ASSESSMENT OF MIXED UNIFORM BOUNDARY CONDITIONS FOR PREDICTING THE MACROSCOPIC MECHANICAL BEHAVIOR OF COMPOSITE MATERIALS

Dieter H. Pahr and Helmut J. Böhm

Institute of Lightweight Design and Structural Biomechanics
Vienna University of Technology
Gusshausstr. 27–29/E317; 1040 Vienna, Austria
pahr@ilsb.tuwien.ac.at

ABSTRACT

Finite Element models can be used to study the macroscopic mechanical properties of inhomogeneous materials in more detail than experiments. Appropriate boundary conditions have to be applied to volume elements (VE) and "apparent" instead of "effective" overall elastic properties are usually computed ([1]). Typical BCs used in such works are kinematic uniform (KUBC), static uniform (SUBC), and periodic boundary (PBC) conditions. Less well known are uniform displacement-traction (orthogonal mixed) BCs (MUBC) first prosed by [2], [3] and used by [4], [5]. Special MUBCs are proposed in [6]. This set of mixed BCs was found to be an excellent choice for extracting the full apparent elasticity tensors of nearly orthotropic cellular materials. Simulations of periodic and microscopically orthotropic volume elements give exactly the same overall elastic properties as those obtained by periodic BCs. Therefore, they are called periodic compatible MUBC (PMUBC). The advantage of PMUBCs is that they can be used for non-periodic inhomogeneous media at lower numerical costs and less modelling effort as periodic BCs. But in this case they provide only apparent overall properties. The objective of this study is to show how mixed uniform BCs work. Furthermore, existing volume elements from [7] (periodic micro geometries of particle and short fiber reinforced composites), [6] (trabecular bone, a biological cellular material) and [8] (woven fabric laminate) are investigated in the linear elastic regime using PMUBCs, PBCs, as well as KUBCs. In that way "apparent" and "effective" predictions for the macroscopic elastic tensors are obtained and can be compared in order to assess the accuracy of PMUBCs. In addition, some elastoplastic load cases involving PMUBCs and PBCs are studied.

1 Introduction

Continuum mechanics considerations are often based on the concept of a Representative Volume Element (RVE) which plays the role of a point of a continuum field approximating the true micro-structured material. The RVE is very clearly defined in two situations only [4] :

1. a unit cell in a periodic micro structure, and
2. a volume containing a very large (mathematically infinite) set of microscale elements,

possessing statistically homogeneous properties. In the case of an RVE, Hill [9] stated that the apparent moduli are effectively independent of the surface values of traction and displacement, as long as these values are macroscopically uniform. For a bounded space domain (denoted as volume element VE) the surface values influence the predictions. In such a case Hill [9] showed that the necessary and sufficient conditions for equivalence between the energetically and mechanically defined properties of elastic materials are contained in the so-called Hill condition (Hill-Mandel macrohomogeneity condition). This condition is satisfied by three different types of uniform boundary conditions for heterogeneous media [2], [4]:

1. uniform displacement (Dirichlet, kinematic, KUBC) boundary condition:

2. uniform traction (Neumann, static, SUBC) boundary condition:

3. uniform displacement-traction (orthogonal mixed, MUBC) boundary condition:

For a bounded space domain each of these mixed BCs yields different "apparent" but energetically and mechanically consistent stiffness tensors. Periodic boundary conditions (PBC) fulfill the Hill condition in the case of periodic micro structures [10], [11], [12] and effective properties are obtained also for a bounded space domain. In that case the VE becomes a unit cell and RVE, respectively.
Special MUBCs for non-periodic volume elements were recently proposed in [6]. There, it was found that the proposed mixed BCs give exactly the same effective elastic properties as periodic BCs if a material with orthotropic symmetry of phase arrangements (micro structure) is used and thus denoted as periodicity compatible MUBCs (PMUBCs). Unfortunately PMUBCs have some limitations which can be summarized as:

1. Mixed uniform boundary conditions in the sense of Hill must be orthogonal. They can be realized only in materials having at least orthotropic elastic symmetry at the macroscale and the volume elements have to be aligned in the axes of orthotropy [2], [3].

2. In order to fulfill the Hill condition the matrices of average stresses and strains need to be symmetric ([6]).

3. If the overall elastic properties of periodic BCs ([6]) should be obtained the micro structures have to be symmetric with respect to the axes of orthotropy (microscopically orthotropic material).

4. In the case of porous micro structures, displacement based boundary conditions are required in order to be able to obtain the average strains directly from the applied a priori strains ([6]).

The objective of this study is to demonstrate the applicability of PMUBCs to a wide range of composite materials if the first and third above statement are not fullfilled exactly. Therefore, a number of existing volume elements that describe periodic micro geometries pertinent to woven composites, particle and short fiber reinforced composites, and cellular materials are investigated. They are subjected to Finite Element analysis with PMUBCs, PBCs and in some case to KUBCs. Predictions for the macroscopic elasticity tensors and non-linear macroscopic responses under uniaxial load cases are also compared.

2 Methods and Materials

A special set of mixed boundary conditions - so called "periodicity compatible" MUBCs (PMUBCs) - are introduced for trabecular bone in a previous work ([6]). This set of BCs is summarized in Table 1 and describe six independent uni-axial strain load cases. ${}^0\varepsilon$ are a priori applied strains, u_i are the displacements at the boundary, t_i are the tractions at the boundary, and l_i the dimensions of a cubical volume element.

Table 1: Periodicity compatible mixed boundary conditions (PMUBC) applied on the sides of a volume element for six independent uniform strain load cases. East, West, North, South, Top, and Bottom denote the sides of the VE (from [6]).

	East	West	North	South	Top	Bottom
Tensile 1	$u_1 = {}^0\varepsilon_{11}\frac{l_1}{2}$ $t_2 = t_3 = 0$	$u_1 = -{}^0\varepsilon_{11}\frac{l_1}{2}$ $t_2 = t_3 = 0$	$u_2 = 0$ $t_1 = t_3 = 0$	$u_2 = 0$ $t_1 = t_3 = 0$	$u_3 = 0$ $t_1 = t_2 = 0$	$u_3 = 0$ $t_1 = t_2 = 0$
Tensile 2	$u_1 = 0$ $t_2 = t_3 = 0$	$u_1 = 0$ $t_2 = t_3 = 0$	$u_2 = {}^0\varepsilon_{22}\frac{l_2}{2}$ $t_1 = t_3 = 0$	$u_2 = -{}^0\varepsilon_{22}\frac{l_2}{2}$ $t_1 = t_3 = 0$	$u_3 = 0$ $t_1 = t_2 = 0$	$u_3 = 0$ $t_1 = t_2 = 0$
Tensile 3	$u_1 = 0$ $t_2 = t_3 = 0$	$u_1 = 0$ $t_2 = t_3 = 0$	$u_2 = 0$ $t_1 = t_3 = 0$	$u_2 = 0$ $t_1 = t_3 = 0$	$u_3 = {}^0\varepsilon_{33}\frac{l_3}{2}$ $t_1 = t_2 = 0$	$u_3 = -{}^0\varepsilon_{33}\frac{l_3}{2}$ $t_1 = t_2 = 0$
Shear 12	$u_2 = {}^0\varepsilon_{21}\frac{l_1}{2}$ $u_3 = 0,\ t_1 = 0$	$u_2 = -{}^0\varepsilon_{21}\frac{l_1}{2}$ $u_3 = 0,\ t_1 = 0$	$u_1 = {}^0\varepsilon_{12}\frac{l_2}{2}$ $u_3 = 0,\ t_2 = 0$	$u_1 = -{}^0\varepsilon_{12}\frac{l_2}{2}$ $u_3 = 0,\ t_2 = 0$	$u_3 = 0$ $t_1 = t_2 = 0$	$u_3 = 0$ $t_1 = t_2 = 0$
Shear 13	$u_3 = {}^0\varepsilon_{31}\frac{l_1}{2}$ $u_2 = 0,\ t_1 = 0$	$u_3 = -{}^0\varepsilon_{31}\frac{l_1}{2}$ $u_2 = 0,\ t_1 = 0$	$u_2 = 0$ $t_1 = t_3 = 0$	$u_2 = 0$ $t_1 = t_3 = 0$	$u_1 = {}^0\varepsilon_{13}\frac{l_3}{2}$ $u_2 = 0,\ t_3 = 0$	$u_1 = -{}^0\varepsilon_{13}\frac{l_3}{2}$ $u_2 = 0,\ t_3 = 0$
Shear 23	$u_1 = 0$ $t_2 = t_3 = 0$	$u_1 = 0$ $t_2 = t_3 = 0$	$u_3 = {}^0\varepsilon_{32}\frac{l_2}{2}$ $u_1 = 0,\ t_2 = 0$	$u_3 = -{}^0\varepsilon_{32}\frac{l_2}{2}$ $u_1 = 0,\ t_2 = 0$	$u_2 = {}^0\varepsilon_{23}\frac{l_3}{2}$ $u_1 = 0,\ t_3 = 0$	$u_2 = -{}^0\varepsilon_{23}\frac{l_3}{2}$ $u_1 = 0,\ t_3 = 0$

2.1 Simplified Models

In order to show the basic nature of these BCs a simple geometry (Figure 1, left) is studied. It is selected such that the microstructure of the VE is not symmetric with respect to the axes of orthotropy but an increasing number of basic pattern decreases this error. The white areas are modelled with E =10GPa, ν =0.15 and the black regions with E =10/20/160/640 GPa, ν =0.3. In order to explain the effect of the BCs two pattern types (Figure 1, right) are sketched and denoted with "Geometry 1" and "Geometry 2". The FEM models (4×4 cells) are shown in black/white. The blue/white pattern indicate the neighborhood implied by the BCs. In case of PBCs the cells are shifted (translated) but PMUBCs feel mirrored volume elements. This results in a different investigated pattern (Figure 1, right, top). If the pattern would be rotated by 45° (Figure 1, right, bottom) a microscopically orthotropic and periodic micro structure is obtained. Thus the overall mechanical properties predicted by PBCs and PMUBCs would coincide. In case of the first (not-rotated) pattern PMUBCs can only give apparent elastic properties and the prediction of PMUBCs will be improved if the size of the investigated volume element increases.

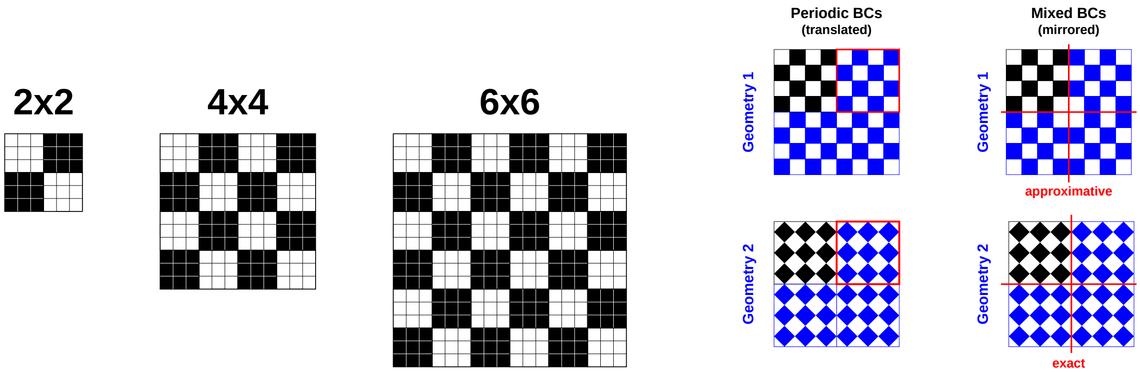

Figure 1: Simple micro geometry (chessboard pattern) with increasing number of basic pattern (left) and different micro geometries with assumed neighborhood by the BCs (right).

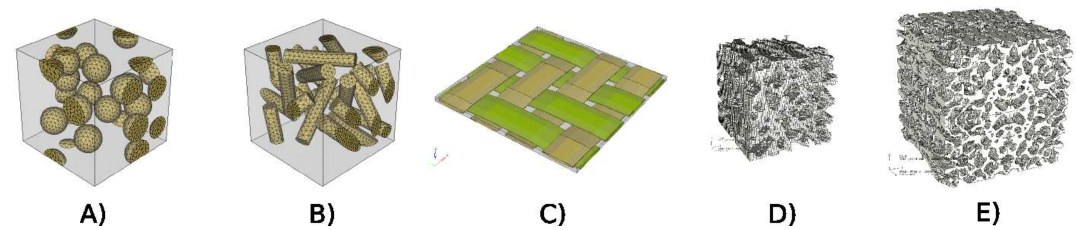

Figure 2: Investigated periodic unit cell model geometries: Unit cells A) of 15 spherical particles, B) 15 randomly oriented cylindrical fibers, C) 2/2 twill weave fabric, D) cube of trabecular bone, E) mirrored trabecular bone cube

2.2 Models of Cellular and Composite Materials

In a second step more realistic periodic but microscopically non-symmetric micro geometries (Figure 2) are investigated. Due to the periodic micro geometries effective material parameters are obtained from PBCs and can be used as references for the overall mechanical properties proposed by other BCs.

The material parameters used for model A and B are summarized in Table 2. All nonlinear analyses are done with s_{R}=5. A detailed description of the modelling can be found in [7].

The 2/2 twill weave fabric models (C in Figure 2) are explained in [8]. Details of the trabecular bone models (D and E in Figure 2) can be found in [6]. Six different bone samples with bone volume fractions of 6.52%, 10.7%, 12.25%, 15.76%, 20.76%, and 37.61% are investigated. The volume element corresponding to real bone (D in Figure 2) is investigated with KUBCs and PMUBCS. In order to be able to compare these results with effective elastic predictions, the bone models are mirrored to obtain a periodic micro structure (E in Figure 2) which can be investigated with PBCs.

Table 2: Material properties used for model A and B in Figure 2. Five different stiffness ratios ($s_R = E_I/E_M$) and two different hardening moduli E_H are investigated (E_H=1 MPa corresponds to the "no hardening" case).

Property	Inclusion	Matrix (s_R=2/5/10/20/30)
Elastic (s_R=2/5/10/20/30)		
E (GPa)	400	200/80/40/20/13.3
ν	0.17	0.3
Plastic		
σ_Y (MPa)	-	100
E_H (MPa)	-	1

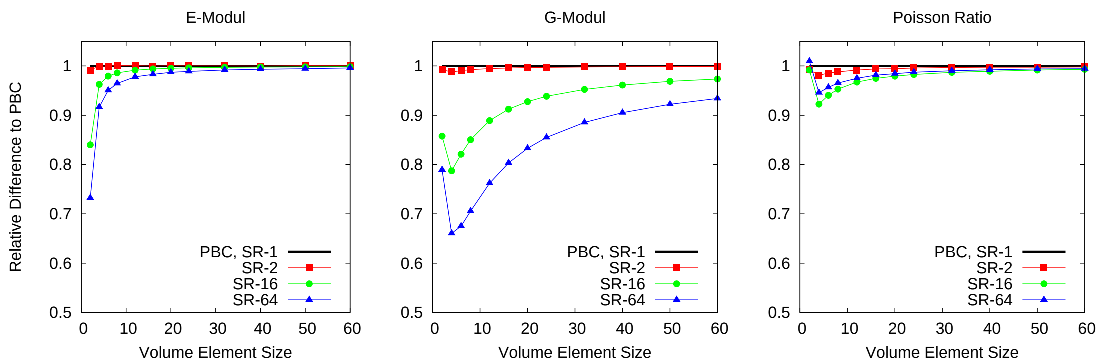

Figure 3: Size and stiffness ratio effect of a simplified geometry (Figure 1, left) analyzed with PBCs and PMUBCs on the the predicted homogenized Young's modulus (left), shear modulus (middle), and Poisson ratio (right).

3 Results

3.1 Simplified Models

2D models of different size (as shown in Figure 1, left) are analyzed with periodic BCs (PBCs) and periodic compatible mixed uniform BCs (PMUBCs). The homogenized elasticity tensor are computed. The Young's moduli, shear moduli, and Poisson ratios are compared (Figure 3) for different stiffness ratios between matrix and inclusion material as well as different volume element sizes. An increased sensitivity in case of high stiffness ratios is visible. For bigger volume elements the error between PBCs and PMUBCs predictions is decreased. In case of the G modulus it is found that for high stiffness ratios relatively big RVEs are needed to bring the error below 10%. This goes hand in hand with [13], where it was shown that the RVE size for accurate predictions depends on the material property to be studied.

3.2 MMC with Spherical Reinforcements

The elastic responses of the investigated volume elements are summarized in Figure 4. Six linearly independent load cases are analyzed and the full elasticity tensor

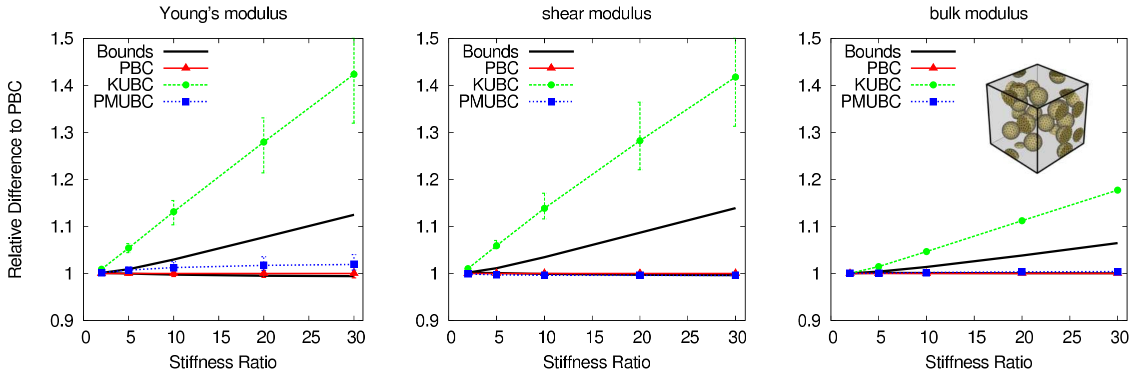

Figure 4: Elastic response of sphere reinforced composites: Relative difference between periodic BCs and KUBCs/PMUBCs for the Young's (left), shear (center), and bulk modulus (right). The bounds correspond to 3-point bounds of [14].

is computed. The error bars in case of the Young's and shear moduli indicate the maximum and minimum values and the lines the mean value of the corresponding modulus. In the case of spherical inclusions (Figure 4) PBCs and PMUBCs are within or close to the 3-point bounds of [14], KUBCs are always outside. They give a distinctly anisotropic material behavior. Such BCs overestimate the Young's modulus E and shear modulus G up to 50%, where the bulk modul K is less influenced. PBC show no marked differences in E and G which indicates that the volume element is nearly isotropic. The difference of PBC and PMUBCs is small (a few percent) for all material parameters and stiffness ratios. Young's moduli obtained from PMUBCs are stiffer and shear moduli slightly softer than PBC based values.

An elastic - ideally plastic material was used to obtain the 3 stress-strain curves in Figure 5 for three different loading scenarios. The stress-strain curves are volume averages from true stress (Cauchy) and true strain (logarithmic) obtained from ABAQUS at integration point level. The computations are done for two different stiffness ratios between matrix and inclusion, s_r=5 and s_r=30. Only PBCs and PMUBCs are compared. The agreement between both is very good (Figure 5).

3.3 MMC with Cylindrical Reinforcements

The volume elements containing randomly cylindrical reinforcements (Figure 6) show similar results to the sphere reinforced composite. But the overestimation with KUBCs is not as significant (only up to 30%). A second difference is that this volume element shows more anisotropy (up to 7%), which is visible from the larger differences of the moduli (error bars in Figure 6).

The elastic-plastic response of this composite (Figure 7) is also similar to the one wiht spherical reinforcements. The differences between the results obtained with the two sets of BCs is very small.

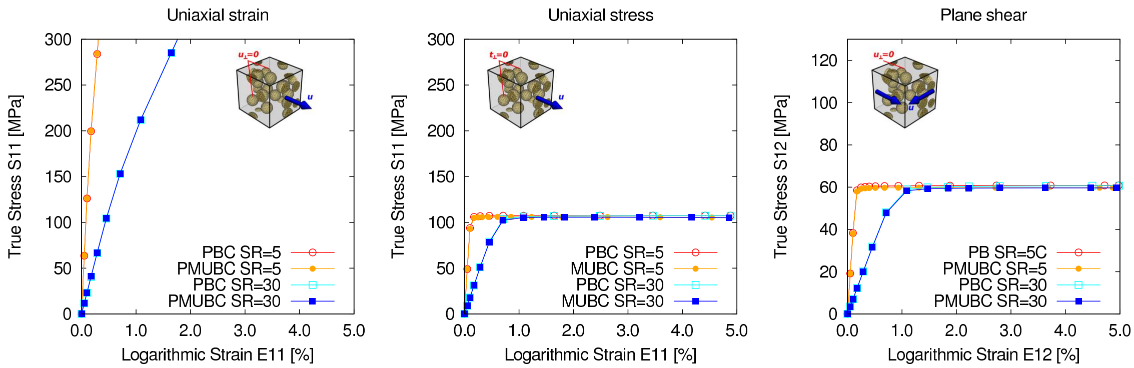

Figure 5: Elastic-plastic response of sphere reinforced composites with weak hardening: Relative difference between periodic BCs and PMUBCs for two different stiffness ratios and three different loading scenarios. Uniaxial tension with constraint faces (left), free faces (center) and shear load case (right).

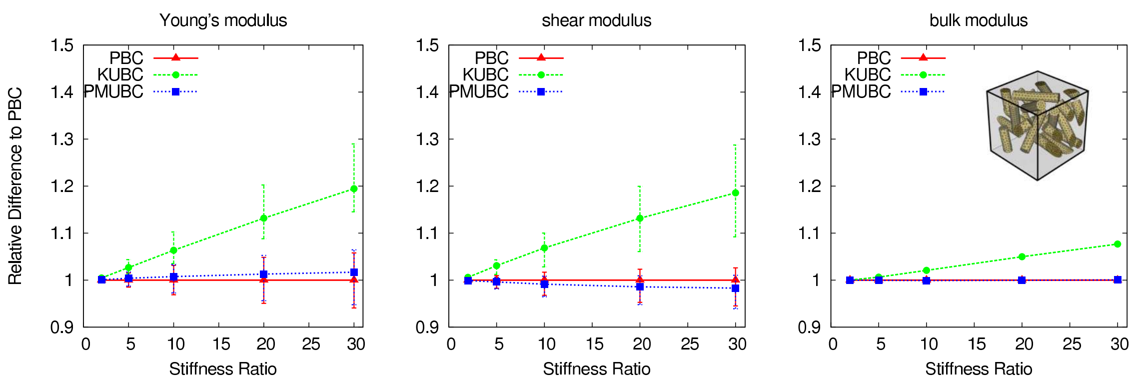

Figure 6: Elastic response of composites with randomly oriented cylindrical reinforcements: Relative difference between periodic BCs and KUBCs/PMUBCs for Young's (left), shear (center), and bulk modulus (right).

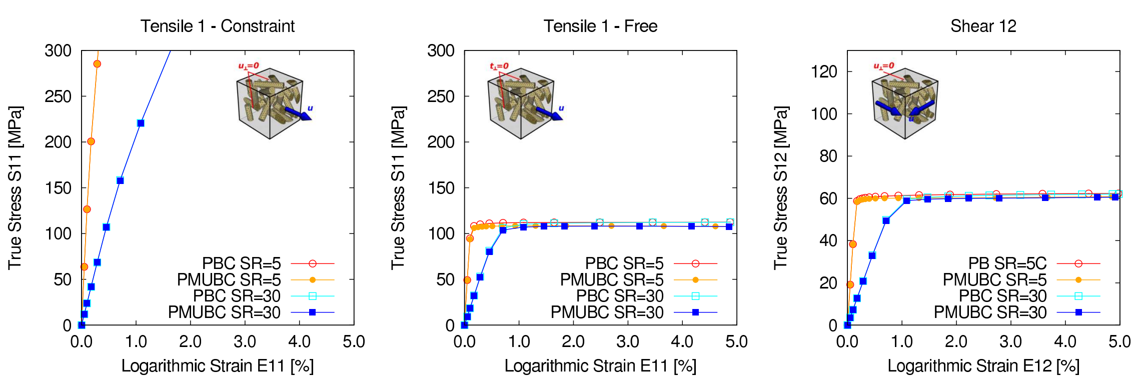

Figure 7: Elastic-plastic response of composites with randomly oriented cylindrical reinforcements without hardening: Relative difference between periodic BCs and PMUBCs for two different stiffness ratios and three different loading scenarios. Uniaxial tension with constraint faces (left), free faces (center) and shear load case (right).

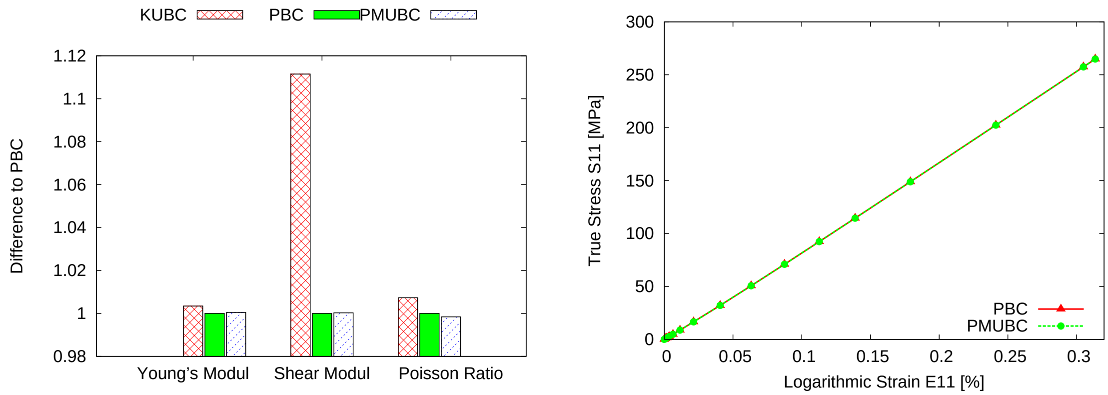

Figure 8: Differences in elastic properties of a woven fabric ply based on KUBC, PBC, and PMUBC boundary conditions (left) and geometrically non-linear analysis of the same model under uniaxial strain (right).

3.4 2/2 Twill Woven Fabric

Results for the elastic behavior of 2/2 twill woven fabric plies are summarized in Figure 8, left. KUBC, PBC, and PMUBC are compared with respect to some in-plane elastic constants (note $E_1 = E_2$). KUBC show a considerable overestimation in case of the shear modulus. All other mechanical material parameters are predicted within a accuracy of 1%. PMUBC closely approach the effective material properties for this type of composite material. In the geometrically non-linear regime a very good agreement is obtained for the uniaxial strain load case between PBC and PMUBC (Figure 8, right).

3.5 Cellular Materials - Trabecular Bone

Figure 9 shows a comparison of the Young's moduli, shear moduli, and Poisson's ratios of six different real bone models (D in Figure 2) with KUBCs and PMUBCs. These results are compared to the predictions from mirrored models (E in Figure 2) based on PBCs. The correlation in the case of PMUBC is nearly perfect but only moderate for KUBCs. In order to quantify these results the concordance correlation coefficient (i.e. correlation with the 45° line, [15]) for E, G, ν is equal to 1.000, 1.000, 0.998 (PMUBCs) and 0.968, 0.923, 0.759 (KUBCs). Figure 9 also shows a wide range of Young's/shear moduli going over two order of magnitudes. In this figure the slight differences between the periodic and PMUBCs in the case of a small volume element are visible.

4 Discussion and Summary

Periodic Mixed BCs are suitable for use in predicting the behavior of various composite materials in the elastic regime although the assumption of microscopic and macroscopic orthotropic symmetry is not met exactly. The overall elastic properties predicted with PMUBCs are close to those obtained with PBCs, with the difference

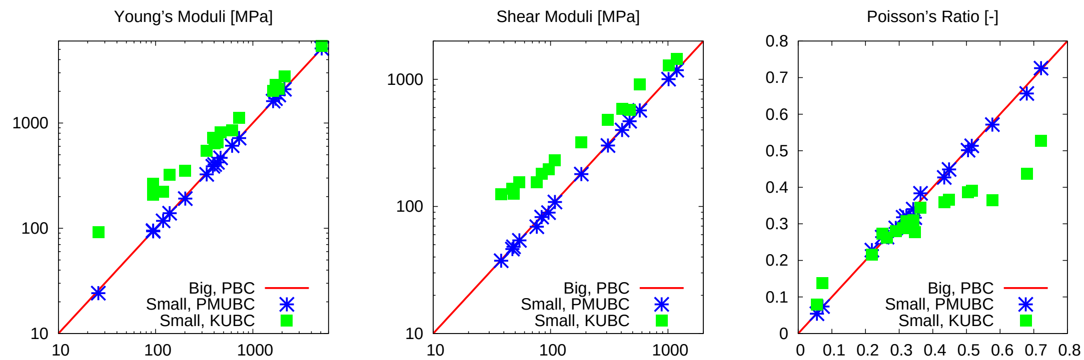

Figure 9: Comparison of Young's moduli (left), shear moduli (middle), and Poisson's ratio (right) of the models with two different BCs (KUBC, MUBC) and the big model with PBC.

that much simpler boundary conditions are applied on the faces of the volume element in case of PMUBCs. In contrast to that KUBCs in many load to marked overetimates of hte moduli.

In the non-linear range also a good correlation between results obtained with PMUBCs and PBCs is found. However, the investigated elasto-plastic load cases show a weakness of the PMUBCs: Only certain boundary conditions can be realized. For the computation of the elasticity tensors this is no limitation because only six independent load cases - force or displacement driven - have to be analyzed. But for non-linear simulation path dependency requires certain loading paths. For this application PBCs are easier to handle than PMUBCs.

It was found that that for displacement controlled loading PMUBCs are more efficient than PBCs with respect to computational resources (memory requirement and CPU time). A further advantages lies in the modelling effort. PBCs required consistent meshes at opposite sides and special software is needed to apply the multi-point-constraint automatically. KUBCs need also an essential modelling effort. Uniform displacements can not be applied by using standard tools because they depend on the nodal locations. In case of PMUBCs no consistent meshes or position dependent BCs are required. Only node sets of the surface of the volume element are necessary. Such information can be simply obtained by standard pre-processing tools.

A special set of mixed uniform boundary conditions proposed [6] are applied to composite materials in the linear and non-linear regime. The usage of PMUBCs for all investigated simulation model could be validated, which indicates that PMUBCs can be a powerful alternative to periodic BCs in the future.

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