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A study on the influence of boundary conditions in computational homogenization of periodic structures with application to woven composites

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A B S T R A C T

The influence of boundary conditions (BCs) in the estimation of elastic properties of periodic structures is investigated using computational homogenization with special focus on planar structures. Uniform displacement, uniform traction, periodic, in-plane periodic and a proposed mix of periodic and traction BCs are used. First, the effect of the BCs is demonstrated in structures with one-, two- and three-dimensional periodicity. Mixed BCs are shown to most accurately represent the behavior of layered structures with a small number of repeating unit cells. Then, BCs are imposed on a twill woven composite architecture. Special attention is devoted to investigate the sensitivity of the estimated properties with respect to the BCs and to show differences when considering a single lamina or a laminate. High sensitivity of the in-plane extensional modulus and Poisson's ratio with respect to the type of BCs is found. Moreover, it is shown that the mix of BCs and in-plane periodic BCs are capable to represent an experimental strain field.

1. Introduction

The use of computational homogenization to estimate mechanical properties of heterogeneous materials is widely accepted cf. [1,2]. This finite element-based approach can be used in periodic and non-periodic structures. It can be performed using different types of boundary conditions (BCs), uniform displacement boundary conditions (UDBCs), uniform traction boundary conditions (UTBCs), periodic boundary conditions (PBCs) and also a combination of these. It has been shown that using UDBCs and UTBCs a large number of repeating unit cells (RUCs) is required to accurately represent periodic structures, while a low number is needed when PBCs are used. For a small number of RUCs, UDBCs overestimates and UTBCs underestimates the stiffness in comparison to PBCs [2–4].

Due to the complex microstructure of woven composites, computational homogenization is commonly used for the estimation of their elastic constants. This is typically performed with PBCs [5–7] or UDBCs [8,9]. When using PBCs, selection of the RUC is not unique and the solution is independent of its choice [10]. This becomes important if periodicity of a single lamina or a laminate want to be represented with a RUC. This might be one of the underlying reasons for discrepancies reported in literature between numerical-experimental results and also between numerical techniques.

Zhang and Harding [8] used homogenization with UDBCs in a plain woven composite and reported over-prediction of experimental results. Also, Byström [7] compared homogenization techniques also in a plain woven composite, and results were compared with experimental data of laminates. The source of discrepancies between numerical and experimental data was reported unknown. Angioni et al. [6] compared a computational homogenization technique based on asymptotic expansion with four analytical methods. They used PBCs in RUCs of different woven architectures and their results were compared with experimental data of laminates. All theoretical results underestimated the experimental data, even when idealizations in the model (such as perfect bonding of matrix-fibers and zero structural defects) was made. They found in a woven composite with a so-called 8H fabric architecture differences in the in-plane modulus of elasticity of about 70%. For a so-called 5H architecture, differences of roughly 400% in the in-plane Poisson's ratio were found. These differences were attributed to the fact that the model was for a single lamina while the available data was for laminates. Moreover, in-plane properties of laminates of different number of layers have been

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compared experimentally for a 2×2 twill architecture [11], finding negligible differences. To the best of our knowledge, Jekabsons and Byström [12] have reported probably the only work that has compared experimentally the in-plane properties of a single lamina and those for a laminate of a plain woven composite. They found significant differences, specially in the Poisson's ratios. They used homogenization with PBCs and concluded that the exact localization of the boundary between a lamina and a laminate was unknown. Matveev [13] made a comparison of the in-plane modulus of elasticity of a twill composite using UDBCs, PBCs and a mix of UDBCs and PBCs, finding differences of about 20%. However, UTBCs and the effect in the other elastic properties was not reported.

The effect of performing homogenization using UTBCs in woven composites is lacking in literature, and in the best of our knowledge, a formal study devoted to investigate the sensitivity of the estimated properties with respect to the BCs in a single lamina and a laminate has not been done. Therefore, this study first investigates the effect of BCs in the estimated properties of structures with one-, two- and three-dimensional periodicity. A mix of PBCs and UTBCs (Mixed-BCs) is proposed, overcoming some of the drawbacks presented by the other types of BCs in planar structures. Then, such BCs are applied to a single lamina and up to a three-layered woven composite laminate with a 2×2 twill architecture. Sensitivity of the estimated properties with respect to the BCs is shown and differences between a single lamina and a laminate are illustrated. Finally, strain fields produced with the different BCs are compared with experimental data reported in literature.

2. Computational homogenization of composite media

2.1. Constitutive relations

The general aim of the computational homogenization in this study is to find the constitutive relation between stresses and strains. This is done by calculating average stresses ($\bar{\sigma}_{ij}$) by given average strains ($\bar{\varepsilon}_{ij}$), or conversely, by given $\bar{\sigma}_{ij}$, calculate $\bar{\varepsilon}_{ij}$. Hence, a linear elastic constitutive relation (considered herein) can be written in matrix–vector form using Voigt notation as,

$$\bar{\boldsymbol{\sigma}} = \bar{\mathbf{C}}\bar{\boldsymbol{\varepsilon}} \tag{1}$$

where $\bar{\mathbf{C}} = \bar{\mathbf{S}}^{-1}$ is the stiffness matrix or the inverse of the compliance matrix [14]. Elastic constants are more easily written in terms of the components of $\bar{\mathbf{S}}$. Then, the problem is reduced to find the components of $\bar{\mathbf{S}}$ by either imposing 6 independent strain vectors ($\bar{\varepsilon}$) and calculate the corresponding stresses ($\bar{\boldsymbol{\sigma}}$) or vice versa. To generate such state of average strain or stress, different BCs can be used, as discussed later in Section 2.3. Under plane-stress conditions, given the in-plane directions 1–2 and the out-of-plane, 3, $\bar{\sigma}_{33} = \bar{\gamma}_{13} = \bar{\gamma}_{23} = 0$. This leads to a constitutive relation between in-plane stresses and strains through a reduced compliance matrix $\bar{\mathbf{S}}_r$ and a reduced stiffness matrix $\bar{\mathbf{Q}}$ such that $\bar{\mathbf{Q}} = \bar{\mathbf{S}}_r^{-1}$. It is worth to mention that while components of $\bar{\mathbf{S}}_r$ have direct correspondence with $\bar{\mathbf{S}}$, it is not the case for $\bar{\mathbf{Q}}$ with $\bar{\mathbf{C}}$, see [14] for further details. Thus, under plane-stress conditions, the problem is reduced to impose three vectors of average stress or strain. However, an inconvenience is that only the four independent constants related with in-plane properties can be calculated, i.e. $E_{11}, E_{22}, \nu_{12}, G_{12}$.

2.2. Equilibrium, compatibility and the Hill–Mandel principle

Computational analysis of heterogeneous structures is done through a selection of a RUC with domain V. Equilibrium of such a RUC can be written in terms of the Cauchy stress tensor on the microscopic scale σ_{ij} and considering that it is subjected to a surface traction t_i with normal n_j on its boundary Γ [15], i.e.,

$$\sigma_{ij,j} + b_i = 0 \quad \text{on } V \tag{2a}$$

$$t_i = \sigma_{ij} n_j \quad \text{on } \Gamma \tag{2b}$$

where b_i are body forces, the comma means differentiation and Einstein's summation convention prevails. Moreover, for linear elastic materials and small deformations, the macroscopic stresses ($\bar{\sigma}_{ij}$) and strains ($\bar{\varepsilon}_{ij}$) can be expressed as averages of the corresponding microscopic parts σ_{ij} and ε_{ij}, respectively as [16],

$$\bar{\sigma}_{ij} = \frac{1}{V}\int_V \sigma_{ij} dV \tag{3a}$$

$$\bar{\varepsilon}_{ij} = \frac{1}{V}\int_V \varepsilon_{ij} dV \tag{3b}$$

Considering the position vector of a point x_j and symmetry of the Cauchy stress tensor, this can be written as $\sigma_{ij} = \delta_{jk}\sigma_{ki} = (\partial x_j/\partial x_k)\sigma_{ki} = x_{j,k}\sigma_{ki}$, where δ_{ij} is the Kronecker delta. Thus, from Eq. (2a) we derive that in the absence of body forces, such a tensor can also be written as $\sigma_{ij} = (\sigma_{ki}x_j)_{,k}$. Hence, using this last relation with Eq. (2b) and the Gauss divergence theorem, Eq. (3a) can be re-written as,

$$\bar{\sigma}_{ij} = \frac{1}{V}\oint_\Gamma t_i x_j dS \tag{4}$$

In Eq. (4) the contour integral is to emphasize the fact that integration is over a closed surface, S. In a similar fashion, considering the Cauchy infinitesimal strain tensor $\varepsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i})$ and with the aid of the Gauss divergence theorem, Eq. (3b) can be written as,

$$\bar{\varepsilon}_{ij} = \frac{1}{V}\oint_\Gamma \frac{1}{2}(u_i n_j + u_j n_i) dS \tag{5}$$

where u_i are the displacements. A basic assumption in computational homogenization is based on energy equivalences, by stating that the strain energy density in the macro level is equal to that one on the micro level, leading to the so-called Hill–Mandel relation [16],

$$\bar{\sigma}_{ij}\bar{\varepsilon}_{ij} = \frac{1}{V}\int_V \sigma_{ij}\varepsilon_{ij} dV \tag{6}$$

Moreover, due to the balance between strain and potential energy, in the absence of body forces,

$$\frac{1}{V}\int_V \sigma_{ij}\varepsilon_{ij} dV = \frac{1}{V}\oint_\Gamma t_i u_i dS \tag{7}$$

For convenience, the expression $\bar{\sigma}_{ij}\bar{\varepsilon}_{ij}$ can be re-written through the use of the Eq. (4) as,

$$\bar{\sigma}_{ij}\bar{\varepsilon}_{ij} = \frac{1}{V}\oint_\Gamma t_i \bar{\varepsilon}_{ij} x_j dS \tag{8}$$

$\bar{\sigma}_{ij}\bar{\varepsilon}_{ij}$ can also be written through the use of Eq. (5) as,

$$\bar{\sigma}_{ij}\bar{\varepsilon}_{ij} = \frac{1}{V}\oint_\Gamma u_i \bar{\sigma}_{ij} n_j dS \tag{9}$$

Also, since $\bar{\sigma}_{ij}\bar{\varepsilon}_{ij} = \bar{\sigma}_{ij}\bar{\varepsilon}_{ik}\delta_{kj} = \bar{\sigma}_{ij}\bar{\varepsilon}_{ik}x_{k,j}$, together with the Gauss divergence theorem, $\bar{\sigma}_{ij}\bar{\varepsilon}_{ij}$ can be written as,

$$\bar{\sigma}_{ij}\bar{\varepsilon}_{ij} = \frac{1}{V}\oint_\Gamma n_j \bar{\varepsilon}_{ik}\bar{\sigma}_{ij} x_k dS \tag{10}$$

Hence, combining Eqs. (7)–(10), an alternative expression for the Hill–Mandel principle can be obtained as,