Application of the multiscale FEM to the modeling of nonlinear composites with a random microstructure

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Abstract

In this contribution the properties and application of the multiscale finite element program MS-FEAP are presented. This code is developed on basis of the coupling the homogenization theory with the finite element method. According to this concept, the investigation of an appropriately chosen representative volume element yields the material parameters needed for the simulation of a macroscopic body. The connection of scales is based on the principle of volume averaging and the Hill-Mandel macrohomogeneity condition. The latter leads to the determination of different types of boundary conditions for the representative volume element and in this way to the postulation of a well-posed problem at this level. The numerical examples presented in the contribution investigate the effective material behavior of microporous media. An isotropic and a transversally anisotropic microstructure are simulated by choosing an appropriate orientation and geometry of the representative volume element in each Gauss point. The results are verified by comparing them with Hashin-Shtrikman’s analytic bounds. However, the chosen examples should just be understood as an illustration of the program application, while its main feature is a modular structure suitable for further development.

1 Introduction

In contrast to linear composite materials, whose modeling is already well investigated [2, 5, 6, 10, 11, 20, 22, 29], the modeling of nonlinear composites is a relatively new subject. The first results in this field were obtained by Talbot and Willis [28] whose procedure is an extension of the Hashin-Shtrikman method [7, 8, 9] developed for linear composites. The approach of Talbot and Willis suggests the energy bounds of a nonlinear composite by using the concept of a comparison linear homogeneous body. The main disadvantage arising here is the duality gap between the bounds obtained by using principles of minimum potential energy and minimum complementary energy. This problem is overcome in the work by Castañeda presenting the so-called new variational principle [3, 4]. Here the idea of the linear heterogeneous comparison body is introduced but the construction of the upper bound still is an open issue. Note that these and similar analytic solutions have just a limited field of application, due to their complexity. This gives rise to the intensive development of numerical methods such as the secant method [23, 27], the partitioning method [13, 14, 15], the adaptive hierarchical modeling method [24, 31] and the micro-macro domain decomposition method [32, 33].

In the scope of this contribution, attention is particularly paid on the concept and application of the multiscale finite element (FEM) [16, 18, 21, 25]. This method shows two important advantages in comparison with other numerical approaches. It is applicable for the solution of problems where finite deformations occur and for the limit cases when the ratio of the characteristic lengths of the scales tends to zero. The method will be presented in the following way: Sec. 2 briefly explains the idea of the homogenization theory, the field of its application, and a possible limitation. After the definition
of macroscopic quantities depending on the microscopic ones, the periodic boundary conditions for a 
representative volume element (RVE) are discussed. The chapter also includes the description of the 
corresponding program code. Sec. 3 and 4 deal with the application of the method for the particular 
case of energy functional in three-field description. Sec. 3 explains in detail the standard, single-
scale formulation while Sec. 4 focuses on the multiscale formulation by emphasizing the differences 
between the scales. Finally, the effective material parameters of randomly microporous media as 
an example of the practical application are investigated in Sec. 5. To this end, a square RVE with 
an elliptic void is proposed and the change of the effective material parameters with the increasing 
porosity is studied. A further elucidating example considers transversal anisotropy and is presented 
in Sec. 6. The paper closes with a brief outlook and conclusions.

2 Concept of the homogenization theory 
and structure of the program

As a kind of homogenization method, the multiscale FEM is applied for statistically uniform mate-
rials. This notion is strongly related to the notion of RVE which should be understood as a material 
sample whose investigation yields the effective material properties. However, in order to define an 
RVE, attention must be paid on a few limitations: the ratio of the characteristic lengths of the assumed 
RVE and of a corresponding homogeneous macroscopic body must tend to zero, but simultaneously 
the RVE must be big enough to contain all necessary information on the material microstructure. 
If such an RVE can be defined, it is possible to give the following definitions for the macroscopic 
quantities [12, 21, 25]

\[ \bar{F} = \frac{1}{V} \int_{B} F dV - \int_{L} x \otimes N dA = \frac{1}{V} \int_{\partial B} x \otimes N dA, \]  
(1)

\[ \bar{P} = \frac{1}{V} \int_{B} P dV = \frac{1}{V} \int_{\partial B} T \otimes X dA, \]  
(2)

where the notation typical for the theory of the finite deformations is used. \( X \) is the position vector, 
\( N \) is the normal vector to the surface, \( F \) is the deformation gradient, \( P \) the first Piola Kirchhoff stress 
tensor and \( T \) the traction. The uppercase letters are related to the reference configuration and the 
lower case letters to the current configuration. The averaging is performed over the volume \( V \) of the 
RVE \( B \) with the boundary \( \partial B \) and the boundary of the voids inside the RVE \( L \). The definitions satisfy 
the Hill postulate that the macroquantities have to be defined depending on the microquantities acting 
on the boundary of the RVE. The connection of the scales also requires the equality of the macropower 
with the volume average of the micropower, which can be expressed in two different ways

\[ P : F = \frac{1}{V} \int_{B} P : F dV \quad \Leftrightarrow \quad \frac{1}{V} \int_{\partial B} (T - \bar{P} N) \cdot (x - \bar{F} X) dA = 0. \]  
(3)

The previous condition is known as Hill-Mandel macrohomogeneity condition and it is used to define 
the possible boundary conditions on the microlevel. Two of them, the static and the kinematic one, 
can be determined directly from (3)_2

\[ T = \bar{P} \cdot N \quad \text{on } \partial B \quad \text{- static b.c.} \]  
(4)

\[ x = \bar{F} \cdot X \quad \text{on } \partial B \quad \text{- kinematic b.c.} \]  
(5)
but for the purposes of this contribution only the periodic boundary conditions shall be considered. In this case the deformation takes the form dependent on the macrodeformation gradient $\bar{F}$ and microfluctuations $\tilde{w}$

$$x = \bar{F}X + \tilde{w}$$  \hspace{1cm} (6)

which after the implementation in (3) yields the conclusion that the microfluctuations $\tilde{w}$ have to be periodic and the tractions $T$ antiperiodic on the periodic boundary of the RVE in order to fulfill Hill macrohomogeneity condition:

$$\tilde{w}^+ = \tilde{w}^- \text{ and } T^+ = -T^-$$  \hspace{1cm} (7)

Assumption (6) for the deformation leads to the additive decomposition of the microdeformation gradient

$$F = \text{Grad } x = \bar{F} + \text{Grad } \tilde{w} = \bar{F} + \tilde{F}.$$  \hspace{1cm} (8)

The described concept (1)-(8) and the standard FEM program FEAPpv [30] are also used in order to write a multiscale FEM-program whose simplified structure is shown in Fig. 1.

**Figure 1: The structure of the multiscale finite element program MSFEAP.**

This figure shows that the standard structure of the program is kept on the macrolevel up to the moment when the definition of the constitutive law inside the element subroutine is needed. As this definition is not available, macrolevel calculations are necessary. To this end, a bridging subroutine makes a backup of the data used on the macrolevel, and the subroutines identical to those on the macrolevel can be called for the microlevel calculations. The macrodeformation gradient on this level...
is understood as a given quantity while the primary results are the distribution of the microfluctuations \( \tilde{w} \) and the first Piola Kirchhoff microstress tensor \( \mathbf{P} \). The volume average of the latter is the sought counterpart on the macrolevel. After finishing the calculations at the microlevel the data related to this level can be deleted and the bridging subroutine recalls the data needed for the macrolevel. In this way macroscale calculations can be continued. The microscale subprogram is called for calculating the effective stresses as well as their derivatives (see Chap. 4). Such calculations are repeated in each Gauss point for each step of the Newton-Raphson iteration (nonlinear materials) and if necessary, for each step of the time iteration (time dependent problems). In the case of the linear material, the procedure is much simpler [17]. Here the effective elasticity tensor must be calculated only once as it is independent from deformation.

Flow chart (Fig. 1) shows the flexible structure of the program, allowing for a simple implementation of the new elements at both levels, and accordingly possible implementations in many different fields. Moreover, it shows that all commands needed for the pre- and postprocessing can be applied at two levels. Their transcription as well as the user interface remain as in the original program FEAPpv. Finally, it is important to note that the program can still be used for single-scale calculations by choosing original elements of the program FEAPpv at the macrolevel. These elements are not connected with the bridging subroutine and they do not activate the program part responsible for microscale calculations.

3 Standard formulation of the P0Q1 element

The implementation of the method will be shown in a particular example concerning the energy potential in a three-field description as proposed by Simo, Taylor and Pister [26]

\[
\Pi(\mathbf{u}, \Theta, p) = \int_V \left[ \psi_{\text{vol}}(\Theta) + \psi_{\text{dev}}(\mathbf{C}^*(\mathbf{u})) + p(J(u) - \Theta) \right] dV + \Pi^{\text{ext}}. \tag{9}
\]

Apart from the displacements which are primary variables, this formulation also depends on the volume change \( \Theta \) and the pressure \( p \). The functional is split in a volumetric and a deviatoric part where the volumetric part only depends on the volume change \( \Theta \) and the deviatoric part on the deviatoric right Cauchy-Green deformation tensor \( \mathbf{C}^* = J^{-2/3} \mathbf{C} \) where \( J = \det \mathbf{F} \) represents the Jacobian. The last part of (9) represents the Lagrange term introduced in order to stipulate the equality of the determinant of the Jacobian and the volume change. For the purpose of formulating the corresponding finite element, the second variation of (9) is needed

\[
\begin{align*}
\int_V \text{Grad} \delta \mathbf{u} : [\text{Grad} \Delta \mathbf{u} \cdot (\mathbf{S}_{\text{dev}} + \mathbf{S}_{\text{vol}})]dV \\
+ \int_V (\text{Grad}^T \delta \mathbf{u} \cdot \mathbf{F}) : (\mathbf{A}_{\text{dev}} + \mathbf{A}_{\text{vol}}) : (\mathbf{F}^T \cdot \text{Grad} \Delta \mathbf{u}) dV \\
+ \int_V (\text{Grad}^T \delta \mathbf{u} \cdot \mathbf{F}) : J \mathbf{C}^{-1} dV \left( \frac{1}{V} \frac{\partial^2 \psi_{\text{vol}}}{\partial \Theta^2} \right) \int_V J \mathbf{C}^{-1} : (\mathbf{F}^T \cdot \text{Grad} \Delta \mathbf{u}) dV \\
+ \Delta \delta \mathbf{u} \Pi^{\text{ext}} = -\delta \Pi^{\text{ext}}. \tag{10}
\end{align*}
\]

Keep in mind that the first variation is necessary in order to satisfy the stationarity condition and the second one in order to linearize the problem. The elasticity tensors \( \mathbf{A}_{\text{dev}} \) and \( \mathbf{A}_{\text{vol}} \) appearing in (10) are defined in the terms of the second Piola Kirchhoff stress tensors \( \mathbf{S}_{\text{dev}} \) and \( \mathbf{S}_{\text{vol}} \) as follows

\[
\begin{align*}
\mathbf{A}_{\text{dev}} &= 2 \frac{\partial \mathbf{S}_{\text{dev}}}{\partial \mathbf{C}}, & \mathbf{A}_{\text{vol}} &= 2 \frac{\partial \mathbf{S}_{\text{vol}}}{\partial \mathbf{C}}. \tag{11}
\end{align*}
\]
and the derivative of pressure has to be calculated according to
\[
\frac{\partial^2 \Psi}{\partial \Theta^2} = \frac{\partial p}{\partial J} = \frac{2}{3} J \frac{\partial p}{\partial C} : C^*.
\] (12)

The final step in the formulation of the element is the implementation of the approximation dependent on the shape functions and nodal values. Without going into details, which can be found in the literature about the FEM [1, 19, 30], this approximation can be expressed in the following way
\[
\begin{align*}
u &= N \cdot \hat{u}^e, \\
B &= \text{Grad } N, \\
\text{Grad } \Delta u &= B \cdot \Delta \hat{u}^e, \\
\text{Grad } \delta u &= B \cdot \delta \hat{u}^e.
\end{align*}
\] (13)

Here \(N\) is a matrix containing the shape functions and \(B\) is a matrix containing the derivatives of the shape functions. A hat symbol denotes the nodal values and \(e\) indicates that all the DOFs of an element are considered. The implementation of (13) into (10) leads to the final form of the stiffness matrix \(K^e\)
\[
K^e = \int_{V^e} G^T \cdot (S_{dev} + S_{vol}) \cdot G \, dV
\]
\[
+ \int_{V^e} (B^T \cdot F) : A : (F^T \cdot B) \, dV
\]
\[
+ \int_{V^e} (B^T \cdot F) : J C^{-1} dV \left( \frac{1}{V} \frac{\partial^2 \Psi_{vol}}{\partial \Theta^2} \right) \int_{V^e} J C^{-1} : (F^T \cdot B) \, dV
\] (14)

with matrix \(G\) being defined in the following way
\[
\int_{V^e} \text{Grad } \delta \hat{u} : [\text{Grad } \Delta u \cdot (S_{dev} + S_{vol})] dV = \delta \hat{u} \cdot \int_{V^e} [G^T \cdot (S_{dev} + S_{vol}) \cdot G] dV \cdot \Delta \hat{u}.
\] (15)

4 Multiscale formulation

Relating now the theory explained in Chap. 2 with the formulation given in Chap. 3, the following formulation of the problem of the simulation of a heterogeneous body can be given. At the macroscale, expression (10) remains unchanged except that the typical notation (overbar symbol) has to be used. The completion of the problem still requires that Dirichlet and Neumann boundary conditions are satisfied
\[
\int_{\bar{V}} \text{Grad } \delta \bar{u} : [\text{Grad } \Delta \bar{u} \cdot (\bar{S}_{dev} + \bar{S}_{vol})] d\bar{V}
\]
\[
+ \int_{\bar{V}} (\text{Grad}^T \delta \bar{u} \cdot \bar{F}) : (\bar{A}_{dev} + \bar{A}_{vol}) : (\bar{F}^T \cdot \text{Grad} \Delta \bar{u}) d\bar{V}
\]
\[
+ \int_{\bar{V}} (\text{Grad}^T \delta \bar{u} \cdot \bar{F}) : J \bar{C}^{-1} d\bar{V} \left( \frac{1}{\bar{V}} \frac{\partial^2 \bar{\Psi}_{vol}}{\partial \bar{\Theta}^2} \right) \int_{\bar{V}} J \bar{C}^{-1} : (\bar{F}^T \cdot \text{Grad} \Delta \bar{u}) d\bar{V}
\]
\[
+ \Delta \delta \bar{u} \bar{\Pi}^{res} = -\delta \bar{u} \bar{\Pi}^{res}
\]
\[
\bar{u} = \bar{u}_0, \quad \delta \bar{u} = 0, \quad \Delta \bar{u} = 0 \quad \text{on } \partial \bar{B}_u.
\] (16)
Contrary to the situation in the case of the standard single-scale method, here the terms dependent on the constitutive law \((\bar{S}_{\text{dev}}, \bar{S}_{\text{vol}}, \bar{A}_{\text{dev}}, \bar{A}_{\text{vol}}, \frac{\partial^2 \Psi_{\text{vol}}}{\partial \Theta^2})\) cannot be calculated directly but by using the data from the microscale. The formulation at this level is similar to (16) and consequently to (10) but it is not identical:

\[
\int_V \text{Grad} \delta \tilde{w} : (\text{Grad} \Delta \tilde{w} \cdot (\bar{S}_{\text{dev}} + \bar{S}_{\text{vol}}))dV \\
+ \int_V (\text{Grad}^T \delta \tilde{w} \cdot F) : (\bar{A}_{\text{dev}} + \bar{A}_{\text{vol}}) : (F^T \cdot \text{Grad} \Delta \tilde{w})dV \\
+ \int_V (\text{Grad}^T \delta \tilde{w} \cdot F) : J C^{-1} \int_V \frac{1}{V} \frac{\partial^2 \Psi_{\text{vol}}}{\partial \Theta^2} \int_V J C^{-1} : (F^T \cdot \text{Grad} \Delta \tilde{w})dV \\
+ \delta \tilde{w} \Pi_{\text{res}} = -\delta \tilde{w} \Pi_{\text{res}} \\
\tilde{w}^+ = \tilde{w}^-, \quad \tilde{w} = 0, \quad \Delta \tilde{w} = 0 \quad \text{on} \quad \partial B; \quad \delta \tilde{w} \Pi_{\text{res}} = f(\bar{F}).
\]

Here the problem depends on the microfluctuations \(\tilde{w}\), and the macrodeformation gradient \(\bar{F}\) is responsible for the residual part \(\delta \tilde{w} \Pi_{\text{res}}\) which should be treated analogously to the residual due to the deformation from the previous step of the Newton-Raphson iteration. The influences of the body forces are neglected and the periodic boundary conditions have to be satisfied.

## 5 Simulation of random microporous media

### 5.1 Tension and shear test of a plate

The application of the method is illustrated by simulating the tension test of a square plate with a side length 40 mm and the vertical uniform load \(p = 1\) kN/mm acting on the horizontal boundaries of the plate. Due to the double symmetry, it is sufficient to simulate only one fourth of the plate where the vertical displacements on the lower boundary and the horizontal displacements on the left boundary are constrained (Fig. 2).

![Figure 2: Tension test of a plate with a random microporous structure.](image)

A periodic microstructure is assumed in the surrounding area of each Gauss point, while the RVEs with different orientations correspond to different Gauss points. This simulates a random microporous structure. The RVE is chosen to be a unit square with an elliptical pore and its geometry is shown in Fig. 3a. Here the side length is denoted by \(2d=1\) mm, the major axis of the pore by \(2a\) and its minor axis by \(2b\).
Figure 3: a) RVE with an elliptical pore. Three groups of tests with a fixed major axis are simulated: b) \( a = d/4 \), c) \( a = 2d/4 \), d) \( a = 3d/4 \). The ellipticity \( b/a \) takes values in the interval \([0,1]\) for each group of tests.

For an exact definition of the matrix material at the microlevel, the Neo Hook constitutive law

\[
\Psi = \Psi_{\text{dev}} + \Psi_{\text{vol}} = \frac{1}{2} \mu (\text{tr} \, C^* - 3) + K (J \ln J - J + 1)
\]  

(18)

and the material parameters \( E = 1000 \text{ N/mm}^2 \), \( \nu = 0.3 \) are assumed in all examples.

Subsequently, the results of three groups of tests with different lengths of the major axis (Fig. 3b-d) will be discussed. In the first case, the major axis is fixed as \( a = d/4 \), \( a = 2d/4 \) in the second, and as \( a = 3d/4 \) in the last case. Ellipticity \( b/a \) changes in each group of tests, taking values from 0 to 1. Ellipticity 0 means that a pore has just appeared and its width is equal to zero, ellipticity 1 corresponds to circular voids. Some of the intermediate results at the microscale are shown in Fig. 4, just as an illustration.

Figure 4: Presentation of the random microstructure and plot of the 11-term of the first Piola Kirchhoff stress tensor at the microlevel. The first Piola Kirchhoff stress tensor is an intermediate result of a tension test for a plate with a random orientation of RVEs.

The final results, the macromaterial parameters \( E \) and \( \nu \), are calculated using displacements on the unconstrained boundaries of the plate at the macrolevel. These results are shown in Fig. 5, where both parameters are seen decreasing with the appearance of pores, while Young’s modulus decreases and Poisson’s ratio increases with their growth. Naturally the pores with the bigger major axis have a more significant influence.
Similar tests are conducted in order to calculate the shear modulus. This time a square plate with a side length of 20 mm is considered under the horizontal load \( p = 1 \, \text{kN/mm} \). Because of the horizontal symmetry, one half of the plate having constrained horizontal and vertical displacements on the lower horizontal boundary is sufficient for a simulation. In order to avoid effects of buckling, vertical displacements are also constrained along all remaining boundaries (Fig. 6a). As in the case of the tension test, three groups of tests are simulated for the fixed major axis \( a \) and the changeable ellipticity \( b/a \). Figure 6b shows that the shear modulus \( \mu \) behaves similarly to Young’s modulus (Fig. 5a). With the appearance of pores it decreases at once and with growing pore size it decreases gradually. The values of the shear modulus obtained by the shear test are compared with the shear modulus calculated with Young’s modulus \( E \) and Poisson’s ratio \( \nu \) from the tension test. This comparison shows that the difference is almost negligible, being 0.4% for the smallest major axis and 1.5% for the longest one.

Figure 5: Changes in Young’s modulus and Poisson’s ratio for different pore sizes.

5.2 Comparison with the Hashin-Shtrikman bounds

In order to verify the quality of the simulations, the results shown in Figs. 5 and 6b are compared with the analytical Hashin-Shtrikman bounds. Here, in order to simplify the check procedure, we assumed that the structural element remains in the domain of small deformations. In contrast to the general
case, the Hashin-Shtrikman bounds for two-phase materials have a much simpler form

\[
K_l = K_1 + \frac{c_2}{K_2 - K_1} \frac{1}{3K_1 + 4\mu_1}, \quad \text{a)} \\
K_u = K_2 + \frac{c_1}{K_1 - K_2} \frac{1}{3K_2 + 4\mu_2}, \quad \text{b)}
\]

(19)

\[
\mu_l = \mu_1 + \frac{c_2}{\mu_2 - \mu_1} \frac{6(K_1 + 2\mu_1)c_1}{5\mu_1(3K_1 + 4\mu_1)}, \quad \text{a)} \\
\mu_u = \mu_2 + \frac{c_1}{\mu_1 - \mu_2} \frac{6(K_2 + 2\mu_2)c_2}{5\mu_2(3K_2 + 4\mu_2)}.
\]

(20)

Here, the subscripts \(l, u\) denote the lower and upper bound respectively, and phases are chosen so that \(K_2 > K_1\) and \(\mu_2 > \mu_1\). Their volume concentrations are denoted by \(c_1\) and \(c_2\). The microporous material represents a two-phase material so that the expressions above can be applied directly. However, as the material parameters of voids are equal to zero, the lower bounds (19)a and (20)a reduce to zero and only the upper bounds remain.

Figure 7 shows the change in the bulk modulus \(K\) and the shear modulus \(\mu\) with respect to the porosity \(p\) which is equal to the volume faction of voids \(p = c_1 = \frac{V_1}{V}\). The diagrams show that the values obtained by the homogenization procedure really lie beneath the upper Hashin-Shtrikman bound, endorsing that the results are in the allowed domain. In each of the diagrams, the diagram representing the data obtained by the multiscale method has three separate parts, one for each group of tests in which the major axis \(a\) is fixed. The line on the top corresponds to the RVE with a pore of width \(a = d/4\), the middle one to the RVE with a pore of width \(a = d/2\), and the bottom most one corresponds to case \(a = 3d/4\). This shows that materials with the same porosity but different shapes of micropores have different material parameters. More precisely, the strength of materials with the same porosity decreases more significantly for elongated voids than for circular voids.

Figure 7: Comparison with the Hashin-Shtrikman upper bound for the bulk and shear modulus.

A diagram for Young’s modulus is shown in Fig. 8, where the lower bound also reduces to zero. The Hashin-Shtrikman method is not appropriate for the Poisson’s ratio, as the standard constraint \(0 < \nu < 0.5\) is stricter than the Hashin-Shtrikman bounds.

### 6 Transversal anisotropy

A further application example is concerned with the modeling of materials with transversal anisotropy and to this end, the situation presented in Fig. 9 is considered. Here, a macroplate is assumed like in Chap. 5. The difference is that the orientation of the RVEs for all Gauss points is constant. As the material behavior is expected to be different in the directions \(x_1\) and \(x_2\), two tension tests are
simulated. In the first case, the load direction is perpendicular to the direction of the major axis of pores (Fig 9a), and in the second case the load is parallel with it (Fig. 9b).

![Figure 9: Two tension tests for a macroplate with a polarized microstructure.](image)

The final results of the tests are displacements of the unconstrained boundaries of the macroplate, and their dependency on the pore size is shown in Fig. 10. The increasing porosity is simulated by increasing the ellipticity in the range [0,1] while the semimajor axis of the micropore is kept constant: \( a = d/2 \). Figure 10a shows the displacements of the loaded edges of the macroscopic plate and Figure 10b the displacements of the free boundaries. As expected, the values of the displacements get closed with increasing ellipticity and finally, for the circular shape of pores, they become equal to each other. Note that index 1 denotes the horizontal and 2 the vertical direction.

The limit case previously described occurs rarely in reality. Such a regular structure might be met in some synthetic, man-made materials. In the case of natural materials, it can almost be excluded. The orientation of the RVEs having a predominant direction in the sense of the middle value is a more realistic case. The following example considers a case where the orientation is taken from the Gauss distribution defined by the expression

\[
f(x, \mu, \sigma) = \frac{1}{\sigma \sqrt{2\pi}} \exp\left(-\frac{(x - \mu)^2}{2\sigma^2}\right)
\]  

(21)
where \( x \) is a variable, \( \mu \) is the average and \( \sigma \) is the deviation. Our final tests consider the situation presented in Fig. 9 where, as has been shown, orientation of the RVEs corresponds to zero for the middle value of the Gauss distribution. In different tests, the deviation takes values from the range \([0,100]\) with step 10. Only one type of RVE, with the geometrical parameters \( d=0.5\text{mm}, a=d/2 \) and \( b=a/2 \), represents the microstructure in all cases.

The calculated displacements for the unconstrained boundaries of the macroplate are shown in Fig. 11. Here the first diagram (Fig. 11a) shows that the vertical displacements of the loaded boundary in the first test decrease and that the horizontal displacements of the loaded edge in the second test increase. The displacement change is fast in the range between \(10^\circ\)–60\(^\circ\) and moderate elsewhere. The displacements of the free boundaries (Fig. 11b) change rapidly for deviations of \(0^\circ\)–30\(^\circ\) and after that the values of the displacements stagnate and get closer to each other. By the deviation of \(90^\circ\)–100\(^\circ\), for the loaded as well as for the unloaded boundary, the displacements obtained in the different tests become nearly equal. This was to be expected as the variation of \(90^\circ\) means that the orientation can vary with a relatively high expectation in the range from -90\(^\circ\) up to 90\(^\circ\) which, because of the symmetry of the RVE, corresponds to the completely random microstructure and uniform distribution of the orientation. This is also endorsed by a comparison with the values of displacements that are obtained using the model explained in Chap. 5.1. The values obtained in these two ways are practically the same: a uniform distribution yields the displacements 0.02460 mm for the loaded and -0.00958 mm for the free boundary and the simulation with the orientation taken from the Gauss distribution by the deviation 90\(^\circ\), reads the corresponding values 0.02460 mm and -0.00957 mm.

Figure 11: Displacements on the loaded (a) and the free boundary (b). Change wrt. deviation is considered.
7 Conclusions

In this contribution, the main features and some examples of application of the multiscale finite element code MSFEAP are presented. The underlying procedure belongs to the group of homogenization methods according to which the problem of modeling a heterogeneous body is split into two parts. The first part represents an analysis of the RVE leading to the effective material parameters, and the second part consists in the application of the so obtained effective values for the simulation of the macroscopic, now homogenized body. These two parts known as the macro and micro boundary value problem are bridged by the Hill macrohomogeneity condition and the concept of the volume average. The presented program has a modular structure which allows a simple adaptation for the use in different fields. Another advantage is the possibility of the application of commands typical for an FE software at two levels.

An illustrative example concerns the simulation of a macroscopic plate under tension and shear load. In all examples the unit square-shaped RVE with the elliptical pore represents the microstructure. The influence of the RVE orientation and the pore size on the effective behavior are especially considered. The first group of tests elaborates the isotropic material behavior which is achieved choosing an arbitrary orientation of RVE in each Gauss point. The here obtained results show that increasing porosity induces a decreasing Young’s and shear modulus and an increasing Poisson’s ratio. By the same porosity, the pores with a smaller ellipticity have a stronger influence on the parameter change. A comparison with the Hashin-Shtrikman bounds shows that all results are in the permitted domain. The further examples concern the transversal anisotropy. To this end the orientation of RVEs is constant or taken from the Gauss distribution. The final results provide an insight in the macroscopic deformation and its dependency on the deviation of the RVE-orientation.

References


