3$ with $\boldsymbol{X}$. The nonlinear deformation map on the micro-scale is denoted as $\boldsymbol{\varphi}_t(\boldsymbol{X})$, which maps points $\boldsymbol{X}$ of the reference placement onto points $\boldsymbol{x}$ of the current placement B_t.

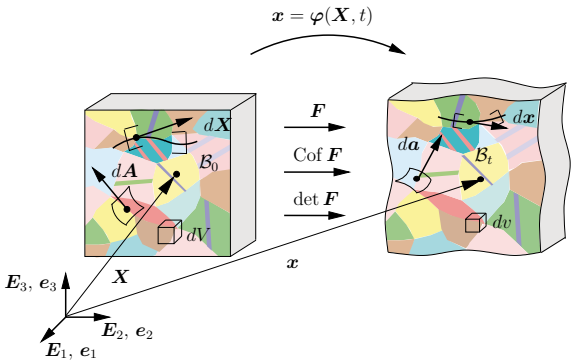

Figure 3. Transport theorems at the micro-scale: Mapping of infinitesimal geometrical elements from the reference to the actual configuration.

The microscopic deformation gradient is defined by

$$\boldsymbol{F}(\boldsymbol{X}) := \mathrm{Grad}_X[\boldsymbol{\varphi}_t(\boldsymbol{X})] \quad \text{with} \quad F^a{}_A := \frac{\partial x^a}{\partial X^A}\,, \tag{13}$$

which maps microscopic infinitesimal line elements $d\boldsymbol{X}$ from the reference configuration to the current configuration, i.e.,

$$d\boldsymbol{x} = \boldsymbol{F}\, d\boldsymbol{X}\,. \tag{14}$$

The transformation of the infinitesimal vectorial area elements of the reference configuration $d\boldsymbol{A} = \boldsymbol{N}\, dA$ to the area elements of the current configuration $d\boldsymbol{a} = \boldsymbol{n}\, da$ is given by

$$d\boldsymbol{a} = [\mathrm{Cof}\, \boldsymbol{F}]d\boldsymbol{A} \quad \text{with} \quad \mathrm{Cof}\, \boldsymbol{F} = J\, \boldsymbol{F}^{-T}\,, \tag{15}$$

using the abbreviation $J = \det \boldsymbol{F}$. The microscopic infinitesimal volume elements dV and dv of the reference and current configuration, respectively, transform with

$$dv = J\, dV\,. \tag{16}$$

As further deformation measures, we introduce the microscopic right Cauchy-Green tensor and the microscopic Finger tensor

$$\boldsymbol{C} := \boldsymbol{F}^T \boldsymbol{F} \quad \text{and} \quad \boldsymbol{b} := \boldsymbol{F} \boldsymbol{F}^T , \tag{17}$$

respectively. Starting from the microscopic first Piola-Kirchhoff stress tensor $\boldsymbol{P}$, we can compute the microscopic Kirchhoff-, Cauchy- and second Piola-Kirchhoff stresses by

$$\boldsymbol{\tau} = \boldsymbol{P} \boldsymbol{F}^T , \quad \boldsymbol{\sigma} = \frac{1}{J} \boldsymbol{\tau} \quad \text{and} \quad \boldsymbol{S} = \boldsymbol{F}^{-1} \boldsymbol{P} , \tag{18}$$

respectively. The balance of linear momentum, neglecting body forces, is given by

$$\mathrm{Div}_X \boldsymbol{P} = \boldsymbol{0} \quad \text{or} \quad \mathrm{div}_x \boldsymbol{\sigma} = \boldsymbol{0} , \tag{19}$$

with respect to the reference and actual placement, respectively. Equation $(19)_2$ is derived from $(19)_1$ by setting $\boldsymbol{P} = \boldsymbol{\sigma} \mathrm{Cof} \boldsymbol{F}$ and applying the Piola identity

$$\mathrm{Div}_X [\mathrm{Cof} \boldsymbol{F}] = \boldsymbol{0} . \tag{20}$$

The balance of moment of momentum

$$\boldsymbol{P} \boldsymbol{F}^T = \boldsymbol{F} \boldsymbol{P}^T . \tag{21}$$

is assumed to be satisfied a priori by symmetry requirements of the Kirchhoff stress tensor, which are guaranteed by the constitutive modeling.

2.3 Macro-variables and microscopic counterparts

An extension of the micro-macro transition framework from small to finite strains has been given in Hill (1972). The determinant $\overline{J}$ of the macroscopic deformation gradient is related to its microscopic counterpart by the volume averages

$$\overline{J} = \frac{1}{V} \int_{\mathcal{B}_0} J \, dV = \frac{1}{V} \int_{\mathcal{B}_t} dv = \frac{v}{V} , \tag{22}$$

here V denotes the reference and v the actual volume of the $\mathcal{RVE}$. Let us assume that the $\mathcal{RVE}$ in its reference placement has a hole $\mathcal{L}_0$ with boundary $\partial \mathcal{L}_0$, then the volume average of deformation gradient can be expressed by

$$\frac{1}{V} \int_{\mathcal{B}_0} \boldsymbol{F} \, dV = \frac{1}{V} \int_{\partial \mathcal{B}_0} \boldsymbol{x} \otimes \boldsymbol{N} \, dA + \frac{1}{V} \int_{\partial \mathcal{L}_0} \boldsymbol{x} \otimes \boldsymbol{N} \, dA . \tag{23}$$

Furthermore, the volume average of the first Piola-Kirchhoff stress tensor is then given by the surface integrals

$$\frac{1}{V}\int_{\mathcal{B}_0} \boldsymbol{P}\, dV = \frac{1}{V}\int_{\partial\mathcal{B}_0} \boldsymbol{t}_0 \otimes \boldsymbol{X}\, dA + \frac{1}{V}\int_{\partial\mathcal{L}_0} \boldsymbol{t}_0 \otimes \boldsymbol{X}\, dA\,, \tag{24}$$

with $\boldsymbol{t}_0 = \boldsymbol{P}\boldsymbol{N}$ and the outward unit normal $\boldsymbol{N}$. In order to get a simple correlation of the macroscopic quantities in terms of suitable integrals over the $\mathcal{RVE}$ with experimental set-ups, we define the macroscopic deformation gradient and the first Piola-Kirchhoff stress tensor in terms of surface integrals over the boundary $\partial\mathcal{B}_0$ of the $\mathcal{RVE}$:

$$\overline{\boldsymbol{F}} = \frac{1}{V}\int_{\partial\mathcal{B}_0} \boldsymbol{x} \otimes \boldsymbol{N}\, dA\,, \qquad \overline{\boldsymbol{P}} = \frac{1}{V}\int_{\partial\mathcal{B}_0} \boldsymbol{t}_0 \otimes \boldsymbol{X}\, dA\,. \tag{25}$$

By analogy with the previous relations, we obtain

$$\dot{\overline{\boldsymbol{F}}} = \frac{1}{V}\int_{\partial\mathcal{B}_0} \dot{\boldsymbol{x}} \otimes \boldsymbol{N}\, dA\,, \qquad \dot{\overline{\boldsymbol{P}}} = \frac{1}{V}\int_{\partial\mathcal{B}_0} \dot{\boldsymbol{t}}_0 \otimes \boldsymbol{X}\, dA\,. \tag{26}$$

In the following, we neglect holes $\mathcal{L}_0$, then the surface integrals (25, 26) are identical to their volume averages. Similar arguments have to be applied if singular surfaces are taken into account, see e.g. Schröder (2000).

For the following algebraic manipulations we introduce an additive decomposition of the microscopic deformation gradient in a constant and a fluctuation part, i.e.,

$$\boldsymbol{F} = \overline{\boldsymbol{F}} + \widetilde{\boldsymbol{F}}\,. \tag{27}$$

Integration of (27) over the representative volume element yields

$$\overline{\boldsymbol{F}} = \frac{1}{V}\int_{\mathcal{B}_0} \boldsymbol{F}\, dV = \frac{1}{V}\int_{\mathcal{B}_0} (\overline{\boldsymbol{F}} + \widetilde{\boldsymbol{F}})\, dV = \overline{\boldsymbol{F}} + \frac{1}{V}\int_{\mathcal{B}_0} \widetilde{\boldsymbol{F}}\, dV\,. \tag{28}$$

The implication of the latter relation is that the volume averages of the fluctuation part $\widetilde{\boldsymbol{F}}$ vanish, i.e.,

$$\frac{1}{V}\int_{\mathcal{B}_0} \widetilde{\boldsymbol{F}}\, dV = \boldsymbol{0}\,. \tag{29}$$

If we further assume that the fluctuation part of the microscopic deformation gradient can be computed by $\widetilde{\boldsymbol{F}} = \mathrm{Grad}_X \widetilde{\boldsymbol{w}}$, where $\widetilde{\boldsymbol{w}}$ represents the fluctuation part of the deformation field on the micro-scale, then the following condition holds:

$$\frac{1}{V}\int_{\partial\mathcal{B}_0} \widetilde{\boldsymbol{w}} \otimes \boldsymbol{N}\, dA = \boldsymbol{0}\,. \tag{30}$$

By analogy with the decomposition of the microscopic deformation gradient, we introduce an additive decomposition of the microscopic first Piola-Kirchhoff stresses in a constant and a fluctuation part, i.e.,

$$\boldsymbol{P} = \overline{\boldsymbol{P}} + \widetilde{\boldsymbol{P}} \,. \tag{31}$$

The evaluation of the integral of the decomposition (31) over the $\mathcal{RVE}$ yields

$$\overline{\boldsymbol{P}} = \frac{1}{V} \int_{\mathcal{B}_0} \boldsymbol{P} \, dV = \frac{1}{V} \int_{\mathcal{B}_0} (\overline{\boldsymbol{P}} + \widetilde{\boldsymbol{P}}) \, dV = \overline{\boldsymbol{P}} + \frac{1}{V} \int_{\mathcal{B}_0} \widetilde{\boldsymbol{P}} \, dV \,, \tag{32}$$

which implies

$$\frac{1}{V} \int_{\mathcal{B}_0} \widetilde{\boldsymbol{P}} \, dV = \boldsymbol{0} \,. \tag{33}$$

Based on the definition of the traction vector $\boldsymbol{t}_0 = \boldsymbol{P}\boldsymbol{N} = (\overline{\boldsymbol{P}} + \widetilde{\boldsymbol{P}})\boldsymbol{N}$ we introduce the abbreviation $\boldsymbol{t}_0 = \overline{\boldsymbol{t}}_0 + \widetilde{\boldsymbol{t}}_0$ with $\overline{\boldsymbol{t}}_0 = \overline{\boldsymbol{P}}\boldsymbol{N}$ and $\widetilde{\boldsymbol{t}}_0 = \widetilde{\boldsymbol{P}}\boldsymbol{N}$. Inserting these quantities in $(25)_2$ yields

$$\overline{\boldsymbol{P}} = \frac{1}{V} \int_{\partial \mathcal{B}_0} (\overline{\boldsymbol{t}}_0 + \widetilde{\boldsymbol{t}}_0) \otimes \boldsymbol{X} \, dA \,. \tag{34}$$

From one part of the surface integral we derive the relation

$$\frac{1}{V} \int_{\partial \mathcal{B}_0} \overline{\boldsymbol{t}}_0 \otimes \boldsymbol{X} \, dA = \frac{1}{V} \int_{\partial \mathcal{B}_0} (\overline{\boldsymbol{P}}\boldsymbol{N}) \otimes \boldsymbol{X} \, dA = \overline{\boldsymbol{P}} \, \frac{1}{V} \int_{\partial \mathcal{B}_0} \boldsymbol{N} \otimes \boldsymbol{X} \, dA \,, \tag{35}$$

which yields with the relation $\dfrac{1}{V} \displaystyle\int_{\partial \mathcal{B}_0} \boldsymbol{N} \otimes \boldsymbol{X} \, dA = \boldsymbol{1}$ the identity

$$\frac{1}{V} \int_{\partial \mathcal{B}_0} \overline{\boldsymbol{t}}_0 \otimes \boldsymbol{X} \, dA = \overline{\boldsymbol{P}} \,. \tag{36}$$

Therefore, we conclude from (34) that for an equilibrium state

$$\frac{1}{V} \int_{\partial \mathcal{B}_0} \widetilde{\boldsymbol{t}}_0 \otimes \boldsymbol{X} \, dA = \boldsymbol{0} \tag{37}$$

holds. In general, other macroscopic quantities are defined by the standard transformations using the macroscopic stress- and deformation tensors. Thus, the macroscopic Kirchhoff stresses $\overline{\boldsymbol{\tau}}$ are defined as

$$\overline{\boldsymbol{\tau}} = \overline{\boldsymbol{P}} \, \overline{\boldsymbol{F}}^T = \frac{1}{V} \int_{\mathcal{B}_0} \boldsymbol{P} \, dV \quad \left(\frac{1}{V} \int_{\mathcal{B}_0} \boldsymbol{F} \, dV \right)^T \,. \tag{38}$$

In a similar way, we define the macroscopic Cauchy stresses by the transformation

$$\overline{\boldsymbol{\sigma}} = \frac{1}{\overline{J}} \overline{\boldsymbol{P}}\, \overline{\boldsymbol{F}}^T = \frac{1}{\overline{J}} \overline{\boldsymbol{\tau}} = \frac{1}{\overline{J}} \left(\frac{1}{V} \int_{\mathcal{B}_0} \boldsymbol{P}\, dV \right) \left(\frac{1}{V} \int_{\mathcal{B}_0} \boldsymbol{F}\, dV \right)^T . \tag{39}$$

Also the definition of the macroscopic Cauchy-Green tensor is based on the product of the macroscopic deformation gradient, i.e.,

$$\overline{\boldsymbol{C}} = \overline{\boldsymbol{F}}^T \overline{\boldsymbol{F}} = \left(\frac{1}{V} \int_{\mathcal{B}_0} \boldsymbol{F}\, dV \right)^T \left(\frac{1}{V} \int_{\mathcal{B}_0} \boldsymbol{F}\, dV \right) , \tag{40}$$

A simple volume averaging of the microscopic Cauchy-Green tensor

$$\frac{1}{V} \int_{\mathcal{B}_0} \boldsymbol{C}\, dV = \frac{1}{V} \int_{\mathcal{B}_0} \boldsymbol{F}^T \boldsymbol{F}\, dV , \tag{41}$$

leads with the decomposition $\boldsymbol{F} = \overline{\boldsymbol{F}} + \widetilde{\boldsymbol{F}}$ to the expression

$$\begin{aligned} \frac{1}{V} \int_{\mathcal{B}_0} (\overline{\boldsymbol{F}} + \widetilde{\boldsymbol{F}})^T (\overline{\boldsymbol{F}} + \widetilde{\boldsymbol{F}})\, dV = \;& \overline{\boldsymbol{F}}^T \overline{\boldsymbol{F}} + \frac{1}{V} \int_{\mathcal{B}_0} \widetilde{\boldsymbol{F}}^T \widetilde{\boldsymbol{F}}\, dV \\ + \;& \frac{1}{V} \int_{\mathcal{B}_0} (\widetilde{\boldsymbol{F}}^T \overline{\boldsymbol{F}} + \overline{\boldsymbol{F}}^T \widetilde{\boldsymbol{F}})\, dV . \end{aligned} \tag{42}$$

The integral term on the right-hand side

$$\int_{\mathcal{B}_0} (\widetilde{\boldsymbol{F}}^T \overline{\boldsymbol{F}} + \overline{\boldsymbol{F}}^T \widetilde{\boldsymbol{F}})\, dV = \int_{\mathcal{B}_0} \widetilde{\boldsymbol{F}}^T\, dV\, \overline{\boldsymbol{F}} + \overline{\boldsymbol{F}}^T \int_{\mathcal{B}_0} \widetilde{\boldsymbol{F}}\, dV \tag{43}$$

vanishes obviously, thus the remaining expression of (41) is

$$\frac{1}{V} \int_{\mathcal{B}_0} \boldsymbol{C}\, dV = \overline{\boldsymbol{F}}^T \overline{\boldsymbol{F}} + \frac{1}{V} \int_{\mathcal{B}_0} \widetilde{\boldsymbol{F}}^T \widetilde{\boldsymbol{F}}\, dV , \tag{44}$$

which differs from (40) by the integral term on the right-hand side in (44).

Equivalences between the definitions (38) and (39) and direct averages of $\boldsymbol{\tau}$ and $\boldsymbol{\sigma}$ with respect to the volume of the $\mathcal{RVE}$ in the reference and actual placement, respectively, i.e.

$$\overline{\boldsymbol{\tau}} \equiv \frac{1}{V} \int_{\mathcal{B}_0} \boldsymbol{\tau}\, dV , \qquad \overline{\boldsymbol{\sigma}} \equiv \frac{1}{v} \int_{\mathcal{B}_t} \boldsymbol{\sigma}\, dv \tag{45}$$

hold only for specific boundary conditions and geometries, see e.g. de Souza Neto and Feijoo (2008). If the conditions are satisfied, we obtain for the Kirchhoff stresses and by analogy for the Cauchy stresses, assuming (19):

$$\frac{1}{V} \int_{\mathcal{B}_0} \boldsymbol{\tau}\, dV = \frac{1}{V} \int_{\partial \mathcal{B}_0} \boldsymbol{t}_0 \otimes \boldsymbol{x}\, dA , \qquad \frac{1}{v} \int_{\mathcal{B}_t} \boldsymbol{\sigma}\, dv = \frac{1}{v} \int_{\partial \mathcal{B}_t} \boldsymbol{t} \otimes \boldsymbol{x}\, da \tag{46}$$

with $\boldsymbol{t} = \boldsymbol{\sigma}\boldsymbol{n}$ and the outward unit normal $\boldsymbol{n}$ on $\partial\mathcal{B}_t$. Useful relations for further kinematical quantities and stress measures in finite deformation plasticity are given in Nemat-Nasser (1999); for the elastoplasticity of polycrystals see Clayton and McDowell (2003).

2.4 Macro-homogeneity condition

One of the most important relations in micro-macro transition schemes is the *macro-homogeneity condition* (also denoted as Hill's condition or Hill-Mandel condition), Hill (1965a) and Mandel (1972). In the finite strain setting, we define the condition as

$$\overline{\boldsymbol{P}} : \dot{\overline{\boldsymbol{F}}} = \frac{1}{V} \int_{\partial\mathcal{B}_0} \boldsymbol{t}_0 \cdot \dot{\boldsymbol{x}} \, dA \,, \tag{47}$$

which leads with the algebraic manipulations

$$\frac{1}{V} \int_{\partial\mathcal{B}_0} \boldsymbol{t}_0 \cdot \dot{\boldsymbol{x}} \, dA = \frac{1}{V} \int_{\partial\mathcal{B}_0} (\boldsymbol{P}\boldsymbol{N}) \cdot \dot{\boldsymbol{x}} \, dA = \frac{1}{V} \int_{\partial\mathcal{B}_0} \boldsymbol{P} : \dot{\boldsymbol{x}} \otimes \boldsymbol{N} \, dA$$

and the application of the Gaussian integral theorem

$$\int_{\partial\mathcal{B}_0} \boldsymbol{P} : \dot{\boldsymbol{x}} \otimes \boldsymbol{N} \, dA = \int_{\mathcal{B}_0} \mathrm{Div}_X [\dot{\boldsymbol{x}}\boldsymbol{P}] \, dV = \int_{\mathcal{B}_0} (\boldsymbol{P} : \mathrm{Grad}_X \dot{\boldsymbol{x}} + \dot{\boldsymbol{x}} \mathrm{Div}_X \boldsymbol{P}) \, dV$$

and taking into account the equilibrium condition (19) to the volume average

$$\overline{\boldsymbol{P}} : \dot{\overline{\boldsymbol{F}}} = \frac{1}{V} \int_{\mathcal{B}_0} \boldsymbol{P} : \dot{\boldsymbol{F}} \, dV \,, \tag{48}$$

with $\dot{\boldsymbol{F}} = \mathrm{Grad}_X \dot{\boldsymbol{x}}$. It should be noted that the macro-homogeneity condition of Hill and Mandel is written as the volume average of the scalar product of first Piola-Kirchhoff stresses and the deformation gradient with respect to the parametrization of the $\mathcal{RVE}$ in the reference placement.

2.5 Constraint/Boundary conditions on the micro-scale

Following the explanations of Hill (1984), we write the identity

$$\frac{1}{V} \int_{\mathcal{B}_0} \boldsymbol{P} : \dot{\boldsymbol{F}} \, dV - \overline{\boldsymbol{P}} : \dot{\overline{\boldsymbol{F}}} = \frac{1}{V} \int_{\mathcal{B}_0} ((\boldsymbol{P} - \overline{\boldsymbol{P}}) : (\dot{\boldsymbol{F}} - \dot{\overline{\boldsymbol{F}}})) \, dV \,. \tag{49}$$

If the right-hand side of the latter equation vanishes, the theorem of product averages (48) is satisfied. Two simple solutions are obtained by setting

$$\boldsymbol{P} = \overline{\boldsymbol{P}} \quad \forall \boldsymbol{X} \in \mathcal{B}_0 \quad \text{or} \quad \dot{\boldsymbol{F}} = \dot{\overline{\boldsymbol{F}}} \quad \forall \boldsymbol{X} \in \mathcal{B}_0 \,, \tag{50}$$

where the first assumption of constant stresses over the $\mathcal{RVE}$ is associated to the estimate of Reuss and the second of a constant deformation gradient to the estimate of Voigt. In the following, we denote the implications in (50) as constraint conditions.

Let us now consider the right-hand side of (49); with the definition of the microscopic deformation gradient (13) and the relation $\mathrm{Grad}_X \boldsymbol{X} = \mathbf{1}$, we obtain

$$\int_{\mathcal{B}_0} (\boldsymbol{P} - \overline{\boldsymbol{P}}) : (\mathrm{Grad}_X \dot{\boldsymbol{x}} - \dot{\overline{\boldsymbol{F}}}\, \mathrm{Grad}_X \boldsymbol{X})\, dV\,. \tag{51}$$

With the equilibrium requirement $\mathrm{Div}_X(\boldsymbol{P} - \overline{\boldsymbol{P}}) = \mathbf{0}$ and the Cauchy theorem $\boldsymbol{t}_0 = \boldsymbol{P}\boldsymbol{N}$, we derive the following equivalent expression of (48):

$$\int_{\partial\mathcal{B}_0} (\boldsymbol{t}_0 - \overline{\boldsymbol{P}}\boldsymbol{N}) \cdot (\dot{\boldsymbol{x}} - \dot{\overline{\boldsymbol{F}}}\boldsymbol{X})\, dA = 0\,. \tag{52}$$

The above relations do not only hold for $\mathrm{Grad}_X \dot{\boldsymbol{x}} = \dot{\boldsymbol{F}}$, but also for $\delta\boldsymbol{F}$ as well as for $\boldsymbol{F}$, etc.; therefore, we can replace $\dot{\overline{\boldsymbol{F}}}$ by $\delta\overline{\boldsymbol{F}}$ and $\overline{\boldsymbol{F}}$. *Dirichlet boundary conditions* are defined by setting the second bracket term in (52) equal to zero, it follows

$$\boldsymbol{x} = \overline{\boldsymbol{F}}\boldsymbol{X} \quad \forall \boldsymbol{X} \in \partial\mathcal{B}_0\,. \tag{53}$$

Analogously, enforcing the first bracket term in (52) to be zero yields the *Neumann boundary conditions*

$$\boldsymbol{t}_0 = \overline{\boldsymbol{P}}\boldsymbol{N} \quad \forall \boldsymbol{X} \in \partial\mathcal{B}_0\,. \tag{54}$$

For the derivation of *periodic boundary conditions* we decompose the boundary of the microstructure ∂B_0 into two associated parts

$$\partial\mathcal{B}_0 = \partial\mathcal{B}_0^- \cup \partial\mathcal{B}_0^+\,. \tag{55}$$

Every point $\boldsymbol{X}^+ \in \partial\mathcal{B}^+$ is assumed to have an associated point $\boldsymbol{X}^- \in \partial\mathcal{B}^-$ with outward unit normals $\boldsymbol{N}^+$ and $\boldsymbol{N}^-$, respectively. Since $\overline{\boldsymbol{F}}$ as well as $\boldsymbol{X}$ are assumed to be given quantities, we define the fluctuation field

$$\widetilde{\boldsymbol{w}} := \boldsymbol{x} - \overline{\boldsymbol{F}}\boldsymbol{X}\,. \tag{56}$$

Thus, the macro-homogeneity condition (52) appears as

$$\begin{aligned}\int_{\partial\mathcal{B}_0} (\boldsymbol{t}_0 - \overline{\boldsymbol{P}}\boldsymbol{N}) \cdot \widetilde{\boldsymbol{w}}\, dA = &\int_{\partial\mathcal{B}_0^+} (\boldsymbol{t}_0^+ - \overline{\boldsymbol{P}}\boldsymbol{N}^+) \cdot \widetilde{\boldsymbol{w}}^+\, dA \\ &+ \int_{\partial\mathcal{B}_0^-} (\boldsymbol{t}_0^- - \overline{\boldsymbol{P}}\boldsymbol{N}^-) \cdot \widetilde{\boldsymbol{w}}^-\, dA\,.\end{aligned} \tag{57}$$

Table 1. constraint conditions & boundary conditions (bcs)

Reuss	$\boldsymbol{P} = \overline{\boldsymbol{P}}$	$\forall \boldsymbol{X} \in \mathcal{B}_0$
Voigt	$\boldsymbol{F} = \overline{\boldsymbol{F}}$	$\forall \boldsymbol{X} \in \mathcal{B}_0$
Dirichlet bcs	$\boldsymbol{x} = \overline{\boldsymbol{F}}\boldsymbol{X}$	$\forall \boldsymbol{X} \in \partial\mathcal{B}_0$
Neumann bcs	$\boldsymbol{t}_0 = \overline{\boldsymbol{P}}\boldsymbol{N}$	$\forall \boldsymbol{X} \in \partial\mathcal{B}_0$
periodic bcs	$\widetilde{\boldsymbol{w}} = \boldsymbol{x} - \overline{\boldsymbol{F}}\boldsymbol{X}$ $\widetilde{\boldsymbol{w}}^+ = \widetilde{\boldsymbol{w}}^-$ $\boldsymbol{t}_0^+ = -\boldsymbol{t}_0^-$	$\forall \boldsymbol{X}^+ \in \partial\mathcal{B}_0^+$ and $\boldsymbol{X}^- \in \partial\mathcal{B}_0^-$

A periodic fluctuation field is characterized by $\widetilde{\boldsymbol{w}}^+ = \widetilde{\boldsymbol{w}}^-$ at associated points, with the essential requirement $\boldsymbol{N}^+ = -\boldsymbol{N}^-$ it follows

$$\int_{\partial\mathcal{B}_0^+} \left\{ (\boldsymbol{t}_0^+ - \overline{\boldsymbol{P}}\boldsymbol{N}^+) \cdot \widetilde{\boldsymbol{w}}^+ + (\boldsymbol{t}_0^- + \overline{\boldsymbol{P}}\boldsymbol{N}^+) \cdot \widetilde{\boldsymbol{w}}^+ \right\} dA = \int_{\partial\mathcal{B}_0^+} (\boldsymbol{t}_0^+ + \boldsymbol{t}_0^-) \cdot \widetilde{\boldsymbol{w}}^+ \, dA \,. \tag{58}$$

The latter expression is identical to zero if $\boldsymbol{t}_0^+ = -\boldsymbol{t}_0^-$ holds.

An appropriate requirement for the type of the boundary condition to be used can be rephrased as follows

- Suquet (1987): *"The boundary conditions must reproduce, as closely as possible, the in situ state of the $\mathcal{RVE}$ inside the material".*

It should be noted that linear boundary displacements yield an energetically upper bound, whereas uniform boundary tractions provide a lower bound of the homogenized system. Nevertheless, the choice of the boundary condition influences the mechanical response in many cases:

- Xia et al. (2003): *"... 'homogeneous boundary conditions' are not only over-constrained but they may also violate the boundary traction periodicity conditions.".*

For periodic media, a natural course of action are periodic boundary conditions. They can be realized in a *strong format*, i.e., one part of the discretized boundary of the $\mathcal{RVE}$ (the *image boundary*, e.g. $\partial\mathcal{B}_0^-$) must be completely mirrored to the nodes on the associated part of the boundary (the *mirror boundary* $\partial\mathcal{B}_0^+$). Alternatively, a *weak format* of the periodic boundary conditions is proposed in Larsson et al. (2011). In this context, we also refer to Miehe and Bayreuther (2007).

In order to discuss the influence of the different boundary conditions on the mechanical response, we consider a periodic microstructure with stiff inclusions embedded in a weak matrix, as shown in Fig. 4a.

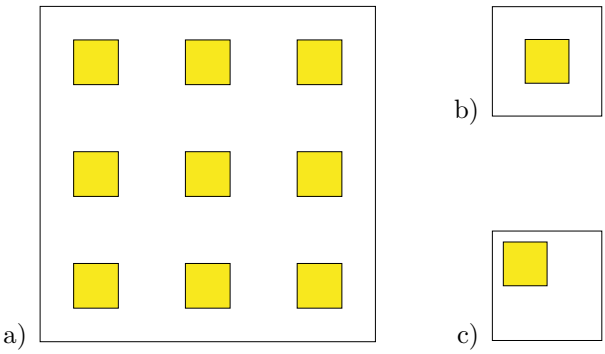

Figure 4. Periodic microstructure: a) Continuous matrix with periodically distributed inclusions. $\mathcal{RVE}s$ with b) a centric and c) an eccentric inclusion, see Schröder (2000).

For the analysis we choose unit cells which are discretized with 20×20 equal-sized quadrilateral elements, the inclusion is discretized with 8×8 elements. We choose a unit cell with a centric inclusion, as depicted in Fig. 4b and one unit cell with an eccentric inclusion, cf. Fig. 4c. The simulation is carried out for small strains under plain strain conditions and we apply an isotropic constitutive law for both, the weak matrix and the stiffer inclusion material. As mentioned above, for the considered periodic media the natural choice are periodic boundary conditions. That means, that for both unit cells, cf. Fig. 4b,c, the periodic boundary conditions must yield identical results. For the macroscopic loading

$$\overline{\boldsymbol{F}} = \text{diag}[\, 1.0005 \,;\; 1.0 \,;\; 1.0 \,]\,, \tag{59}$$

we obtain the stress distribution as depicted in Fig. 5. In both cases, the macroscopic Cauchy stress tensor has only non-vanishing and identical diagonal components, as expected; the values of the components of the stress tensor (in consistent units) are

$$\overline{\boldsymbol{\sigma}}^{per} = \text{diag}[\, 837.4 \,;\; 490.7 \,;\; 530.7 \,]\,. \tag{60}$$

These stress values will be applied to the unit cells when we analyze the Neumann boundary conditions. The stress response for the Dirichlet boundary conditions is depicted in Fig. 6. For the unit cell with centered inclusion, the macroscopic stress tensor is also diagonal and the values differ

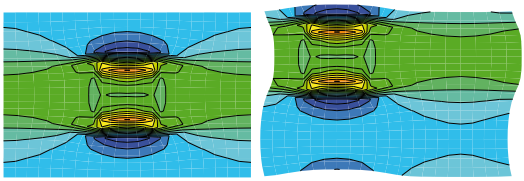

Figure 5. Stress σ_{11} in the unit cells with centric (left) and eccentric (right) inclusion under periodic boundary conditions, see Schröder (2000).

approximately by 1% compared to (60) and the local stress distribution is comparable to the ones in Fig. 5. Considering the unit cell with the eccentric inclusion, we observe a symmetry-break in the stress distribution. Nevertheless, the stress components deviate from the components in (60) by approx. 3%, in addition the off-diagonal element of $\overline{\boldsymbol{\sigma}}$ is not vanishing.

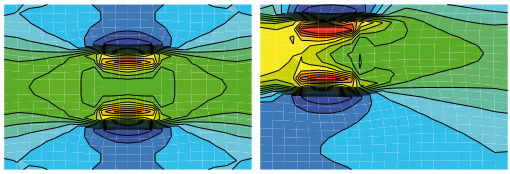

Figure 6. Stress σ_{11} in the unit cells with centric (left) and eccentric (right) inclusion under Dirichlet boundary conditions, see Schröder (2000).

Applying the stress values of (60) as loading conditions for the Neumann boundary conditions, we get the results shown in Fig. 7. The macroscopic deformation gradient should be close to (59). The deviation for both unit cells is approximately up to 8% and again we observe a symmetry-break in the local stress distribution for the unit cell with the eccentric inclusion.
Sum up: As expected, periodic boundary conditions yield the best results.

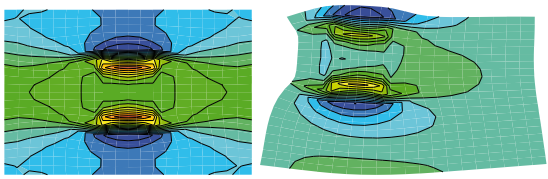

Figure 7. Stress σ_{11} in the unit cells with centric (left) and eccentric (right) inclusion under Neumann boundary conditions, see Schröder (2000).

2.6 Remarks on the Choice of the $\mathcal{RVE}$

The choice of the representative volume element ($\mathcal{RVE}$) for the application to a two-scale homogenization scheme is an ongoing research topic. In general, the $\mathcal{RVE}$ should be a partial volume of the material, which is statistically homogeneous from the macroscopic point of view. Furthermore, the choice of a $\mathcal{RVE}$ is not unique, see Fig. 8.

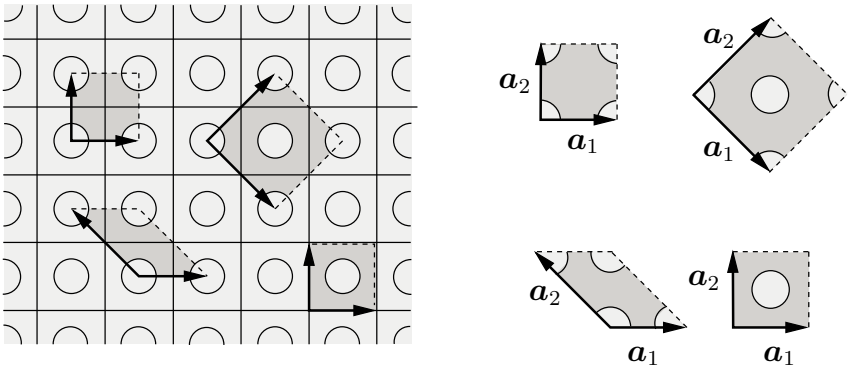

Figure 8. Non-uniqueness of the $\mathcal{RVE}$s of a periodically arranged microstructure. The dashed boxed regions represent four possible $\mathcal{RVE}$s, see Schröder (2000).

In Zeman (2003), several properties for the definition of a $\mathcal{RVE}$, taken from the literature, are summarized:

- Hill (1963): *"This phrase (the $\mathcal{RVE}$) will be used when referring to a sample that (a) is structurally entirely typical of the whole structure on average, and (b) contains sufficient number of inclusions for the apparent overall moduli to be effectively independent of the surface value of traction and displacement, so long as these values are "macroscopically uniform""*

- Hashin (1983): *"The RVE is a model of the material to be used to determine the corresponding effective properties of the homogenized macroscopic model. The RVE should be large enough to contain sufficient information about the microstructure in order to be representative, however it should be much smaller than the macroscopic body."*

- Drugan and Willis (1996): *"The RVE is the smallest material volume element of the composite for which the usual spatially constant "over-*

all modulus" macroscopic constitutive representation is a sufficiently accurate model to represent the mean constitutive response."

- Ostoja-Starzewski (2001): *"The RVE is very clearly defined in two situations only: (i) it is a unit cell of a periodic microstructure, and (ii) volume containing a very large set of micro-scale elements, possessing statistically homogeneous and ergodic properties."*

- Stroeven et al. (2002): *"The determination of the RVE size is by no means straightforward. It depends on the material under consideration, but also on the structure sensitivity of the physical quantity that is measured. Normally, elastic moduli are taken as the governing parameter, however, other quantities can also be taken, such as energy dissipation in case of microstructural cracking."*

A note on periodic unit cells: In periodic media, typically unit cells, which are translationally symmetric, are used as $\mathcal{RVE}$s. In order to design (sub-) unit cells with a lower number of degrees of freedom, Ohno et al. (2001) exploited the point symmetrical distribution of the mechanical field quantities with respect to the center of the considered unit cell. Substantial savings in computer time can also be realized when the unit cell possesses further special symmetries, see Flores and de Souza Neto (2010).

A note on random microstructures: Capturing the random nature of microstructures is a challenge in homogenization (effective macroscopic description). The lack of microstructural periodicity implies that we have to analyze statistical volume elements ($\mathcal{SVE}s$) instead of $\mathcal{RVE}s$. Mathematical tools for the characterization of random microstructures are discussed in Ohser and Mücklich (2000). A brief introduction of basic morphological measurements for a quantitative characterization of the geometry of random microstructures is given in Jeulin and Ostoja-Starzewski (2001). From the viewpoint of stochastical mechanics, we could consider ensemble averages over several realizations of the microstructure. From the practical point of view, we are interested in only one realization of the microstructure in order to achieve a sufficient estimate of the macroscopic mechanical response. Furthermore, the interchangeability of the ensemble averaging and volume averaging (in general for sufficiently large microstructures) is a key assumption in this field, which is based on the concepts of statistical homogeneity and ergodicity, see Jeulin and Ostoja-Starzewski (2001) and Ostoja-Starzweski (2008).

3 Algorithmic Treatment

This chapter concerns the theoretical and numerical treatment of a discrete two-scale homogenization scheme, also known as the FE^2-method or direct micro-macro transition approach. A major role plays the coupled numerical solution of the boundary value problems on both scales. Especially the consistent linearization of the effective macroscopic response function can be seen as a crucial part in this numerical scheme. In the following, the (matrix) approximations of the field quantities are denoted by a superscript h, e.g., the discrete counterpart of $\boldsymbol{x}$ is denoted as $\boldsymbol{x}^h$.

3.1 Boundary Value Problems on the Macro- and Micro-Scale

The *balance of linear momentum at the macro-scale* (11) can be written in its weak form as

$$\overline{G} = -\int_{\overline{\mathcal{B}}_0} \delta\overline{\boldsymbol{x}} \cdot \left(\mathrm{Div}_{\overline{X}}\overline{\boldsymbol{P}} + \overline{\boldsymbol{f}}\right) \, dV \tag{61}$$

with $\overline{G} = 0$ at the equilibrium state. Application of the relation

$$\delta\overline{\boldsymbol{x}} \cdot \mathrm{Div}_{\overline{X}}\,\overline{\boldsymbol{P}} = \mathrm{Div}_{\overline{X}}[\delta\overline{\boldsymbol{x}}\,\overline{\boldsymbol{P}}] - \mathrm{Grad}_{\overline{X}}\delta\overline{\boldsymbol{x}} : \overline{\boldsymbol{P}} \tag{62}$$

and the Gauss integral theorem yields the modified expression

$$\overline{G} = \underbrace{\int_{\overline{\mathcal{B}}_0} \delta\overline{\boldsymbol{F}} : \overline{\boldsymbol{P}} \, dV}_{=:\,\overline{G}^{int}} - \underbrace{\left\{ \int_{\overline{\mathcal{B}}_0} \delta\overline{\boldsymbol{x}} \cdot \overline{\boldsymbol{f}} \, dV + \int_{\partial\overline{\mathcal{B}}_0} \delta\overline{\boldsymbol{x}} \cdot \overline{\boldsymbol{t}}_0 \, dA \right\}}_{=:\,\overline{G}^{ext}} \tag{63}$$

with $\overline{\boldsymbol{t}}_0 = \overline{\boldsymbol{P}}\,\overline{\boldsymbol{N}}$. For the discretization of the *macroscopic boundary value problem*, we apply the following discretizations for the actual, virtual and incremental deformation within a typical finite element

$$\overline{\boldsymbol{x}}^h = \overline{\boldsymbol{X}}^h + \mathbb{N}^e\overline{\boldsymbol{d}}\,, \quad \delta\overline{\boldsymbol{x}}^h = \mathbb{N}^e\delta\overline{\boldsymbol{d}}\,, \qquad \Delta\overline{\boldsymbol{x}}^h = \mathbb{N}^e\Delta\overline{\boldsymbol{d}}\,, \tag{64}$$

respectively. Here the matrix $\mathbb{N}^e$ contains the classical ansatz-functions and the vectors $\{\overline{\boldsymbol{d}}\,, \delta\overline{\boldsymbol{d}}\,, \Delta\overline{\boldsymbol{d}}\}$ represent the actual, virtual and incremental nodal displacements. With the $\mathbb{B}^e$-matrices containing the partial derivatives of the ansatz functions with respect to reference coordinates, we define the approximations of the actual, virtual and incremental deformation tensors

$$\overline{\boldsymbol{F}}^h = \mathbf{1}^h + \mathbb{B}^e\overline{\boldsymbol{d}}\,, \qquad \delta\overline{\boldsymbol{F}}^h = \mathbb{B}^e\delta\overline{\boldsymbol{d}}\,, \qquad \Delta\overline{\boldsymbol{F}}^h = \mathbb{B}^e\Delta\overline{\boldsymbol{d}}\,. \tag{65}$$

Inserting the approximations for the virtual fields (64) and (65) in Eq. (63) yields the approximation of $\overline{G}(\overline{\boldsymbol{x}}, \delta\overline{\boldsymbol{x}})$ by $\overline{G}^h(\overline{\boldsymbol{x}}^h, \delta\overline{\boldsymbol{x}}^h)$, i.e.

$$\overline{G}^h = \sum_e \overline{G}^e(\overline{\boldsymbol{x}}^h, \delta\overline{\boldsymbol{x}}^h) = \sum_e \overline{G}^{e,int}(\overline{\boldsymbol{x}}^h, \delta\overline{\boldsymbol{x}}^h) - \sum_e \overline{G}^{e,ext}(\overline{\boldsymbol{x}}^h, \delta\overline{\boldsymbol{x}}^h) \,. \quad (66)$$

If the weak form (63) is associated with a typical finite element, we get the expressions for the internal and external parts

$$\overline{G}^{e,int}(\overline{\boldsymbol{x}}^h, \delta\overline{\boldsymbol{x}}^h) = \delta\overline{\boldsymbol{d}}^T \underbrace{\int_{\overline{\mathcal{B}}_0^e} \mathbb{B}^{eT} \overline{\boldsymbol{P}}^h \, dV}_{=:\,\overline{\boldsymbol{r}}^{e,int}} \,, \quad (67)$$

and

$$\overline{G}^{e,ext}(\overline{\boldsymbol{x}}^h, \delta\overline{\boldsymbol{x}}^h) = \delta\overline{\boldsymbol{d}}^T \underbrace{\left\{ \int_{\overline{\mathcal{B}}_0^e} \mathbb{N}^e \overline{\boldsymbol{f}}^h \, dV + \int_{\partial\overline{\mathcal{B}}_0^e} \mathbb{N}^e \overline{\boldsymbol{t}}_0^h \, dA \right\}}_{=:\,\overline{\boldsymbol{r}}^{e,ext}} \,. \quad (68)$$

With this, the element residual vector $\overline{\boldsymbol{r}}^e$ is computed by $\overline{\boldsymbol{r}}^e = \overline{\boldsymbol{r}}^{e,int} - \overline{\boldsymbol{r}}^{e,ext}$. To solve the nonlinear weak form $\overline{G}^h(\overline{\boldsymbol{x}}^h, \delta\overline{\boldsymbol{x}}^h)$ we apply the Newton-Raphson iteration scheme. Therefore, the linerization of $\overline{G}^h(\overline{\boldsymbol{x}}^h, \delta\overline{\boldsymbol{x}}^h)$ at $\overline{\boldsymbol{x}}^h = \overline{\boldsymbol{x}}^{h*}$ has to be computed:

$$\mathrm{Lin}\, \overline{G}^h(\overline{\boldsymbol{x}}^{h*}, \delta\overline{\boldsymbol{x}}^h, \Delta\overline{\boldsymbol{x}}^h) = \overline{G}^h(\overline{\boldsymbol{x}}^{h*}, \delta\overline{\boldsymbol{x}}^h) + \Delta\overline{G}^h(\overline{\boldsymbol{x}}^{h*}, \delta\overline{\boldsymbol{x}}^h, \Delta\overline{\boldsymbol{x}}^h) \,. \quad (69)$$

The linear increment is defined as the directional derivative of $\overline{G}^h$ at $\overline{\boldsymbol{x}}^h$ in the direction of the incremental deformation $\Delta\overline{\boldsymbol{x}}^h$, i.e.,

$$\Delta\overline{G}^h(\overline{\boldsymbol{x}}^{h*}, \delta\overline{\boldsymbol{x}}^h, \Delta\overline{\boldsymbol{x}}^h) = \frac{d}{d\epsilon} \left[\overline{G}^h(\overline{\boldsymbol{x}}^{h*} + \epsilon\Delta\overline{\boldsymbol{x}}^h, \delta\overline{\boldsymbol{x}}^h) \right] \Big|_{\epsilon=0} \,. \quad (70)$$

For dead-loaded systems the linear increment of the discrete form of $\overline{G}$ is formally given by

$$\Delta\overline{G}^h = \sum_e \Delta\overline{G}^{e,int} \quad (71)$$

and the linear increment for a typical element is calculated by

$$\Delta\overline{G}^{e,int} = \int_{\overline{\mathcal{B}}_0^e} \delta\overline{\boldsymbol{F}}^{hT} \overline{\mathbb{A}}^h \Delta\overline{\boldsymbol{F}}^h \, dV = \delta\overline{\boldsymbol{d}}^T \underbrace{\int_{\overline{\mathcal{B}}_0^e} \mathbb{B}^{eT} \overline{\mathbb{A}}^h \mathbb{B}^e \, dV}_{=:\,\overline{\boldsymbol{k}}^e} \Delta\overline{\boldsymbol{d}} \,. \quad (72)$$

For the computation of the stiffness matrix $\overline{\boldsymbol{k}}^e$ for a macroscopic element, we need the macroscopic (overall) algorithmic consistent moduli $\overline{\mathbb{A}}$, which is formally defined by the partial derivative

$$\overline{\mathbb{A}} = \frac{\partial \overline{\boldsymbol{P}}}{\partial \overline{\boldsymbol{F}}} \quad \text{with} \quad \overline{\boldsymbol{P}} = \frac{1}{V} \int_{\mathcal{B}_0} \boldsymbol{P}(\boldsymbol{F})\, dV \ . \tag{73}$$

This fourth-order tensor cannot be computed directly, becauce we have no explicit expression of the macroscopic first Piola-Kirchhoff stress tensor $\overline{\boldsymbol{P}}$ as a function of its work-conjugated variable, the macroscopic deformation gradient $\overline{\boldsymbol{F}}$. An efficient algorithmic treatment of handling this is presented in the next chapter; therefore, we assume the algorithmic consistent moduli $\overline{\mathbb{A}}$ as known at this point. Thus, the linearization yields

$$\sum_{e=1}^{\overline{num}_{ele}} \left\{ \delta \overline{\boldsymbol{d}}^T \left(\overline{\boldsymbol{k}}^e \Delta \overline{\boldsymbol{d}} + \overline{\boldsymbol{r}}^e \right) \right\} = 0 \ , \tag{74}$$

where $\overline{num}_{ele}$ denotes the number of macroscopic finite elements. The application of the assembling procedure yields the system of equations

$$\overline{\boldsymbol{K}} \Delta \overline{\boldsymbol{D}} = -\overline{\boldsymbol{R}} \quad \text{with} \quad \overline{\boldsymbol{K}} = \mathop{\mathsf{A}}_{e=1}^{\overline{num}_{ele}} \overline{\boldsymbol{k}}^e \quad \text{and} \quad \overline{\boldsymbol{R}} = \mathop{\mathsf{A}}_{e=1}^{\overline{num}_{ele}} \overline{\boldsymbol{r}}^e \, , \tag{75}$$

where A denote the standard assembling operators. The solution of the latter system of equations yields an increment of the actual deformation field. This procedure has to be repeated until an equilibrium state of the macroscopic boundary value problem has been reached, i.e. $\overline{G}^h(\overline{\boldsymbol{x}}, \delta \overline{\boldsymbol{x}}) \approx 0$.

The weak form of the *balance of linear momentum at the microscale*, based on the expression $(19)_1$, is given by

$$G = -\int_{\mathcal{B}_0} \delta \boldsymbol{x} \cdot \mathrm{Div}_X \boldsymbol{P}\, dV \tag{76}$$

with $G = 0$. Here, we are neglecting the volume acceleration and inertia terms. Taking into account the additive split of the deformation into a linear map $\overline{\boldsymbol{F}}\boldsymbol{X}$ and a fluctuation part $\widetilde{\boldsymbol{w}}$, we obtain the following representation of the microscopic deformation tensor $\boldsymbol{F} = \mathrm{Grad}_X \boldsymbol{x}$:

$$\boldsymbol{F} = \overline{\boldsymbol{F}} + \widetilde{\boldsymbol{F}} \quad \text{with} \quad \widetilde{\boldsymbol{F}} = \mathrm{Grad}_X \widetilde{\boldsymbol{w}} \ . \tag{77}$$

With this in hand, we get the modified expression

$$G = \int_{\mathcal{B}_0} \delta \widetilde{\boldsymbol{F}} : \boldsymbol{P}\, dV \ . \tag{78}$$

Note that the part $\overline{\boldsymbol{F}}$ of the microscopic deformation gradient $\boldsymbol{F}$ is given and constant over the $\mathcal{RVE}$.

For the discretization of the *microscopic boundary value problem*, we apply the following discretizations for the actual, virtual and incremental fluctuation within a typical finite element

$$\widetilde{\boldsymbol{w}}^h = \mathbb{N}^e \widetilde{\boldsymbol{d}}, \qquad \delta\widetilde{\boldsymbol{w}}^h = \mathbb{N}^e \delta\widetilde{\boldsymbol{d}}, \qquad \Delta\widetilde{\boldsymbol{w}}^h = \mathbb{N}^e \Delta\widetilde{\boldsymbol{d}}, \tag{79}$$

respectively. Here, the matrix $\mathbb{N}^e$ contains the classical ansatz-functions and the vectors $\{\widetilde{\boldsymbol{d}}, \delta\widetilde{\boldsymbol{d}}, \Delta\widetilde{\boldsymbol{d}}\}$ represent the actual, virtual and incremental nodal fluctuations. With the $\mathbb{B}^e$-matrices containing the partial derivatives of the ansatz functions with respect to reference coordinates, we define the approximations of the actual, virtual and incremental deformation tensors

$$\widetilde{\boldsymbol{F}}^h = \mathbb{B}^e \widetilde{\boldsymbol{d}}, \qquad \delta\widetilde{\boldsymbol{F}}^h = \mathbb{B}^e \delta\widetilde{\boldsymbol{d}}, \qquad \Delta\widetilde{\boldsymbol{F}}^h = \mathbb{B}^e \Delta\widetilde{\boldsymbol{d}}\,. \tag{80}$$

Inserting the approximations for the virtual fields (79) and (80) in (78) leads to the discrete counterpart G^h of G:

$$G^h(\boldsymbol{x}^h, \delta\boldsymbol{x}^h) = \sum_e G^e(\boldsymbol{x}^h, \delta\boldsymbol{x}^h) \tag{81}$$

with

$$G^e(\boldsymbol{x}^h, \delta\boldsymbol{x}^h) = \delta\boldsymbol{d}^T \underbrace{\int_{\mathcal{B}_0^e} \mathbb{B}^{eT} \boldsymbol{P}^h \, dV}_{=:\,\boldsymbol{r}^e}\,. \tag{82}$$

To solve the nonlinear discrete weak form $G^h(\boldsymbol{x}^h, \delta\boldsymbol{x}^h)$, we apply the Newton-Raphson iteration scheme and apply the linerization analogously to the procedure at the macro-scale described above. Finally, we obtain the linear increment for a typical microscopic finite element

$$\Delta G^e = \int_{\mathcal{B}_0^e} \delta\widetilde{\boldsymbol{F}}^{h\,T} \mathbb{A}^h \Delta\widetilde{\boldsymbol{F}}^h \, dV = \delta\widetilde{\boldsymbol{d}}^T \underbrace{\int_{\mathcal{B}_0^e} \mathbb{B}^{eT} \mathbb{A}^h \mathbb{B}^e \, dV}_{=:\,\boldsymbol{k}^e} \Delta\widetilde{\boldsymbol{d}}\,. \tag{83}$$

The application of the standard assembling operator, cf. Eq. (75), to the microscopic stiffness matrices and the residual vectors result in the system of equations

$$\boldsymbol{K}\Delta\widetilde{\boldsymbol{D}} + \boldsymbol{R} = 0\,. \tag{84}$$

From this system of equations, we obtain an update of the discrete fluctuation field and evaluate the discrete weak form (82). If the euclidian norm of $\boldsymbol{R}$ is higher than a given tolerance, we apply further Newton iteration steps until convergence is achieved.

3.2 Computation of Algorithmic Consistent Overall Moduli

In the previous section, we assumed that the macroscopic overall moduli $\overline{\mathbb{A}}$ was given during the solution process at the macro-scale. However, in contrast to the macroscopic stress tensor $\overline{\boldsymbol{P}}$, which can be calculated directly as the volume average of the microscopic counterparts, the macroscopic moduli cannot be consistently computed solely by volumetric averaging. Starting from the incremental constitutive relation at the macro-scale

$$\Delta\overline{\boldsymbol{P}} = \left\{ \frac{1}{V} \frac{\partial}{\partial \overline{\boldsymbol{F}}} \int_{\mathcal{B}} \boldsymbol{P}(\boldsymbol{F})\, dV \right\} : \Delta\overline{\boldsymbol{F}} =: \overline{\mathbb{A}} : \Delta\overline{\boldsymbol{F}} \,, \tag{85}$$

we define the overall (effective) nominal moduli as follows

$$\overline{\mathbb{A}} = \frac{1}{V} \int_{\mathcal{B}} \frac{\partial}{\partial \overline{\boldsymbol{F}}} \boldsymbol{P}(\boldsymbol{F})\, dV = \frac{1}{V} \int_{\mathcal{B}} \frac{\partial \boldsymbol{P}(\boldsymbol{F})}{\partial \boldsymbol{F}} : \frac{\partial \boldsymbol{F}}{\partial \overline{\boldsymbol{F}}}\, dV \,. \tag{86}$$

Let us now exploit the additive decomposition of $\boldsymbol{F}$ into a constant and a fluctuating part. Substituting

$$\boldsymbol{F} = \overline{\boldsymbol{F}} + \widetilde{\boldsymbol{F}} \,, \tag{87}$$

in Equation (86) yields

$$\overline{\mathbb{A}} = \frac{1}{V} \int_{\mathcal{B}} \frac{\partial \boldsymbol{P}(\boldsymbol{F})}{\partial \boldsymbol{F}} : \frac{\partial (\overline{\boldsymbol{F}} + \widetilde{\boldsymbol{F}})}{\partial \overline{\boldsymbol{F}}}\, dV \,. \tag{88}$$

Thus, we obtain with the abbreviation $\mathbb{A} := \partial_F \boldsymbol{P}(\boldsymbol{F})$

$$\overline{\mathbb{A}} = \frac{1}{V} \int_{\mathcal{B}} \mathbb{A}\, dV + \frac{1}{V} \int_{\mathcal{B}} \mathbb{A} : \frac{\partial \widetilde{\boldsymbol{F}}}{\partial \overline{\boldsymbol{F}}}\, dV \,. \tag{89}$$

In the latter equation, the computation of the sensitivity of $\widetilde{\boldsymbol{F}}$ with respect to $\overline{\boldsymbol{F}}$ is the crucial part. Starting from the weak form of the balance of linear momentum at the micro-scale (78) at an equilibrium state, i.e., $G = 0$, then the linearization yields

$$\int_{\mathcal{B}} \delta\widetilde{\boldsymbol{F}} : \mathbb{A} : \Delta\boldsymbol{F}\, dV = 0 \,. \tag{90}$$

Substituting the additive split (87) in (90) yields

$$\underbrace{\int_{\mathcal{B}_0} \delta\widetilde{\boldsymbol{F}} : \mathbb{A} : \Delta\overline{\boldsymbol{F}}\, dV}_{\int_{\mathcal{B}_0} \delta\widetilde{\boldsymbol{F}} : \mathbb{A}\, dV \; : \Delta\overline{\boldsymbol{F}}} + \int_{\mathcal{B}_0} \delta\widetilde{\boldsymbol{F}} : \mathbb{A} : \Delta\widetilde{\boldsymbol{F}}\, dV = 0 \,. \tag{91}$$

The discrete counterpart of the latter equation appears after inserting the approximations of the fluctuation part of the deformation gradient (80) as

$$\sum_{e=1}^{num_{ele}} \delta\widetilde{\boldsymbol{d}}^T \left\{ \underbrace{\int_{\mathcal{B}_0^e} \mathbb{B}^{eT} \mathbb{A}^h \, dV}_{\boldsymbol{l}^e} \, \Delta\overline{\boldsymbol{F}}^h + \underbrace{\int_{\mathcal{B}_0^e} \mathbb{B}^{eT} \mathbb{A}^h \mathbb{B}^e \, dV}_{\boldsymbol{k}^e} \, \Delta\widetilde{\boldsymbol{d}} \right\} = 0 \,, \tag{92}$$

where num_{ele} denotes the number of microscopic finite elements, $\boldsymbol{k}^e$ the element stiffness matrices, see also (83), and $\boldsymbol{l}^e$ the matrices, which take into account the sensitivity of the moduli of the individual finite elements. Thus, in contracted matrix notation, we obtain

$$\sum_{e=1}^{num_{ele}} \left\{ \delta\widetilde{\boldsymbol{d}}^T \left(\boldsymbol{l}^e \, \Delta\overline{\boldsymbol{F}}^h + \boldsymbol{k}^e \Delta\widetilde{\boldsymbol{d}} \right) \right\} = 0 \,. \tag{93}$$

Application of a standard assembling procedure, cf. Eq. (75), yields

$$\delta\widetilde{\boldsymbol{D}}^T \left(\boldsymbol{K} \Delta\widetilde{\boldsymbol{D}} + \boldsymbol{L} \, \Delta\overline{\boldsymbol{F}} \right) = 0 \,. \tag{94}$$

The global stiffness matrix $\boldsymbol{K}$ and the generalized right hand sides $\boldsymbol{L}$ are defined as

$$\boldsymbol{K} = \mathop{\mathsf{A}}_{e=1}^{num_{ele}} \boldsymbol{k}^e \,, \qquad \boldsymbol{L} = \mathop{\mathsf{A}}_{e=1}^{num_{ele}} \boldsymbol{l}^e \,. \tag{95}$$

Formally, the solution of Eq. (94) is achieved by

$$\Delta\widetilde{\boldsymbol{D}} = -\boldsymbol{K}^{-1} \boldsymbol{L} \, \Delta\overline{\boldsymbol{F}}^h \,, \tag{96}$$

which represents the incremental fluctuation field as a consequence of an incremental macroscopic deformation gradient. Inserting the elementwise solutions $\Delta\widetilde{\boldsymbol{d}}$ of (96) in $(80)_3$ and substituting this result into Eq. (89) yields

$$\overline{\mathbb{A}}^h = \underbrace{\frac{1}{V} \sum_{e=1}^{num_{ele}} \int_{\mathcal{B}^e} \mathbb{A}^h \, dV}_{\mathbb{A}^{\text{Voigt}}} + \frac{1}{V} \sum_{e=1}^{num_{ele}} \int_{\mathcal{B}^e} \mathbb{A}^h \, \frac{\partial(\mathbb{B}^e \Delta\widetilde{\boldsymbol{d}})}{\partial\overline{\boldsymbol{F}}^h} \, dV \,, \tag{97}$$

where $\mathbb{A}^{\text{Voigt}}$ denotes the (numerical approximation of the) Voigt upper bound. The second integral term in (97) can be reformulated as

$$\frac{1}{V} \sum_{e=1}^{num_{ele}} \int_{\mathcal{B}^e} \mathbb{A}^h \, \frac{\partial(\mathbb{B}^e \Delta\widetilde{\boldsymbol{d}})}{\partial\overline{\boldsymbol{F}}^h} \, dV = \frac{1}{V} \sum_{e=1}^{num_{ele}} \underbrace{\int_{\mathcal{B}^e} \mathbb{A}^h \mathbb{B}^e \, dV}_{\boldsymbol{l}^{e\star}} \, \frac{\partial\Delta\widetilde{\boldsymbol{d}}}{\partial\overline{\boldsymbol{F}}^h} \,, \tag{98}$$

where $\boldsymbol{l}^{e\star} = \boldsymbol{l}^{eT}$ if $\mathbb{A}$ fullfills the major symmetries, i.e., $\mathbb{A}_{ijkl} = \mathbb{A}_{klij}$. This symmetry relation is provided in the following. After assembling the discrete form, we get with (96) and the linear increment

$$\Delta\overline{\boldsymbol{F}}^h = \overline{\boldsymbol{F}}^h - \overline{\boldsymbol{F}}^h_n \,, \tag{99}$$

based on the nomenclature

$$\overline{\boldsymbol{F}}^h = \overline{\boldsymbol{F}}^h(t_{n+1}) \quad \text{and} \quad \overline{\boldsymbol{F}}^h_n = \overline{\boldsymbol{F}}^h(t_n) \,, \tag{100}$$

the algebraic expression

$$\frac{1}{V}\boldsymbol{L}^T \frac{\partial \Delta\widetilde{\boldsymbol{D}}}{\partial \overline{\boldsymbol{F}}^h} = -\frac{1}{V}\boldsymbol{L}^T\, \boldsymbol{K}^{-1}\boldsymbol{L}\, \frac{\partial \Delta\overline{\boldsymbol{F}}}{\partial \overline{\boldsymbol{F}}^h} = -\frac{1}{V}\boldsymbol{L}^T\, \boldsymbol{K}^{-1}\boldsymbol{L} \,. \tag{101}$$

Thus, the final result for the algorithmic consistent overall moduli is

$$\boxed{\overline{\mathbb{A}} = \mathbb{A}^{\text{Voigt}} - \frac{1}{V}\boldsymbol{L}^T\boldsymbol{K}^{-1}\boldsymbol{L} \quad \text{with} \quad \mathbb{A}^{\text{Voigt}} = \frac{1}{V}\sum_e \int_{\mathcal{B}^e} \mathbb{A}^h \, dV} \,, \tag{102}$$

see Miehe et al. (1999a,b).

In general, huge computational costs in typical direct nonlinear homogenization schemes are governed by using the Newton-Raphson iteration on both scales at each quadrature point. For the efficient computation of the second term in $(102)_1$, we identify

$$\boldsymbol{L}^T\boldsymbol{K}^{-1}\boldsymbol{L} = \boldsymbol{L}^T\mathbb{X}. \tag{103}$$

Here, $\mathbb{X}$ is the solution of a system of equations with several, e.g. nine in 3D, right hand sides which are organized in the matrix $\boldsymbol{L}$:

$$\boldsymbol{K}\mathbb{X} = \boldsymbol{L} \,. \tag{104}$$

For the solution of (103) as well as for the solutions of the weak forms, the sparse structure of all matrices is taken into account.
A study of efficient two-scale homogenization algorithms for nonlinear problems using approximations of the Schur-Complement of the microscopic stiffness matrix based on e.g. LU factorizations is presented in Okada et al. (2010). Several works in the literature are concerned with the derivation of the overall tangent moduli as well as with different approaches (associated to Schur complement computation, perturbation techniques, penalty formulations, Lagrange multiplier methods) useful for efficient computations, in this context we refer to Miehe et al. (1999a), Schröder (2000), Kouznetsova et al. (2001), Miehe and Koch (2002), Miehe (2003), Miehe and Bayreuther (2007), Temizer and Wriggers (2008) and Schröder and Keip (2012).

4 Stability Problems at Different Scales

A challenge in two-scale homogenization techniques is the consideration of instability problems on the different scales, cf. Abeyaratne and Triantafyllidis (1984), Triantafyllidis and Maker (1985), Müller (1987), Geymonat et al. (1993), Miehe et al. (2002), Schröder (2010). In the following, we restrict ourselves to hyperelastic materials and distinguish between structural instabilities and material instabilities. Let

$$\overline{\Pi}(\overline{\boldsymbol{x}}) = \overline{\Pi}^{int}(\overline{\boldsymbol{F}}) + \overline{\Pi}^{ext}(\overline{\boldsymbol{x}}) \tag{105}$$

be the total potential energy of the body of interest on the macro-scale, with

$$\overline{\Pi}^{int}(\overline{\boldsymbol{F}}) = \int_{\overline{\mathcal{B}}_0} \overline{\psi}(\overline{\boldsymbol{F}})\, dV \tag{106}$$

and

$$\overline{\Pi}^{ext}(\overline{\boldsymbol{x}}) = -\int_{\overline{\mathcal{B}}_0} \overline{\boldsymbol{x}} \cdot \overline{\boldsymbol{f}}\, dV - \int_{\partial\overline{\mathcal{B}}_{0,t}} \overline{\boldsymbol{x}} \cdot \overline{\boldsymbol{t}}_0\, dA\ . \tag{107}$$

An equilibrium state, denoted by $\overline{\boldsymbol{x}}^{eq}$, is characterized by an infimum of the total potential energy in the space of admissible functions. The deformation state $\overline{\boldsymbol{x}}^{eq}$ is stable if the inequality

$$\overline{\Pi}(\overline{\boldsymbol{x}}^{ka}) \geq \overline{\Pi}(\overline{\boldsymbol{x}}^{eq}) \quad \forall \text{ kinematically admissible } \overline{\boldsymbol{x}}^{ka} \tag{108}$$

holds and the equality sign only holds for some $\overline{\boldsymbol{x}}^{ka} \neq \overline{\boldsymbol{x}}^{eq}$, see Ogden (1984). The inequality (108) is a sufficient (global) condition for the stability of the equilibrium state $\overline{\boldsymbol{x}}^{eq}$.

For a more suitable criterion, especially from the computational point of view, we restrict our analysis to kinematically admissible functions in the vicinity of $\overline{\boldsymbol{x}}^{eq}$. This means that Eq. (108) becomes an infinitesimal stability criterion, see Truesdell and Noll (1965), chapter 68. The deviation of the total potential energy between an equilibrium state $\overline{\boldsymbol{x}}^{eq}$ and $\overline{\boldsymbol{x}}^{ka}$ is

$$\Delta\overline{\Pi} := \overline{\Pi}(\boldsymbol{x}^{ka}) - \overline{\Pi}(\overline{\boldsymbol{x}}^{eq})\ . \tag{109}$$

For the following remarks, let us recapitulate the first directional derivative of $\overline{\Pi}$ in the direction of $\delta\overline{\boldsymbol{x}}$

$$\frac{d}{d\epsilon}\overline{\Pi}(\overline{\boldsymbol{x}}^{eq} + \epsilon\, \delta\overline{\boldsymbol{x}})\bigg|_{\epsilon=0} =: \overline{G}(\overline{\boldsymbol{x}}^{eq}, \delta\overline{\boldsymbol{x}}^{eq})\ . \tag{110}$$

The second directional derivative of $\overline{\Pi}$, or equivalently the directional derivative of $\overline{G}$, is

$$\frac{d}{d\epsilon}\overline{G}(\overline{\boldsymbol{x}}^{eq}, \delta\overline{\boldsymbol{x}}, \epsilon\, \Delta\overline{\boldsymbol{x}})\bigg|_{\epsilon=0} := \Delta\overline{G}(\overline{\boldsymbol{x}}^{eq}, \delta\overline{\boldsymbol{x}}, \Delta\overline{\boldsymbol{x}})\ . \tag{111}$$

Let us now write $\Delta\overline{\Pi}$, see (109), in terms of a classical Taylor expansion, then we obtain

$$\Delta\overline{\Pi} = \overline{G}(\overline{\boldsymbol{x}}^{eq}, \delta\overline{\boldsymbol{x}}) + \frac{1}{2!}\Delta G(\overline{\boldsymbol{x}}^{eq}, \delta\overline{\boldsymbol{x}}, \Delta\overline{\boldsymbol{x}}) + \frac{1}{3!}\dots \,. \tag{112}$$

In an equilibrium state, $\overline{G}$ is per definition identical to zero, thus, the equilibrium state is stable if

$$\Delta\overline{G}(\overline{\boldsymbol{x}}^{eq}, \delta\overline{\boldsymbol{x}}^{eq}, \Delta\overline{\boldsymbol{x}}) = \int_{\overline{\mathcal{B}}_0} \delta\overline{\boldsymbol{F}} : \overline{\mathbb{A}} : \Delta\overline{\boldsymbol{F}} > 0 \tag{113}$$

holds. More general overviews in this field can be found e.g. in Pflüger (1975) and Thompson and Hunt (1984).

Generalized Convexity Conditions play a major role for the proofs of the existence of minimizing deformations $\boldsymbol{x}$ of the elastic free energy $\psi(\boldsymbol{F})$ of boundary value problems subjected to specific boundary value conditions. A sufficient condition for the existence of minimizers is the sequential-weak lower semicontinuity (s.w.l.s.) and the coercivity of the free energy function. Morrey (1952, 1966) introduced the concept of quasiconvexity, which is formulated as an integral inequality over an arbitrary domain subjected to affine Dirichlet boundary conditions:

[Definition of Quasiconvexity] An elastic stored energy is quasiconvex whenever for all $\mathcal{B} \subset \mathbb{R}^3$, all constant deformation gradients $\overline{\boldsymbol{F}} \in \mathbb{R}^{3\times3}$ and all superposed fluctuation fields $\boldsymbol{w} \in C_0^\infty(\mathcal{B})$ (i.e. with $\boldsymbol{w} = \boldsymbol{0}$ on $\partial\mathcal{B}$) the integral inequality

$$\int_{\mathcal{B}} W(\overline{\boldsymbol{F}} + \mathrm{Grad}\boldsymbol{w})\, dV \geq \int_{\mathcal{B}} W(\overline{\boldsymbol{F}})\, dV = W(\overline{\boldsymbol{F}}) \times \mathrm{Vol}(\mathcal{B}) \tag{114}$$

is valid, Morrey (1952). □

The sequential-lower semicontinuity condition is ensured if the elastic stored energy is quasiconvex and an additional growth condition is fulfilled.

Another very important concept is the polyconvexity introduced by Ball (1977a,b):

[Definition of Polyconvexity] $\boldsymbol{F} \mapsto W(\boldsymbol{F})$ is polyconvex if and only if there exists a function $P : \mathbb{R}^{3\times3} \times \mathbb{R}^{3\times3} \times \mathbb{R} \mapsto \mathbb{R}$ (in general non-unique) such that

$$W(\boldsymbol{F}) = P(\boldsymbol{F}, \mathrm{Cof}\boldsymbol{F}, \det\boldsymbol{F}) \tag{115}$$

and the function $(\boldsymbol{F}, \mathrm{Cof}\boldsymbol{F}, \det\boldsymbol{F}) \in \mathbb{R}^{19} \mapsto P(\boldsymbol{F}, \mathrm{Cof}\boldsymbol{F}, \det\boldsymbol{F}) \in \mathbb{R}$ is convex for all points $\boldsymbol{X} \in \mathbb{R}^3$. □

Polyconvex functions are always s.w.l.s.. Finally, let us recapitulate the notion of Rank-one-convexity and ellipticity:

[Definition of Rank-one convexity] An elastic stored energy is rank-one convex whenever

$$W(\boldsymbol{F} + \lambda \boldsymbol{m} \otimes \boldsymbol{N}_0) \leq \lambda W(\boldsymbol{F} + \boldsymbol{m} \otimes \boldsymbol{N}_0) + (1 - \lambda) W(\boldsymbol{F}) \tag{116}$$

holds for all $\lambda \in [0, 1]$, $\boldsymbol{F} \in \mathbb{R}^{3\times3}$ and all $\boldsymbol{m} \in \mathbb{R}^3, \boldsymbol{N}_0 \in \mathbb{R}^3$ with $\det(\boldsymbol{F} + \lambda \boldsymbol{m} \otimes \boldsymbol{N}_0) > 0$. □

[Definition of Ellipticity] We say that the stored energy $W(\boldsymbol{F}) = \psi(\boldsymbol{C})$ leads to a uniformly elliptical equilibrium system whenever the uniform Legendre-Hadamard condition

$$\exists\, c^+ > 0\,, \forall\, \boldsymbol{F} \in \mathbb{R}^{3\times3}\,, \forall\, \boldsymbol{m}, \boldsymbol{N}_0 \in \mathbb{R}^3 \backslash \{\boldsymbol{0}\} : \\ (\boldsymbol{m} \otimes \boldsymbol{N}_0) : \mathbb{A} : (\boldsymbol{m} \otimes \boldsymbol{N}_0) \geq c^+ \, \|\boldsymbol{m}\|^2 \|\boldsymbol{N}_0\|^2$$

holds. We state that W gives rise to an (strictly) elliptical system if and only if the Legendre-Hadamard condition is valid:

$$\forall\, \boldsymbol{F} \in \mathbb{R}^{3\times3}\,, \forall\, \boldsymbol{m}, \boldsymbol{N}_0 \in \mathbb{R}^3 \backslash \{\boldsymbol{0}\} : \; (\boldsymbol{m} \otimes \boldsymbol{N}_0) : \mathbb{A} : (\boldsymbol{m} \otimes \boldsymbol{N}_0) \geq 0 \; (> 0). \; \square$$

Note that for smooth stored energy functions W strict rank-one convexity implies the strict Legendre-Hadamard condition. A physical interpretation of the aforementioned conditions can be obtained in the context in the field of wave propagation, for more details we refer e.g. to Schröder (2010).

A free energy is materially stable if it is elliptic. A reformulation of the Legendre-Hadamard condition yields

$$(\boldsymbol{m} \otimes \boldsymbol{N}_0) : \mathbb{A} : (\boldsymbol{m} \otimes \boldsymbol{N}_0) = \boldsymbol{m} \cdot \overline{\boldsymbol{Q}}(\boldsymbol{N}_0)\boldsymbol{m} > 0\,, \tag{117}$$

with the accoustic tensor $\overline{\boldsymbol{Q}}$, which is given in index notation by

$$\overline{Q}^{ab} = \mathbb{A}^{aBbD} N_{0B} N_{0D}\,. \tag{118}$$

This means that the accoustic tensor must be positive definite if we want to ensure material stability.

The non-uniqueness of solutions is an inherent feature in finite deformation continuum mechanics. Such problems could occur on both scales, the micro- and the macro-scale. In the following, we focus on microscopic structural instabilities, i.e. on non-stable equilibrium states on the micro-scale, in the context of the micro to macro transition. These phenomena are

associated to convexity properties of the boundary value problems on both scales and their interactions. Following Müller (1987) and Geymonat et al. (1993), we summarize that (i) in case of convex functionals we compute macroscopic energies by

$$\overline{\psi}(\overline{\boldsymbol{F}}) := \inf_{\widetilde{\boldsymbol{w}}} \frac{1}{V_0} \int_{\overline{B}_0} \psi(\overline{\boldsymbol{F}} + \nabla \widetilde{\boldsymbol{w}})\, dV\,, \tag{119}$$

with the fluctuation field $\widetilde{\boldsymbol{w}}$ on *one* unit cell $\mathcal{B}_0$. (ii) Structural instability problems on the micro-scale are associated to the homogenization of a nonconvex boundary value problem on the micro-scale. However, for non-convex functions we have to find in addition the critical size of the representative volume element $\mathcal{B}_0^{crit}$, i.e.

$$\overline{\psi}(\overline{\boldsymbol{F}}) := \inf_{\mathcal{B}_0^{crit}} \left\{ \inf_{\widetilde{\boldsymbol{w}}} \frac{1}{V_0^{crit}} \int_{\mathcal{B}_0^{crit}} \psi(\overline{\boldsymbol{F}} + \nabla \widetilde{\boldsymbol{w}}) dV \right\}\,, \tag{120}$$

with the fluctuation field $\widetilde{\boldsymbol{w}}$ on the representative volume element $\mathcal{B}_0^{crit}$ of critical size. It should be noted that for micro-heterogeneous structures, e.g. for fiber-reinforced matrix materials, the concept of quasiconvexity may not hold. As an illustrative example, we consider the system depicted in Fig. 9 and assume Dirichlet boundary conditions at the outer boundary. Even under affine boundary deformations, as indicated in Fig. 9, we are not able to expect an infimum of the stored energy of the whole system for a constant deformation gradient. On the contrary, we observe a buckling of the fiber for a specific compression state in horizontal direction, which should represent a post-critical stable deformation state.

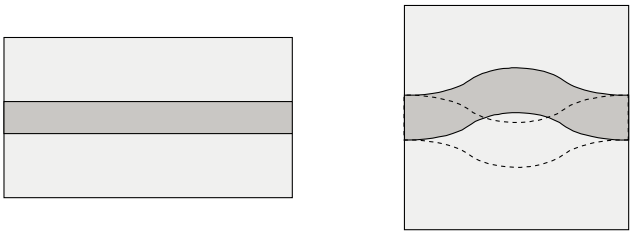

Figure 9. Fiber-reinforced matrix material: Unloaded reference configuration (left) versus buckling of the elastically bedded rod under horizontal compression (right), cf. Marsden and Hughes (1983).

In the following we analyze the influence of the size of the representative volume element (RVE) of a fiber-reinforced microstructure on the macroscopic response at microscopic buckling problems, as discussed in Schröder (2000). A more detailed analysis of instabilities on both scales as well as their interactions are given in Miehe et al. (2002). We consider a homogeneous deformation state at the macro-scale. The considered microstructure consists of a weak matrix (volume faction 80%) with fibers, which are reinforced in horizontal direction, as depicted in Fig. 10a. We expect two classical bifurcation modes, an out-of-phase buckling (Fig. 10b) and an in-phase buckling (Fig. 10c) of the fibers.

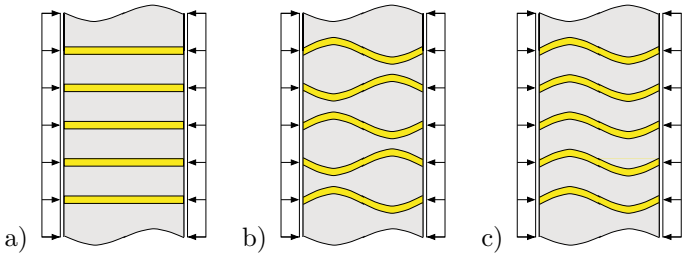

Figure 10. Horizontally loaded fiber reinforced composites: a) reference configuration, b) symmetric (out-of-phase) and c) unsymmetric (in-phase) buckling of the fibers, cf. Schröder (2000).

For simplicity, we apply a standard isotropic St. Venant-Kirchhoff material for the matrix and the fibers and apply periodic boundary conditions. The matrix material has a compression modulus of $\kappa_M = 49.98\, N/mm^2$ and a shear modulus of $\mu_M = 74.97\, N/mm^2$; for the reinforcement we consider the parameters $\kappa_I = 10^4\, \kappa_M$ and $\mu_I = 10^4\, \mu_M$. Applying the macroscopic deformation gradient $\overline{\boldsymbol{F}}$ with

$$\bar{\boldsymbol{F}} = \begin{bmatrix} 1-\lambda & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{121}$$

represents a horizontal compression state. For the considered compression case, we distinguish, as mentioned above, between two characteristic failure modes: buckling of the reinforcement in-phase (unsymmetric case) and buckling out-of-phase (symmetric case). For the unsymmetric case, we consider a finite-element discretization of an $\mathcal{RVE}$ with one fiber and for the symmetric case a finite-element discretization of an $\mathcal{RVE}$ with two fibers arranged in parallel. The crucial part is the yet unknown size of the $\mathcal{RVE}s$.

Thus, in order to find the critical load value as a function of the length of the discretized microstructure we have to modify the length of the $\mathcal{RVE}s$. For the finite element simulation of the in-phase buckling we discretize the system with 120×20 and for the out-of-phase buckling with 60×40 four-noded standard displacement elements. We start the simulation with a length of $l = 12$ (in consistent units) and increase the length by increments of $\Delta l = 12$ until the value $l = 60$ is reached. Two typical post-critical deformation states for the lengths $l = 6$ and $l = 2$ at the compressions $\lambda = 0.04$ and $\lambda = 0.01$, respectively, are shown in Fig. 11a,b.

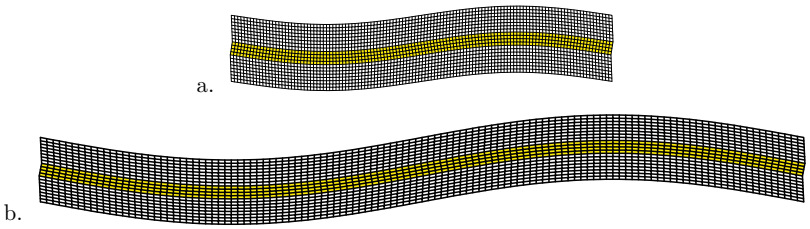

Figure 11. In-phase buckling of the fiber: post-critical deformation state of a) $l = 6$ at a compression parameter $\lambda = 0.04$ and b) $l = 12$ at a compression parameter $\lambda = 0.01$, see Schröder (2000).

The macroscopic Kirchhoff-stresses $\overline{\tau}_{11}$ with respect to the compression parameter λ are depicted in Fig. 12 for different lengths l. With increasing length l, the load-displacement curves are decreasing. Fig. 12b represents the critical stress components $\overline{\tau}_{11,crit}$ at the onset of the microscopic instability. The critical load converges against the lower bound.

For the stability analysis of the out-of-phase buckling mode, we start the simulation with a length $l = 3$ and increase the length stepwise using the increment $\Delta l = 1$ until $l = 12$ is reached.
Fig. 13a shows the macroscopic Kirchhoff-stresses $\overline{\tau}_{11}$ versus the loading paramter λ for eight different lengths. In contrast to the previously discussed in-phase buckling mode, the change of the characteristic curve shape is significant with increasing length. In Fig. 13b, the critical macroscopic stresses $\overline{\tau}_{11,crit}$ are depicted for the onset of the buckling of the fibers. The minimum of the critical stress $\overline{\tau}_{11,crit}$ is obtained at approximately $l = 7$.
Postcritical deformation states for the $\mathcal{RVE}$ of length $l = 5$ at the compression values $\lambda = 0.02$ and $\lambda = 0.03$ are depicted in Fig. 14a,b. A sequence of deformation states for the length $l = 12$ is documented in Fig. 15a–c, for

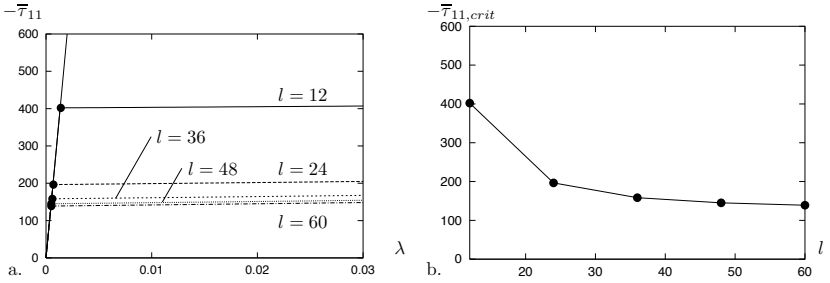

Figure 12. In-phase buckling of the fiber: a) macroscopic Kirchhoff-stresses $\overline{\tau}_{11}$ versus the compression parameter λ and b) critical stress $\overline{\tau}_{11,crit}$ at the onset of the structural instability at the micro-scale versus the length l of the considered microstructure, see Schröder (2000).

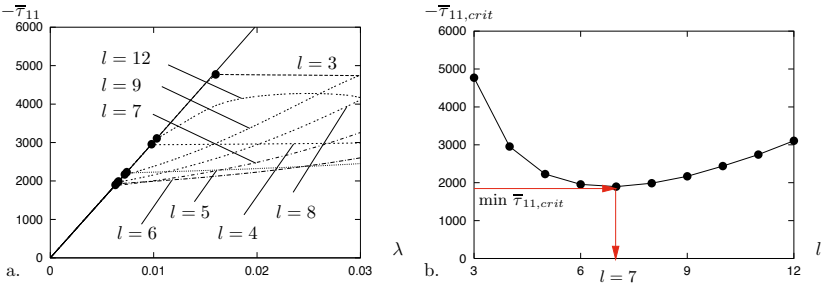

Figure 13. Out-of-phase buckling of the fibers: a) macroscopic Kirchhoff-stresses $\overline{\tau}_{11}$ versus the compression parameter λ for different lengths l and b) critical stress $\overline{\tau}_{11,crit}$ at the onset of the structural instability versus the length l, see Schröder (2000).

the load parameters $\lambda = 0.011, 0.017$ and 0.035, respectively. Additionally, Fig. 15c shows that higher-order buckling modes occur in the case where the length $\mathcal{RVE}$ becomes large enough. Here, three repeating characteristic deformation patterns are observable within the $\mathcal{RVE}$.

The two classical bifurcation modes, in-phase and out-of-phase, show different characteristics in the postcritical regime. In case of the out-of-phase buckling, the fibers support each other at a specific misalignment,