



Virtual testing of micro-heterogeneous composites for constructing macroscale yield surfaces Master's thesis in Solid and Fluid Mechanics

A. ESMAEILI, S. ASADI

Department of Applied Mechanics Division of Material and Computational Mechanics CHALMERS UNIVERSITY OF TECHNOLOGY Gothenburg, Sweden 2012 Master's thesis 2012:06

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Master's thesis 2012:06 ISSN 1652-8557 Department of Applied Mechanics Division of Material and Computational Mechanics Chalmers University of Technology SE-412 96 Gothenburg Sweden Telephone: +46 (0)31-772 1000

Cover:

von-Mises effective stress distribution within a mechanically loaded composite with circular inclusions

Chalmers Reproservice Gothenburg, Sweden 2012 Virtual testing of micro-heterogeneous composites for constructing macroscale yield surfaces Master's thesis in Solid and Fluid Mechanics A. ESMAEILI, S. ASADI Department of Applied Mechanics Division of Material and Computational Mechanics Chalmers University of Technology

Abstract

This thesis discusses an approach based on computational homogenization to establish macroscopic yield surfaces for virtual elastic-plastic composites using an adopted "offset point" yield criterion. A material consisting of randomly distributed cylindrical (circular in 2D) inclusions embedded in a monolithic matrix is studied. The considered material model in each of the composite's micro-constituents is of elastic-plastic type, whereby the concept of internal variables is adopted to account for dissipative effects.

The macroscopic stress-strain response of the material is determined from virtual testing on representative volume elements (RVEs) for given volume fraction and statistical distribution of inclusions. A strategy is proposed for the determination of the macroscopic yield surface via a novel stress-driven algorithm. Numerical results obtained by imposing two classical prolongation conditions of Dirichlet and Neumann boundary conditions are compared. Key parts in the proposed strategy is the choice of the proper RVE-size and the number of essential realizations needed for establishing the microscopic yield surface.

A more elaborate technique for estimating statistical bounds for the yield surface of the virtual composite is applied and compared to the results generated by classical Dirichlet and Neumann assumptions.

Keywords: Homogenization, yield surface, Representative volume element, Multiscale problem, Dirichlet boundary condition, Neumann boundary condition

Preface

In this study, a novel development within the area of micromechanics, Computational Homogenization, is employed in order to determine a heterogenous material's yield surface numerically. The project is carried out as a master's thesis in cooperation with the division of Material and Computational Mechanics at Chalmers University of Technology under supervision of Dr. F. Larsson.

Acknowledgements

We would like to exploit this opportunity to express our sincere gratitude to Dr. Fredrik Larsson and Prof. Kenneth Runesson for their advice and support. Without their helps this project would not have been possible.

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1 Introduction

1.1 Background

Due to growing interest in determining the macroscopic overall behavior of heterogeneous materials, computational methods are becoming increasingly concerned with the application of homogenization technique.

The macroscopic mechanical description of heterogeneous material can be based on the introduction of at least two different phenomenological scales, namely the Macroscale and the Microscale. The Macroscale is usually associated with homogenized continuous media undergoing smooth stress and strain states. The Microscale, on the other hand, is often characterized by a statistically representative volume which contains different microstructural constituents [13]. The microstructure of the composite in this thesis consists of distribution of circular inclusions representing particles or fibers in 3D within a binding matrix. The purpose of those inclusions is Often to stiffen the material [12].

In this context, a complete scale separation is assumed in order to account for the effect of material substructure in constitutive modeling such that the microscale solution interacts with the macroscale response only via its homogenized results.



Figure 1.1.1: Illustration of computational homogenization strategy for stress problems.

Determining the behavior of the material on one length scale by information from other length scales is known as multiscale modeling. One of the advantages of multiscale modeling is that microscale phenomenon can be revealed which leads to a deeper understanding of the mechanisms that determine the material behavior, cf. Nilenius et al.[4].

A classical approach in order to account for subscale heterogeneities is averaging the influence of subscale properties to obtain their effective counterparts that holds on the macroscale. This process is called homogenization, cf. Besson et al. [8], Roters et al. [7], Ostoja-Starzewski [6] and Geers et al. [5].

In order to perform the computational homogenization, a unit cell, called "RVE", that statistically represents the microscale heterogeneities is considered. A Representative Volume Element "RVE" is a computational domain of the material, which possesses microstructure, contains adequate statistical information about the heterogeneous medium in order to be a representative of the material's microstructure.

Apart from the basic assumption on scale separation, a number of other model assumptions are (implicitly or explicitly) made as part of the computations. One particular model assumption is represented by the choice of boundary (or loading) conditions on the RVE. A proper choice means that convergence is obtained as the RVE size is increased [10]. In order to assure an appropriate choice, the Hill-Mandel macro-homogeneity condition must be fulfilled.

In this thesis the focus is on stress-driven loadings, where the macroscopic stress (\bar{P}) is controlled. In this context, two classical choices of boundary conditions are investigated; Dirichlet and Neumann boundary conditions. Having the suitable boundary condition and a constitutive driver corresponding to the mechanical behavior of the given composite's microconstituents, the static equilibrium state of the RVE for a certain stage of loading process is solved. Obtaining the solution, it is possible to define the macroscopic effective properties as volume averages of associated variables over the unit cell at the current loading stage.

Upon driving the equilibrium equations pertinent to different length scale combined with constitutive equations and boundary conditions a system of partial differential equations is constructed. This system is often non-linear due to geometrical and/or material non-linearities. Analytical solutions can be obtained only for extremely simple geometries and loading conditions. Therefore, for the analysis of practical multi-dimensional problems with complex geometries and loading conditions approximate, numerical methods are required. In practice, Finite Element Analysis (FEA) is often used to solve problems in solid mechanics. The same methodology can be used for the numerical solution of multiscale models. But in this case, discretization is often carried out in different levels for different length scales, in terms of the element size and type, cf. Geers et al. [5], Kouznetsova et al. [15].

The thesis presents a theoretical and computational framework in order to establish approximate bounds for the macroscopic yield surface of a micro-heterogeneous elastic-plastic composite, with random distribution of constituents, undergoing in-elastic deformation at small strains. The main focus of the thesis is put on the possibility to construct two consistent and distinguished bounds on the macroscopic yield surface.

In order to establish a criterion for "macroscopic yielding" in the principal stress space, it is assumed that the effective yield stress is defined as the state when the magnitude of the macroscopic plastic strain has reached a given predefined proportionality limit called "offset yield point".

1.2 Purpose and scope

The main purposes of this paper is summarized as follows :

• Establish the microscale model in terms of topology and constitutive models for the heterogeneous material based on plasticity with mixed isotropic and kinematic hardening.

• Investigate the optimum RVE size and number of realizations in order to construct the sharpest possible bounds on the macroscopic yield surface.

• Develop a strategy to bound the macroscopic yield surface(stress response on the principal stress space), employing sufficient number of realizations with a given confidence interval.

The report is organized in a manner that first some theoretical backgrounds and concepts are introduced and explained briefly, then the material model prototype is proposed. The computational strategy and utilized yield criterion is described in virtual testing section.

Then the algorithms are presented in details. Furthermore, the proper size of the RVE and number of realizations which leads to optimum convergence in the indicated parameter is investigated. Then, the upper and lower bound of macroscopic yield surface is defined based on stress response for a given composite according to elasto-plastic model prototype. The final part of the report consists of conclusions and some suggestions concerning the possible future work.

2 Multiscale formulations

2.1 Quasistatic stress problem

Assuming that static equilibrium is fulfilled at any given time, the equilibrium equation may be expressed in the reference (or material) configuration in terms of the first Piola-Kirchhoff stress tensor as:

$$-P \cdot \nabla = f \qquad on \quad \Omega, \qquad (2.1.1)$$

$$u = u_p, \qquad on \quad \partial \Omega_D,$$

$$t \doteq P \cdot N = t_p, \qquad on \quad \partial \Omega_N$$

¹ Where, the computational domain occupies the spatial domain Ω with the boundary $\partial \Omega$ in the reference configuration, P in the above equation denotes the 1st Piola-Kirchhoff stress, ∇ is the Divergence operator and f is the body force.

As, the relevant classical boundary conditions on $\partial\Omega$ are defined in equation (2.1.1), namely, the Dirichlet boundary condition and the Neumann boundary condition, where in the equation $(2.1.1)_c t$ denotes the reference boundary traction (boundary force per unit reference area) and N is a reference unit normal vector. A constitutive model is required in order to determine P in terms of the macroscale displacement field u. Subsequently, the stress-deformation relation P(H)is obtained, where the displacement gradient $H[u] \doteq u \otimes \nabla$ is related to the deformation gradient F[u] as H[u] = F[u] - I.

Remark 1. We note that small strain kinematics imply that:

(i) P is symmetric,

(ii) it is only the symmetric part of H that effects P.

For finite deformation kinematics, corresponding constraints apply.

Introducing the space of admissible displacements

$$\mathbb{U} = \{ u | u = u_p \text{ on } \partial\Omega_D, {}^2 (\int \left[\nabla u \right]^2 d\Omega)^{\frac{1}{2}} < \infty \}$$

$$(2.1.2)$$

The corresponding space of test functions is

$$\mathbb{U}^0 = \{ u | u = 0 \text{ on } \partial\Omega_D, (\int [\nabla u]^2 d\Omega)^{\frac{1}{2}} < \infty \}$$

$$(2.1.3)$$

The standard variational format then reads: Find $u \in \mathbb{U}$ that solves

$$a(u;\delta u) = l(\delta u) \qquad \forall \delta u \in \mathbb{U}^0$$
 (2.1.4)

where

$$a(u;\delta u) \doteq \int_{\Omega} P : H[\delta u] dV, \qquad (2.1.5)$$
$$l(\delta u) \doteq \int_{\Omega} f \cdot \delta u dV + \int_{\partial \Omega_N} t_p \cdot \delta u dS,$$

It is noted that $a(u; \delta u)$ is a semilinear form (that is nonlinear in the first argument, while it is always linear in the last argument). Moreover, $l(\delta u)$ is a linear functional.

 $^{^{1}}$ Equation (2.1.1) is referred to as the strong, local or pointwise form of the equilibrium equation.

²The condition corresponds to the sufficiently regularity of the given function.

2.2 Classical (Model based) homogenization

2.2.1 Preliminaries

The "model-based homogenization" represents an attempt to solve the problems in which the macrocontinuum problem is numerically unresolvable using, say, straight forward FE-discretization, in the sense that resolving the fine scale representation, embedded in U, in presence of heterogeneities is numerically expensive.

Hence, the viewpoint adopted is a complete scale separation meaning that there are two sets of scales; one associated with the macroscopic scales (Macroscale) and the other with microscopic scales (Microscale).

The main concept is to replace the heterogenous macro-continuum by a homogenous medium with mechanical properties that have to be determined. So, the strategy is to approximate the macroscopic field y, positioned at the macroscale position \bar{X}_i , with the spatially homogenized field (as a smoothing approximation) that is computed on the associated representative microstructure. In practice, numerical quadrature is employed at the evaluation of integrals in the spatial domain. Hence, homogenization on the RVE's is carried out (only) in these macroscale quadrature points [1].

The key step of the strategy is to perform an accurate computation on representative microstructures as resolvable scales and assure a precise incorporation of the effects of the microscales upon the constitutive model.

In this numerical method the fine scale fields are discretized on representative microstructures namely, Representative Volume Elements (RVE) which provide detailed information on fine scale mechanisms. The introduced RVE is assumed to occupy the subscale region $\Omega_{\Box,i}$. Besides, it is also assumed to be centered at the macroscale position \bar{X}_i (The Gauss point), i.e. $\langle X - \bar{X}_i \rangle_{\Box,i} = 0$ for any $\bar{X}_i \in \Omega$.

The macroscopic extensive fields are then defined by "volume averages" of their microscopic counterparts when the microstructure is in the equilibrium state, s.t.:

$$y(\bar{X}_i) \mapsto \langle y \rangle_{\square}(\bar{X}_i) \qquad \bar{X}_i \in \Omega$$
 (2.2.1)

Similarly, we introduce homogenization on the boundary surface $\partial \Omega$ as

$$y(\bar{X}_i) \mapsto \langle \langle y \rangle \rangle_{\square}(\bar{X}_i) \qquad \bar{X}_i \in \partial \Omega \tag{2.2.2}$$

where the Representative Surface Element(RSE) occupies the subscale region $\partial \Omega$.

The volume average of the quantity of interest pertinent to the RVEs on Ω_{\Box} is then introduced as:

$$\langle \bullet \rangle_{\Box} \doteq \frac{1}{|\Omega_{\Box}|} \int_{\Omega_{\Box}} \bullet d\Omega \tag{2.2.3}$$

and it's associated surface average on γ_{\Box} is denoted:

$$\langle \langle \bullet \rangle \rangle_{\Box} \doteq \frac{1}{|\gamma_{\Box}|} \int_{\gamma_{\Box}} \bullet \, d\gamma \tag{2.2.4}$$

where \bullet denotes the property of interest.

In brief, this strategy implies a numerical implementation, based in general setting, on a nonlinear finite element analysis of the macro-continuum, which is locally coupled at each Gauss point with a nonlinear finite element analysis of the attached microstructure.

Upon introducing the homogenization approach, the original problem formulation of the standard variational format remains formally unchanged if the integrands are replaced by their homogenized counterparts in all space-variational forms [2].

Hence,(2.1.4) is replaced by:

$$a(u;\delta u) \doteq \int_{\Omega} \langle P: H[\delta u] \rangle_{\Box} dV, \qquad (2.2.5)$$
$$l(\delta u) \doteq \int_{\Omega} \langle f \cdot \delta u \rangle_{\Box} dV + \int_{\partial \Omega_N} \langle \langle t_p \cdot \delta u \rangle \rangle_{\Box} dS, \qquad (2.2.6)$$

This method allows the analysis of all possible geometries and constitutive models, regarding a typical heterogeneous material.

2.2.2 Separation of scales

The key assumption in the model-based homogenization is that a Multiscale system can be decomposed, a priori, into two sets of scales namely, the Macroscale and the Microscale, in order to account for the microstructure effects into constitutive model.

2.2.3 The Representative Volume Element (RVE)

The Representative Volume Element (RVE) is generally regarded to a volume Ω_{\Box} (in this thesis a surface of a infinitesimal thickness) which is a statistical representation of the properties of a typical heterogeneous material. On the other hand, RVE plays the role of a mathematical point of a continuum field, approximating the true material microstructure [3].

In this regard, the RVE size must be chosen in a manner to realistically represent the microstructure. This perspective leads to the condition that the smallest RVE size for which a macroscopic "effective" constitutive theory can be applied is one that is sufficiently large to include effectively a sampling of all possible microstructural configurations yet small enough to keep the computational costs in a minimum possible level.

2.2.4 Prolongation conditions

Inside each RVE, the total solution of the RVE, $u(\bar{X}, X)$ is split into a smooth part, u^M , and a fluctuating part, u^s ; Hence,

$$u(\bar{X}, X) = u^{M}(\bar{X}, X) + u^{s}(\bar{X}, X)$$
(2.2.7)



Figure 2.2.1: Relation between U, U^M and U^s

The separated scales are linked by setting $u^M(\bar{X}, X) = \bar{u}(\bar{X})$ inside each RVE, where $u^M \in \mathbb{U}^M$ is the smooth (macroscale) solution on Ω_{\Box} and $\bar{u} \in \overline{\mathbb{U}}$ is the (global) macroscale displacement field [1].

The assumptions that are imposed on the problem in order to establish a relation between macrosolution u^M , where $u^M \approx \bar{u}$, and the fluctuating part of microscale solution $u^s \doteq u^s \{u^M\}$ defines prolongation conditions. Different model assumptions are possible with respect to the choice of prolongation conditions for the RVE, i.e. the imposed boundary condition and the appropriate variational format of the RVE problem. In this context, two different prolongation conditions are investigated in the present paper namely, the classical Dirichlet and Neumann boundary conditions, which are considered in detail in the following sections.

2.2.5 Variationally consistent first order homogenization

As to the definition of prolongation conditions, the relation of the macroscale field u^M inside the RVE with respect to the (global) macroscale displacement field \bar{u} and its derivatives is required to be established. The task of correlating these two variable fields is called "Prolongation". Hence, for macroscale prolongation to Ω_{\Box} , For given $\bar{X} \in \Omega$, $X \in \Omega_{\Box}$

$$u^{M}(X) = u^{M}(\bar{H}^{(0)} \doteq \bar{u}, \bar{H}^{(1)} \doteq \bar{H}, \bar{H}^{(2)}, ..., \bar{H}^{(K)}; X)$$
(2.2.8)

With higher order gradients (K=order of homogenization)

$$\bar{H}^{(k)} \doteq \bar{u} \otimes \underbrace{\bar{\nabla} \otimes \bar{\nabla} \otimes \dots \otimes \bar{\nabla}}_{k}$$
(2.2.9)

where we introduced the macroscale gradient $\overline{\nabla}$ with respect to the coordinate \overline{X} . 1st order (conventional):

$$u^{M}(X) = \bar{u} + \bar{H} \cdot [X - \bar{X}]$$
(2.2.10)

2nd order:

$$u^{M}(X) = \bar{u} + \bar{H} \cdot [X - \bar{X}] + \frac{1}{2} [X - \bar{X}] \cdot \bar{H}^{(2)} \cdot [X - \bar{X}]$$
(2.2.11)

In this thesis, the standard (model-based) first order homogenization based on a proper assumption about the smoothness of the macroscale field (linear variation of u^M) within the RVE is applied. Where $\bar{u} \in \bar{\mathbb{U}}$ is the (global) macroscale displacement field, and $\bar{H} \doteq \bar{u} \otimes \bar{\nabla}$ is the macroscale displacement gradient.

Remark 2. $\overline{H} = \langle G[u^M] \rangle_{\Box} \neq \langle G[u] \rangle_{\Box} \doteq \langle H \rangle_{\Box}$, unless further assumptions or conditions are imposed on the fluctuation field.

Next, it is possible to introduce the space \mathbb{U}^M as follows:

$$\mathbb{U}^{M} = \{ u^{M} | u^{M}(\bar{X}, X) = \bar{u}(\bar{X}) + \bar{H}.[X - \bar{X}], \bar{u} \in \bar{\mathbb{U}} \}$$
(2.2.12)

Remark 3. A possible drawback of the first order homogenization technique is that it does not account for the absolute size of the microstructure, thus failing to represent geometrical size effects. Moreover, an ambiguity concerns the assumption of uniform macroscopic fields across the microstructure, which works well in regions where the macroscopic fields vary smoothly, but it does, in fact, not work well in regions where steep gradients occur at e.g. corners, boundary layers, cracks, inclusions etc. The proper consideration of these issues requires (at least) a second order homogenization technique along with a matching higher order continuum formulation [14].

2.2.6 Variational multiscale problem

Following the computational implementation of Multiscale theories which is mentioned so far, it is possible to replace the single-scale problem of equation (2.1.4) with a variational Multiscale problem as:

Find $u^M \in \mathbb{U}^M$ that solves:

$$a(u\{u^M\};\delta u) = l(\delta u) \qquad \forall \delta u^M \in \mathbb{U}^{M,0}$$
(2.2.13)

where we introduce the space of test functions $\mathbb{U}^{M,0}$ as:

$$\mathbb{U}^{M,0} = \{ u^M | u^M = 0 \text{ on } \partial\Omega_D, (\int [\nabla u^M]^2 d\Omega)^{\frac{1}{2}} < \infty \}$$
(2.2.14)

Then, regarding the decomposition of displacement fields

$$u\{u^M\} = u^M + u^s\{u^M\}$$
(2.2.15)

We may conclude that

$$\delta u = \delta u^M + (u^s)' \{ u^M; \delta u^M \}$$
(2.2.16)

whereby, it is tacitly used that δu can be defined implicitly as a linear functional in terms of δu^M [2].

Expanding the variational macroscale problem of equation (2.2.13) by substituting the variation δu with it's definition in equation (2.2.16), the balance equation may be obtained as decomposed form of δu^M and δu^s as:

Find $u^M \in \mathbb{U}^M$ that is the solution of

$$a(u\{u^{M}\};\delta u^{M}) - R(u\{u^{M}\};(u^{s})'\{u^{M};\delta u^{M}\}) = l(\delta u^{M}) \qquad \forall \delta u^{M} \in \mathbb{U}^{M,0}$$
(2.2.17)

Where,

$$R(u\{u^{M}\}; (u^{s})'\{u^{M}; \delta u^{M}\}) = R(u; \delta u^{s}) \doteq \int_{\Omega} R_{\Box}(u; \delta u^{s}) dV$$
(2.2.18)

Next, it is assumed that for the chosen prolongation condition, the "local" version of Hill-Mandel macrohomogeneity condition, which is considered in detail in the following subsections, is satisfied.

$$R_{\Box}(u\{u^{M}\};(u^{s})'\{u^{M};\delta u^{M}\}) = 0 \qquad \forall \delta u^{M} \in \mathbb{U}^{M,0}$$
(2.2.19)

Upon applying the local variationally consistent macrohomogeneity condition on each RVE, the global Hill-Mandel condition is consequently satisfied and the residual in (2.2.17) vanishes as:

$$R(u\{u^{M}\}; (u^{s})'\{u^{M}; \delta u^{M}\}) = 0 \qquad \forall \delta u^{M} \in \mathbb{U}^{M,0}$$
(2.2.20)

Accordingly, the variational macroscale problem of eq. (2.2.17) reduces to a simpler problem as follows: Find $u^M \in \mathbb{U}^M$ s.t.,

$$a(u\{u^M\}; \delta u^M) = l(\delta u^M) \qquad \forall \delta u^M \in \mathbb{U}^{M,0}$$
(2.2.21)

2.2.7 Hill-Mandel macro-homogeneity condition

As mentioned earlier, so as to vanishing the residual associated with any test function δu^s , equation (2.2.20), the so-called Hill-Mandel microhomogeneity condition must be fulfilled. Generally speaking, the condition states that the microscopic volume average of the virtual work performed on the RVE is coincide to the local virtual work on the macroscale, i.e.,

$$\langle P: H[\delta u] \rangle_{\Box} = \langle P \rangle_{\Box} : \langle H[\delta u] \rangle_{\Box} = \bar{P} : \delta \bar{H}$$
(2.2.22)

Which is formulated in terms of a work conjugated set of deformation gradient tensor and the first Piola-Kirchhoff stress tensor. Then, the virtual work on the subscale can be rewritten as:

$$\langle P: H[\delta u] \rangle_{\Box} = \frac{1}{|\Omega_{\Box}|} \int_{\Omega_{\Box}} P: H[\delta u] d\Omega = \frac{1}{|\Omega_{\Box}|} [\int_{\Omega_{\Box}} f \cdot u d\Omega + \int_{\partial\Omega_{\Box}} t \cdot u dS]$$
(2.2.23)

Where the Gauss' theorem is used in order to drive the right hand side of the equation. Note that body is perfectly bounded and there are no body force, so the equation reduces to :

$$\langle P: H[\delta u] \rangle_{\Box} = \frac{1}{|\Omega_{\Box}|} \int_{\partial \Omega_{\Box}} t \cdot \delta u dS \tag{2.2.24}$$

Applying the decomposition introduced in (2.2.16) implies:

$$H[\delta u] = \delta \bar{H} + H[\delta u^s], \qquad (2.2.25)$$

Upon inserting (2.2.25) into equation (2.2.22) the local Hill-Mandel microhomogeneity condition reads;

$$\bar{P}:\delta\bar{H}-\langle P:H[\delta u]\rangle_{\Box} = \underbrace{\bar{P}:\delta\bar{H}-\langle P\rangle_{\Box}:\delta\bar{H}}_{=0} -\langle P:H[\delta u^{s}]\rangle_{\Box} = (2.2.26)$$
$$\frac{1}{|\Omega_{\Box}|} \int_{\partial\Omega_{\Box}} t \cdot \delta u^{s} dS \doteq R_{\Box}(u\{u^{M}\};\delta u^{s}),$$

2.2.8 Subscale modeling-RVE problem

Assuming the standard continuum relations are applied everywhere, on the macro-continuum down to the microscale, the subscale (local) quasi-static problem on a RVE, occupying the computational domain Ω_{\Box} with the boundary $\partial \Omega_{\Box}$, reads,

$$-P \cdot \nabla = f \qquad on \quad \Omega_{\Box} \tag{2.2.27}$$

As to the solution of the problem, regarding the definition of macroscale displacement in the first order homogenization format in equation (2.2.10), to obtain a unique solution for u^M , it is required to restrict the displacement solution in order to prevent the rigid body motion. In this context, we introduce the space of admissible displacements as:

$$\mathbb{U}_{\Box} = \{ (\int [\nabla u]^2 d\Omega)^{\frac{1}{2}} < \infty \quad in \quad \Omega_{\Box} \quad , u(X_0) = 0 \}$$
 (2.2.28)

Where $X_0 \in \Omega_{\Box}$ denotes a single and arbitrarily chosen point within the RVE. The corresponding space of test functions then introduced as:

$$\mathbb{U}_{\square}^{0} = \{ u | u = 0 \text{ on } \partial\Omega_{\square,D}, (\int \left[\nabla u\right]^{2} d\Omega)^{\frac{1}{2}} < \infty \}$$

$$(2.2.29)$$

It is noteworthy that it is possible to reduce the eq.(2.2.10) to $u^M(X) = \overline{H} \cdot [X - \overline{X}]$ by setting $X_0 = \overline{X}$, where, \overline{X} is the macroscale position as the RVE is centered $\langle X - \overline{X} \rangle = 0$. Moreover, upon setting $\overline{X} = 0$, this expression can be reduced even more such that: $u^M(X) = \overline{H} \cdot X$. Therefore, the space of macroscale displacement field (2.2.12) may be reintroduced as:

$$\mathbb{U}^{M} = \{ u^{M} | u^{M}(\bar{X}, X) = \bar{H}. X, \bar{u} \in \bar{\mathbb{U}} \}$$
(2.2.30)

The subscale variational format then reads: Find $u \in \mathbb{U}_{\Box}$ that solves

$$a_{\Box}(u;\delta u) - \frac{1}{|\Omega_{\Box}|} \int_{\partial\Omega_{\Box}} t \cdot \delta u dS = \langle f \cdot \delta u \rangle_{\Box} \qquad \forall \delta u \in \mathbb{U}_{\Box}^{0}$$
(2.2.31)

where

$$a_{\Box}(u;\delta u) \doteq \langle P: H[\delta u] \rangle_{\Box} \tag{2.2.32}$$

The microscale formulation is complete upon imposing the "loading" on the RVE in terms of the prescribed homogenized (macroscale) displacement gradient \bar{H} ; Therefore, we enforce the following condition, as:

 $\frac{1}{|\Omega_{\Box}|} \int_{\Omega_{\Box}} H dV = \frac{1}{|\Omega_{\Box}|} \int_{\Gamma_{\Box}} u \otimes N dS = \bar{H}$ (2.2.33)

for given \overline{H} .

Given the microscale stress P, it is also possible to compute the macroscale (homogenized) stress \bar{P} [10]:

$$\bar{P} \doteq \frac{1}{|\Omega_{\Box}|} \int_{\Omega_{\Box}} P dV = \frac{1}{|\Omega_{\Box}|} \int_{\Gamma_{\Box}} t \otimes X dS + \frac{1}{|\Omega_{\Box}|} \int_{\Omega_{\Box}} f \otimes X dV$$
(2.2.34)

Then, we assume the special case in which the body forces are vanished, which is a common assumption in microscale computations.

The manipulations leading to (2.2.34) involve using the identity $I = \nabla \otimes X$, Gauss's theorem and the equilibrium equation (2.2.27)

2.2.9 Approximation of the RVE's response

As to the approximation of the RVE's response of a heterogeneous material, an approach based on ensemble averaging is employed. Let α be a particular realization in the set \mathcal{P}_{α} of equiprobable realizations and let y be a random field, statistically homogeneous and ergodic³. Then the expectation of y is defined by $\langle y \rangle_{\Box}^{\mathcal{P}_{\alpha}} = \int_{\mathcal{P}_{\alpha}} y(\alpha) d\alpha$ approximated by a Monte-carlo computation [9].

$$\langle y \rangle_{\Box}^{\mathcal{P}_{\alpha}} \approx \frac{1}{N_{\Box,\alpha}} \sum_{i=1}^{N_{\alpha}} y(\alpha_i)$$
 (2.2.35)

with N_{α} being the number of unit cell realizations. The ergodicity assumption then implies that the expectation of y is equal to the volume average of y over Ω_{\Box}

$$\langle y \rangle_{\Box} \doteq \frac{1}{|\Omega_{\Box}|} \int_{\Omega_{\Box}} y d\Omega_{\Box}$$
 (2.2.36)

2.2.10 Macroscale problem

As mentioned earlier, the macroscopic extensive fields are defined by volume averages of their microscopic counterparts, computed on the associated RVE , represented by the auxiliary form:

$$\bar{y} \doteq \langle y \rangle_{\square} \tag{2.2.37}$$

In this context, the variational macroscale forms of eq.(2.2.21) are evaluated as:

$$\int_{\Omega} \langle P : G[\delta u^{M}] \rangle_{\Box} d\bar{V} = \int_{\Omega} \bar{P} : \delta \bar{H} d\bar{V}, \qquad (2.2.38)$$
$$\int_{\Omega} \langle f \cdot \delta u^{M} \rangle_{\Box} d\bar{V} = \int_{\Omega} \bar{f} \cdot \delta \bar{u} d\bar{V}, \\\int_{\partial \Omega_{N}} \langle \langle t_{p} \cdot \delta u^{M} \rangle_{\Box} d\bar{S} = \int_{\partial \Omega_{N}} \bar{t_{p}} \cdot \delta \bar{u} d\bar{S},$$

Consequently, the macroscale variational format reads;

$$\bar{a}\{\bar{u};\delta\bar{u}\} = \bar{l}\{\delta\bar{u}\} \qquad \forall \delta\bar{u} \in \bar{\mathbb{U}}^0 \tag{2.2.39}$$

where,

$$\bar{a}\{\bar{u};\delta\bar{u}\} \doteq \int_{\Omega} \bar{P}:\delta\bar{H}d\bar{V},$$

$$\bar{l}\{\delta\bar{u}\} \doteq \int_{\Omega} \bar{f}\cdot\delta\bar{u}d\bar{V} + \int_{\partial\Omega_N} \bar{t_p}\cdot\delta\bar{u}d\bar{S},$$
(2.2.40)

 $^{^{3}}$ A system is said to be ergodic when in the case of it's statical homogeneous fields, the moving average and the ensemble average are constant and also equal.

2.3 Boundary Conditions

According to the subsection (2.2.4), in order to establish a relation between two separated scales (macroscale and microscale), it is necessary to specify the fluctuation part of the microscale solution $u^s\{u^M\}$ in terms of the macro-solution u^M by imposing the prolongation condition on the RVE. In this regard, two types of boundary conditions on the RVE are considered in the present study, namely Dirichlet (essential) boundary condition where the displacements on the boundaries are prescribed and Neumann (Natural) boundary condition where the tractions on the boundaries are prescribed.

Remark: It must be noted that the solution space associated with both cases of boundary conditions are restricted by imposing the condition of plane stress loading.

2.3.1 Dirichlet boundary condition

Continuous format

To begin with, in order to specify the subscale displacement field $u = u^M + u^s$, whereby the linearly varying part $u^M = \hat{H} \cdot X$ is parameterized in terms of the constant tensor \hat{H} by the first order homogenization assumption, it only remains to introduce the fluctuation field. As the definition of Dirichlet boundary condition implies, $u^s = 0$ is a proper choice on $\partial \Omega_{\Box}$ to define piecewise linear displacements on the sides of Ω_{\Box} .

$$u = \hat{H} \cdot X$$
 on $\partial \Omega_{\Box}$ (2.3.1)

Inserting u in (2.2.33) gives:

$$\bar{H} = \frac{1}{|\Omega_{\Box}|} \int_{\partial\Omega_{\Box}} \underbrace{\hat{H} \cdot X}_{u} \otimes NdS = \hat{H} \cdot \frac{1}{|\Omega_{\Box}|} \int_{\partial\Omega_{\Box}} X \otimes NdS = \hat{H}$$
(2.3.2)

where, it is used that $\int_{\partial\Omega_{\square}} X \otimes N dS = |\Omega_{\square}|I.$

Hence, it implies that $\hat{H} = \bar{H}$. Where, as a direct result, it is concluded that the Hill-Mandel microhomogeneity condition is satisfied, s.t.:

$$\frac{1}{|\Omega_{\Box}|} \int_{\partial \Omega_{\Box}} t \cdot \underbrace{[\delta \hat{H} \cdot X]}_{\delta u} dS = \left(\frac{1}{|\Omega_{\Box}|} \int_{\partial \Omega_{\Box}} t \otimes X dS\right) : \delta \bar{H} = \bar{P} : \delta \bar{H},$$
(2.3.3)

Next, we introduce the space of admissible microscale displacements

$$\mathbb{U}_{(D)} = \{ u | u = \overline{H} \cdot X \text{ on } \partial\Omega_{\Box}, (\int [\nabla u]^2 dV)^{\frac{1}{2}} < \infty \}$$

$$(2.3.4)$$

and the corresponding space of test functions

$$\mathbb{U}^{0}_{(D)} = \{ u | u = 0 \text{ on } \partial\Omega_{\Box}, (\int [\nabla u]^{2} dV)^{\frac{1}{2}} < \infty \}$$
(2.3.5)

where, Dirichlet boundary condition restricts the space as $\mathbb{U}_{\square}^{D} \subseteq \mathbb{U}_{\square}$, but the traction space is remained unrestricted $\mathbb{T}_{\square}^{D} = \mathbb{T}_{\square}$.

The pertinent standard variational format then reads;

For given value of the macroscale \bar{P} , find $(u^s, \bar{H}) \in (\mathbb{U}(0)_{(D)}, R^{2 \times 2^{sym}})$ that solves

$$\begin{cases} a_{\Box}(u;\delta u) = 0 & \forall \delta u \in \mathbb{U}_{(D)}(0) \doteq \mathbb{U}_{(D)}^{0} \\ \langle P \rangle_{\Box} : \delta \bar{H} = \bar{P} : \delta \bar{H} & \forall \delta \bar{H} \in \mathbb{R}^{3x3} \end{cases}$$
(2.3.6)

Where we introduced the variational form as:

$$a_{\Box}(u;\delta u) \doteq \frac{1}{|\Omega_{\Box}|} \int_{\Omega_{\Box}} P(H[u]) : H[\delta u] d\Omega$$
(2.3.7)

The above relation is obtained considering a special common case of vanishing body forces f = 0. Furthermore, since the test function is zero on the boundaries, the right hand side of the equation $(2.3.6)_a$ vanishes completely.

The macroscale algorithmic tangent compliance tensor

Next, the purpose is to establish the algorithmic compliance tensor \bar{C}_{\Box} , defined by

$$d\bar{H}^{sym} = \bar{C}_{\Box} : d\bar{P}, \tag{2.3.8}$$

for variations $d\bar{P}$ of the macroscopic stress \bar{P} .

Remark 4. Henceforth, we assume small strain kinematics, whereby \bar{P} will be symmetric and the rigid body deformation is characterized by $\bar{H}^{sym} = 0$, we point out that the skew-symmetric part of \bar{H} will be indeterminate for given \bar{P} .

In this respect, as a preliminary it is first assumed that the state equation $(2.3.6)_a$ must hold for $u \in \mathbb{U}_{(D)}$ as well as for $u + du \in \mathbb{U}_{(D)}$, i.e.,

$$a_{\Box}(u;\delta u) = 0 \quad \forall \delta u \in \mathbb{U}^0_{(D)} \tag{2.3.9}$$

$$a_{\Box}(u+du;\delta u) = 0 \quad \forall \delta u \in \mathbb{U}^0_{(D)}$$

$$(2.3.10)$$

Subsequently, the difference of equations (2.3.9) and (2.3.10) can be expressed as:

$$a_{\Box}(u+du;\delta u) - a_{\Box}(u;\delta u) = 0 \quad \forall \delta u \in \mathbb{U}^0_{(D)}$$
(2.3.11)

Since variations du are small expression (2.3.11) reduces to it's tangential format of: Finding $du \in \mathbb{U}_{(D)}$ such that:

$$a'_{\Box}(u;\delta u,du) = 0 \quad \forall \delta u \in \mathbb{U}^0_{(D)}$$

$$(2.3.12)$$

According to the decomposition of the subscale displacement field $u = u^M + u^s$ with $u^M = \overline{H} \cdot X$, c.f. continuous format, its associative decomposition of variations gives:

$$du = du^M + du^s, (2.3.13)$$

With $du^M \doteq d\bar{H} \cdot X \in \mathbb{U}_{(D)}(d\bar{H})$ and $du^s \in \mathbb{U}^0_{(D)}$. Expanding the tangential format of equation (2.3.12) by substituting the variation du by it's decomposed alternative expression gives;

$$a'_{\square}(u;\delta u, d\bar{H} \cdot X + du^s) = 0 \quad \forall \delta u \in \mathbb{U}^0_{(D)}$$

$$(2.3.14)$$

Successively, by manipulating equation $(2.3.6)_b$, it gives:

$$\left\langle \frac{\delta P}{\delta H} : \left[d\bar{H} + u^s \otimes \nabla \right] \right\rangle_{\Box} : \delta\bar{H} = d\bar{P} : \delta\bar{H}$$
(2.3.15)

Furthermore, we introduce nodal variable $\bar{H}^{(ij)}$ that corresponds to "unit macroscale stress gradient", i.e. nodal displacement gradients that correspond to $\bar{P}_{ij} = 1$ which are defined as,

$$d\bar{H} = \sum_{i,j} \bar{H}^{(ij)} d\bar{P}_{ij}, \qquad \text{and} \qquad d\bar{P} = \sum_{i,j} e_i \otimes e_j d\bar{P}_{ij} \qquad (2.3.16)$$

Using the linearity in the tangential format (2.3.14) and (2.3.15), we arrive at the problem of solving for displacement gradient field as: find $\bar{H}^{(i)} \in \mathbb{D}^{373}$ such that:

find $\bar{H}^{(ij)} \in \mathbb{R}^{3x3}$ such that:

$$\begin{cases}
 a'_{\Box}(u; \delta u, \bar{H}^{(ij)} \cdot X + u^{s(ij)}) = 0 & \forall \delta u \in \mathbb{U}^{0}_{(D)} \\
 \langle \frac{\delta P}{\delta H} : [\bar{H}^{(ij)} + u^{s(ij)} \otimes \nabla] \rangle_{\Box} : \delta \bar{H} = e_i \otimes e_j : \delta \bar{H} \quad \forall \delta \bar{H} \in \mathbb{R}^{3x3}
\end{cases}$$
(2.3.17)

Hence, the algorithmic compliance tensor reads:

$$d\bar{H} = \underbrace{\left(\sum_{i,j} \bar{H}^{(ij)} e_i \otimes e_j\right)}_{\bar{C}_{\square}} : d\bar{P}$$
(2.3.18)

Remark 5. In practice, we again remark that the relation in (2.3.18) must be solved together with restricts on $d\bar{H}$ and $d\bar{P}$. To be more specific, for small strain kinematics, the relation in (2.3.18) only relate $d\bar{P}$ to the symmetric part of $d\bar{H}$.

Furthermore, dP must be symmetric for the same special case.

2.3.2 Neumann boundary condition

Continuous format

The subscale stress field P can be decomposed into a constant tensor \hat{P} and a fluctuation field P'(X) as $P = \hat{P} + P'$. In this context, the choice $P' \cdot N = 0$ on $\partial \Omega_{\Box}$ defines a piecewise constant traction on the sides of Ω_{\Box} , where it is assumed that traction due to fluctuation field P' is vanished on the $\partial \Omega_{\Box}$. Hence, the boundary condition of Neuman type reduces to:

$$t \doteq P \cdot N = \hat{P} \cdot N \quad \text{on} \quad \partial \Omega_{\Box} \tag{2.3.19}$$

Now, inserting the definition for traction t in (2.2.34) gives:

$$\bar{P} = \frac{1}{|\Omega_{\Box}|} \int_{\partial\Omega_{\Box}} \underbrace{\hat{P} \cdot N}_{t} \otimes X dS = \hat{P} \cdot \frac{1}{|\Omega_{\Box}|} \int_{\partial\Omega_{\Box}} N \otimes X dS = \hat{P}$$
(2.3.20)

where, it is used that $\int_{\partial\Omega_{\square}} N \otimes X dS = |\Omega_{\square}|I.$

Hence, it implies that $\hat{P} = \bar{P}$. Where, as a direct result, it is concluded that the Hill-Mandel microhomogeneity condition is satisfied, s.t.:

$$\frac{1}{|\Omega_{\Box}|} \int_{\partial\Omega_{\Box}} \underbrace{(\bar{P} \cdot N)}_{t} \cdot \delta u dS = \bar{P} : \left(\frac{1}{|\Omega_{\Box}|} \int_{\partial\Omega_{\Box}} \delta u \otimes N dS\right) = \bar{P} : \delta \bar{H},$$
(2.3.21)

In order to establish the appropriate variational format, we introduce the space of admissible microscale displacements

$$\mathbb{U}_{(N)} = \{ u | \int_{\Omega_{\Box}} u d\Omega = 0, (\int [\nabla u]^2 d\Omega)^{\frac{1}{2}} < \infty \}$$
(2.3.22)

and the corresponding space of test functions

$$\mathbb{U}_{(N)}^{0} = \{ u | u = 0 \text{ on } \partial\Omega_{\Box}, (\int [\nabla u]^{2} d\Omega)^{\frac{1}{2}} < \infty \}$$
(2.3.23)

When, the space of constant mean-stress tensors is remained unrestricted as $\mathbb{P}_{(N)} = \mathbb{R}^{3x^3}$. Then, we introduce the variational form:

$$a_{\Box}(u;\delta u) \doteq \frac{1}{|\Omega_{\Box}|} \int_{\Omega_{\Box}} P(H[u]) : H[\delta u] d\Omega, \qquad (2.3.24)$$

The pertinent standard variational format then reads;

For given value of the macroscale \overline{P} , find $u \in \mathbb{U}_{(N)}$ that solves

$$a_{\Box}(u;\delta u) = \bar{P} : \langle H[\delta u] \rangle_{\Box} \quad \forall \delta u \in \mathbb{U}^{0}_{(N)}$$
(2.3.25)

The macroscale algorithmic tangent compliance tensor

Next, it is possible to establish the algorithmic compliance tensor \bar{C}_{\Box} for variation $d\bar{P}$ such that:

$$d\bar{H}^{sym} = \bar{C}_{\Box} : d\bar{P} \tag{2.3.26}$$

In this context, it is concluded that the state equation (2.3.25) must hold for $u \in \mathbb{U}_{(N)}$ as well as $u + du \in \mathbb{U}_{(N)}$, under the condition of variation of $\bar{P} \in \mathbb{R}^{3x3}$ to $\bar{P} + d\bar{P} \in \mathbb{R}^{3x3}$. Hence, it gives:

$$a_{\Box}(u;\delta u) = \bar{P} : \langle H[\delta u] \rangle_{\Box} \quad \forall \delta u \in \mathbb{U}^{0}_{(N)}$$

$$(2.3.27)$$

and,

$$a_{\Box}(u+du;\delta u) = (\bar{P}+d\bar{P}): \langle H[\delta u] \rangle_{\Box} \quad \forall \delta u \in \mathbb{U}^{0}_{(N)}$$
(2.3.28)

Upon subtracting (2.3.27) and (2.3.28) we have;

$$a_{\Box}(u+du;\delta u) - a_{\Box}(u;\delta u) = d\bar{P} : \langle H[\delta u] \rangle_{\Box} \quad \forall \delta u \in \mathbb{U}^{0}_{(N)}$$
(2.3.29)

Since the perturbations du are small the equation (2.3.29) reduces to its tangential format as;

$$a'_{\Box}(u;\delta u,du) = d\bar{P}: \langle H[\delta u] \rangle_{\Box} \quad \forall \delta u \in \mathbb{U}^{0}_{(N)}$$
(2.3.30)

Besides, we introduce nodal variables $\hat{u}^{(ij)}$ that corresponds to "unit macroscale stress gradient", i.e. nodal displacements that correspond to $\bar{P}_{ij} = 1$ which are defined as,

$$du = \sum_{i,j} \hat{u}^{(ij)} d\bar{P}_{ij}, \qquad \text{and} \qquad d\bar{P} = \sum_{i,j} e_i \otimes e_j d\bar{P}_{ij} \qquad (2.3.31)$$

Using the linearity in the tangential format (2.3.30), we arrive at the problem of solving for displacement field as:

find $\hat{u}^{(ij)} \in \mathbb{U}_{(N)}$ such that:

$$a'_{\Box}(u;\delta u,\hat{u}^{(ij)}) = e_i \otimes e_j : \langle H[\delta u] \rangle_{\Box} \quad \forall \delta u \in \mathbb{U}^0_{(N)}$$

$$(2.3.32)$$

Hence, the algorithmic compliance tensor reads:

$$d\bar{H} = \underbrace{\left(\sum_{i,j} \langle H[\hat{u}^{ij}] \rangle_{\Box} e_i \otimes e_j\right)}_{\bar{C}_{\Box}(\bar{P})} : d\bar{P}$$
(2.3.33)

3 Microscale features

3.1 Preliminaries

The representative volume element (RVE) of a material microstructure plays an important role in the analysis of heterogeneous materials, such as composites. A key point in such models is the determination of the appropriate geometry, material model and the RVE size, in order to get a precise representation of materials heterogeneities. Hence, they can take realistic distributions of phases and constitutive models of the heterogeneities into account. In the following sections, the method of subscale simulation consisting of constitutive modeling and RVE generation is described.

3.2 Geometric features

The special case of two dimensional RVE problems are investigated. This simplification leads to computations of surface integrals instead of volume integrals, surface fractions instead of volume fractions and so on.

The heterogeneity of the microstructure is manifested by the presence of "circular inclusions" embedded in a square matrix as a typical RVE. The RVEs are chosen in a 2D square form (cubic in 3D) in order to be able to simply depict a uniform periodically repetitive array of heterogeneities. Upon parametrization of the microstructure's geometry, numbers of typical morphological parameters consisting of volume fraction (V_f) (inclusion volume/total volume), standard deviation of the inclusion radius (σ_r), V_p (total volume/number of inclusions) and RVE size (L_{\Box}) are introduced. In numerical computations, it is required to keep the volume fraction of inclusions fixed to a prescribed percentage. But, since the volume fraction value fluctuates due to the statistical nature of the inclusion sizes, we introduce the expected value for the volume fraction $E[V_f]$ as:

$$E[V_f] = E[\frac{1}{\Omega_{\Box}} \sum_{i=1}^{n_{inc}} \pi r_i^2] = \frac{1}{\Omega_{\Box}} n_{inc} \pi E[r_i^2] =$$

$$\frac{1}{\Omega_{\Box}} n_{inc} \pi E[(r - \mu_r)^2 + 2\mu_r r - \mu_r^2] = \frac{1}{\Omega_{\Box}} n_{inc} \pi [E[(r - \mu_r)^2] + 2\underbrace{E[r]}_{\mu_r} \mu_r - \mu_r^2]$$
(3.2.1)

Whereby $r_i \doteq \mu_r + \sigma_r$ is the radius of the i^{th} inclusion and μ_r and σ_r are the sample mean and the standard deviation, respectively.

Thus the volume fraction is defined based on the mean value μ_r and standard deviation σ_r of the radius of the inclusions, as follows

$$\bar{V}_f \doteq \frac{1}{\Omega_{\Box}} n_{inc} \pi [\sigma_r^2 + \mu_r^2], \qquad (3.2.2)$$

According to the random positions of inclusions inside the RVE, a proportion of inclusions volume might be not taken into account in the volume fraction due to the intersection of the inclusions and the RVE's boundaries.

To avoid this inconvenience, a special procedure is applied for RVE generation which is explained in detail as following c.f [11].

To this end, a large RVE is generated from where the window was centered in the middle on a offset distance R_{max} , which makes it assured that all the inclusions center are coordinated inside the window. Then, it is possible to compute the RVE size as follows:

- $1.V_f$, σ_r , l_{\Box} is chosen.
- 2. Given V_f , σ_r , the expected value of inclusions radius, E[R] is computed. 2. Given E[R] and σ_r the effect distance R_r is obtained
- 3.Given E[R] and σ_r , the offset distance R_{max} is obtained.

4. Given R_{max} , the required number of inclusions $\left(N_{inc}\right)$ is computed.

5.Given (N_{inc}) , the side length of the RVE, L_{\Box} is finally determined.

Consequently, a unit cell of the side length L_{\Box} is obtained on which the computations is carried out.

The unit cells are then meshed using "Constant Strain Triangles (CST)" which is the simplest possible 2D finite element.



Figure 3.2.1: RVE generation's parameter {Left}, meshed unit cell {Right}

Hence, in order to maintain the accuracy of results as well as to retrieve the prescribed volume fraction the mesh size should be chosen small but yet coarse enough to keep the computational costs reasonable.

3.3 Constitutive model

The constitutive relations

As the prototype model, the "flow plasticity theory" (mixed isotropic and kinematic hardening) is employed, see e.g. [16], in conjunction with the von-Mises yield surface which is the most widely used model within metal plasticity.

Using,

$$\sigma = E^e : \epsilon^e \tag{3.3.1}$$

With

$$E^e = 2GI_{dev}^{sym} + KI \otimes I \tag{3.3.2}$$

 σ may be split as follows:

$$\sigma = \sigma_{dev} + \sigma_m I \tag{3.3.3}$$

Where $\sigma_{dev} = 2G\epsilon^{e}_{dev}$, $\sigma_m = K\epsilon^{e}_{vol}$. In addition, the free energy representing hardening is chosen as follow

$$\psi^{p} = \frac{1}{2}rHk^{2} + \frac{1}{2}[1-r]Ha_{e}^{2} \qquad \text{with} \qquad a_{e} = \sqrt{\frac{2}{3}}|a_{dev}| \qquad (3.3.4)$$

where k and a are isotropic and kinematic hardening variables, respectively. Moreover, H is the constant hardening modulus of the uniaxial stress-strain curve (which is assumed to be bilinear), whereas r is a parameter that controls the relation between isotropic and kinematic hardening. The von Mises yield function with mixed hardening is defined as

$$\Phi = \sigma_e^{red} - \sigma_y - \kappa, \quad \sigma_e^{red} = \sqrt{\frac{3}{2}} |\sigma_{dev}^{red}| \quad with \quad \sigma^{red} \doteq \sigma - \alpha \tag{3.3.5}$$

where σ_e^{red} is the (reduced) equivalent stress, σ_y is the initial yield stress, κ is the "drag stress" due to isotropic hardening, and α is the "back stress" due to the kinematic hardening. Whereas the dissipative stresses are defined as;

$$\kappa = -\frac{\partial \psi^p}{\partial k} = -rHk, \qquad \qquad \alpha = -\frac{\partial \psi^p}{\partial a} = -\frac{2}{3}[1-r]Ha_{dev} \qquad (3.3.6)$$

Associative flow and hardening rules

The associative flow and hardening rules for the considered model are give as:

$$\dot{\boldsymbol{\epsilon}}^{p} = \lambda \boldsymbol{\nu} \quad \text{with} \quad \boldsymbol{\nu} \doteq \frac{\partial \Phi}{\partial \boldsymbol{\sigma}} = \frac{3}{2\sigma_{e}^{red}} \boldsymbol{\sigma}_{dev}^{red}$$
 (3.3.7)

$$\dot{k} = \lambda \zeta_k \quad \text{with} \quad \zeta_k \doteq \frac{\partial \Phi}{\partial \kappa} = -1$$
 (3.3.8)

$$\dot{\alpha} = \lambda \zeta_{\alpha} \quad \text{with} \quad \zeta_{\alpha} \doteq \frac{\partial \Phi}{\partial \alpha} = -\frac{3}{2\sigma_e^{red}} \sigma_{dev}^{red} = -\nu$$
 (3.3.9)

or

$$\dot{\boldsymbol{\epsilon}}^{p} = \lambda \frac{3}{2\sigma_{e}^{red}} \boldsymbol{\sigma}_{dev}^{red}, \qquad \dot{\boldsymbol{k}} = -\lambda, \qquad \dot{\boldsymbol{\alpha}} = -\lambda \frac{3}{2\sigma_{e}^{red}} \boldsymbol{\sigma}_{dev}^{red} = -\dot{\boldsymbol{\epsilon}}^{p} \qquad (3.3.10)$$

Where the plastic multiplier λ is determined by complementarity conditions

$$\lambda \ge 0,$$
 $\Phi(\boldsymbol{\sigma}) \le 0,$ $\lambda \Phi(\boldsymbol{\sigma}) = 0,$ (3.3.11)

By introduction of kinematic hardening, it is possible to simulate the Bauschinger effect, i.e. that the yield stress in compression, upon reversed loading from tension, is smaller than it was in tension.

4 Construction of yield surface

4.1 Preliminaries

The "yield strength" of a material is defined as a stress level at which the material begins to deform plastically. Prior to this point the material deformation returns to its original configuration, after removing the applied stress or on the other hand it deforms Elastically. But, as the stress reaches the yield strength the material deformation becomes plastic, i.e. some fractions of deformation remains at the loading stage configuration after the stress removal.

In three dimensional space of the principal stresses (P_1, P_2, P_3) , an infinite sets of yield strength points forms together a yield surface. In this paper for simplicity's sake, the principal stresses space is reduced to a two dimensional space (P_1, P_2) by imposing plane stress scenario on the microscale problem.

Knowledge

an upper limit to the load that can be applied, before plastic deformation. It is also important for the control of many materials production techniques such as forging, rolling or pressing.

The following section describes an approach which is used, in order to construct computable upper and lower bounds for the macroscopic yield surfaces associated with two imposed (Dirichlet and Neumann) boundary conditions .

4.2 Computational strategy based on random realizations on finite-sized RVE

4.2.1 Preliminaries

In this section, we consider a realization on Ω_{\Box} with a priori chosen RVE size on which the following described computations are carried out for two different cases of Dirichlet an Neumann boundary conditions.

As mentioned earlier, in order to construct the yield surface in the plane of principal stresses it is required to specify infinite numbers of yield strength points on the plane. To this end, sufficiently large numbers of straight stress paths corresponding to various angles α are defined in the principal stress space (P_1, P_2) by incrementing the applied stress, until a certain predefined criterion of yielding is satisfied. These obtained yield points can then be combined to render the initial yield surface.

For the given realization, the macroscale stress \bar{P} with angle α is defined as:

$$\bar{P}(\alpha, \hat{P}) = \mathbb{I}_{\alpha} \cdot \hat{P} \tag{4.2.1}$$

whereby, \mathbb{I}_{α} is introduced as :

$$\mathbb{I}_{\alpha} \doteq \cos(\alpha) e_I \otimes e_I + \sin(\alpha) e_{II} \otimes e_{II} \tag{4.2.2}$$

so that tensor \mathbb{I}_{α} , with $||\mathbb{I}_{\alpha}|| = 1$, represents the given direction and \hat{P} denotes the corresponding stress magnitude.

4.2.2 Offset Yield Point criterion

The next step is to introduce a criterion, in order to calculate the macroscopic yield point. According to the given material model, it is noticed that the yield point is not easily defined based on the shape of stress strain curve, as shown in Fig.(4.2.1). In this regard, the "Offset yield point" is arbitrarily defined. The value for this is commonly set at 0.2% of the macroscopic plastic strain. It is assumed that all constituents have entered the plastic regime when this stress is reached.



Figure 4.2.1: "Offset Yield Strength" criterion for the deformation of the yield stress.

Hence, for a given angle α , it is assumed that \hat{P}_y is defined as the state, when the effective plastic strain, denoted by $||\bar{H}^p||$, reaches the offset yield point \bar{H}^p_y , see Fig.(4.2.2) Then, it is possible to define the macroscopic plastic strain by "Offset-length" as:

$$\bar{\epsilon}^p(\bar{H},\hat{P}) \doteq ||\bar{H}^p|| \tag{4.2.3}$$

where the measure $\bar{\epsilon}^p$ is defined as:

$$\bar{\epsilon}^p(\bar{H},\hat{P}) \doteq ||\bar{H} - \bar{C}_{\Box,(0)}:\bar{P}||^1$$
(4.2.4)

for $\bar{P} = \mathbb{I}_{\alpha} \cdot \hat{P}$. whereby, $\bar{C}_{\Box,(0)} \doteq \bar{C}_{\Box}(0)$ is the (constant) elastic compliance tensor, obtained as $\hat{P} = 0$ for the given realization.

Remark 6. The strain tensor $\overline{C}_{\Box,(0)}$: \overline{P} is the elastic strain provided that no reversed plastic loading occurs on the subscale upon removal of the applied stress \overline{P} .

4.2.3 In-elastic strain control algorithm

In order to compute the macroscopic plastic strain corresponding to the yield point, it is possible to treat \bar{H}^p as a "time-like" variable, $0 \leq ||\bar{H}^p|| \leq \bar{H}^p_y$. In this context, since $||\bar{H}^p||$ is zero until a certain stage of loading is reached, we just increase the stress by predefined loading steps until $||\bar{H}^p||$ reaches a point where $||\bar{H}^p|| \geq 0$.

Thereafter, it is possible to compute the targeted value of \hat{P} that corresponds exactly to the value of \bar{H}_{y}^{p} , by implementing a Newton-Raphson method.

¹All the norms used in the thesis are of L_2 type.



Figure 4.2.2: Development of plastic strain \bar{H}^p vs \hat{P} associated with Dirichlet and Neumann conditions, $\hat{P} \leq \hat{P}_{el}$ when $||\bar{H}^p|| = 0$ and $\hat{P} = \hat{P}_y$ when $||\bar{H}^p|| = \bar{H}_y^p$, angle $\alpha = 0$.

Remark 7. The load magnitude \hat{P}_{el} when $||\bar{H}^p|| = 0$ denotes the elastic limit load, which corresponds to the state when plastic yielding first occurs anywhere within the RVE.

4.2.4 Tangent formula

Upon employing the Newton-Raphson method, to solve the In-elastic strain control problem, we introduce a residual associated with the state when the Offset-length is equal to 0.2% of the macroscopic plastic strain as;

For given angle α , find $\hat{P} \in \mathbb{R}^{2x^2}$ that solves:

$$\operatorname{Res} = \|\bar{H}_{\Box}(\mathbb{I}_{\alpha} \cdot \hat{P}) - \bar{C}_{\Box,(0)} : \mathbb{I}_{\alpha} \cdot \hat{P}\| - 0.002$$
(4.2.5)

For small variation of $d\hat{P} \in \mathbb{R}^{2x^2}$ the tangent form then reads;

$$J(\bar{P}) = \frac{\bar{H}_{\Box}(\mathbb{I}_{\alpha} \cdot \bar{H}) - \bar{C}_{\Box,(0)} : \mathbb{I}_{\alpha} \cdot \hat{P}}{\|\bar{H}_{\Box}(\mathbb{I}_{\alpha} \cdot \bar{H}) - \bar{C}_{\Box,(0)} : \mathbb{I}_{\alpha} \cdot \hat{P}\|} : \left(\left[\bar{C}_{\Box}(\mathbb{I}_{\alpha} \cdot \hat{P}) - \bar{C}_{\Box,(0)} \right] : \mathbb{I}_{\alpha} \right),$$
(4.2.6)

Where \bar{C}_{\Box} denotes the macroscale algorithmic compliance tensor, which is computed for two different cases of Dirichlet and Neumann boundary conditions c.f (2.3.18) and (B.2.4).

4.3 Alternative bounds

As it can be seen later, the order of constructed upper and lower bounds on the yield surface, associated with the prolongation conditions, is sensitive to the combination of material properties of the constituents which compose the composite under consideration. Therefore, these bounds don't satisfy the requirements based on having two consistent bounds on the yield surface. furthermore, there may be intersections between these bounds for specific combinations of material properties. In order to investigate the possibility to establish two consistent bounds on the yield surface, we resort to the definition of Offset-length (eq. 4.2.4) as:

$$\bar{\epsilon}^{p}(\bar{H},\hat{P}) \doteq ||\bar{H}^{p}|| = ||\bar{H} - \bar{C}_{\Box,(0)} : \bar{P}||$$
(4.3.1)

squaring of both sides of the equation gives:

$$||\bar{H}^{p}||^{2} = ||\bar{H} - \bar{C}_{\Box,(0)} : \bar{P}||^{2} = \underbrace{||\bar{H}||^{2}}_{\bar{H}^{tot}} - \underbrace{2\bar{H} : \bar{C}_{\Box,(0)} : \bar{P}}_{assume=2||\bar{H}|| \ ||\bar{C}_{\Box,(0)} : \bar{P}||} + \underbrace{||\bar{C}_{\Box,(0)} : \bar{P}||^{2}}_{\bar{H}^{el}}$$
(4.3.2)

where, it is assumed that the term $\overline{H}: \overline{C}_{\Box,(0)}: \overline{P}$ is greater than zero.

Then, considering the results associated with imposing two classical prolongation condition, the widest possible bounds on the yield surface can be constructed, such as:

$$||\bar{H}_{min}^{tot}||^{2} - 2||\bar{H}_{max}^{tot}|| ||\bar{H}_{max}^{el}|| + ||\bar{H}_{min}^{el}||^{2} \le ||\bar{H}^{p}||^{2} \le ||\bar{H}_{max}^{tot}||^{2} - 2||\bar{H}_{min}^{tot}|| ||\bar{H}_{min}^{el}|| + ||\bar{H}_{max}^{el}||^{2}$$

$$(4.3.3)$$

where the maximum and minimum values of strain in equation (4.3.3) are obtained by comparison between associated effective values in Dirichlet and Neumann boundary condition computations. From now on we're calling these bounds "Extremum alternative bounds".

Next, it remains to compute the yield point \hat{P}_y as the state, when the macroscopic plastic strain, \bar{H}^P reaches the offset yield point. To this end, again the "time-like" approach, discussed in section (4.2.3), is employed in the sense that we increase the applied stress by predefined loading steps and obtain the development of plastic strain \bar{H}^p versus the applied stresses. Then, interpolating the plastic strain's path for the offset yield point, we calculate the corresponding yield stress \hat{P}_y .

In order to investigate the possibility of constructing two sharper bounds which are still consistent, we consider the behavior of two other alternative bounds by replacing the average strain in the bound's definitions as:

$$||\bar{H}_{min}^{tot}||^{2} - 2||\bar{H}_{avg}^{tot}|| ||\bar{H}_{avg}^{el}|| + ||\bar{H}_{min}^{el}||^{2} \le ||\bar{H}_{max}^{tot}||^{2} - 2||\bar{H}_{avg}^{tot}|| ||\bar{H}_{avg}^{el}|| + ||\bar{H}_{max}^{el}||^{2}$$

$$(4.3.4)$$

where $\bar{H}_{avg}^{tot} = \frac{\bar{H}_{max}^{tot} + \bar{H}_{min}^{tot}}{2}$ and $\bar{H}_{avg}^{el} = \frac{\bar{H}_{max}^{el} + \bar{H}_{min}^{el}}{2}$. From now on we're calling these bounds "Averaged alternative bounds".

Again, adopting the same strategy as already discussed we calculate the yield point corresponding each angle in the principle stress plane.

Remark 8. One drawback concerning the construction of the alternative bounds is the more expensive computational costs might be spent than the regular bounds, which is due to employing interpolation technique instead of Newton-Raphson method in order to compute the value of \hat{P}^{y} corresponding to the value of \overline{H}_{μ}^{p} .

4.4 Construction of a macroscopic yield surface

After defining the yield surface construction algorithm for a single realization, we thus aim at studying the macroscopic upper and lower bounds associated with the two prolongation conditions and also the alternative bounds introduced earlier, c.f section (4.3).

Since the yield surfaces can not be defined analytically, therefore, it is not possible to predict their behavior associated with each bound a priori. Thus it is only possible to study the surfaces numerically by computing the pertinent mean value surface and corresponding upper and lower bounds for the given confidence interval.

Mean value and Confidence interval

Upon performing numerical evaluation of the yield value of \hat{P} , denoted \hat{P}_y , based on finite number of random realizations of the RVE topology, it is required to investigate the reliability of our estimate for the given confidence. To this end, we aim at studying the macroscopic upper \hat{P}_{y}^{UB} and the lower bound \hat{P}_{y}^{LB} such that, independently for each of bounds we obtain;



$$\hat{P}_y^{LB} \le \hat{P}_y \le \hat{P}_y^{UB} \tag{4.4.1}$$

Figure 4.4.1: Example of the mean value yield surface and corresponding bounds associated with the Dirichlet boundary condition (the bounds reflect a 99% confidence level)

The surfaces can be specified as the statistical averaging of sufficiently large number of realization. Upon using the following statistical equation :

$$|E[\bar{P}_y\{\bar{P},\tilde{\omega}\}] - \mu[\bar{P}_y\{\bar{P},\omega_i\}_{i=1}^N]| \le c\left[[\bar{P}_y\{\bar{P},\omega_i\}_{i=1}^N],P\right],$$
(4.4.2)

where ω_i denotes one realization of the stochastic process $\tilde{\omega}$ and E is the expected value for the macroscopic yield stress which is defined as follows:

$$E[\bar{P}_y\{\bar{P},\tilde{\omega}\}] \doteq \lim_{N \to +\infty} \frac{1}{N} \sum_{i=1}^N \bar{P}_{y,i}\{\bar{P},\tilde{\omega}\}$$
(4.4.3)

The direct result of the above equality leads to the bounding of E as:

$$\bar{P}_y^{LB} \le E[\bar{P}^y\{\bar{P},\tilde{\omega}\}] \le \bar{P}_y^{UB},\tag{4.4.4}$$

where the upper bound(UB) and the lower bound(LB) are defined as follows :

$$\bar{P}_{y}^{UB} \doteq \mu[\bar{P}_{y}\{\bar{P},\omega_{i}\}_{i=1}^{N}] + c\left[[\bar{P}_{y}\{\bar{P},\omega_{i}\}_{i=1}^{N}],P\right],$$

$$\bar{P}_{y}^{LB} \doteq \mu[\bar{P}_{y}\{\bar{P},\omega_{i}\}_{i=1}^{N}] - c\left[[\bar{P}_{y}\{\bar{P},\omega_{i}\}_{i=1}^{N}],P\right],$$
(4.4.5)

Note that if the number of realization increases the equality holds for smaller values of confidence interval, which leads us to the sharper and more rigorous bounds. In the optimum case $(N \to \infty)$, the expected value, E, will be equal to the mean value, $\mu(c[\bullet, P] = 0)$, where $c[\bar{P}_i^y, P]$ denotes confidence interval which assures that the certain probability (P) of the realizations are inside the specified bounds. At the present paper the confidence interval is set to 99%.

5 Numerical results

Subscale modeling

As discussed earlier we consider a microstructure composed of a matrix with monolithic material into which circular (in 2D) particles embedded, where the flow plasticity theory is employed to model both of microconstituent's material behavior. In the present examples, the materials under consideration composed of stiffer inclusions than the matrix it is embedded in. It is noted that the material properties adopted herein the examples are just for numerical purposes.

In order to investigate a proper size and number of realizations of RVEs, to be able to approximate the true material's macrostructure, we consider the behavior of yield stress response, pertinent to a specific angle in the principal stress plane, versus various RVE sizes and also various number of realizations, respectively.

Successively, the introduced bounds are constructed on the yield surface of the given heterogenous material and compared to find the most consistent and accurate of them.

5.1 Computational example 1

Material properties of the microstructure

The isotropic bulk material of the composite's matrix is modeled using young's modulus $E_m = 200Gpa$, poisson's ratio $\nu_m = 0.3$, constant hardening modulus $H_m = (0.2 \cdot E_m)$ and the control variable $r_m = 0.8$, where the inclusions as the stiffer components are modeled using young's modulus $E_i = 300Gpa$, poisson's ratio $\nu_i = 0.202$, constant hardening modulus $H_i = (0.2 \cdot E_i)$ and the control variable $r_i = 0.8$.

Both materials are assumed to satisfy the von-Mises yield criterion with mixed isotropic and kinematic hardening and associated flow rules when yield strength for matrix and inclusion's materials are $\sigma_m^y = 300Mpa$ and $\sigma_i^y = 1000Mpa$, respectively.

Statistical properties of the microstructure

In order to establish the statistical properties of an RVE's topology, we introduce the predefined morphological parameters of the unit cell according to the section (3.2) as:

Volume fraction $V_f = 30\%$, standard deviation of inclusion's radius $\sigma_r = 0.01 \mu m$ and centered windows's side length (according to section's computation) $l_{\Box} = 2\mu m$ which gives the unit cell's side length $L_{\Box} \simeq 2.27 \mu m$.



Figure 5.1.1: Example of microstructure on an RVE with random distribution of particles $\{Right\}$ and statistical parameter's presentation of an RVE's topology $\{Left\}$

The key point in the proposed strategy is the choice of the proper RVE-size and number of realizations of the unit cell's topology in order to obtain the sharpest (most accurate) possible bounds on the yield surface where the computational costs are still reasonable. Owing to study the accuracy of results, we evaluate the expected yield stress response versus different RVE's sizes and different number of realizations, respectively.

It is expected that for sufficiently large unit cells, the prolongation conditions responses converge to the same results. The same behavior is anticipated for increasing in the number of realizations. To this end, we proceed by studying the expected mean value of the yield strength response from RVEs of different sizes based on 25 realizations of the topology when the stress's path angle in the principal plane stress is set on $\alpha = 0$.

The figure (5.1.2) shows that the bounds constructed on the yield surface tend to create sharper bounds as the size of RVE increases. It can be seen that increasing the RVE's side length, the desired accuracy for responses occurs when $L_{\Box} \simeq 2.27$.

The same strategy is employed in order to investigate the proper realization number, in the sense that this time we evaluate the expected mean value of the yield strength response versus different number of realizations when the stress path and RVE length side are set to $\alpha = 0$ and $L_{\Box} \simeq 2.27$, respectively.

As can be seen in Fig. (5.1.3), if we use sufficiently large numbers of realizations, which is $N_{\alpha} = 25$ in this case, the results converge to very close responses.

Also note that σ_{ref} were chosen so that the upper confidence bound is one at the fourth data point. Similarly, \mathbf{L}_{ref} is chosen so that the side length of the unit cell is ten at the last data point.



Figure 5.1.2: The figure shows the sensitivity of yield strength to RVE sizes. Number of realizations $N_{\alpha} = 25$, angle $\alpha = 0$. The upper blue solid line represents the sample mean value for the Dirichlet boundary condition and the red solid line corresponds to the sample mean value for the Neumann boundary condition. The black diamond-marked line represents the upper confidence interval and the circle-marked line represents the lower confidence interval associated with the upper and lower bounds introduced in equation (4.3.3).



Figure 5.1.3: The figure shows the sensitivity of yield strength to number of realizations. RVE side length $L_{\Box} \simeq 2.27$, angle $\alpha = 0$. The blue solid line represents the sample mean value for the Dirichlet boundary condition and the red solid line corresponds to the sample mean value for the Neumann boundary condition. The black diamond-marked line represents the upper confidence interval and the circle-marked line represents the lower confidence interval associated with the upper and lower bounds introduced in equation (4.3.3).

Computational results

Therefore, in order to perform ensemble averages and constructing the bounds on the yield surface, concerning every angle's computations, we generate $N_{\alpha} = 25$ unit cell realizations of side length $L_{\Box} \simeq 2.27$. Rendering the obtained yield points according to sufficiently large number of stress paths, the associated yield bounds are constructed, Fig. (5.1.4).



Figure 5.1.4: Yield surface bounds. The upper blue solid line represents the sample mean value for the Dirichlet boundary condition and the red solid line corresponds to the sample mean value for the Neumann boundary condition. The black diamond-marked line represents the upper confidence interval and the circle-marked line represents the lower confidence interval associated with the upper and lower bounds introduced in equation (4.3.3) {left} and equation(4.3.4) {right}, respectively.

Concerning the shape of the yield surface, our investigation highlights the fact that the generated macroscopic probability yield bounds do generally follow a von Mises-type criterion.

However, according to Fig. (5.1.4), it is concluded that the surface associated with Dirichlet boundary condition yields the outer surface (upper bound) relative to the surface constructed by imposing the Neumann boundary condition.

Obviously, this results is case sensitive, in the sense that if we consider a composite with different combinations of matrix and particle's material properties, the bounds order concerning two prolongation conditions may be different.

In order to investigate this phenomena we present the next example where the composite composed of particles of higher stiffness with low yield strength and a monolithic compliant matrix with high yield strength.

Generally, the main concern in constructing the bounds is establishing two consistent and distinguished upper and lower bound without any risk of intersection between them for various combination of constituent's material properties.

To this end, we also observe the behavior of bounds introduced in equations (4.3.3) and (4.3.4) in comparison with the prolongation condition's yield surfaces.

5.2 Computational example 2

Material properties of the microstructure

The isotropic bulk material of the heterogeneous material's matrix is modeled using young's modulus $E_m = 200Gpa$, poisson's ratio $\nu_m = 0.3$, constant hardening modulus $H_m = (0.2 \cdot E_m)$ and the control variable $r_m = 0.8$, where the inclusions are modeled using young's modulus $E_i = 900Gpa$, poisson's ratio $\nu_i = 0.202$, constant hardening modulus $H_i = (0.2 \cdot E_i)$ and the control variable $r_i = 0.8$.

Also, similar to example 1, both materials are assumed to satisfy the Von-mises yield criterion with mixed isotropic and kinematic hardening when yield strength for matrix and inclusions are $\sigma_m^y = 2000Mpa$ and $\sigma_i^y = 200Mpa$, respectively.

Statistical properties of the microstructure

In this example, we introduce similar morphological parameters of the unit cell as in example 1, so that:

Volume fraction $V_f = 30\%$, standard deviation of inclusion's radius $\sigma_r = 0.01 \mu m$ and centered windows's side length (according to section's computation) $l_{\Box} = 2\mu m$ which gives the unit cell's side length $L_{\Box} \simeq 2.27 \mu m$.

Besides, investigating the proper RVE size and number of realizations leads to the same result as the previous example, such that; $L\Box \simeq 2.27$ and $N_{\alpha} = 25$. See figures (5.2.1) and (5.2.2).

Also note that σ_{ref} were chosen so that the upper confidence bound is one at the fourth data point. Similarly, L_{ref} is chosen so that the side length of the unit cell is ten at the last data point.



Figure 5.2.1: The figure shows the sensitivity of yield strength to RVE sizes. Number of realizations $N_{\alpha} = 25$, angle $\alpha = 0$. The blue solid line represents the sample mean value for Dirichlet boundary conditions and the red solid line corresponds to the sample mean value for Neumann boundary conditions. The black diamond-marked line represents the upper confidence interval and the circle-marked line represents the lower confidence interval associated with the upper and lower bounds introduced in equation (4.3.3)



Figure 5.2.2: The figure shows the sensitivity of yield strength to number of realizations. RVE side length $L_{\Box} \simeq 2.27$, angle $\alpha = 0$. The blue solid line represents the sample mean value for the Dirichlet boundary condition and the red solid line corresponds to the sample mean value for the Neumann boundary condition. The black diamond-marked line represents the upper confidence interval and the circle-marked line represents the lower confidence interval associated with the upper and lower bounds introduced in equation (4.3.3)

Computational results

We successively construct the bounds as we treated in the previous example with $N_{\alpha} = 25$ unit cell realizations of side length $L_{\Box} \simeq 2.27$ concerning every angle's computations, Fig. (5.2.3).



Figure 5.2.3: Yield surface bounds. The upper blue solid line represents the sample mean value for the Dirichlet boundary condition and the red solid line corresponds to the sample mean value for the Neumann boundary condition. The black diamond-marked line represent the upper confidence interval and the circle-marked line represent the lower confidence interval associated with the upper and lower bounds introduced in equation (4.3.3) {left} and equation(4.3.4) {right}, respectively.

We observe that this time, unlike the results in example 1, the surface associated with Neumann

boundary condition yields the outer surface (upper bound) relative to the surface established by imposing the Dirichlet boundary condition.

But, investigating the introduced bounds of equations (4.3.3) and (4.3.4) in figures (5.1.4) and (5.2.3), we realize that they behave consistently, in the sense that the sequence of bounds doesn't change for various composites.

Although, these bounds are not as sharp as the bounds associated with two prolongation conditions are but it is noticed that bounds related with equation (4.3.4) are sharper than those introduced in equation (4.3.3).

6 Conclusions and outlook

We have developed a strategy to establish macroscopic yield surfaces for a heterogeneous material, with non-uniform distribution of constituents, undergoing in-elastic deformation at small strains. Adopting conventional first order homogenization, the effective properties of the material is characterized via subscale boundary value problems on Representative Volume Elements (RVE's). In this context, two classical choices of prolongation conditions are investigated; Dirichlet boundary condition and Neumann boundary condition. The main focus was put on the possibility to construct two consistent and distinguished bounds on the macroscopic yield surface employing these two classical boundary conditions. From the numerical results we choose a proper RVE size and number of realizations, in order to satisfy the required accuracy of the results.

Successively, we investigate the results in two examples. The examples considered here, made the differences between two different combination of material properties apparent, in the sense that evaluating surfaces with assumed material properties in Example 1, yields the Dirichlet associated surface as the upper bound. Whereas, the combination of material properties in Example 2 represent a different sequence of bounds.

In this context considering the Extremum and Averaged alternative bounds, we realize that in spite of being wider and consequently less accurate bounds compare to those associated with prolongation condition bounds, we have consistent and reliable bounds on the yield surface.

According to the results, since the Averaged alternative bounds construct sharper surfaces than those created by Extremum alternative bounds, it is concluded that we can use the former surfaces as the alternative bounds for the prolongation condition bounds.

Besides, upon constructing the bounds, we observe that the generated macroscopic yield bounds generally follow a von Mises-type criterion which is in accordance with the employed criterion in the microconstituents material's models.

The developed strategy provides a unified computational tools for the determination of macroscopic yield surface for virtual materials with heterogenous microstructures.

However, several issues remain to be studied in future works. An important one is to investigate more rigorous and/or sharper bounds. Furthermore, validation for "real" material constituents and topology (microscopy pictures,...) including real testing is of a great interest.

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A Appendix A

A.1 Box.I

Compute yield limit along the direction α :

$$\bar{\sigma}(\alpha) \doteq I_{\alpha},$$

 $I_{\alpha} \doteq \left[\cos\alpha, \sin\alpha, 0\right]^{T},$

for $\alpha \in [0, 2\pi]$ 1.Compute initial guess $\bar{\sigma}_{0,2}^{(0)}$ and elastic compliance :

1.1. Until
 $\bar{\epsilon}>0$

$$\bar{\sigma}_{0.2}^{(0)} = \bar{\sigma},$$
 (A.1.1)

1.1.1.Compute $\bar{\epsilon}^p = \bar{\epsilon}^p(\bar{\sigma}, I_\alpha)$

1.1.1.1.Compute $\bar{\sigma}_{\Box}$, $\bar{\epsilon}_{\Box}$,

 $\label{eq:constraint} \begin{array}{cc} 1.1.1.2. \text{if} \ \bar{\sigma} = 0 & \text{then}, \quad C_0 = C \\ 2. \text{Until} \ \bar{\epsilon}^p = 0.2\% \end{array}$

2.1. Compute $\bar{\epsilon}^p = \bar{\epsilon}^p(\bar{\sigma}, I_\alpha)$

2.1.1.Compute $\bar{\sigma}_{\Box}$, $\bar{\epsilon}_{\Box}$,

2.2.Update $\bar{\sigma}_{0.2} \Leftarrow \bar{\sigma}_{0.2} + \Delta \bar{\sigma}_{0.2}$

$$\Delta \bar{\sigma}_{0.2} \doteq -(R^{-1})J,\tag{A.1.2}$$

A.2 Dirichlet boundary condition Algorithm

1.Box.I 2.Initial Guess $u^{(0)}$ 3.Until ||R|| < TOL3.1.Compute $Res = \begin{bmatrix} f_{int,I} \\ B_{\epsilon}^T f_{int,c} \end{bmatrix} - \begin{bmatrix} \underline{0} \\ \overline{\sigma} \end{bmatrix}$ 3.2.Update $u = u + \Delta u$, $\Delta u = -[\mathbb{K}_t]^{-1}Res$, $\mathbb{K}_t = \begin{bmatrix} \mathbb{K}_{II} & \mathbb{K}_{IB}B_{\epsilon} \\ B_{\epsilon}^T \mathbb{K}_{BI} & B_{\epsilon}^T \mathbb{K}_{BI}B_{\epsilon} \end{bmatrix}$, $K = K_{global}$,

4. Compute $\bar{\sigma}_{\Box}$, $\bar{\epsilon}_{\Box}$, C where

$$C = -[E]^{-1},$$

$$E = B_{\epsilon}{}^{T} \mathbb{K}_{BI} \hat{u}_{i} + \mathbb{K}_{BB} B_{\epsilon},$$

$$\hat{u}_{i} = -[\mathbb{K}_{II}]^{-1} \mathbb{K}_{IB} B_{\epsilon},$$

A.3 Neumann boundary condition Algorithm

1.Box. I 2.Initial Guess $u^{(0)}$ 3.Until
 $||{\cal R}|| < TOL$

3.1.Compute
$$Res = f_{int,I}C_H[I_\alpha \bar{\sigma}]$$

3.2. Update
 $u=u+\Delta u$,

$$\Delta u = -[K_{global}]^{-1} Res,$$

4. Compute $\bar{\sigma}_{\Box}$, $\bar{\epsilon}_{\Box}$, C where

$$C = C_{H}{}^{T} [\tilde{K}_{BB}]^{-1} C_{H},$$

$$\tilde{K}_{BB} \doteq K_{BB} - K_{BI} K_{II}{}^{-1} K_{IB},$$

$$\bar{\sigma}_{\Box} \doteq \frac{1}{|\Omega_{\Box}|} \sum_{n=1}^{nrelem} \sigma_{e} |\Omega_{e}|,$$

$$\bar{\epsilon}_{\Box} \doteq \frac{1}{|\Omega_{\Box}|} \sum_{n=1}^{nrelem} \epsilon_{e} |\Omega_{e}|,$$

B Appendix B

B.1 Matrix Discretization DBC

The following chapter considers the discrete form of RVE problem equations.

First the displacement field is divided into two parts associated with internal nodes (u_I) and the boundary nodes (u_B) , as shown :

$$u = \begin{bmatrix} u_I \\ u_B \end{bmatrix},\tag{B.1.1}$$

(Considering $u_I \in \Omega$ and $u_B \in \partial \Omega$)

Introducing the sensitivity field denoting by $\hat{\bullet}$, (which means the change of value of interest by corresponding unit perturbation).

Thus the displacement field can be written as follows :

$$u = \begin{bmatrix} u_I \\ \hat{u}_M \bar{H}^{sym} \end{bmatrix}, \tag{B.1.2}$$

Respectively, the force vector and associated tangent of discretized microstructure can be discretized in a same manner :

$$f = \begin{bmatrix} f_I \\ f_B \end{bmatrix}, \tag{B.1.3}$$

$$\mathbb{K} = \begin{bmatrix} \mathbb{K}_{II} & \mathbb{K}_{IB} \\ \mathbb{K}_{BI} & \mathbb{K}_{BB} \end{bmatrix},$$
(B.1.4)

Here the displacement field changes are stated in forms of the macroscopic strain change by utilizing the sensitivity field.

$$du^{M,i} = \hat{u}^{M,i} d\bar{H},\tag{B.1.5}$$

$$du^{M,b} = \hat{u}^{M,b} d\bar{H},\tag{B.1.6}$$

$$du^{s,i} = \hat{u}^{s,i} d\bar{H},\tag{B.1.7}$$

$$du^{s,b} = 0, (B.1.8)$$

As indicated before, $u^{s,b} = 0$, which means there is no fluctuation field in the boundary nodes according to D.B.C.

Considering that the displacement field can be split down additively, the total displacement for both internal and the boundary nodes can be stated as:

$$du^{i} = \left[du^{M,i} + du^{s,i} \right] = \left[\hat{u}^{M,i} + \hat{u}^{s,i} \right] d\bar{H}, \tag{B.1.9}$$

$$du^{b} = \left[du^{M,b}\right] = \left[\hat{u}^{M,b}\right] d\bar{H},\tag{B.1.10}$$

Note that there is no internal forces (f_{int}^I) related to the free nodes inside the RVE.

Ultimately, the linearized form of the discretization of equation regarding to internal force imposed to the RVE can be specified as:

$$\begin{bmatrix} \mathbb{K}_{II} & \mathbb{K}_{IB}\hat{U}^M \\ (\hat{U}^M)^T \mathbb{K}_{BI} & (\hat{U}^M)^T \mathbb{K}_{BB}\hat{U}^M \end{bmatrix} \begin{bmatrix} U_I \\ \bar{H} \end{bmatrix} = \begin{bmatrix} 0 \\ \bar{P} \end{bmatrix},$$
(B.1.11)

Besides, the internal force related to the free nodes remain constant, such that $(d\underline{f}^i = 0)$. Therefore, two equations extracted form matrix form must be satisfied :

$$\mathbb{K}_{II}U_I + \mathbb{K}_{IB}\hat{U}^M\bar{H} = f^I_{int} = 0, \qquad (B.1.12)$$

$$\mathbb{K}_{BI}U_I + \mathbb{K}_{BB}\hat{U}^M\bar{H} = f^B_{int},\tag{B.1.13}$$

The value of $\hat{U}^{M,(ij)}$ is given explicitly from the coordinates of the nodal points. Consider a typical node located at the local position X_p and the nodal variable $\hat{U}^{\bullet,(ij)}$ associated with the displacement in the direction of e_l for $l \in \{1, 2, ..., NDIM\}$. For instance, $\hat{U}^{M,(ij)}$ can be computed explicitly as:

$$\hat{U}^{M,(ij)} = \left[(X_P)_j - \bar{X}_j \right] e_i.e_l,$$
 (B.1.14)

respectively, it leads us:

$$\hat{U}^{M,(11)} = \left[(X_P)_1 - \bar{X}_1 \right], \tag{B.1.15}$$

$$\hat{U}^{M,(12)} = \left[(X_P)_2 - \bar{X}_2 \right],$$
 (B.1.16)

$$\hat{U}^{M,(21)} = 0, \tag{B.1.17}$$

$$\hat{U}^{M,(22)} = 0, \tag{B.1.18}$$

The last two arguments are set to be zero, since we only study the effects of uniaxial loading imposed in the direction of e_1 , also for K_{BI} and f_{int} we have :

$$\mathbb{K}_{BI} = \frac{1}{|\Omega_{\Box}|} \int B^T D B d\Omega, \qquad (B.1.19)$$

$$f_{int} = \frac{1}{|\Omega_{\Box}|} \int f d\Omega, \qquad (B.1.20)$$

Since $[\hat{U}^M]^T f^B_{int} = \bar{P}$, the second equation can be written as:

$$[\hat{U}^{M}]^{T} \mathbb{K}_{BI} U_{I} + [\hat{U}^{M}]^{T} \mathbb{K}_{BB} \hat{U}^{M} \bar{H} = [\hat{U}^{M}]^{T} f_{int}^{B} = \bar{P},$$
(B.1.21)

Based on what the ATS-tensor definition is, \bar{L} can be defined as shown :

$$d\bar{P} = \bar{L} : d\bar{H},\tag{B.1.22}$$

$$d\bar{P} = [\hat{U}^{M}]^{T} f_{int}^{B} = \underbrace{[\hat{U}^{M}]^{T} [\mathbb{K}_{BI} \hat{U}_{I} + \mathbb{K}_{BB}] \hat{U}^{M}]}_{\bar{L}} : d\bar{H},$$
(B.1.23)

$$\bar{L} = \left[\hat{U}^{M}\right]^{T} f_{int}^{B} = \left[\hat{U}^{M}\right]^{T} \underbrace{\left[\mathbb{K}_{BB} - \mathbb{K}_{BI}\mathbb{K}_{II}^{-1}\mathbb{K}_{IB}\right]}_{\tilde{\mathbb{K}}_{BB}} \left[\hat{U}^{M}\right], \tag{B.1.24}$$

After defining the reduced matrix $\tilde{\mathbb{K}}_{BB}$, the ATS-tensor can be represented in more simplified form as:

$$\bar{L} = [\hat{U}^{M}]^{T} f^{B}_{int} = [\hat{U}^{M}]^{T} \tilde{\mathbb{K}}_{BB} [\hat{U}^{M}], \qquad (B.1.25)$$

B.2 Matrix Discretization NBC

Upon inserting the compliance tensor, the sensitivity fields are identical to DBC format, thus, the perturbation on strain field can be specified as follows:

$$d\bar{H}^{sym} = \bar{\mathbb{C}}_{\square} : d\bar{P} \tag{B.2.1}$$

Moreover, the macroscopic stress tensor perturbation can be characterized in 2D as :

$$d\bar{P} = \sum_{i,j} e_i \otimes e_j d\bar{P}_{ij} \tag{B.2.2}$$

The applied displacement sensitivity field, to define the corresponding compliance tensor is:

$$du = \sum_{i,j} \hat{u}^{(ij)} d\bar{H}_{ij} \tag{B.2.3}$$

Which ultimately gives the definition for $\overline{\mathbb{C}}_{\Box}$ as stated:

$$d\bar{H} = \underbrace{\left(\sum_{i,j} \langle H[\hat{u}^{ij}] \rangle_{\Box} e_i \otimes e_j\right)}_{\bar{\mathbb{C}}_{\Box}(\bar{P})} : d\bar{P}$$
(B.2.4)

We express $\overline{\mathbb{C}}_{\Box}(u; \overline{P})$ in matrix format when macroscopic stress control situation is governing:

$$\bar{\mathbb{C}}_{\Box}(u;\delta\bar{P}) \doteq \langle H \rangle_{\Box} : \delta\bar{P}, \tag{B.2.5}$$

$$= \left[\frac{1}{|\Omega_{\Box}|} \int_{\Gamma_{\Box}} u \otimes N dS\right] : \delta \bar{P}, \tag{B.2.6}$$

$$=\sum_{k=1}^{NVAR_{u,b}} (u^b)_k \left[\underbrace{\frac{1}{|\Omega_{\Box}|} \int_{\Gamma_{\Box}} \phi^b_{\ k} \otimes NdS}_{\mathbb{C}_k} \right] : \delta\bar{P}, \tag{B.2.7}$$

$$=\sum_{k=1}^{NVAR_{u,b}} (\underline{u}^b)_k \underline{C}_k \delta \underline{\overline{P}},$$
(B.2.8)

Thus

$$\bar{\mathbb{C}}_{\Box}(u;\delta\bar{P}) = \sum_{k=1}^{NVAR_{u,b}} \delta\underline{\bar{P}}^T \underline{C}_k(\underline{u}^b)^T, \qquad (B.2.9)$$

¹ Introduce \mathbb{C}_k representation considering that $\dim(\mathbb{C}_k) = 4 \times 4$ as :

$$\underline{C}_{k} = [(\mathbb{C}_{k})_{11} \quad (\mathbb{C}_{k})_{12} \quad (\mathbb{C}_{k})_{21} \quad (\mathbb{C}_{k})_{22}], \qquad (B.2.10)$$

with definition stated as follows:

$$\mathbb{C}_{k} \doteq \left[\frac{1}{|\Omega_{\Box}|} \int_{\Gamma_{\Box}} \phi^{b}{}_{k} \otimes NdS\right], \tag{B.2.11}$$

Respectively, the matrix \mathbb{C} can be defined as:

$$\underline{C}(i,:) \doteq \begin{bmatrix} (\mathbb{C}_i)_{11} & (\mathbb{C}_i)_{12} & (\mathbb{C}_i)_{21} & (\mathbb{C}_i)_{22} \end{bmatrix}, \quad where \quad 1 \leq i \leq NVAR_{u,b} \quad (B.2.12)$$

¹The definition of \mathbb{C} matrix refers to Voigt form of the displacement gradient when multiplying with nodal displacements