

HOMOGENIZATION OF COMPOSITES EMBEDDING GENERAL IMPERFECT INTERFACES

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By
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Homogenization of composites embedding general imperfect interfaces

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We certify that we have read this thesis and that in our opinion it is fully adequate, in scope and in quality, as a thesis for the degree of Master of Science.



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ABSTRACT

HOMOGENIZATION OF COMPOSITES EMBEDDING GENERAL IMPERFECT INTERFACES

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The objective of this work is to present a systematic study on the overall behavior of composites embedding general interfaces between the constituents. The zero-thickness interface model represents a finite-thickness interphase between the constituents. The term *general interface* refers to an interface model that allows for both displacement and traction jumps, unlike cohesive or elastic interface models. To set the stage, a comprehensive study on homogenization is carried out to examine the effects of various representative volume elements (RVE) and boundary conditions on the overall response of composites. Next, we extend the homogenization framework to account for interfaces hence, capturing size effects in both particulate and fiber composites. Two new analytical approaches are developed to determine the overall size-dependent response of composites. The first approach extends the composite sphere assemblage (CSA), composite cylinder assemblage (CCA) and the generalized self-consistent method (GSCM) resulting in bounds and estimates on the macroscopic properties of composites. In the second approach, we generalize the Mori-Tanaka method that not only determines the effective properties but also provides the state of the stress and strain in each phase of the medium including the interface. The proposed analytical results are thoroughly verified via a series of numerical examples using the finite element method.

Keywords: Composites, Homogenization, General interface, Size effects.

ÖZET

GENEL KUŞURLU ARAYÜZ KONULMASI İLE KOMPOZİTLERİN TÜRDEŞLEŞTİRİLMESİ

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Bu çalışmanın amacı, bileşenleri arasına bir genel arayüz koyarak kompozit malzemelerin bir bütün olarak davranışları üzerine sistematik bir çalışma sunmaktır. Sıfır-kalınlıklı arayüz modeli bileşenler arasındaki sonlu-kalınlıklı bir arayüzü temsil etmektedir. *Genel arayüz* modeli, birleştirici veya elastik arayüz modellerinin aksine hem yerdeğişim, hem de çekiş süreksizliğine izin veren bir arayüz modelidir. İlk olarak, birçok farklı temsili hacim ögesinin ve sınır koşullarının, kompozit malzemelerin bir bütün olarak davranışları üzerindeki etkisini inceleme amacıyla türdeşleştirme üzerine kapsamlı bir çalışma yapılmıştır. Daha sonra, türdeşleştirme çerçevesi arayüzleri dahil etmek üzere genişletilmiş, bu sayede iri parçacıklı ve fiber kompozitlerdeki boyut etkileri de yakalanmıştır. Kompozitlerin, bir bütün olarak boyuta bağlı tepkisini belirleyebilmek için iki yeni analitik yaklaşım geliştirilmiştir. Birinci yaklaşım, kompozit küre bir araya getirilmesi, kompozit silindir bir araya getirilmesi ve genel istikrarlı metodu ileri taşıyarak, kompozitlerin makroskopik özellikleri için tahminler ve sınırlar elde edilmesini sağlamıştır. İkinci yaklaşımda ise sadece bütün üzerinde etki eden özellikleri belirlemekle beraber, aynı zamanda arayüz dahil maddenin her fazında gerilme ve gerinim durumlarını tespit eden Mori-Tanaka metodu genelleştirilmiştir. İleri sürülen analitik sonuçlar, sonlu eleman metodunun kullanıldığı bir dizi numerik örnek ile detaylı bir şekilde doğrulanmıştır.

Anahtar sözcükler: Kompozitler, Türdeşleştirme, Genel arayüz, Boyut etkileri.

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Chapter 1

Introduction

Almost all materials possess heterogeneous structures at certain length-scales. Heterogeneous materials possess more complex behavior compared to their associated constituents. Therefore, composites have been the subject of an increasing interest in many engineering applications over the past decades. The mechanical behavior of composites is highly dependent on their micro-structural characteristics such as volume fraction, shape, orientation and distribution of their constituents. Conducting experiments on numerous materials with various phases is not practical. Also, performing a direct numerical simulation on the whole macro-structure with all the heterogeneities would include a huge number of variables which is extremely complicated, if not impossible. As a result, multi-scale methods have been developed to determine the overall response of heterogeneous media in terms of the constitutive behavior of their underlying microstructures. Multi-scale methods are categorized into concurrent methods and homogenization methods. In the concurrent methods [1–4], the problems at the microscopic and macroscopic scales are solved simultaneously, which requires a strong coupling between the two scales. On the other hand, in the homogenization method [5–7], the micro-problem and macro-problem are solved separately. The two main assumptions in the homogenization method are (i) the separation of the length scale between the micro- and macro-problem and (ii) the

energy equivalence between the two scales also known as the Hill–Mandel condition [5, 8]. The homogenization method falls into analytical homogenization and computational homogenization. Pioneering contributions in analytical homogenization include [9–20] and later extended in [21–28]. Despite providing useful information, the analytical homogenization approach requires certain simplifications on the microstructure such as its geometry and distribution pattern. On the contrary, the computational homogenization method is capable of dealing with such complexities, thus it has been widely adopted in the past decades, see [29–43] among others. Detailed reviews on the computational homogenization have been conducted in [44–47]. Computational homogenization is essentially based on calculating the macroscopic quantities from the solution of a boundary value problem at the micro-scale. The average-field theory [48, 49] is employed in order to bridge the microscopic quantities to their macroscopic counterparts. In doing so, the boundary conditions at the micro-scale are chosen such that the Hill–Mandel condition is satisfied. Firooz et al. [50] has conducted a detailed study on both computational and analytical homogenization as well as the influence of boundary conditions and RVE types on the overall behavior of composites. For further details on the formulation, implementation and application of appropriate boundary conditions in the context of the computational homogenization, see [51–57].

A major shortcoming of the classical computational homogenization is that it fails to account for size-dependent material behavior, often referred to as *size effects*. On the other hand, the size effects in composites are essentially attributed to surface [58] and interface effects [59, 60]. As the characteristic length of a heterogeneous structure decreases as in nano-composites, owing to the large area-to-volume ratio, the effects of the surface and interface energy on the overall material response become significant and no longer negligible [61–73], see Fig. 1.1. Comparisons with experiments and atomistic simulations in [74–79] justify that the size effects due to interfaces are physically meaningful. Therefore, it is of great importance to extend the homogenization method to account for the interfaces between the constituents of a micro-structure so as to capture the size effects.

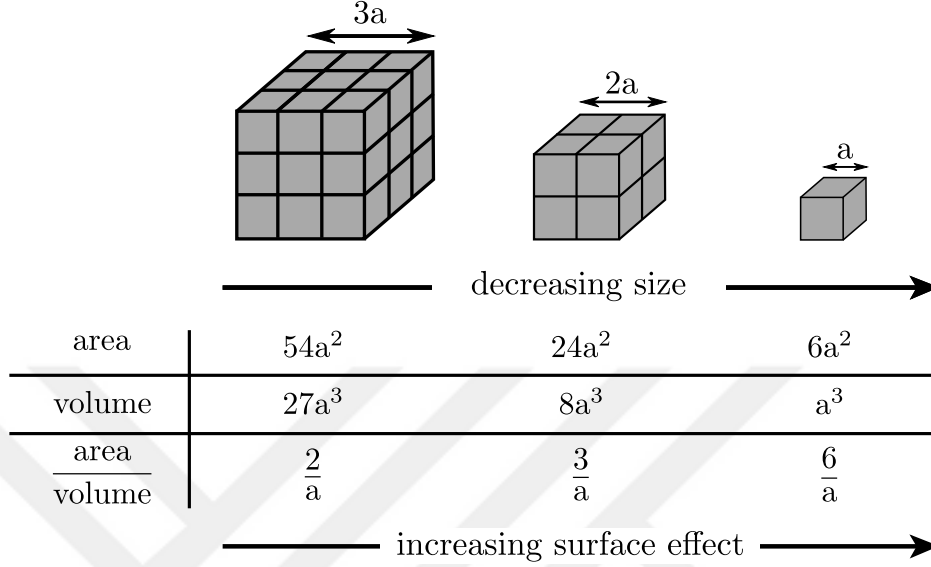


Figure 1.1: Illustration of increasing surface effects when decreasing size.

The term interface here refers to a zero-thickness model characterized by displacement and traction jumps that can sufficiently represent a finite-thickness interphase region. Figure 1.2 illustrates a finite-thickness interphase with its associated zero-thickness interface model for fiber composites and particulate composites. A trivial approach to describe the bonding between the constituents at the micro-scale is to assume perfect bonding. However, the assumption of perfect bonding between the constituents is usually inadequate to describe the mechanical behavior and physical nature of interfaces and therefore, imperfect interface models have been developed. The imperfect interface models can be divided into three categories of cohesive, elastic and general interfaces based on their mechanical behavior as shown in Fig. 1.3. The *elastic interface model* [80–83] allows for a traction jump across the interface due to elasticity along the interface [84] but the interface remains geometrically coherent. Benveniste and Miloh [85], derived the elastic interface conditions based on a formal asymptotic expansion for the stresses and displacements of a thin interphase layer. Sharma et al. [86] used a variational formulation to derive explicit expressions for the elastic state of eigenstrained spherical inclusions embedded in a matrix with elastic interfaces. Later, Sharma and Ganti [87] proposed closed-form expressions for the modified Eshelby’s tensor for cylindrical and spherical inclusions in composites

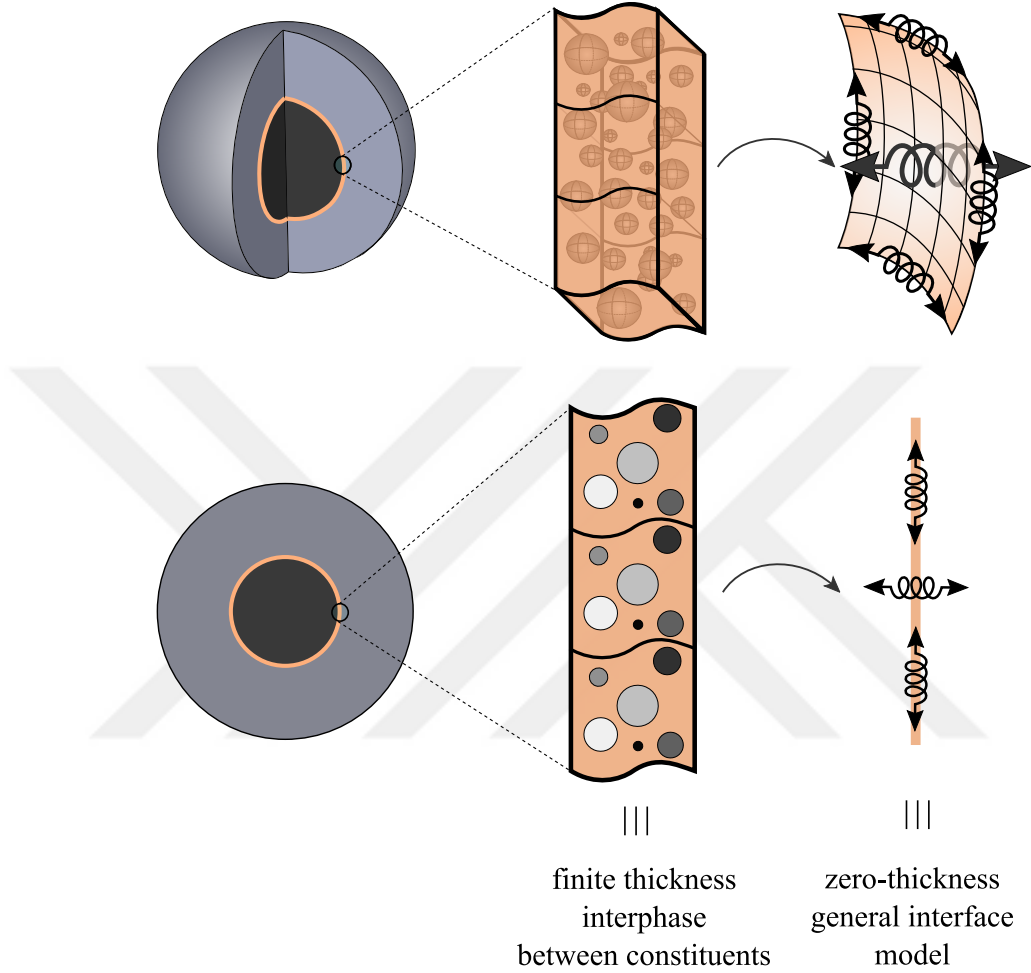


Figure 1.2: Illustration of a finite-thickness interphase with a zero-thickness interface model for both two-dimensional and three-dimensional analysis.

with elastic interfaces, followed by Duan et al. [64]. Exploiting the composite sphere assemblage (CSA) method, the Mori–Tanaka method and the generalized self-consistent method, Duan et al. [88] established a generalized micro-mechanical framework to account for interface stress effects on the effective moduli of composites containing nano-inhomogeneities, see also [89] for nano-voids. Huang and Sun [90] obtained analytical expressions for the effective moduli of particulate composites with elastic interfaces via linearizing a finite deformation theory. Yvonnet et al. [73] established a numerical approach via combining the extended finite element method (XFEM) and the level set method to capture the elastic interface effects. The elastic interface model including three phases

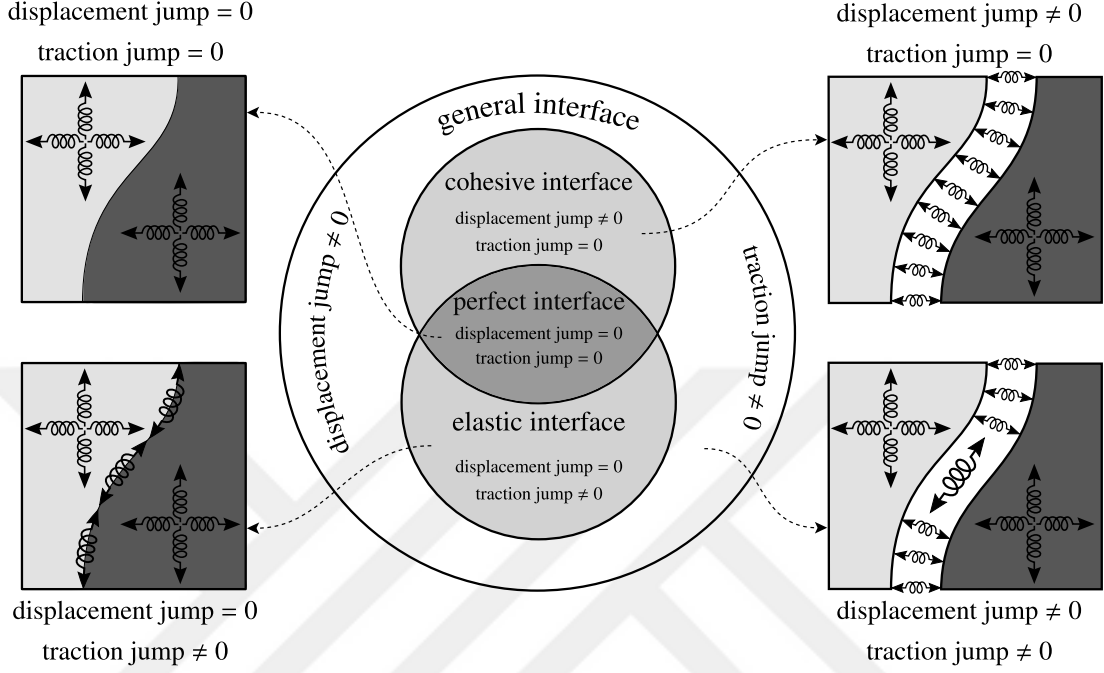


Figure 1.3: Categorization of interface models.

was addressed by Le-Quang and He [91] and closed-form first-order upper and lower bounds for the macroscopic elastic moduli were derived. Brisard et al. [61] applied a variational framework for polarization methods in nano-composites to determine a lower-bound on the shear modulus of a nano-composites with elastic interfaces. Mogilevskaya et al. [92] presented a new technique to evaluate the effective properties of linearly elastic fiber reinforced composites embedding elastic interfaces with hexagonal arrangement. Kushch et al. [93] obtained a complete solution via vectorial spherical harmonics for the problem of multiple interacting spherical inclusions. Chatzigeorgiou et al. [62], using the theory of surface elasticity, developed a homogenization framework to account for size effects at small scales via endowing the interfaces with their own energetic structure. Dai et al. [94] used a complex variable method to obtain the effective shear modulus and the corresponding stress distribution in a composite embedding an elastic interface. Gao et al. [95] studied the effects of a curvature-dependent interfacial energy on the overall elastic properties of nano-composites. The *cohesive interface model* [96–98] allows for a displacement jump across the interface while enforcing the traction continuity [99]. Benveniste [100] extended “direct” and

“energy” approaches in composite to derive the effective shear modulus of particulate composites with cohesive interfaces. Achenbach and Zhu [101] studied a composite medium with cohesive interfaces between the fibers and the matrix and obtained numerical results for the stresses in the constituents. Hashin [102, 103] determined the effective elastic moduli of particulate composites with cohesive interfaces on the basis of the generalized self-consistent scheme and the composite sphere assemblage method. Lipton and Vernescu [104] introduced new variational principles and bounds for the effective elastic moduli of anisotropic two-phase composites with cohesive interfaces. Fan and Wang [105] utilized a linear spring model to study cohesive interfaces where displacement jumps are present and formulated the interaction of a screw dislocation with an imperfect interface. Duan et al. [106] derived local and average stress concentration tensors for the inhomogeneities with cohesive and elastic interface effects based on the solutions of the elastostatic problems. Tan et al. [107] determined the effective constitutive relations of particulate composites with a piecewise linear cohesive law at the interface under hydrostatic tension. Later, Duan et al. [63, 108] proposed a unified framework based on the generalized self-consistent method and a replacement procedure to predict the overall properties of particulate and fiber composites embedding elastic and cohesive interfaces. An efficient three-dimensional numerical approach based on the extended finite element method to model the cohesive interfaces model was proposed by Zhu et al. [109]. Fritzen and Leuschner [70] developed a reduced order model to predict the nonlinear response of a heterogeneous medium embedding cohesive interfaces. Both the cohesive and elastic interface models can be interpreted as the two limit cases of a *general interface model* [110, 111] allowing for both the displacement and traction jumps across the interface. Benveniste [112] generalized the Bövik’s model [113] to an arbitrarily curved three-dimensional thin anisotropic layer between the two anisotropic constituents of a composite medium and obtained a more compact form of the interface model, see also [114, 115]. Gu and He [116] derived a general interface model for coupled multifield phenomena via applying Taylor’s expansion to a three-dimensional curved thin interphase. Later, Gu et al. [117] derived estimates for the size-dependent effective elastic moduli of particle-reinforced composites

with general interfaces. Chatzigeorgiou et al. [118] extended the composite cylinder assemblage (CCA) approach to account for general interfaces and derived a closed-form analytical solution to compute the effective interface-enhanced material response. Firooz and Javili [119] performed a thorough numerical study and pinpointed some uncommon characteristics of composites due to the presence of general interfaces. Later Firooz et al. [120, 121] extended the composite cylinder assemblage, composite sphere assemblage and generalized self-consistent method to account for general interfaces and developed closed form expressions for the bounds and estimates on the overall bulk and shear modulus of fiber and particulate composites. They also developed an interface-enhanced Mori–Tanaka method which provided the stress/strain relation in each phase of the medium including the interfaces. Comparison of their solution with the computational results obtained from the finite element method showed a remarkable agreement. Further details on thermodynamics of interfaces can be found in [122–124].

In summary, the main objective of this work is *to develop novel analytical approaches to determine the overall response of fiber-reinforced and particle-reinforced composites embedding general interfaces and provide thorough comparisons with computational simulations*. Substantial portions of the work presented here are contained in the following publications [50, 119–121]:

- S. Firooz, S. Saeb, G. Chatzigeorgiou, F. Meraghni, P. Steinmann, A. Javili, Systematic study of homogenization and the utility of circular simplified representative volume element, *Mathematics and Mechanics of Solids* doi:10.1177/1081286518823834.
- S. Firooz, A. Javili, Understanding the role of general interfaces in the overall behavior of composites and size effects, *Computational Materials Science* 162 (2019) 245–254.
- S. Firooz, G. Chatzigeorgiou, F. Meraghni, A. Javili, Bounds on size effects in composites via homogenization accounting for general interfaces, *Continuum Mechanics and Thermodynamics* doi:10.1007/s00161-019-00796-w.

- S. Firooz, G. Chatzigeorgiou, F. Meraghni, A. Javili, Homogenization accounting for size effects in particulate composites due to general interfaces, Mechanics of Materials (under review).

Throughout this manuscript, the inclusion is identified by index 1 and matrix by index 2. The macroscopic quantities are distinguished from their microscopic counterparts by a left superscript “M”. For instance, $^M\{\bullet\}$ is a macroscopic quantity with its counterpart being $\{\bullet\}$ at the micro-scale. Interface quantities are distinguished from the bulk quantities by a bar placed on top. That is, $\{\bar{\bullet}\}$ denotes an interface quantity with its bulk counterpart $\{\bullet\}$. Moreover, the average and the jump operators across the interface are denoted by $\{\{\bullet\}\}$ and $[\{\bullet\}]$, respectively. The scalar product of two vectors $\mathbf{a}$ and $\mathbf{b}$ is denoted $\mathbf{a} \cdot \mathbf{b} = a_i b_i$ and the scalar product of two second-order tensors $\mathbf{A}$ and $\mathbf{B}$ is denoted $\mathbf{A} : \mathbf{B} = A_{ij} B_{ij}$. The dyadic product of two vectors $\mathbf{a}$ and $\mathbf{b}$ is a second-order tensor $\mathbf{C} = \mathbf{a} \otimes \mathbf{b}$ with $C_{ij} = a_i b_j$ and the dyadic product of two second-order tensors $\mathbf{A}$ and $\mathbf{B}$ is a fourth-order tensor $\mathbb{D} = \mathbf{A} \otimes \mathbf{B}$ with $D_{ijkl} = A_{ij} B_{kl}$. The composition of two second-order tensors $\mathbf{A}$ and $\mathbf{B}$ is a second-order tensor $\mathbf{E} = \mathbf{A} \cdot \mathbf{B}$ with $E_{ij} = A_{im} B_{mj}$. The action of a second-order tensors $\mathbf{A}$ on a vector $\mathbf{b}$ is a vector $\mathbf{c} = \mathbf{A} \cdot \mathbf{b}$ with $c_i = A_{ij} b_j$. The non-standard tensor products $\overline{\otimes}$ and $\underline{\otimes}$ of two second-order tensors $\mathbf{A}$ and $\mathbf{B}$ are the forth order tensors $\mathbb{C} = \mathbf{A} \overline{\otimes} \mathbf{B}$ and $\mathbb{D} = \mathbf{A} \underline{\otimes} \mathbf{B}$, respectively, with the components $C_{ijkl} = A_{ik} B_{jl}$ and $D_{ijkl} = A_{il} B_{jk}$. The non-standard dyadic product of a vector $\mathbf{a}$ and a second-order tensor $\mathbf{B}$ is a third-order tensor $\mathcal{C} = \mathbf{B} \overline{\otimes} \mathbf{a}$ with $C_{ijk} = B_{ik} a_j$. The non-standard dot product of a fourth-order tensor $\mathbb{A}$ on a vector $\mathbf{b}$ is a third-order tensor $\mathcal{C} = \mathbf{b} \cdot \mathbb{A}$ with $C_{ijk} = A_{isjk} b_s$.

The rest of this manuscript is organized as follows. Section 2 provides a comprehensive study on classical homogenization. The interface-enhanced homogenization technique is developed in Section 3, followed by a set of numerical examples to illustrate the role of the interfaces on the overall response of composites. Section 4 concludes this work and provides further outlook.

Chapter 2

Homogenization

The objective of this section is provide a systematic study on the homogenization technique from both theoretical and computational points of view. The theoretical aspects of homogenization are detailed in Section 2.1. Section 2.2 elaborates on the finite element implementation of homogenization. Next, several established analytical estimates on the overall properties composites are presented in Section 2.3. Finally, Section 2.4 provides a set of numerical examples to compare the analytical and computational results as well as a comprehensive study on the effects of the RVE type and boundary condition on the overall behavior of composites.

2.1 Theory

In homogenization, the problem is separated into micro- and macro-problems based on the assumption of the separation of length-scales. Moreover, the Hill–Mandel condition [6, 8] is imposed to guarantee the energy equivalence between the scales. At the micro-scale, the boundary value problem often corresponds to a representative domain, referred to as the representative volume element (RVE). A proper RVE must be selected such that it contains enough details to sufficiently

represent the microstructure of the material and it has to be small enough to fulfill the assumption of scale separation, see [125–129] for more details on the definition of the RVE. Since the macro-structure is heterogeneous, it is not possible to associate a constitutive material behavior to the macro-problem. To overcome this problem, it is assumed that the constitutive material response at the micro-scale is known and via solving the associated boundary value problem at the micro-scale and proper averaging over the RVE, the overall response at the macro-scale is obtained. Two different approaches are available to address the micro-problem. In strain-driven homogenization, the macroscopic deformation gradient is prescribed and the macroscopic stress is calculated. On the contrary, the macroscopic stress is prescribed in stress-driven homogenization for an unknown macroscopic deformation gradient. The framework presented here is based on first-order strain-driven computational homogenization.

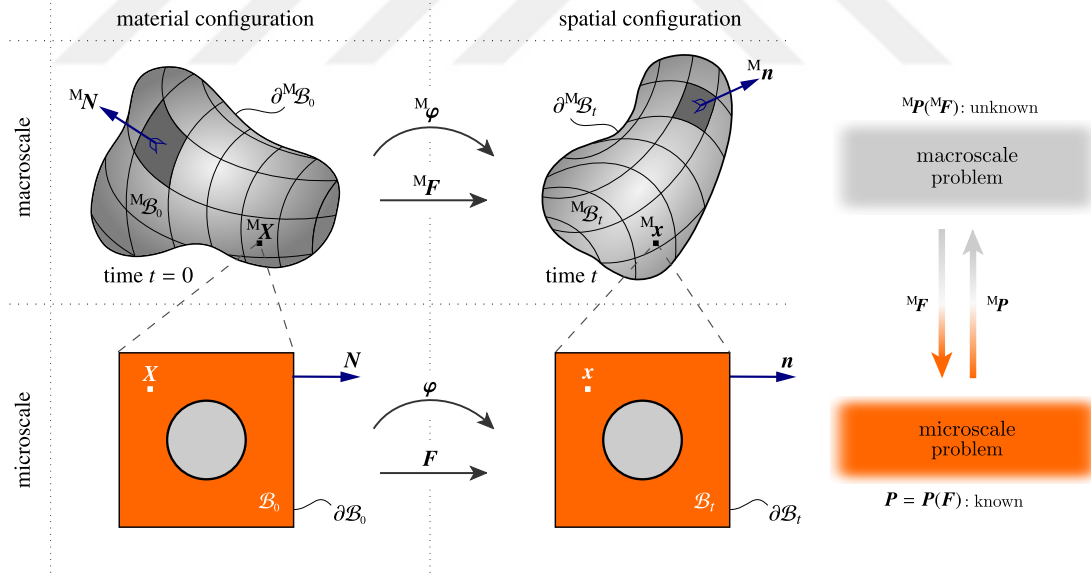


Figure 2.1: Computational homogenization graphical summary.

2.1.1 Macro-problem

Let a macroscopic continuum body take the material configuration ${}^M\mathcal{B}_0$ at time $t = 0$ and the spatial configuration ${}^M\mathcal{B}_t$ at time $t > 0$, as shown in Fig. 2.1. The boundaries of the body in the material and the spatial configuration are denoted

as $\partial^M \mathcal{B}_0$ and $\partial^M \mathcal{B}_t$, respectively. Moreover, ${}^M \mathbf{N}$ and ${}^M \mathbf{n}$ define the material and spatial outward unit normal vectors to the boundaries. The material point ${}^M \mathbf{X}$ is mapped to its spatial counterpart ${}^M \mathbf{x}$ via the nonlinear deformation map ${}^M \boldsymbol{\varphi}$ as ${}^M \mathbf{x} = {}^M \boldsymbol{\varphi}({}^M \mathbf{X})$. The infinitesimal line element $d^M \mathbf{X}$ from the material configuration is mapped to $d^M \mathbf{x}$ in the spatial configuration via the linear map ${}^M \mathbf{F}$ as $d^M \mathbf{x} = {}^M \mathbf{F} \cdot d^M \mathbf{X}$ where ${}^M \mathbf{F} = {}^M \text{Grad} {}^M \boldsymbol{\varphi}$ is the macroscopic deformation gradient. In addition, the Jacobian determinant ${}^M J = \det {}^M \mathbf{F}$ maps the infinitesimal material volume element $d^M V$ to its spatial counterpart $d^M v$ via $d^M v = {}^M J d^M V$. Finally, the normal map ${}^M J {}^M \mathbf{F}^{-t}$ transforms the directional surface element from the material configuration $d^M \mathbf{S} = d^M S {}^M \mathbf{N}$ to the directional surface element in the spatial configuration $d^M \mathbf{s} = d^M s {}^M \mathbf{n}$ as $d^M \mathbf{s} = {}^M J {}^M \mathbf{F}^{-t} \cdot d^M \mathbf{S}$. The governing equations for the macro-problem are the balances of linear and angular momentum. For a quasi-static case, the balance of linear momentum reads

$${}^M \text{Div} {}^M \mathbf{P} + {}^M \mathbf{b}_0^p = \mathbf{0} \quad \text{in} \quad {}^M \mathcal{B}_0 \quad \text{subject to} \quad {}^M \mathbf{P} \cdot {}^M \mathbf{N} = {}^M \mathbf{t}_0 \quad \text{on} \quad \partial^M \mathcal{B}_0,$$

with

$${}^M \mathbf{t}_0 = {}^M \mathbf{t}_0^p \quad \text{on} \quad \partial^M \mathcal{B}_{0,N} \quad \text{and} \quad {}^M \boldsymbol{\varphi} = {}^M \boldsymbol{\varphi}^p \quad \text{on} \quad \partial^M \mathcal{B}_{0,D},$$

where ${}^M \mathbf{b}_0^p$ represents the body force density in the material configuration and ${}^M \mathbf{P}$ defines the macroscopic Piola stress. The traction ${}^M \mathbf{t}_0$ acts on the boundary $\partial^M \mathcal{B}_0$. The prescribed traction that acts on the Neumann portion of the boundary $\partial^M \mathcal{B}_{0,N} \subset \partial^M \mathcal{B}_0$ is denoted as ${}^M \mathbf{t}_0^p$. The displacement that is applied to the boundary $\partial^M \mathcal{B}_0$ is ${}^M \boldsymbol{\varphi}$. The prescribed displacement ${}^M \boldsymbol{\varphi}^p$ acts on the Dirichlet part of the boundary $\partial^M \mathcal{B}_{0,D} \subset \partial^M \mathcal{B}_0$. The balance of the angular momentum at the macro-scale reads ${}^M \mathbf{P} \cdot {}^M \mathbf{F}^t = {}^M \mathbf{F} \cdot {}^M \mathbf{P}^t$.

2.1.2 Micro-problem

As illustrated in Fig. 2.1, the notations for the micro-problem mimic the macro-problem without the left superscript “M”. The kinematics of the micro-problem such as points, line elements, surface elements and volume elements from the

material to spatial configuration read

$$\mathbf{x} = \boldsymbol{\varphi}(\mathbf{X}), \quad \mathrm{d}\mathbf{x} = \mathbf{F} \cdot \mathrm{d}\mathbf{X}, \quad \mathrm{d}\mathbf{s} = J \mathbf{F}^{-t} \cdot \mathrm{d}\mathbf{S}, \quad \mathrm{d}v = J \mathrm{d}V.$$

Due to the scale separation assumption, the body forces vanish at the micro-scale. The balance of linear momentum for the micro-problem is

$$\operatorname{Div} \mathbf{P} = \mathbf{0} \quad \text{in } \mathcal{B}_0 \quad \text{subject to } \mathbf{P} \cdot \mathbf{N} = \mathbf{t}_0 \quad \text{on } \partial \mathcal{B}_0, \quad (2.1)$$

with

$$\mathbf{t}_0 = \mathbf{t}_0^p \quad \text{on } \partial \mathcal{B}_{0,N} \quad \text{and} \quad \boldsymbol{\varphi} = \boldsymbol{\varphi}^p \quad \text{on } \partial \mathcal{B}_{0,D}.$$

Moreover, the balance of angular momentum reads $\mathbf{P} \cdot \mathbf{F}^t = \mathbf{F} \cdot \mathbf{P}^t$.

2.1.3 Micro-to-macro transition

The micro-to-macro transition is essentially a proper averaging of the quantities at the micro-scale to link them with their counterparts at the macro-scale. This method is capable of incorporating geometrical and physical nonlinearities without additional effort. As it is depicted in Fig. 2.1, the macroscopic deformation gradient is imposed onto the microstructure and the micro-problem is solved as a classical boundary value problem. To proceed, it proves convenient to define the volume average operator $\langle \{\bullet\} \rangle$ as

$$\langle \{\bullet\} \rangle := \frac{1}{\mathcal{V}_0} \int_{\mathcal{B}_0} \{\bullet\} \mathrm{d}V \quad \text{with} \quad \mathcal{V}_0 = \int_{\mathcal{B}_0} \mathrm{d}V.$$

Average deformation gradient theorem Assume that $\mathbf{F}_c$ is a constant tensor and $\partial \mathcal{B}_0$ is the boundary of the domain $\mathcal{B}_0$ with the outward unit normal $\mathbf{N}$. The average deformation gradient theorem states that if $\boldsymbol{\varphi} = \mathbf{F}_c \cdot \mathbf{X}$ is prescribed on the boundary, then $\langle \mathbf{F} \rangle = \mathbf{F}_c$. To prove this theorem, we exploit the gradient

theorem and $\mathbf{F} = \text{Grad}\boldsymbol{\varphi}$ which yield

$$\begin{aligned}\langle \mathbf{F} \rangle &= \frac{1}{\mathcal{V}_0} \int_{\mathcal{B}_0} \mathbf{F} \, dV = \frac{1}{\mathcal{V}_0} \int_{\mathcal{B}_0} \text{Grad}\boldsymbol{\varphi} \, dV = \frac{1}{\mathcal{V}_0} \int_{\partial\mathcal{B}_0} \boldsymbol{\varphi} \otimes \mathbf{N} \, dA \\ &= \frac{1}{\mathcal{V}_0} \int_{\partial\mathcal{B}_0} [\mathbf{F}_c \cdot \mathbf{X}] \otimes \mathbf{N} \, dA = \frac{1}{\mathcal{V}_0} \mathbf{F}_c \cdot \int_{\partial\mathcal{B}_0} \mathbf{X} \otimes \mathbf{N} \, dA.\end{aligned}$$

The last integral simplifies to

$$\int_{\partial\mathcal{B}_0} \mathbf{X} \otimes \mathbf{N} \, dA = \int_{\mathcal{B}_0} \text{Grad}\mathbf{X} \, dV = \int_{\mathcal{B}_0} \mathbf{I} \, dV = \mathbf{I} \int_{\mathcal{B}_0} dV = \mathcal{V}_0 \mathbf{I}. \quad (2.2)$$

Therefore we conclude that

$$\langle \mathbf{F} \rangle = \frac{1}{\mathcal{V}_0} \mathbf{F}_c \cdot [\mathcal{V}_0 \mathbf{I}] = \mathbf{F}_c \cdot \mathbf{I} = \mathbf{F}_c.$$

More precisely, the average deformation gradient theorem states that if a deformation $\mathbf{F}_c \cdot \mathbf{X}$ is prescribed on the boundary of a domain $\partial\mathcal{B}_0$, the average deformation gradient in the domain will be equal to $\mathbf{F}_c$ regardless of how complex the deformation gradient is throughout the domain. As a result, within the context of micro-to-macro transition, we can define the macroscopic deformation gradient as the average of the microscopic deformation gradient as

$${}^M\mathbf{F} = \langle \mathbf{F} \rangle = \frac{1}{\mathcal{V}_0} \int_{\mathcal{B}_0} \mathbf{F} \, dV = \frac{1}{\mathcal{V}_0} \int_{\partial\mathcal{B}_0} \boldsymbol{\varphi} \otimes \mathbf{N} \, dA.$$

Average Piola stress theorem Assume that $\mathbf{P}_c$ is a constant tensor and $\partial\mathcal{B}_0$ is the boundary of the domain $\mathcal{B}_0$ with the outward unit normal $\mathbf{N}$. The average Piola stress theorem states that if $\mathbf{t}_0 = \mathbf{P}_c \cdot \mathbf{N}$ is prescribed on the boundary, then $\langle \mathbf{P} \rangle = \mathbf{P}_c$. To prove this theorem we can write

$$\langle \mathbf{P} \rangle = \frac{1}{\mathcal{V}_0} \int_{\mathcal{B}_0} \mathbf{P} \, dV = \frac{1}{\mathcal{V}_0} \int_{\mathcal{B}_0} \mathbf{P} \cdot \mathbf{I} \, dV = \frac{1}{\mathcal{V}_0} \int_{\mathcal{B}_0} \mathbf{P} \cdot \text{Grad}\mathbf{X} \, dV,$$

which can be restated as

$$\frac{1}{\mathcal{V}_0} \int_{\mathcal{B}_0} \mathbf{P} \cdot \text{Grad}\mathbf{X} \, dV = \frac{1}{\mathcal{V}_0} \int_{\mathcal{B}_0} \text{Div}(\mathbf{P} \otimes \mathbf{X}) \, dV - \frac{1}{\mathcal{V}_0} \int_{\mathcal{B}_0} \text{Div}\mathbf{P} \otimes \mathbf{X} \, dV.$$

Imposing the linear momentum balance $\text{Div} \mathbf{P} = \mathbf{0}$,

$$\langle \mathbf{P} \rangle = \frac{1}{\mathcal{V}_0} \int_{\mathcal{B}_0} \text{Div}(\mathbf{P} \otimes \mathbf{X}) \, dV,$$

which can be transformed to an integral over the boundary using the divergence theorem as

$$\langle \mathbf{P} \rangle = \frac{1}{\mathcal{V}_0} \int_{\partial \mathcal{B}_0} [\mathbf{P} \otimes \mathbf{X}] \cdot \mathbf{N} \, dA = \frac{1}{\mathcal{V}_0} \int_{\partial \mathcal{B}_0} \mathbf{P} \cdot \mathbf{N} \otimes \mathbf{X} \, dA = \frac{1}{\mathcal{V}_0} \int_{\partial \mathcal{B}_0} \mathbf{t}_0 \otimes \mathbf{X} \, dA.$$

Using the assumption $\mathbf{t}_0 = \mathbf{P}_c \cdot \mathbf{N}$, we have

$$\langle \mathbf{P} \rangle = \frac{1}{\mathcal{V}_0} \int_{\partial \mathcal{B}_0} \mathbf{t}_0 \otimes \mathbf{X} \, dA = \frac{1}{\mathcal{V}_0} \int_{\partial \mathcal{B}_0} \mathbf{P}_c \cdot \mathbf{N} \otimes \mathbf{X} \, dA = \frac{1}{\mathcal{V}_0} \mathbf{P}_c \cdot \underbrace{\int_{\partial \mathcal{B}_0} \mathbf{N} \otimes \mathbf{X} \, dA}_{\mathcal{V}_0 \mathbf{I}},$$

and thus,

$$\langle \mathbf{P} \rangle = \frac{1}{\mathcal{V}_0} \mathbf{P}_c \cdot [\mathcal{V}_0 \mathbf{I}] = \mathbf{P}_c.$$

More precisely, the average Piola stress theorem states that if a traction $\mathbf{P}_c \cdot \mathbf{N}$ is prescribed on the boundary of a domain $\partial \mathcal{B}_0$, the average Piola stress in the domain will be equal to the $\mathbf{P}_c$ regardless of how complex the stress is throughout the domain. As a result, within the context of micro-to-macro transition, we can define the macroscopic Piola stress as the average of the microscopic Piola stress as

$${}^M \mathbf{P} = \langle \mathbf{P} \rangle = \frac{1}{\mathcal{V}_0} \int_{\mathcal{B}_0} \mathbf{P} \, dV = \frac{1}{\mathcal{V}_0} \int_{\partial \mathcal{B}_0} \mathbf{t}_0 \otimes \mathbf{X} \, dA.$$

Hill–Mandel condition The Hill–Mandel condition necessitates the incremental energy equivalence between the two scales as

$${}^M \mathbf{P} : \delta {}^M \mathbf{F} \stackrel{!}{=} \frac{1}{\mathcal{V}_0} \int_{\mathcal{B}_0} \mathbf{P} : \delta \mathbf{F} \, dV. \quad (2.3)$$

Hill’s lemma, transforms the above relation into a surface integral

$$\frac{1}{\mathcal{V}_0} \int_{\mathcal{B}_0} \mathbf{P} : \delta \mathbf{F} \, dV - {}^M \mathbf{P} : \delta {}^M \mathbf{F} = \int_{\partial \mathcal{B}_0} [\delta \boldsymbol{\varphi} - \delta {}^M \mathbf{F} \cdot \mathbf{X}] \cdot [\mathbf{t}_0 - {}^M \mathbf{P} \cdot \mathbf{N}] \, dA, \quad (2.4)$$

which is proven in Appendix A. Inserting Hill's lemma (2.4) into the Hill–Mandel condition (2.3) yields

$$\int_{\partial\mathcal{B}_0} [\delta\varphi - \delta^{\mathbf{M}}\mathbf{F} \cdot \mathbf{X}] \cdot [\mathbf{t}_0 - {}^{\mathbf{M}}\mathbf{P} \cdot \mathbf{N}] \, dA \stackrel{!}{=} 0, \quad (2.5)$$

which shall be understood as the Hill–Mandel condition in terms of a surface integral over the boundary of the RVE. Various boundary conditions can fulfill the Hill–Mandel condition a priori, see [130, 131]. Among all the boundary conditions that satisfy the Hill–Mandel condition, the canonical ones are

- Constant deformation condition in $\mathcal{B}_0$ known as Taylor's assumption

$$\varphi = {}^{\mathbf{M}}\mathbf{F} \cdot \mathbf{X} \quad \text{in } \mathcal{B}_0,$$

- linear displacement boundary condition (DBC)

$$\varphi = {}^{\mathbf{M}}\mathbf{F} \cdot \mathbf{X} \quad \text{on } \partial\mathcal{B}_0,$$

- uniform traction boundary condition (TBC)

$$\mathbf{t}_0 = {}^{\mathbf{M}}\mathbf{P} \cdot \mathbf{N} \quad \text{on } \partial\mathcal{B}_0,$$

- periodic displacement and anti-periodic traction (PBC)

$$[\varphi - {}^{\mathbf{M}}\mathbf{F} \cdot \mathbf{X}] + [\mathbf{t}_0 - {}^{\mathbf{M}}\mathbf{P} \cdot \mathbf{N}] = 0 \quad \text{on } \partial\mathcal{B}_0,$$

- Constant stress condition in $\mathcal{B}_0$ known as Sach's assumption

$$\mathbf{P} = {}^{\mathbf{M}}\mathbf{P} \quad \text{in } \mathcal{B}_0.$$

For strain-driven computational homogenization the condition ${}^{\mathbf{M}}\mathbf{F} = \langle \mathbf{F} \rangle$ is a priori satisfied for both DBC and PBC. However, this is not the case for TBC and the condition ${}^{\mathbf{M}}\mathbf{F} = \langle \mathbf{F} \rangle$ shall be regarded as an additional constraint. All the above boundary conditions satisfy the balance of angular momentum at the macro-scale.

It is commonly accepted that DBC and TBC overestimate and underestimate PBC, respectively.

2.2 Finite element implementation

The aim of this section is to provide a general finite element formulation to solve the boundary value problem at the micro-scale. For the sake of generality, we write the equations in terms of $\mathbf{P}$ and $\mathbf{F}$. Further simplifications of this framework recovers the small-strain linear elasticity. The material model is assumed to be hyperelastic hence nondissipative. Thus, the micro free energy density is only a function of the deformation gradient as $\psi = \psi(\mathbf{F})$. The micro Piola stress and micro Piola tangent read

$$\mathbf{P} = \frac{\partial \psi}{\partial \mathbf{F}}, \quad \mathbb{A} = \frac{\partial \mathbf{P}}{\partial \mathbf{F}}. \quad (2.6)$$

Further details on the definition of the bulk energy density ψ and derivation of the Piola stress and Piola tangent is available in Appendix B.1. In order to find the weak form of the balance equation (2.1), a vector-valued test function $\delta \boldsymbol{\varphi}$ is contracted from left. Knowing that the test function vanishes at the Dirichlet portion of the boundary and using the divergence theorem, the global weak form of the linear momentum balance reads

$$\int_{\mathcal{B}_0} \mathbf{P} : \text{Grad} \delta \boldsymbol{\varphi} \, dV - \int_{\partial \mathcal{B}_{0,N}} \delta \boldsymbol{\varphi} \cdot \mathbf{t}_0 \, dA \stackrel{!}{=} 0 \quad \forall \delta \boldsymbol{\varphi} \in \mathcal{H}_0^1(\mathcal{B}_0),$$

with $\mathcal{H}_0^1$ denoting the Sobolev space of order 1 where the test functions are zero on the Dirichlet part of the boundary.

The next step is to discretize the weak form in space. The domain is discretized into a set of bulk and surface elements as

$$\mathbf{A} \int_{e=1}^{\#be} \mathcal{B}_0^e \mathbf{P} : \text{Grad} \delta \boldsymbol{\varphi} \, dV - \mathbf{A} \int_{e=1}^{\#se} \partial \mathcal{B}_{0,N}^e \delta \boldsymbol{\varphi} \cdot \mathbf{t}_0 \, dA \stackrel{!}{=} 0$$

where $\#be$ denotes the number of bulk elements and $\#se$ represents the number of surface elements. Employing the isoparametric concept and the Bubnov–Galerkin finite element method, the bulk and surface geometries are approximated using the natural coordinates $\boldsymbol{\xi}$ as follows

$$\begin{aligned} \mathbf{X}|_{B_0^i} &\approx \mathbf{X}(\boldsymbol{\xi}) = \sum_{i=1}^{\#nbe} N^i(\boldsymbol{\xi}) \mathbf{X}^i, & \mathbf{X}|_{\partial B_{0,N}^i} &\approx \mathbf{X}(\boldsymbol{\xi}) = \sum_{i=1}^{\#nse} N^i(\boldsymbol{\xi}) \mathbf{X}^i, \\ \mathbf{x}|_{B_0^i} &\approx \mathbf{x}(\boldsymbol{\xi}) = \sum_{i=1}^{\#nbe} N^i(\boldsymbol{\xi}) \mathbf{x}^i, & \mathbf{x}|_{\partial B_{0,N}^i} &\approx \mathbf{x}(\boldsymbol{\xi}) = \sum_{i=1}^{\#nse} N^i(\boldsymbol{\xi}) \mathbf{x}^i, \\ \delta\boldsymbol{\varphi}|_{B_0^i} &\approx \delta\boldsymbol{\varphi}(\boldsymbol{\xi}) = \sum_{i=1}^{\#nbe} N^i(\boldsymbol{\xi}) \delta\boldsymbol{\varphi}^i, & \delta\boldsymbol{\varphi}|_{\partial B_{0,N}^i} &\approx \delta\boldsymbol{\varphi}(\boldsymbol{\xi}) = \sum_{i=1}^{\#nse} N^i(\boldsymbol{\xi}) \delta\boldsymbol{\varphi}^i, \end{aligned}$$

with N being the shape functions, $\#nbe$ denoting number of nodes per bulk element and $\#nse$ denoting number of nodes per surface element. Figure 2.2 depicts the discretized two- and three-dimensional domains. Substituting the test functions with their spatial approximations renders the residual vector corresponding to a global node I

$$\mathbf{R}^I := \mathbf{A} \int_{B_0^e} \mathbf{P} \cdot \text{Grad} N^i \, dV - \mathbf{A} \int_{\partial B_{0,N}^e} \mathbf{t}_0 \cdot N^i \, dA,$$

in which i is the local node corresponding to the global node I . Putting all the unknown coordinates $\mathbf{d}$ into the global unknown coordinate vector $[\boldsymbol{\varphi}]$ and assembling the global nodal residual vectors $\mathbf{R}^I$ into the global residual vector $[\mathbf{R}]$ results in the non-linear system of equations $[\mathbf{R}] \stackrel{!}{=} 0$ which can be solved

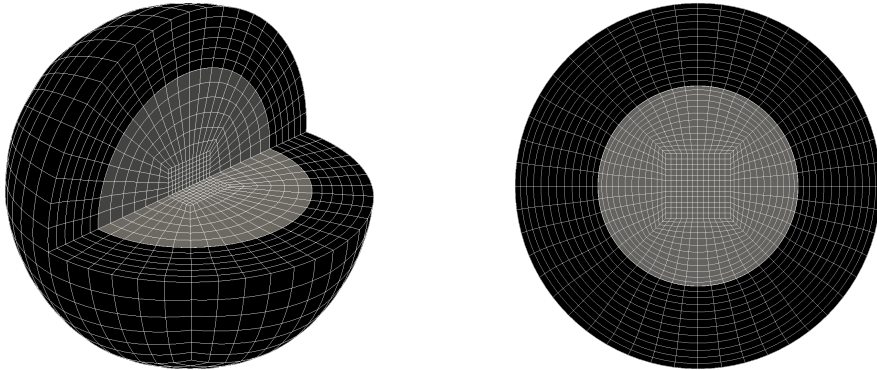


Figure 2.2: Discretization two- and three-dimensional domains.

using the Newton–Raphson scheme as

$$[\mathbf{R}]_{n+1} \stackrel{!}{=} \mathbf{0} \quad \Rightarrow \quad [\mathbf{R}]_{n+1} = [\mathbf{R}]_n + [\mathbf{K}]_n \Delta[\boldsymbol{\varphi}]_n \stackrel{!}{=} \mathbf{0} \quad \text{with} \quad [\mathbf{K}]_n := \frac{\partial[\mathbf{R}]_n}{\partial[\boldsymbol{\varphi}]_n},$$

that yields the incremental updates $[\boldsymbol{\varphi}]_{n+1} = [\boldsymbol{\varphi}]_n + \Delta[\boldsymbol{\varphi}]_n$. Here $[\mathbf{K}]_n$ denotes the tangent stiffness and n is the iteration step.

2.3 Analytical estimates

Analytical methods in homogenization have been established to derive explicit analytical solutions for the overall response of heterogeneous media and thus, require certain simplifying assumptions. As a result, analytical homogenization is, in general, limited to small strain linear elasticity theory. In this section the most significant and extensively used analytical estimates on the overall behavior of composites are listed. Note, for the sake of brevity, only the final form of each estimate is stated here. The balance equations of linear small-strain elasticity are $\text{Div} \boldsymbol{\sigma} = 0$ and $\boldsymbol{\sigma} = \boldsymbol{\sigma}^t$ with $\boldsymbol{\sigma}$ being the linear stress measure. The strain field $\boldsymbol{\varepsilon}$ is the symmetric gradient of displacement $\mathbf{u}$ as $\boldsymbol{\varepsilon} = \text{Grad}^{\text{sym}} \mathbf{u}$. Small-strain linear elasticity relates the stress $\boldsymbol{\sigma}$ to the strain $\boldsymbol{\varepsilon}$ according to the linear relation $\boldsymbol{\sigma} = \mathbb{C} : \boldsymbol{\varepsilon}$ in which the fourth-order constitutive tensor $\mathbb{C} = \mu [\mathbf{I} \otimes \mathbf{I} + \mathbf{I} \otimes \mathbf{I}] + \lambda [\mathbf{I} \otimes \mathbf{I}]$, with λ and μ being the first and second Lamé parameters of the material. See Appendix B.1 for further details regarding the linearization of the material response.

2.3.1 Fiber composites

Figure 2.3 demonstrates the heterogeneous medium corresponding to a fiber composite with its underlying simplified micro-structure of two concentric cylinders corresponding to the fiber (phase 1) and matrix (phase 2). To examine such a medium, a two-dimensional plain-strain problem with transverse isotropy is

employed.

Voigt bounds correspond to a uniform strain field within the RVE resulting in the upper limit for the effective overall response of the material as

$$M_{\kappa} = [1 - f]\kappa_2 + f\kappa_1 \quad \text{and} \quad M_{\mu} = [1 - f]\mu_2 + f\mu_1 ,$$

where f is the inclusion volume fraction and κ is the material bulk modulus and relates to the Lamé parameters as $\kappa = \lambda + \mu$ in plane strain linear elasticity. Note that the uniform-strain assumption violates the balance of linear momentum, in general. Thus, Voigt bounds shall only be understood as upper *unreachable* bounds.

Reuss bounds correspond to a uniform stress field within the RVE leading to the lower limit for the effective response of the material as

$$M_{\kappa} = \frac{\kappa_2\kappa_1}{[1 - f]\kappa_1 + f\kappa_2} \quad \text{and} \quad M_{\mu} = \frac{\mu_2\mu_1}{[1 - f]\mu_1 + f\mu_2} .$$

The uniform-stress assumption violates the compatibility of the strain field and thus, Reuss bounds shall only be understood as lower *unreachable* bounds.

Hashin and Rosen [15] proposed a predictive model based on a Composite Cylinder Assemblage (CCA) to obtain the bulk and shear moduli of transversely isotropic composites having circular inclusions in hexagonal and random arrays. The effective coefficients in this approach are frequently used to date. In this

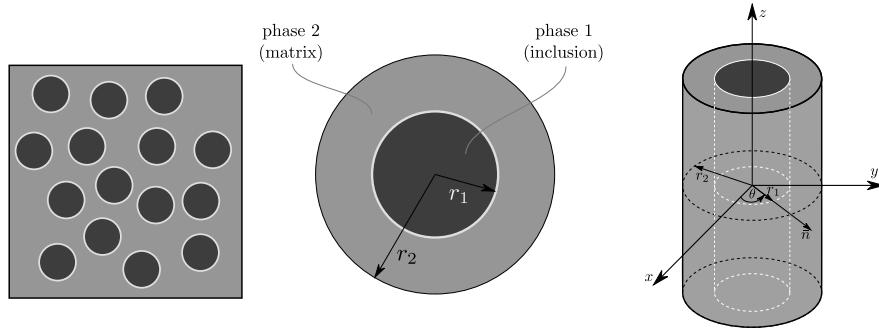


Figure 2.3: Heterogeneous medium and its corresponding simplified RVE.

method, the upper and lower bounds on the bulk modulus coincide and read

$$M_{\kappa_U} = M_{\kappa_L} = \frac{\kappa_2 [\mu_2 + \kappa_1] + f \mu_2 [\kappa_1 - \kappa_2]}{\mu_2 + \kappa_1 + f [\kappa_2 - \kappa_1]},$$

where the subscripts “U” and “L” denote the upper and the lower bounds, respectively. While the mathematical procedure of determination of bounds for the shear modulus has been addressed precisely in [15], closed form expressions for the bounds for the shear modulus, for the first time, are given here as

$$M_{\mu_U} = \mu_2 \left[\frac{2f [\kappa_2 + \mu_2] \left[\frac{\mu_1 - \mu_2}{\mu_1 \kappa_2 + \mu_2 \kappa_2 + 2\mu_2 \mu_1} \right]}{\frac{f [\mu_1 - \mu_2] [\kappa_2 + 2\mu_2]}{\mu_1 \kappa_2 + \mu_2 \kappa_2 + 2\mu_2 \mu_1} \left[\frac{3[1-f]^2 \left[\frac{\kappa_2}{\kappa_2 + 2\mu_2} \right]^2}{f^3 \left[\frac{\mu_1 \kappa_1 [\kappa_2 + 2\mu_2] - \mu_2 \kappa_2 [\kappa_1 + 2\mu_1]}{[\kappa_2 + 2\mu_2] [\kappa_1 \mu_1 + \mu_2 (\kappa_1 + 2\mu_1)]} \right] - 1} - 1 \right] + 1} + 1 \right],$$

$$M_{\mu_L} = \mu_2 \left[\frac{2f [\kappa_2 + \mu_2] \left[\frac{\mu_1 - \mu_2}{\mu_1 \kappa_2 + \mu_2 \kappa_2 + 2\mu_2 \mu_1} \right]}{\frac{f [\mu_1 - \mu_2] [\kappa_2 + 2\mu_2]}{\mu_1 \kappa_2 + \mu_2 \kappa_2 + 2\mu_2 \mu_1} \left[\frac{3[1-f]^2 \left[\frac{\kappa_2}{\kappa_2 + 2\mu_2} \right]^2}{f^3 \left[\frac{\mu_1 \kappa_1 [\kappa_2 + 2\mu_2] - \mu_2 \kappa_2 [\kappa_1 + 2\mu_1]}{[\kappa_2 + 2\mu_2] [\kappa_1 \mu_1 + \mu_2 (\kappa_1 + 2\mu_1)]} \right] + \frac{\kappa_2}{\kappa_2 + 2\mu_2} - 1 \right] + 1} + 1 \right].$$

Hashin [132] used the variational approach developed by Hashin and Shtrikman [133] to derive bounds on the overall response of fiber composites with transverse isotropy. The aim of this approach was to tighten the bounds proposed by Reuss and Voigt. The Hashin–Shtrikman bounds (HSB) for the overall bulk and shear moduli read

$$M_{\kappa_U} = \kappa_2 + \frac{f}{\frac{1}{\kappa_1 - \kappa_2} + \frac{1-f}{\kappa_2 + \mu_2}}, \quad M_{\kappa_L} = \kappa_1 + \frac{[1-f]}{\frac{1}{\kappa_2 - \kappa_1} + \frac{f}{\kappa_1 + \mu_1}},$$

$$M_{\mu_U} = \mu_2 + \frac{f}{\frac{1}{\mu_1 - \mu_2} + \frac{[1-f][\kappa_2 + 2\mu_2]}{2\mu_2[\kappa_2 + \mu_2]}}, \quad M_{\mu_L} = \mu_1 + \frac{[1-f]}{\frac{1}{\mu_2 - \mu_1} + \frac{f[\kappa_1 + 2\mu_1]}{2\mu_1[\kappa_1 + \mu_1]}},$$

for stiffness ratios less than one. The upper and the lower bound switch for

stiffness ratios more than one.

Christensen and Lo [134] developed a new scheme called generalized self-consistent method (GSCM) to determine the overall shear modulus of composites. In this method, an equivalent medium whose properties are unknown is assumed to surround the RVE and via solving the boundary value problem, the overall shear modulus of the medium is determined. The positive solution of the below quadratic equation renders the effective shear modulus of fiber composites

$$A \left[\frac{\mu^M}{\mu_2} \right]^2 + 2B \frac{\mu^M}{\mu_2} + C = 0,$$

where

$$\begin{aligned} A &= \phi + \left[\frac{\mu_1}{\mu_2} \eta_2 + \eta_1 \eta_2 - \left[\frac{\mu_1}{\mu_2} \eta_2 - \eta_1 \right] f^3 \right] \left[c \eta_2 \left[\frac{\mu_1}{\mu_2} - 1 \right] - \left[\frac{\mu_1}{\mu_2} \eta_2 + 1 \right] \right], \\ B &= -\phi + \frac{1}{2} \left[\frac{\mu_1}{\mu_2} \eta_2 + \left[\frac{\mu_1}{\mu_2} - 1 \right] f + 1 \right] \left[\left[\eta_2 - 1 \right] \left[\frac{\mu_1}{\mu_2} + \eta_1 \right] - 2 \left[\frac{\mu_1}{\mu_2} \eta_2 - \eta_1 \right] f^3 \right] \\ &\quad + \frac{f}{2} \left[\eta_2 + 1 \right] \left[\frac{\mu_1}{\mu_2} - 1 \right] \left[\frac{\mu_1}{\mu_2} + \eta_1 + \left[\frac{\mu_1}{\mu_2} \eta_2 - \eta_1 \right] f^3 \right], \\ C &= \phi + \left[\frac{\mu_1}{\mu_2} \eta_2 + \left[\frac{\mu_1}{\mu_2} - 1 \right] f + 1 \right] \left[\frac{\mu_1}{\mu_2} + \eta_1 + \left[\frac{\mu_1}{\mu_2} \eta_2 - \eta_1 \right] f^3 \right], \end{aligned}$$

with

$$\phi = 3f[1-f]^2 \left[\frac{\mu_1}{\mu_2} - 1 \right] \left[\frac{\mu_1}{\mu_2} + \eta_1 \right], \quad \eta_1 = 3 - \frac{2[\kappa_1 - \mu_1]}{\kappa_1}, \quad \eta_2 = 3 - \frac{2[\kappa_2 - \mu_2]}{\kappa_2}.$$

The Hashin and Shtrikman variational principle [132, 133] is well-known to provide the best bounds independent of the phase geometry and are formulated only in terms of the phase properties and inclusion volume fraction. Hill [16] also derived bounds on five different effective properties of composites with transversely isotropic geometry. Walpole [18, 135] utilized piece-wise uniform polarization and rederived these bounds in a more general fashion. His method also includes anisotropic constituents and disk-shape fiber composites. All aforementioned

bounds were independent of phase geometry and they were only applicable on three types of geometries; laminated, isotropic and transversely isotropic. Later, Willis [20] modified the Hashin–Shtrikman bounds by inserting the two-point correlation function to account for more general cases of phase geometry. If the two-point correlation function involves radial, cylindrical or disk symmetry, the above mentioned bounds could be recovered. See [136] for more details on the derivation of explicit forms for the Willis bounds.

2.3.2 Particulate composites

Figure 2.4 shows a heterogeneous medium corresponding to a particulate composite with its underlying RVE as well as a proper coordinate system to examine such a medium. The simplified RVE consists of two concentric spheres corresponding to the particle (phase 1) and the matrix (phase 2).

Voigt and **Reuss** bounds are independent of the composite type thus, for particulate composites they remain the same and read

$$\text{Voigt: } \begin{cases} M_{\kappa} = [1 - f]\kappa_2 + f\kappa_1, \\ M_{\mu} = [1 - f]\mu_2 + f\mu_1, \end{cases} \quad \text{Reuss: } \begin{cases} M_{\kappa} = \frac{\kappa_2\kappa_1}{[1 - f]\kappa_1 + f\kappa_2}, \\ M_{\mu} = \frac{\mu_2\mu_1}{[1 - f]\mu_1 + f\mu_2}, \end{cases}$$

where κ is the material bulk modulus and relates to the Lamé parameters as $\kappa = \lambda + 2\mu/3$.

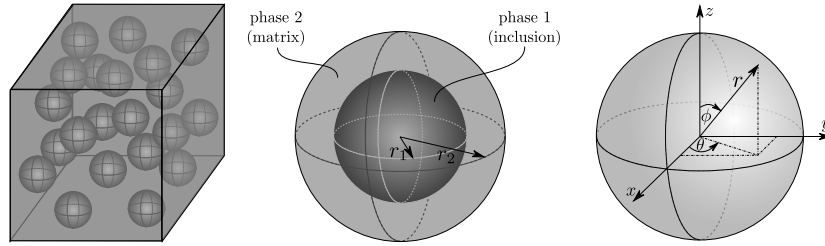


Figure 2.4: Heterogeneous medium (left) with its simplified RVE (middle) and the proper coordinates system (right) to examine such medium.

Hashin [12] developed the Composite Sphere Assemblage (CSA) to obtain the bulk and shear moduli of particulate composites. In this method, the upper and lower bounds on the bulk modulus coincide and read

$$^M\kappa_U = ^M\kappa_L = \kappa_2 + \frac{[\kappa_1 - \kappa_2][4\mu_2 + 3\kappa_2]f}{4\mu_2 + 3\kappa_1 + 3f[\kappa_2 - \kappa_1]},$$

where the subscripts “U” and “L” denote the upper and the lower bounds, respectively. While the mathematical procedure of determination of bounds for the shear modulus has been addressed precisely in [12], closed form expressions for the bounds for the shear modulus, for the first time, are given here as

$$^M\mu_U = \frac{\mu_2}{f \left[1 - \frac{\mu_1}{\mu_2} \right]} + 1, \\ \frac{\mu_1}{\mu_2} + \frac{[7 - 5\nu_2][1 - f] \left[\frac{\mu_1}{\mu_2} - 1 \right]}{15[\nu_2 - 1]} + \frac{21\phi \left[\frac{1}{f^{2/3}} - 1 \right] [f^2 - f^4] \left[\frac{2\mu_1}{\mu_2} - 2 \right]}{5[\nu_2 - 1] \left[4f^4 [\phi[10\nu_2 - 7] - 10\nu_1 + 7] - \phi[5\nu_2 + 7] \right]} \\ ^M\mu_L = \mu_2 \left[\frac{f \left[\frac{\mu_1}{\mu_2} - 1 \right]}{\frac{\mu_1}{\mu_2} - \frac{[\frac{\mu_1}{\mu_2} - 1][5\nu_2 - 7] + f[10\nu_2 - 8]}{15[\nu_2 - 1]} + \frac{21\phi \left[\frac{1}{f^{2/3}} - 1 \right] [f^2 - f^4] \left[\frac{2\mu_1}{\mu_2} - 2 \right]}{5[\nu_2 - 1] \left[4f^4 [\phi[10\nu_2 - 7] - 10\nu_1 + 7] - \phi[10\nu_2 - 7] \right]}} + 1 \right],$$

where

$$\phi = \frac{40\nu_1 - \frac{\mu_1[5\nu_1 + 7]}{\mu_2} - 28}{35[\nu_2 - 1]},$$

and ν_1 and ν_2 are the Poisson’s ratios of the particle and the matrix, respectively. The Poisson’s ratio relates to the Lamé parameters as $\nu = \lambda/2(\lambda + \mu)$.

Hashin and Shtrikman used a variational approach in [133] to derive bounds on the overall response of particulate composites. The aim of this approach was to tighten the bounds proposed by Reuss and Voigt. The Hashin–Shtrikman

bounds for the overall bulk and shear moduli read

$$\begin{aligned} {}^M\kappa_U &= \kappa_2 + \frac{f}{\frac{1}{\kappa_1 - \kappa_2} + \frac{3[1-f]}{3\kappa_2 + 4\mu_2}}, & {}^M\kappa_L &= \kappa_1 + \frac{[1-f]}{\frac{1}{\kappa_2 - \kappa_1} + \frac{3f}{3\kappa_1 + 4\mu_1}}, \\ {}^M\mu_U &= \mu_2 + \frac{f}{\frac{1}{\mu_1 - \mu_2} + \frac{6[1-f][\kappa_2 + 2\mu_2]}{5\mu_2[3\kappa_2 + 4\mu_2]}}, & {}^M\mu_L &= \mu_1 + \frac{[1-f]}{\frac{1}{\mu_2 - \mu_1} + \frac{6f[\kappa_1 + 2\mu_1]}{5\mu_1[3\kappa_1 + 4\mu_1]}}, \end{aligned}$$

for stiffness ratios less than one. The upper and the lower bound switch for stiffness ratios more than one.

Christensen and Lo [134] developed the generalized self-consistent method (GSCM) to determine the overall shear modulus of composites via considering an effective medium surrounding the matrix. The positive solution of the below quadratic equation renders the effective shear modulus of particulate composites

$$A \left[\frac{{}^M\mu}{\mu_2} \right]^2 + B \frac{{}^M\mu}{\mu_2} + C = 0$$

where

$$\begin{aligned} A &= 8 \left[\frac{\mu_1}{\mu_2} - 1 \right] \left[4 - 5\nu_2 \right] \eta_1 f^{10/3} - 2 \left[63 \left[\frac{\mu_1}{\mu_2} - 1 \right] \eta_2 + 2\eta_1 \eta_3 \right] f^{7/3} \\ &\quad + 252 \left[\frac{\mu_1}{\mu_2} - 1 \right] \eta_2 f^{5/3} - 25 \left[\frac{\mu_1}{\mu_2} - 1 \right] \left[7 - 12\nu_2 + 8\nu_2^2 \right] \eta_2 f + 4 \left[7 - 10\nu_2 \right] \eta_2 \eta_3, \\ B &= -4 \left[\frac{\mu_1}{\mu_2} - 1 \right] \left[1 - 5\nu_2 \right] \eta_1 f^{10/3} + 4 \left[63 \left[\frac{\mu_1}{\mu_2} - 1 \right] \eta_2 + 2\eta_1 \eta_3 \right] f^{7/3} \\ &\quad - 504 \left[\frac{\mu_1}{\mu_2} - 1 \right] \eta_2 f^{5/3} + 150 \left[\frac{\mu_1}{\mu_2} - 1 \right] \left[3 - \nu_2 \right] \nu_2 \eta_2 f + 3 \left[15\nu_2 - 7 \right] \eta_2 \eta_3, \\ C &= 4 \left[\frac{\mu_1}{\mu_2} - 1 \right] \left[5\nu_2 - 7 \right] \eta_1 f^{10/3} - 2 \left[63 \left[\frac{\mu_1}{\mu_2} - 1 \right] \eta_2 + 2\eta_1 \eta_3 \right] f^{7/3} \\ &\quad + 252 \left[\frac{\mu_1}{\mu_2} - 1 \right] \eta_2 f^{5/3} + 25 \left[\frac{\mu_1}{\mu_2} - 1 \right] \left[\nu_2^2 - 7 \right] \eta_2 f - \left[-7 + 5\nu_2 \right] \eta_2 \eta_3, \end{aligned}$$

with

$$\begin{aligned} \eta_1 &= \left[\frac{\mu_1}{\mu_2} - 1 \right] \left[49 - 50\nu_1 \nu_2 \right] + 35 \frac{\mu_1}{\mu_2} \left[\nu_1 - 2\nu_2 \right] + 35 \left[2\nu_1 - \nu_2 \right], \\ \eta_2 &= 5\nu_1 \left[\frac{\mu_1}{\mu_2} - 8 \right] + 7 \left[\frac{\mu_1}{\mu_2} + 4 \right], \\ \eta_3 &= \frac{\mu_1}{\mu_2} \left[8 - 10\nu_2 \right] + \left[7 - 5\nu_2 \right], \end{aligned}$$

where ν_1 and ν_2 are the Poisson's ratios of the particle and the matrix, respectively.

2.4 Numerical examples

This section provides a comprehensive comparison between the analytical estimates and computational results through a series of numerical examples. The overall behavior of composites under various boundary conditions and with different RVE shapes are examined thoroughly. Note, we limit our discussions to a two-dimensional analysis corresponding to fiber composites. Extension of the work to a three-dimensional model would be straightforward and does not provide any new significant insight thus, not addressed here for the sake of brevity. All the computational results are obtained using our in-house finite element code. In a finite deformation setting, the Newton–Raphson scheme is employed to solve the system of non-linear equations. Our numerical simulations are robust and render quadratic convergence.

Figure 2.5 depicts the RVEs of interest in this study. The cutout of a real microstructure with random distribution of inclusions can eventually result in isotropic effective behavior. While tetragonal and hexagonal packings are space-filling, they cannot capture the isotropic response of a material. On the other hand, the circular RVE can furnish isotropic effective behavior suitable for comparing with

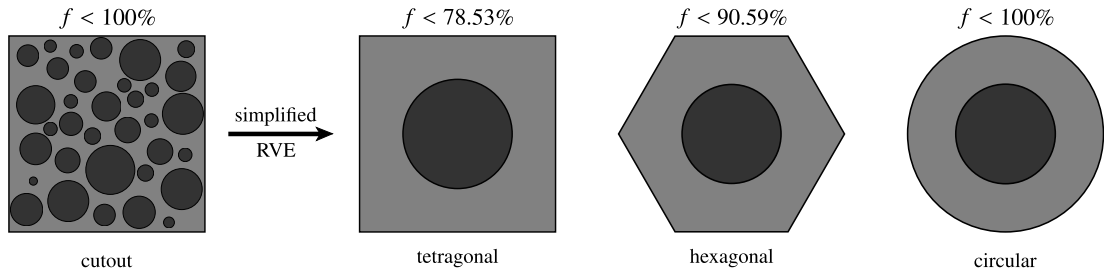


Figure 2.5: Complex RVE and its *simplified* counterparts. The inclusion volume fraction of a cutout could reach 100%. The cutout (left) shall be understood as the RVE. Three *simplified* RVEs are suggested to replace the cutout. The cutout of the real micro-structure can eventually result in isotropic effective behavior.

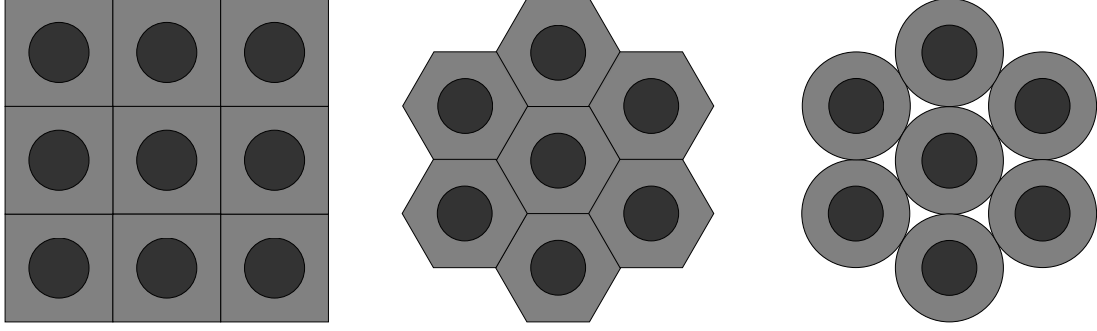


Figure 2.6: Packing network for each RVE.

analytical solutions here and it is the only RVE that could reach the maximum volume fraction of a real cutout of a material. Figure 2.6 shows the packing of these RVEs. The area of each RVE is set to 1 so that the inclusion area corresponds to the volume fraction f . Obviously, the volume fraction f could not exceed a certain value for the tetragonal and hexagonal RVEs, see Fig. 2.7.

In order to provide a thorough comparison of the numerical and analytical results, the overall bulk modulus $^M\kappa$, shear modulus $^M\mu$ and Poisson's ratio $^M\nu$ of transversely isotropic fiber composites are examined. Five different stiffness ratios of 0.01, 0.1, 1, 10 and 100 are considered for each RVE. The stiffness ratio represents the ratio of the inclusion to matrix (incl./matr.) Lamé parameters. A stiffness ratio less than one corresponds to a more compliant inclusion than the matrix and in the limit of incl./matr. $\rightarrow 0$, the inclusion represents a void. On the contrary, the stiffness ratio more than one corresponds to a stiffer inclusion compared to matrix and in the limit of incl./matr. $\rightarrow \infty$, the inclusion acts as a rigid fiber. Throughout all the examples, the matrix properties are set to $\lambda_2 = 10$, $\mu_2 = 10$ while the inclusion parameters vary to generate the predefined stiffness

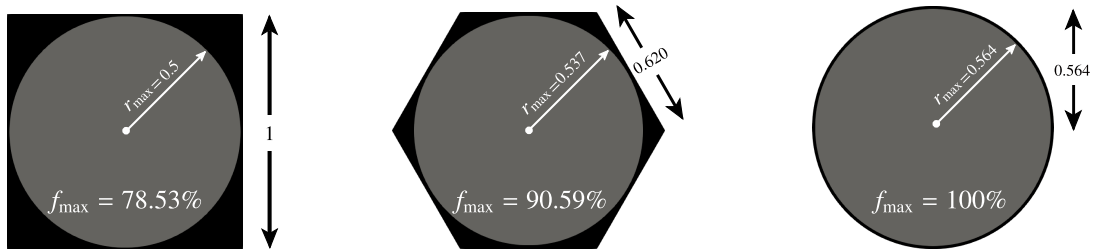


Figure 2.7: Maximum reachable volume fraction for each RVE.

ratios.

Figure 2.8 shows the effective bulk modulus $^M\kappa$ with respect to the volume fraction f for all the RVEs with various stiffness ratios. For the tetragonal and hexagonal RVEs, five lines on each graph represent the analytical estimates of Voigt and Reuss together with the numerical results corresponding to DBC, PBC and TBC. The RVEs in tetragonal and hexagonal packings are space-filling but cannot capture the isotropic behavior of the effective material. On the contrary, the circular RVE renders isotropic behavior and thus, comparison with the associated analytical estimates is justifiable. Voigt and Reuss bounds always provide reliable bounds. As expected, PBC is bounded with TBC from below and DBC from above. Moving from the tetragonal RVE towards the circular RVE, we observe that the numerical results tend to converge until they totally coincide at the circular RVE. Therefore, different boundary conditions result in the same responses when the RVE is circular. Less difference between the numerical results is observed for low volume fractions. As previously mentioned, the CCA upper and lower bounds coincide while the Hashin–Shtirkman bounds do not. For $\text{incl./matr.} < 1$, a remarkable agreement is observed between the numerical results, CCA and the upper HSB (Hashin–Shtrikman bound) and for $\text{incl./matr.} > 1$, the numerical results, CCA and the lower HSB coincide. For $\text{incl./matr.} = 1$, all the results coincide since the domain is uniform.

Figure 2.9 shows the effective shear modulus $^M\mu$ versus the volume fraction for different RVEs as well as stiffness ratios. It is observed that different boundary conditions, in general, provide more distinguishable effective values compared to the previous case. Another solution corresponding to the generalized self-consistent method (GSCM) is added to the results for the sake of completeness. Nevertheless, as we move from the tetragonal RVE towards the circular RVE, PBC moves towards DBC and ultimately coincides with it. Thus, prescribing PBC and DBC to the circular RVE yield identical response. PBC renders the most sensitive boundary condition to the RVE type for shear deformation. In contrast to the previous case, there is no coincidence between CCA and Hashin–Shtrikman bounds. Moreover, GSCM lies within the CCA and Hashin–Shtrikman bounds for all cases. A striking agreement is observed between CCA lower bound and TBC

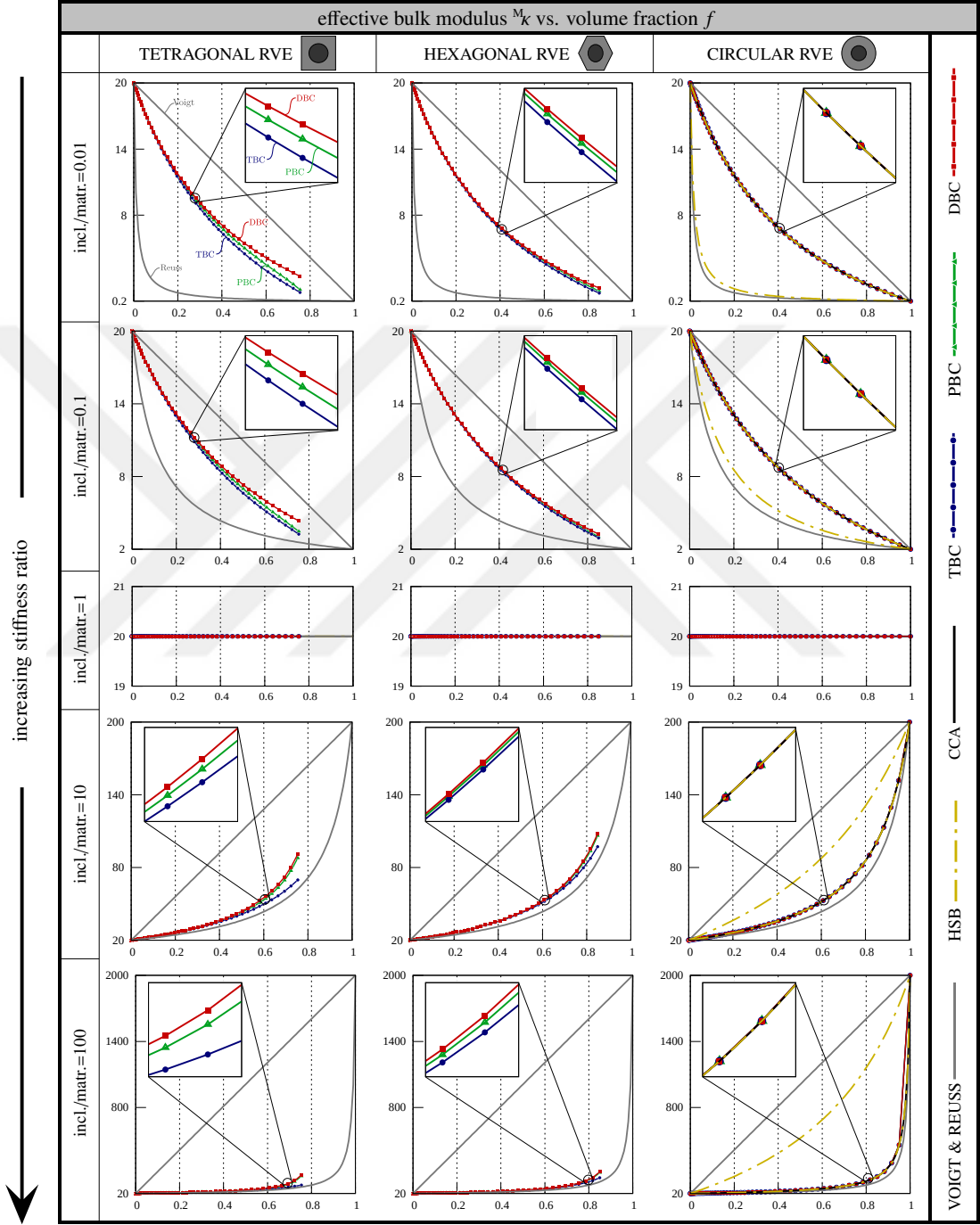


Figure 2.8: Effective bulk modulus versus volume fraction f . The numerical results are shown by lines with points on top of them whereas the analytical results are shown using lines solely. HSB stands for Hashin–Shtrikman bounds. Composite cylinder assemblage is denoted as CCA.

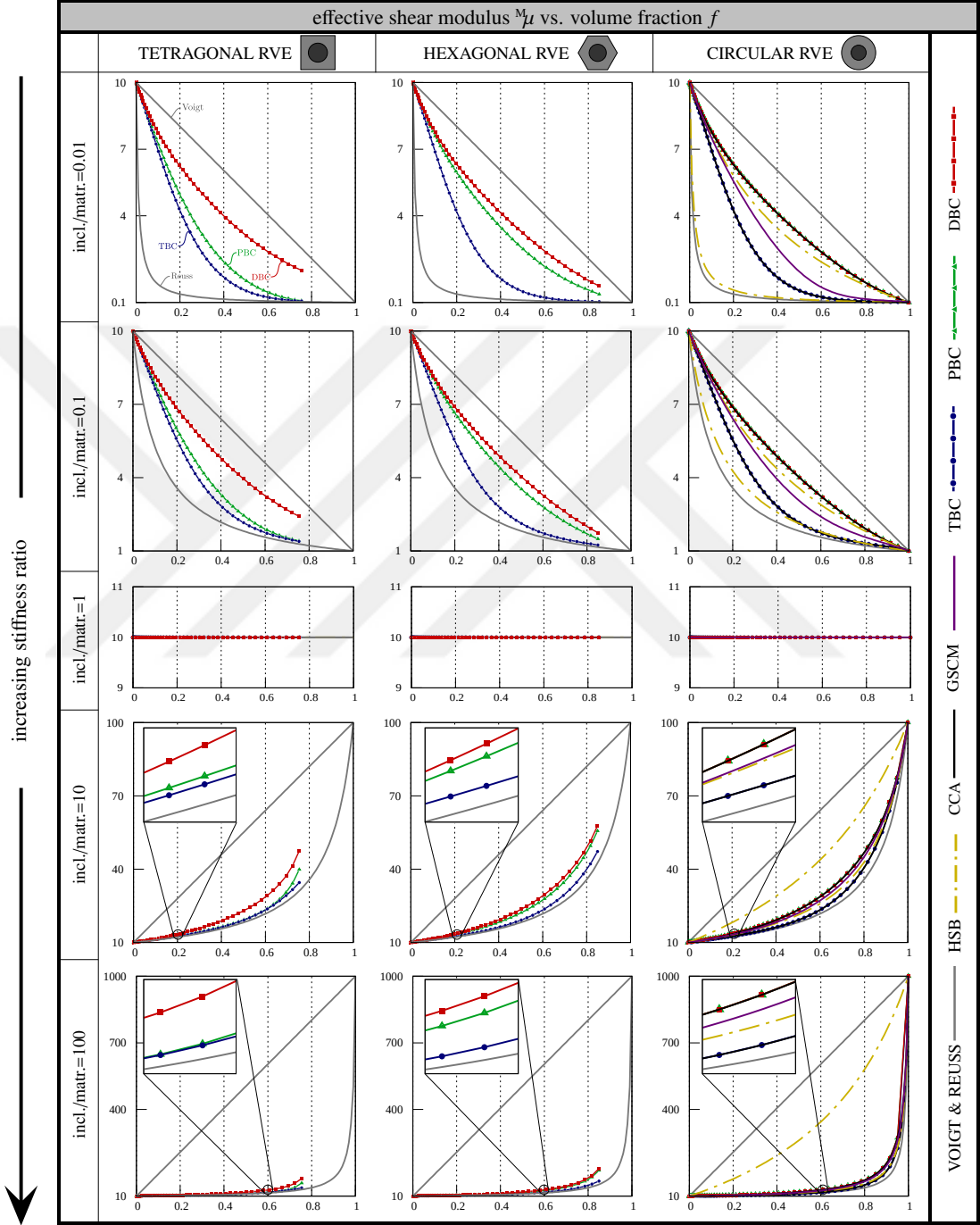


Figure 2.9: Effective shear modulus versus volume fraction f . The numerical results are shown by lines with points on top of them whereas the analytical results are shown using lines solely. HSB stands for Hashin–Shtrikman bounds. Composite cylinder assemblage is denoted as CCA. Generalized self-consistent method is denoted as GSCM.

and between CCA upper bound and DBC/PBC. A counterintuitive observation is that for incl./matr. < 1 , DBC and PBC together with CCA upper bound overestimate the upper HSB and for incl./matr. > 1 , TBC together with CCA lower bound underestimate the lower HSB.

Another shortcoming of the Hashin–Shtrikman bounds is that similar to Voigt and Reuss bounds, they cannot distinguish between the matrix and the fiber. Figure 2.10 sheds light on this issue by providing a comparison of the analytical estimates and the numerical results obtained using the circular RVE. The first column correspond to a certain properties for the matrix and fiber. In the second column, the properties are switched and the results are illustrated with respect to matrix volume fraction $1 - f$. The third column shows the subtraction of the

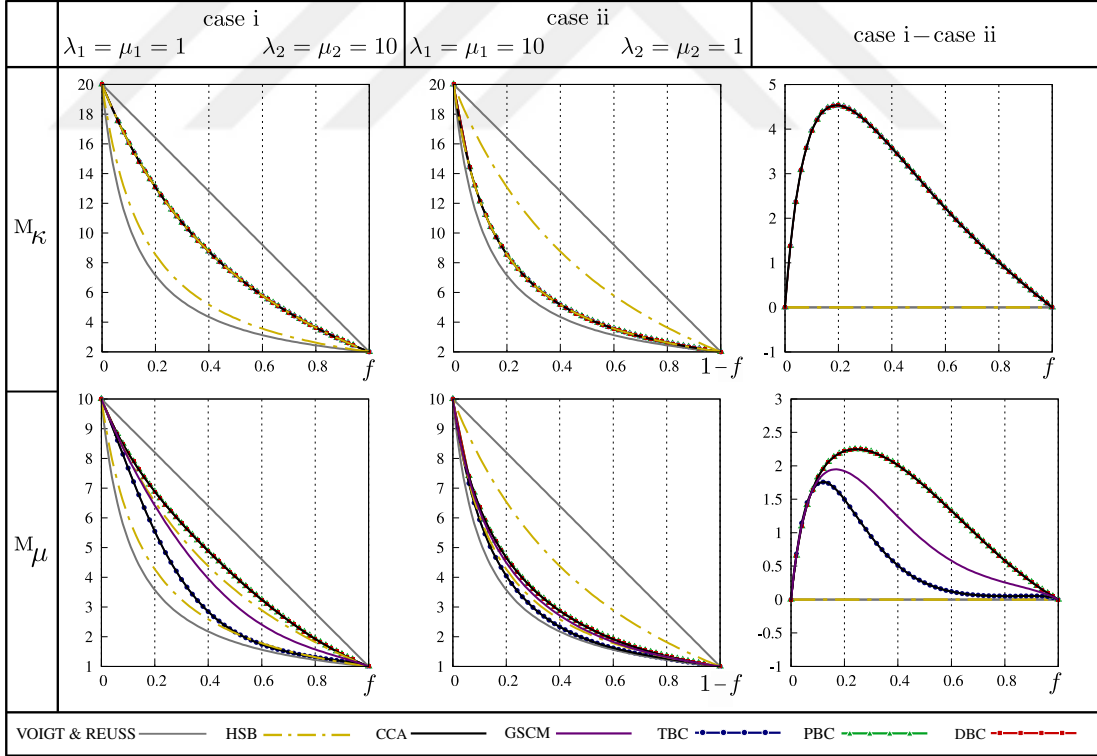


Figure 2.10: Illustration of the insensitivity of the Hashin–Shtrikman bounds to micro-structure’s constituents. Voigt and Reuss bounds do not distinguish between the fiber and matrix. Numerical results correspond to the circular RVE. CCA solution agrees with the numerical results. The first column shows incl./matr = 0.1 and the fiber’s volume fraction is f . The second column corresponds to incl./matr = 10 and the x-axis shows $1 - f$ instead of f . The third column shows the difference of the results in the first and the second column.

results associated with the first and second column. We observe that in contrast to the numerical results, CCA and GSCM, the Voigt, Reuss and Hashin–Shtrikman bounds are incapable of distinguishing between the matrix and the fiber hence, the difference between the responses vanishes in the right column.

Figure 2.11 illustrates the numerical results of various material properties with respect to volume fraction for the circular RVE. As observed previously, when the RVE is circular, DBC and PBC always render identical response. For the bulk modulus, DBC coincides with TBC while for the shear modulus, TBC underestimates DBC, as expected. For the Poisson’s ratio, TBC overestimates DBC. Another counterintuitive observation is that although the Poisson’s ratio of the fiber and matrix are identical, the overall Poisson’s ratio is dependent to the fiber volume fraction and is not constant.

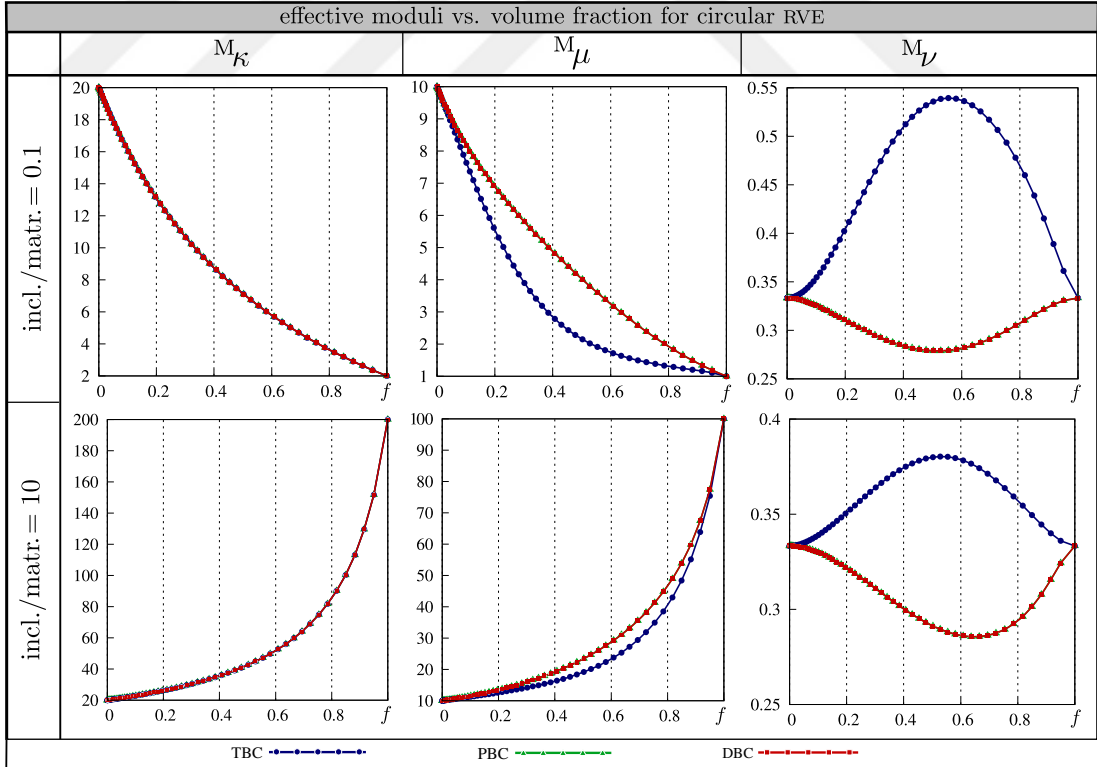


Figure 2.11: Illustration of different moduli versus volume fraction for two different stiffness ratios. The numerical results depicted in this figure correspond to the circular RVE. Each column corresponds to a specific material property and each row stands for specific stiffness ratio.

Heterogeneous materials generally possess non-periodic or random composition to some extents. Clearly, the distribution pattern of the inclusions influences the overall material response, see [137, 138]. The next set of numerical studies aims to highlight the effects of different morphologies of the micro-structures on the effective properties. To do so, we consider several RVEs with identical volume fractions of $f = 15\%$ and with random and periodic distribution of inclusions undergone the three canonical boundary conditions. The periodic micro-structure is modeled such that the inclusions of the same size are uniformly distributed throughout the RVE whereas the random micro-structures contain inclusions with different sizes and no specific order. The numerical results corresponding to the circular RVE with the same volume fraction as well as CCA and Hashin–Shtrikman bounds are also included for the sake of completeness. This study is performed for two stiffness ratios of 0.1 and 10 and the results are depicted in Figs. 2.12 and 2.13. The variation of the effective bulk modulus, shear modulus and Poisson’s ratio with respect to increasing the number of inclusions within the microstructure are examined. The lower Hashin–Shtrikman bound in Fig. 2.12 and the upper Hashin–Shtrikman bound in Fig. 2.13 are eliminated since they do not fit within the given range. We shall highlight that for each level of the random micro-structure, almost ten samples with different distribution patterns are investigated. That is, the effective responses shown in Figs. 2.12 and 2.13 do not correspond only to the micro-structures depicted at the bottom but reflect the average of the effective responses obtained from ten samples.

In both types of the microstructures and for both stiffness ratios, the results from DBC, PBC and TBC tend to converge to an *effective* response as the number of inclusions increases sufficiently. This trend is smoother for the periodic micro-structure compared to the random micro-structure where some fluctuations are present. We observe that due to the periodicity of the periodic micro-structure, PBC remains constant unlike TBC and DBC tend to approach to it from below and above, respectively. Somewhat interestingly, for the bulk modulus, the numerical results indicate that for random micro-structures and for both stiffness ratios, the circular RVE provides closer overall response to the overall response of the *true* RVE obtained by PBC. This is justified by the fact that increasing the

number of inclusions within the random micro-structure resembles increasing the level of isotropy. Nonetheless, for the periodic micro-structure, increasing the number of inclusions does not alter the anisotropy of the material due to the uniform distribution of the inclusions. To be more precise, a proper case that

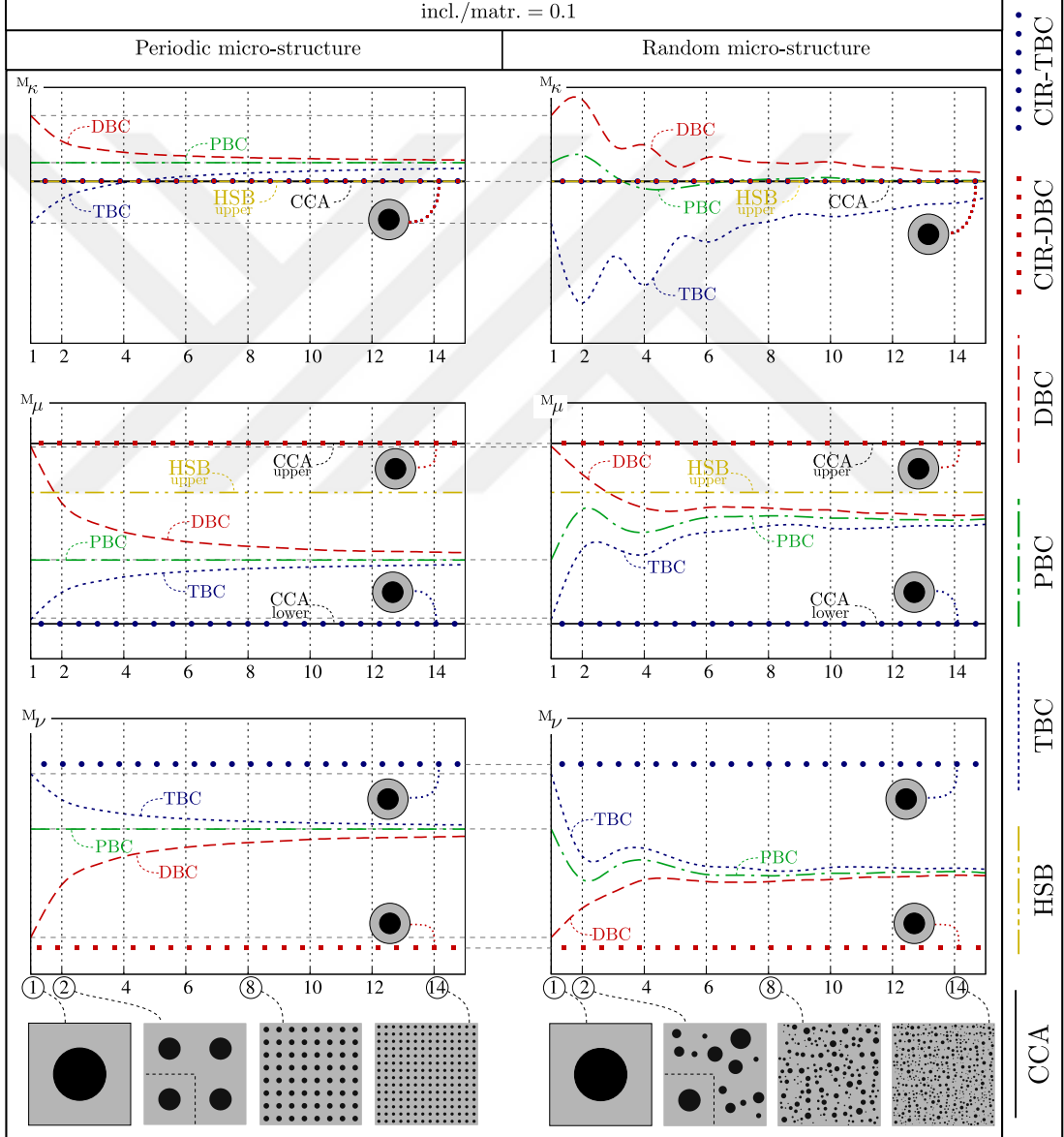


Figure 2.12: Illustration of the evolution of the effective properties versus the degree of periodicity and randomness for periodic and random macro-structures for stiffness ratio of 0.1. The size of the RVE remains constant as we increase the level of periodicity or randomness. The horizontal axis shows the degree of periodicity and randomness for the periodic and random microstructure, respectively. The micro-structures for some levels are depicted at the bottom of the figure.

could resemble an isotropic material suitable to be compared with analytical bounds is the random micro-structure with a large number of inclusions and randomness. Looking at the shear modulus, for the random micro-structure with large number of inclusions, the material response lies within the Hashin–Shtrikman

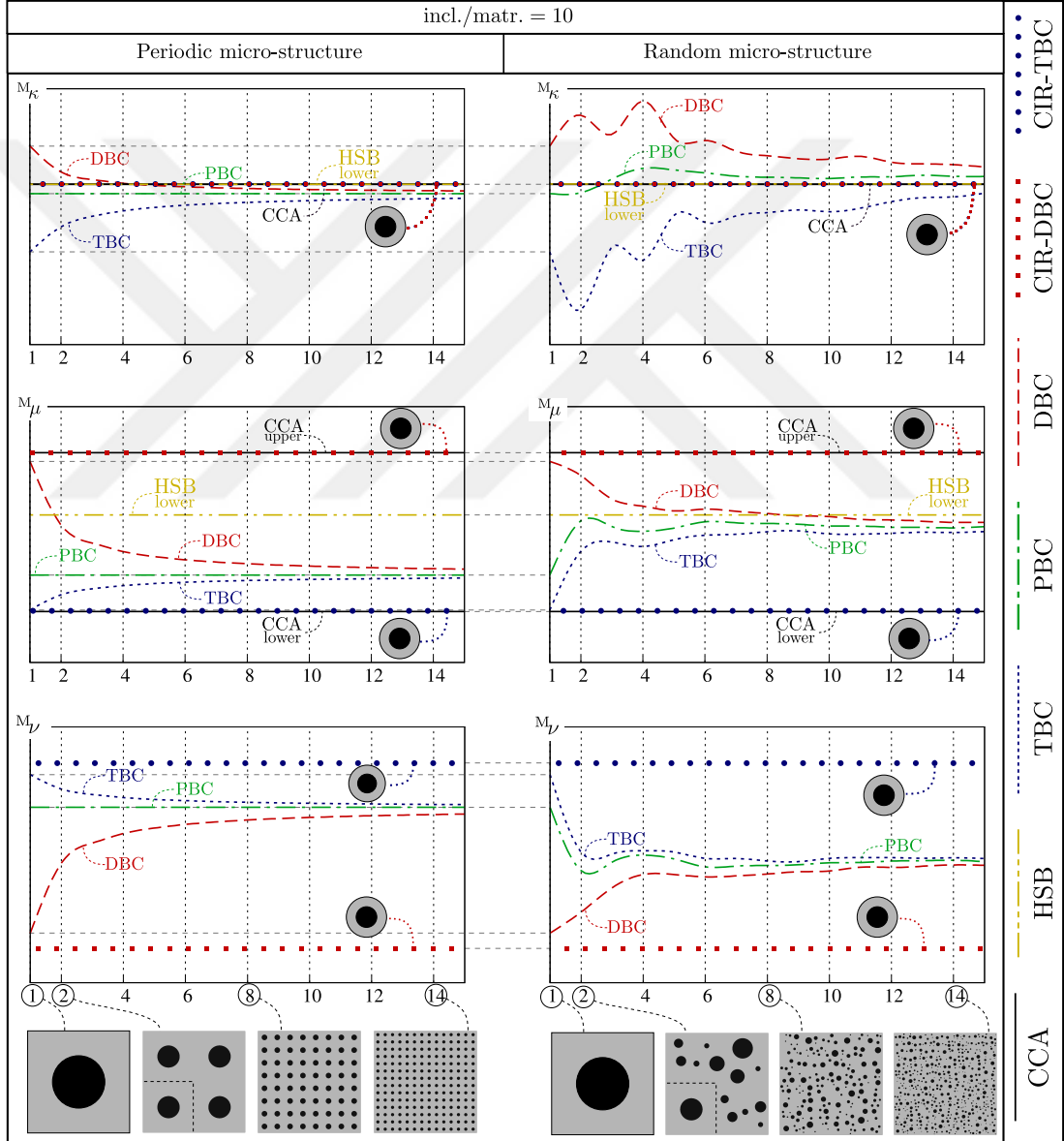


Figure 2.13: Illustration of the evolution of the effective properties versus the degree of periodicity and randomness for periodic and random macro-structures for stiffness ratio of 10. The size of the RVE remains constant as we increase the level of periodicity or randomness. The horizontal axis shows the degree of periodicity and randomness for the periodic and random microstructure, respectively. The micro-structures for some levels are depicted at the bottom of the figure.

bounds for $\text{incl./matr.} = 0.1$. However, for $\text{incl./matr.} = 10$, the lower Hashin–Shtrikman bound is violated and fails to provide a proper bound on the shear modulus. *This observation shall be compared with Hashin’s remark in [139] that it has never been shown that his bounds on shear modulus are the best possible bounds. Clearly, we observe that his bounds on shear modulus do not serve as “bounds” at least not in the sense of CCA, Voigt and Reuss bounds.* For the Poisson’s ratio, unlike the shear modulus and the bulk modulus, TBC provides the stiffest response whereas DBC renders the most compliant response.

All the previous examples were only valid at small strains. Our computational framework is capable to carry out finite deformation analysis. Here, we extend the numerical studies to finite deformations setting. The examples carefully analyze the overall material response for various boundary conditions and RVE type. Unlike small-strain linear elasticity, for finite deformations it is not possible to define an effective material parameter such as bulk modulus or shear modulus. Therefore, in what follows the apparent macroscopic quantities of interest are Piola stress and deformation gradient. For instance, for volumetric expansion, the xx -component and for simple shear, the xy -component of the Piola stress or deformation gradient are the macroscopic properties of interest. Figure 2.14 exhibits the distribution of the deformation gradient throughout the RVEs when simple shear with magnitude of 50% is prescribed. The stiffness ratio is $\text{incl./matr.} = 0.1$ and the inclusion volume fraction is 20%. The deformed RVEs are depicted at every 10% increment. Note, even for finite deformation analysis our numerical simulation does not lose its robustness and quadratic convergence is obtained. Moreover, Fig. 2.15 compares the distribution of the deformation gradient for RVEs with centric and off-centric inclusions under three different boundary conditions when simple shear is prescribed. The inclusion volume fraction in this study is assumed to be 30% and the stiffness ratio is $\text{incl./matr.} = 0.1$. Evidently, eccentricity of the inclusion results in non-symmetric distribution and some local concentrations. Larger values of the deformation gradient is observed for the off-centric cases. A counterintuitive observation is that, in contrast to the centric case, PBC and DBC do not render the same response for the circular RVE when the inclusion is off-centric.

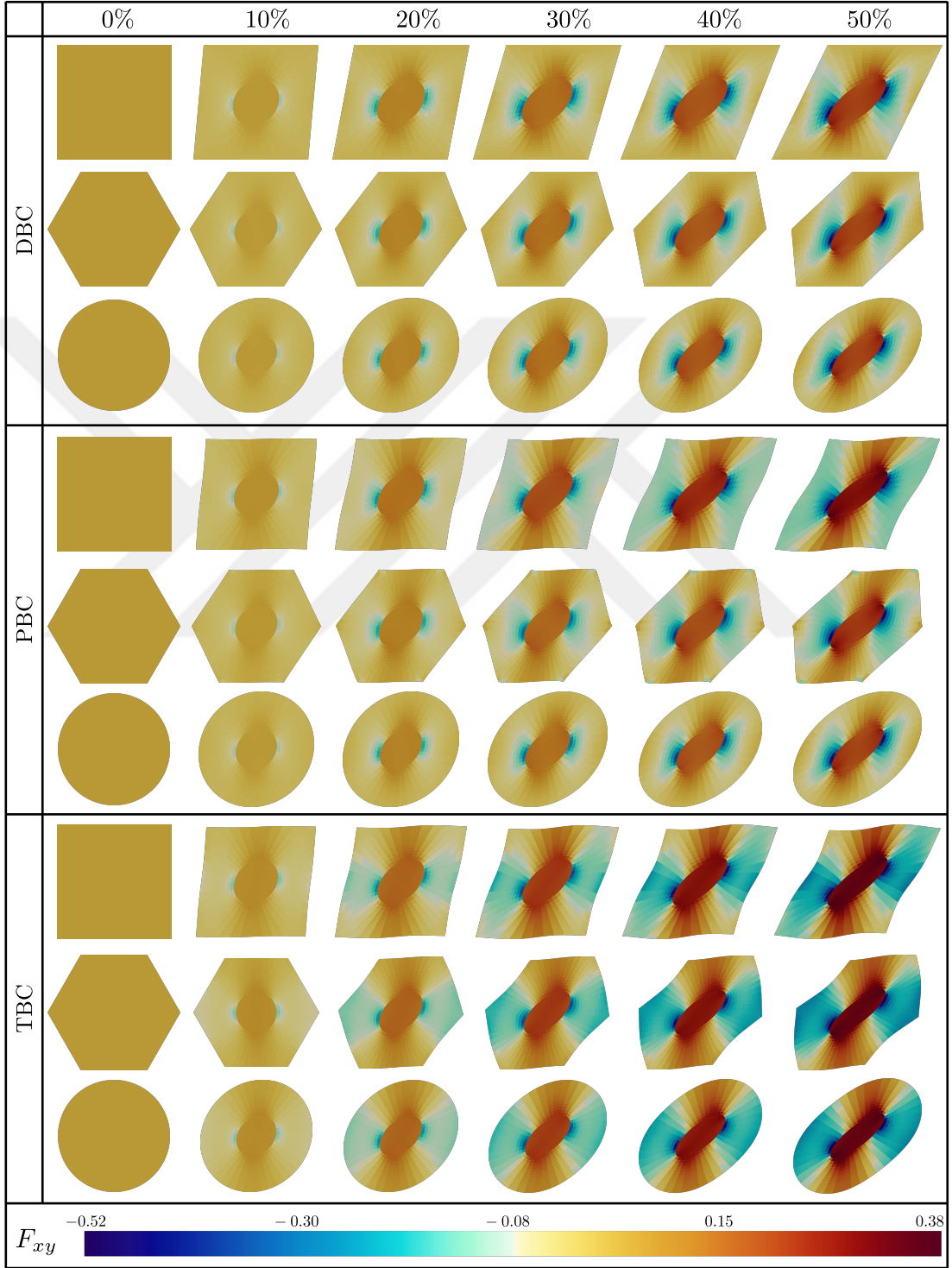


Figure 2.14: Deformation gradient throughout the RVEs at finite deformations under simple shear for the stiffness ratio of incl./matr. = 0.1.

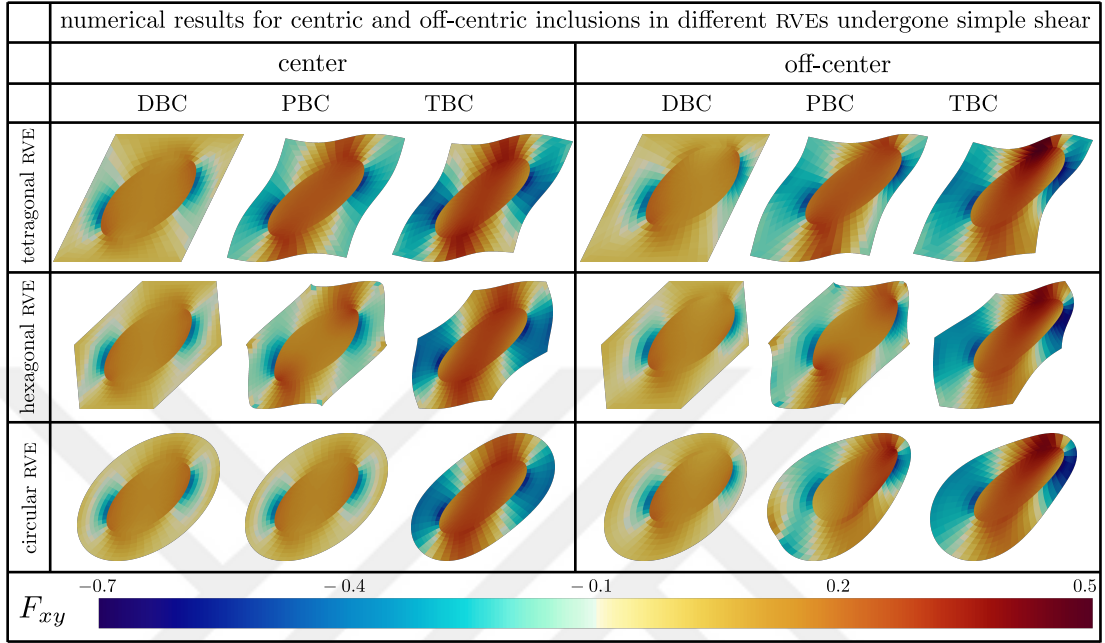


Figure 2.15: Deformation gradient throughout the RVEs at finite deformations under simple shear for both centric and off-centric inclusions with stiffness ratio of incl./matr. = 0.1.

Chapter 3

Interface-enhanced homogenization

The objective of this chapter is to extend the homogenization framework to account for interfaces hence capturing size effects. The theoretical aspects of homogenization incorporating interfaces are detailed in Section 3.1. This is then followed by elaborating on the finite element implementation of such problems in Section 3.2. Section 3.3 elaborates the new analytical schemes to determine the overall response of composites. Section 3.4 compares the computational and analytical results through a set of numerical examples.

3.1 Theory

This section establishes the governing equations of continua embedding a general interface within the framework of homogenization. Similar to Section 2.1, the problem is decomposed into two separate macro- and micro-problems. The separation of the length scales has two important outcomes for our study. First, the unknown macroscopic behavior of the medium can be calculated by homogenization of the underlying micro-structure whose constitutive laws are assumed

to be known. Second, the influence of the interface would no longer be negligible due to the large area-to-volume ratio and thus, the micro-scale possesses a physical length-scale. Note, the following study mainly focuses on the incorporation of the general interfaces into the homogenization framework. That is, our RVE is assumed to be composed of a matrix containing an inclusion with a general imperfect interface in between. Further details on the formulation of the general interface model in the context of continuum mechanics can be found in [140–142]. To proceed, the following frequently used interface operators need to be defined

$$\begin{aligned}\bar{\mathbf{I}} &:= \mathbf{I} - \bar{\mathbf{N}} \otimes \bar{\mathbf{N}}, & \overline{\text{Grad}}\{\bar{\bullet}\} &:= \text{Grad}\{\bar{\bullet}\} \cdot \bar{\mathbf{I}}, \\ \overline{\text{Div}}\{\bar{\bullet}\} &:= \overline{\text{Grad}}\{\bar{\bullet}\} : \bar{\mathbf{I}}, & \overline{\text{Det}}\{\bar{\bullet}\} &:= \frac{|[\{\bar{\bullet}\} \cdot \bar{\mathbf{G}}_1] \times [\{\bar{\bullet}\} \cdot \bar{\mathbf{G}}_2]|}{|\bar{\mathbf{G}}_1 \times \bar{\mathbf{G}}_2|}.\end{aligned}$$

3.1.1 Macro-problem

The kinematics of the macro-problem here is similar to Section 2.1.1 and is not detailed here for the sake of brevity. The balance equations in the macro-problem are the balances of linear and angular momentum which read

$$\begin{aligned}{}^{\text{M}}\text{Div} {}^{\text{M}}\mathbf{P} + {}^{\text{M}}\mathbf{b}_0^{\text{p}} &= 0 \quad \text{in} \quad {}^{\text{M}}\mathcal{B}_0 \quad \text{subject to} \quad {}^{\text{M}}\mathbf{P} \cdot {}^{\text{M}}\mathbf{N} = {}^{\text{M}}\mathbf{t}_0 \quad \text{on} \quad \partial {}^{\text{M}}\mathcal{B}_0, \\ {}^{\text{M}}\mathbf{t}_0 &= {}^{\text{M}}\mathbf{t}_0^{\text{p}} \quad \text{on} \quad \partial {}^{\text{M}}\mathcal{B}_{0,\text{N}} \quad \text{and} \quad {}^{\text{M}}\boldsymbol{\varphi} = {}^{\text{M}}\boldsymbol{\varphi}^{\text{p}} \quad \text{on} \quad \partial {}^{\text{M}}\mathcal{B}_{0,\text{D}}.\end{aligned}$$

and

$${}^{\text{M}}\mathbf{P} \cdot {}^{\text{M}}\mathbf{F}^t = {}^{\text{M}}\mathbf{F} \cdot {}^{\text{M}}\mathbf{P}^t.$$

3.1.2 Micro-problem

The definition of the micro-problem is nearly identical to Section 2.1.2, however, due to the presence of the interface, the interface related relations shall be discussed. The configuration $\mathcal{B}_0$ at the micro-scale is assumed to be the RVE with its boundary denoted $\partial \mathcal{B}_0$. The interface $\mathcal{I}_0$ in the material configuration, splits the micro-structure into two sub-domains $\mathcal{B}_0^+$ and $\mathcal{B}_0^-$ associated with the plus

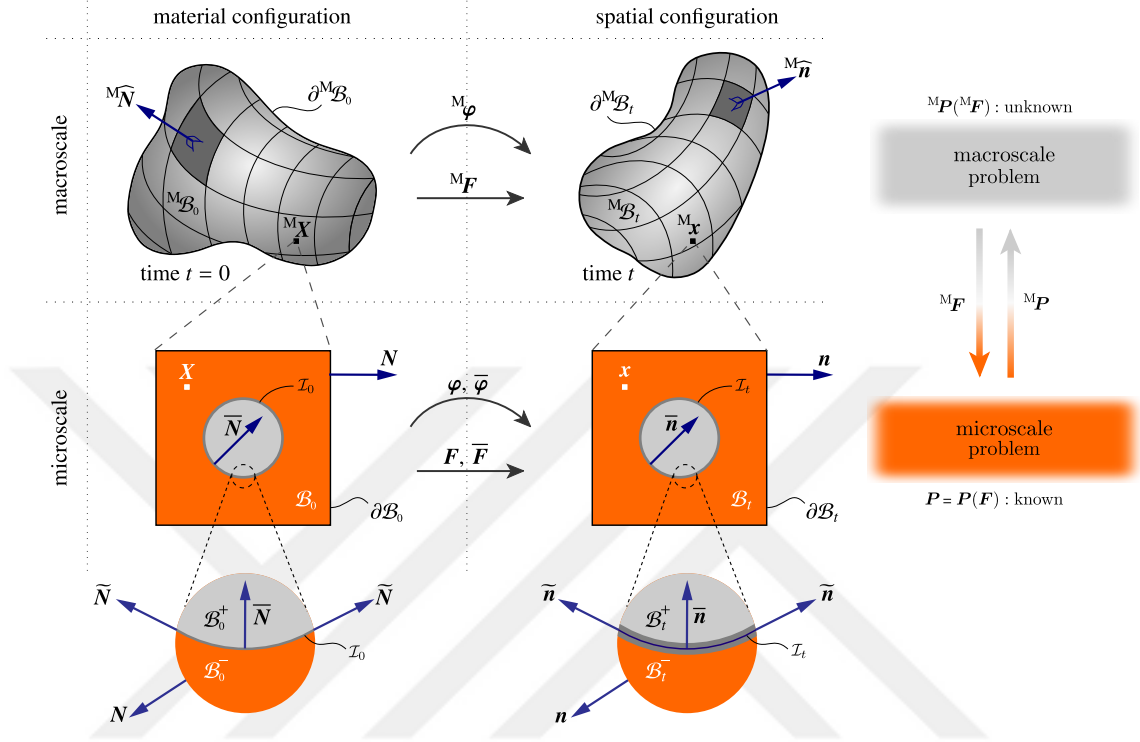


Figure 3.1: Computational interface-enhanced homogenization graphical summary. The interface $\mathcal{I}$ splits the domain into $\mathcal{B}_0^+$ and $\mathcal{B}_0^-$ corresponding to the plus and minus sides of the interface. The non-linear map $\bar{\varphi}$ maps the interfacial points $\bar{\mathbf{X}}$ from the material configuration to $\bar{\mathbf{x}}$ in the spatial configuration. Interface line elements are mapped from the material configuration to the spatial configuration via $\bar{\mathbf{F}}$. The interface unit normal $\bar{\mathbf{N}}$ points from the minus side of the interface to its plus side.

and minus sides of the interface, respectively. In other words, the sub-domains $\mathcal{B}_0^+$ and $\mathcal{B}_0^-$ correspond to the inclusion and the matrix, respectively and the interface can be regarded as the boundary of the inclusion. In the material and spatial configurations, the unit normals to the interface are denoted as $\bar{\mathbf{N}}$ and $\bar{\mathbf{n}}$, respectively. Note, the interface unit normal points from the minus side of the interface to its plus side. In this manuscript, we assume that the inclusion and consequently the interface are entirely enclosed within the RVE and do not have any intersection with the boundary $\partial\mathcal{B}_0$. It is of great importance to mention that the plus and minus sides of the interface coincide geometrically in the material configuration whereas this is not the case in the spatial configuration.

The points on the interface in the material configuration $\bar{\mathbf{X}}$ map to their spatial

counterparts $\bar{\mathbf{x}}$ via the non-linear interfacial map $\bar{\boldsymbol{\varphi}} = \llbracket \boldsymbol{\varphi} \rrbracket$. The interface deformation gradient $\bar{\mathbf{F}}$ maps the interface line elements in the material configuration $d\bar{\mathbf{X}}$ to the spatial interface line elements $d\bar{\mathbf{x}}$. The interface deformation gradient relates to the interface non-linear map via $\bar{\mathbf{F}} = \overline{\text{Grad}} \bar{\boldsymbol{\varphi}} = \mathbf{F} \cdot \bar{\mathbf{I}}$, where $\bar{\mathbf{I}}$ is the interface identity tensor.

At the micro-scale, for a quasi-static problem, the balance equations in the bulk and on the interface read

$$\begin{aligned} \text{bulk:} & \quad \begin{cases} \text{linear momentum :} & \text{Div} \mathbf{P} = \mathbf{0}, \\ \text{angular momentum :} & \mathbf{P} \cdot \mathbf{F}^t = \mathbf{F} \cdot \mathbf{P}^t, \end{cases} \\ \text{interface:} & \quad \begin{cases} \text{linear momentum :} & \overline{\text{Div}} \bar{\mathbf{P}} + \llbracket \mathbf{P} \rrbracket \cdot \bar{\mathbf{N}} = \mathbf{0}, \\ \text{angular momentum :} & \boldsymbol{\epsilon} : \left[\llbracket \boldsymbol{\varphi} \rrbracket \otimes \left[\llbracket \mathbf{P} \rrbracket \cdot \bar{\mathbf{N}} \right] + \bar{\mathbf{F}} \cdot \bar{\mathbf{P}}^t \right] = \mathbf{0}, \end{cases} \end{aligned} \quad (3.1)$$

where $\boldsymbol{\epsilon}$ is the Levi-Civita permutation symbol. Moreover the tractions read

$$\begin{aligned} \mathbf{P} \cdot \mathbf{N} &= \mathbf{t}_0 \quad \text{on} \quad \partial \mathcal{B}_0, \\ \llbracket \mathbf{P} \rrbracket \cdot \bar{\mathbf{N}} &= \llbracket \mathbf{t} \rrbracket \quad \text{on} \quad \mathcal{I}_0, \\ \llbracket \mathbf{P} \rrbracket \cdot \bar{\mathbf{N}} &=: \bar{\mathbf{t}} \quad \text{on} \quad \mathcal{I}_0, \end{aligned}$$

with $\mathbf{t}_0$ being the prescribed traction on the boundary $\partial \mathcal{B}_0$ and $\llbracket \mathbf{t} \rrbracket$ and $\bar{\mathbf{t}}$ being the traction jump across the interface and the interface traction, respectively.

3.1.3 Micro-to-macro transition

In the computational homogenization framework, at the micro-scale, the constitutive behavior of each phase is assumed to be known and the overall macroscopic material response is obtained via solving the associated boundary value problem and proper averaging over the RVE [44, 47, 143–145]. To proceed, the following

average definitions prove to be helpful for the upcoming calculations

$$\begin{aligned}
\langle \{\bullet\} \rangle_{\mathcal{B}_0^-} &:= \frac{1}{\mathcal{V}_0} \int_{\mathcal{B}_0^-} \{\bullet\} dV, & \langle \{\bullet\} \rangle_{\mathcal{B}_0^+} &:= \frac{1}{\mathcal{V}_0} \int_{\mathcal{B}_0^+} \{\bullet\} dV, \\
\langle \{\bullet\} \rangle_{\partial \mathcal{B}_0} &:= \frac{1}{\mathcal{V}_0} \int_{\partial \mathcal{B}_0} \{\bullet\} dV, & \langle \{\bullet\} \rangle_{\mathcal{I}_0} &:= \frac{1}{\mathcal{V}_0} \int_{\mathcal{I}_0} \{\bullet\} dA, \\
\langle \{\bullet\} \rangle &= \langle \{\bullet\} \rangle_{\mathcal{B}_0} = \frac{1}{\mathcal{V}_0} \int_{\mathcal{B}_0^-} \{\bullet\} dV + \frac{1}{\mathcal{V}_0} \int_{\mathcal{B}_0^+} \{\bullet\} dV.
\end{aligned}$$

Extended average deformation gradient theorem In order to relate the micro and macro deformation gradients in our problem, the classical average deformation gradient theorem is extended to incorporate interfaces. Assume that $\mathbf{F}_c$ is a constant tensor and $\partial \mathcal{B}_0$ is the boundary of the domain $\mathcal{B}_0$ with the outward unit normal $\mathbf{N}$. The average deformation gradient theorem states that if $\boldsymbol{\varphi} = \mathbf{F}_c \cdot \mathbf{X}$ is prescribed on the boundary $\partial \mathcal{B}_0$, then $\langle \mathbf{F} \rangle_{\mathcal{B}_0} + \langle \llbracket \boldsymbol{\varphi} \rrbracket \otimes \overline{\mathbf{N}} \rangle_{\mathcal{I}_0} = \mathbf{F}_c$. To prove this theorem, employing $\llbracket \boldsymbol{\varphi} \rrbracket = \boldsymbol{\varphi}^+ - \boldsymbol{\varphi}^-$ and applying the gradient theorem yield

$$\begin{aligned}
\frac{1}{\mathcal{V}_0} \int_{\partial \mathcal{B}_0} \boldsymbol{\varphi} \otimes \mathbf{N} dA &= \frac{1}{\mathcal{V}_0} \int_{\mathcal{B}_0^-} \text{Grad} \boldsymbol{\varphi} dV + \frac{1}{\mathcal{V}_0} \int_{\mathcal{I}_0} \llbracket \boldsymbol{\varphi} \rrbracket \otimes \overline{\mathbf{N}} dA + \frac{1}{\mathcal{V}_0} \int_{\mathcal{B}_0^+} \text{Grad} \boldsymbol{\varphi} dV \\
&= \frac{1}{\mathcal{V}_0} \int_{\mathcal{B}_0^-} \mathbf{F} dV + \frac{1}{\mathcal{V}_0} \int_{\mathcal{I}_0} \llbracket \boldsymbol{\varphi} \rrbracket \otimes \overline{\mathbf{N}} dA + \frac{1}{\mathcal{V}_0} \int_{\mathcal{B}_0^+} \mathbf{F} dV \\
&= \langle \mathbf{F} \rangle_{\mathcal{B}_0^-} + \frac{1}{\mathcal{V}_0} \int_{\mathcal{I}_0} \llbracket \boldsymbol{\varphi} \rrbracket \otimes \overline{\mathbf{N}} dA + \langle \mathbf{F} \rangle_{\mathcal{B}_0^+} \\
&= \langle \mathbf{F} \rangle_{\mathcal{B}_0} + \langle \llbracket \boldsymbol{\varphi} \rrbracket \otimes \overline{\mathbf{N}} \rangle_{\mathcal{I}_0}.
\end{aligned}$$

Finally, replacing $\boldsymbol{\varphi} = \mathbf{F}_c \cdot \mathbf{X}$ renders the theorem

$$\begin{aligned}
\langle \mathbf{F} \rangle_{\mathcal{B}_0} + \langle \llbracket \boldsymbol{\varphi} \rrbracket \otimes \overline{\mathbf{N}} \rangle_{\mathcal{I}_0} &= \langle \boldsymbol{\varphi} \otimes \mathbf{N} \rangle_{\partial \mathcal{B}_0} \\
&= \langle \mathbf{F}_c \cdot \mathbf{X} \otimes \mathbf{N} \rangle_{\partial \mathcal{B}_0} = \mathbf{F}_c \cdot \langle \mathbf{X} \otimes \mathbf{N} \rangle_{\partial \mathcal{B}_0} = \mathbf{F}_c \cdot \mathbf{I} = \mathbf{F}_c.
\end{aligned}$$

The extended deformation gradient theorem encompasses the additional terms due to the deformation jump across the interface and not the deformation gradient along the interface. The average deformation gradient theorem states if a deformation $\mathbf{F}_c \cdot \mathbf{X}$ is prescribed on a boundary of a body, the bulk average of the deformation gradient plus the boundary average of the projection of the jump

of the deformation gradient onto the interface is equal to $\mathbf{F}_c$ regardless of how complex the deformation gradient is throughout the domain. Motivated by the average deformation gradient theorem, in view of the micro-to-macro transition, the macroscopic deformation gradient can be written as

$${}^M\mathbf{F} := \langle \mathbf{F} \rangle_{\mathcal{B}_0} + \langle [\![\boldsymbol{\varphi}]\!] \otimes \overline{\mathbf{N}} \rangle_{\mathcal{I}_0} = \langle \boldsymbol{\varphi} \otimes \mathbf{N} \rangle_{\partial\mathcal{B}_0} . \quad (3.2)$$

Extended average Piola stress theorem Assume that $\mathbf{P}_c$ is a constant tensor and $\partial\mathcal{B}_0$ is the boundary of the domain $\mathcal{B}_0$ with the outward unit normal $\mathbf{N}$. The average Piola stress theorem states that if $\mathbf{t}_0 = \mathbf{P}_c \cdot \mathbf{N}$ is prescribed on the boundary, then $\langle \mathbf{P} \rangle_{\mathcal{B}_0} + \langle \overline{\mathbf{P}} \rangle_{\mathcal{I}_0} = \mathbf{P}_c$. To prove , using $\mathbf{t}_0 = \mathbf{P} \cdot \mathbf{N}$ we can write

$$\frac{1}{\mathcal{V}_0} \int_{\partial\mathcal{B}_0} \mathbf{t}_0 \otimes \mathbf{X} \, dA = \frac{1}{\mathcal{V}_0} \int_{\partial\mathcal{B}_0} [\mathbf{P} \cdot \mathbf{N}] \otimes \mathbf{X} \, dA .$$

Adding and subtracting an integral as follows

$$\begin{aligned} \frac{1}{\mathcal{V}_0} \int_{\partial\mathcal{B}_0} \mathbf{t}_0 \otimes \mathbf{X} \, dA &= \frac{1}{\mathcal{V}_0} \int_{\partial\mathcal{B}_0} [\mathbf{P} \cdot \mathbf{N}] \otimes \mathbf{X} \, dA + \frac{1}{\mathcal{V}_0} \int_{\mathcal{I}_0^-} [\mathbf{P} \cdot \mathbf{N}] \otimes \overline{\mathbf{X}} \, dA \\ &\quad - \frac{1}{\mathcal{V}_0} \int_{\mathcal{I}_0^-} [\mathbf{P} \cdot \mathbf{N}] \otimes \overline{\mathbf{X}} \, dA . \end{aligned}$$

Employing the divergence theorem yields

$$\begin{aligned} \frac{1}{\mathcal{V}_0} \int_{\partial\mathcal{B}_0} \mathbf{t}_0 \otimes \mathbf{X} \, dA &= \frac{1}{\mathcal{V}_0} \int_{\mathcal{B}_0^-} \text{Div}(\mathbf{X} \overline{\otimes} \mathbf{P}) \, dV - \frac{1}{\mathcal{V}_0} \int_{\mathcal{I}_0} \overline{\text{Div}}(\overline{\mathbf{X}} \overline{\otimes} \overline{\mathbf{P}}) \, dA \\ &\quad + \frac{1}{\mathcal{V}_0} \int_{\mathcal{I}_0} \overline{\mathbf{P}} \, dA + \frac{1}{\mathcal{V}_0} \int_{\mathcal{B}_0^+} \text{Div}(\mathbf{X} \overline{\otimes} \mathbf{P}) \, dV . \end{aligned}$$

Then, using the identity $\text{Div}(\mathbf{X} \overline{\otimes} \mathbf{P}) = \text{Div} \mathbf{P} \otimes \mathbf{X} + \mathbf{P} \cdot \text{Grad} \mathbf{X}$ and applying the divergence theorem on the second term we have

$$\begin{aligned} \frac{1}{\mathcal{V}_0} \int_{\partial\mathcal{B}_0} \mathbf{t}_0 \otimes \mathbf{X} \, dA &= \frac{1}{\mathcal{V}_0} \int_{\mathcal{B}_0^-} \mathbf{P} \, dV - \frac{1}{\mathcal{V}_0} \int_{\partial\mathcal{I}_0} [\overline{\mathbf{X}} \overline{\otimes} \overline{\mathbf{P}}] \cdot \widetilde{\mathbf{N}} \, dL \\ &\quad + \frac{1}{\mathcal{V}_0} \int_{\mathcal{I}_0} \overline{\mathbf{K}} [\overline{\mathbf{X}} \overline{\otimes} \overline{\mathbf{P}}] \cdot \overline{\mathbf{N}} \, dA + \frac{1}{\mathcal{V}_0} \int_{\mathcal{I}_0} \overline{\mathbf{P}} \, dA + \frac{1}{\mathcal{V}_0} \int_{\mathcal{B}_0^+} \mathbf{P} \, dV , \end{aligned}$$

where $\overline{K} = -\overline{\text{Div}} \overline{\mathbf{N}}$ and $\widetilde{\mathbf{N}}$ is the normal at the boundary of the interface but along the interface itself. Since we assumed that the interface does not intersect with the boundary $\partial\mathcal{I}_0 = \emptyset$, the second integral vanishes. Moreover, due to the superficiality of the interface, $\overline{\mathbf{P}} \cdot \overline{\mathbf{N}} = 0$ and the third integral vanishes and consequently

$$\langle \mathbf{P} \rangle_{\mathcal{B}_0} + \langle \overline{\mathbf{P}} \rangle_{\mathcal{I}_0} = \langle \mathbf{t}_0 \otimes \mathbf{X} \rangle_{\partial\mathcal{B}_0} .$$

Finally, we can deduce

$$\begin{aligned} \langle \mathbf{P} \rangle_{\mathcal{B}_0} + \langle \overline{\mathbf{P}} \rangle_{\mathcal{I}_0} &= \langle \mathbf{t}_0 \otimes \mathbf{X} \rangle_{\partial\mathcal{B}_0} = \langle \mathbf{P}_c \cdot \mathbf{N} \otimes \mathbf{X} \rangle_{\partial\mathcal{B}_0} \\ &= \mathbf{P}_c \cdot \langle \mathbf{N} \otimes \mathbf{X} \rangle_{\partial\mathcal{B}_0} = \mathbf{P}_c \cdot \mathbf{I} = \mathbf{P}_c . \end{aligned}$$

The average Piola stress theorem states if a traction $\mathbf{P}_c \cdot \mathbf{N}$ is prescribed on a boundary of a body, the bulk average of the Piola stress plus the interface average of the interface stress is equal to $\mathbf{P}_c$ regardless of how complex the stress is throughout the domain. Motivated by the average Piola stress theorem, in view of the micro-to-macro transition, the macroscopic Piola stress can be written as

$${}^{\text{M}}\mathbf{P} := \langle \mathbf{P} \rangle_{\mathcal{B}_0} + \langle \overline{\mathbf{P}} \rangle_{\mathcal{I}_0} = \langle \mathbf{t}_0 \otimes \mathbf{X} \rangle_{\partial\mathcal{B}_0} . \quad (3.3)$$

Extended Hill–Mandel condition Equipped with the macroscopic Piola stress and deformation gradient, the next step is to impose the incremental energy equivalence between the micro- and macro-scales in an interface-enhanced fashion. The incremental energy equivalence is also known as the Hill–Mandel condition. The Hill–Mandel condition in terms of the surface integrals reads

$${}^{\text{M}}\mathbf{P} : \delta^{\text{M}}\mathbf{F} - \langle \mathbf{t}_0 \cdot \delta\boldsymbol{\varphi} \rangle_{\partial\mathcal{B}_0} \stackrel{!}{=} 0 , \quad (3.4)$$

that can be expressed alternatively as

$$\langle \mathbf{t}_0 \cdot \delta\boldsymbol{\varphi} \rangle_{\partial\mathcal{B}_0} = \langle \mathbf{P} : \delta\mathbf{F} \rangle_{\mathcal{B}_0} + \langle \overline{\mathbf{P}} : \delta\overline{\mathbf{F}} \rangle_{\mathcal{I}_0} + \langle \overline{\mathbf{t}} \cdot \llbracket \delta\boldsymbol{\varphi} \rrbracket \rangle_{\mathcal{I}_0} .$$

Inserting Hill's lemma into the Hill–Mandel condition (3.4) yields

$$\int_{\partial\mathcal{B}_0} [\delta\boldsymbol{\varphi} - \delta^{\text{M}}\mathbf{F} \cdot \mathbf{X}] \cdot [\mathbf{t}_0 - {}^{\text{M}}\mathbf{P} \cdot \mathbf{N}] \, \text{d}A \stackrel{!}{=} 0,$$

which is identical to the Hill–Mandel condition in the absence of the interface, given in the previous chapter. Therefore, the boundary conditions here remain identical to those in the absence of the interfaces. More precisely, we imposed DBC, PBC and TBC in the following discussions.

3.2 Finite element implementation

The goal of this section is to briefly elaborate on the computational aspects of general interfaces within the framework of the finite element method. See [141] for more details on the finite element implementation of interface-enhanced homogenization. The material model for the bulk is similar to Section 2.2 and thus, definition of the Piola stress and Piola tangent is identical to Eq. (2.6). Moreover, interface elasticity theory, suggests an independent energy density to be assigned to the interface. For the interface material response, we additively decompose the material response into an orthogonal response across the interface and a tangential response along the interface. As a result, the interface free energy density for a hyperelastic behavior depends on both the interface deformation gradient and the jump of the motion across the interface as

$$\bar{\psi}(\bar{\mathbf{F}}, \llbracket \boldsymbol{\varphi} \rrbracket) = \bar{\psi}^{\parallel}(\bar{\mathbf{F}}) + \bar{\psi}^{\perp}(\llbracket \boldsymbol{\varphi} \rrbracket).$$

Accordingly, the interface Piola stress and Piola tangent read

$$\bar{\mathbf{P}} = \frac{\partial \bar{\psi}^{\parallel}}{\partial \bar{\mathbf{F}}}, \quad \bar{\mathbf{A}}_{\parallel} = \frac{\partial \bar{\mathbf{P}}}{\partial \bar{\mathbf{F}}}, \quad \bar{\mathbf{t}} = \frac{\partial \bar{\psi}^{\parallel}}{\partial \llbracket \boldsymbol{\varphi} \rrbracket}, \quad \bar{\mathbf{A}}_{\perp} = \frac{\partial \bar{\mathbf{t}}}{\partial \llbracket \boldsymbol{\varphi} \rrbracket},$$

and consequently we have

$$\frac{\partial \bar{\mathbf{t}}}{\partial \bar{\mathbf{F}}} = \mathbf{0}, \quad \frac{\partial \bar{\mathbf{P}}}{\partial \llbracket \boldsymbol{\varphi} \rrbracket} = \mathbf{0}.$$

Further details on the definition of the interface energy density $\bar{\psi}$ and the corresponding derivations are available in Appendix B.2.

The first step for the finite element implementation of the theory is to derive the weak form. In doing so, the strong form of the linear momentum balance equations (3.1) for the bulk and interface are tested with a vector-valued test function $\delta\varphi$. Using the divergence theorem, the weak form of the balance of linear momentum in the absence of the body forces read

$$\int_{\mathcal{B}_0} \mathbf{P} : \text{Grad} \delta\varphi \, dV + \int_{\mathcal{I}_0} \bar{\mathbf{P}} : \overline{\text{Grad}} \delta\bar{\varphi} \, dA + \int_{\mathcal{I}_0} \bar{\mathbf{t}} \cdot \llbracket \delta\varphi \rrbracket \, dA = 0, \quad (3.5)$$

where the test functions belong to the Sobolev space $\mathcal{H}_0^1$.

Next step is to discretize the weak form. In order to have an efficient and straightforward finite element method implementation, we take the interface elements to be consistent with the bulk elements. With this strategy, the facets of two adjacent bulk elements can be considered as the two sides of the interface and no further interpolation is required. In the material configuration, the bulk $\mathcal{B}_0$ and the interface $\mathcal{I}_0$ are discretized into a set of elements as

$$\mathcal{B}_0 \approx \mathcal{B}_0^h = \mathbf{A}_{e=1}^{\#be} \mathcal{B}_0^e, \quad \mathcal{I}_0 \approx \mathcal{I}_0^h = \mathbf{A}_{e=1}^{\#ie} \mathcal{I}_0^e,$$

where $\#be$ denotes the number of bulk elements and $\#ie$ represents the number of interface elements. Employing the isoparametric concept and the Bubnov–Galerkin finite element method, the geometries are approximated using the natural coordinates $\boldsymbol{\xi}$ according to

$$\begin{aligned} \mathbf{X} \Big|_{\mathcal{B}_0^i} &\approx \mathbf{X}^h(\boldsymbol{\xi}) = \sum_{i=1}^{\#nbe} N^i(\boldsymbol{\xi}) \mathbf{X}^i, & \bar{\mathbf{X}} \Big|_{\mathcal{I}_0^i} &\approx \bar{\mathbf{X}}^h(\bar{\boldsymbol{\xi}}) = \sum_{i=1}^{\#nie} \bar{N}^i(\bar{\boldsymbol{\xi}}) \bar{\mathbf{X}}^i, \\ \delta\varphi \Big|_{\mathcal{B}_0^i} &\approx \delta\varphi^h(\boldsymbol{\xi}) = \sum_{i=1}^{\#nbe} N^i(\boldsymbol{\xi}) \delta\varphi^i, & \delta\bar{\varphi} \Big|_{\mathcal{I}_0^i} &\approx \delta\bar{\varphi}^h(\bar{\boldsymbol{\xi}}) = \sum_{i=1}^{\#nie} \bar{N}^i(\bar{\boldsymbol{\xi}}) \delta\bar{\varphi}^i, \end{aligned} \quad (3.6)$$

where N^i is the shape function for the bulk and $\bar{N}^i$ is the shape function for the interface. Number of nodes per bulk element is denoted as $\#nbe$ and $\#nie$ denotes number of nodes per interface element. Note, the natural coordinates

for the interface is one order less than that of the bulk. That is, the interface natural coordinates follows $\boldsymbol{\xi} \in [-1, 1]^{\text{PD}-1}$ and the bulk natural coordinates follows $\boldsymbol{\xi} \in [-1, 1]^{\text{PD}}$, with PD being the problem dimension. Applying the approximations (3.6) to the weak form (3.5) yields

$$\begin{aligned} & \mathbf{A}_{e=1}^{\#be} \int_{\mathcal{B}_0^e} \mathbf{P} : \left[\sum_{i=1}^{\#nbe} \delta \boldsymbol{\varphi}^i \otimes \text{Grad} N^i \right] dV \\ & + \mathbf{A}_{e=1}^{\#ie} \int_{\mathcal{I}_0^e} \overline{\mathbf{P}} : \left[\frac{1}{2} \sum_{i=1}^{\#nie} [\delta \boldsymbol{\varphi}^+]^i \otimes \overline{\text{Grad}} \overline{N}^i + \frac{1}{2} \sum_{i=1}^{\#nie} [\delta \boldsymbol{\varphi}^-]^i \otimes \overline{\text{Grad}} \overline{N}^i \right] dA \\ & + \mathbf{A}_{e=1}^{\#ie} \int_{\mathcal{I}_0^e} \bar{\mathbf{t}} \cdot \left[\sum_{i=1}^{\#nie} [\delta \boldsymbol{\varphi}^+]^i \overline{N}^i - \sum_{i=1}^{\#nie} [\delta \boldsymbol{\varphi}^-]^i \overline{N}^i \right] dA = 0. \end{aligned}$$

As a result, the global nodal residual vector $\mathbf{R}^I$ for a global node I reads

$$\begin{aligned} \mathbf{R}^I(\boldsymbol{\varphi}) &= \mathbf{A}_{e=1}^{\#be} \int_{\mathcal{B}_0^e} \mathbf{P} \cdot \text{Grad} N^i dV \\ &+ \mathbf{A}_{e=1}^{\#ie} \int_{\mathcal{I}_0^{+e}} \frac{1}{2} \overline{\mathbf{P}} \cdot \overline{\text{Grad}} \overline{N}^i dA + \mathbf{A}_{e=1}^{\#ie} \int_{\mathcal{I}_0^{-e}} \frac{1}{2} \overline{\mathbf{P}} \cdot \overline{\text{Grad}} \overline{N}^i dA \\ &+ \mathbf{A}_{e=1}^{\#ie} \int_{\mathcal{I}_0^{+e}} \bar{\mathbf{t}} \overline{N}^i dA - \mathbf{A}_{e=1}^{\#ie} \int_{\mathcal{I}_0^{-e}} \bar{\mathbf{t}} \overline{N}^i dA \stackrel{!}{=} 0. \end{aligned}$$

Putting all the unknown coordinates into the global coordinate vector $[\boldsymbol{\varphi}]$ and assembling the global nodal residual vectors $\mathbf{R}^I$ into the global residual vector $[\mathbf{R}]$ results in the fully discrete non-linear system of equations which can be solved using the Newton–Raphson scheme as follows

$$[\mathbf{R}]_{n+1} \stackrel{!}{=} \mathbf{0} \quad \Rightarrow \quad [\mathbf{R}]_{n+1} = [\mathbf{R}]_n + [\mathbf{K}]_n \Delta[\boldsymbol{\varphi}]_n \stackrel{!}{=} \mathbf{0} \quad \text{with} \quad [\mathbf{K}] := \frac{\partial [\mathbf{R}]}{\partial [\boldsymbol{\varphi}]},$$

that yields the incremental updates $[\boldsymbol{\varphi}]_{n+1} = [\boldsymbol{\varphi}]_n + \Delta[\boldsymbol{\varphi}]_n$. Here $\mathbf{K}$ denotes the tangent stiffness and n is the iteration step. The next step is to determine the residual and stiffness elements. To proceed, it would be extremely helpful to decompose the residual into three parts of contributions of the bulk, plus side of

the interface and minus side of the interface as

$$\mathbf{R}^I = \mathbf{R}^I + \mathbf{R}_+^I + \mathbf{R}_-^I \stackrel{!}{=} 0,$$

with

$$\begin{aligned}\mathbf{R}^I &= \int_{\mathcal{B}_0} \mathbf{P} \cdot \text{Grad} N^I \, dV, \\ \overline{\mathbf{R}}_+^I &= \int_{\mathcal{I}_0} \frac{1}{2} \overline{\mathbf{P}} \cdot \overline{\text{Grad}} \overline{N}^I + \overline{\mathbf{t}} \overline{N}^I \, dA, \\ \overline{\mathbf{R}}_-^I &= \int_{\mathcal{I}_0} \frac{1}{2} \overline{\mathbf{P}} \cdot \overline{\text{Grad}} \overline{N}^I - \overline{\mathbf{t}} \overline{N}^I \, dA.\end{aligned}$$

Determination of the elements of the tangent stiffness for the bulk is straightforward and reads

$$\mathbf{K}^{IJ} = \frac{\partial \mathbf{R}^I}{\partial \varphi^J} = \int_{\mathcal{B}_0} \text{Grad} N^I \cdot \mathbb{A} \cdot \text{Grad} N^J \, dV \quad \text{with} \quad \mathbb{A} := \frac{\partial \mathbf{P}}{\partial \mathbf{F}}.$$

However, for the interface elements, the residual and tangent stiffness are slightly more complex and requires certain treatments since they both encompass the contribution of the plus and minus side of the interface as

$$\overline{\mathbf{R}}^I = \begin{bmatrix} \overline{\mathbf{R}}_-^I \\ \overline{\mathbf{R}}_+^I \end{bmatrix}, \quad \overline{\mathbf{K}}^{IJ} = \begin{bmatrix} \frac{\partial \overline{\mathbf{R}}_-^I}{\partial \varphi_-^J} & \frac{\partial \overline{\mathbf{R}}_-^I}{\partial \varphi_+^J} \\ \frac{\partial \overline{\mathbf{R}}_+^I}{\partial \varphi_-^J} & \frac{\partial \overline{\mathbf{R}}_+^I}{\partial \varphi_+^J} \end{bmatrix}.$$

Finally the different elements of the tangent stiffness are determined as follows

$$\begin{aligned}\frac{\partial \overline{\mathbf{R}}_-^I}{\partial \varphi_-^J} &= \int_{\mathcal{I}_0} \frac{1}{4} \overline{\text{Grad}} \overline{N}^I \cdot \overline{\mathbb{A}}_{\parallel} \cdot \overline{\text{Grad}} \overline{N}^J + \overline{N}^I \overline{\mathbb{A}}_{\perp} \overline{N}^J \, dA, \\ \frac{\partial \overline{\mathbf{R}}_-^I}{\partial \varphi_+^J} &= \int_{\mathcal{I}_0} \frac{1}{4} \overline{\text{Grad}} \overline{N}^I \cdot \overline{\mathbb{A}}_{\parallel} \cdot \overline{\text{Grad}} \overline{N}^J - \overline{N}^I \overline{\mathbb{A}}_{\perp} \overline{N}^J \, dA, \\ \frac{\partial \overline{\mathbf{R}}_+^I}{\partial \varphi_-^J} &= \int_{\mathcal{I}_0} \frac{1}{4} \overline{\text{Grad}} \overline{N}^I \cdot \overline{\mathbb{A}}_{\parallel} \cdot \overline{\text{Grad}} \overline{N}^J - \overline{N}^I \overline{\mathbb{A}}_{\perp} \overline{N}^J \, dA, \\ \frac{\partial \overline{\mathbf{R}}_+^I}{\partial \varphi_+^J} &= \int_{\mathcal{I}_0} \frac{1}{4} \overline{\text{Grad}} \overline{N}^I \cdot \overline{\mathbb{A}}_{\parallel} \cdot \overline{\text{Grad}} \overline{N}^J + \overline{N}^I \overline{\mathbb{A}}_{\perp} \overline{N}^J \, dA.\end{aligned}$$

3.3 Analytical estimates

The objective of this section is to develop the two new analytical approaches to determine the overall behavior of composites embedding general interfaces. The first analytical approach is a direct extension of the composite cylinder assemblage (CCA) approach, composite sphere assemblage (CSA) approach and the generalized self-consistent method (GSCM) to account for general interfaces. This approach results in bounds and estimates on the macroscopic properties. In the second approach, using the modified Eshelby's heterogeneity problem, we establish a generalized interface-enhanced Mori–Tanaka method that not only determines the effective properties but also provides the interaction tensors in each phase of the medium. Consequently, using the interaction tensors, the state of the stress and strain in each phase of the medium including the interface can be determined. In the absence of external forces, the balance equations in the bulk and on the interface for linear small-strain elasticity problems read

$$\begin{cases} \text{Div} \boldsymbol{\sigma} = \mathbf{0} & \text{in } \mathcal{B}_0, \\ \boldsymbol{\sigma} \cdot \mathbf{n} = \mathbf{t}_0 & \text{on } \partial \mathcal{B}_0. \end{cases} \quad \begin{cases} \overline{\text{Div}} \bar{\boldsymbol{\sigma}} + \llbracket \boldsymbol{\sigma} \rrbracket \cdot \bar{\mathbf{n}} = \mathbf{0} & \text{along } \mathcal{I}_0, \\ \llbracket \boldsymbol{\sigma} \rrbracket \cdot \bar{\mathbf{n}} = \bar{\mathbf{t}} & \text{across } \mathcal{I}_0, \end{cases} \quad (3.7)$$

where $\mathbf{t}$ is the traction on the boundary $\partial \mathcal{B}_0$. The displacement average and the displacement jump across the interface are defined by

$$\llbracket \mathbf{u} \rrbracket := \frac{1}{2} [\mathbf{u}^+ + \mathbf{u}^-] \quad \text{and} \quad \llbracket \mathbf{u} \rrbracket := \mathbf{u}^+ - \mathbf{u}^-,$$

where $\mathbf{u}^+$ and $\mathbf{u}^-$ are the displacement of the plus and minus side of the interface, respectively. Unlike the bulk strain field, the interface strain field is not the symmetric gradient of the interface displacement but also its projection onto the interface and read

$$\bar{\boldsymbol{\varepsilon}} = \frac{1}{2} \left[\bar{\mathbf{I}} \cdot \overline{\text{Grad}} \bar{\mathbf{u}} + [\overline{\text{Grad}} \bar{\mathbf{u}}]^t \cdot \bar{\mathbf{I}} \right].$$

The material behavior for the bulk is assumed to be standard and isotropic elastic taking the form $\boldsymbol{\sigma} = 2\mu\boldsymbol{\varepsilon} + \lambda[\boldsymbol{\varepsilon} : \mathbf{I}]\mathbf{I}$ where λ and μ are the bulk Lamé parameters. For the interface, the orthogonal response across the interface and a tangential response along the interface read $\bar{\mathbf{t}} = \bar{k}[\![\mathbf{u}]\!]$ and $\bar{\boldsymbol{\sigma}} = 2\bar{\mu}\bar{\boldsymbol{\varepsilon}} + \bar{\lambda}[\bar{\boldsymbol{\varepsilon}} : \bar{\mathbf{I}}]\bar{\mathbf{I}}$ respectively. Here $\bar{\lambda}$ and $\bar{\mu}$ are the interface Lamé parameters representing the interface resistance against in-plane stretches and $\bar{k}$ is the interface orthogonal resistance against opening. Further details regarding the interface constitutive law can be found in Appendix B.2. Figure 3.2 categorizes the main interface models based on the orthogonal and tangential response of the interface. The elastic interface model is recovered when $\bar{\lambda} \neq 0$, $\bar{\mu} \neq 0$ and $\bar{k} \rightarrow \infty$. The conditions

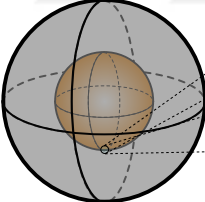
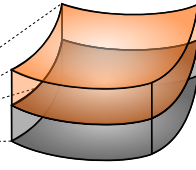
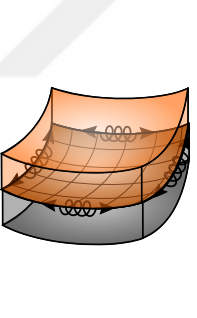
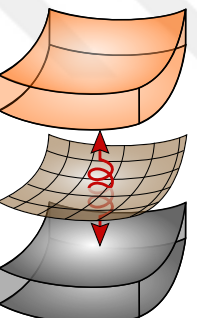
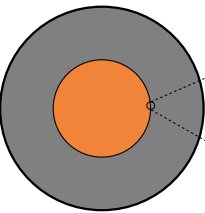
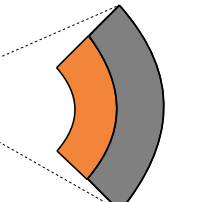
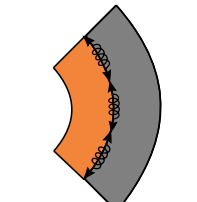
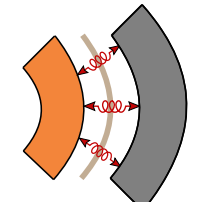
	perfect interface	elastic interface	cohesive interface	general interface
	displacement jump = 0 traction jump = 0	displacement jump = 0 traction jump $\neq 0$	displacement jump $\neq 0$ traction jump = 0	displacement jump $\neq 0$ traction jump $\neq 0$
				
	$\bar{\lambda} = 0, \bar{\mu} = 0, \bar{k} \rightarrow \infty$	$\bar{\lambda} \neq 0, \bar{\mu} \neq 0, \bar{k} \rightarrow \infty$	$\bar{\lambda} = 0, \bar{\mu} = 0, \bar{k} \rightarrow \infty$	$\bar{\lambda} \neq 0, \bar{\mu} \neq 0, \bar{k} \rightarrow \infty$
				
	$\bar{\mu} = 0, \bar{k} \rightarrow \infty$	$\bar{\mu} \neq 0, \bar{k} \rightarrow \infty$	$\bar{\mu} = 0, \bar{k} \rightarrow \infty$	$\bar{\mu} \neq 0, \bar{k} \rightarrow \infty$
tangential stiffness (resistance against stretch)	= 0	$\neq 0$	= 0	$\neq 0$
orthogonal stiffness (resistance against opening)	$\rightarrow \infty$	$\rightarrow \infty$	$\rightarrow \infty$	$\rightarrow \infty$

Figure 3.2: Interfaces based on their tangential and orthogonal behavior.

$\bar{\lambda} = 0$ and $\bar{\mu} = 0$ recover the cohesive interface model when $\bar{k} \rightarrow \infty$. Finally, the perfect interface model can be considered as the coincidence of the cohesive and the elastic interface models with $\bar{\lambda} = 0$, $\bar{\mu} = 0$ and $\bar{k} \rightarrow \infty$.

Finally, in a small-strain linear elasticity setting, the macroscopic stress and strain fields can be defined as

$$\begin{aligned}\mathbf{M}\boldsymbol{\varepsilon} &= \frac{1}{\mathcal{V}} \int_{\partial\mathcal{B}_0} \frac{1}{2} [\mathbf{u} \otimes \mathbf{n} + \mathbf{n} \otimes \mathbf{u}] \, dA, \\ \mathbf{M}\boldsymbol{\sigma} &= \frac{1}{\mathcal{V}} \int_{\partial\mathcal{B}_0} \mathbf{t}_0 \otimes \mathbf{x} \, dA,\end{aligned}$$

that, using the extended divergence theorem [141], transform to

$$\begin{aligned}\mathbf{M}\boldsymbol{\varepsilon} &= \frac{1}{\mathcal{V}} \int_{\mathcal{B}_0} \boldsymbol{\varepsilon} \, dV + \frac{1}{\mathcal{V}} \int_{\mathcal{I}_0} \frac{1}{2} [\llbracket \mathbf{u} \rrbracket \otimes \bar{\mathbf{n}} + \bar{\mathbf{n}} \otimes \llbracket \mathbf{u} \rrbracket] \, dA, \\ \mathbf{M}\boldsymbol{\sigma} &= \frac{1}{\mathcal{V}} \int_{\mathcal{B}_0} \boldsymbol{\sigma} \, dV + \frac{1}{\mathcal{V}} \int_{\mathcal{I}_0} \bar{\boldsymbol{\sigma}} \, dA.\end{aligned}\tag{3.8}$$

3.3.1 Fiber composites

Figure 3.3 demonstrates the heterogeneous medium and its underlying RVE consisting of two concentric cylinders corresponding to the fiber (phase 1) and matrix (phase 2) with the interface lying at $r = r_1$. The volume fraction of the fiber is $f = r_1^2/r_2^2$. Obviously, for the problem of interest here, it is more convenient to express the equilibrium equations and the constitutive laws in cylindrical coordinate system with coordinates r , θ and z . The term *size* here refers to the physical size of the micro-structure. The definition of the size is schematically illustrated in Fig. 3.4. The volume fraction of the inclusion is denoted f . The radii of the inclusion and matrix can be calculated for a given volume fraction f and size ℓ .

Table 3.1 gathers the relations between the material parameters for a generic case and for a transversely isotropic case. For transversely isotropic materials,

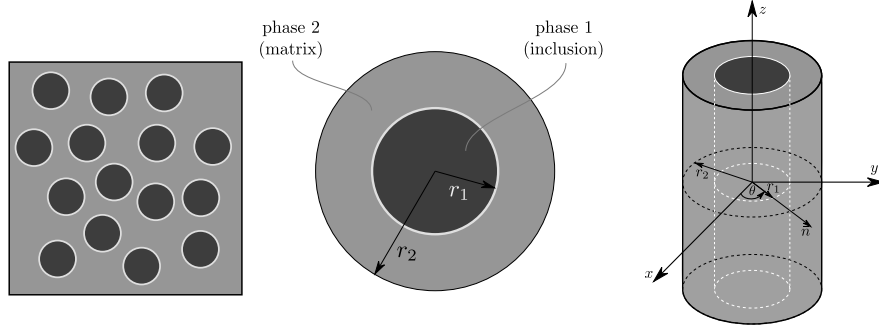


Figure 3.3: Heterogeneous medium and its corresponding simplified RVE considered in our problem. The inner radius shows the radius of the fiber whereas the outer one shows the radius of the matrix. The interface lies at $r = r_1$.

the constitutive material behavior in Voigt notation reads

$$\begin{bmatrix} \sigma_{rr} \\ \sigma_{\theta\theta} \\ \sigma_{zz} \\ \sigma_{r\theta} \\ \sigma_{rz} \\ \sigma_{\theta z} \end{bmatrix} = \begin{bmatrix} \kappa_{tr} + \mu_{tr} & \kappa_{tr} - \mu_{tr} & l & 0 & 0 & 0 \\ \kappa_{tr} - \mu_{tr} & \kappa_{tr} + \mu_{tr} & l & 0 & 0 & 0 \\ l & l & n & 0 & 0 & 0 \\ 0 & 0 & 0 & \mu_{tr} & 0 & 0 \\ 0 & 0 & 0 & 0 & \mu_{ax} & 0 \\ 0 & 0 & 0 & 0 & 0 & \mu_{ax} \end{bmatrix} \begin{bmatrix} \varepsilon_{rr} \\ \varepsilon_{\theta\theta} \\ \varepsilon_{zz} \\ 2\varepsilon_{r\theta} \\ 2\varepsilon_{rz} \\ 2\varepsilon_{\theta z} \end{bmatrix},$$

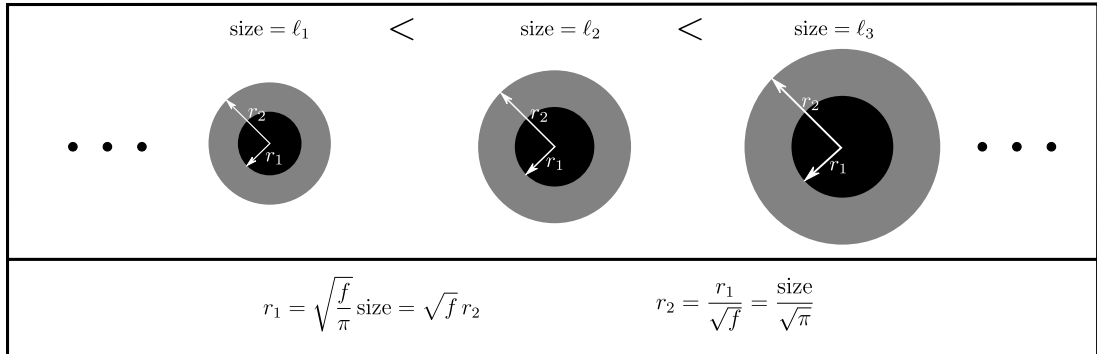


Figure 3.4: Illustration of the term “size”.

Table 3.1: The relations between the material parameters for a generic case and a transversely isotropic case. The parameters in the first row correspond to a generic case but in the second row correspond to a more specific (transversely isotropic) case of interest here.

bulk					interface						
μ_{ax}	μ_{tr}	κ_{tr}	l	n	$\bar{\mu}_{\text{ax}}$	$\bar{m}$	$\bar{n}$	$\bar{l}$	$\bar{k}_r$	$\bar{k}_\theta$	$\bar{k}_z$
μ	μ	$\lambda + \mu$	λ	$\lambda + 2\mu$	$\bar{\mu}$	$2\bar{\mu}$	$2\bar{\mu}$	0	$\bar{k}$	$\bar{k}$	$\bar{k}$
μ_{ax} : axial shear modulus					$\bar{\mu}_{\text{ax}}$: interface axial shear modulus						
μ_{tr} : transverse shear modulus					$\bar{m}$: interface transverse shear parameter						
κ_{tr} : transverse bulk modulus					$\bar{n}$: interface axial stiffness						
l : stiffness in rz and θz directions					$\bar{l}$: interface stiffness in θz direction						
n : axial stiffness					$\bar{k}_r$: interface orthogonal resistance in r						
μ : shear modulus					$\bar{k}_\theta$: interface orthogonal resistance in θ						
λ : first Lamé parameter					$\bar{k}_z$: interface orthogonal resistance in z						
					$\bar{\mu}$: interface in-plane resistance						
					$\bar{k}$: interface orthogonal resistance						

with

$$\begin{aligned}
\varepsilon_{rr} &= \frac{\partial u_r}{\partial r}, & 2\varepsilon_{r\theta} &= \frac{\partial u_\theta}{\partial r} + \frac{1}{r} \frac{\partial u_r}{\partial \theta} - \frac{u_\theta}{r}, \\
\varepsilon_{\theta\theta} &= \frac{1}{r} \frac{\partial u_\theta}{\partial \theta} + \frac{u_r}{r}, & 2\varepsilon_{rz} &= \frac{\partial u_z}{\partial r} + \frac{\partial u_r}{\partial z}, \\
\varepsilon_{zz} &= \frac{\partial u_z}{\partial z}, & 2\varepsilon_{\theta z} &= \frac{1}{r} \frac{\partial u_z}{\partial \theta} + \frac{\partial u_\theta}{\partial z},
\end{aligned} \tag{3.9}$$

the equilibrium equations in the bulk

$$\left\{ \begin{aligned} & \frac{\partial \sigma_{rr}}{\partial r} + \frac{1}{r} \frac{\partial \sigma_{r\theta}}{\partial \theta} + \frac{\partial \sigma_{rz}}{\partial z} + \frac{\sigma_{rr} - \sigma_{\theta\theta}}{r} = 0, \\ & \frac{\partial \sigma_{r\theta}}{\partial r} + \frac{1}{r} \frac{\partial \sigma_{\theta\theta}}{\partial \theta} + \frac{\partial \sigma_{\theta z}}{\partial z} + \frac{2}{r} \sigma_{r\theta} = 0, \\ & \frac{\partial \sigma_{rz}}{\partial r} + \frac{1}{r} \frac{\partial \sigma_{\theta z}}{\partial \theta} + \frac{\partial \sigma_{zz}}{\partial z} + \frac{1}{r} \sigma_{rz} = 0. \end{aligned} \right.$$

The constitutive relations for the general interface model at $r = r_1$ is characterized by four parameters for the traction jump ($\bar{m}$, $\bar{l}$, $\bar{n}$ and $\bar{\mu}_{\text{ax}}$) and three parameters

for the displacement jump ($\bar{k}_r$, $\bar{k}_\theta$ and $\bar{k}_z$) as

$$\begin{bmatrix} \bar{\sigma}_{\theta\theta} \\ \bar{\sigma}_{zz} \\ \bar{\sigma}_{\theta z} \end{bmatrix} = \begin{bmatrix} \bar{m} & \bar{l} & 0 \\ \bar{l} & \bar{n} & 0 \\ 0 & 0 & \bar{\mu}_{ax} \end{bmatrix} \begin{bmatrix} \bar{\varepsilon}_{\theta\theta} \\ \bar{\varepsilon}_{zz} \\ 2\bar{\varepsilon}_{\theta z} \end{bmatrix} \quad \text{with} \quad \begin{aligned} \bar{\varepsilon}_{\theta\theta} &= \frac{1}{r_1} \frac{\partial \bar{u}_\theta}{\partial \theta} + \frac{\bar{u}_r}{r_1}, \\ \bar{\varepsilon}_{zz} &= \frac{\partial \bar{u}_z}{\partial z}, \\ 2\bar{\varepsilon}_{\theta z} &= \frac{1}{r_1} \frac{\partial \bar{u}_z}{\partial \theta} + \frac{\partial \bar{u}_\theta}{\partial z}. \end{aligned}$$

For the interface orthogonal behavior we have

$$\begin{bmatrix} \bar{t}_r \\ \bar{t}_\theta \\ \bar{t}_z \end{bmatrix} = \begin{bmatrix} \bar{k}_r \llbracket u_r \rrbracket \\ \bar{k}_\theta \llbracket u_\theta \rrbracket \\ \bar{k}_z \llbracket u_z \rrbracket \end{bmatrix}.$$

The equilibrium equations at the interface are

$$\begin{cases} -\frac{\bar{\sigma}_{\theta\theta}}{r_1} + \llbracket \sigma_{rr} \rrbracket = 0, \\ \frac{1}{r_1} \frac{\partial \bar{\sigma}_{\theta\theta}}{\partial \theta} + \frac{\partial \bar{\sigma}_{\theta z}}{\partial z} + \llbracket \sigma_{r\theta} \rrbracket = 0, \\ \frac{1}{r_1} \frac{\partial \bar{\sigma}_{\theta z}}{\partial \theta} + \frac{\partial \bar{\sigma}_{zz}}{\partial z} + \llbracket \sigma_{rz} \rrbracket = 0. \end{cases}$$

The three normal vectors in cylindrical coordinates read

$$\mathbf{n}_r = \begin{bmatrix} \cos \theta \\ \sin \theta \\ 0 \end{bmatrix}, \quad \mathbf{n}_\theta = \begin{bmatrix} -\sin \theta \\ \cos \theta \\ 0 \end{bmatrix}, \quad \mathbf{n}_z = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix},$$

and therefore, the displacements and stresses can be represented in tensorial forms as

$$\begin{aligned} \mathbf{u} &= u_r \mathbf{n}_r + u_\theta \mathbf{n}_\theta + u_z \mathbf{n}_z, \\ \boldsymbol{\sigma} &= \sigma_{rr} \mathbf{n}_r \otimes \mathbf{n}_r + \sigma_{\theta\theta} \mathbf{n}_\theta \otimes \mathbf{n}_\theta + \sigma_{zz} \mathbf{n}_z \otimes \mathbf{n}_z + \frac{1}{2} \sigma_{r\theta} [\mathbf{n}_r \otimes \mathbf{n}_\theta + \mathbf{n}_\theta \otimes \mathbf{n}_r] \\ &\quad + \frac{1}{2} \sigma_{rz} [\mathbf{n}_r \otimes \mathbf{n}_z + \mathbf{n}_z \otimes \mathbf{n}_r] + \frac{1}{2} \sigma_{\theta z} [\mathbf{n}_\theta \otimes \mathbf{n}_z + \mathbf{n}_z \otimes \mathbf{n}_\theta], \\ \bar{\boldsymbol{\sigma}} &= \bar{\sigma}_{\theta\theta} \mathbf{n}_\theta \otimes \mathbf{n}_\theta + \bar{\sigma}_{zz} \mathbf{n}_z \otimes \mathbf{n}_z + \frac{1}{2} \bar{\sigma}_{\theta z} [\mathbf{n}_\theta \otimes \mathbf{n}_z + \mathbf{n}_z \otimes \mathbf{n}_\theta]. \end{aligned}$$

The divergence theorem for our problem can be written as

$$\begin{aligned} \text{bulk :} \quad & \int_{\mathcal{B}_0} \operatorname{div}\{\bullet\} \, dV + \int_{\mathcal{I}_0} \llbracket \{\bullet\} \rrbracket \cdot \bar{\mathbf{n}} \, dA = \int_{\partial\mathcal{B}_0} \{\bullet\} \cdot \mathbf{n} \, dA, \\ \text{interface :} \quad & \int_{\mathcal{I}_0} \overline{\operatorname{div}\{\bullet\}} \, dA - \int_{\mathcal{I}_0} \overline{\operatorname{div}\bar{\mathbf{n}}} \{\bullet\} \cdot \bar{\mathbf{n}} \, dA = \int_{\partial\mathcal{I}_0} \{\bullet\} \cdot \tilde{\mathbf{n}} \, dL, \end{aligned}$$

where $\tilde{\mathbf{n}}$ is the normal at the boundary of the interface but along the interface itself. Using the above theorems, the average mechanical energy in the composite reads

$$\begin{aligned} U &= \frac{1}{2\mathcal{V}} \int_{\mathcal{B}_0} \boldsymbol{\sigma} : \boldsymbol{\varepsilon} \, dV + \frac{1}{2\mathcal{V}} \int_{\mathcal{I}_0} \bar{\boldsymbol{\sigma}} : \bar{\boldsymbol{\varepsilon}} \, dA \\ &= \frac{1}{2\mathcal{V}} \underbrace{\left[\int_{\mathcal{B}_0} \operatorname{div}[\mathbf{u} \cdot \boldsymbol{\sigma}] \, dV + \int_{\mathcal{I}_0} \bar{\mathbf{u}} \cdot \llbracket \boldsymbol{\sigma} \rrbracket \cdot \bar{\mathbf{n}} \, dA \right]}_{\int_{\partial\mathcal{B}_0} \boldsymbol{\sigma} \cdot \mathbf{n} \cdot \mathbf{u} \, dA} + \frac{1}{2\mathcal{V}} \underbrace{\int_{\mathcal{I}_0} \overline{\operatorname{div}[\bar{\mathbf{u}} \cdot \bar{\boldsymbol{\sigma}}]} \, dA}_{\int_{\partial\mathcal{I}_0} \bar{\boldsymbol{\sigma}} \cdot \tilde{\mathbf{n}} \cdot \bar{\mathbf{u}} \, dL = 0}. \end{aligned}$$

The volume element in cylindrical coordinates is $dv = r dr d\theta dz$, the (vertical) surface element at a constant radius r is $ds_r = r d\theta dz$, the (horizontal) surface element at a constant height z is $ds_z = r dr d\theta$ and the line element at a constant radius r and height z is $dl = r d\theta$. Finally, the average mechanical energy in the RVE and in equivalent homogeneous medium read

$$\begin{aligned} U^{\text{RVE}} &= \frac{1}{2\mathcal{V}} \int_0^{2\pi} \int_0^{r_2} \left[\sigma_{rz} u_r + \sigma_{\theta z} u_\theta + \sigma_{zz} u_z \right]_{z=L} r \, dr \, d\theta \\ &\quad - \frac{1}{2\mathcal{V}} \int_0^{2\pi} \int_0^{r_2} \left[\sigma_{rz} u_r + \sigma_{\theta z} u_\theta + \sigma_{zz} u_z \right]_{z=-L} r \, dr \, d\theta \\ &\quad + \frac{1}{2\mathcal{V}} \int_{-L}^L \int_0^{2\pi} \left[\sigma_{rr} u_r + \sigma_{\theta r} u_\theta + \sigma_{zr} u_z \right]_{r=r_2} r_2 \, d\theta \, dz \\ &\quad + \frac{1}{2\mathcal{V}} \int_0^{2\pi} \left[\left[\bar{\sigma}_{\theta z} \bar{u}_\theta + \bar{\sigma}_{zz} \bar{u}_z \right]_{z=L} - \left[\bar{\sigma}_{\theta z} \bar{u}_\theta + \bar{\sigma}_{zz} \bar{u}_z \right]_{z=-L} \right]_{r=r_1} r_1 \, d\theta, \\ U^{\text{eq}} &= \frac{1}{2\mathcal{V}} \int_0^{2\pi} \int_0^{r_2} \left[\sigma_{rz}^{\text{eq}} u_r^{\text{eq}} + \sigma_{\theta z}^{\text{eq}} u_\theta^{\text{eq}} + \sigma_{zz}^{\text{eq}} u_z^{\text{eq}} \right]_{z=L} dr \, d\theta \\ &\quad - \frac{1}{2\mathcal{V}} \int_0^{2\pi} \int_0^{r_2} \left[\sigma_{rz}^{\text{eq}} u_r^{\text{eq}} + \sigma_{\theta z}^{\text{eq}} u_\theta^{\text{eq}} + \sigma_{zz}^{\text{eq}} u_z^{\text{eq}} \right]_{z=-L} dr \, d\theta \\ &\quad + \frac{1}{2\mathcal{V}} \int_{-L}^L \int_0^{2\pi} \left[\sigma_{rr}^{\text{eq}} u_r^{\text{eq}} + \sigma_{\theta r}^{\text{eq}} u_\theta^{\text{eq}} + \sigma_{zr}^{\text{eq}} u_z^{\text{eq}} \right]_{r=r_2} r_2 \, d\theta \, dz. \end{aligned}$$

As we will see later, for the expansion and the in-plane shear boundary value problems, all the quantities with index z vanish and the above relations simplify to

$$\begin{aligned} U^{\text{RVE}} &= \frac{1}{4\pi r_2^2 L} \int_{-L}^L \int_0^{2\pi} \left[\sigma_{rr}^{(2)} u_r^{(2)} + \sigma_{r\theta}^{(2)} u_\theta^{(2)} \right]_{r=r_2} r_2 d\theta dz, \\ U^{\text{eq}} &= \frac{1}{4\pi r_2^2 L} \int_{-L}^L \int_0^{2\pi} \left[\sigma_{rr}^{\text{eq}} u_r^{\text{eq}} + \sigma_{r\theta}^{\text{eq}} u_\theta^{\text{eq}} \right]_{r=r_2} r_2 d\theta dz. \end{aligned} \quad (3.10)$$

3.3.1.1 Composite cylinder assemblage (CCA) approach and the generalized self-consistent method (GSCM)

The original CCA approach was developed by Hashin and Rosen [15] where he provided analytical solution strategies to estimate the macroscopic bulk modulus $^M\kappa$ and the macroscopic shear modulus $^M\mu$ of particulate composites. While the original CCA approach can accurately calculate the effective bulk modulus, it can only provide bounds on the effective shear modulus. Christensen and Lo [134] resolved this issue via solving the boundary value problem using the generalized self consistent method and obtained an estimation of the effective shear modulus. In this case, the RVE is assumed as a set of three concentric cylinders where the external layer is an unknown effective medium. Recently, Chatzigeorgiou et al. [118] proposed an extension of the generalized self-consistent method (GSCM) [134] and the composite cylinders assemblage (CCA) approach [15] to determine the effective shear modulus and bulk modulus of fiber composites embedding general interfaces. Motivated by these observations, here the original formalism of Hashin and Rosen [15] is extended to account for the general interface to determine bounds on the overall shear modulus $^M\mu$. Note that the same methodology can be employed to obtain bounds for the effective bulk modulus $^M\kappa$. However, the upper and lower bounds on the bulk modulus coincide. Therefore, the bounds and estimates for the bulk modulus are identical. The derivations of the effective bulk and shear modulus developed in [118] are briefly stated here for the sake of completeness.

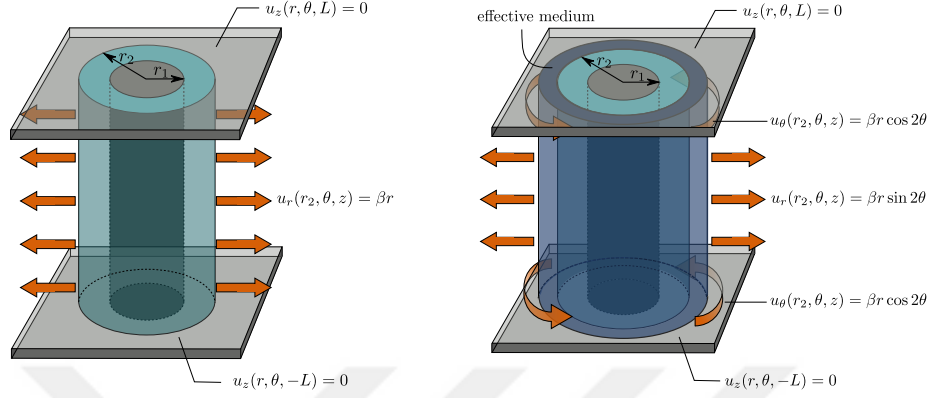


Figure 3.5: Boundary value problems for obtaining the macroscopic bulk modulus (left) and the macroscopic shear modulus (right).

Effective bulk modulus Assume that the RVE is subject to a radial expansion with its upper and lower surfaces fixed as depicted in Fig. 3.5 (left). The displacement field in cylindrical coordinates reads

$$\mathbf{u}_{(r,\theta,z)}^0 = \begin{bmatrix} \beta r \\ 0 \\ 0 \end{bmatrix}. \quad (3.11)$$

Hashin and Rosen [15] showed that the displacement field within each constituent reads

$$u_r^{(i)} = \beta \Xi_1^{(i)} r + \beta \Xi_2^{(i)} \frac{1}{r} \quad \text{and} \quad u_\theta^{(i)} = u_z^{(i)} = 0, \quad (3.12)$$

for $i = 1, 2$ where $i = 1$ corresponds to the fiber and $i = 2$ corresponds to the matrix. The unknowns $\Xi_1^1, \Xi_1^2, \Xi_2^1$ and Ξ_2^2 can be calculated using the boundary and interface conditions

- finite displacement at $r = 0$

$$u_r^{(1)} \text{ finite at } r = 0 \rightarrow \Xi_2^{(1)} = 0, \quad (3.13)$$

- traction average at $r = r_1$

$$\bar{t}_r = \bar{k}_r \llbracket u_r \rrbracket \rightarrow \frac{\sigma_{rr}^{(2)}(r_1) + \sigma_{rr}^{(1)}(r_1)}{2} = \bar{k}_r [u_r^{(2)}(r_1) - u_r^{(1)}(r_1)], \quad (3.14)$$

- traction equilibrium at $r = r_1$

$$[\overline{\text{div}} \bar{\sigma}]_r + \llbracket t_r \rrbracket = 0 \rightarrow -\frac{\bar{\sigma}_{\theta\theta}}{r_1} + \sigma_{rr}^{(2)}(r_1) - \sigma_{rr}^{(1)}(r_1) = 0, \quad (3.15)$$

- prescribed displacement at $r = r_2$

$$u_r^{(2)}(r_2) = \beta r, \quad (3.16)$$

leading to the system

$$\begin{bmatrix} 0 & 1 & \frac{1}{r_2^2} \\ -\lambda_1 - \mu_1 - \frac{\bar{\mu}}{2r_1} & \lambda_2 + \mu_2 - \frac{\bar{\mu}}{2r_1} & -\frac{2\mu_2 r_1 + \bar{\mu}}{2r_1^3} \\ \frac{\lambda_1 + \mu_1}{\bar{k}} + r_1 & \frac{\lambda_2 + \mu_2}{\bar{k}} - r_1 & -\frac{\mu_2 + \bar{k}r_1}{\bar{k}r_1^2} \end{bmatrix} \begin{bmatrix} \Xi_1^{(1)} \\ \Xi_1^{(2)} \\ \Xi_2^{(2)} \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}. \quad (3.17)$$

If the RVE is substituted by an equivalent homogeneous medium, applying the boundary condition (3.11) yields the displacement field $u_r^{\text{eq}} = \beta r$ and $u_\theta^{\text{eq}} = u_z^{\text{eq}} = 0$. Using Eq. (3.10), the overall energy in the bulk and in the RVE read

$$U^{\text{RVE}} = 2\beta^2 \left[\Xi_1^{(2)} [\lambda_2 + \mu_2] - \frac{\Xi_2^{(2)} \mu_2}{r_2^2} \right] \quad \text{and} \quad U^{\text{eq}} = 2\beta^2 M_\kappa,$$

where $\Xi_1^{(2)}$ and $\Xi_2^{(2)}$ are the solutions of the system (3.17). The above energies should be equal according to Hill–Mandel condition. Therefore, we can obtain an explicit expression for the overall bulk modulus M_κ of fiber composites embedding general interfaces

$$M_\kappa = \lambda_2 + \mu_2 + \frac{f}{\frac{\left[\frac{2r_1 \lambda_1 + 2r_1 \mu_1 + \bar{\mu}}{4r_1^2} \left[\frac{2\bar{k}r_1^2 - \bar{\mu}}{2\lambda_1 + 2\mu_1 + \bar{k}r_1} \right] + 2r_1 \bar{\mu} \right] - \left[\lambda_2 + \mu_2 \right] + \frac{\bar{\mu}}{2r_1}} + \frac{1-f}{\lambda_2 + 2\mu_2}}.$$

Effective shear modulus In order to determine the effective shear modulus of fiber composites, Christensen and Lo [134] proposed to consider an infinite effective medium surrounding the matrix whose properties are indeed the unknowns of the problem. Therefore, the composite cylinder assemblage approach is transformed to the generalized self-consistent method. To obtain the effective shear modulus, a deviatoric displacement is applied to the RVE as depicted in Fig. 3.5 (right). The displacement field in cylindrical coordinates reads

$$\mathbf{u}_{(r,\theta,z)}^0 = \begin{bmatrix} \beta r \sin 2\theta \\ \beta r \cos 2\theta \\ 0 \end{bmatrix}.$$

Considering the above boundary value problem and following the procedures in [134], the developed displacement fields in the medium follow as

$$\begin{aligned} u_r^{(i)} &= \sum_{j=1}^4 a_j^{(i)} \Xi_j^{(i)} r^{n_j^{(i)}} \sin(2\theta), & u_\theta^{(i)} &= \sum_{j=1}^4 \Xi_j^{(i)} r^{n_j^{(i)}} \cos(2\theta), \\ u_r^{(\text{eff})} &= \beta \frac{r_2}{4^{\text{M}\mu}} \left[\frac{2r}{r_2} + \Xi_3^{(\text{eff})} \frac{r_2^3}{r^3} + 2 \left[1 + \frac{\text{M}\mu}{\text{M}\kappa} \right] \Xi_4^{(\text{eff})} \frac{r_2}{r} \right] \sin(2\theta), \\ u_\theta^{(\text{eff})} &= \beta \frac{r_2}{4^{\text{M}\mu}} \left[\frac{2r}{r_2} - \Xi_3^{(\text{eff})} \frac{r_2^3}{r^3} + 2 \frac{\text{M}\mu}{\text{M}\kappa} \Xi_4^{(\text{eff})} \frac{r_2}{r} \right] \cos(2\theta), \end{aligned} \quad (3.18)$$

for $i = 1, 2$ where $i = 1$ corresponds to the fiber and $i = 2$ corresponds to the matrix. The constants $a_j^{(i)}$ read

$$a_j^{(i)} = \frac{2\lambda^{(i)} + 6\mu^{(i)} - 2n_j^{(i)}[\lambda^{(i)} + \mu^{(i)}]}{\lambda^{(i)} + 6\mu^{(i)} + [n_j^{(i)}]^2[\lambda^{(i)} + 2\mu^{(i)}]}, \quad (3.19)$$

with $n_j^{(i)}$ being the solutions of the polynomial $n^4 - 10n^2 + 9 = 0$. The constants $n_1^{(i)}$ and $n_2^{(i)}$ are taken to be the positive solutions and $n_3^{(i)}$ and $n_4^{(i)}$ are taken to be the negative solutions as $n_1^{(i)} = 3$, $n_2^{(i)} = 1$, $n_3^{(i)} = -3$ and $n_4^{(i)} = -1$. The ten unknowns $\Xi_1^{(1)}$, $\Xi_2^{(1)}$, $\Xi_3^{(1)}$, $\Xi_4^{(1)}$, $\Xi_1^{(2)}$, $\Xi_2^{(2)}$, $\Xi_3^{(2)}$, $\Xi_4^{(2)}$, $\Xi_3^{(\text{eff})}$ and $\Xi_4^{(\text{eff})}$ can be determined via applying the interface and boundary conditions. The boundary and interface conditions that hold for the RVE in this problem are

- finite displacement at $r = 0$

$$u_r^{(1)}, u_\theta^{(1)} \text{ finite at } r = 0 \rightarrow \Xi_3^{(1)} = \Xi_4^{(1)} = 0, \quad (3.20)$$

- traction average at $r = r_1$ in r direction

$$\bar{t}_r = \bar{k}_r \llbracket u_r \rrbracket \rightarrow \sigma_{rr}^{(2)}(r_1) + \sigma_{rr}^{(1)}(r_1) = 2\bar{k}_r [u_r^{(2)}(r_1) - u_r^{(1)}(r_1)], \quad (3.21)$$

- traction average at $r = r_1$ in θ direction

$$\bar{t}_\theta = \bar{k}_\theta \llbracket u_\theta \rrbracket \rightarrow \sigma_{r\theta}^{(2)}(r_1) + \sigma_{r\theta}^{(1)}(r_1) = 2\bar{k}_\theta [u_\theta^{(2)}(r_1) - u_\theta^{(1)}(r_1)], \quad (3.22)$$

- traction equilibrium at $r = r_1$ in r direction

$$[\overline{\text{div}} \bar{\sigma}]_r + \llbracket t_r \rrbracket = 0 \rightarrow -\frac{\bar{\sigma}_{\theta\theta}}{r_1} + \sigma_{rr}^{(2)}(r_1) - \sigma_{rr}^{(1)}(r_1) = 0, \quad (3.23)$$

- traction equilibrium at $r = r_1$ in θ direction

$$[\overline{\text{div}} \bar{\sigma}]_\theta + \llbracket t_\theta \rrbracket = 0 \rightarrow \frac{1}{r_1} \frac{\partial \bar{\sigma}_{\theta\theta}}{\partial \theta} + \sigma_{r\theta}^{(2)}(r_1) - \sigma_{r\theta}^{(1)}(r_1) = 0, \quad (3.24)$$

- traction continuity at $r = r_2$

$$\sigma_{rr}^{(2)}(r_2) = \sigma_{rr}^{(\text{eff})}(r_2) \quad \text{and} \quad \sigma_{r\theta}^{(2)}(r_2) = \sigma_{r\theta}^{(\text{eff})}(r_2) \quad (3.25)$$

- displacement continuity at $r = r_2$

$$u_r^{(2)}(r_2) = u_r^{(\text{eff})}(r_2) \quad \text{and} \quad u_\theta^{(2)}(r_2) = u_\theta^{(\text{eff})}(r_2). \quad (3.26)$$

In order to find the unknowns using the above system of equations, an additional energetic criterion expressed in [134] must be imposed which is deduced from the Eshelby's energy principle

$$\int_0^{2\pi} \left[\sigma_{rr}^{(\text{eff})} u_r^{\text{eq}} + \sigma_{r\theta}^{(\text{eff})} u_\theta^{\text{eq}} - \sigma_{rr}^{\text{eq}} u_r^{(\text{eff})} - \sigma_{r\theta}^{\text{eq}} u_\theta^{(\text{eff})} \right]_{r=r_2} d\theta = 0, \quad (3.27)$$

that yields $\Xi_4^{(\text{eff})} = 0$. The remaining unknowns are calculated by solving the system (3.20)–(3.26). Further details regarding the solution of the system are available in Appendix C.1.1. Unlike the effective bulk modulus, it is not possible to furnish an explicit expression for the effective shear modulus. Nevertheless, a semi-explicit expression is attainable which reads

$$[a_6 b_5 - a_5 b_6]^M \mu^2 - [b_5 c_5 - b_6 c_5 + a_5 c_6 + a_6 c_6]^M \mu + 2c_5 c_6 = 0.$$

Between the two roots obtained from the above relation, the positive one is the effective shear modulus. The parameters a_5 , a_6 , b_5 , b_6 , c_5 and c_6 are obtained from Eq. (C.4), see Appendix C.1.1 for more details.

Upper bound on shear modulus To obtain the *upper bound* on the overall in-plane shear modulus, shear displacement is applied on the boundary of the RVE as shown in Fig. 3.6 (left) according to

$$\mathbf{u}_{(r,\theta,z)}^0 = \begin{bmatrix} \beta r \sin 2\theta \\ \beta r \cos 2\theta \\ 0 \end{bmatrix}.$$

Similar to the previous case, the developed displacement fields in the medium result in the analytical form

$$u_r^{(i)} = \sum_{j=1}^4 a_j^{(i)} \Xi_j^{(i)} r^{n_j^{(i)}} \sin(2\theta), \quad u_\theta^{(i)} = \sum_{j=1}^4 \Xi_j^{(i)} r^{n_j^{(i)}} \cos(2\theta), \quad (3.28)$$

where the superscripts $i = 1, 2$ correspond to the fiber and matrix, respectively. The constants $a_j^{(i)}$ are obtained similar to Eq. (3.19).

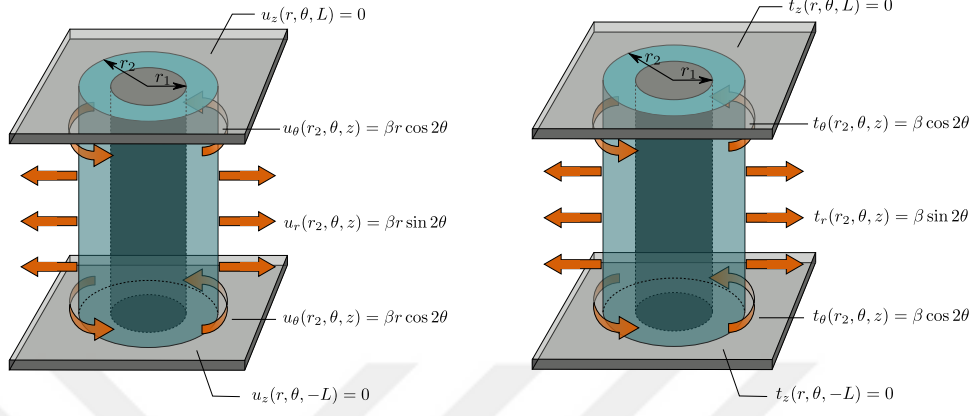


Figure 3.6: Boundary value problems for obtaining bounds on the macroscopic shear modulus of a fiber composite. Strain boundary condition (left) and stress boundary condition (right).

The eight unknowns $\Xi_1^{(1)}$, $\Xi_2^{(1)}$, $\Xi_3^{(1)}$, $\Xi_4^{(1)}$, $\Xi_1^{(2)}$, $\Xi_2^{(2)}$, $\Xi_3^{(2)}$ and $\Xi_4^{(2)}$ can be determined via applying the boundary and interface conditions as

- finite displacement at $r = 0$

$$u_r^{(1)}, u_\theta^{(1)} \text{ finite at } r = 0 \rightarrow \Xi_3^{(1)} = \Xi_4^{(1)} = 0, \quad (3.29)$$

- traction average at $r = r_1$ in r direction

$$\bar{t}_r = \bar{k}_r \llbracket u_r \rrbracket \rightarrow \sigma_{rr}^{(2)}(r_1) + \sigma_{rr}^{(1)}(r_1) = 2\bar{k}_r [u_r^{(2)}(r_1) - u_r^{(1)}(r_1)], \quad (3.30)$$

- traction average at $r = r_1$ in θ direction

$$\bar{t}_\theta = \bar{k}_\theta \llbracket u_\theta \rrbracket \rightarrow \sigma_{r\theta}^{(2)}(r_1) + \sigma_{r\theta}^{(1)}(r_1) = 2\bar{k}_\theta [u_\theta^{(2)}(r_1) - u_\theta^{(1)}(r_1)], \quad (3.31)$$

- traction equilibrium at $r = r_1$ in r direction

$$[\overline{\text{div } \bar{\sigma}}]_r + \llbracket t_r \rrbracket = 0 \rightarrow -\frac{\bar{\sigma}_{\theta\theta}}{r_1} + \sigma_{rr}^{(2)}(r_1) - \sigma_{rr}^{(1)}(r_1) = 0 \quad (3.32)$$

- traction equilibrium at $r = r_1$ in θ direction

$$[\overline{\text{div}} \bar{\sigma}]_{\theta} + \llbracket t_{\theta} \rrbracket = 0 \rightarrow \frac{1}{r_1} \frac{\partial \bar{\sigma}_{\theta\theta}}{\partial \theta} + \sigma_{r\theta}^{(2)}(r_1) - \sigma_{r\theta}^{(1)}(r_1) = 0, \quad (3.33)$$

- prescribed displacement at $r = r_2$ in r and θ direction

$$u_r^{(2)}(r_2) = \beta r \sin 2\theta, \quad \text{and} \quad u_{\theta}^{(2)}(r_2) = \beta r \cos 2\theta. \quad (3.34)$$

Further details regarding the construction of the system of equations are available in Appendix C.1.2. For an equivalent homogeneous medium with the same boundary conditions, the displacement field reads $u_r^{\text{eq}}(r) = \beta r \sin(2\theta)$ and $u_{\theta}^{\text{eq}}(r) = \beta r \cos(2\theta)$. Having the stress and displacement fields, using Eq. (3.10), one can calculate the average mechanical energy in the RVE and in the equivalent homogeneous medium

$$U^{\text{RVE}} = \frac{\beta^2}{2} \left[\frac{6\mu_2[\lambda_2 + \mu_2]r_2^2}{2\lambda_2 + 3\mu_2} \Xi_1^{(2)} + 4\mu_2 \Xi_2^{(2)} - \frac{2[\lambda_2 + \mu_2]}{r_2^2} \Xi_4^{(2)} \right],$$

$$U^{\text{eq}} = 2\beta^2 \mu.$$

Considering $U^{\text{RVE}} = U^{\text{eq}}$ results in a semi-explicit expression for the upper bound on the effective in-plane shear modulus

$$\mu_{\text{UB}} = \frac{1}{4} \left[\frac{6\mu_2[\lambda_2 + \mu_2]r_2^2}{2\lambda_2 + 3\mu_2} \Xi_1^{(2)} + 4\mu_2 \Xi_2^{(2)} - \frac{2[\lambda_2 + \mu_2]}{r_2^2} \Xi_4^{(2)} \right].$$

where $\Xi_1^{(2)}$, $\Xi_2^{(2)}$, $\Xi_3^{(2)}$ and $\Xi_4^{(2)}$ are the solution of the system of equations (C.5), see Appendix C.1.2 for more details.

Lower bound on the shear modulus Following the same methodology for the boundary value problem of Fig. 3.6 (right), the *lower bound* on the macroscopic in-plane shear modulus can be obtained. Consider an RVE subject to the

traction field

$$\mathbf{t}_{(r,\theta,z)}^0 = \begin{bmatrix} \beta \sin 2\theta \\ \beta \cos 2\theta \\ 0 \end{bmatrix}.$$

The displacement fields in the constituents due to this boundary conditions are similar to Eq. (3.28). The eight unknowns $\Xi_1^{(1)}$, $\Xi_2^{(1)}$, $\Xi_3^{(1)}$, $\Xi_4^{(1)}$, $\Xi_1^{(2)}$, $\Xi_2^{(2)}$, $\Xi_3^{(2)}$ and $\Xi_4^{(2)}$ can be determined via applying the boundary and interface conditions

- finite displacement at $r = 0$

$$u_r^{(1)}, u_\theta^{(1)} \text{ finite at } r = 0 \rightarrow \Xi_3^{(1)} = \Xi_4^{(1)} = 0, \quad (3.35)$$

- traction average at $r = r_1$ in r direction

$$\bar{t}_r = \bar{k}_r \llbracket u_r \rrbracket \rightarrow \sigma_{rr}^{(2)}(r_1) + \sigma_{rr}^{(1)}(r_1) = 2\bar{k}_r [u_r^{(2)}(r_1) - u_r^{(1)}(r_1)], \quad (3.36)$$

- traction average at $r = r_1$ in θ direction

$$\bar{t}_\theta = \bar{k}_\theta \llbracket u_\theta \rrbracket \rightarrow \sigma_{r\theta}^{(2)}(r_1) + \sigma_{r\theta}^{(1)}(r_1) = 2\bar{k}_\theta [u_\theta^{(2)}(r_1) - u_\theta^{(1)}(r_1)], \quad (3.37)$$

- traction equilibrium at $r = r_1$ in r direction

$$[\overline{\text{div } \bar{\sigma}}]_r + \llbracket t_r \rrbracket = 0 \rightarrow -\frac{\bar{\sigma}_{\theta\theta}}{r_1} + \sigma_{rr}^{(2)}(r_1) - \sigma_{rr}^{(1)}(r_1) = 0, \quad (3.38)$$

- traction equilibrium at $r = r_1$ in θ direction

$$[\overline{\text{div } \bar{\sigma}}]_\theta + \llbracket t_\theta \rrbracket = 0 \rightarrow \frac{1}{r_1} \frac{\partial \bar{\sigma}_{\theta\theta}}{\partial \theta} + \sigma_{r\theta}^{(2)}(r_1) - \sigma_{r\theta}^{(1)}(r_1) = 0, \quad (3.39)$$

- prescribed traction at $r = r_2$ in r and θ direction

$$\sigma_{rr}^{(2)}(r_2) = \beta \sin(2\theta) \quad \text{and} \quad \sigma_{r\theta}^{(2)}(r_2) = \beta \cos(2\theta). \quad (3.40)$$

Further details regarding the construction of the system of equations are available in Appendix C.1.3. For an equivalent homogeneous medium with the same boundary conditions, the displacement field reads

$$u_r^{\text{eq}}(r) = \frac{\beta}{2M_\mu} r \sin(2\theta), \quad u_\theta^{\text{eq}}(r) = \frac{\beta}{2M_\mu} r \cos(2\theta), \quad u_z^{\text{eq}}(r) = 0.$$

Using Eq. (3.10), the same strategy can be employed to define the energy stored in the RVE and the equivalent homogeneous medium.

$$U^{\text{RVE}} = \frac{\beta^2}{2} \left[\frac{3[\lambda_2 + \mu_2]r_2^2}{2\lambda_2 + 3\mu_2} \Xi_1^{(2)} + 2\Xi_2^{(2)} + \frac{\lambda_2 + 3\mu_2}{\mu_2 r_2^2} \Xi_4^{(2)} \right],$$

$$U^{\text{eq}} = \frac{\beta^2}{2M_\mu}.$$

Considering $U^{\text{RVE}} = U^{\text{eq}}$ results in a semi-explicit expression for the lower bound on the effective in-plane shear modulus

$$M_{\text{LB}} = \left[\frac{3[\lambda_2 + \mu_2]r_2^2}{2\lambda_2 + 3\mu_2} \Xi_1^{(2)} + 2\Xi_2^{(2)} + \frac{\lambda_2 + 3\mu_2}{\mu_2 r_2^2} \Xi_4^{(2)} \right]^{-1},$$

where $\Xi_1^{(2)}$, $\Xi_2^{(2)}$, $\Xi_3^{(2)}$ and $\Xi_4^{(2)}$ are the solution of the system of equations (C.6), see Appendix C.1.3 for more details..

3.3.1.2 Modified Mori–Tanaka method

Analytical estimates for the effective properties of fiber composites with general interfaces have been developed so far. Also, using energy principles, Duan et al. [146] proposed to substitute the fiber/interface system with an equivalent fiber to predict the overall behavior of the medium. Both methodologies provide reasonable estimates compared to full field homogenization strategies, like the periodic homogenization framework, but they cannot provide information about the local fields that are developed in various phases of the medium, including the interface. *Our new methodology here not only obtains the effective properties, but also defines the concentration tensors in each phase.* The primary advantage of

the concentration tensors is that they link the macroscopic fields with the average fields in the matrix, fiber and interface hence, furnishing better insights into the micro-structural response of composites. For composites with interfaces, the main idea is to identify the global interaction tensors for the fiber/interface system by solving the Eshelby's inhomogeneity problem [11]. Such investigation is motivated by similar techniques in the literature for coated particles or fibers [47, 147–149]. Admittedly, the Mori–Tanaka estimates can lose major symmetry and thus results in physically meaningless estimates. However, the loss of symmetry in the Mori–Tanaka estimates appears in composites with different shapes of fibers, or fibers of the same shape but different orientation (non-uniform orientation distribution function). For aligned long fiber composites, it has been shown analytically that Mori–Tanaka continues to produce effective properties that respect the major symmetry [150].

General framework Figure 3.10 (left) illustrates an inhomogeneity with general ellipsoidal shape occupying the space Ω_1 with elasticity modulus $\mathbf{L}^{(1)}$ surrounded by a general interface $\mathcal{I}$. An infinite matrix occupying the space Ω_2 with elasticity tensor $\mathbf{L}^{(2)}$ is embedding the inhomogeneity/interface system. The matrix is subjected to a far field linear displacement condition $\mathbf{u}^0 = \boldsymbol{\varepsilon}^0 \cdot \mathbf{x}$. The equilibrium equations throughout the medium are given in Eq. (3.7), further detailed in [118]. Here, similar to [146] we propose to treat the fiber/interface system as a unique phase, but instead of identifying the response, we identify a

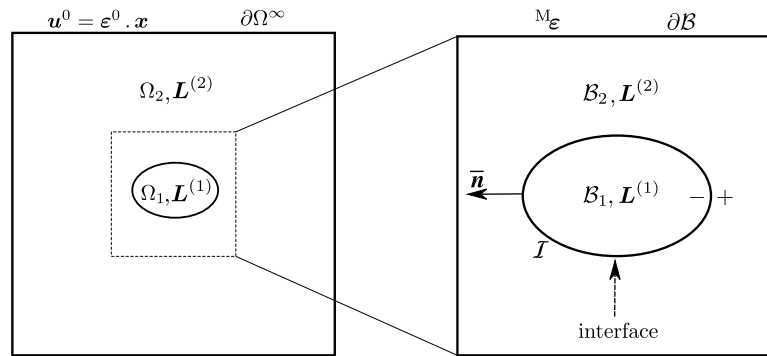


Figure 3.7: Illustration of inhomogeneity with general interface inside an infinite matrix (left) and RVE of fiber composite with general interface (right).

strain interaction tensor $\mathbf{T}$ and a stress-strain interaction tensor $\mathbf{H}$ as

$$\begin{aligned}\langle \boldsymbol{\varepsilon} \rangle_{\Omega_1}^+ &= \mathbf{T} : \boldsymbol{\varepsilon}^0 = \frac{1}{2|\Omega_1|} \int_{\mathcal{I}_0} [\mathbf{u}^+ \otimes \bar{\mathbf{n}} + \bar{\mathbf{n}} \otimes \mathbf{u}^+] dA, \\ \langle \boldsymbol{\sigma} \rangle_{\Omega_1}^+ &= \mathbf{H} : \boldsymbol{\varepsilon}^0 = \frac{1}{|\Omega_1|} \int_{\Omega_1} \boldsymbol{\sigma}^- dV + \frac{1}{|\Omega_1|} \int_{\mathcal{I}_0} \bar{\boldsymbol{\sigma}} dA.\end{aligned}\tag{3.41}$$

In addition, one can identify the pure fiber's concentration tensor as

$$\langle \boldsymbol{\varepsilon} \rangle_{\Omega_1}^- = \mathbf{T}^{(1)} : \boldsymbol{\varepsilon}^0 = \frac{1}{2|\Omega_1|} \int_{\mathcal{I}_0} [\mathbf{u}^- \otimes \bar{\mathbf{n}} + \bar{\mathbf{n}} \otimes \mathbf{u}^-] dA.\tag{3.42}$$

More precisely, $\langle \boldsymbol{\varepsilon} \rangle_{\Omega_1}^-$ corresponds to the strain field in the fiber itself whereas $\langle \boldsymbol{\varepsilon} \rangle_{\Omega_1}^+$ corresponds to the strain field in the fiber/interface system. This case study is an extension of the Eshelby's inhomogeneity problem and the tensors $\mathbf{T}$ and $\mathbf{H}$ are extremely useful to develop the mean field theories for composites [47]. Consider an RVE of fiber composite with the volume of $\mathcal{V}$ and the boundary of $\partial\mathcal{B}_0$ occupying the space $\mathcal{B}$ shown in Fig. 3.10 (right). The RVE is subject to a macroscopic strain ${}^M\boldsymbol{\varepsilon}$. The fiber with the volume of $\mathcal{V}_1$ occupies the space $\mathcal{B}_1$ and the matrix with the volume of $\mathcal{V}_2$ occupies the space $\mathcal{B}_2$. Obviously, $\mathcal{B} = \mathcal{B}_1 \cup \mathcal{B}_2$ and $\mathcal{V} = \mathcal{V}_1 + \mathcal{V}_2$. The fiber volume fraction is $f = \mathcal{V}_1/\mathcal{V}$ and accordingly, Eq. (3.8) can be rewritten as

$$\begin{aligned}{}^M\boldsymbol{\varepsilon} &= \frac{1}{\mathcal{V}} \int_{\mathcal{B}_0} \boldsymbol{\varepsilon} dV + \frac{1}{2\mathcal{V}} \int_{\mathcal{I}_0} [[\mathbf{u}]] \otimes \bar{\mathbf{n}} + \bar{\mathbf{n}} \otimes [[\mathbf{u}]] dA = [1-f]\boldsymbol{\varepsilon}^{(2)} + f\boldsymbol{\varepsilon}^{(1)} + \hat{\boldsymbol{\varepsilon}}, \\ {}^M\boldsymbol{\sigma} &= \frac{1}{\mathcal{V}} \int_{\mathcal{B}_0} \boldsymbol{\sigma} dV + \frac{1}{\mathcal{V}} \int_{\mathcal{I}_0} \bar{\boldsymbol{\sigma}} dA = [1-f]\mathbf{L}^{(2)} : \boldsymbol{\varepsilon}^{(2)} + f\mathbf{L}^{(1)} : \boldsymbol{\varepsilon}^{(1)} + \hat{\boldsymbol{\sigma}},\end{aligned}\tag{3.43}$$

in which

$$\begin{aligned}\boldsymbol{\varepsilon}^{(1)} &= \frac{1}{\mathcal{V}_1} \int_{\mathcal{B}_1} \boldsymbol{\varepsilon} dV, \\ \boldsymbol{\varepsilon}^{(2)} &= \frac{1}{\mathcal{V}_2} \int_{\mathcal{B}_2} \boldsymbol{\varepsilon} dV \\ \hat{\boldsymbol{\varepsilon}} &= \frac{1}{2\mathcal{V}} \int_{\mathcal{I}_0} [[\mathbf{u}]] \otimes \bar{\mathbf{n}} + \bar{\mathbf{n}} \otimes [[\mathbf{u}]] dA,\end{aligned}$$

are the average strains in the fiber, matrix and interface, respectively. The average stress on the interface reads

$$\widehat{\boldsymbol{\sigma}} = \frac{1}{\mathcal{V}} \int_{\mathcal{I}_0} \overline{\boldsymbol{\sigma}} \, dA.$$

Exploiting the interaction tensors (3.41) and (3.42), the Mori-Tanaka scheme reads

$$\boldsymbol{\varepsilon}^{(1)} = \mathbf{T}^{(1)} : \boldsymbol{\varepsilon}^{(2)}, \quad \boldsymbol{\varepsilon}^{(1)} + \frac{1}{f} \widehat{\boldsymbol{\varepsilon}} = \mathbf{T} : \boldsymbol{\varepsilon}^{(2)}, \quad \mathbf{L}^{(1)} : \boldsymbol{\varepsilon}^{(1)} + \frac{1}{f} \widehat{\boldsymbol{\sigma}} = \mathbf{H} : \boldsymbol{\varepsilon}^{(2)}. \quad (3.44)$$

Thus, Eq. (3.43)₁ yields

$${}^M\boldsymbol{\varepsilon} = \left[[1-f]\mathbb{I} + f\mathbf{T} \right] : \boldsymbol{\varepsilon}^{(2)} \quad \text{or} \quad \boldsymbol{\varepsilon}^{(2)} = \mathbf{A}^{(2)} : {}^M\boldsymbol{\varepsilon},$$

where $\mathbb{I}$ is the fourth order identity tensor and $\mathbf{A}^{(2)} = [[1-f]\mathbb{I} + f\mathbf{T}]^{-1}$. On the other hand, Eq. (3.43)₂ yields

$${}^M\boldsymbol{\sigma} = \left[[1-f]\mathbf{L}^{(2)} + f\mathbf{H} \right] : \boldsymbol{\varepsilon}^{(2)} = \left[[1-f]\mathbf{L}^{(2)} + f\mathbf{H} \right] : \mathbf{A}^{(2)} : {}^M\boldsymbol{\varepsilon}.$$

Thus, the macroscopic stiffness tensor is given by the expression

$${}^M\mathbf{L} = \left[[1-f]\mathbf{L}^{(2)} + f\mathbf{H} \right] : \mathbf{A}^{(2)}.$$

The properties of the equivalent fiber employed in [117] can be recovered according to

$$\mathbf{L}^{\text{eq}} = \mathbf{H} : \mathbf{T}^{-1}.$$

The macroscopic elasticity tensors obtained by our proposed method are formally identical to those given in [146]. The conceptual difference is that instead of seeking the properties of the equivalent fiber, the target is to identify the global strain and stress tensors of the fiber/interface system. For a given macroscopic strain ${}^M\boldsymbol{\varepsilon}$, the average strain and stress in the fiber and matrix read

$$\begin{aligned} \boldsymbol{\varepsilon}^{(1)} &= \mathbf{T}^{(1)} : \mathbf{A}^{(2)} : {}^M\boldsymbol{\varepsilon}, & \boldsymbol{\sigma}^{(1)} &= \mathbf{L}^{(1)} : \boldsymbol{\varepsilon}^{(1)} = \mathbf{L}^{(1)} : \mathbf{T}^{(1)} : \mathbf{A}^{(2)} : {}^M\boldsymbol{\varepsilon}, \\ \boldsymbol{\varepsilon}^{(2)} &= \mathbf{A}^{(2)} : {}^M\boldsymbol{\varepsilon}, & \boldsymbol{\sigma}^{(2)} &= \mathbf{L}^{(2)} : \boldsymbol{\varepsilon}^{(2)} = \mathbf{L}^{(2)} : \mathbf{A}^{(2)} : {}^M\boldsymbol{\varepsilon}. \end{aligned}$$

Using Eq. (3.44), the average strain and stress on the interface read

$$\widehat{\boldsymbol{\varepsilon}} = f \left[\boldsymbol{T} - \boldsymbol{T}^{(1)} \right] : \boldsymbol{A}^{(2)} : {}^M \boldsymbol{\varepsilon}, \quad \widehat{\boldsymbol{\sigma}} = f \left[\boldsymbol{H} - \boldsymbol{L}^{(1)} : \boldsymbol{T}^{(1)} \right] : \boldsymbol{A}^{(2)} : {}^M \boldsymbol{\varepsilon}.$$

So far, the only missing parts to complete the homogenization framework are the interaction tensors $\boldsymbol{T}$, $\boldsymbol{H}$ and $\boldsymbol{T}^{(1)}$. To this end, the extended Eshelby's problem is solved analytically for three boundary value problems similar to those described by Hashin [151] in the Composite Cylinders Assemblage approach. In fiber composites with isotropic or transversely isotropic phases, the strain and stress-strain interaction tensors present transverse isotropy. In Voigt notation, they take the forms

$$\begin{aligned} \boldsymbol{T} &= \begin{bmatrix} T_{11} & T_{11} - T_{44} & T_{13} & 0 & 0 & 0 \\ T_{11} - T_{44} & T_{11} & T_{13} & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & T_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & T_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & T_{55} \end{bmatrix}, \\ \boldsymbol{H} &= \begin{bmatrix} H_{11} & H_{11} - 2H_{44} & H_{13} & 0 & 0 & 0 \\ H_{11} - 2H_{44} & H_{11} & H_{13} & 0 & 0 & 0 \\ H_{31} & H_{31} & H_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & H_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & H_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & H_{55} \end{bmatrix}, \end{aligned} \quad (3.45)$$

see [149] for more details on $\boldsymbol{T}$. Note that $\boldsymbol{T}^{(1)}$ has similar structure with $\boldsymbol{T}$. Using this general representation, the three boundary value problems to identify the interaction tensors will be introduced.

Axial shear conditions For this case, the far field displacement and strain fields applied to the RVE in cylindrical coordinates read

$$\boldsymbol{u}_{(r,\theta,z)}^0 = \begin{bmatrix} 0 \\ 0 \\ \beta r \cos \theta \end{bmatrix}, \quad \boldsymbol{\varepsilon}_{(r,\theta,z)}^0 = \begin{bmatrix} 0 & 0 & \frac{\beta}{2} \cos \theta \\ 0 & 0 & -\frac{\beta}{2} \sin \theta \\ \frac{\beta}{2} \cos \theta & -\frac{\beta}{2} \sin \theta & 0 \end{bmatrix}.$$

For these boundary conditions, the important displacements and stresses in the matrix, fiber and interface are given by

$$\begin{aligned} u_z^{(i)}(r, \theta) &= \beta r U_z^{(i)}(r) \cos \theta \quad \text{with} \quad U_z^{(i)}(r) = \Xi_1^{(i)} + \Xi_2^{(i)} \frac{1}{[r/r_1]^2}, \\ \sigma_{rz}^{(i)}(r, \theta) &= \beta \Sigma_{rz}^{(i)}(r) \cos \theta \quad \text{with} \quad \Sigma_{rz}^{(i)}(r) = \mu_{\text{ax}}^{(i)} \left[\Xi_1^{(i)} - \Xi_2^{(i)} \frac{1}{[r/r_1]^2} \right], \\ \bar{\sigma}_{\theta z}(\theta) &= \beta \bar{\Sigma}_{\theta z} \sin \theta \quad \text{with} \quad \bar{\Sigma}_{\theta z} = -\frac{\bar{\mu}_{\text{ax}}}{2} \left[\Xi_1^{(1)} + \Xi_1^{(2)} + \Xi_2^{(1)} + \Xi_2^{(2)} \right], \end{aligned}$$

for $i = 1, 2$ where $i = 1$ corresponds to the fiber and $i = 2$ corresponds to the matrix. The unknowns that need to be defined are $\Xi_1^{(1)}$, $\Xi_2^{(1)}$, $\Xi_1^{(2)}$, $\Xi_2^{(2)}$. The boundary and interface conditions lead to the equations

- finite displacement at $r = r_1$

$$u_z^{(1)} \text{ finite at } r = 0 \rightarrow \Xi_2^{(1)} = 0, \quad (3.46)$$

- traction average at $r = r_1$ in z direction

$$\bar{t}_z = \bar{k}_z \llbracket u_z \rrbracket \rightarrow \Sigma_{rz}^{(2)}(r_1) + \Sigma_{rz}^{(1)}(r_1) = 2\bar{k}_z r_1 [U_z^{(2)}(r_1) - U_z^{(1)}(r_1)], \quad (3.47)$$

- traction equilibrium at $r = r_1$ in z direction

$$\begin{aligned} [\overline{\text{div}} \bar{\sigma}]_z + \llbracket t_z \rrbracket &= 0 \rightarrow \frac{1}{r_1} \frac{\partial \bar{\sigma}_{\theta z}(\theta)}{\partial \theta} + \sigma_{rz}^{(2)}(r_1) - \sigma_{rz}^{(1)}(r_1) = 0 \\ &\rightarrow \frac{\bar{\Sigma}_{\theta z}}{r_1} + \Sigma_{rz}^{(2)}(r_1) - \Sigma_{rz}^{(1)}(r_1) = 0, \end{aligned} \quad (3.48)$$

- Prescribed displacement at the boundary

$$u_z^{(2)}(r \rightarrow \infty) = \beta r \cos \theta \rightarrow \Xi_1^{(2)} = 1, \quad (3.49)$$

Solving the above linear system, the average strain and stress in the fiber/interface system read

$$\langle \epsilon \rangle_{\Omega_1}^- = U_z^{(1)}(r_1) \epsilon^0, \quad \langle \epsilon \rangle_{\Omega_1}^+ = U_z^{(2)}(r_1) \epsilon^0, \quad \langle \sigma \rangle_{\Omega_1}^+ = \Sigma_{rz}^{(2)}(r_1) \epsilon^0.$$

Since $\mathbf{H}$ is a stress-type tensor and the applied shear angle is β , the term H_{55} must be equal to the generated stress on the fiber/interface system. Consequently, the axial shear interaction terms are

$$T_{55}^{(1)} = \Xi_1^{(1)}, \quad T_{55} = 1 + \Xi_2^{(2)}, \quad H_{55} = \mu_{\text{ax}}^{(2)} \left[1 - \Xi_2^{(2)} \right]. \quad (3.50)$$

Transverse shear conditions For this case, the far field displacement and strain fields applied to the RVE in the cylindrical coordinates read

$$\mathbf{u}_{(r,\theta,z)}^0 = \begin{bmatrix} \beta r \sin 2\theta \\ \beta r \cos 2\theta \\ 0 \end{bmatrix}, \quad \boldsymbol{\epsilon}_{(r,\theta,z)}^0 = \begin{bmatrix} \beta \sin 2\theta & \beta \cos 2\theta & 0 \\ \beta \cos 2\theta & -\beta \sin 2\theta & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

For these boundary conditions, the important displacements and stresses at each phase are given by the general expressions

$$\begin{aligned} u_r^{(i)}(r, \theta) &= \beta r U_r^{(i)}(r) \sin 2\theta \quad \text{with} \quad U_r^{(i)}(r) = \frac{\kappa_{\text{tr}}^{(i)} - \mu_{\text{tr}}^{(i)}}{2\kappa_{\text{tr}}^{(i)} + \mu_{\text{tr}}^{(i)}} [r/r_1]^2 \Xi_1^{(i)} + \Xi_2^{(i)} \\ &\quad - \frac{1}{[r/r_1]^4} \Xi_3^{(i)} + \frac{\kappa_{\text{tr}}^{(i)} + \mu_{\text{tr}}^{(i)}}{\mu_{\text{tr}}^{(i)}} \frac{1}{[r/r_1]^2} \Xi_4^{(i)}, \\ u_\theta^{(i)}(r, \theta) &= \beta r U_\theta^{(i)}(r) \cos 2\theta \quad \text{with} \quad U_\theta^{(i)}(r) = [r/r_1]^2 \Xi_1^{(i)} + \Xi_2^{(i)} + \frac{1}{[r/r_1]^4} \Xi_3^{(i)} \\ &\quad + \frac{1}{[r/r_1]^2} \Xi_4^{(i)}, \\ \sigma_{rr}^{(i)}(r, \theta) &= \beta \Sigma_{rr}^{(i)}(r) \sin 2\theta \quad \text{with} \quad \Sigma_{rr}^{(i)}(r) = 2\mu_{\text{tr}}^{(i)} \Xi_2^{(i)} + 6\mu_{\text{tr}}^{(i)} \frac{1}{[r/r_1]^4} \Xi_3^{(i)} \\ &\quad - 4\kappa_{\text{tr}}^{(i)} \frac{1}{[r/r_1]^2} \Xi_4^{(i)}, \\ \sigma_{r\theta}^{(i)}(r, \theta) &= \beta \Sigma_{r\theta}^{(i)}(r) \cos 2\theta \quad \text{with} \quad \Sigma_{r\theta}^{(i)}(r) = \frac{6\kappa_{\text{tr}}^{(i)} \mu_{\text{tr}}^{(i)}}{2\kappa_{\text{tr}}^{(i)} + \mu_{\text{tr}}^{(i)}} [r/r_1]^2 \Xi_1^{(i)} + 2\mu_{\text{tr}}^{(i)} \Xi_2^{(i)} \\ &\quad - 6\mu_{\text{tr}}^{(i)} \frac{1}{[r/r_1]^4} \Xi_3^{(i)} + 2\kappa_{\text{tr}}^{(i)} \frac{1}{[r/r_1]^2} \Xi_4^{(i)}, \\ \bar{u}_r(\theta) &= \beta r_1 \bar{U}_r \sin 2\theta \quad \text{with} \quad \bar{U}_r = \frac{U_r^{(1)}(r_1) + U_r^{(2)}(r_1)}{2}, \end{aligned}$$

$$\begin{aligned}\bar{u}_\theta(\theta) &= \beta r_1 \bar{U}_\theta \cos 2\theta \quad \text{with} \quad \bar{U}_\theta = \frac{U_\theta^{(1)}(r_1) + U_\theta^{(2)}(r_1)}{2}, \\ \bar{\sigma}_{\theta\theta}(\theta) &= \beta \bar{\Sigma}_{\theta\theta} \sin 2\theta \quad \text{with} \quad \bar{\Sigma}_{\theta\theta} = \bar{m} [\bar{U}_r - 2\bar{U}_\theta],\end{aligned}$$

for $i = 1, 2$ where $i = 1$ corresponds to the fiber and $i = 2$ corresponds to the matrix. The unknowns that need to be defined are $\Xi_1^{(1)}, \Xi_2^{(1)}, \Xi_3^{(1)}, \Xi_4^{(1)}, \Xi_1^{(2)}, \Xi_2^{(2)}, \Xi_3^{(2)}, \Xi_4^{(2)}$. The boundary and interface conditions necessitate the relations

- finite displacement at $r = 0$

$$u_r^{(1)}, u_\theta^{(1)} \text{ finite at } r = 0 \rightarrow \Xi_3^{(1)} = \Xi_4^{(1)} = 0, \quad (3.51)$$

- traction average at $r = r_1$ in r direction

$$\bar{t}_r = \bar{k}_r \llbracket u_r \rrbracket \rightarrow \Sigma_{rr}^{(2)}(r_1) + \Sigma_{rr}^{(1)}(r_1) = 2\bar{k}_r r_1 [U_r^{(2)}(r_1) - U_r^{(1)}(r_1)], \quad (3.52)$$

- traction average at $r = r_1$ in θ direction

$$\bar{t}_\theta = \bar{k}_\theta \llbracket u_\theta \rrbracket \rightarrow \Sigma_{r\theta}^{(2)}(r_1) + \Sigma_{r\theta}^{(1)}(r_1) = 2\bar{k}_\theta r_1 [U_\theta^{(2)}(r_1) - U_\theta^{(1)}(r_1)], \quad (3.53)$$

- traction equilibrium at $r = r_1$ in r direction

$$\begin{aligned}[\overline{\text{div } \bar{\sigma}}]_r + \llbracket t_r \rrbracket &= 0 \rightarrow -\frac{\bar{\sigma}_{\theta\theta}(\theta)}{r_1} + \sigma_{rr}^{(2)}(r_1) - \sigma_{rr}^{(1)}(r_1) = 0 \\ &\rightarrow -\frac{\bar{\Sigma}_{\theta\theta}}{r_1} + \Sigma_{rr}^{(2)}(r_1) - \Sigma_{rr}^{(1)}(r_1) = 0,\end{aligned} \quad (3.54)$$

- traction equilibrium at $r = r_1$ in θ direction

$$\begin{aligned}[\overline{\text{div } \bar{\sigma}}]_\theta + \llbracket t_\theta \rrbracket &= 0 \rightarrow \frac{1}{r_1} \frac{\partial \bar{\sigma}_{\theta\theta}(\theta)}{\partial \theta} + \sigma_{r\theta}^{(2)}(r_1) - \sigma_{r\theta}^{(1)}(r_1) = 0 \\ &\rightarrow \frac{2}{r_1} \bar{\Sigma}_{\theta\theta} + \Sigma_{r\theta}^{(2)}(r_1) - \Sigma_{r\theta}^{(1)}(r_1) = 0,\end{aligned} \quad (3.55)$$

- prescribed displacement at the boundary in r direction

$$u_r^{(2)}(r \rightarrow \infty) = \beta r \sin 2\theta \rightarrow \Xi_1^{(2)} = 0, \quad (3.56)$$

- prescribed displacement at the boundary in θ direction

$$u_\theta^{(2)}(r \rightarrow \infty) = \beta r \cos 2\theta \rightarrow \Xi_2^{(2)} = 1. \quad (3.57)$$

Solving the above linear system, the average strain and stress in the fiber/interface system are

$$\begin{aligned} \langle \boldsymbol{\varepsilon} \rangle_{\Omega_1}^- &= \frac{1}{2} \left[U_r^{(1)}(r_1) + U_\theta^{(1)}(r_1) \right] \boldsymbol{\varepsilon}^0, \\ \langle \boldsymbol{\varepsilon} \rangle_{\Omega_1}^+ &= \frac{1}{2} \left[U_r^{(2)}(r_1) + U_\theta^{(2)}(r_1) \right] \boldsymbol{\varepsilon}^0, \\ \langle \boldsymbol{\sigma} \rangle_{\Omega_1}^+ &= \frac{1}{2} \left[\Sigma_{rr}^{(2)}(r_1) + \Sigma_{r\theta}^{(2)}(r_1) \right] \boldsymbol{\varepsilon}^0. \end{aligned}$$

Again, since $\mathbf{H}$ is a stress-type tensor and the applied shear angle is 2β , the term H_{44} must be equal to the half of the generated stress on the fiber/interface system. Consequently, the transverse shear interaction terms are

$$\begin{aligned} T_{44}^{(1)} &= \frac{3\kappa_{\text{tr}}^{(1)}}{4\kappa_{\text{tr}}^{(1)} + 2\mu_{\text{tr}}^{(1)}} \Xi_1^{(1)} + \Xi_2^{(1)}, \\ T_{44} &= 1 + \frac{\kappa_{\text{tr}}^{(2)} + 2\mu_{\text{tr}}^{(2)}}{2\mu_{\text{tr}}^{(2)}} \Xi_4^{(2)}, \\ H_{44} &= \mu_{\text{tr}}^{(2)} - \frac{\kappa_{\text{tr}}^{(2)}}{2} \Xi_4^{(2)}. \end{aligned} \quad (3.58)$$

Axisymmetric conditions For this case, the far field displacement and strain fields applied to the RVE in the cylindrical coordinates read

$$\mathbf{u}_{(r,\theta,z)}^0 = \begin{bmatrix} e^T r \\ 0 \\ e^A z \end{bmatrix}, \quad \boldsymbol{\varepsilon}_{(r,\theta,z)}^0 = \begin{bmatrix} e^T & 0 & 0 \\ 0 & e^T & 0 \\ 0 & 0 & e^A \end{bmatrix}.$$

For these boundary conditions, the important displacements and stresses in the matrix, fiber and the interface are given by

$$\begin{aligned}
u_z^{(i)}(z) &= e^A z, \\
u_r^{(i)}(r) &= e^T r U_r^{(i)}(r) \quad \text{with} \quad U_r^{(i)}(r) = \left[\Xi_1^{(i)} + \Xi_2^{(i)} \frac{1}{[r/r_1]^2} \right], \\
\sigma_{rr}^{(i)}(r) &= e^T \Sigma_{rr}^{(i)}(r) + e^A l^{(i)} \quad \text{with} \quad \Sigma_{rr}^{(i)}(r) = 2\kappa_{\text{tr}}^{(i)} \Xi_1^{(i)} - 2\mu_{\text{tr}}^{(i)} \Xi_2^{(i)} \frac{1}{[r/r_1]^2}, \\
\sigma_{zz}^{(i)} &= e^T \Sigma_{zz}^{(i)} + e^A n^{(i)} \quad \text{with} \quad \Sigma_{zz}^{(i)} = 2l^{(i)} \Xi_1^{(i)}, \\
\bar{\sigma}_{\theta\theta} &= e^T \bar{\Sigma}_{\theta\theta} + e^A \bar{l} \quad \text{with} \quad \bar{\Sigma}_{\theta\theta} = \frac{\bar{m}}{2} \left[\Xi_1^{(1)} + \Xi_1^{(2)} + \Xi_2^{(1)} + \Xi_2^{(2)} \right], \\
\bar{\sigma}_{zz} &= e^T \bar{\Sigma}_{zz} + e^A \bar{n} \quad \text{with} \quad \bar{\Sigma}_{zz} = \frac{\bar{l}}{2} \left[\Xi_1^{(1)} + \Xi_1^{(2)} + \Xi_2^{(1)} + \Xi_2^{(2)} \right],
\end{aligned}$$

for $i = 1, 2$ where $i = 1$ corresponds to the fiber and $i = 2$ corresponds to the matrix. The unknowns that need to be defined are $\Xi_1^{(1)}, \Xi_2^{(1)}, \Xi_1^{(2)}, \Xi_2^{(2)}$. The boundary and interface conditions necessitate

- finite displacement at $r = 0$

$$u_r^{(1)} \text{ finite at } r = 0 \rightarrow \Xi_2^{(1)} = 0, \quad (3.59)$$

- traction average at $r = r_1$ in r direction

$$\bar{t}_r = \bar{k}_r \llbracket u_r \rrbracket \rightarrow \sigma_{rr}^{(2)}(r_1) + \sigma_{rr}^{(1)}(r_1) = 2\bar{k}_r [u_r^{(2)}(r_1) - u_r^{(1)}(r_1)], \quad (3.60)$$

- traction equilibrium at $r = r_1$ in r direction

$$[\overline{\text{div}} \bar{\sigma}]_r + \llbracket t_r \rrbracket = 0 \rightarrow -\frac{\bar{\sigma}_{\theta\theta}}{r_1} + \sigma_{rr}^{(2)}(r_1) - \sigma_{rr}^{(1)}(r_1) = 0, \quad (3.61)$$

- Prescribed displacement at the boundary

$$u_r^{(2)}(r \rightarrow \infty) = e^T r \rightarrow \Xi_1^{(2)} = 1. \quad (3.62)$$

Solving the above linear system, the average strain and stress in the fiber/interface system are

$$\begin{aligned}
\langle \boldsymbol{\varepsilon} \rangle_{\Omega_1}^- &= \begin{bmatrix} U_r^{(1)}(r_1) e^T & 0 & 0 \\ 0 & U_r^{(1)}(r_1) e^T & 0 \\ 0 & 0 & e^A \end{bmatrix}, \quad \langle \boldsymbol{\varepsilon} \rangle_{\Omega_1}^+ = \begin{bmatrix} U_r^{(2)}(r_1) e^T & 0 & 0 \\ 0 & U_r^{(2)}(r_1) e^T & 0 \\ 0 & 0 & e^A \end{bmatrix}, \\
\langle \boldsymbol{\sigma} \rangle_{\Omega_1}^+ &= \begin{bmatrix} \Sigma_{rr}^{(2)}(r_1) & 0 & 0 \\ 0 & \Sigma_{rr}^{(2)}(r_1) & 0 \\ 0 & 0 & \Sigma_{zz}^{(1)} + \frac{2\bar{\Sigma}_{zz}}{r_1} \end{bmatrix} e^T + \begin{bmatrix} l^{(2)} & 0 & 0 \\ 0 & l^{(2)} & 0 \\ 0 & 0 & n^{(1)} + \frac{2\bar{n}}{r_1} \end{bmatrix} e^A.
\end{aligned} \tag{3.63}$$

At this stage two cases are examined.

case I: $e^A = 0$ and $e^T = 1$. The constants from the solution of the linear system are denoted as $\Xi_{11}^{(1)}$ and $\Xi_{21}^{(2)}$. For this condition, the general forms of the dilute concentration tensors in Eq. (3.45) permits to write

$$\begin{aligned}
\langle \varepsilon_{xx} \rangle_{\Omega_1}^- &= T_{11}^{(1)} + [T_{11}^{(1)} - T_{44}^{(1)}], & \langle \varepsilon_{xx} \rangle_{\Omega_1}^+ &= T_{11} + [T_{11} - T_{44}], \\
\langle \sigma_{xx} \rangle_{\Omega_1}^+ &= H_{11} + [H_{11} - 2H_{44}], & \langle \sigma_{zz} \rangle_{\Omega_1}^+ &= 2H_{31}.
\end{aligned}$$

From (3.63), clearly we have

$$\begin{aligned}
T_{11}^{(1)} &= \frac{1}{2} [\Xi_{11}^{(1)} + T_{44}^{(1)}], & T_{11} &= \frac{1}{2} [1 + \Xi_{21}^{(2)} + T_{44}], \\
H_{11} &= \kappa_{\text{tr}}^{(2)} - \mu_{\text{tr}}^{(2)} \Xi_{21}^{(2)} + H_{44}, & H_{31} &= l^{(1)} \Xi_{11}^{(1)} + \frac{\bar{l}}{2r_1} [1 + \Xi_{11}^{(1)} + \Xi_{21}^{(2)}].
\end{aligned} \tag{3.64}$$

case II: $e^A = e^T = 1$. The constants from the solution of the linear system are denoted as $\Xi_{12}^{(1)}$ and $\Xi_{22}^{(2)}$. For this condition, the general forms of the dilute

concentration tensors in Eq. (3.45) permits to write

$$\begin{aligned}
\langle \varepsilon_{xx} \rangle_{\Omega_1}^- &= T_{11}^{(1)} + [T_{11}^{(1)} - T_{44}^{(1)}] + T_{13}^{(1)}, \\
\langle \varepsilon_{xx} \rangle_{\Omega_1}^+ &= T_{11} + [T_{11} - T_{44}] + T_{13}, \\
\langle \sigma_{xx} \rangle_{\Omega_1}^+ &= H_{11} + [H_{11} - 2H_{44}] + H_{13}, \\
\langle \sigma_{zz} \rangle_{\Omega_1}^+ &= 2H_{31} + H_{33}.
\end{aligned}$$

Combining the last expression with (3.63) and (3.64) yields

$$\begin{aligned}
T_{13}^{(1)} &= \Xi_{12}^{(1)} + T_{44}^{(1)} - 2T_{11}^{(1)}, \\
T_{13} &= 1 + \Xi_{22}^{(2)} + T_{44} - 2T_{11}, \\
H_{13} &= 2\kappa_{\text{tr}}^{(2)} - 2\mu_{\text{tr}}^{(2)}\Xi_{22}^{(2)} + l^{(2)} + 2H_{44} - 2H_{11}, \\
H_{33} &= 2l^{(1)}\Xi_{12}^{(1)} + \frac{\bar{l}}{r_1} \left[1 + \Xi_{12}^{(1)} + \Xi_{22}^{(2)} \right] + n^{(1)} + \frac{2\bar{n}}{r_1} - 2H_{31}.
\end{aligned} \tag{3.65}$$

Expressions (3.50), (3.58), (3.64) and (3.65) provide all the required coefficients for the interaction tensors, which in turn can be implemented in the Mori–Tanaka scheme to identify the macroscopic elasticity tensor of fiber composites. The components of ${}^M\mathbf{L}$ are expressed as given in Eq. (3.9).

3.3.2 Particulate composites

Figure 3.8 shows a heterogeneous medium with its underlying micro-structure as well as a proper coordinate system to examine such medium. The simplified RVE consists of two concentric spheres corresponding to the matrix (phase 2) and the particle (phase 1) with the general interface lying at $r = r_1$. It proves convenient to express the homogenization problem in this medium in spherical coordinate system with the coordinates r , θ and ϕ . The volume fraction of the particle is $f = r_1^3/r_2^3$. The term *size* here refers to the physical size of the micro-structure. The definition of the size is schematically illustrated in Fig. 3.9 for both particle-reinforced composites. The radii of the inclusion and the matrix can be calculated for a given volume fraction f and size ℓ .

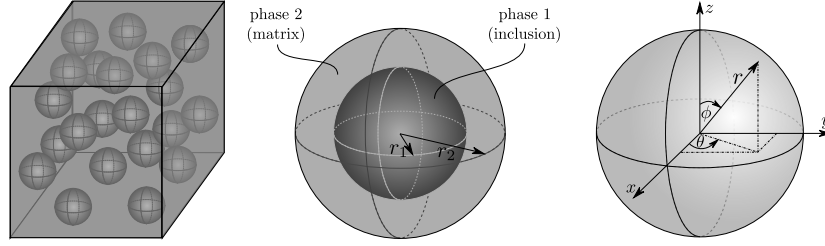


Figure 3.8: Heterogeneous medium (left) with its simplified RVE (middle) and the proper coordinate system (right) to examine such medium.

The constitutive material behavior in Voigt notation reads

$$\begin{bmatrix} \sigma_{rr} \\ \sigma_{\theta\theta} \\ \sigma_{\phi\phi} \\ \sigma_{r\theta} \\ \sigma_{r\phi} \\ \sigma_{\theta\phi} \end{bmatrix} = \begin{bmatrix} \kappa + 4\mu/3 & \kappa - 2\mu/3 & \kappa - 2\mu/3 & 0 & 0 & 0 \\ \kappa - 2\mu/3 & \kappa + 4\mu/3 & \kappa - 2\mu/3 & 0 & 0 & 0 \\ \kappa - 2\mu/3 & \kappa - 2\mu/3 & \kappa + 4\mu/3 & 0 & 0 & 0 \\ 0 & 0 & 0 & \mu & 0 & 0 \\ 0 & 0 & 0 & 0 & \mu & 0 \\ 0 & 0 & 0 & 0 & 0 & \mu \end{bmatrix} \begin{bmatrix} \varepsilon_{rr} \\ \varepsilon_{\theta\theta} \\ \varepsilon_{\phi\phi} \\ 2\varepsilon_{r\theta} \\ 2\varepsilon_{r\phi} \\ 2\varepsilon_{\theta\phi} \end{bmatrix},$$

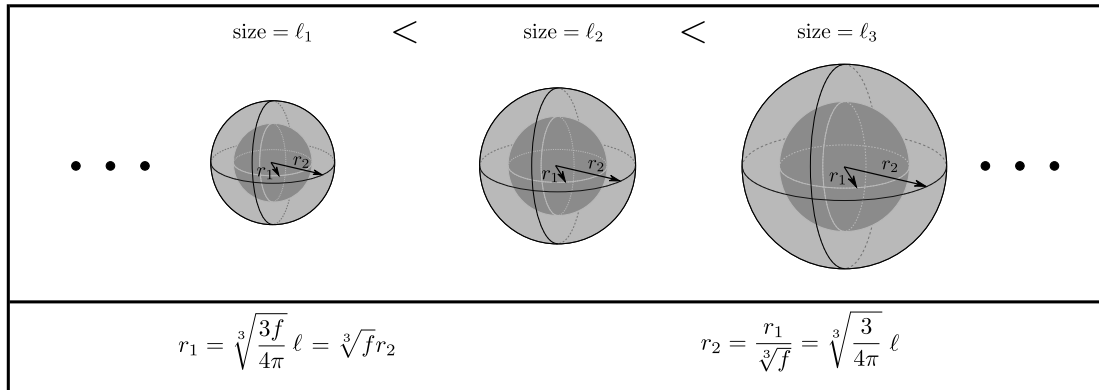


Figure 3.9: Illustration of the term “size”. Having the volume fraction, the radius of the inclusion and the matrix can be obtained for each specific size. As a result, size is proportional to the radius of the inclusion or that of the matrix.

with

$$\begin{aligned}
\varepsilon_{rr} &= \frac{\partial u_r}{\partial r}, & 2\varepsilon_{r\phi} &= \frac{\partial u_\phi}{\partial r} + \frac{1}{r \sin \theta} \frac{\partial u_r}{\partial \phi} - \frac{u_\phi}{r}, \\
\varepsilon_{\theta\theta} &= \frac{1}{r} \frac{\partial u_\theta}{\partial \theta} + \frac{u_r}{r}, & 2\varepsilon_{\theta\phi} &= \frac{1}{r} \frac{\partial u_\phi}{\partial \theta} + \frac{1}{r \sin \theta} \frac{\partial u_\theta}{\partial \phi} - \frac{u_\phi \cos \theta}{r \sin \theta}, \\
\varepsilon_{\phi\phi} &= \frac{1}{r \sin \theta} \frac{\partial u_\phi}{\partial \phi} + \frac{u_r}{r} + \frac{u_\theta \cos \theta}{r \sin \theta}, & 2\varepsilon_{r\theta} &= \frac{\partial u_\theta}{\partial r} + \frac{1}{r} \frac{\partial u_r}{\partial \theta} - \frac{u_\theta}{r}.
\end{aligned}$$

The equilibrium equations in the bulk are

$$\begin{aligned}
\frac{\partial \sigma_{rr}}{\partial r} + \frac{1}{r} \frac{\partial \sigma_{r\theta}}{\partial \theta} + \frac{\sigma_{r\theta} \cos \theta}{r \sin \theta} + \frac{2\sigma_{rr} - \sigma_{\theta\theta} - \sigma_{\phi\phi}}{r} + \frac{1}{r \sin \theta} \frac{\partial \sigma_{r\phi}}{\partial \phi} &= 0, \\
\frac{\partial \sigma_{r\theta}}{\partial r} + \frac{1}{r} \frac{\partial \sigma_{\theta\theta}}{\partial \theta} + \frac{3\sigma_{r\theta}}{r} + \frac{[\sigma_{\theta\theta} - \sigma_{\phi\phi}] \cos \theta}{r \sin \theta} + \frac{1}{r \sin \theta} \frac{\partial \sigma_{\theta\phi}}{\partial \phi} &= 0, \\
\frac{\partial \sigma_{r\phi}}{\partial r} + \frac{1}{r} \frac{\partial \sigma_{\theta\phi}}{\partial \theta} + \frac{3\sigma_{r\phi}}{r} + \frac{2\sigma_{\theta\phi} \cos \theta}{r \sin \theta} + \frac{1}{r \sin \theta} \frac{\partial \sigma_{\phi\phi}}{\partial \phi} &= 0.
\end{aligned} \tag{3.66}$$

Considering the spherical particles having the radius $r = r_1$, the constitutive relations at the interface read

$$\begin{bmatrix} \bar{\sigma}_{\theta\theta} \\ \bar{\sigma}_{\phi\phi} \\ \bar{\sigma}_{\theta\phi} \end{bmatrix} = \begin{bmatrix} \bar{\lambda} + 2\bar{\mu} & \bar{\lambda} & 0 \\ \bar{\lambda} & \bar{\lambda} + 2\bar{\mu} & 0 \\ 0 & 0 & \bar{\mu} \end{bmatrix} \begin{bmatrix} \bar{\varepsilon}_{\theta\theta} \\ \bar{\varepsilon}_{\phi\phi} \\ 2\bar{\varepsilon}_{\theta\phi} \end{bmatrix},$$

with

$$\begin{aligned}
\bar{\varepsilon}_{\theta\theta} &= \frac{1}{r_1} \frac{\partial \bar{u}_\theta}{\partial \theta} + \frac{\bar{u}_r}{r_1}, \\
\bar{\varepsilon}_{\phi\phi} &= \frac{1}{r_1 \sin \theta} \frac{\partial \bar{u}_\phi}{\partial \phi} + \frac{\bar{u}_r}{r_1} + \frac{\bar{u}_\theta \cos \theta}{r_1 \sin \theta}, \\
2\bar{\varepsilon}_{\theta\phi} &= \frac{1}{r_1} \frac{\partial \bar{u}_\phi}{\partial \theta} + \frac{1}{r_1 \sin \theta} \frac{\partial \bar{u}_\theta}{\partial \phi} - \frac{\bar{u}_\phi \cos \theta}{r_1 \sin \theta}.
\end{aligned}$$

For the interface orthogonal behavior we have

$$\begin{bmatrix} \bar{t}_r \\ \bar{t}_\theta \\ \bar{t}_\phi \end{bmatrix} = \bar{k} \begin{bmatrix} \llbracket u_r \rrbracket \\ \llbracket u_\theta \rrbracket \\ \llbracket u_\phi \rrbracket \end{bmatrix}. \tag{3.67}$$

The interface equilibrium equations read

$$\begin{aligned}
& -\frac{\bar{\sigma}_{\theta\theta} + \bar{\sigma}_{\phi\phi}}{r_1} + \llbracket \sigma_{rr} \rrbracket = 0, \\
& \frac{1}{r_1} \frac{\partial \bar{\sigma}_{\theta\theta}}{\partial \theta} + \frac{1}{r_1 \sin \theta} \frac{\partial \bar{\sigma}_{\theta\phi}}{\partial \phi} + \frac{[\bar{\sigma}_{\theta\theta} - \bar{\sigma}_{\phi\phi}] \cos \theta}{r_1 \sin \theta} + \llbracket \sigma_{r\theta} \rrbracket = 0, \\
& \frac{1}{r_1} \frac{\partial \bar{\sigma}_{\theta\phi}}{\partial \theta} + \frac{1}{r_1 \sin \theta} \frac{\partial \bar{\sigma}_{\phi\phi}}{\partial \phi} + \frac{2\bar{\sigma}_{\theta\phi} \cos \theta}{r_1 \sin \theta} + \llbracket \sigma_{r\phi} \rrbracket = 0.
\end{aligned} \tag{3.68}$$

The displacements and stresses can be presented more precisely as

$$\begin{aligned}
\mathbf{u} &= u_r \mathbf{n}_r + u_\theta \mathbf{n}_\theta + u_\phi \mathbf{n}_\phi, \\
\boldsymbol{\sigma} &= \sigma_{rr} \mathbf{n}_r \otimes \mathbf{n}_r + \sigma_{\theta\theta} \mathbf{n}_\theta \otimes \mathbf{n}_\theta + \sigma_{\phi\phi} \mathbf{n}_\phi \otimes \mathbf{n}_\phi + \frac{1}{2} \sigma_{r\theta} [\mathbf{n}_r \otimes \mathbf{n}_\theta + \mathbf{n}_\theta \otimes \mathbf{n}_r] \\
&\quad + \frac{1}{2} \sigma_{r\phi} [\mathbf{n}_r \otimes \mathbf{n}_\phi + \mathbf{n}_\phi \otimes \mathbf{n}_r] + \frac{1}{2} \sigma_{\theta\phi} [\mathbf{n}_\theta \otimes \mathbf{n}_\phi + \mathbf{n}_\phi \otimes \mathbf{n}_\theta], \\
\bar{\boldsymbol{\sigma}} &= \bar{\sigma}_{\theta\theta} \mathbf{n}_\theta \otimes \mathbf{n}_\theta + \bar{\sigma}_{\phi\phi} \mathbf{n}_\phi \otimes \mathbf{n}_\phi + \frac{1}{2} \bar{\sigma}_{\theta\phi} [\mathbf{n}_\theta \otimes \mathbf{n}_z + \mathbf{n}_z \otimes \mathbf{n}_\theta],
\end{aligned}$$

with the normal vectors in spherical coordinates

$$\mathbf{n}_r = \begin{bmatrix} \sin \theta \cos \phi \\ \sin \theta \sin \phi \\ \cos \theta \end{bmatrix}, \quad \mathbf{n}_\theta = \begin{bmatrix} \cos \theta \cos \phi \\ \cos \theta \sin \phi \\ -\sin \theta \end{bmatrix}, \quad \mathbf{n}_\phi = \begin{bmatrix} -\sin \phi \\ \cos \phi \\ 0 \end{bmatrix}.$$

Finally, the overall mechanical energy stored in the RVE and in equivalent homogeneous medium read

$$\begin{aligned}
U^{\text{RVE}} &= \frac{1}{2\mathcal{V}} \int_{\mathcal{B}_0} \boldsymbol{\sigma} : \boldsymbol{\varepsilon} \, dV = \frac{3}{8\pi r_2} \int_0^{2\pi} \int_0^\pi \left[\sigma_{rr}^{(2)} u_r^{(2)} + \sigma_{r\theta}^{(2)} u_\theta^{(2)} + \sigma_{r\phi}^{(2)} u_\phi^{(2)} \right]_{r=r_2} \sin \theta \, d\theta \, d\phi, \\
U^{\text{eq}} &= \frac{1}{2\mathcal{V}} \int_{\mathcal{B}_0} \boldsymbol{\sigma} : \boldsymbol{\varepsilon} \, dV = \frac{3}{8\pi r_2} \int_0^{2\pi} \int_0^\pi \left[\sigma_{rr}^{\text{eq}} u_r^{\text{eq}} + \sigma_{r\theta}^{\text{eq}} u_\theta^{\text{eq}} + \sigma_{r\phi}^{\text{eq}} u_\phi^{\text{eq}} \right]_{r=r_2} \sin \theta \, d\theta \, d\phi.
\end{aligned} \tag{3.69}$$

3.3.2.1 Composite sphere assemblage (CSA) approach and the generalized self-consistent method (GSCM)

The original CSA approach was developed by Hashin [12] where he provided analytical solution strategies to estimate the macroscopic bulk modulus ${}^M\kappa$ and the macroscopic shear modulus ${}^M\mu$ of a particulate composite. While the original CSA approach can accurately calculate the effective bulk modulus, it can only provide bounds on the effective shear modulus. Similar to fiber composites, Christensen and Lo [134] resolved this issue via solving the boundary value problem using the generalized self consistent method and obtained an estimation of the effective shear modulus. Here, we extend these two approaches to account for the general interfaces and derive explicit expressions for the overall bulk modulus ${}^M\kappa$ and semi-explicit expressions for the upper bound, lower bound and an estimate for the overall shear modulus ${}^M\mu$ of particle reinforced composites. Note that the same methodology can be employed to obtain bounds for the effective bulk modulus ${}^M\kappa$. However, the upper and lower bounds on the bulk modulus coincide. Therefore, the bounds and estimates for the bulk modulus yield identical results.

Effective Bulk modulus Assume that the RVE is subject to a far field hydrostatic displacement field. The displacement in both Cartesian and spherical coordinates read

$$\mathbf{u}_{(x,y,z)}^0 = \begin{bmatrix} \beta x \\ \beta y \\ \beta z \end{bmatrix} \quad \text{and} \quad \mathbf{u}_{(r,\theta,\phi)}^0 = \begin{bmatrix} \beta r \\ 0 \\ 0 \end{bmatrix}. \quad (3.70)$$

For this type of boundary condition, Hashin [12] has demonstrated that at every phase the displacement field that satisfies the equilibrium equations (3.66) reads

$$u_r^{(i)} = \beta r U_r^{(i)}(r), \quad u_\theta^{(i)} = u_\phi^{(i)} = 0 \quad \text{with} \quad U_r^{(i)}(r) = \Xi_1^{(i)} + \Xi_2^{(i)} \frac{1}{[r/r_1]^3}, \quad (3.71)$$

for $i = 1, 2$ where $i = 1$ corresponds to the particle and $i = 2$ corresponds to the matrix. The unknowns $\Xi_1^{(2)}$, $\Xi_2^{(2)}$, $\Xi_1^{(1)}$ and $\Xi_2^{(1)}$ can be calculated using the boundary and interface conditions

- finite displacement at $r = 0$

$$u_r^{(1)} \text{ finite at } r = 0 \rightarrow \Xi_2^{(1)} = 0, \quad (3.72)$$

- traction average at $r = r_1$

$$\bar{t}_r = \bar{k}_r \llbracket u_r \rrbracket \rightarrow \frac{\sigma_{rr}^{(2)}(r_1) + \sigma_{rr}^{(1)}(r_1)}{2} = \bar{k}_r [u_r^{(2)}(r_1) - u_r^{(1)}(r_1)], \quad (3.73)$$

- traction equilibrium at $r = r_1$

$$[\overline{\text{div } \bar{\sigma}}]_r + \llbracket t_r \rrbracket = 0 \rightarrow -\frac{\bar{\sigma}_{\theta\theta} + \bar{\sigma}_{\phi\phi}}{r_1} + \sigma_{rr}^{(2)}(r_1) - \sigma_{rr}^{(1)}(r_1) = 0, \quad (3.74)$$

- prescribed displacement at $r = r_2$

$$u_r^{(2)}(r_2) = \beta r, \quad (3.75)$$

which leads to the system

$$\begin{bmatrix} 1 + \frac{3\kappa_1}{2\bar{k}r_1} & -1 + \frac{3\kappa_2}{2\bar{k}r_1} & -1 - \frac{2\mu_2}{\bar{k}r_1} \\ 3\kappa_1 + \frac{2[\bar{\lambda} + \bar{\mu}]}{r_1} & -3\kappa_2 + \frac{2[\bar{\lambda} + \bar{\mu}]}{r_1} & 4\mu_2 + \frac{2[\bar{\lambda} + \bar{\mu}]}{r_1} \\ 0 & 1 & f \end{bmatrix} \begin{bmatrix} \Xi_1^{(1)} \\ \Xi_1^{(2)} \\ \Xi_2^{(2)} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}. \quad (3.76)$$

If the RVE is substituted by an equivalent homogeneous medium, applying the boundary condition (3.70), yields the displacement field $u_r^{\text{eq}} = \beta r$ and $u_\theta^{\text{eq}} = u_\phi^{\text{eq}} = 0$. Using Eq. (3.69), the overall energy in both the RVE and the equivalent

homogeneous medium read

$$U^{\text{RVE}} = \frac{3\beta^2}{2} \left[3\kappa_2 \Xi_1^{(2)} - 4f\mu_2 \Xi_2^{(2)} \right] \quad \text{and} \quad U^{\text{eq}} = \frac{9\beta^2}{2} M_\kappa,$$

where the unknowns $\Xi_1^{(2)}$ and $\Xi_2^{(2)}$ are determined from the system (3.76). According to the Hill–Mandel condition, the above energies should be equal. Therefore, we obtain a closed-form expression for the macroscopic bulk modulus M_κ of particulate composites with general interfaces

$$M_\kappa = \frac{3\kappa_2\xi + 4\mu_2\eta}{3[\xi - f\eta]}, \quad \text{with} \quad \begin{cases} \xi = \left[\frac{\bar{\lambda} + \bar{\mu}}{r_1} + \bar{k}r_1 \right] [3\kappa_1 + 4\mu_2] + 4\bar{k}r_1 \left[\frac{\bar{\lambda} + \bar{\mu}}{r_1} \right] + 12\kappa_1\mu_2, \\ \eta = \left[\frac{\bar{\lambda} + \bar{\mu}}{r_1} + \bar{k}r_1 \right] [3\kappa_1 - 3\kappa_2] + 4\bar{k}r_1 \left[\frac{\bar{\lambda} + \bar{\mu}}{r_1} \right] - 9\kappa_1\kappa_2. \end{cases}$$

Effective Shear modulus In order to obtain the effective shear modulus M_μ of a particle reinforced composite, we employ the method proposed by Christensen and Lo [134] considering an infinite effective medium surrounding the matrix whose properties are the unknowns of our problem. Consider the RVE subject to a deviatoric displacement field

$$u_{(r,\theta,\phi)}^0 = \begin{bmatrix} \beta r \sin^2 \theta \cos 2\phi \\ \beta r \sin \theta \cos \theta \cos 2\phi \\ -\beta r \sin \theta \sin 2\phi \end{bmatrix}.$$

For this type of boundary condition, Christensen and Lo [134] have demonstrated that at every phase the displacement field that satisfies the equilibrium equations (3.66) reads

$$\begin{aligned} u_r^{(i)} &= \beta r U_r^{(i)}(r) \sin^2 \theta \cos 2\phi, \\ u_\theta^{(i)} &= \beta r U_\theta^{(i)}(r) \sin \theta \cos \theta \cos 2\phi, \\ u_\phi^{(i)} &= -\beta r U_\theta^{(i)}(r) \sin \theta \sin 2\phi, \end{aligned}$$

with

$$\begin{aligned} U_r^{(i)}(r) &= \Xi_1^{(i)} + \left[2 - 3 \frac{\kappa_i}{\mu_i} \right] [r/r_1]^2 \Xi_2^{(i)} + \frac{3\Xi_3^{(i)}}{[r/r_1]^5} + \left[3 + 3 \frac{\kappa_i}{\mu_i} \right] \frac{\Xi_4^{(i)}}{[r/r_1]^3}, \\ U_\theta^{(i)}(r) &= \Xi_1^{(i)} - \left[\frac{11}{3} + 5 \frac{\kappa_i}{\mu_i} \right] [r/r_1]^2 \Xi_2^{(i)} - \frac{2\Xi_3^{(i)}}{[r/r_1]^5} + \frac{2\Xi_4^{(i)}}{[r/r_1]^3}. \end{aligned} \quad (3.77)$$

The displacement field in the effective medium reads

$$\begin{aligned} u_r^{(\text{eff})}(r, \theta, \phi) &= \beta r U_r^{(\text{eff})}(r) \sin^2 \theta \cos 2\phi, \\ u_\theta^{(\text{eff})}(r, \theta, \phi) &= \beta r U_\theta^{(\text{eff})}(r) \sin \theta \cos \theta \cos 2\phi, \\ u_\phi^{(\text{eff})}(r, \theta, \phi) &= -\beta r U_\theta^{(\text{eff})}(r) \sin \theta \sin 2\phi, \end{aligned}$$

with

$$\begin{aligned} U_r^{(\text{eff})}(r) &= \frac{3\Xi_3^{(\text{eff})}}{[r/r_1]^5} + \left[3 + 3 \frac{\kappa}{\mu} \right] \frac{\Xi_4^{(\text{eff})}}{[r/r_1]^3}, \\ U_\theta^{(\text{eff})}(r) &= -\frac{2\Xi_3^{(\text{eff})}}{[r/r_1]^5} + \frac{2\Xi_4^{(\text{eff})}}{[r/r_1]^3}. \end{aligned} \quad (3.78)$$

Perfect bonding between the effective medium and the matrix is assumed which renders

$$\begin{aligned} u_r^{(2)}(r_2, \theta, \phi) &= u_r^{(\text{eff})}(r_2, \theta, \phi), \quad \sigma_{rr}^{(2)}(r_2, \theta, \phi) = \sigma_{rr}^{(\text{eff})}(r_2, \theta, \phi), \\ u_\theta^{(2)}(r_2, \theta, \phi) &= u_\theta^{(\text{eff})}(r_2, \theta, \phi), \quad \sigma_{r\theta}^{(2)}(r_2, \theta, \phi) = \sigma_{r\theta}^{(\text{eff})}(r_2, \theta, \phi), \\ u_\phi^{(2)}(r_2, \theta, \phi) &= u_\phi^{(\text{eff})}(r_2, \theta, \phi), \quad \sigma_{r\phi}^{(2)}(r_2, \theta, \phi) = \sigma_{r\phi}^{(\text{eff})}(r_2, \theta, \phi). \end{aligned} \quad (3.79)$$

So far our problem contains ten unknowns of $\Xi_1^{(1)}, \Xi_2^{(1)}, \Xi_3^{(1)}, \Xi_4^{(1)}, \Xi_1^{(2)}, \Xi_2^{(2)}, \Xi_3^{(2)}, \Xi_4^{(2)}, \Xi_3^{(\text{eff})}$ and $\Xi_4^{(\text{eff})}$. These unknowns can be calculated using the boundary and interface conditions

- finite displacement at $r = 0$

$$u_r^{(1)}, u_\theta^{(1)} \text{ finite at } r = 0 \rightarrow \Xi_3^{(1)} = \Xi_4^{(1)} = 0, \quad (3.80)$$

- traction average at $r = r_1$ in r direction

$$\bar{t}_r = \bar{k}_r \llbracket u_r \rrbracket \rightarrow \sigma_{rr}^{(2)}(r_1) + \sigma_{rr}^{(1)}(r_1) = 2\bar{k}_r [u_r^{(2)}(r_1) - u_r^{(1)}(r_1)] , \quad (3.81)$$

- traction average at $r = r_1$ in θ direction

$$\bar{t}_\theta = \bar{k}_\theta \llbracket u_\theta \rrbracket \rightarrow \sigma_{r\theta}^{(2)}(r_1) + \sigma_{r\theta}^{(1)}(r_1) = 2\bar{k}_\theta [u_\theta^{(2)}(r_1) - u_\theta^{(1)}(r_1)] , \quad (3.82)$$

- traction equilibrium at $r = r_1$ in r direction

$$[\overline{\text{div } \bar{\sigma}}]_r + \llbracket t_r \rrbracket = 0 \rightarrow -\frac{\bar{\sigma}_{\theta\theta} + \bar{\sigma}_{\phi\phi}}{r_1} + \sigma_{rr}^{(2)}(r_1) - \sigma_{rr}^{(1)}(r_1) = 0 , \quad (3.83)$$

- traction equilibrium at $r = r_1$ in θ direction

$$[\overline{\text{div } \bar{\sigma}}]_\theta + \llbracket t_\theta \rrbracket = 0 \rightarrow \frac{1}{r_1} \frac{\partial \bar{\sigma}_{\theta\theta}}{\partial \theta} + \frac{1}{r_1 \sin \theta} \frac{\partial \bar{\sigma}_{\theta\phi}}{\partial \phi} + \frac{[\bar{\sigma}_{\theta\theta} - \bar{\sigma}_{\phi\phi}] \cos \theta}{r_1 \sin \theta} + \sigma_{r\theta}^{(2)}(r_1) - \sigma_{r\theta}^{(1)}(r_1) = 0 , \quad (3.84)$$

- traction continuity at $r = r_2$

$$\sigma_{rr}^{(2)}(r_2) = \sigma_{rr}^{(\text{eff})}(r_2) \quad \text{and} \quad \sigma_{r\theta}^{(2)}(r_2) = \sigma_{r\theta}^{(\text{eff})}(r_2) \quad (3.85)$$

- displacement continuity at $r = r_2$

$$u_r^{(2)}(r_2) = u_r^{(\text{eff})}(r_2) \quad \text{and} \quad u_\theta^{(2)}(r_2) = u_\theta^{(\text{eff})}(r_2) . \quad (3.86)$$

Considering a homogeneous equivalent medium under the same boundary condition, the displacement field in the medium is similar to Eq. (3.95). From the Eshelby's energy principle, we can deduce

$$\int_0^{2\pi} \int_0^\pi \left[\sigma_{rr}^{(\text{eff})} u_r^{\text{eq}} + \sigma_{r\theta}^{(\text{eff})} u_\theta^{\text{eq}} + \sigma_{r\phi}^{(\text{eff})} u_\phi^{\text{eq}} - \sigma_{rr}^{\text{eq}} u_r^{(\text{eff})} - \sigma_{r\theta}^{\text{eq}} u_\theta^{(\text{eff})} - \sigma_{r\phi}^{\text{eq}} u_\phi^{(\text{eff})} \right] \sin \theta \, d\theta \, d\phi = 0 . \quad (3.87)$$

Substituting the stress and displacement fields of the RVE and equivalent homogeneous medium at $r = r_2$ in this integral results in $\Xi_4^{(\text{eff})} = 0$. The remaining

seven unknowns are calculated by solving the system of equations (3.80)–(3.86). Further details regarding the construction of the system of equations are available in Appendix C.2.1. Unlike the macroscopic bulk modulus ${}^M\kappa$, it is not possible to provide an explicit expression for the effective shear modulus ${}^M\mu$ and identify its simplified forms for various interface types. Nonetheless, we have developed the following *semi-explicit* expression to obtain the macroscopic shear modulus ${}^M\mu$

$${}^M\mu = \frac{1}{80} \left[b_6 - b_5 + 12a_6 + 8a_5 + \sqrt{\Delta} \right] ,$$

with

$$\Delta = [b_6 - b_5 + 12a_6 + 8a_5]^2 - 80[a_5b_6 - b_5a_6] ,$$

where the constants $a_i, b_i, i = 1, \dots, 6$ are obtained from the solution of the system of equations (C.7) and using Eqs.(C.8) and (C.10), see Appendix C.2.1 for more details.

Upper bound on shear modulus To obtain the *upper bound* on the overall shear modulus, shear displacement is applied on the boundary of the RVE according to

$$\mathbf{u}_{(r,\theta,\phi)}^0 = \begin{bmatrix} \beta r \sin^2 \theta \cos 2\phi \\ \beta r \sin \theta \cos \theta \cos 2\phi \\ -\beta r \sin \theta \sin 2\phi \end{bmatrix} .$$

For this type of boundary condition, Christensen and Lo [134] have demonstrated that at every phase the displacement field that satisfies the equilibrium equations (3.66) reads

$$\begin{aligned} u_r^{(i)} &= \beta r U_r^{(i)}(r) \sin^2 \theta \cos 2\phi , \\ u_\theta^{(i)} &= \beta r U_\theta^{(i)}(r) \sin \theta \cos \theta \cos 2\phi , \\ u_\phi^{(i)} &= -\beta r U_\theta^{(i)}(r) \sin \theta \sin 2\phi , \end{aligned}$$

with

$$\begin{aligned} U_r^{(i)}(r) &= \Xi_1^{(i)} + \left[2 - 3 \frac{\kappa_i}{\mu_i} \right] [r/r_1]^2 \Xi_2^{(i)} + \frac{3\Xi_3^{(i)}}{[r/r_1]^5} + \left[3 + 3 \frac{\kappa_i}{\mu_i} \right] \frac{\Xi_4^{(i)}}{[r/r_1]^3}, \\ U_\theta^{(i)}(r) &= \Xi_1^{(i)} - \left[\frac{11}{3} + 5 \frac{\kappa_i}{\mu_i} \right] [r/r_1]^2 \Xi_2^{(i)} - \frac{2\Xi_3^{(i)}}{[r/r_1]^5} + \frac{2\Xi_4^{(i)}}{[r/r_1]^3}. \end{aligned} \quad (3.88)$$

The eight unknowns $\Xi_1^{(1)}, \Xi_2^{(1)}, \Xi_3^{(1)}, \Xi_4^{(1)}, \Xi_1^{(2)}, \Xi_2^{(2)}, \Xi_3^{(2)}, \Xi_4^{(2)}$ can be calculated using the boundary and interface conditions

- finite displacement at $r = 0$

$$u_r^{(1)}, u_\theta^{(1)} \text{ finite at } r = 0 \rightarrow \Xi_3^{(1)} = \Xi_4^{(1)} = 0, \quad (3.89)$$

- traction average at $r = r_1$ in r direction

$$\bar{t}_r = \bar{k}_r \llbracket u_r \rrbracket \rightarrow \sigma_{rr}^{(2)}(r_1) + \sigma_{rr}^{(1)}(r_1) = 2\bar{k}_r [u_r^{(2)}(r_1) - u_r^{(1)}(r_1)], \quad (3.90)$$

- traction average at $r = r_1$ in θ direction

$$\bar{t}_\theta = \bar{k}_\theta \llbracket u_\theta \rrbracket \rightarrow \sigma_{r\theta}^{(2)}(r_1) + \sigma_{r\theta}^{(1)}(r_1) = 2\bar{k}_\theta [u_\theta^{(2)}(r_1) - u_\theta^{(1)}(r_1)], \quad (3.91)$$

- traction equilibrium at $r = r_1$ in r direction

$$[\overline{\text{div } \bar{\sigma}}]_r + \llbracket t_r \rrbracket = 0 \rightarrow -\frac{\bar{\sigma}_{\theta\theta} + \bar{\sigma}_{\phi\phi}}{r_1} + \sigma_{rr}^{(2)}(r_1) - \sigma_{rr}^{(1)}(r_1) = 0, \quad (3.92)$$

- traction equilibrium at $r = r_1$ in θ direction

$$\begin{aligned} [\overline{\text{div } \bar{\sigma}}]_\theta + \llbracket t_\theta \rrbracket = 0 \rightarrow & \frac{1}{r_1} \frac{\partial \bar{\sigma}_{\theta\theta}}{\partial \theta} + \frac{1}{r_1 \sin \theta} \frac{\partial \bar{\sigma}_{\theta\phi}}{\partial \phi} + \frac{[\bar{\sigma}_{\theta\theta} - \bar{\sigma}_{\phi\phi}] \cos \theta}{r_1 \sin \theta} \\ & + \sigma_{r\theta}^{(2)}(r_1) - \sigma_{r\theta}^{(1)}(r_1) = 0, \end{aligned} \quad (3.93)$$

- prescribed displacement at $r = r_2$ in r and θ direction

$$u_r^{(2)}(r = r_2) = \beta r \sin^2 \theta \cos 2\phi, \quad \text{and} \quad u_\theta^{(2)}(r = r_2) = \beta r \sin \theta \cos \theta \cos 2\phi. \quad (3.94)$$

Further details regarding the construction of the system of equations are available in Appendix C.2.2. If the RVE is substituted by an equivalent homogeneous medium, applying the same boundary condition leads to the displacement field

$$u_r^{\text{eq}} = \beta r \sin^2 \theta \cos 2\phi, \quad u_\theta^{\text{eq}} = \beta r \sin \theta \cos \theta \cos 2\phi, \quad u_\phi^{\text{eq}} = -\beta r \sin \theta \sin 2\phi. \quad (3.95)$$

Equipped with all the displacement and stress fields, the overall energy according to Eq. (3.69) in both RVE and the equivalent homogeneous medium read

$$U^{\text{RVE}} = \frac{\beta^2}{5} \left[10\mu_2 \Xi_1^{(2)} - 14[3\kappa_2 + \mu_2] f^{-2/3} \Xi_2^{(2)} - 2[9\kappa_2 + 8\mu_2] f \Xi_4^{(2)} \right] \\ U^{\text{eq}} = 2\beta^2 \mu.$$

Considering $U^{\text{RVE}} = U^{\text{eq}}$ results in a *semi-explicit* expression for the upper bound on the macroscopic shear modulus

$$\mu_{\text{UB}}^{\text{M}} = \frac{1}{10} \left[10\mu_2 \Xi_1^{(2)} - 14[3\kappa_2 + \mu_2] f^{-2/3} \Xi_2^{(2)} - 2[9\kappa_2 + 8\mu_2] f \Xi_4^{(2)} \right],$$

where $\Xi_1^{(2)}$, $\Xi_2^{(2)}$ and $\Xi_4^{(2)}$ are the solutions of the system of equations (C.11), see Appendix C.2.2 for more details..

Lower bound on shear modulus In order to obtain *lower bound*, unlike the upper bound due to prescribed displacements, we prescribe traction on the RVE according to

$$\mathbf{t}_{(r,\theta,\phi)}^0 = \begin{bmatrix} \sigma_{rr}^0 \\ \sigma_{r\theta}^0 \\ \sigma_{r\phi}^0 \end{bmatrix} = \begin{bmatrix} \beta \sin^2 \theta \cos 2\phi \\ \beta \sin \theta \cos \theta \cos 2\phi \\ -\beta \sin \theta \sin 2\phi \end{bmatrix}. \quad (3.96)$$

The solution of the boundary value problem for this case is similar to Eq. (3.88) and the eight unknowns $\Xi_1^{(1)}$, $\Xi_2^{(1)}$, $\Xi_3^{(1)}$, $\Xi_4^{(1)}$, $\Xi_1^{(2)}$, $\Xi_2^{(2)}$, $\Xi_3^{(2)}$ and $\Xi_4^{(2)}$ can be calculated using the boundary and interface conditions

- finite displacement at $r = 0$

$$u_r^{(1)}, u_\theta^{(1)} \text{ finite at } r = 0 \rightarrow \Xi_3^{(1)} = \Xi_4^{(1)} = 0, \quad (3.97)$$

- traction average at $r = r_1$ in r direction

$$\bar{t}_r = \bar{k}_r \llbracket u_r \rrbracket \rightarrow \sigma_{rr}^{(2)}(r_1) + \sigma_{rr}^{(1)}(r_1) = 2\bar{k}_r [u_r^{(2)}(r_1) - u_r^{(1)}(r_1)], \quad (3.98)$$

- traction average at $r = r_1$ in θ direction

$$\bar{t}_\theta = \bar{k}_\theta \llbracket u_\theta \rrbracket \rightarrow \sigma_{r\theta}^{(2)}(r_1) + \sigma_{r\theta}^{(1)}(r_1) = 2\bar{k}_\theta [u_\theta^{(2)}(r_1) - u_\theta^{(1)}(r_1)], \quad (3.99)$$

- traction equilibrium at $r = r_1$ in r direction

$$[\overline{\text{div } \bar{\sigma}}]_r + \llbracket t_r \rrbracket = 0 \rightarrow -\frac{\bar{\sigma}_{\theta\theta} + \bar{\sigma}_{\phi\phi}}{r_1} + \sigma_{rr}^{(2)}(r_1) - \sigma_{rr}^{(1)}(r_1) = 0, \quad (3.100)$$

- traction equilibrium at $r = r_1$ in θ direction

$$\begin{aligned} [\overline{\text{div } \bar{\sigma}}]_\theta + \llbracket t_\theta \rrbracket = 0 \rightarrow & \frac{1}{r_1} \frac{\partial \bar{\sigma}_{\theta\theta}}{\partial \theta} + \frac{1}{r_1 \sin \theta} \frac{\partial \bar{\sigma}_{\theta\phi}}{\partial \phi} + \frac{[\bar{\sigma}_{\theta\theta} - \bar{\sigma}_{\phi\phi}] \cos \theta}{r_1 \sin \theta} \\ & + \sigma_{r\theta}^{(2)}(r_1) - \sigma_{r\theta}^{(1)}(r_1) = 0, \end{aligned} \quad (3.101)$$

- prescribed traction at $r = r_2$ in r and θ direction

$$\sigma_{rr}^{(2)}(r_2) = \beta \sin^2 \theta \cos 2\phi \quad \text{and} \quad \sigma_{r\theta}^{(2)}(r_2) = \beta \sin \theta \cos \theta \cos 2\phi. \quad (3.102)$$

Further details regarding the construction of the system of equations are available in Appendix C.2.3. If the RVE is substituted by an equivalent homogeneous

medium, applying the boundary condition (3.96) results in the displacement field

$$u_r^{\text{eq}} = \frac{\beta}{2M_\mu} r \sin^2 \theta \cos 2\phi, \quad u_\theta^{\text{eq}} = \frac{\beta}{2M_\mu} r \sin \theta \cos \theta \cos 2\phi, \quad u_\phi^{\text{eq}} = -\frac{\beta}{2M_\mu} r \sin \theta \sin 2\phi.$$

Having all the displacement and stress fields, according to Eq. (3.69), the overall energy in both RVE and the equivalent homogeneous medium read

$$U^{\text{RVE}} = \frac{\beta^2}{5} \left[5\Xi_1^{(2)} - 7 \left[1 + 3\frac{\kappa_2}{\mu_2} \right] f^{-2/3} \Xi_2^{(2)} + 6 \left[2 + \frac{\kappa_2}{\mu_2} \right] f \Xi_4^{(2)} \right],$$

$$U^{\text{eq}} = \frac{\beta^2}{2M_\mu},$$

resulting in a *semi-explicit* expression for the lower bound on the effective shear modulus

$$M_{\mu_{\text{LB}}} = \frac{5}{2} \left[5\Xi_1^{(2)} - 7 \left[1 + 3\frac{\kappa_2}{\mu_2} \right] f^{-2/3} \Xi_2^{(2)} + 6 \left[2 + \frac{\kappa_2}{\mu_2} \right] f \Xi_4^{(2)} \right]^{-1},$$

where $\Xi_1^{(2)}$, $\Xi_2^{(2)}$ and $\Xi_4^{(2)}$ are the solutions of the system of equations (C.12), see Appendix C.2.3 for more details.

3.3.2.2 Modified Mori-Tanaka approach

In this section we elaborate the modified Mori–Tanaka method for particulate composites. As we mentioned earlier, the most significant advantage of this method is that in addition to the overall macroscopic properties, it also determines the concentrations tensors thus, the state of the stress and strain in each phase of the medium can be obtained.

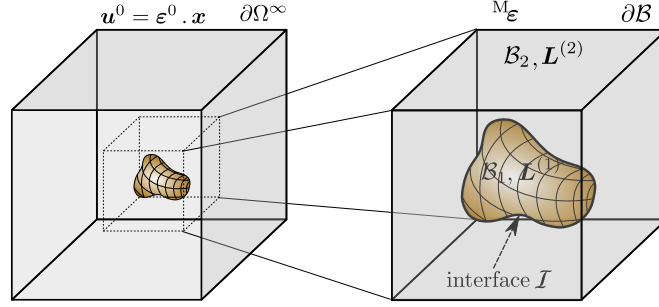


Figure 3.10: Inhomogeneity with imperfect interface inside an infinite matrix (left) and the RVE consisting of the inhomogeneity with imperfect interface inside a matrix material (right).

3.3.2.2.1 General framework The general framework of the Mori–Tanaka method for fiber and particle composites is the same therefore, is not discussed here to avoid repetition. The only difference between the two problems is the structure of the matrices $\mathbf{H}$, $\mathbf{T}$ and $\mathbf{T}^{(1)}$. For a particle reinforced composite with isotropic constituents, the interaction tensors are isotropic and can be written as

$$\mathbf{T}^{(1)} = 3T^{b(1)}\mathcal{I}^h + 2T^{s(1)}\mathcal{I}^d, \quad \mathbf{T} = 3T^b\mathcal{I}^h + 2T^s\mathcal{I}^d, \quad \mathbf{H} = 3H^b\mathcal{I}^h + 2H^s\mathcal{I}^d$$

with

$$\mathcal{I}^h = \frac{1}{3}\mathbf{I} \otimes \mathbf{I}, \quad \mathcal{I}^d = \mathcal{I} - \mathcal{I}^h.$$

In order to complete the homogenization framework, we must determine the interaction tensors $\mathbf{H}$, $\mathbf{T}$ and $\mathbf{T}^{(1)}$. In doing so, we employ the Eshelby’s inhomogeneity problem for *isochoric* and *deviatoric* conditions.

3.3.2.2.2 Isochoric conditions Assume an RVE consisting of an infinite matrix with a spherical inhomogeneity subject to a hydrostatic far field displacement field according to

$$\mathbf{u}_{(x,y,z)}^0 = \begin{bmatrix} \beta x \\ \beta y \\ \beta z \end{bmatrix} \quad \text{and} \quad \mathbf{u}_{(r,\theta,\phi)}^0 = \begin{bmatrix} \beta r \\ 0 \\ 0 \end{bmatrix}. \quad (3.103)$$

The displacement fields in the particle and the matrix are similar to Eq. (3.71) resulting in four unknowns of $\Xi_1^{(1)}$, $\Xi_2^{(1)}$, $\Xi_1^{(2)}$ and $\Xi_2^{(2)}$. The boundary and interface conditions read

- finite displacement at $r = 0$

$$u_r^{(1)} \text{ finite at } r = 0 \rightarrow \Xi_2^{(1)} = 0, \quad (3.104)$$

- traction average at $r = r_1$

$$\bar{t}_r = \bar{k}_r \llbracket u_r \rrbracket \rightarrow \frac{\sigma_{rr}^{(2)}(r_1) + \sigma_{rr}^{(1)}(r_1)}{2} = \bar{k}_r [u_r^{(2)}(r_1) - u_r^{(1)}(r_1)], \quad (3.105)$$

- traction equilibrium at $r = r_1$

$$[\overline{\text{div}} \bar{\sigma}]_r + \llbracket t_r \rrbracket = 0 \rightarrow -\frac{\bar{\sigma}_{\theta\theta} + \bar{\sigma}_{\phi\phi}}{r_1} + \sigma_{rr}^{(2)}(r_1) - \sigma_{rr}^{(1)}(r_1) = 0, \quad (3.106)$$

- prescribed displacement at $r = r_2$

$$u_r^{(2)}(r \rightarrow \infty) = \beta r, \quad \rightarrow \quad \Xi_1^{(2)} = 1. \quad (3.107)$$

result in the linear system of equations

$$\begin{bmatrix} 1 + \frac{3\kappa_1}{2\bar{k}r_1} & -1 - \frac{2\mu_2}{\bar{k}r_1} \\ 3\kappa_1 + \frac{2\bar{k}}{r_1} & 4\mu_2 + \frac{2[\bar{\lambda} + \bar{\mu}]}{r_1} \end{bmatrix} \begin{bmatrix} \Xi_1^{(1)} \\ \Xi_2^{(2)} \end{bmatrix} = \begin{bmatrix} 1 - \frac{3\kappa_2}{2\bar{k}r_1} \\ 3\kappa_2 - \frac{2[\bar{\lambda} + \bar{\mu}]}{r_1} \end{bmatrix}. \quad (3.108)$$

Solving this system, the average strain in the particle and the strain and stress fields in the particle+interface system are obtained as

$$\int_B \boldsymbol{\epsilon}_{\Omega_1}^- dV = \Xi_1^{(1)} \boldsymbol{\epsilon}^0, \quad \int_B \boldsymbol{\epsilon}_{\Omega_1}^+ dV = [1 + \Xi_2^{(2)}] \boldsymbol{\epsilon}^0, \quad \int_B \boldsymbol{\sigma}_{\Omega_1}^+ dV = [3\kappa_2 - 4\mu_2 \Xi_2^{(2)}] \boldsymbol{\epsilon}^0.$$

Consequently, the bulk interaction terms read

$$3T^{b(1)} = \Xi_1^{(1)}, \quad 3T^b = 1 + \Xi_2^{(2)}, \quad 3H^b = 3\kappa_2 - 4\mu_2 \Xi_2^{(2)},$$

where $\Xi_1^{(1)}$ and $\Xi_2^{(2)}$ are obtained from the solution of the linear system (3.108).

3.3.2.2.3 Deviatoric conditions Assume the RVE is subject to a deviatoric far field displacement field

$$\mathbf{u}_{(x,y,z)}^0 = \begin{bmatrix} \beta y \\ -\beta x \\ 0 \end{bmatrix} \quad \text{and} \quad u_{(r,\theta,\phi)}^0 = \begin{bmatrix} \beta r \sin^2 \theta \cos 2\phi \\ \beta r \sin \theta \cos \theta \cos 2\phi \\ -\beta r \sin \theta \sin 2\phi \end{bmatrix}. \quad (3.109)$$

The displacement fields in the particle and the matrix are similar to Eq. (3.88) resulting in eight unknowns of with the unknowns $\Xi_1^{(1)}$, $\Xi_2^{(1)}$, $\Xi_3^{(1)}$, $\Xi_4^{(1)}$, $\Xi_1^{(2)}$, $\Xi_2^{(2)}$, $\Xi_3^{(2)}$ and $\Xi_4^{(2)}$. The boundary and interface conditions read

- finite displacement at $r = 0$

$$u_r^{(1)}, u_\theta^{(1)} \text{ finite at } r = 0 \rightarrow \Xi_3^{(1)} = \Xi_4^{(1)} = 0, \quad (3.110)$$

- traction average at $r = r_1$ in r direction

$$\bar{t}_r = \bar{k}_r \llbracket u_r \rrbracket \rightarrow \sigma_{rr}^{(2)}(r_1) + \sigma_{rr}^{(1)}(r_1) = 2\bar{k}_r \left[u_r^{(2)}(r_1) - u_r^{(1)}(r_1) \right], \quad (3.111)$$

- traction average at $r = r_1$ in θ direction

$$\bar{t}_\theta = \bar{k}_\theta \llbracket u_\theta \rrbracket \rightarrow \sigma_{r\theta}^{(2)}(r_1) + \sigma_{r\theta}^{(1)}(r_1) = 2\bar{k}_\theta \left[u_\theta^{(2)}(r_1) - u_\theta^{(1)}(r_1) \right], \quad (3.112)$$

- traction equilibrium at $r = r_1$ in r direction

$$\left[\overline{\text{div } \bar{\sigma}} \right]_r + \llbracket t_r \rrbracket = 0 \rightarrow -\frac{\bar{\sigma}_{\theta\theta} + \bar{\sigma}_{\phi\phi}}{r_1} + \sigma_{rr}^{(2)}(r_1) - \sigma_{rr}^{(1)}(r_1) = 0, \quad (3.113)$$

- traction equilibrium at $r = r_1$ in θ direction

$$\begin{aligned} [\overline{\text{div}} \bar{\sigma}]_\theta + \llbracket t_\theta \rrbracket = 0 \rightarrow & \frac{1}{r_1} \frac{\partial \bar{\sigma}_{\theta\theta}}{\partial \theta} + \frac{1}{r_1 \sin \theta} \frac{\partial \bar{\sigma}_{\theta\phi}}{\partial \phi} + \frac{[\bar{\sigma}_{\theta\theta} - \bar{\sigma}_{\phi\phi}] \cos \theta}{r_1 \sin \theta} \\ & + \sigma_{r\theta}^{(2)}(r_1) - \sigma_{r\theta}^{(1)}(r_1) = 0, \end{aligned} \quad (3.114)$$

- prescribed displacement at $r = r_2$ in r direction

$$u_r^{(2)}(r = r_2) = \beta r \sin^2 \theta \cos 2\phi, \quad \rightarrow \quad \Xi_1^{(2)} = 1, \quad \Xi_2^{(2)} = 0, \quad (3.115)$$

- prescribed displacement at $r = r_2$ in θ direction

$$u_\theta^{(2)}(r = r_2) = \beta r \sin \theta \cos \theta \cos 2\phi \quad \rightarrow \quad \Xi_1^{(2)} = 1, \quad \Xi_2^{(2)} = 0. \quad (3.116)$$

resulting in the system of equations

$$\begin{bmatrix} 1 + \frac{\mu_1}{\bar{k}r_1} & 2 - 3\frac{\kappa_1}{\mu_1} + \zeta_1 & -3 - \frac{12\mu_2}{\bar{k}r_1} & -3 - 3\frac{\kappa_2}{\mu_2} + \zeta_2 \\ 1 + \frac{\mu_1}{\bar{k}r_1} & -\frac{11}{3} - 5\frac{\kappa_1}{\mu_1} + \zeta_3 & 2 + \frac{8\mu_2}{\bar{k}r_1} & -2 + \frac{3\kappa_2}{\bar{k}r_1} \\ 2\mu_1 - \zeta_9 & 3\kappa_1 - 2\mu_1 + \zeta_4 & 24\mu_2 + 12\zeta_9 & \zeta_{10} + \frac{6\kappa_2\zeta_9}{\mu_2} \\ 2\mu_1 + \zeta_5 & -16\kappa_1 - \frac{10}{3}\mu_1 + \zeta_6 & -16\mu_2 + \zeta_7 & -6\kappa_2 + \zeta_8 \end{bmatrix} \begin{bmatrix} \Xi_1^{(1)} \\ \Xi_2^{(1)} \\ \Xi_3^{(2)} \\ \Xi_4^{(2)} \end{bmatrix} = \begin{bmatrix} 1 - \frac{\mu_2}{\bar{k}r_1} \\ 1 - \frac{\mu_2}{\bar{k}r_1} \\ 2\mu_2 + \zeta_9 \\ 2\mu_2 - \zeta_5 \end{bmatrix},$$

with

$$\begin{aligned} \zeta_1 &= \frac{3\kappa_1 - 2\mu_1}{2\bar{k}r_1}, & \zeta_6 &= -\frac{\kappa_1 [9\bar{\lambda} + 19\bar{\mu}]}{\mu_1 r_1} - \frac{[45\bar{\lambda} + 67\bar{\mu}]}{3r_1}, \\ \zeta_2 &= -\frac{9\kappa_2 + 4\mu_2}{\bar{k}r_1}, & \zeta_7 &= -\frac{4[3\bar{\lambda} + 4\bar{\mu}]}{r_1}, \\ \zeta_3 &= -\frac{24\kappa_1 + 5\mu_1}{3\bar{k}r_1}, & \zeta_8 &= \frac{-6\kappa_2 [\bar{\lambda} + \bar{\mu}] + 4\mu_2 \bar{\mu}}{\mu_2 r_1}, \\ \zeta_4 &= \frac{[9\kappa_1 + 15\mu_1] [\bar{\lambda} + \bar{\mu}]}{\mu_1 r_1}, & \zeta_9 &= \frac{[\bar{\lambda} + \bar{\mu}]}{r_1}, \\ \zeta_5 &= \frac{[\bar{\lambda} + 3\bar{\mu}]}{r_1}, & \zeta_{10} &= 18\kappa_2 + 8\mu_2. \end{aligned}$$

Solving this system, the average strain in the particle and the strain and stress in the particle+interface system are determined as

$$\begin{aligned}\int_{\mathcal{B}} \boldsymbol{\varepsilon}_{\Omega_1}^- dV &= \frac{1}{5} \left[5\Xi_1^{(1)} - 7 \left[1 + 3 \frac{\kappa_1}{\mu_1} \right] \Xi_2^{(1)} \right] \boldsymbol{\varepsilon}^0, \\ \int_{\mathcal{B}} \boldsymbol{\varepsilon}_{\Omega_1}^+ dV &= \frac{1}{5} \left[5 + 6 \left[2 + \frac{\kappa_2}{\mu_2} \right] \Xi_4^{(2)} \right] \boldsymbol{\varepsilon}^0, \\ \int_{\mathcal{B}} \boldsymbol{\sigma}_{\Omega_1}^+ dV &= \frac{1}{5} \left[10\mu_2 - 2 [9\kappa_2 + 8\mu_2] \Xi_4^{(2)} \right] \boldsymbol{\varepsilon}^0.\end{aligned}$$

Consequently, the shear interaction terms read

$$\begin{aligned}2T^{s(1)} &= \frac{1}{5} \left[5\Xi_1^{(1)} - 7 \left[1 + 3 \frac{\kappa_1}{\mu_1} \right] \Xi_2^{(1)} \right], \\ 2T^s &= \frac{1}{5} \left[5 + 6 \left[2 + \frac{\kappa_2}{\mu_2} \right] \Xi_4^{(2)} \right], \\ 2H^s &= \frac{1}{5} \left[10\mu_2 - 2 [9\kappa_2 + 8\mu_2] \Xi_4^{(2)} \right].\end{aligned}$$

3.4 Numerical examples

In this section, through a set of numerical examples, the analytical solutions are evaluated via comparison with the computational results using the finite element method. In doing so, the overall material response of fiber composites and particulate composites embedding general interfaces is investigated. It shall be emphasized that the results obtained by the computational analysis are regarded as the “exact” solution and the analytical solutions are understood as “approximations”. The RVE in our computational study is simplified to a spherical micro-structure for the particulate composites and to a circular micro-structure for fiber composites in order to capture isotropic response inherent to the analytical solutions. Throughout the examples, the inclusion volume fraction is assumed $f = 30\%$. Three different stiffness ratios of 0.1, 1 and 10 are examined. The stiffness ratio denoted as incl./matr. is the ratio of the inclusion Lamé parameters to the matrix Lamé parameters. The stiffness ratio 0.1 indicates a 10 times more compliant inclusion compared to the matrix whereas the stiffness ratio 10 corresponds to a 10

times stiffer inclusion than the matrix. Obviously, the stiffness ratio 1 represents identical inclusion and matrix. In particular, the limit case of $\text{incl./matr.} \rightarrow \infty$ indicates a rigid inclusion whereas $\text{incl./matr.} = 0$ is the limit case where the inclusion resembles a void. In this study, we set the matrix material parameters to $\lambda_2 = \mu_2 = 1$ and the inclusion material parameters vary in accordance with the predefined stiffness ratios. In order to highlight the role of the general interface in the overall material response, two values of $\bar{\lambda} = \bar{\mu} = 1$ and $\bar{\lambda} = \bar{\mu} = 100$ are considered for the general interface in-plane parameters indicating a low and a high elastic resistance against in-plane stretches, respectively. On the other hand, the two considered values for the general interface orthogonal resistance against opening are $\bar{k} = 1$ indicating a low stiffness and $\bar{k} = 100$ indicating a high orthogonal resistance. In the limit of $\bar{k} = 0$, the interface shows no opening resistance resembling a totally detached matrix and particle. In contrast, the limit of $\bar{k} \rightarrow \infty$ corresponds to a coherent interface. Note, for the fiber composites, we set $\bar{\lambda} = 0$ since only one interface in-plane parameter is sufficient to represent the tangential response of the interface.

Figures 3.11–3.13 illustrate the effective bulk modulus M_K and shear modulus M_μ versus size for different stiffness ratios for both fiber and particulate composites. Each column corresponds to a specific in-plane resistance $\bar{\mu}$ and each row corresponds to a specific orthogonal resistance $\bar{k}$. Lines indicate the analytical solutions corresponding to the analytical approaches developed in Section 3.3. Red circular points and blue rectangular points correspond to computational results using the finite element method obtained via prescribing DBC and TBC, respectively. The solid straight black line shows the effective response due to the perfect interface. A remarkable agreement between the analytical solutions and the computational results are consistently observed for all the examples. For all the cases, a size-dependent response is observed due to the presence of the general interface. For the bulk modulus, all the solutions render a consistent behavior with respect to the perfect interface solution. The results coincide with the perfect interface solution at small sizes. Increasing the size results in deviation from the perfect interface solution until a critical size at which an extremum is reached. Further increase in size yields asymptotic convergence of the results

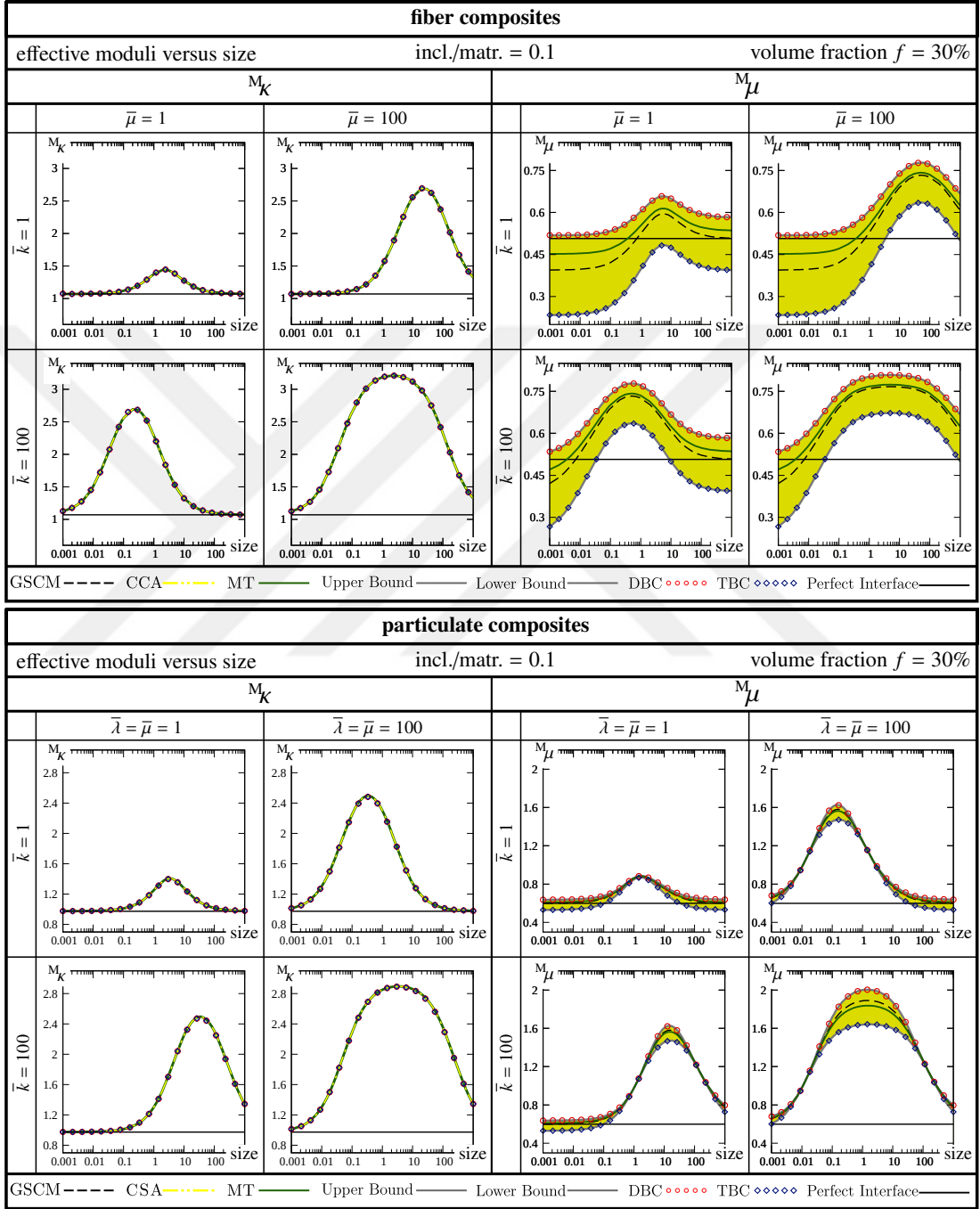


Figure 3.11: The effective bulk and shear moduli versus size for $\text{incl./matr.} = 0.1$. The lines correspond to the analytical solutions and dots correspond to the numerical results using the finite element method. “GSCM” corresponds to the generalized self-consistent method. “CCA” corresponds to the composite cylinder assemblage method. “CSA” corresponds to the composite sphere assemblage method.

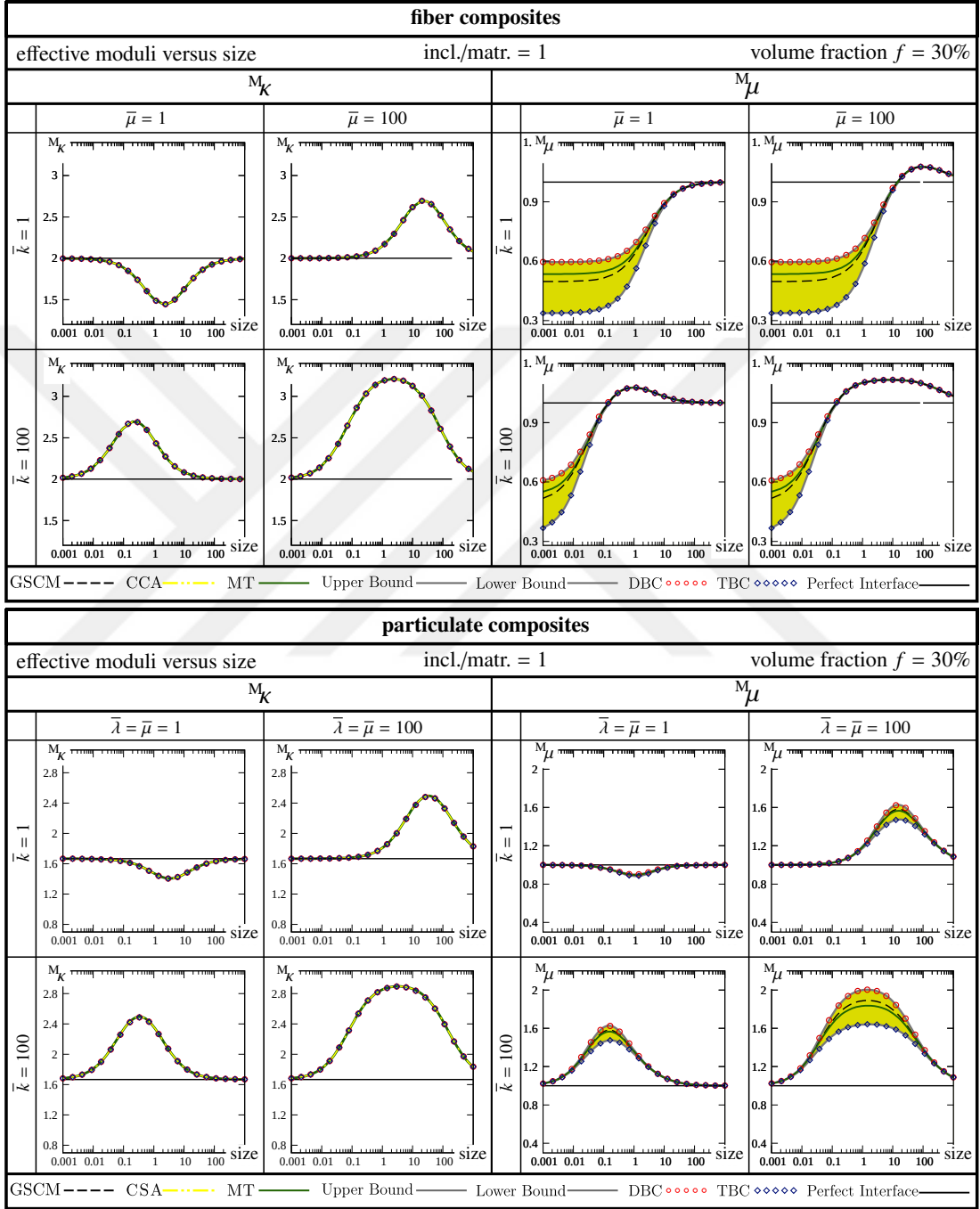


Figure 3.12: The effective bulk and shear moduli versus size for incl./matr. = 1. The lines correspond to the analytical solutions and dots correspond to the numerical results using the finite element method. “GSCM” corresponds to the generalized self-consistent method. “CCA” corresponds to the composite cylinder assemblage method. “CSA” corresponds to the composite sphere assemblage method.

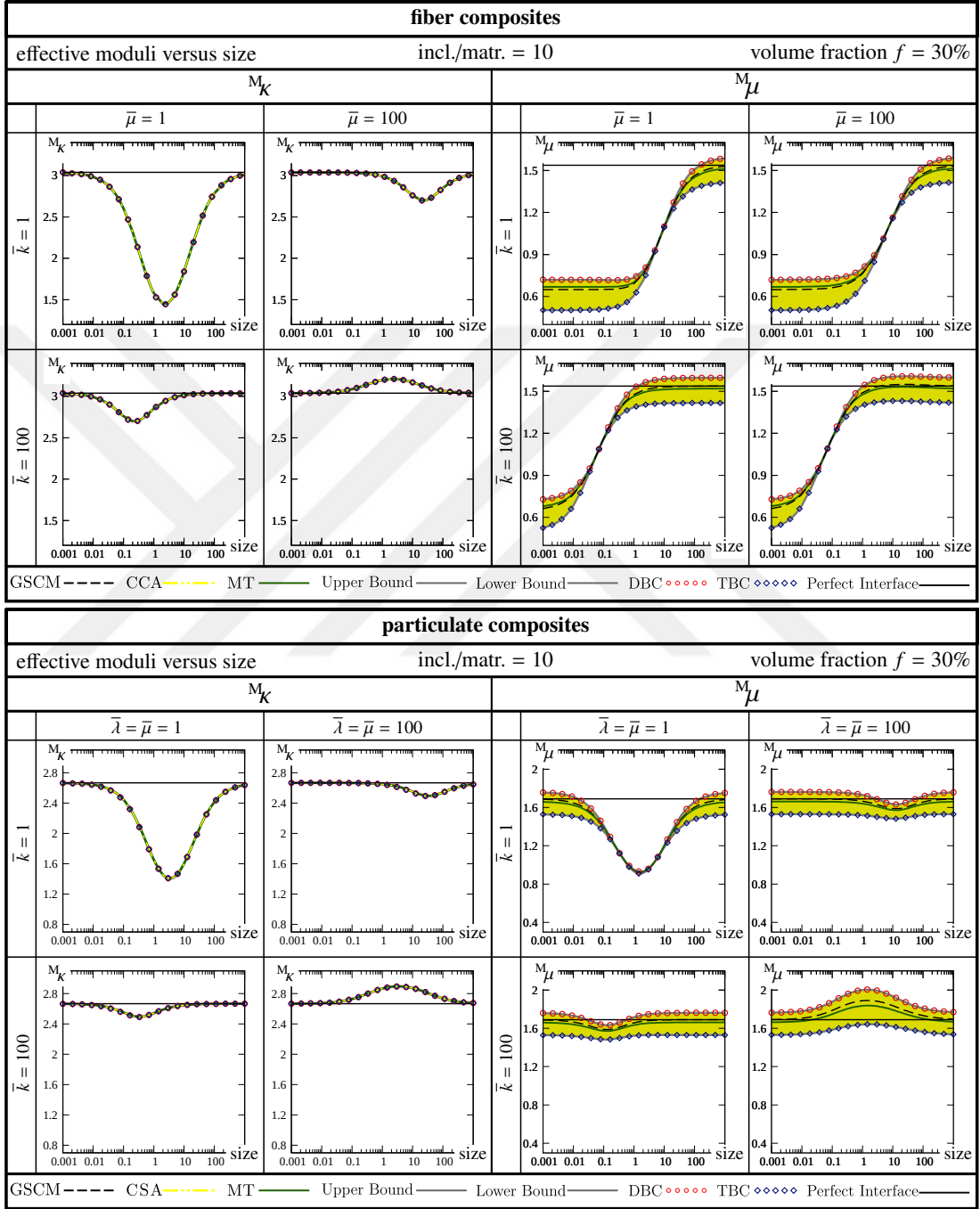


Figure 3.13: The effective bulk and shear moduli versus size for $\text{incl./matr.} = 10$. The lines correspond to the analytical solutions and dots correspond to the numerical results using the finite element method. “GSCM” corresponds to the generalized self-consistent method. “CCA” corresponds to the composite cylinder assemblage method. “CSA” corresponds to the composite sphere assemblage method.

to the perfect interface solution which is due to the diminished interface effects at large sizes. For $\text{incl./matr.} = 0.1$, the results corresponding to the general interface always overestimate those obtained from the perfect interface model. However, for the other stiffness ratios, depending on the interface parameters, the results render either a weaker or a stronger response compared to the perfect interface solution. Evidently, if the interface parameters are large enough, the response due to the general interface is stiffer than those of the perfect interface. Overall, an important observation and especially useful for computational material design is that in the presence of interfaces, even if the inclusion is identical to the matrix, various combinations of parameters could result in substantially different but also size-dependent overall material behavior. For the shear modulus, there is a perfect agreement between the upper bound and DBC and the lower bound and TBC. For fiber composites, when $\text{incl./matr.} = 0.1$, the bounds never coincide, when $\text{incl./matr.} = 1$, the upper and the lower bounds *converge* at larger sizes and when $\text{incl./matr.} = 10$, the bounds tend to approach to each other until they coincide at a specific sizes and then they distant from each other as size increases. For particulate composites, the bounds coincide at small and large sizes for $\text{incl./matr.} = 1$. More complex behavior is observed for the other stiffness ratios. A particular observation is that the generalized self-consistent method and the modified Mori–Tanaka method do not provide similar estimates for the effective shear modulus. For fiber composites, when $\text{incl./matr.} = 0.1$ and $\text{incl./matr.} = 1$, the response obtained from GSCM underestimates that of MT method. However, when $\text{incl./matr.} = 10$, the results corresponding to GSCM underestimate the ones obtained from MT before the bounds coincide whereas the opposite story holds after the bounds coincidence. For particulate composites, when $\text{incl./matr.} = 0.1$ Mori–Tanaka overestimates GSCM at very small and very large sizes. However, when $\text{incl./matr.} = 1$ and $\text{incl./matr.} = 10$, it is the solution due to GSCM that overestimates that of Mori–Tanaka.

Inspired by the observations made throughout the numerical examples, it is possible to distinguish between two dissimilar bounds on the overall behavior of the micro-structure, namely *size-dependent bounds* and *ultimate bounds*. Size-dependent bounds are the bounds on the effective behavior of the micro-structure

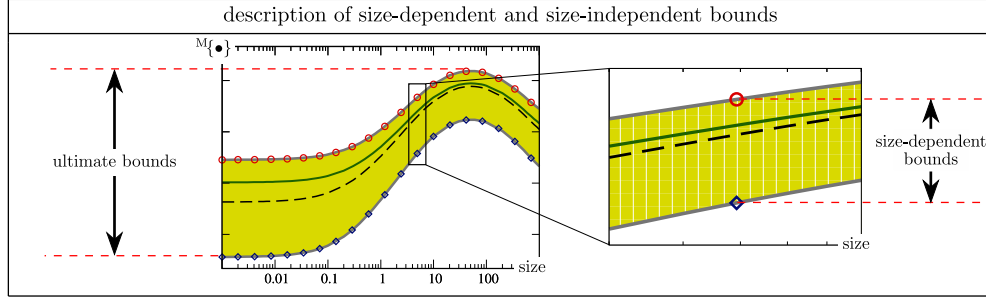


Figure 3.14: Schematic illustration of size-dependent and ultimate bounds.

at any given size. The upper and lower size-dependent bounds correspond to the solution of the boundary value problem associated with DBC and TBC, respectively. On the other hand, we also observe that the macroscopic response is always bounded between two specific values regardless of the size of the micro-structure and thus, we refer to them as ultimate bounds. In the case of a stiff inclusion within a more compliant matrix such as $\text{incl./matr.} = 10$ shown in Fig. 3.13 for fiber composites, the ultimate bounds are reached at extreme sizes. However, the ultimate bounds may be reached at critical sizes and not necessarily at the limits, see for instance Fig. 3.11. Figure. 3.14 elucidate the notions of ultimate and size-dependent bounds schematically. Size-dependent bounds are local in the sense that for a specific interface and material parameters, they vary with respect to size. In contrast, the ultimate bounds are independent of size and they entirely depend on the interface and bulk material properties. As pointed out earlier, the size-dependent bounds coincide in the case of the effective bulk modulus M_{κ} and are only distinct in the case of the effective shear modulus M_{μ} . This conclusion for general interface is in agreement with that derived by Hashin and Rosen for the case of a perfect interface [15].

Figures 3.15 and 3.16 provide a generic comparison of the elastic, cohesive and general interfaces at different sizes and stiffness ratios. For Fig. 3.15 the interface parameters are $\bar{k} = 1$, $\bar{\mu} = 100$ and for Fig. 3.16 the interface parameters are $\bar{k} = 100$, $\bar{\mu} = 1$. The stiffness ratio is $\text{incl./matr.} = 0.1$ for both figure. The top boxes correspond to the effective bulk modulus M_{κ} and the bottom boxes correspond to the effective shear modulus is M_{μ} . The left graphs in each box show the effective modulus of interest versus size for three different stiffness ratios of

0.1 (top), 1 (middle) and 10 (bottom). The solid black lines represent the effective response associated with the general interface model and the dashed red and blue lines correspond to the overall response due to the elastic and cohesive interface models, respectively. The middle micro-structures render the stress distribution throughout the RVEs for various interface types at size = 0.01. The graphs on the right show the effective moduli versus stiffness ratio and size. It is observed

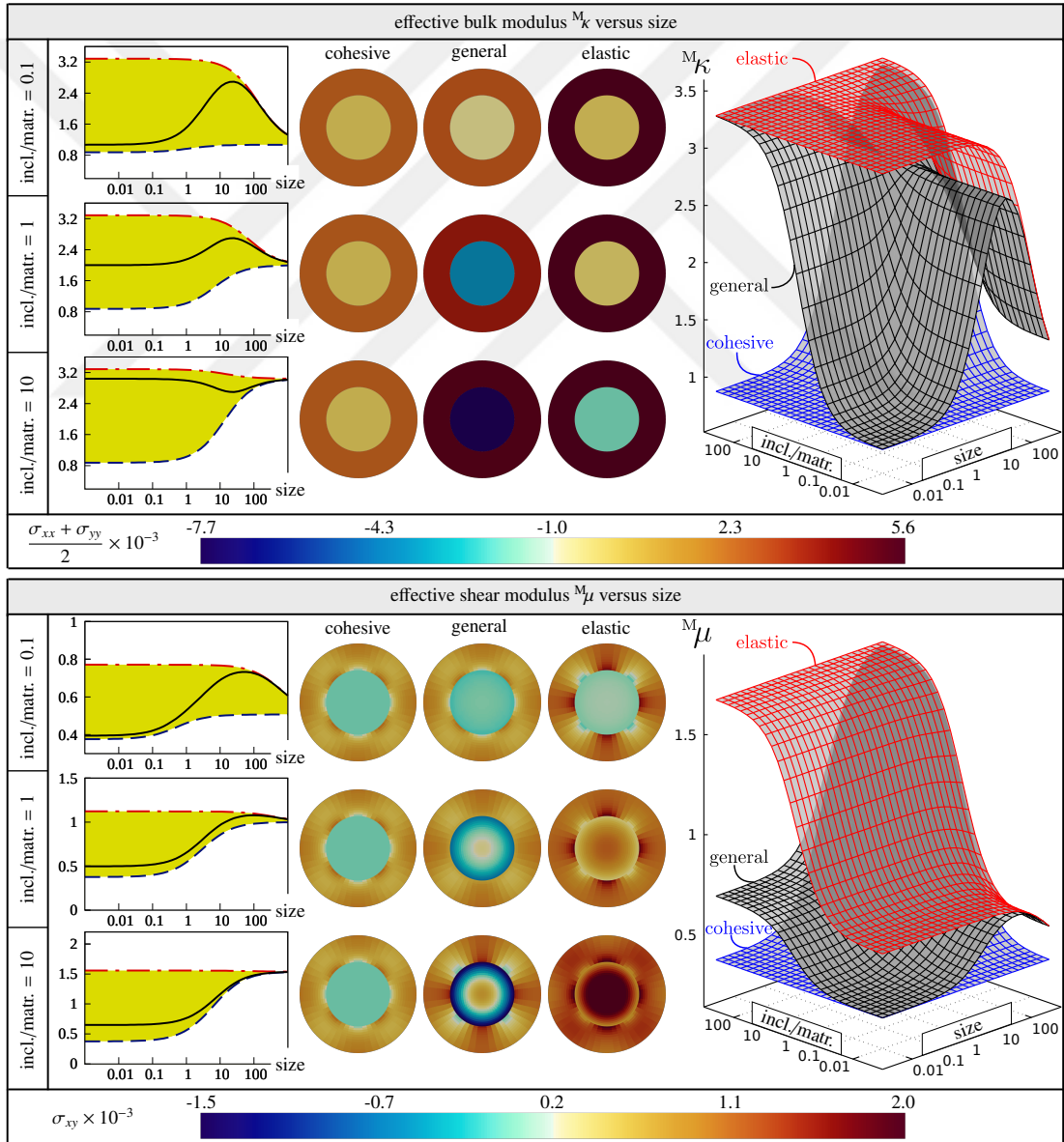


Figure 3.15: Effective bulk and shear modulus versus the stiffness ratio and size for different interface types. The interface parameters are $\bar{k} = 1$ and $\bar{\mu} = 100$. The stiffness ratio is incl./matr. = 0.1.

that for a fixed set of interface parameters, the overall response due to the general interface model is bounded between those associated with the cohesive and elastic interfaces from top and bottom, respectively. Therefore, the elastic and cohesive interface models can be interpreted as the upper and lower bounds of the general interface model, respectively. Furthermore, all the effective responses coincide when the size of the micro-structure is very large. This is expected since the

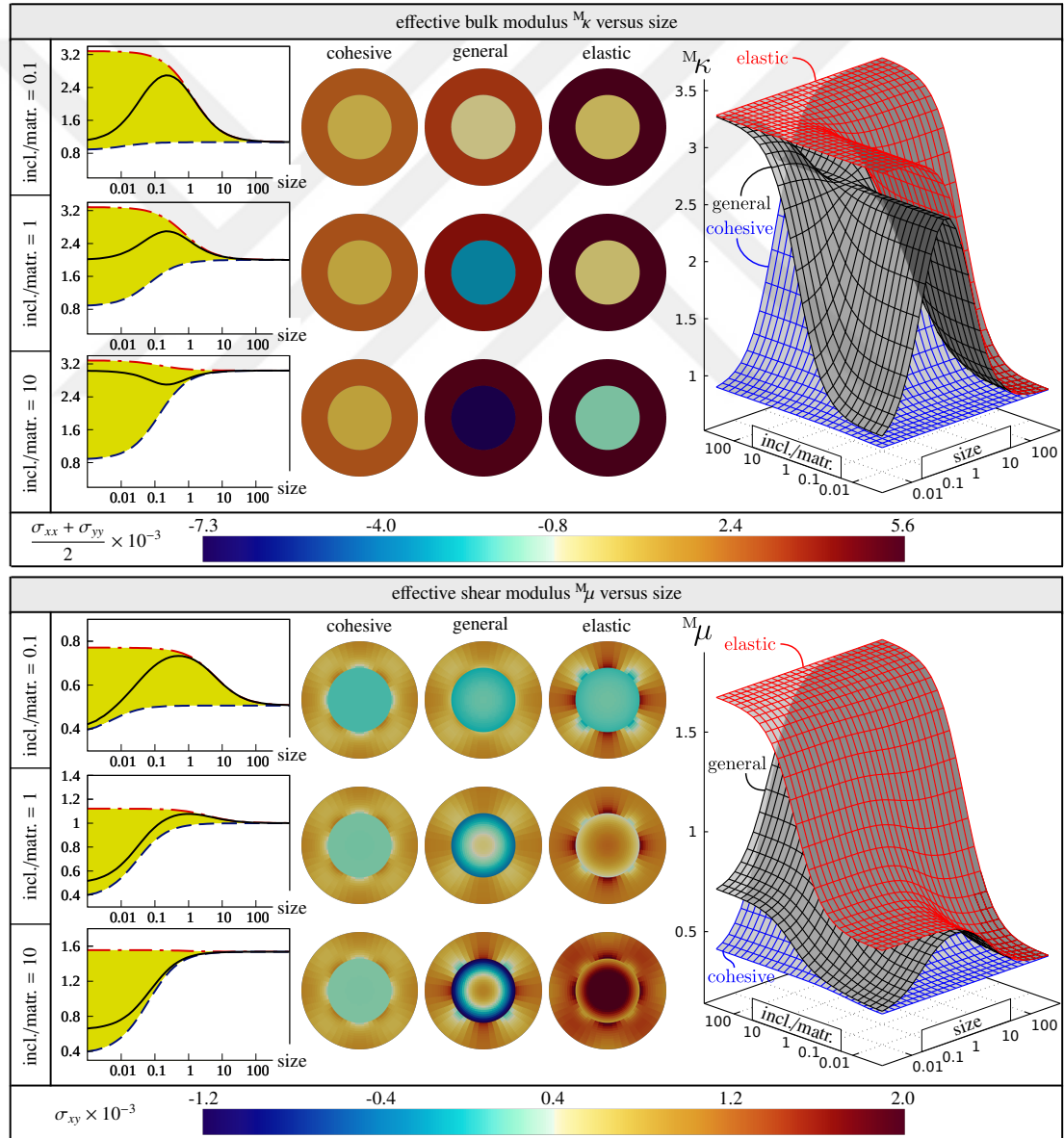


Figure 3.16: Effective bulk and shear modulus versus the stiffness ratio and size for different interface types. The interface parameters are $\bar{k} = 100$ and $\bar{\mu} = 1$. The stiffness ratio is $\text{incl./matr.} = 0.1$.

interface effects are proportional to the area-to-volume ratio, hence diminishing at large sizes of the micro-structure. On the other hand, at very small sizes,

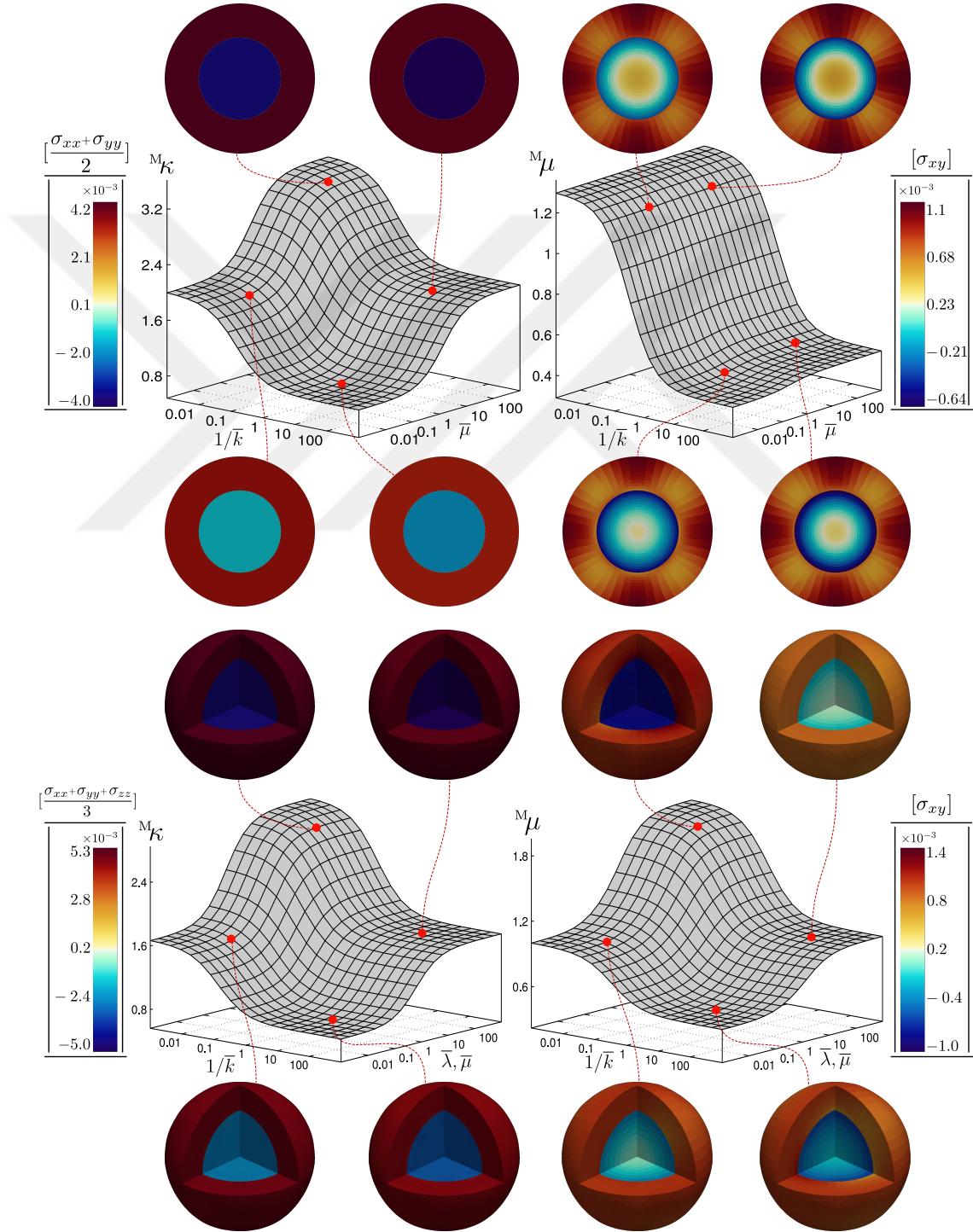


Figure 3.17: Effective moduli versus the interface parameters for fiber composites and particulate composites.

elastic and cohesive interfaces render the same response regardless of the stiffness ratio whereas the response due to the general interface model tends to distant from the cohesive and approach the elastic solution as we increase the stiffness ratio. According to the results throughout Figs. 3.15 and 3.16, the elastic interface model shows a smaller-stiffer trend opposite to the cohesive interface model that leads to larger-stiffer behavior regardless of the stiffness ratio. However, this is not the case for the general interface model. The general interface model shows both the smaller-stiffer and larger-stiffer trends resulting in a *critical size* at which its trend reverses. As it can be seen, the overall response due to the general interface model is highly non-linear, relatively complicated and in principle unpredictable.

To pinpoint the effects of the general interface parameters on the overall properties of composites, Fig. 3.17 renders the effective moduli versus the interface orthogonal resistance $\bar{k}$ and the interface tangential coefficients $\bar{\lambda}$ and $\bar{\mu}$. The two top figures correspond to the effective bulk and shear modulus of the fiber composites whereas the two bottom figures render the effective bulk and shear modulus of particulate composites. The stiffness ratio is set to $\text{incl./matr.} = 1$. For fiber composites, when bulk modulus is studied, increasing any of the interface parameters result in stiffer response. However, when shear modulus is examined, the results show almost no sensitivity with respect to the interface in-plane resistance while increasing the orthogonal resistance stiffens the response. For particulate composites the interface parameters are essentially stiffness-like parameters in the sense that larger values of the interface parameters result in stiffer macroscopic behavior. More precisely, larger $\bar{k}$ results in larger effective parameters $^M\kappa$ and $^M\mu$ for any set of $\bar{\lambda}$ and $\bar{\mu}$. Similarly, larger $\bar{\lambda}$ and $\bar{\mu}$ result in larger effective parameters $^M\kappa$ and $^M\mu$ for any $\bar{k}$. That is, the most compliant overall behavior can be obtained if all the interface parameters vanish altogether or oppositely, the larger the interface parameters, the stiffer the effective response.

As pointed out earlier, a key feature of our proposed modified Mori–Tanaka approach is that in addition to the overall material properties, it determines the interaction tensors and consequently the stress and strain fields within each phase of the medium. The next set of examples are devised to demonstrate the utility of our modified Mori–Tanaka method to calculate the stress state in the medium

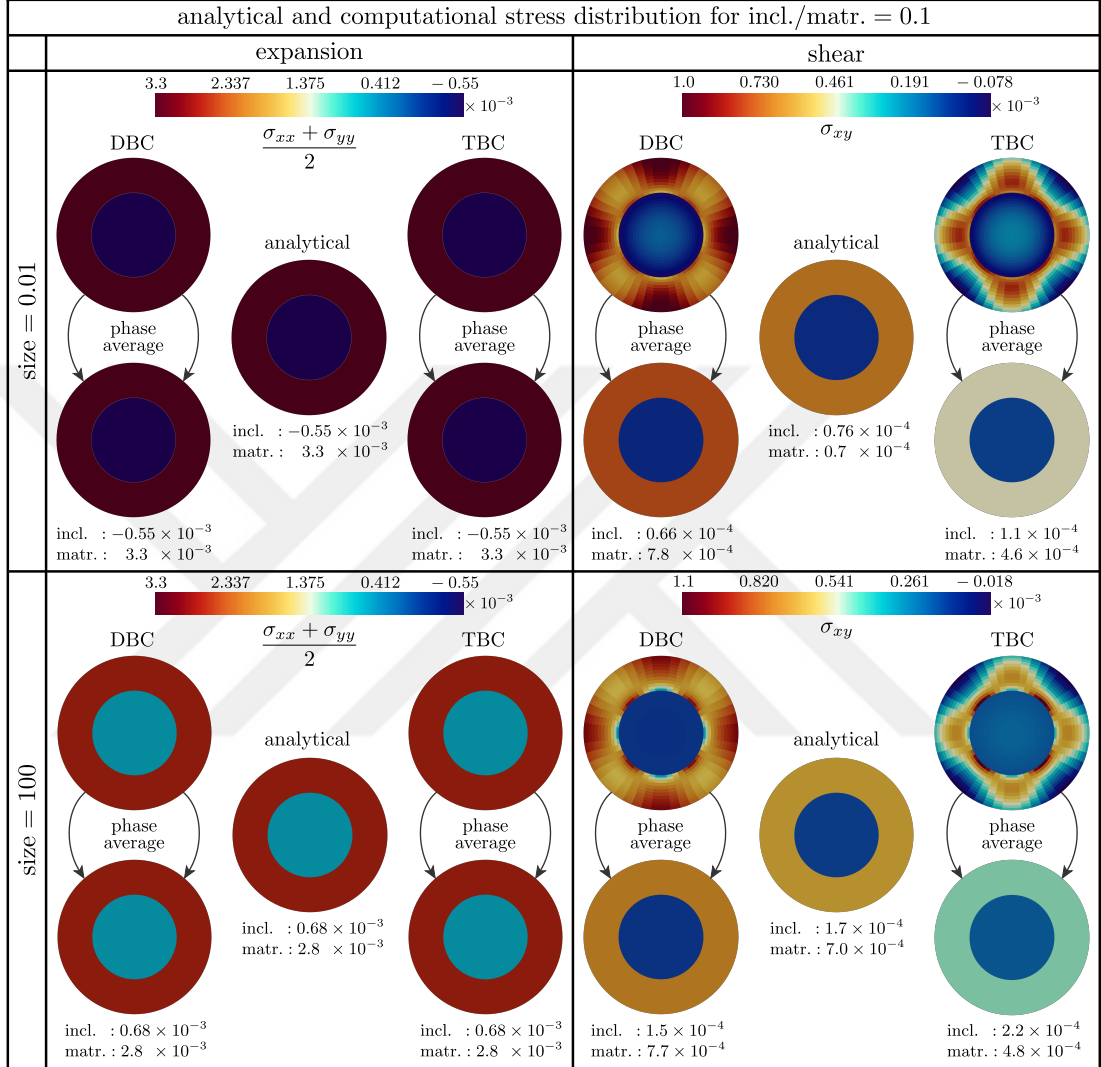


Figure 3.18: Comparison of 2D analytical and numerical stress distributions for incl./matr. = 0.1.

subject to volumetric expansion and simple shear. Figures 3.18–3.23 show the analytical and computational stress distributions throughout the micro-structure for different sizes as well as different stiffness ratios for both fiber- and particle-reinforced composites. All of the micro-structures are schematically scaled to the same size for better illustration. On the left columns, volumetric expansion is applied to the micro-structure and the pressure-like quantity $[\sigma_{xx} + \sigma_{yy} + \sigma_{zz}]/3$ for the three-dimensional analysis and $[\sigma_{xx} + \sigma_{yy}]/2$ for the two dimensional analysis are more relevant to study. On the other hand, on the right columns, simple shear

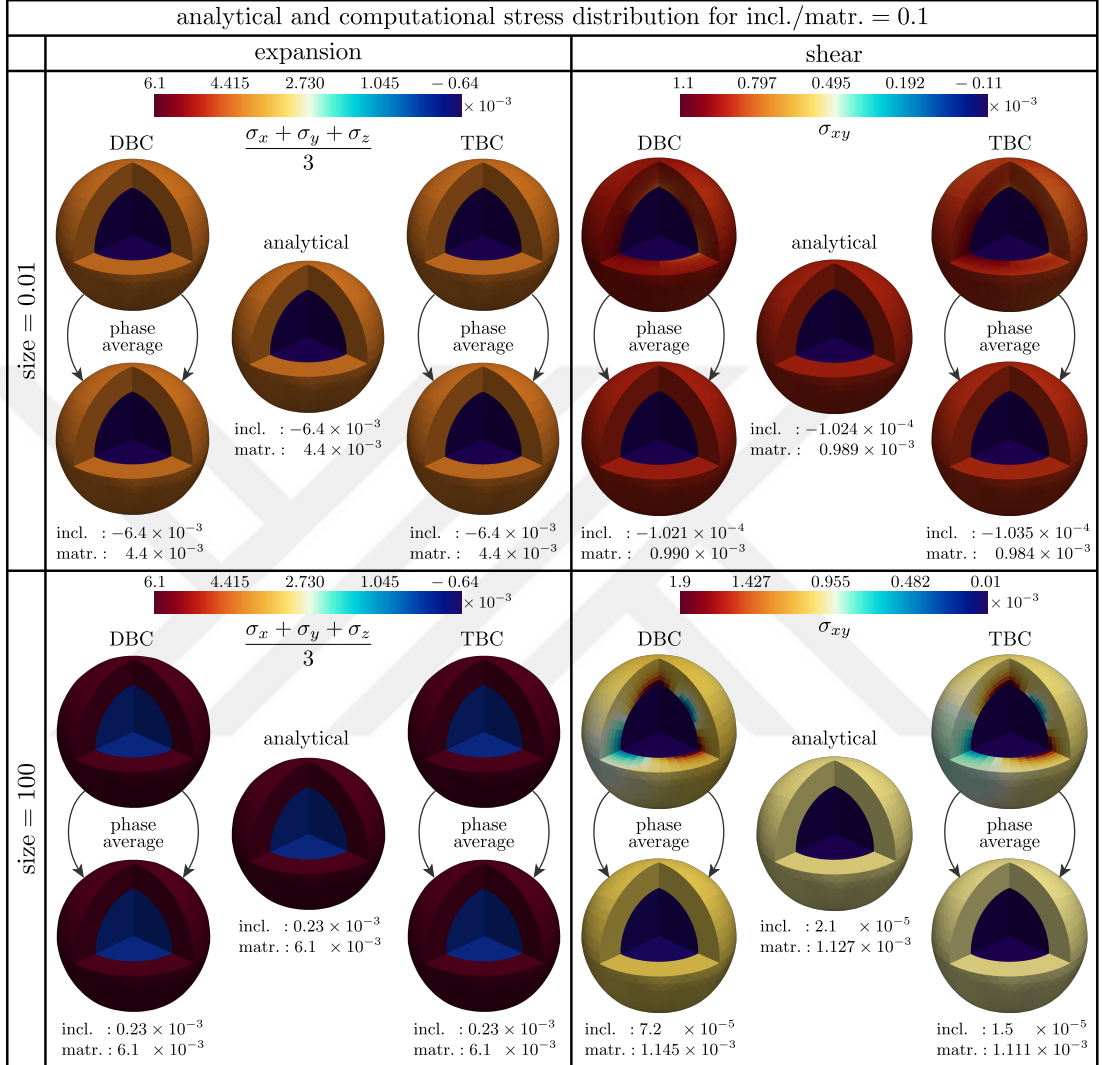


Figure 3.19: Comparison of 3D analytical and numerical stress distributions for incl./matr. = 0.1.

in xy -plane is applied to the RVE in which case the stress component of interest is σ_{xy} . In each box, the top micro-structures correspond to the computational local stress distributions due to DBC and TBC and the analytical stress distribution is shown at the center. Since our proposed analytical scheme determines the average stresses in the constituents of the medium, the bottom micro-structures in each box render the average computational stress due to DBC and TBC suitable for comparison with the analytical stresses. The average stresses in the particle and the matrix are stated below each case for the sake of clarity. For the expansion

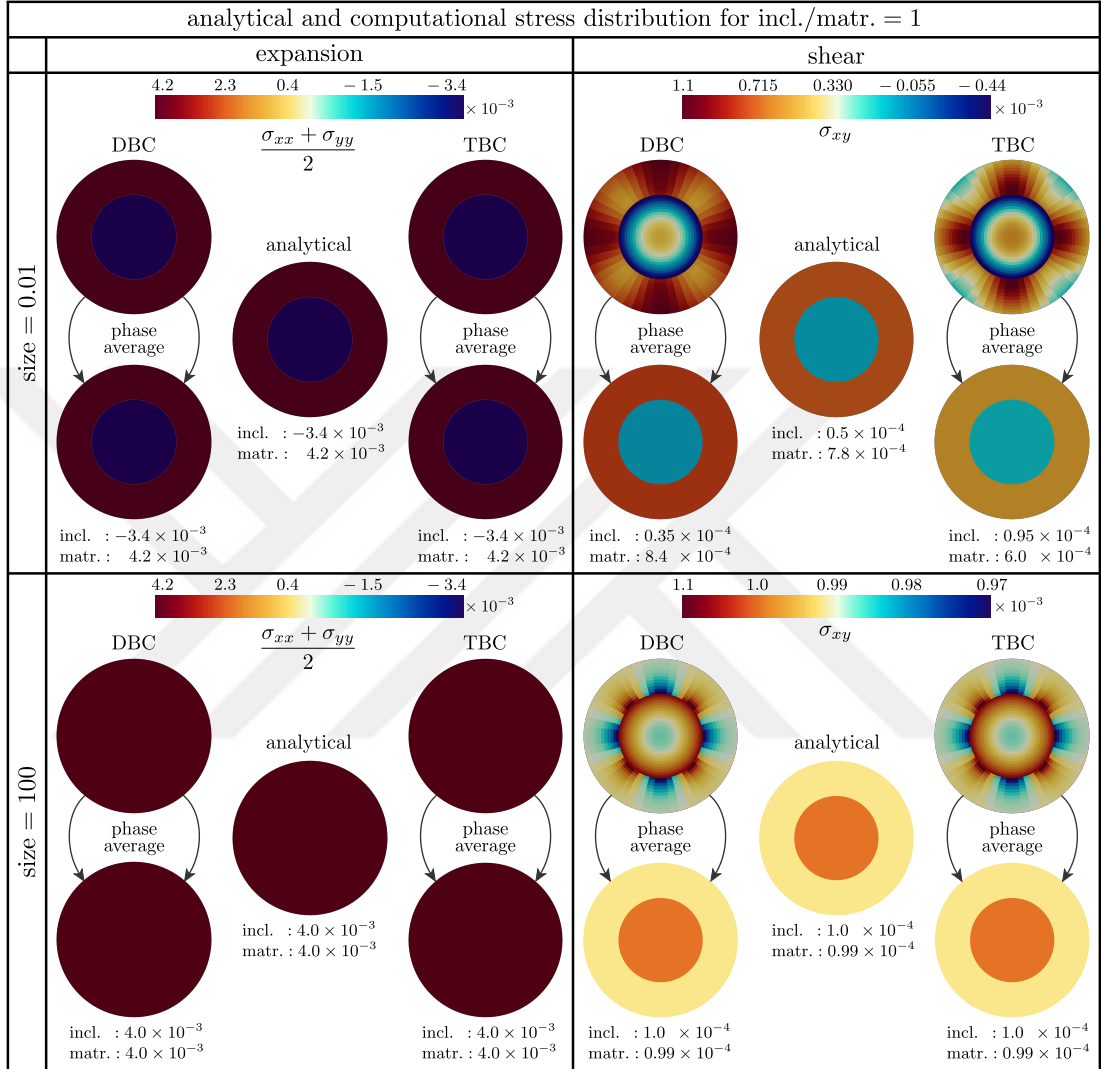


Figure 3.20: Comparison of 2D analytical and numerical stress distributions for incl./matr. = 1.

case, the analytical stress field is exact and the stress distribution completely resembles the computational and average computational stresses. However, for the shear case various conclusions can be drawn. For incl./matr. = 0.1, the average stresses due to DBC overestimate the analytical stresses both in the matrix and particle. On the other hand, the average stresses due to TBC underestimate the analytical stresses both in the matrix and particle. When incl./matr. = 1, for size = 0.01, the computational average stresses due to DBC and TBC, overestimate and

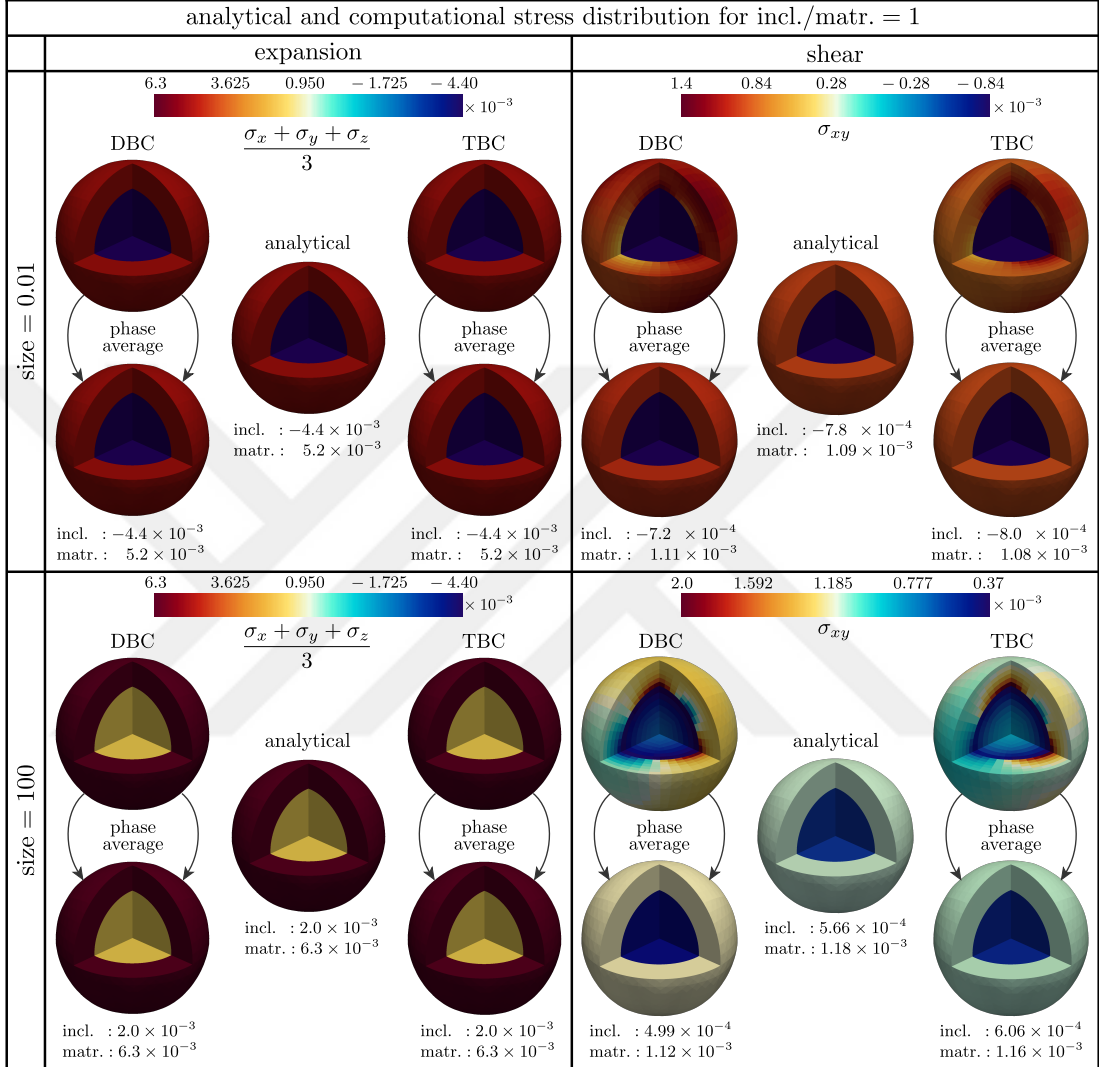


Figure 3.21: Comparison of 3D analytical and numerical stress distributions for incl./matr. = 1.

underestimate the analytical stresses in both phases for both fiber and particulate composites. When size = 100, the same observation is made for the average stress in the matrix. However, for particulate composites the average stress in the fiber due to TBC overestimate the analytical stress with DBC underestimating it. For the fiber composites, analytical and computational results render exact values the stress averages in both fiber and matrix. Finally for incl./matr. = 10, in fiber composites, the average stress in the fiber due to TBC overestimates that of analytical solution and DBC at size = 0.01 while the opposite story holds for

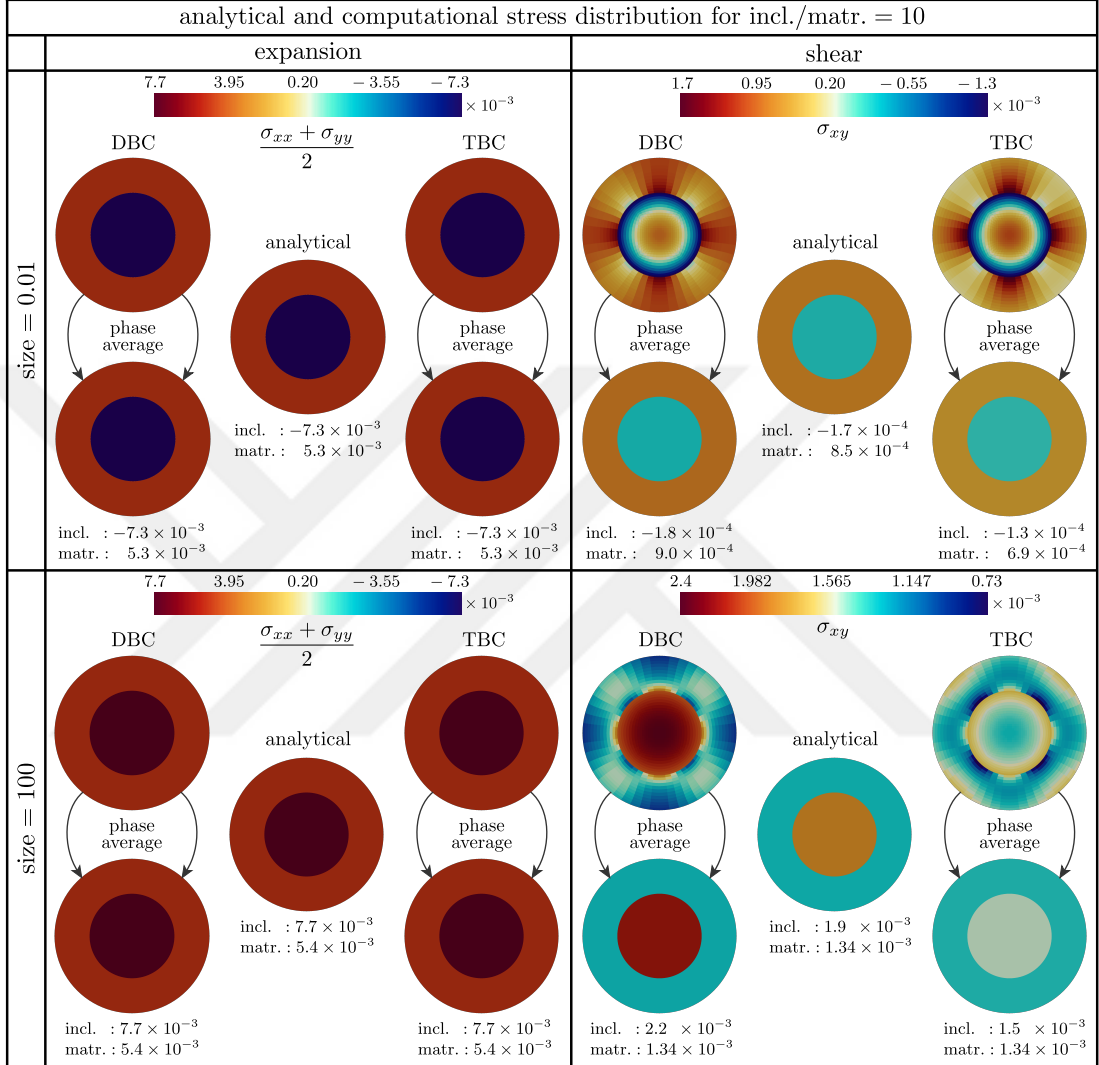


Figure 3.22: Comparison of 2D analytical and numerical stress distributions for incl./matr. = 10.

the stress in the matrix. On the other hand, for size = 100, the average stress in the matrix is identical for all solutions whereas the average stress in the fiber due to DBC and TBC, overestimate and underestimate the analytical stress, respectively. For particulate composites when incl./matr. = 10, the computational average stresses similarly overestimate and underestimate the analytical stresses when size = 0.01. DBC results in the least average stress in the matrix whereas TBC yields the highest value when size = 100. In order to have a better insight towards the analytical and computational stresses, the overall average stress in

the matrix and inclusion for each case shall be calculated and compared to the overall moduli.

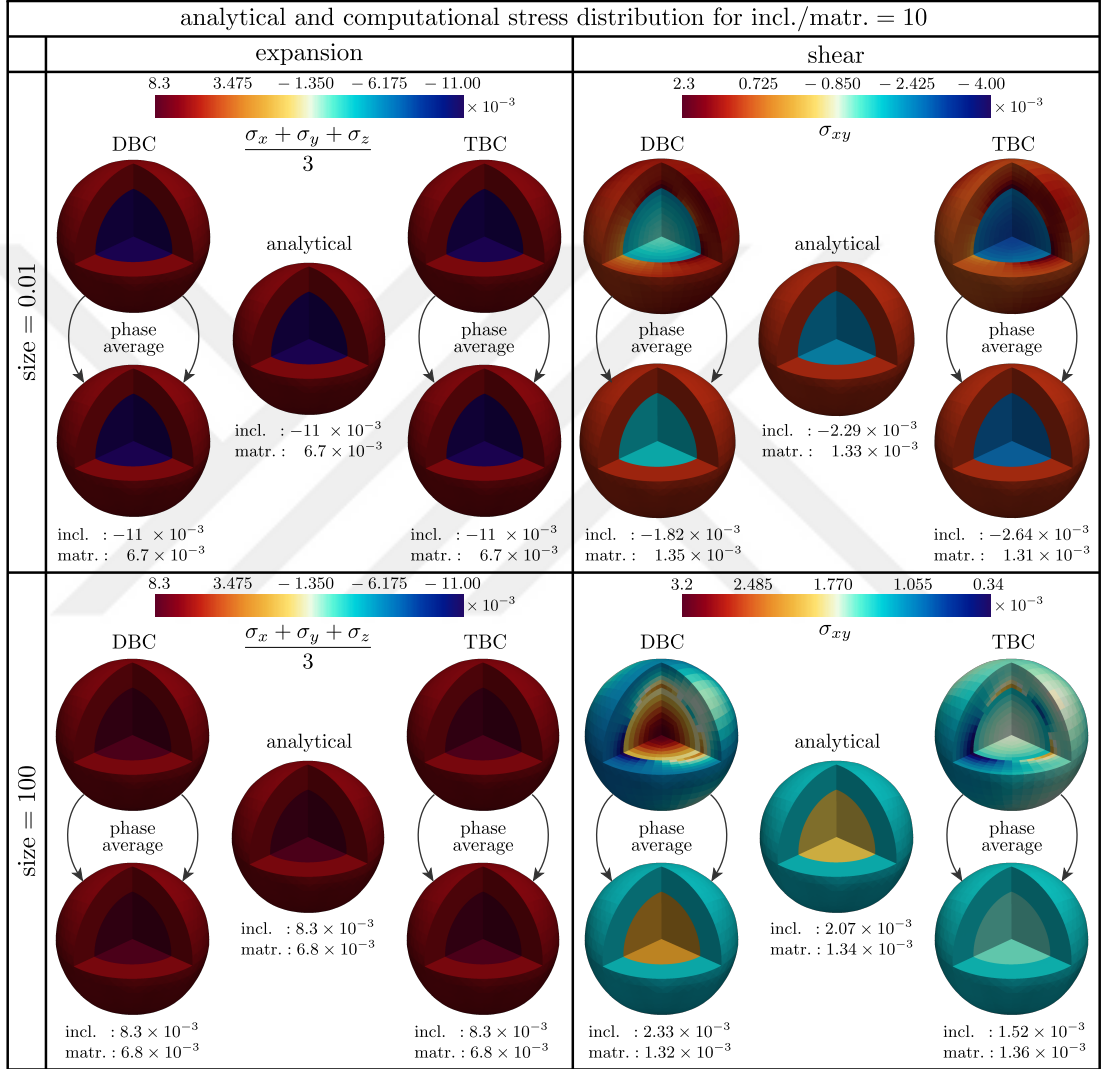


Figure 3.23: Comparison of 3D analytical and numerical stress distributions for incl./matr. = 10.

Chapter 4

Conclusion

A comprehensive study on homogenization was carried out and the effects of RVE type and boundary conditions on the overall response of fiber composites were investigated. Analytical estimates and computational results in homogenization were compared thoroughly and it was found that Hashin–Shtirkman bounds on shear modulus can be violated. Via extending the homogenization scheme to account for interfaces, we established a new framework to determine the overall properties of composites embedding general interfaces. Two new analytical approaches to determine the overall behavior of fiber- and particle-reinforced composites were developed. First, an interface-enhanced composite cylinder assemblage (CCA) approach, composite cylinder assemblage (CSA) approach and generalized self-consistent method (GSCM) were developed resulting in new estimates and bounds for the effective properties of composites. Explicit formulations for the overall bulk modulus and semi-explicit formulations for estimate and bounds on the overall shear modulus of particulate and fiber composites were presented for the first time. Second, we modified the Mori–Tanaka approach to incorporate general interfaces. This approach not only provides estimates for the overall properties, but also it determines the interaction tensors in the medium. Therefore, the state of stress and strain in each phase of the composite including the interface can be determined. This provides a significant insight into the computational design of composites accounting for generalized interfaces and size

effects. Our proposed analytical estimates are in excellent agreement with computational results using the finite element method. Our methodology can readily recover any of cohesive, elastic or perfect interface models. The responses due to the general interface model were bounded between the cohesive and elastic interface models. All of the observations demonstrate that the overall material response in presence of the general interface is complex and in principle not intuitive.

The work presented here could be extended in various possible ways. A first immediate extension of this work could be conducting the same study for thermal or electrical problems. Interface inelasticity and the effects of interface curvature has not been taken into account in this study. Another extension would be to study interface-enhanced homogenization in mechanical problems at finite deformation regime so as to capture the non-linear effects. One can also perform homogenization where the gradient of the strain is taken into account and distinguish between the size effects due to interfaces and those caused by the strain gradient.

Bibliography

- [1] J. Q. Broughton, F. F. Abraham, N. Bernstein, and E. Kaxiras, “Concurrent coupling of length scales: Methodology and application,” *Physical Review B*, vol. 60, pp. 2391–2403, 1999.
- [2] J. T. Oden, K. Vemaganti, and N. Moës, “Hierarchical modeling of heterogeneous solids,” *Computer Methods in Applied Mechanics and Engineering*, vol. 172, pp. 3–25, 1999.
- [3] S. Ghosh, J. Bai, and P. Raghavan, “Concurrent multi-level model for damage evolution in microstructurally debonding composites,” *Mechanics of Materials*, vol. 39, pp. 241–266, 2007.
- [4] A. R. Khoei, F. Jahanbakhshi, and A. Aramoon, “A concurrent multi-scale technique in modeling heterogeneous FCC nano-crystalline structures,” *Mechanics of Materials*, vol. 83, pp. 40–65, 2015.
- [5] R. Hill, “Elastic properties of reinforced solids: Some theoretical principles,” *Journal of the Mechanics and Physics of Solids*, vol. 11, pp. 357–372, 1963.
- [6] R. Hill, “On Constitutive Macro-Variables for Heterogeneous Solids at Finite Strain,” *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, vol. 326, pp. 131–147, 1972.
- [7] R. W. Ogden, “On the overall moduli of non-linear elastic composite materials,” *Journal of the Mechanics and Physics of Solids*, vol. 22, pp. 541–553, 1974.

- [8] J. Mandel, “Contribution theorique a l’etude de l’ecrouissage et des lois de l’ecoulement plastique,” in *Applied Mechanics*, pp. 502–509, Springer, 1966.
- [9] W. Voigt, “Ueber die Beziehung zwischen den beiden Elasticitätsconstanten isotroper Körper,” *Annalen der physik*, vol. 274, pp. 573–578, 1889.
- [10] V. A. Reuss, “Berechnung der Fliehgrenze von Mischkristallen auf Grund der Plastizitätsbedingung für Einkristalle,” *Z. Angew. Math. Mech*, vol. 9, pp. 49–58, 1929.
- [11] J. D. Eshelby, “The Determination of the Elastic Field of an Ellipsoidal Inclusion, and Related Problems,” *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, vol. 241, pp. 376–396, 1957.
- [12] Z. Hashin, “The Elastic Moduli of Heterogeneous Materials,” *Journal of Applied Mechanics*, vol. 29, pp. 143–150, 1962.
- [13] Z. Hashin and S. Shtrikman, “A variational approach to the theory of the elastic behaviour of polycrystals,” *Journal of the Mechanics and Physics of Solids*, vol. 10, pp. 343–352, 1962.
- [14] Z. Hashin and S. Shtrikman, “On some variational principles in anisotropic and nonhomogeneous elasticity,” *Journal of the Mechanics and Physics of Solids*, vol. 10, pp. 335–342, 1962.
- [15] Z. Hashin and B. W. Rosen, “The Elastic Moduli of Fiber-Reinforced Materials,” *Journal of Applied Mechanics*, vol. 31, pp. 223–232, 1964.
- [16] R. Hill, “Theory of mechanical properties of fibre-strengthened materials: I. Elastic behaviour,” *Journal of the Mechanics and Physics of Solids*, vol. 12, pp. 199–212, 1964.
- [17] R. Hill, “A self-consistent mechanics of composite materials,” *Journal of the Mechanics and Physics of Solids*, vol. 13, pp. 213–222, 1965.
- [18] L. J. Walpole, “On the overall elastic moduli of composite materials,” *Journal of the Mechanics and Physics of Solids*, vol. 17, pp. 235–251, 1969.

- [19] T. Mori and K. Tanaka, “Average stress in matrix and average elastic energy of materials with misfitting inclusions,” *Acta Metallurgica*, vol. 21, pp. 571–574, 1973.
- [20] J. R. Willis, “Bounds and self-consistent estimates for the overall properties of anisotropic composites,” *Journal of the Mechanics and Physics of Solids*, vol. 25, pp. 185–202, 1977.
- [21] S. Nemat-Nasser and T. Iwakuma, “Elastic-plastic composites at finite strains,” *International Journal of Solids and Structures*, vol. 21, pp. 55–65, 1985.
- [22] J. R. Willis, “On methods for bounding the overall properties of nonlinear composites,” *Journal of the Mechanics and Physics of Solids*, vol. 39, pp. 73–86, 1991.
- [23] P. Ponte Castañeda, “The effective mechanical properties of nonlinear isotropic composites,” *Journal of the Mechanics and Physics of Solids*, vol. 39, pp. 45–71, 1991.
- [24] S. Torquato, “Random Heterogeneous Media: Microstructure and Improved Bounds on Effective Properties,” *Applied Mechanics Reviews*, vol. 44, pp. 37–76, 1991.
- [25] P. Ponte Castañeda, G. DeBotton, and G. Li, “Effective properties of nonlinear inhomogeneous dielectrics,” *Physical Review B*, vol. 46, pp. 4387–4394, 1992.
- [26] S. Nemat-Nasser, N. Yu, and M. Hori, “Bounds and estimates of overall moduli of composites with periodic microstructure,” *Mechanics of Materials*, vol. 15, pp. 163–181, 1993.
- [27] B. Balendran and S. Nemat-Nasser, “Bounds on Elastic Moduli of Composites,” *Journal of the Mechanics and Physics of Solids*, vol. 43, pp. 1825–1853, 1995.

- [28] D. M. Kochmann and G. W. Milton, “Rigorous bounds on the effective moduli of composites and inhomogeneous bodies with negative-stiffness phases,” *Journal of the Mechanics and Physics of Solids*, vol. 71, pp. 46–63, 2014.
- [29] L. C. Brinson and W. S. Lin, “Comparison of micromechanics methods for effective properties of multiphase viscoelastic composites,” *Composite Structures*, vol. 41, pp. 353–367, 1998.
- [30] K. Terada and N. Kikuchi, “A class of general algorithms for multi-scale analyses of heterogeneous media,” *Computer Methods in Applied Mechanics and Engineering*, vol. 190, pp. 5427–5464, 2001.
- [31] T. I. Zohdi and P. Wriggers, “Archives of Computational Methods in Engineering Computational Micro-macro Material Testing,” *Archives of Computational Methods in Engineering*, vol. 8, pp. 131–228, 2001.
- [32] C. Miehe, “Strain-driven homogenization of inelastic microstructures and composites based on an incremental variational formulation,” *International Journal for Numerical Methods in Engineering*, vol. 55, pp. 1285–1322, 2002.
- [33] F. Feyel, “A multilevel finite element method (FE²) to describe the response of highly non-linear structures using generalized continua,” *Computer Methods in Applied Mechanics and Engineering*, vol. 192, pp. 3233–3244, 2003.
- [34] N. Moës, M. Cloirec, P. Cartraud, and J. F. Remacle, “A computational approach to handle complex microstructure geometries,” *Computer Methods in Applied Mechanics and Engineering*, vol. 192, pp. 3163–3177, 2003.
- [35] I. Özdemir, W. A. M. Brekelmans, and M. G. D. Geers, “Computational homogenization for heat conduction in heterogeneous solids,” *International Journal for Numerical Methods in Engineering*, vol. 73, pp. 185–204, 2008.
- [36] F. Fritzen and M. Leuschner, “Reduced basis hybrid computational homogenization based on a mixed incremental formulation,” *Computer Methods in Applied Mechanics and Engineering*, vol. 260, pp. 143–154, 2013.

- [37] A. Javili, G. Chatzigeorgiou, and P. Steinmann, “Computational homogenization in magneto-mechanics,” *International Journal of Solids and Structures*, vol. 50, pp. 4197–4216, 2013.
- [38] D. M. Kochmann and G. N. Venturini, “Homogenized mechanical properties of auxetic composite materials in finite-strain elasticity,” *Smart Materials and Structures*, vol. 22, p. 084004, 2013.
- [39] R. Biswas and L. H. Poh, “A micromorphic computational homogenization framework for heterogeneous materials,” *Journal of the Mechanics and Physics of Solids*, vol. 102, pp. 187–208, 2017.
- [40] F. Larsson, K. Runesson, and F. Su, “Variationally consistent computational homogenization of transient heat flow Fredrik,” *International Journal for Numerical Methods in Engineering*, vol. 81, pp. 1659–1686, 2010.
- [41] S. Göktepe and C. Miehe, “A micro-macro approach to rubber-like materials. Part III: The micro-sphere model of anisotropic Mullins-type damage,” *Journal of the Mechanics and Physics of Solids*, vol. 53, pp. 2259–2283, 2005.
- [42] C. Miehe and S. Göktepe, “A micro-macro approach to rubber-like materials. Part II: The micro-sphere model of finite rubber viscoelasticity,” *Journal of the Mechanics and Physics of Solids*, vol. 53, pp. 2231–2258, 2005.
- [43] C. Miehe, S. Göktepe, and F. Lulei, “A micro-macro approach to rubber-like materials - Part I: The non-affine micro-sphere model of rubber elasticity,” *Journal of the Mechanics and Physics of Solids*, vol. 52, pp. 2617–2660, 2004.
- [44] S. Saeb, P. Steinmann, and A. Javili, “Aspects of Computational Homogenization at Finite Deformations: A Unifying Review From Reuss’ to Voigt’s Bound,” *Applied Mechanics Reviews*, vol. 68, p. 050801, 2016.
- [45] M. G. D. Geers, V. G. Kouznetsova, and W. A. M. Brekelmans, “Multi-scale computational homogenization: Trends and challenges,” *Journal of Computational and Applied Mathematics*, vol. 234, pp. 2175–2182, 2010.

- [46] N. Charalambakis, “Homogenization Techniques and Micromechanics. A Survey and Perspectives,” *Applied Mechanics Reviews*, vol. 63, p. 030803, 2010.
- [47] M. J. Pindera, H. Khatam, A. S. Drago, and Y. Bansal, “Micromechanics of spatially uniform heterogeneous media: A critical review and emerging approaches,” *Composites Part B: Engineering*, vol. 40, pp. 349–378, 2009.
- [48] P. Suquet, “Local and global aspects in the mathematical theory of plasticity,” *Plasticity today*, pp. 279–309, 1985.
- [49] O. Pierard, C. Friebel, and I. Doghri, “Mean-field homogenization of multi-phase thermo-elastic composites: A general framework and its validation,” *Composites Science and Technology*, vol. 64, pp. 1587–1603, 2004.
- [50] S. Firooz, S. Saeb, G. Chatzigeorgiou, F. Meraghni, P. Steinmann, and A. Javili, “Systematic study of homogenization and the utility of circular simplified representative volume element,” *Mathematics and Mechanics of Solids*, 2019.
- [51] K. Terada, M. Hori, T. Kyoya, and N. Kikuchi, “Simulation of the multi-scale convergence in computational homogenization approaches,” *International Journal of Solids and Structures*, vol. 37, pp. 2285–2311, 2000.
- [52] X. Yuan and Y. Tomita, “Effective properties of cosserat composites with periodic microstructure,” *Mechanics Research Communications*, vol. 28, pp. 265–270, 2001.
- [53] M. Jiang, K. Alzebdeh, I. Jasiuk, and M. Ostoja-Starzewski, “Scale and boundary conditions effects in elastic properties of random composites,” *Acta Mechanica*, vol. 148, pp. 63–78, 2001.
- [54] M. Ostoja-Starzewski, “Material spatial randomness: From statistical to representative volume element,” *Probabilistic Engineering Mechanics*, vol. 21, pp. 112–132, 2006.

- [55] A. Drago and M. J. Pindera, “Micro-macromechanical analysis of heterogeneous materials: Macroscopically homogeneous vs periodic microstructures,” *Composites Science and Technology*, vol. 67, pp. 1243–1263, 2007.
- [56] S. Saroukhani, R. Vafadari, R. Andersson, F. Larsson, and K. Runesson, “On statistical strain and stress energy bounds from homogenization and virtual testing,” *European Journal of Mechanics, A/Solids*, vol. 51, pp. 77–95, 2015.
- [57] V. D. Nguyen, L. Wu, and L. Noels, “Unified treatment of microscopic boundary conditions and efficient algorithms for estimating tangent operators of the homogenized behavior in the computational homogenization method,” *Computational Mechanics*, vol. 59, pp. 483–505, 2017.
- [58] N. Daher and G. A. Maugin, “The method of virtual power in continuum mechanics application to media presenting singular surfaces and interfaces,” *Acta Mechanica*, vol. 60, pp. 217–240, 1986.
- [59] E. Sanchez-Palencia, “Comportement limite d’un probleme de transmission travers une plaque faiblement conductrice,” *Comptes Rendus Mathematique Academie des Sciences*, vol. 270, pp. 1026–1028, 1970.
- [60] H. P. Huy and E. Sanchez-Palencia, “Phénomènes de transmission à travers des couches minces de conductivité élevée,” *Journal of Mathematical Analysis and Applications*, vol. 47, pp. 284–309, 1974.
- [61] S. Brisard, L. Dormieux, and D. Kondo, “Hashin-Shtrikman bounds on the shear modulus of a nanocomposite with spherical inclusions and interface effects,” *Computational Materials Science*, vol. 50, pp. 403–410, 2010.
- [62] G. Chatzigeorgiou, A. Javili, and P. Steinmann, “Multiscale modelling for composites with energetic interfaces at the micro- or nanoscale,” *Mathematics and Mechanics of Solids*, vol. 20, pp. 1130–1145, 2015.
- [63] H. L. Duan, X. Yi, Z. P. Huang, and J. Wang, “A unified scheme for prediction of effective moduli of multiphase composites with interface effects. Part I: Theoretical framework,” *Mechanics of Materials*, vol. 39, pp. 81–93, 2007.

- [64] H. L. Duan, J. Wang, Z. P. Huang, and B. L. Karimhaloo, “Eshelby formalism for nano-inhomogeneities,” *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, vol. 461, pp. 3335–3353, 2005.
- [65] S. G. Mogilevskaya, S. L. Crouch, and H. K. Stolarski, “Multiple interacting circular nano-inhomogeneities with surface/interface effects,” *Journal of the Mechanics and Physics of Solids*, vol. 56, pp. 2298–2327, 2008.
- [66] L. Nazarenko, S. Bargmann, and H. Stolarski, “Closed-form formulas for the effective properties of random particulate nanocomposites with complete Gurtin–Murdoch model of material surfaces,” *Continuum Mechanics and Thermodynamics*, vol. 29, pp. 77–96, 2017.
- [67] P. Sharma and S. Ganti, “Size-Dependent Eshelby’s Tensor for Embedded Nano-Inclusions Incorporating Surface/Interface Energies,” *Journal of Applied Mechanics*, vol. 71, pp. 663–671, 2004.
- [68] P. Sharma and L. T. Wheeler, “Size-Dependent Elastic State of Ellipsoidal Nano-Inclusions Incorporating Surface/Interface Tension,” *Journal of Applied Mechanics*, vol. 74, pp. 447–454, 2007.
- [69] L. Tian and R. K. N. D. Rajapakse, “Analytical Solution for Size-Dependent Elastic Field of a Nanoscale Circular Inhomogeneity,” *Journal of Applied Mechanics*, vol. 74, pp. 568–574, 2007.
- [70] F. Fritzen and M. Leuschner, “Nonlinear reduced order homogenization of materials including cohesive interfaces,” *Computational Mechanics*, vol. 56, pp. 131–151, 2015.
- [71] A. Javili, F. Dell’Isola, and P. Steinmann, “Geometrically nonlinear higher-gradient elasticity with energetic boundaries,” *Journal of the Mechanics and Physics of Solids*, vol. 61, pp. 2381–2401, 2013.
- [72] E. Monteiro, Q. C. He, and J. Yvonnet, “Hyperelastic large deformations of two-phase composites with membrane-type interface,” *International Journal of Engineering Science*, vol. 49, pp. 985–1000, 2011.

- [73] J. Yvonnet, H. Le Quang, and Q. C. He, “An XFEM/level set approach to modelling surface/interface effects and to computing the size-dependent effective properties of nanocomposites,” *Computational Mechanics*, vol. 42, pp. 119–131, 2008.
- [74] D. Davydov, A. Javili, and P. Steinmann, “On molecular statics and surface-enhanced continuum modeling of nano-structures,” *Computational Materials Science*, vol. 69, pp. 510–519, 2013.
- [75] B. A. M. Elsner, S. Müller, S. Bargmann, and J. Weissmüller, “Surface excess elasticity of gold: Ab initio coefficients and impact on the effective elastic response of nanowires,” *Acta Materialia*, vol. 124, pp. 468–477, 2017.
- [76] J. He and C. M. Lilley, “Surface effect on the elastic behavior of static bending nanowires,” *Nano Letters*, vol. 8, pp. 1798–1802, 2008.
- [77] V. I. Levitas and K. Samani, “Size and mechanics effects in surface-induced melting of nanoparticles,” *Nature Communications*, vol. 2, pp. 284–286, 2011.
- [78] P. A. T. Olsson and H. S. Park, “On the importance of surface elastic contributions to the flexural rigidity of nanowires,” *Journal of the Mechanics and Physics of Solids*, vol. 60, pp. 2064–2083, 2012.
- [79] H. S. Park and P. A. Klein, “Surface stress effects on the resonant properties of metal nanowires: The importance of finite deformation kinematics and the impact of the residual surface stress,” *Journal of the Mechanics and Physics of Solids*, vol. 56, pp. 3144–3166, 2008.
- [80] M. E. Gurtin and A. I. Murdoch, “A continuum theory of elastic material surfaces,” *Archive for Rational Mechanics and Analysis*, vol. 57, pp. 291–323, 1975.
- [81] M. E. Gurtin and A. I. Murdoch, “Surface stress in solids,” *International Journal of Solids and Structures*, vol. 14, pp. 431–440, 1978.

- [82] A. I. Murdoch, “A thermodynamical theory of elastic material interfaces,” *Quarterly Journal of Mechanics and Applied Mathematics*, vol. 29, pp. 245–275, 1976.
- [83] D. J. Steigmann and R. W. Ogden, “Plane deformations of elastic solids with intrinsic boundary elasticity,” *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, vol. 453, pp. 853–877, 1997.
- [84] Z. Han, S. G. Mogilevskaya, and D. Schillinger, “Local fields and overall transverse properties of unidirectional composite materials with multiple nanofibers and Steigmann–Ogden interfaces,” *International Journal of Solids and Structures*, vol. 147, pp. 166–182, 2018.
- [85] Y. Benveniste and T. Miloh, “Imperfect soft and stiff interfaces in two-dimensional elasticity,” *Mechanics of Materials*, vol. 33, pp. 309–323, 2001.
- [86] P. Sharma, S. Ganti, and N. Bhate, “Effect of surfaces on the size-dependent elastic state of nano-inhomogeneities,” *Applied Physics Letters*, vol. 82, pp. 535–537, 2003.
- [87] P. Sharma, “Size-dependent elastic fields of embedded inclusions in isotropic chiral solids,” *International Journal of Solids and Structures*, vol. 41, pp. 6317–6333, 2004.
- [88] H. L. Duan, J. Wang, Z. P. Huang, and B. L. Karihaloo, “Size-dependent effective elastic constants of solids containing nano-inhomogeneities with interface stress,” *Journal of the Mechanics and Physics of Solids*, vol. 53, pp. 1574–1596, 2005.
- [89] L. H. He, “Self-strain of solids with spherical nanovoids,” *Applied Physics Letters*, vol. 88, pp. 12–15, 2006.
- [90] Z. P. Huang and L. Sun, “Size-dependent effective properties of a heterogeneous material with interface energy effect: From finite deformation theory to infinitesimal strain analysis,” *Acta Mechanica*, vol. 190, pp. 151–163, 2007.

- [91] H. Le Quang and Q. C. He, “Variational principles and bounds for elastic inhomogeneous materials with coherent imperfect interfaces,” *Mechanics of Materials*, vol. 40, pp. 865–884, 2008.
- [92] S. G. Mogilevskaya, S. L. Crouch, A. La Grotta, and H. K. Stolarski, “The effects of surface elasticity and surface tension on the transverse overall elastic behavior of unidirectional nano-composites,” *Composites Science and Technology*, vol. 70, pp. 427–434, 2010.
- [93] V. I. Kushch, S. G. Mogilevskaya, H. K. Stolarski, and S. L. Crouch, “Elastic interaction of spherical nanoinhomogeneities with GurtinMurdoch type interfaces,” *Journal of the Mechanics and Physics of Solids*, vol. 59, pp. 1702–1716, 2011.
- [94] M. Dai, P. Schiavone, and C. F. Gao, “Prediction of the Stress Field and Effective Shear Modulus of Composites Containing Periodic Inclusions Incorporating Interface Effects in Anti-plane Shear,” *Journal of Elasticity*, vol. 125, pp. 217–230, 2016.
- [95] X. Gao, Z. Huang, and D. Fang, “Curvature-dependent interfacial energy and its effects on the elastic properties of nanomaterials,” *International Journal of Solids and Structures*, vol. 113-114, pp. 100–107, 2017.
- [96] D. S. Dudgale, “Yielding of steel sheets containing slits,” *Journal of the Mechanics and Physics of Solids*, vol. 8, pp. 100–104, 1960.
- [97] G. I. Barenblatt, “The mathematical theory of equilibrium cracks in brittle materials.,” in *Advances in Applied Mechanics*, vol. 7, pp. 55–129, 1962.
- [98] A. Needleman, “A Continuum Model for Void Nucleation by Inclusion Debonding,” *Journal of Applied Mechanics*, vol. 54, pp. 525–531, 1987.
- [99] A. Javili, “A note on traction continuity across an interface in a geometrically non-linear framework,” *Mathematics and Mechanics of Solids*.
- [100] Y. Benveniste, “The effective mechanical behaviour of composite materials with imperfect contact between the constituents,” *Mechanics of Materials*, vol. 4, pp. 197–208, 1985.

- [101] J. D. Achenbach and H. Zhu, “Effect of interfacial zone on mechanical behavior and failure of fiber-reinforced composites,” *Journal of the Mechanics and Physics of Solids*, vol. 37, pp. 381–393, 1989.
- [102] Z. Hashin, “Thermoelastic properties of particulate composites with imperfect interface,” *Journal of the Mechanics and Physics of Solids*, vol. 39, pp. 745–762, 1991.
- [103] Z. Hashin, “Thermoelastic properties of fiber composites with imperfect interface,” *Mechanics of Materials*, vol. 8, pp. 333–348, 1990.
- [104] R. Lipton and B. Vernescu, “Variational methods, size effects and extremal microgeometries for elastic composites with imperfect interface,” *Mathematical Models and Methods in Applied Science*, vol. 5, pp. 1139–1173, 1995.
- [105] H. Fan and G. F. Wang, “Screw dislocation interacting with imperfect interface,” *Mechanics of Materials*, vol. 35, pp. 943–953, 2003.
- [106] H. L. Duan, J. Wang, Z. P. Huang, and Z. Y. Luo, “Stress concentration tensors of inhomogeneities with interface effects,” *Mechanics of Materials*, vol. 37, pp. 723–736, 2005.
- [107] H. Tan, Y. Huang, C. Liu, and P. H. Geubelle, “The Mori-Tanaka method for composite materials with nonlinear interface debonding,” *International Journal of Plasticity*, vol. 21, pp. 1890–1918, 2005.
- [108] H. L. Duan, X. Yi, Z. P. Huang, and J. Wang, “A unified scheme for prediction of effective moduli of multiphase composites with interface effects: Part II-Application and scaling laws,” *Mechanics of Materials*, vol. 39, pp. 94–103, 2007.
- [109] Q. Zhu, S. Gu, J. Yvonnet, J. Shao, and Q. He, “Three-dimensional numerical modelling by XFEM of spring-layer imperfect curved interfaces with applications to linearly elastic composite materials,” *International Journal for Numerical Methods in Engineering*, vol. 88, pp. 307–328, 2011.

- [110] Z. Hashin, “Thin interphase/imperfect interface in elasticity with application to coated fiber composites,” *Journal of the Mechanics and Physics of Solids*, vol. 50, pp. 2509–2537, 2002.
- [111] Y. Benveniste, “Models of thin interphases and the effective medium approximation in composite media with curvilinearly anisotropic coated inclusions,” *International Journal of Engineering Science*, vol. 72, pp. 140–154, 2013.
- [112] Y. Benveniste, “A general interface model for a three-dimensional curved thin anisotropic interphase between two anisotropic media,” *Journal of the Mechanics and Physics of Solids*, vol. 54, pp. 708–734, 2006.
- [113] P. Bövik, “On the modelling of thin interface layers in elastic and acoustic scattering problems,” *The Quarterly Journal of Mechanics and Applied Mathematics*, vol. 47, pp. 17–42, 1994.
- [114] J. Wang, H. L. Duan, Z. Zhang, and Z. P. Huang, “An anti-interpenetration model and connections between interphase and interface models in particle-reinforced composites,” *International Journal of Mechanical Sciences*, vol. 47, pp. 701–718, 2005.
- [115] Y. Koutsawa, A. Karatrantos, W. Yu, and D. Ruch, “A micromechanics approach for the effective thermal conductivity of composite materials with general linear imperfect interfaces,” *Composite Structures*, vol. 200, pp. 747–756, 2018.
- [116] S. T. Gu and Q. C. He, “Interfacial discontinuity relations for coupled multifield phenomena and their application to the modeling of thin interphases as imperfect interfaces,” *Journal of the Mechanics and Physics of Solids*, vol. 59, pp. 1413–1426, 2011.
- [117] S. T. Gu, J. T. Liu, and Q. C. He, “Size-dependent effective elastic moduli of particulate composites with interfacial displacement and traction discontinuities,” *International Journal of Solids and Structures*, vol. 51, pp. 2283–2296, 2014.

- [118] G. Chatzigeorgiou, F. Meraghni, and A. Javili, “Generalized interfacial energy and size effects in composites,” *Journal of the Mechanics and Physics of Solids*, vol. 106, pp. 257–282, 2017.
- [119] S. Firooz and A. Javili, “Understanding the role of general interfaces in the overall behavior of composites and size effects,” *Computational Materials Science*, vol. 162, pp. 245–254, 2019.
- [120] S. Firooz, G. Chatzigeorgiou, F. Meraghni, and A. Javili, “Bounds on size effects in composites via homogenization accounting for general interfaces,” *Continuum Mechanics and Thermodynamics*, 2019.
- [121] S. Firooz, G. Chatzigeorgiou, F. Meraghni, and A. Javili, “Analytical homogenization schemes accounting for size effects in particulate composites due to general interfaces,” *Mechanics of Materials (in review)*, 2019.
- [122] F. Dell’Isola and A. Romano, “On the derivation of thermomechanical balance equations for continuous systems with a nonmaterial interface,” *International Journal of Engineering Science*, vol. 25, pp. 1459–1468, 1987.
- [123] E. Fried and M. E. Gurtin, “Thermomechanics of the interface between a body and its environment,” *Continuum Mechanics and Thermodynamics*, vol. 19, pp. 253–271, 2007.
- [124] A. Javili, A. McBride, and P. Steinmann, “Thermomechanics of Solids With Lower-Dimensional Energetics: On the Importance of Surface, Interface, and Curve Structures at the Nanoscale. A Unifying Review,” *Applied Mechanics Reviews*, vol. 65, p. 010802, 2013.
- [125] I. M. Gitman, H. Askes, and E. C. Aifantis, “The representative volume size in static and dynamic micro-macro transitions,” *International Journal of Fracture*, vol. 135, pp. 3–9, 2005.
- [126] Z. F. Khisaeva and M. Ostoja-Starzewski, “On the size of RVE in finite elasticity of random composites,” *Journal of Elasticity*, vol. 85, pp. 153–173, 2006.

- [127] I. Temizer, T. Wu, and P. Wriggers, “On the optimality of the window method in computational homogenization,” *International Journal of Engineering Science*, vol. 64, pp. 66–73, 2013.
- [128] M. Thomas, N. Boyard, L. Perez, Y. Jarny, and D. Delaunay, “Representative volume element of anisotropic unidirectional carbon-epoxy composite with high-fibre volume fraction,” *Composites Science and Technology*, vol. 68, pp. 3184–3192, 2008.
- [129] I. Temizer and T. I. Zohdi, “A numerical method for homogenization in non-linear elasticity,” *Computational Mechanics*, vol. 40, pp. 281–298, 2007.
- [130] F. Larsson, K. Runesson, S. Saroukhani, and R. Vafadari, “Computational homogenization based on a weak format of micro-periodicity for RVE-problems,” *Computer Methods in Applied Mechanics and Engineering*, vol. 200, pp. 11–26, 2011.
- [131] A. Javili, P. Steinmann, and J. Mosler, “Micro-to-macro transition accounting for general imperfect interfaces,” *Computer Methods in Applied Mechanics and Engineering*, vol. 317, pp. 274–317, 2017.
- [132] Z. Hashin, “On Elastic Materials Behaviour of Arbitrary of Fibre Reinforced Phase Transverse Geometry,” *Journal of the Mechanics and Physics of Solids*, vol. 13, pp. 119–134, 1965.
- [133] Z. Hashin and S. Shtrikman, “A variational approach to the theory of the elastic behaviour of multiphase materials,” *Journal of the Mechanics and Physics of Solids*, vol. 11, pp. 127–140, 1963.
- [134] R. M. Christensen and K. H. Lo, “Solutions for effective shear properties in three phase sphere and cylinder models,” *Journal of the Mechanics and Physics of Solids*, vol. 27, pp. 315–330, 1979.
- [135] L. J. Walpole, “On bounds for the overall elastic moduli of inhomogeneous systmes-I,” *Journal of the Mechanics and Physics of Solids*, vol. 14, pp. 151–162, 1966.

- [136] G. J. Weng, “Explicit evaluation of Willis’ bounds with ellipsoidal inclusions,” *International Journal of Engineering Science*, vol. 30, pp. 83–92, 1992.
- [137] D. Savvas, G. Stefanou, M. Papadrakakis, and G. Deodatis, “Homogenization of random heterogeneous media with inclusions of arbitrary shape modeled by XFEM,” *Computational Mechanics*, vol. 54, pp. 1221–1235, 2014.
- [138] S. Ghosh, K. Lee, and S. Moorthy, “Multiple scale analysis of heterogeneous elastic structures using homogenization theory and voronoi cell finite element method,” *International Journal of Solids and Structures*, vol. 32, pp. 27–62, 1995.
- [139] Z. Hashin, “Analysis of composite materials—a survey,” *Journal of Applied Mechanics*, vol. 50, pp. 481–505, 1983.
- [140] A. Javili, “Variational formulation of generalized interfaces for finite deformation elasticity,” *Mathematics and Mechanics of Solids*, vol. 23, pp. 1303–1322, 2018.
- [141] A. Javili, P. Steinmann, and J. Mosler, “Micro-to-macro transition accounting for general imperfect interfaces,” *Computer Methods in Applied Mechanics and Engineering*, vol. 317, pp. 274–317, 2017.
- [142] A. Javili, S. Kaessmair, and P. Steinmann, “General imperfect interfaces,” *Computer Methods in Applied Mechanics and Engineering*, vol. 275, pp. 76–97, 2014.
- [143] P. Kanouté, D. P. Boso, J. L. Chaboche, and B. A. Schrefler, “Multiscale methods for composites: A review,” *Archives of Computational Methods in Engineering*, vol. 16, pp. 31–75, 2009.
- [144] N. Charalambakis, G. Chatzigeorgiou, Y. Chemisky, and F. Meraghni, “Mathematical homogenization of inelastic dissipative materials: a survey and recent progress,” *Continuum Mechanics and Thermodynamics*, vol. 30, pp. 1–51, 2018.

- [145] K. Matous, M. G. D. Geers, V. G. Kouznetsova, and A. Gillman, “A review of predictive nonlinear theories for multiscale modeling of heterogeneous materials,” *Journal of Computational Physics*, vol. 330, pp. 192–220, 2017.
- [146] H. L. Duan and B. L. Karihaloo, “Effective thermal conductivities of heterogeneous media containing multiple imperfectly bonded inclusions,” *Physical Review B*, vol. 75, p. 064206, 2007.
- [147] Y. Benveniste, G. J. Dvorak, and T. Chen, “Stress fields in composites with coated inclusions,” *Mechanics of Materials*, vol. 7, pp. 305–317, 1989.
- [148] Z. Wang, R. J. Oelkers, K. C. Lee, and F. T. Fisher, “Annular Coated Inclusion model and applications for polymer nanocomposites – Part II: Cylindrical inclusions,” *Mechanics of Materials*, vol. 101, pp. 50–60, 2016.
- [149] Z. Wang, R. J. Oelkers, K. C. Lee, and F. T. Fisher, “Annular Coated Inclusion model and applications for polymer nanocomposites – Part I: Spherical inclusions,” *Mechanics of Materials*, vol. 101, pp. 170–184, 2016.
- [150] Y. Benveniste, G. J. Dvorak, and T. Chen, “On diagonal and elastic symmetry of the approximate effective stiffness tensor of heterogeneous media,” *Journal of the Mechanics and Physics of Solids*, vol. 39, no. 7, pp. 927–946, 1991.
- [151] Z. Hashin, “Thermoelastic properties of fiber composites with imperfect interface,” *Mechanics of Materials*, vol. 8, pp. 333–348, 1990.

Appendix A

Hill's lemma

The Hill's lemma reads

$$\langle \mathbf{P} : \delta^{\mathbf{M}} \mathbf{F} \rangle - {}^{\mathbf{M}}\mathbf{P} : \delta \mathbf{F} = \frac{1}{\mathcal{V}_0} \int_{\partial \mathcal{B}_0} [\delta \varphi - \delta^{\mathbf{M}} \mathbf{F} \cdot \mathbf{X}] \cdot [\mathbf{t}_0 - {}^{\mathbf{M}}\mathbf{P} \cdot \mathbf{N}] \, dA.$$

In order to prove this lemma, we begin the right-hand side of the above equation to obtain the left-hand side. the right-hand side integral can be written as

$$\int_{\partial \mathcal{B}_0} [\delta \varphi - \delta^{\mathbf{M}} \mathbf{F} \cdot \mathbf{X}] \cdot [\mathbf{t}_0 - {}^{\mathbf{M}}\mathbf{P} \cdot \mathbf{N}] \, dA = \int_{\partial \mathcal{B}_0} [\delta \varphi - \delta^{\mathbf{M}} \mathbf{F} \cdot \mathbf{X}] \cdot [\mathbf{P} \cdot \mathbf{N} - {}^{\mathbf{M}}\mathbf{P} \cdot \mathbf{N}] \, dA.$$

Multiplying the two brackets on the right-hand side yields

$$\begin{aligned} \text{RHS} &= \int_{\partial \mathcal{B}_0} \delta \varphi \cdot [\mathbf{P} \cdot \mathbf{N}] \, dA - \int_{\partial \mathcal{B}_0} \delta \varphi \cdot [{}^{\mathbf{M}}\mathbf{P} \cdot \mathbf{N}] \, dA \\ &\quad - \int_{\partial \mathcal{B}_0} [\delta^{\mathbf{M}} \mathbf{F} \cdot \mathbf{X}] \cdot \mathbf{P} \cdot \mathbf{N} \, dA + \int_{\partial \mathcal{B}_0} [\delta^{\mathbf{M}} \mathbf{F} \cdot \mathbf{X}] \cdot {}^{\mathbf{M}}\mathbf{P} \cdot \mathbf{N} \, dA \\ &= \int_{\partial \mathcal{B}_0} [\delta \varphi \cdot \mathbf{P}] \cdot \mathbf{N} \, dA - \int_{\partial \mathcal{B}_0} {}^{\mathbf{M}}\mathbf{P} : [\delta \varphi \otimes \mathbf{N}] \, dA \\ &\quad - \int_{\partial \mathcal{B}_0} \delta^{\mathbf{M}} \mathbf{F} : \left[[\mathbf{P} \cdot \mathbf{N}] \otimes \mathbf{X} \right] \, dA + \int_{\partial \mathcal{B}_0} [\delta^{\mathbf{M}} \mathbf{F} \cdot {}^{\mathbf{M}}\mathbf{P}] : [\mathbf{X} \otimes \mathbf{N}] \, dA. \end{aligned}$$

Taking the constant parts out of the integrals and applying the divergence theorem on the first integral results

$$\begin{aligned} \text{RHS} = & \int_{\mathcal{B}_0} \text{Div}(\delta\boldsymbol{\varphi} \cdot \mathbf{P}) \, dV - {}^{\text{M}}\mathbf{P} : \int_{\partial\mathcal{B}_0} \delta\boldsymbol{\varphi} \otimes \mathbf{N} \, dA \\ & - \delta^{\text{M}}\mathbf{F} : \int_{\partial\mathcal{B}_0} \left[[\mathbf{P} \cdot \mathbf{N}] \otimes \mathbf{X} \right] \, dA + \left[\delta^{\text{M}}\mathbf{F}^t \cdot {}^{\text{M}}\mathbf{P} \right] : \int_{\partial\mathcal{B}_0} \mathbf{X} \otimes \mathbf{N} \, dA. \end{aligned} \quad (\text{A.1})$$

Now each integral is treated individually. The first integral becomes

$$\text{Div}(\delta\boldsymbol{\varphi} \cdot \mathbf{P}) = \delta\boldsymbol{\varphi} \cdot \underbrace{\text{Div}\mathbf{P}}_0 + \mathbf{P} : \underbrace{\text{Grad}\delta\boldsymbol{\varphi}}_{\delta\mathbf{F}} = \mathbf{P} : \delta\mathbf{F}$$

Applying the gradient theorem on the second integral results in

$$\int_{\partial\mathcal{B}_0} \delta\boldsymbol{\varphi} \otimes \mathbf{N} \, dA = \int_{\mathcal{B}_0} \text{Grad}\delta\boldsymbol{\varphi} \, dV.$$

Using the average Piola theorem, the third integral simplifies to

$$\int_{\partial\mathcal{B}_0} \left[[\mathbf{P} \cdot \mathbf{N}] \otimes \mathbf{X} \right] \, dA = \mathcal{V}_0 \langle \mathbf{P} \rangle.$$

Finally, the last integral reduces to

$$\int_{\partial\mathcal{B}_0} \mathbf{X} \otimes \mathbf{N} \, dA = \mathcal{V}_0 \mathbf{I}.$$

Implementing all the above relations in Eq. (A.1) yields

$$\begin{aligned} \text{RHS} = & \int_{\mathcal{B}_0} \mathbf{P} : \delta\mathbf{F} \, dV - {}^{\text{M}}\mathbf{P} : \int_{\mathcal{B}_0} \text{Grad}\delta\boldsymbol{\varphi} \, dV - \delta^{\text{M}}\mathbf{F} : \langle \mathbf{P} \rangle + \left[\delta^{\text{M}}\mathbf{F}^t \cdot {}^{\text{M}}\mathbf{P} \right] : \left[\mathcal{V}_0 \mathbf{I} \right], \\ = & \mathcal{V}_0 \langle \mathbf{P} : \delta\mathbf{F} \rangle - \mathcal{V}_0 {}^{\text{M}}\mathbf{P} : \langle \delta\mathbf{F} \rangle - \mathcal{V}_0 \langle \mathbf{P} \rangle : \delta^{\text{M}}\mathbf{F} + \mathcal{V}_0 {}^{\text{M}}\mathbf{P} : \delta^{\text{M}}\mathbf{F}. \end{aligned}$$

Using the definitions of the average deformation gradient and average Piola stress we conclude

$$\begin{aligned} & = \mathcal{V}_0 \langle \mathbf{P} : \delta\mathbf{F} \rangle - \mathcal{V}_0 {}^{\text{M}}\mathbf{P} : \delta^{\text{M}}\mathbf{F} - \mathcal{V}_0 {}^{\text{M}}\mathbf{P} : \delta^{\text{M}}\mathbf{F} + \mathcal{V}_0 {}^{\text{M}}\mathbf{P} : \delta^{\text{M}}\mathbf{F} \\ & = \mathcal{V}_0 \langle \mathbf{P} : \delta\mathbf{F} \rangle - \mathcal{V}_0 {}^{\text{M}}\mathbf{P} : \delta^{\text{M}}\mathbf{F} = \mathcal{V}_0 \left[\langle \mathbf{P} : \delta\mathbf{F} \rangle - {}^{\text{M}}\mathbf{P} : \delta^{\text{M}}\mathbf{F} \right]. \end{aligned}$$

Appendix B

Material modeling

The main goal of the discussion here is to shed light on the material modeling of the bulk and interface for finite deformation elasticity and also, to elaborate on its linear counterpart for small strain elasticity. Since this contribution deals with fiber composites as well as particulate composites, both two-dimensional and three-dimensional settings are discussed. That is, the two-dimensional setting corresponds to the plane-strain condition associated with fiber composites.

B.1 Bulk

Following the Coleman–Noll procedure, the free energy densities ψ in the bulk for a hyperelastic material must be a function of only the deformation gradient or $\psi = \psi(\mathbf{F})$. From a physical perspective, it is of crucial importance that the energy density ψ satisfies the material frame-indifference in the sense that it remains invariant under rigid body translations and in particular rotations as

$$\psi(\mathbf{F}) = \psi(\mathbf{Q} \cdot \mathbf{F}) \quad \forall \mathbf{Q} \in \mathcal{SO}(3),$$

in which $\mathbf{Q}$ denotes an arbitrary proper orthogonal tensor. It can be shown that the energy density ψ is frame-indifferent if and only if the deformation gradient

$\mathbf{F}$ enters the energy through the right Cauchy–Green tensor $\mathbf{C}$ as

$$\psi = \psi(\mathbf{F}) \quad \xRightarrow{\text{material frame indifference}} \quad \psi = \psi(\mathbf{C}) \quad \text{with} \quad \mathbf{C} := \mathbf{F}^t \cdot \mathbf{F}.$$

Furthermore, Imposing isotropy on the material behavior requires the free energy density to be a function of the invariants of $\mathbf{C}$ as

$$\psi = \psi(\mathbf{C}) \quad \xRightarrow{\text{isotropy}} \quad \psi = \psi(I_1, I_2, I_3) \quad \text{with} \quad \begin{cases} I_1 = \mathbf{C} : \mathbf{I} , \\ I_2 = [\text{Cof } \mathbf{C}] : \mathbf{I} , \\ I_3 = \text{Det } \mathbf{C} . \end{cases}$$

Among various possible choices, we choose a compressible neo-Hookean model with the free energy density

$$\psi = \frac{1}{2} \mu [I_1 - 3 - \ln I_3] + \frac{1}{4} \lambda [I_3 - 1 - \ln I_3] ,$$

with λ and μ being the Lamé parameters. The proposed free energy in terms of $\mathbf{F}$ takes a more familiar format

$$\psi = \frac{1}{2} \mu [\mathbf{F} : \mathbf{F} - 3 - 2 \ln J] + \frac{1}{4} \lambda [J^2 - 1 - 2 \ln J] \quad \text{with} \quad J := \text{Det } \mathbf{F} .$$

For the given bulk energy density, the Piola stress $\mathbf{P}$ and its tangent $\mathbb{A}$ read

$$\begin{aligned} \mathbf{P} &:= \frac{\partial \psi}{\partial \mathbf{F}} = \mu [\mathbf{F} - \mathbf{F}^{-t}] + \frac{1}{2} \lambda [J^2 - 1] \mathbf{F}^{-t} , \\ \mathbb{A} &:= \frac{\partial \mathbf{P}}{\partial \mathbf{F}} = \mu [\mathbb{I} - \mathbb{J}] + \frac{1}{2} \lambda [J^2 - 1] \mathbb{J} + \lambda J^2 \mathbf{F}^{-t} \otimes \mathbf{F}^{-t} , \end{aligned}$$

in which $\mathbb{I}$ and $\mathbb{J}$ are fourth-order tensors defined by

$$\mathbb{I} := \frac{\partial \mathbf{F}}{\partial \mathbf{F}} = \mathbf{I} \otimes \mathbf{I} \quad \text{and} \quad \mathbb{J} := \frac{\partial \mathbf{F}^{-t}}{\partial \mathbf{F}} = -\mathbf{F}^{-t} \underline{\otimes} \mathbf{F}^{-1} ,$$

Linear elasticity The aforementioned non-linear constitutive law is linearized next at the reference configuration to obtain its linear counterpart suitable for

small-strain elasticity. The linear stress measure $\boldsymbol{\sigma}$ reads

$$\boldsymbol{\sigma} := \boldsymbol{P} \big|_I + \mathbb{A} \big|_I : \text{Grad} \boldsymbol{u},$$

in which

$$\boldsymbol{P} \big|_I = \mathbf{0} \quad \text{and} \quad \mathbb{A} \big|_I = \mu [\boldsymbol{I} \overline{\otimes} \boldsymbol{I} + \boldsymbol{I} \underline{\otimes} \boldsymbol{I}] + \lambda \boldsymbol{I} \otimes \boldsymbol{I}.$$

The classical fourth-order constitutive tensor for small-strain elasticity $\mathbb{C}$ is indeed related to $\mathbb{A}$ via $\mathbb{C} := \mathbb{A} \big|_I$ and due to its symmetry properties $\mathbb{C} : \text{Grad} \boldsymbol{u} = \mathbb{C} : \boldsymbol{\varepsilon}$ with $\boldsymbol{\varepsilon} := \text{Grad}^{\text{sym}} \boldsymbol{u}$ and therefore

$$\boldsymbol{\sigma} = \mathbb{C} : \boldsymbol{\varepsilon} \quad \text{with} \quad \mathbb{C} = \mu [\boldsymbol{I} \overline{\otimes} \boldsymbol{I} + \boldsymbol{I} \underline{\otimes} \boldsymbol{I}] + \lambda \boldsymbol{I} \otimes \boldsymbol{I}.$$

or alternatively

$$\boldsymbol{\sigma} = 2\mu \boldsymbol{\varepsilon} + \lambda [\boldsymbol{\varepsilon} : \boldsymbol{I}] \boldsymbol{I}. \quad (\text{B.1})$$

The constitutive tensor $\mathbb{C}$ is often expressed in terms of the symmetric and volumetric identities $\mathbb{I}^{\text{sym}}$ and $\mathbb{I}^{\text{vol}}$, respectively, defined as

$$\mathbb{I}^{\text{sym}} = \frac{1}{2} [\boldsymbol{I} \overline{\otimes} \boldsymbol{I} + \boldsymbol{I} \underline{\otimes} \boldsymbol{I}] \quad \text{and} \quad \mathbb{I}^{\text{vol}} = \frac{1}{3} \boldsymbol{I} \otimes \boldsymbol{I}.$$

Thus, the constitutive relation for small-strain elasticity reads

$$\boldsymbol{\sigma} = \mathbb{C} : \boldsymbol{\varepsilon} \quad \text{with} \quad \mathbb{C} = 2\mu \mathbb{I}^{\text{sym}} + 3\lambda \mathbb{I}^{\text{vol}}.$$

Furthermore, reformulation of the constitutive relation using the fourth-order deviatoric identity $\mathbb{I}^{\text{dev}} = \mathbb{I}^{\text{sym}} - \mathbb{I}^{\text{vol}}$ yields

$$\boldsymbol{\sigma} = \mathbb{C} : \boldsymbol{\varepsilon} \quad \text{with} \quad \mathbb{C} = 2\mu \mathbb{I}^{\text{dev}} + [3\lambda + 2\mu] \mathbb{I}^{\text{vol}} = 2\mu \mathbb{I}^{\text{dev}} + 3\kappa \mathbb{I}^{\text{vol}},$$

with κ indicating the bulk modulus and finally

$$\boldsymbol{\sigma} = 2\mu \boldsymbol{\varepsilon}^{\text{dev}} + 3\kappa \boldsymbol{\varepsilon}^{\text{vol}} \quad \text{with} \quad \kappa = \lambda + \frac{2}{3}\mu.$$

Plane-strain finite deformation elasticity For a two-dimensional plane-strain condition, the deformation gradient $\mathbf{F}$ simplifies to $\mathbf{F} = \mathbf{F}^* + \mathbf{e}_z \otimes \mathbf{e}_z$ with $\mathbf{F}^*$ being the deformation gradient in two dimensions. A direct consequence of such deformations is that the associated Piola stress can also be decomposed into an in-plane part $\mathbf{P}^*$ and an out-of-plane part P_{zz} . Therefore, the two-dimensional Piola stress $\mathbf{P}^*$ and its tangent $\mathbb{A}^*$ read

$$\begin{aligned}\mathbf{P}^* &= \mu [\mathbf{F}^* - [\mathbf{F}^*]^{-t}] + \frac{1}{2} \lambda [[J^*]^2 - 1] [\mathbf{F}^*]^{-t} \quad \text{with} \quad J^* := \text{Det} \mathbf{F}^* = J, \\ \mathbb{A}^* &= \mu [\mathbb{I}^* - \mathbb{J}^*] + \frac{1}{2} \lambda [[J^*]^2 - 1] \mathbb{J}^* + \lambda [J^*]^2 [\mathbf{F}^*]^{-t} \otimes [\mathbf{F}^*]^{-t},\end{aligned}$$

in which $\mathbb{I}^*$ and $\mathbb{J}^*$ are fourth-order tensors defined by

$$\mathbb{I}^* := \frac{\partial \mathbf{F}^*}{\partial \mathbf{F}^*} = \mathbf{I}^* \otimes \mathbf{I}^* \quad \text{and} \quad \mathbb{J}^* := \frac{\partial [\mathbf{F}^*]^{-t}}{\partial \mathbf{F}^*} = -[\mathbf{F}^*]^{-t} \otimes [\mathbf{F}^*]^{-1},$$

with $\mathbf{I}^* = \mathbf{I} - \mathbf{e}_z \otimes \mathbf{e}_z$ being the second-order identity tensor in two dimensions.

Plane-strain linear elasticity Similar to the linearization procedure carried out previously, a linear elasticity theory conforming to plane-strain is established next. To do so, we define the two-dimensional stress $\boldsymbol{\sigma}^*$ as

$$\boldsymbol{\sigma}^* := \mathbf{P}^*|_I + \mathbb{A}^*|_{I^*} : \text{Grad} \mathbf{u}^*,$$

with

$$\mathbf{P}^*|_{I^*} = \mathbf{0} \quad \text{and} \quad \mathbb{A}^*|_{I^*} = \mu [\mathbf{I}^* \otimes \mathbf{I}^* + \mathbf{I}^* \otimes \mathbf{I}^*] + \lambda \mathbf{I}^* \otimes \mathbf{I}^*. \quad (\text{B.2})$$

Via defining the linear elasticity tensor $\mathbb{C}^*$ as $\mathbb{C}^* := \mathbb{A}^*|_{I^*}$ and due to its symmetry properties, $\mathbb{C}^* : \text{Grad} \mathbf{u}^* = \mathbb{C}^* : \boldsymbol{\varepsilon}^*$ with $\boldsymbol{\varepsilon}^*$ being the two-dimensional strain tensor. Therefore the constitutive response reads

$$\boldsymbol{\sigma}^* = \mathbb{C}^* : \boldsymbol{\varepsilon}^* \quad \text{with} \quad \mathbb{C}^* = \mu [\mathbf{I}^* \otimes \mathbf{I}^* + \mathbf{I}^* \otimes \mathbf{I}^*] + \lambda \mathbf{I}^* \otimes \mathbf{I}^*.$$

The constitutive tensor $\mathbb{C}^\star$ can be expressed in terms of the symmetric and volumetric identities $[\mathbb{I}^\star]^{\text{sym}}$ and $[\mathbb{I}^\star]^{\text{vol}}$, respectively, defined as

$$[\mathbb{I}^\star]^{\text{sym}} = \frac{1}{2} [\mathbf{I}^\star \otimes \mathbf{I}^\star + \mathbf{I}^\star \otimes \mathbf{I}^\star] \quad \text{and} \quad [\mathbb{I}^\star]^{\text{vol}} = \frac{1}{2} \mathbf{I}^\star \otimes \mathbf{I}^\star.$$

Thus, the constitutive relation for linear plane-strain elasticity reads

$$\boldsymbol{\sigma}^\star = \mathbb{C}^\star : \boldsymbol{\varepsilon}^\star \quad \text{with} \quad \mathbb{C}^\star = 2\mu [\mathbb{I}^\star]^{\text{sym}} + 2\lambda [\mathbb{I}^\star]^{\text{vol}}.$$

or

$$\boldsymbol{\sigma}^\star = \mathbb{C}^\star : \boldsymbol{\varepsilon}^\star \quad \text{with} \quad \mathbb{C} = 2\mu [\mathbb{I}^\star]^{\text{dev}} + 2\kappa^\star [\mathbb{I}^\star]^{\text{vol}},$$

with $[\mathbb{I}^\star]^{\text{dev}} = [\mathbb{I}^\star]^{\text{sym}} - [\mathbb{I}^\star]^{\text{vol}}$ and $\kappa^\star$ indicating the two-dimensional bulk modulus and finally

$$\boldsymbol{\sigma}^\star = 2\mu [\boldsymbol{\varepsilon}^\star]^{\text{dev}} + 2\kappa^\star [\boldsymbol{\varepsilon}^\star]^{\text{vol}} \quad \text{with} \quad \kappa^\star = \lambda + \mu.$$

B.2 Interface

Similar to the material modeling in the bulk, the constitutive response of the interface can be characterized through its free energy density. Following a Coleman–Noll-like procedure, the interface free energy density $\bar{\psi}$ for hyperelastic material behavior must be a function of the interface deformation gradient as well as the displacement jump across the interface as $\bar{\psi} = \bar{\psi}(\bar{\mathbf{F}}, [\![\boldsymbol{\varphi}]\!])$. The interface free energy density $\bar{\psi}$ must remain invariant with respect to finite rotations as

$$\bar{\psi}(\bar{\mathbf{F}}, [\![\boldsymbol{\varphi}]\!]) = \bar{\psi}(\mathbf{Q} \cdot \bar{\mathbf{F}}, \mathbf{Q} \cdot [\![\boldsymbol{\varphi}]\!]) \quad \forall \mathbf{Q} \in \mathcal{SO}(3).$$

It can be shown that the energy density $\bar{\psi}$ is frame-indifferent if and only if $\bar{\mathbf{F}}$ and $[\![\boldsymbol{\varphi}]\!]$ enter the interface energy through $\bar{\mathbf{C}}$ and $\bar{c}$. That is

$$\bar{\psi} = \bar{\psi}(\bar{\mathbf{F}}, [\![\boldsymbol{\varphi}]\!]) \quad \xrightarrow{\text{material frame indifference}} \quad \bar{\psi} = \bar{\psi}(\bar{\mathbf{C}}, \bar{c}),$$

with

$$\overline{\mathbf{C}} := \overline{\mathbf{F}}^t \cdot \overline{\mathbf{F}} \quad \text{and} \quad \overline{c} := \llbracket \boldsymbol{\varphi} \rrbracket \cdot \llbracket \boldsymbol{\varphi} \rrbracket. \quad (\text{B.3})$$

Imposing isotropy on the material behavior requires the interface free energy density to be a function of the invariants of $\overline{\mathbf{C}}$ and $\overline{c}$ as

$$\overline{\psi} = \overline{\psi}(\overline{\mathbf{C}}, \overline{c}) \quad \xrightarrow{\text{isotropy}} \quad \overline{\psi} = \overline{\psi}(\overline{I}_1, \overline{I}_2, \overline{I}_3) \quad \text{with} \quad \begin{cases} \overline{I}_1 = \overline{\mathbf{C}} : \overline{\mathbf{I}}, \\ \overline{I}_2 = \text{Det } \overline{\mathbf{C}}, \\ \overline{I}_3 = \sqrt{\overline{c}}. \end{cases}$$

Among various possible options and in the spirit of a neo-Hookean material model in the bulk, the interface free energy density is chosen as

$$\overline{\psi} = \frac{1}{2} \overline{\mu} [\overline{I}_1 - 2 - \ln \overline{I}_2] + \frac{1}{4} \overline{\lambda} [\overline{I}_2 - 1 - \ln \overline{I}_2] + \frac{1}{2} \overline{k} \overline{I}_3^2, \quad (\text{B.4})$$

in which $\overline{\mu}$, $\overline{\lambda}$ and $\overline{k}$ are the interface material parameters. Both $\overline{\mu}$ and $\overline{\lambda}$ correspond to the in-plane interface response while $\overline{k}$ determines the orthogonal stiffness of an interface. The in-plane parameters $\overline{\mu}$ and $\overline{\lambda}$ have the unit N/m and shall be understood as interface Lamé parameters. The orthogonal stiffness $\overline{k}$ with the unit N/m³ indicates the resistance of the interface against opening and shall be understood as the isotropic cohesive parameter. In the limit of vanishing $\overline{k}$, the general interface model exhibits no resistance against opening. Increasing $\overline{k}$ strengthens the interface resistance against opening. In the limit of $\overline{k} \rightarrow \infty$, the interface opening ultimately vanishes and thus, the general interface model behaves in a geometrically coherent manner. The interface energy density can be written as a function of the interface deformation gradient $\overline{\mathbf{F}}$ and the interface displacement jump $\llbracket \boldsymbol{\varphi} \rrbracket$ as

$$\overline{\psi} = \frac{1}{2} \overline{\mu} [\overline{\mathbf{F}} : \overline{\mathbf{F}} - 2 - 2 \ln \overline{J}] + \frac{1}{4} \overline{\lambda} [\overline{J}^2 - 1 - 2 \ln \overline{J}] + \frac{1}{2} \overline{k} \llbracket \boldsymbol{\varphi} \rrbracket \cdot \llbracket \boldsymbol{\varphi} \rrbracket,$$

with $\bar{J} = \overline{\text{Det}\mathbf{F}}$. For the given interface energy density, the interface stress $\bar{\mathbf{P}}$, the interface traction $\bar{\mathbf{t}}$ and their tangents read

$$\begin{aligned}\bar{\mathbf{P}} &:= \frac{\partial \bar{\psi}}{\partial \bar{\mathbf{F}}} = \bar{\mu} [\bar{\mathbf{F}} - \bar{\mathbf{F}}^{\text{t}}] + \frac{1}{2} \bar{\lambda} [\bar{J}^2 - 1] \bar{\mathbf{F}}^{\text{t}}, & \bar{\mathbf{t}} &:= \frac{\partial \bar{\psi}}{\partial \llbracket \boldsymbol{\varphi} \rrbracket} = \bar{k} \llbracket \boldsymbol{\varphi} \rrbracket, \\ \bar{\mathbb{A}}_{\parallel} &:= \frac{\partial \bar{\mathbf{P}}}{\partial \bar{\mathbf{F}}} = \bar{\mu} [\bar{\mathbb{I}} - \bar{\mathbb{J}}] + \frac{1}{2} \bar{\lambda} [\bar{J}^2 - 1] \bar{\mathbb{J}} + \bar{\lambda} \bar{J}^2 \bar{\mathbf{F}}^{\text{t}} \otimes \bar{\mathbf{F}}^{\text{t}}, & \bar{\mathbb{A}}_{\perp} &:= \frac{\partial \bar{\mathbf{t}}}{\partial \llbracket \boldsymbol{\varphi} \rrbracket} = \bar{k} \mathbf{I},\end{aligned}$$

in which $\bar{\mathbb{I}}$ and $\bar{\mathbb{J}}$ are fourth-order tensors defined by

$$\bar{\mathbb{I}} := \frac{\partial \bar{\mathbf{F}}}{\partial \bar{\mathbf{F}}} = \mathbf{I} \otimes \bar{\mathbf{I}} \quad \text{and} \quad \bar{\mathbb{J}} := \frac{\partial \bar{\mathbf{F}}^{\text{t}}}{\partial \bar{\mathbf{F}}} = -\bar{\mathbf{F}}^{\text{t}} \otimes \bar{\mathbf{F}}^{\text{t}} + [\bar{\mathbf{n}} \otimes \bar{\mathbf{n}}] \otimes [\bar{\mathbf{F}}^{\text{t}} \cdot \bar{\mathbf{F}}^{\text{t}}].$$

Linear elasticity The aforementioned non-linear constitutive law for the interface is linearized next at the reference configuration to obtain its linear counterpart suitable for small-strain interface elasticity. The interface linear stress measure $\bar{\boldsymbol{\sigma}}$ and interface traction¹ $\bar{\mathbf{t}}$ read

$$\bar{\boldsymbol{\sigma}} := \bar{\mathbf{P}}|_{\bar{\Gamma}} + \bar{\mathbb{A}}_{\parallel}|_{\bar{\Gamma}} : \overline{\text{Grad}} \bar{\mathbf{u}} \quad \text{and} \quad \bar{\mathbf{t}} = \bar{\mathbf{t}}|_{\bar{\Gamma}} + \bar{\mathbb{A}}_{\perp}|_{\bar{\Gamma}} \cdot \llbracket \boldsymbol{\varphi} \rrbracket,$$

in which

$$\bar{\mathbf{P}}|_{\bar{\Gamma}} = \mathbf{0}, \quad \bar{\mathbf{t}}|_{\bar{\Gamma}} = \mathbf{0}, \quad \bar{\mathbb{A}}_{\parallel}|_{\bar{\Gamma}} = \bar{\mu} [\bar{\mathbf{I}} \otimes \bar{\mathbf{I}} + \bar{\mathbf{I}} \otimes \bar{\mathbf{I}}] + \bar{\lambda} \bar{\mathbf{I}} \otimes \bar{\mathbf{I}}, \quad \bar{\mathbb{A}}_{\perp}|_{\bar{\Gamma}} = \bar{k} \mathbf{I}.$$

and therefore

$$\bar{\boldsymbol{\sigma}} = \bar{\mathbb{C}} : \bar{\boldsymbol{\varepsilon}} \quad \text{and} \quad \bar{\mathbf{t}} = \bar{k} \llbracket \boldsymbol{\varphi} \rrbracket.$$

The interface fourth-order constitutive tensor for small-strain elasticity $\bar{\mathbb{C}}$ is indeed related to $\bar{\mathbb{A}}_{\parallel}$ via $\bar{\mathbb{C}} := \bar{\mathbb{A}}_{\parallel}|_{\bar{\Gamma}}$ and $\mathbb{C} = \bar{\mu} [\bar{\mathbf{I}} \otimes \bar{\mathbf{I}} + \bar{\mathbf{I}} \otimes \bar{\mathbf{I}}] + \bar{\lambda} \bar{\mathbf{I}} \otimes \bar{\mathbf{I}}$. This results in $\bar{\boldsymbol{\sigma}} = \bar{\mu} \bar{\boldsymbol{\varepsilon}} + \bar{\lambda} [\bar{\boldsymbol{\varepsilon}} : \bar{\mathbf{I}}] \bar{\mathbf{I}}$. The constitutive tensor $\bar{\mathbb{C}}$ can be expressed in terms of the symmetric and volumetric identities $\bar{\mathbb{I}}^{\text{sym}}$ and $\bar{\mathbb{I}}^{\text{vol}}$, respectively, defined as

$$\bar{\mathbb{I}}^{\text{sym}} = \frac{1}{2} [\bar{\mathbf{I}} \otimes \bar{\mathbf{I}} + \bar{\mathbf{I}} \otimes \bar{\mathbf{I}}] \quad \text{and} \quad \bar{\mathbb{I}}^{\text{vol}} = \frac{1}{2} \bar{\mathbf{I}} \otimes \bar{\mathbf{I}}.$$

¹The interface traction-separation law is linear by definition and thus, we use $\mathbf{t}$ for both small-strain and finite deformation settings.

Thus, the constitutive relation for small-strain elasticity reads

$$\bar{\boldsymbol{\sigma}} = \bar{\mathbb{C}} : \bar{\boldsymbol{\varepsilon}} \quad \text{and} \quad \bar{\mathbf{t}} = \bar{k} \llbracket \boldsymbol{\varphi} \rrbracket \quad \text{with} \quad \bar{\mathbb{C}} = 2\bar{\mu} \bar{\mathbb{I}}^{\text{sym}} + 2\bar{\lambda} \bar{\mathbb{I}}^{\text{vol}}.$$

Furthermore, reformulation of the constitutive relation using the fourth-order deviatoric identity $\bar{\mathbb{I}}^{\text{dev}} = \bar{\mathbb{I}}^{\text{sym}} - \bar{\mathbb{I}}^{\text{vol}}$ yields

$$\bar{\boldsymbol{\sigma}} = \bar{\mathbb{C}} : \bar{\boldsymbol{\varepsilon}} \quad \text{and} \quad \bar{\mathbf{t}} = \bar{k} \llbracket \boldsymbol{\varphi} \rrbracket,$$

with

$$\bar{\mathbb{C}} = 2\bar{\mu} \bar{\mathbb{I}}^{\text{dev}} + [2\bar{\lambda} + 2\bar{\mu}] \bar{\mathbb{I}}^{\text{vol}} = 2\bar{\mu} \bar{\mathbb{I}}^{\text{dev}} + 2\bar{\kappa} \bar{\mathbb{I}}^{\text{vol}}, \quad (\text{B.5})$$

where $\bar{\kappa}$ indicates the interface modulus and finally

$$\bar{\boldsymbol{\sigma}} = 2\bar{\mu} \bar{\boldsymbol{\varepsilon}}^{\text{dev}} + 2\bar{\kappa} \bar{\boldsymbol{\varepsilon}}^{\text{vol}} \quad \text{with} \quad \bar{\kappa} = \bar{\lambda} + \bar{\mu}.$$

Plane-strain finite deformation elasticity For a two-dimensional plane-strain condition, the interface deformation gradient $\bar{\mathbf{F}}$ simplifies to $\bar{\mathbf{F}} = \bar{\mathbf{F}}^* + \mathbf{e}_z \otimes \mathbf{e}_z$ with $\bar{\mathbf{F}}^*$ being the interface deformation gradient in two dimensions or more precisely, a curve deformation gradient. A direct consequence of such deformations is that the associated Piola stress can also be decomposed into an in-plane part $\bar{\mathbf{P}}^*$ and an out-of-plane part P_{zz} . Furthermore, the in-plane part has a tangential component corresponding to the stretch of the interface and an orthogonal component corresponding to the opening of the interface. As such, the tangential component can be captured by only one interface parameter and thus, without loss of generality, we set $\bar{\lambda} = 0$ and therefore

$$\bar{\mathbf{P}}^* = \bar{\mu} [\bar{\mathbf{F}}^* - [\bar{\mathbf{F}}^*]^{-\text{t}}], \quad \bar{\mathbf{t}}^* = \bar{k} \llbracket \boldsymbol{\varphi} \rrbracket^*,$$

$$\bar{\mathbb{A}}_{\parallel}^* = \bar{\mu} [\bar{\mathbb{I}}^* - \bar{\mathbb{J}}^*], \quad \bar{\mathbb{A}}_{\perp}^* = \bar{k} \mathbf{I},$$

in which $\bar{\mathbb{I}}^*$ and $\bar{\mathbb{J}}^*$ are the restrictions of $\bar{\mathbb{I}}$ and $\bar{\mathbb{J}}$, respectively, on to the two-dimensional plane.

Plane-strain linear elasticity Similar to the linearization procedure carried

out previously, an interface linear elasticity theory conforming to plane-strain can be established. Since the interface in general is a two-dimensional surface in a three-dimensional space, its two-dimensional counterpart corresponds to a curve with a tangential resistance identified by $\bar{\mu}$ and an orthogonal resistance identified by $\bar{k}$. As such the derivations are nearly identical to the previous discussion on linearization of the interface response except that now we set $\bar{\lambda} = 0$ and thus

$$\bar{\boldsymbol{\sigma}}^* = 2\bar{\mu} \bar{\boldsymbol{\varepsilon}}^* \quad \text{and} \quad \bar{\boldsymbol{t}}^* = \bar{k} \llbracket \boldsymbol{\varphi} \rrbracket^*.$$

Appendix C

System of equations for the estimate and bounds on the shear modulus

In this section we elaborate on the system of equations used to obtain the estimate and the bounds on the macroscopic shear modulus explained in Sections 3.3.1 and 3.3.2.

C.1 Fiber composites

C.1.1 Effective shear modulus

For this problem, the displacement fields in the matrix, fiber and the effective medium are given in Eq. (3.18) resulting in ten unknowns $\Xi_1^{(1)}$, $\Xi_2^{(1)}$, $\Xi_3^{(1)}$, $\Xi_4^{(1)}$, $\Xi_1^{(2)}$, $\Xi_2^{(2)}$, $\Xi_3^{(2)}$, $\Xi_4^{(2)}$, $\Xi_3^{(\text{eff})}$ and $\Xi_4^{(\text{eff})}$. We concluded that since the displacement at the center of the RVE must be finite, $\Xi_3^{(1)}$ and $\Xi_4^{(1)}$ must vanish. Applying the energetic criterion expressed in Eq. (3.27) yields $\Xi_4^{(\text{eff})}$. The remaining seven unknowns are

determined using the below system which is deduced from Eq. (3.20)–(3.26)

$$\begin{bmatrix} Q_{11} & Q_{12} & Q_{13} & Q_{14} & Q_{15} & Q_{16} \\ Q_{21} & Q_{22} & Q_{23} & Q_{24} & Q_{25} & Q_{26} \\ Q_{31} & Q_{32} & Q_{33} & Q_{34} & Q_{35} & Q_{36} \\ Q_{41} & Q_{42} & Q_{43} & Q_{44} & Q_{45} & Q_{46} \\ Q_{51} & Q_{52} & Q_{53} & Q_{54} & Q_{55} & Q_{56} \\ Q_{61} & Q_{62} & Q_{63} & Q_{64} & Q_{65} & Q_{66} \end{bmatrix} \begin{bmatrix} \Xi_1^{(1)} \\ \Xi_2^{(1)} \\ \Xi_1^{(2)} \\ \Xi_2^{(2)} \\ \Xi_3^{(2)} \\ \Xi_4^{(2)} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 1 \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ -\frac{3}{2} \\ \frac{3}{2} \end{bmatrix} \Xi_3^{(\text{eff})}, \quad (\text{C.1})$$

The components of $\mathbf{Q}$ read

$$\begin{aligned} Q_{11} &= \frac{3\bar{\mu} [\lambda_1 + 2\mu_1] r_1}{[2\lambda_1 + 3\mu_1]}, & Q_{12} &= \frac{\bar{\mu}}{r_1} - 2\mu_1, \\ Q_{13} &= \frac{3\bar{\mu} [\lambda_2 + 2\mu_2] r_1}{[2\lambda_2 + 3\mu_2]}, & Q_{14} &= \frac{\bar{\mu}}{r_1} + 2\mu_2, \\ Q_{15} &= \frac{3\bar{\mu}}{r_1^5} + \frac{6\mu_2}{r_1^4}, & Q_{16} &= -\frac{4[\lambda_2 + \mu_2]}{r_1^2} - \frac{\lambda_2 \bar{\mu}}{\mu_2 r_1^3}, \\ Q_{21} &= -\frac{6[\bar{\mu} [\lambda_1 + 2\mu_1] + \mu_1 [\lambda_1 + \mu_1] r_1] r_1}{[2\lambda_1 + 3\mu_1]}, & Q_{22} &= -\frac{2\bar{\mu}}{r_1} - 2\mu_1, \\ Q_{23} &= -\frac{6[\bar{\mu} [\lambda_2 + 2\mu_2] - \mu_2 [\lambda_2 + \mu_2] r_1] r_1}{[2\lambda_2 + 3\mu_2]}, & Q_{24} &= -\frac{2\bar{\mu}}{r_1} + 2\mu_2, \\ Q_{25} &= -\frac{6\bar{\mu}}{r_1^5} - \frac{6\mu_2}{r_1^4}, & Q_{26} &= \frac{2[\lambda_2 + \mu_2]}{r_1^2} + \frac{2\bar{\mu} \lambda_2}{\mu_2 r_1^3}, \\ Q_{31} &= \frac{\lambda_1 r_1^3}{[2\lambda_1 + 3\mu_1]}, & Q_{32} &= \frac{\mu_1}{\bar{k}} + r_1, \\ Q_{33} &= -\frac{\lambda_2 r_1^3}{[2\lambda_2 + 3\mu_2]}, & Q_{34} &= \frac{\mu_2}{\bar{k}} - r_1, \\ Q_{35} &= -\frac{3\mu_2}{\bar{k} r_1^4} - \frac{1}{r_1^3}, & Q_{36} &= -\frac{2[\lambda_2 + \mu_2]}{\bar{k} r_1^2} - \frac{[\lambda_2 + 2\mu_2]}{\mu_2 r_1}, \\ Q_{41} &= \frac{3\mu_1 [\lambda_1 + \mu_1] r_1^2}{\bar{k} [2\lambda_1 + 3\mu_1]} + r_1^3, & Q_{42} &= \frac{\mu_1}{\bar{k}} + r_1, \\ Q_{43} &= \frac{3\mu_2 [\lambda_2 + \mu_2] r_1^2}{\bar{k} [2\lambda_2 + 3\mu_2]} - r_1^3, & Q_{44} &= \frac{\mu_2}{\bar{k}} - r_1, \\ Q_{45} &= -\frac{3\mu_2}{\bar{k} r_1^4} - \frac{1}{r_1^3}, & Q_{46} &= \frac{[\lambda_2 + \mu_2]}{\bar{k} r_1^2} - \frac{1}{r_1}, \end{aligned}$$

$$\begin{aligned}
Q_{51} &= Q_{52} = Q_{53} = Q_{61} = Q_{62} = 0, & Q_{54} &= 2\mu_2, \\
Q_{55} &= -\frac{1}{r_2^3}, & Q_{65} &= \frac{1}{r_2^3}, \\
Q_{56} &= \frac{[\lambda_2 + 2\mu_2]}{\mu_2 r_2}, & Q_{64} &= 2\mu_2 \\
Q_{63} &= \frac{6\mu_2 \zeta_4 r_2^2}{[2\lambda_2 + 3\mu_2]} & Q_{66} &= \frac{1}{r_2},
\end{aligned}$$

Note, the above system of equations is nonlinear thus, special treatments must be applied. We express the solution of the above system in the form

$$\begin{bmatrix} \Xi_1^{(1)} \\ \Xi_2^{(1)} \\ \Xi_1^{(2)} \\ \Xi_2^{(2)} \\ \Xi_3^{(2)} \\ \Xi_4^{(2)} \end{bmatrix} = \begin{bmatrix} g_1 \\ g_2 \\ a_1 \\ a_2 \\ a_3 \\ a_4 \end{bmatrix} + \begin{bmatrix} h_1 \\ h_2 \\ b_1 \\ b_2 \\ b_3 \\ b_4 \end{bmatrix} \Xi_3^{(\text{eff})}. \quad (\text{C.2})$$

The equations Eq. (3.25) and (3.25) can be written as

$$a_5 + b_5 \Xi_3^{(\text{eff})} = \frac{c_5 + c_6 \Xi_3^{(\text{eff})}}{M_\mu}, \quad a_6 + b_6 \Xi_3^{(\text{eff})} = \frac{c_5 - c_6 \Xi_3^{(\text{eff})}}{M_\mu}. \quad (\text{C.3})$$

with

$$\begin{aligned}
a_5 &= \frac{\lambda_2 r_2^3}{2\lambda_2 + 3\mu_2} a_1 + r_2 a_2 - \frac{1}{r_2^3} a_3 + \frac{\lambda_2 + 2\mu_2}{\mu_2 r_2} a_4, \\
a_6 &= r_2^3 a_1 + r_2 a_2 + \frac{1}{r_2^3} a_3 + \frac{1}{r_2} a_4, \\
b_5 &= \frac{\lambda_2 r_2^3}{2\lambda_2 + 3\mu_2} b_1 + r_2 b_2 - \frac{1}{r_2^3} b_3 + \frac{\lambda_2 + 2\mu_2}{\mu_2 r_2} b_4, \\
b_6 &= r_2^3 b_1 + r_2 b_2 + \frac{1}{r_2^3} b_3 + \frac{1}{r_2} b_4, \\
c_5 &= \frac{r_2}{2}, \\
c_6 &= \frac{r_2}{4}.
\end{aligned} \quad (\text{C.4})$$

Subtracting (C.9)₁ from (C.9)₂ gives

$$\Xi_3^{(\text{eff})} = \frac{[a_5 - a_6]^M \mu}{2c_6 + [b_6 - b_5]^M \mu}.$$

Substituting the final result in (C.9)₁, after some algebra we obtain the below quadratic equation

$$[a_6 b_5 - a_5 b_6]^M \mu^2 - [b_5 c_5 - b_6 c_5 + a_5 c_6 + a_6 c_6]^M \mu + 2c_5 c_6 = 0.$$

From the two possible solutions the positive value is the macroscopic shear modulus.

C.1.2 Upper bound on the shear modulus

For this problem, the displacement fields in the matrix, fiber and the effective medium are given in Eq. (3.28) resulting in ten unknowns $\Xi_1^{(1)}, \Xi_2^{(1)}, \Xi_3^{(1)}, \Xi_4^{(1)}, \Xi_1^{(2)}, \Xi_2^{(2)}, \Xi_3^{(2)}$ and $\Xi_4^{(2)}$. We concluded that since the displacement at the center of the RVE must be finite, $\Xi_3^{(1)}$ and $\Xi_4^{(1)}$ must vanish. The remaining six unknowns are determined using the below system which is deduced from Eqs. (3.29)–(3.34)

$$\begin{bmatrix} Q_{11} & Q_{12} & Q_{13} & Q_{14} & Q_{15} & Q_{16} \\ Q_{21} & Q_{22} & Q_{23} & Q_{24} & Q_{25} & Q_{26} \\ Q_{31} & Q_{32} & Q_{33} & Q_{34} & Q_{35} & Q_{36} \\ Q_{41} & Q_{42} & Q_{43} & Q_{44} & Q_{45} & Q_{46} \\ Q_{51} & Q_{52} & Q_{53} & Q_{54} & Q_{55} & Q_{56} \\ Q_{61} & Q_{62} & Q_{63} & Q_{64} & Q_{65} & Q_{66} \end{bmatrix} \begin{bmatrix} \Xi_1^{(1)} \\ \Xi_2^{(1)} \\ \Xi_1^{(2)} \\ \Xi_2^{(2)} \\ \Xi_3^{(2)} \\ \Xi_4^{(2)} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ r_2 \\ r_2 \end{bmatrix}. \quad (\text{C.5})$$

The components of $\mathbf{Q}$ read

$$\begin{aligned}
Q_{11} &= \frac{3\bar{\mu} [\lambda_1 + 2\mu_1] r_1}{[2\lambda_1 + 3\mu_1]}, & Q_{12} &= \frac{\bar{\mu}}{r_1} - 2\mu_1, \\
Q_{13} &= \frac{3\bar{\mu} [\lambda_2 + 2\mu_2] r_1}{[2\lambda_2 + 3\mu_2]}, & Q_{14} &= \frac{\bar{\mu}}{r_1} + 2\mu_2, \\
Q_{15} &= \frac{3\bar{\mu}}{r_1^5} + \frac{6\mu_2}{r_1^4}, & Q_{16} &= -\frac{4[\lambda_2 + \mu_2]}{r_1^2} - \frac{\lambda_2 \bar{\mu}}{\mu_2 r_1^3}, \\
Q_{21} &= -\frac{6[\bar{\mu} [\lambda_1 + 2\mu_1] + \mu_1 [\lambda_1 + \mu_1] r_1] r_1}{[2\lambda_1 + 3\mu_1]}, & Q_{22} &= -\frac{2\bar{\mu}}{r_1} - 2\mu_1, \\
Q_{23} &= -\frac{6[\bar{\mu} [\lambda_2 + 2\mu_2] - \mu_2 [\lambda_2 + \mu_2] r_1] r_1}{[2\lambda_2 + 3\mu_2]}, & Q_{24} &= -\frac{2\bar{\mu}}{r_1} + 2\mu_2, \\
Q_{25} &= -\frac{6\bar{\mu}}{r_1^5} - \frac{6\mu_2}{r_1^4}, & Q_{26} &= \frac{2[\lambda_2 + \mu_2]}{r_1^2} + \frac{2\bar{\mu} \lambda_2}{\mu_2 r_1^3}, \\
Q_{31} &= \frac{\lambda_1 r_1^3}{[2\lambda_1 + 3\mu_1]}, & Q_{32} &= \frac{\mu_1}{\bar{k}} + r_1, \\
Q_{33} &= -\frac{\lambda_2 r_1^3}{[2\lambda_2 + 3\mu_2]}, & Q_{34} &= \frac{\mu_2}{\bar{k}} - r_1, \\
Q_{35} &= -\frac{3\mu_2}{\bar{k} r_1^4} - \frac{1}{r_1^3}, & Q_{36} &= -\frac{2[\lambda_2 + \mu_2]}{\bar{k} r_1^2} - \frac{[\lambda_2 + 2\mu_2]}{\mu_2 r_1}, \\
Q_{41} &= \frac{3\mu_1 [\lambda_1 + \mu_1] r_1^2}{\bar{k} [2\lambda_1 + 3\mu_1]} + r_1^3, & Q_{42} &= \frac{\mu_1}{\bar{k}} + r_1, \\
Q_{43} &= \frac{3\mu_2 [\lambda_2 + \mu_2] r_1^2}{\bar{k} [2\lambda_2 + 3\mu_2]} - r_1^3, & Q_{44} &= \frac{\mu_2}{\bar{k}} - r_1, \\
Q_{45} &= -\frac{3\mu_2}{\bar{k} r_1^4} - \frac{1}{r_1^3}, & Q_{46} &= \frac{[\lambda_2 + \mu_2]}{\bar{k} r_1^2} - \frac{1}{r_1}, \\
Q_{51} &= Q_{52} = Q_{61} = Q_{62} = 0, & Q_{53} &= \frac{\lambda_2 r_2^3}{[2\lambda_2 + 3\mu_2]}, \\
Q_{54} &= r_2, & Q_{55} &= -Q_{65} = -\frac{1}{r_2^3}, \\
Q_{56} &= \frac{[\lambda_2 + 2\mu_2]}{\mu_2 r_2}, & Q_{63} &= r_2^3, \\
Q_{64} &= r_2, & Q_{66} &= \frac{1}{r_2},
\end{aligned}$$

C.1.3 Lower bound on the shear modulus

For this problem, the displacement fields in the matrix, fiber and the effective medium are given in Eq. (3.28) resulting in ten unknowns $\Xi_1^{(1)}$, $\Xi_2^{(1)}$, $\Xi_3^{(1)}$, $\Xi_4^{(1)}$, $\Xi_1^{(2)}$, $\Xi_2^{(2)}$, $\Xi_3^{(2)}$ and $\Xi_4^{(2)}$. We concluded that since the displacement at the center of the RVE must be finite, $\Xi_3^{(1)}$ and $\Xi_4^{(1)}$ must vanish. The remaining six unknowns are determined using the below system which is deduced from Eqs. (3.35)–(3.40)

$$\begin{bmatrix} Q_{11} & Q_{12} & Q_{13} & Q_{14} & Q_{15} & Q_{16} \\ Q_{21} & Q_{22} & Q_{23} & Q_{24} & Q_{25} & Q_{26} \\ Q_{31} & Q_{32} & Q_{33} & Q_{34} & Q_{35} & Q_{36} \\ Q_{41} & Q_{42} & Q_{43} & Q_{44} & Q_{45} & Q_{46} \\ Q_{51} & Q_{52} & Q_{53} & Q_{54} & Q_{55} & Q_{56} \\ Q_{61} & Q_{62} & Q_{63} & Q_{64} & Q_{65} & Q_{66} \end{bmatrix} \begin{bmatrix} \Xi_1^{(1)} \\ \Xi_2^{(1)} \\ \Xi_1^{(2)} \\ \Xi_2^{(2)} \\ \Xi_3^{(2)} \\ \Xi_4^{(2)} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 1 \end{bmatrix}, \quad (\text{C.6})$$

The components of $\mathbf{Q}$ read

$$\begin{aligned} Q_{11} &= \frac{3\bar{\mu}[\lambda_1 + 2\mu_1]r_1}{[2\lambda_1 + 3\mu_1]}, & Q_{12} &= \frac{\bar{\mu}}{r_1} - 2\mu_1, \\ Q_{13} &= \frac{3\bar{\mu}[\lambda_2 + 2\mu_2]r_1}{[2\lambda_2 + 3\mu_2]}, & Q_{14} &= \frac{\bar{\mu}}{r_1} + 2\mu_2, \\ Q_{15} &= \frac{3\bar{\mu}}{r_1^5} + \frac{6\mu_2}{r_1^4}, & Q_{16} &= -\frac{4[\lambda_2 + \mu_2]}{r_1^2} - \frac{\lambda_2\bar{\mu}}{\mu_2 r_1^3}, \\ Q_{21} &= -\frac{6[\bar{\mu}[\lambda_1 + 2\mu_1] + \mu_1[\lambda_1 + \mu_1]r_1]r_1}{[2\lambda_1 + 3\mu_1]}, & Q_{22} &= -\frac{2\bar{\mu}}{r_1} - 2\mu_1, \\ Q_{23} &= -\frac{6[\bar{\mu}[\lambda_2 + 2\mu_2] - \mu_2[\lambda_2 + \mu_2]r_1]r_1}{[2\lambda_2 + 3\mu_2]}, & Q_{24} &= -\frac{2\bar{\mu}}{r_1} + 2\mu_2, \\ Q_{25} &= -\frac{6\bar{\mu}}{r_1^5} - \frac{6\mu_2}{r_1^4}, & Q_{26} &= \frac{2[\lambda_2 + \mu_2]}{r_1^2} + \frac{2\bar{\mu}\lambda_2}{\mu_2 r_1^3}, \\ Q_{31} &= \frac{\lambda_1 r_1^3}{[2\lambda_1 + 3\mu_1]}, & Q_{32} &= \frac{\mu_1}{k} + r_1, \\ Q_{33} &= -\frac{\lambda_2 r_1^3}{[2\lambda_2 + 3\mu_2]}, & Q_{34} &= \frac{\mu_2}{k} - r_1, \end{aligned}$$

$$\begin{aligned}
Q_{35} &= -\frac{3\mu_2}{\bar{k}r_1^4} - \frac{1}{r_1^3}, & Q_{36} &= -\frac{2[\lambda_2 + \mu_2]}{\bar{k}r_1^2} - \frac{[\lambda_2 + 2\mu_2]}{\mu_2 r_1}, \\
Q_{41} &= \frac{3\mu_1[\lambda_1 + \mu_1]r_1^2}{\bar{k}[2\lambda_1 + 3\mu_1]} + r_1^3, & Q_{42} &= \frac{\mu_1}{\bar{k}} + r_1, \\
Q_{43} &= \frac{3\mu_2[\lambda_2 + \mu_2]r_1^2}{\bar{k}[2\lambda_2 + 3\mu_2]} - r_1^3, & Q_{44} &= \frac{\mu_2}{\bar{k}} - r_1, \\
Q_{45} &= -\frac{3\mu_2}{\bar{k}r_1^4} - \frac{1}{r_1^3}, & Q_{46} &= \frac{[\lambda_2 + \mu_2]}{\bar{k}r_1^2} - \frac{1}{r_1}, \\
Q_{51} &= Q_{52} = Q_{53} = Q_{61} = Q_{62} = 0, & Q_{54} &= 2\mu_2, \\
Q_{55} &= -\frac{1}{r_2^3}, & Q_{65} &= \frac{1}{r_2^3}, \\
Q_{56} &= \frac{[\lambda_2 + 2\mu_2]}{\mu_2 r_2}, & Q_{64} &= 2\mu_2, \\
Q_{63} &= \frac{6\mu_2\zeta_4 r_2^2}{[2\lambda_2 + 3\mu_2]}, & Q_{66} &= \frac{1}{r_2},
\end{aligned}$$

C.2 Particulate composites

C.2.1 Effective shear modulus

For this problem the displacement fields in the particle and the matrix are given in Eq. (3.88) and the displacement field in the effective medium is given in Eq. (3.78). This problem contains ten unknown of $\Xi_1^{(1)}$, $\Xi_2^{(1)}$, $\Xi_3^{(1)}$, $\Xi_4^{(1)}$, $\Xi_1^{(2)}$, $\Xi_2^{(2)}$, $\Xi_3^{(2)}$, $\Xi_4^{(2)}$, $\Xi_3^{(\text{eff})}$ and $\Xi_4^{(\text{eff})}$. We concluded that since at the center of the RVE the displacement field needs to be finite, $\Xi_3^{(1)}$ and $\Xi_4^{(1)}$ must be zero. Substitution of the stress and displacement fields in Eq. (3.87) yielded $\Xi_4^{(\text{eff})} = 0$. The remaining seven unknowns are determined using the below system which is deduced from the

conditions (3.80)–(3.86)

$$\begin{bmatrix} Q_{11} & Q_{12} & Q_{13} & Q_{14} & Q_{15} & Q_{16} \\ Q_{21} & Q_{22} & Q_{23} & Q_{24} & Q_{25} & Q_{26} \\ Q_{31} & Q_{32} & Q_{33} & Q_{34} & Q_{35} & Q_{36} \\ Q_{41} & Q_{42} & Q_{43} & Q_{44} & Q_{45} & Q_{46} \\ Q_{51} & Q_{52} & Q_{53} & Q_{54} & Q_{55} & Q_{56} \\ Q_{61} & Q_{62} & Q_{63} & Q_{64} & Q_{65} & Q_{66} \end{bmatrix} \begin{bmatrix} \Xi_1^{(1)} \\ \Xi_2^{(1)} \\ \Xi_1^{(2)} \\ \Xi_2^{(2)} \\ \Xi_3^{(2)} \\ \Xi_4^{(2)} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 1 \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 3 \\ -2 \end{bmatrix} f^{5/3} \Xi_3^{\text{eff}}, \quad (\text{C.7})$$

The components of $\mathbf{Q}$ read

$$\begin{aligned} Q_{11} &= 1 + \frac{\mu_1}{\bar{k}r_1}, & Q_{12} &= 2 - 3\frac{\kappa_1}{\mu_1} + \frac{3\kappa_1 - 2\mu_1}{2\bar{k}r_1}, \\ Q_{13} &= -1 + \frac{\mu_2}{\bar{k}r_1}, & Q_{14} &= -2 + 3\frac{\kappa_2}{\mu_2} + \frac{3\kappa_2 - 2\mu_2}{2\bar{k}r_1}, \\ Q_{15} &= -3 - \frac{12\mu_2}{\bar{k}r_1}, & Q_{16} &= -3 - 3\frac{\kappa_2}{\mu_2} - \frac{9\kappa_2 + 4\mu_2}{\bar{k}r_1}, \\ Q_{21} &= 1 + \frac{\mu_1}{\bar{k}r_1}, & Q_{22} &= -\frac{11}{3} - 5\frac{\kappa_1}{\mu_1} + \frac{24\kappa_1 + 5\mu_1}{3\bar{k}r_1}, \\ Q_{23} &= -1 + \frac{\mu_2}{\bar{k}r_1}, & Q_{24} &= \frac{11}{3} + 5\frac{\kappa_2}{\mu_2} - \frac{24\kappa_2 + 5\mu_2}{3\bar{k}r_1}, \\ Q_{25} &= 2 + \frac{8\mu_2}{\bar{k}r_1}, & Q_{26} &= -2 + \frac{3\kappa_2}{\bar{k}r_1}, \\ Q_{31} &= 2\mu_1 - \frac{\bar{\lambda} + \bar{\mu}}{r_1}, & Q_{32} &= 3\kappa_1 - 2\mu_1 + \frac{[9\kappa_1 + 15\mu_1][\bar{\lambda} + \bar{\mu}]}{\mu_1 r_1}, \\ Q_{33} &= -2\mu_2 - \frac{\bar{\lambda} + \bar{\mu}}{r_1}, & Q_{34} &= -3\kappa_2 + 2\mu_2 + \frac{[9\kappa_2 + 15\mu_2][\bar{\lambda} + \bar{\mu}]}{\mu_2 r_1}, \\ Q_{35} &= 24\mu_2 + \frac{12[\bar{\lambda} + \bar{\mu}]}{r_1}, & Q_{36} &= 18\kappa_2 + 8\mu_2 + \frac{6\kappa_2[\bar{\lambda} + \bar{\mu}]}{\mu_2 r_1}, \\ Q_{41} &= 2\mu_1 + \frac{[\bar{\lambda} + \bar{\mu}] + 2\bar{\mu}}{r_1}, & Q_{43} &= -2\mu_2 + \frac{[\bar{\lambda} + \bar{\mu}] + 2\bar{\mu}}{\mu_2 r_1}, \\ Q_{45} &= -16\mu_2 + \frac{4[3\bar{\lambda} + 4\bar{\mu}]}{r_1}, & Q_{46} &= -6\kappa_2 + \frac{-6\kappa_2[\bar{\lambda} + \bar{\mu}] + 4\mu_2\bar{\mu}}{\mu_2 r_1}, \end{aligned}$$

$$\begin{aligned}
Q_{51} &= Q_{52} = Q_{61} = Q_{62} = 0, & Q_{53} &= Q_{63} = 1, \\
Q_{54} &= \left[2 - 3 \frac{\kappa_2}{\mu_2} \right] f^{-2/3}, & Q_{55} &= 3f^{5/3}, \\
Q_{56} &= \left[3 + 3 \frac{\kappa_2}{\mu_2} \right] f, & Q_{64} &= - \left[\frac{11}{3} + 5 \frac{\kappa_2}{\mu_2} \right] f^{-2/3}, \\
Q_{65} &= -2f^{5/3}, & Q_{66} &= 2f, \\
Q_{42} &= -16\kappa_1 - \frac{10}{3}\mu_1 + -\frac{\kappa_1 [9\bar{\lambda} + 19\bar{\mu}]}{\mu_1 r_1} - \frac{[45\bar{\lambda} + 67\bar{\mu}]}{3r_1}, \\
Q_{44} &= 16\kappa_2 + \frac{10}{3}\mu_2 + -\frac{\kappa_2 [9\bar{\lambda} + 19\bar{\mu}]}{\mu_2 r_1} - \frac{[45\bar{\lambda} + 67\bar{\mu}]}{3r_1},
\end{aligned}$$

The obtained system of equations though is nonlinear hence, requiring a special treatment. We express the solution of the above system in the form

$$\begin{bmatrix} \Xi_1^{(1)} \\ \Xi_2^{(1)} \\ \Xi_1^{(2)} \\ \Xi_2^{(2)} \\ \Xi_3^{(2)} \\ \Xi_4^{(2)} \end{bmatrix} = \begin{bmatrix} g_1 \\ g_2 \\ a_1 \\ a_2 \\ a_3 \\ a_4 \end{bmatrix} + \begin{bmatrix} h_1 \\ h_2 \\ b_1 \\ b_2 \\ b_3 \\ b_4 \end{bmatrix} f^{5/3} \Xi_3^{(\text{eff})}. \quad (\text{C.8})$$

Using (C.8), the last two conditions of Eq. (3.79) are written as

$$\begin{aligned}
a_5 + b_5 f^{5/3} \Xi_3^{(\text{eff})} &= 2^{\text{M}} \mu - 24^{\text{M}} \mu f^{5/3} \Xi_3^{(\text{eff})}, \\
a_6 + b_6 f^{5/3} \Xi_3^{(\text{eff})} &= 2^{\text{M}} \mu + 16^{\text{M}} \mu f^{5/3} \Xi_3^{(\text{eff})},
\end{aligned} \quad (\text{C.9})$$

with

$$\begin{aligned}
a_5 &= 2\mu_2 a_1 + [3\kappa_2 - 2\mu_2]f^{-2/3}a_2 - 24\mu_2 f^{5/3}a_3 - [18\kappa_2 + 8\mu_2]f a_4, \\
a_6 &= 2\mu_2 a_1 - \left[16\kappa_2 + \frac{10}{3}\mu_2\right] f^{-2/3}a_2 + 16\mu_2 f^{5/3}a_3 + 6\kappa_2 f a_4, \\
b_5 &= 2\mu_2 b_1 + [3\kappa_2 - 2\mu_2]f^{-2/3}b_2 - 24\mu_2 f^{5/3}b_3 - [18\kappa_2 + 8\mu_2]f b_4, \\
b_6 &= 2\mu_2 b_1 - \left[16\kappa_2 + \frac{10}{3}\mu_2\right] f^{-2/3}b_2 + 16\mu_2 f^{5/3}b_3 + 6\kappa_2 f b_4.
\end{aligned} \tag{C.10}$$

Subtracting (C.9)₁ from (C.9)₂ gives

$$f^{5/3}\Xi_3^{(\text{eff})} = \frac{a_6 - a_5}{40^M\mu + b_5 - b_6}.$$

Substituting the final result in (C.9)₁, after some algebra we obtain the below quadratic equation

$$80^M\mu^2 - 2[b_6 - b_5 + 12a_6 + 8a_5]^M\mu + a_5b_6 - b_5a_6 = 0.$$

From the two possible solutions the positive value is the macroscopic shear modulus.

C.2.2 Upper bound on the shear modulus

The displacement fields in the matrix and the particle were given in Eq. (3.88) which has eight unknowns of $\Xi_1^{(1)}$, $\Xi_2^{(1)}$, $\Xi_3^{(1)}$, $\Xi_4^{(1)}$, $\Xi_1^{(2)}$, $\Xi_2^{(2)}$, $\Xi_3^{(2)}$ and $\Xi_4^{(2)}$. We concluded that since the displacement fields at the center of the RVE must be finite, $\Xi_3^{(1)}$ and $\Xi_4^{(1)}$ must vanish. The remaining six unknowns are determined

using the below system which is deduced from the conditions (3.89)–(3.94)

$$\begin{bmatrix} Q_{11} & Q_{12} & Q_{13} & Q_{14} & Q_{15} & Q_{16} \\ Q_{21} & Q_{22} & Q_{23} & Q_{24} & Q_{25} & Q_{26} \\ Q_{31} & Q_{32} & Q_{33} & Q_{34} & Q_{35} & Q_{36} \\ Q_{41} & Q_{42} & Q_{43} & Q_{44} & Q_{45} & Q_{46} \\ Q_{51} & Q_{52} & Q_{53} & Q_{54} & Q_{55} & Q_{56} \\ Q_{61} & Q_{62} & Q_{63} & Q_{64} & Q_{65} & Q_{66} \end{bmatrix} \begin{bmatrix} \Xi_1^{(1)} \\ \Xi_2^{(1)} \\ \Xi_1^{(2)} \\ \Xi_2^{(2)} \\ \Xi_3^{(2)} \\ \Xi_4^{(2)} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 1 \end{bmatrix}, \quad (\text{C.11})$$

The components of $\mathbf{Q}$ read

$$\begin{aligned} Q_{11} &= 1 + \frac{\mu_1}{\bar{k}r_1}, & Q_{12} &= 2 - 3\frac{\kappa_1}{\mu_1} + \frac{3\kappa_1 - 2\mu_1}{2\bar{k}r_1}, \\ Q_{13} &= -1 + \frac{\mu_2}{\bar{k}r_1}, & Q_{14} &= -2 + 3\frac{\kappa_2}{\mu_2} + \frac{3\kappa_2 - 2\mu_2}{2\bar{k}r_1}, \\ Q_{15} &= -3 - \frac{12\mu_2}{\bar{k}r_1}, & Q_{16} &= -3 - 3\frac{\kappa_2}{\mu_2} - \frac{9\kappa_2 + 4\mu_2}{\bar{k}r_1}, \\ Q_{21} &= 1 + \frac{\mu_1}{\bar{k}r_1}, & Q_{22} &= -\frac{11}{3} - 5\frac{\kappa_1}{\mu_1} + \frac{24\kappa_1 + 5\mu_1}{3\bar{k}r_1}, \\ Q_{23} &= -1 + \frac{\mu_2}{\bar{k}r_1}, & Q_{24} &= \frac{11}{3} + 5\frac{\kappa_2}{\mu_2} + \frac{24\kappa_2 + 5\mu_2}{3\bar{k}r_1}, \\ Q_{25} &= 2 + \frac{8\mu_2}{\bar{k}r_1}, & Q_{26} &= -2 + \frac{3\kappa_2}{\bar{k}r_1}, \\ Q_{31} &= 2\mu_1 - \frac{\bar{\lambda} + \bar{\mu}}{r_1}, & Q_{32} &= 3\kappa_1 - 2\mu_1 + \frac{[9\kappa_1 + 15\mu_1][\bar{\lambda} + \bar{\mu}]}{\mu_1 r_1}, \\ Q_{33} &= -2\mu_2 - \frac{\bar{\lambda} + \bar{\mu}}{r_1}, & Q_{34} &= -3\kappa_2 + 2\mu_2 + \frac{[9\kappa_2 + 15\mu_2][\bar{\lambda} + \bar{\mu}]}{\mu_2 r_1}, \\ Q_{35} &= 24\mu_2 + \frac{12[\bar{\lambda} + \bar{\mu}]}{r_1}, & Q_{36} &= 18\kappa_2 + 8\mu_2 + \frac{6\kappa_2[\bar{\lambda} + \bar{\mu}]}{\mu_2 r_1}, \\ Q_{41} &= 2\mu_1 + \frac{[\bar{\lambda} + \bar{\mu}] + 2\bar{\mu}}{r_1}, & Q_{43} &= -2\mu_2 + \frac{[\bar{\lambda} + \bar{\mu}] + 2\bar{\mu}}{\mu_2 r_1}, \\ Q_{45} &= -16\mu_2 + \frac{4[3\bar{\lambda} + 4\bar{\mu}]}{r_1}, & Q_{46} &= -6\kappa_2 + \frac{-6\kappa_2[\bar{\lambda} + \bar{\mu}] + 4\mu_2\bar{\mu}}{\mu_2 r_1}, \end{aligned}$$

$$\begin{aligned}
Q_{51} &= Q_{52} = Q_{61} = Q_{62} = 0, & Q_{53} &= Q_{63} = 1, \\
Q_{54} &= \left[2 - 3 \frac{\kappa_2}{\mu_2} \right] f^{-2/3}, & Q_{55} &= 3f^{5/3}, \\
Q_{56} &= \left[3 + 3 \frac{\kappa_2}{\mu_2} \right] f, & Q_{64} &= - \left[\frac{11}{3} + 5 \frac{\kappa_2}{\mu_2} \right] f^{-2/3}, \\
Q_{65} &= -2f^{5/3}, & Q_{66} &= 2f, \\
Q_{42} &= -16\kappa_1 - \frac{10}{3}\mu_1 + -\frac{\kappa_1 [9\bar{\lambda} + 19\bar{\mu}]}{\mu_1 r_1} - \frac{[45\bar{\lambda} + 67\bar{\mu}]}{3r_1}, \\
Q_{44} &= 16\kappa_2 + \frac{10}{3}\mu_2 + -\frac{\kappa_2 [9\bar{\lambda} + 19\bar{\mu}]}{\mu_2 r_1} - \frac{[45\bar{\lambda} + 67\bar{\mu}]}{3r_1},
\end{aligned}$$

C.2.3 Lower bound on shear modulus

The far field stress field in this case led to the displacement field according to Eq. (3.88) with the eight unknowns $\Xi_1^{(1)}$, $\Xi_2^{(1)}$, $\Xi_3^{(1)}$, $\Xi_4^{(1)}$, $\Xi_1^{(2)}$, $\Xi_2^{(2)}$, $\Xi_3^{(2)}$ and $\Xi_4^{(2)}$. We concluded that since the displacement fields at the center of the RVE must be finite, $\Xi_3^{(1)}$ and $\Xi_4^{(1)}$ must vanish. The remaining six unknowns are determined using the below system which is deduced from the conditions (3.97)–(3.102)

$$\begin{bmatrix}
Q_{11} & Q_{12} & Q_{13} & Q_{14} & Q_{15} & Q_{16} \\
Q_{21} & Q_{22} & Q_{23} & Q_{24} & Q_{25} & Q_{26} \\
Q_{31} & Q_{32} & Q_{33} & Q_{34} & Q_{35} & Q_{36} \\
Q_{41} & Q_{42} & Q_{43} & Q_{44} & Q_{45} & Q_{46} \\
Q_{51} & Q_{52} & Q_{53} & Q_{54} & Q_{55} & Q_{56} \\
Q_{61} & Q_{62} & Q_{63} & Q_{64} & Q_{65} & Q_{66}
\end{bmatrix}
\begin{bmatrix}
\Xi_1^{(1)} \\
\Xi_2^{(1)} \\
\Xi_1^{(2)} \\
\Xi_2^{(2)} \\
\Xi_3^{(2)} \\
\Xi_4^{(2)}
\end{bmatrix}
=
\begin{bmatrix}
0 \\
0 \\
0 \\
0 \\
1 \\
1
\end{bmatrix}, \quad (C.12)$$

The components of $\mathbf{Q}$ read

$$\begin{aligned}
Q_{11} &= 1 + \frac{\mu_1}{\bar{k}r_1}, & Q_{12} &= 2 - 3\frac{\kappa_1}{\mu_1} + \frac{3\kappa_1 - 2\mu_1}{2\bar{k}r_1}, \\
Q_{13} &= -1 + \frac{\mu_2}{\bar{k}r_1}, & Q_{14} &= -2 + 3\frac{\kappa_2}{\mu_2} + \frac{3\kappa_2 - 2\mu_2}{2\bar{k}r_1}, \\
Q_{15} &= -3 - \frac{12\mu_2}{\bar{k}r_1}, & Q_{16} &= -3 - 3\frac{\kappa_2}{\mu_2} + \frac{9\kappa_2 + 4\mu_2}{\bar{k}r_1}, \\
Q_{21} &= 1 + \frac{\mu_1}{\bar{k}r_1}, & Q_{22} &= -\frac{11}{3} - 5\frac{\kappa_1}{\mu_1} + \frac{24\kappa_1 + 5\mu_1}{3\bar{k}r_1}, \\
Q_{23} &= -1 + \frac{\mu_2}{\bar{k}r_1}, & Q_{24} &= \frac{11}{3} + 5\frac{\kappa_2}{\mu_2} + \frac{24\kappa_2 + 5\mu_2}{3\bar{k}r_1}, \\
Q_{25} &= 2 + \frac{8\mu_2}{\bar{k}r_1}, & Q_{26} &= -2 + \frac{3\kappa_2}{\bar{k}r_1}, \\
Q_{31} &= 2\mu_1 - \frac{r_1}{\bar{\lambda} + \bar{\mu}}, & Q_{32} &= 3\kappa_1 - 2\mu_1 + \frac{[9\kappa_1 + 15\mu_1][\bar{\lambda} + \bar{\mu}]}{\mu_1 r_1}, \\
Q_{33} &= -2\mu_2 - \frac{r_1}{\bar{\lambda} + \bar{\mu}}, & Q_{34} &= -3\kappa_2 + 2\mu_2 + \frac{[9\kappa_2 + 15\mu_2][\bar{\lambda} + \bar{\mu}]}{\mu_2 r_1}, \\
Q_{35} &= 24\mu_2 + \frac{12[\bar{\lambda} + \bar{\mu}]}{r_1}, & Q_{36} &= 18\kappa_2 + 8\mu_2 + \frac{6\kappa_2[\bar{\lambda} + \bar{\mu}]}{\mu_2 r_1}, \\
Q_{41} &= 2\mu_1 + \frac{[\bar{\lambda} + \bar{\mu}] + 2\bar{\mu}}{r_1}, & Q_{43} &= -2\mu_2 + \frac{[\bar{\lambda} + \bar{\mu}] + 2\bar{\mu}}{r_1}, \\
Q_{45} &= -16\mu_2 + \frac{4[3\bar{\lambda} + 4\bar{\mu}]}{r_1}, & Q_{46} &= -6\kappa_2 + \frac{-6\kappa_2[\bar{\lambda} + \bar{\mu}] + 4\mu_2\bar{\mu}}{\mu_2 r_1}, \\
Q_{51} &= Q_{52} = Q_{61} = Q_{62} = 0, & Q_{53} &= Q_{63} = 2\mu_2, \\
Q_{54} &= [3\kappa_2 - 2\mu_2]f^{-2/3}, & Q_{55} &= -24\mu_2 f^{5/3}, \\
Q_{56} &= -[18\kappa_2 + 8\mu_2]f, & Q_{64} &= -\left[16\kappa_2 + \frac{10}{3}\mu_2\right]f^{-2/3}, \\
Q_{65} &= 16\mu_2 f^{5/3}, & Q_{66} &= 6\kappa_2 f,
\end{aligned}$$

$$\begin{aligned}
Q_{42} &= -16\kappa_1 - \frac{10}{3}\mu_1 + \frac{\kappa_1[9\bar{\lambda} + 19\bar{\mu}]}{\mu_1 r_1} - \frac{[45\bar{\lambda} + 67\bar{\mu}]}{3r_1}, \\
Q_{44} &= 16\kappa_2 + \frac{10}{3}\mu_2 + \frac{\kappa_2[9\bar{\lambda} + 19\bar{\mu}]}{\mu_2 r_1} - \frac{[45\bar{\lambda} + 67\bar{\mu}]}{3r_1},
\end{aligned}$$