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THE INFLUENCE OF DIFFERENT IMPLEMENTATION OF PERIODIC BOUNDARY CONDITIONS INTO FEM SOFTWARE

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Abstract: *This paper deals with the implementation of periodic boundary conditions in homogenization to determine effective elastic properties of arbitrary composite systems assuming two specific implementation schemes. As an example, the homogenization procedure applied to a composite system with plain weave textile basalt reinforcement was examined. The geometry of the analyzed sample was idealized with the help of statistically equivalent periodic unit cell. The comparison of the effective properties shows consistency of both implementations.*

Keywords: Periodic boundary conditions, Homogenization, Finite element method, Stress control, Strain control.

1. Introduction

Even with a large number of various numerical techniques at hand, the finite element method (FEM) is still considered to be the most universal method for solving variation formulated problems of physics connected to problems of field theory. One of the significant advantages of FEM in the field of continuum mechanics is particularly the possibility of solving tasks for universal geometric shapes of the analysis domain, universal load and support and also for complex constitutive relations of a material. Herein, FEM in adopted to solve the homogenization problem at the level of statistically equivalent periodic unit cell (SEPUC) of a textile reinforced composite formulated at the level of yarns, meso-scale.

In particular, we are concerned with a representative volume element (RVE) having well defined geometry and boundary conditions. Since this RVE is assumed periodic, often termed a periodic unit cell (PUC), the formulation has to be accompanied by so called periodic boundary conditions. In terms of loading, two different approaches can be adopted, stress or strain control loading conditions, to arrive at the estimates of effective properties. In terms of numerical implementation, we compare two specific ways of implementing periodic boundary conditions here linked to FEln and OOFEM software products, respectively (Patzák and Bittnar).

2. Solution in Terms of Fluctuation Fields - FEln

First, we consider the FEln software product that allows for a direct application of the load in the form of macroscopically constant strain $\boldsymbol{E}$, or stress $\boldsymbol{\Sigma}$. Unlike most commercial software, here the primary unknown is the fluctuation part of the displacement field $\boldsymbol{u}^*$, which enables rather straightforward implementation of the periodic boundary conditions. This step will be explained as one particular point of a general 1st order homogenization scheme discussed next.

To that end, suppose that the local strain field can be decomposed into the homogeneous, macroscopically linear part $\boldsymbol{U} = \boldsymbol{E} \cdot x$ and the fluctuation part $\boldsymbol{u}^*$ such that

$$\boldsymbol{u}(x) = \mathbf{E} \cdot x + \boldsymbol{u}^*(x). \qquad (1)$$

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Local strain thus becomes

$$\boldsymbol{\varepsilon}(x) = \boldsymbol{E} + \boldsymbol{\varepsilon}^*(x). \tag{2}$$

The displacements $\boldsymbol{u}^*$ are assumed periodic, the same displacements $\boldsymbol{u}^*$ on opposite sides of the unit cell, to ensure that the fluctuation part of strain disappears up on volume averaging, i.e. $\langle \boldsymbol{\varepsilon}^* \rangle = 0, \langle \boldsymbol{\varepsilon} \rangle = \boldsymbol{E}$. Introduction of local $\boldsymbol{\sigma}(x)$ and macroscopic $\boldsymbol{\Sigma} = \langle \boldsymbol{\sigma} \rangle$ stress fields allows us to express the virtual format of Hill's Lemma as

$$\left\langle \delta\,\boldsymbol{\varepsilon}(\boldsymbol{x})^{\mathsf{T}}\,\boldsymbol{\sigma}(\boldsymbol{x}) \right\rangle = \delta\,\boldsymbol{E}^{\mathsf{T}}\boldsymbol{\Sigma}\,. \tag{3}$$

The local constitutive law reeds

$$\boldsymbol{\sigma}(x) = \mathbf{L}(x)\boldsymbol{\varepsilon}(u(x)). \tag{4}$$

Substituting Eq. (4) into Eq. (3) gives

$$\delta\,\boldsymbol{E}^T \langle \mathbf{L}(x)(\boldsymbol{E} + \boldsymbol{\varepsilon}^*(x)) \rangle + \left\langle \delta\,\boldsymbol{\varepsilon}^*(x)^T \mathbf{L}(x)\boldsymbol{E} \right\rangle + \left\langle \delta\,\boldsymbol{\varepsilon}^*(x)^T \mathbf{L}(x)\boldsymbol{\varepsilon}^*(x) \right\rangle = \delta\,\boldsymbol{E}^T\,\boldsymbol{\Sigma}\,. \tag{5}$$

Since $\delta\,\boldsymbol{E}$ and $\delta\,\boldsymbol{\varepsilon}^*(x)$ are independent, we can split Eq. (5) into two equations

$$\delta\,\boldsymbol{E}^T\,\boldsymbol{\Sigma} = \delta\,\boldsymbol{E}^T \left[\langle \mathbf{L}(x) \rangle \boldsymbol{E} + \langle \mathbf{L}(x)\boldsymbol{\varepsilon}^*(x) \rangle \right], \tag{6}$$

$$0 = \left\langle \delta\,\boldsymbol{\varepsilon}^*(x)^T \mathbf{L}(x) \right\rangle \boldsymbol{E} + \left\langle \delta\,\boldsymbol{\varepsilon}^*(x)^T \mathbf{L}(x)\boldsymbol{\varepsilon}^*(x) \right\rangle. \tag{7}$$

Referring to (Šejnoha and Zeman, 2013) it can be shown that Eq. (6) and (7) are directly applicable when prescribing the overall stress $\boldsymbol{\Sigma}$. In case of prescribed overall strain $\boldsymbol{E}$, Eq. (7) reduces to

$$\Omega \langle \mathbf{L}(x)(\boldsymbol{E} + \boldsymbol{\varepsilon}^*(x)) \delta\,\boldsymbol{\varepsilon}^*(x) \rangle = 0\,. \tag{8}$$

There are two options how to account for the periodic boundary conditions. If starting directly from Eq. (6) and (7) or Eq. (8), the solution is searched in terms of unknown $\boldsymbol{u}^*$. In such a case the periodicity of $\boldsymbol{u}^*$ is enforced simply by assigning the same code numbers to the associated degrees of freedom of $\boldsymbol{u}^*$. However, when using commercial codes implementation of periodic boundary conditions is not that straightforward and will be explained in more detail in the next section.

3. Solution in Terms of Total Fields - OOFEM

To begin with, assume a three-dimensional rectangular SEPUC with dimensions *l* (x-direction), *b* (y-direction) and *h* (z-direction), see Fig. 1.

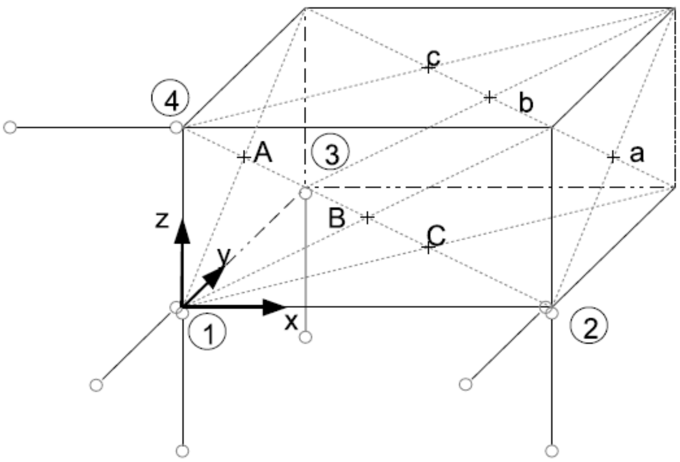

Fig. 1: Scheme of SEPUC.

The macroscopic linear displacements attain the form

$$\begin{Bmatrix} U_{(x,y,z)} \\ V_{(x,y,z)} \\ W_{(x,y,z)} \end{Bmatrix} = \underbrace{\begin{bmatrix} 1-\frac{x}{l}-\frac{y}{b}-\frac{z}{h} & \frac{x}{l} & \frac{y}{b} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{y}{b} & \frac{z}{h} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{z}{h} \end{bmatrix}}_{\mathbf{A}} \underbrace{\begin{Bmatrix} u_1 \\ u_2 \\ u_3 \\ v_3 \\ v_4 \\ w_4 \end{Bmatrix}}_{\boldsymbol{d}}, \tag{9}$$

u_1-w_4 corresponds to free nodal displacements of the supported nodes, see Fig. 1. The associated strain field is then provided by

$$\underbrace{\begin{Bmatrix} E_{xx} \\ E_{yy} \\ E_{zz} \\ 2E_{xy} \\ 2E_{yz} \\ 2E_{xz} \end{Bmatrix}}_{\boldsymbol{E}} = \underbrace{\begin{bmatrix} -\frac{1}{l} & \frac{1}{l} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{b} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{h} \\ -\frac{1}{b} & 0 & \frac{1}{b} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{h} & 0 \\ -\frac{1}{h} & 0 & 0 & 0 & 0 & 0 \end{bmatrix}}_{\mathbf{B}} \underbrace{\begin{Bmatrix} u_1 \\ u_2 \\ u_3 \\ v_3 \\ v_4 \\ w_4 \end{Bmatrix}}_{\boldsymbol{d}} \quad \Rightarrow \quad \boldsymbol{E} = \mathbf{B}\boldsymbol{d} \tag{10}$$

Combining Eqs. (10) and (9) gives

$$U_{(x,y,z)} = E_{xx}x + 2E_{xy}y + 2E_{xz}(z-H) + u^*_{(x,y,z)}, \tag{11}$$

$$V_{(x,y,z)} = E_{yy}y + 2E_{yz}z + v^*_{(x,y,z)}, \tag{12}$$

$$W_{(x,y,z)} = E_{zz}z + w^*_{(x,y,z)}. \tag{13}$$

The assumption of periodic boundary condition leads to

$$u_a = -u_1 + u_2 + u_A, \tag{14}$$

$$v_b = v_3 + v_B, \tag{15}$$

$$w_c = w_4 + w_C. \tag{16}$$

When macroscopic constant strain is prescribed, the control displacements in the form (11) - (13) need to be prescribed while for the stress control conditions, the appropriate averages of stress components can be ensured by applying appropriate concentrated forces according to the next equations

$$\boldsymbol{F} = \mathbf{B}^T \boldsymbol{\Sigma}\, lhb. \tag{17}$$

4. Evaluation of Effective Properties Using Periodic Boundary Conditions

As an example, we consider the composite reinforced by plain weave basalt reinforcement, see Fig. 2.

The actual analysis was performed exploiting the SEPUC in Fig. 1, see (Šejnoha and Zeman, 2013, Vorel et al., 2013) for more details.

The analyzed composite consists of three materials – pores, matrix and basalt reinforcements. At the level of SEPUC (meso-scale), the reinforcements are introduced through the homogenized properties of yarns. These in turn are found from an independent homogenization procedure carried out first at the level of fibers (micro-scale) here employing the Mori-Tanaka averaging scheme (Šejnoha and Zeman, 2013). This method builds upon the knowledge of the shape and orientation of the reinforcements, their material properties and volume fractions. The resulting homogenized properties of the basalt yarn together with the assumed matrix properties are listed in Tab.1. Tab. 2 then summarizes the effective stiffnesses of the entire system obtained for the two loading conditions and the used software products.

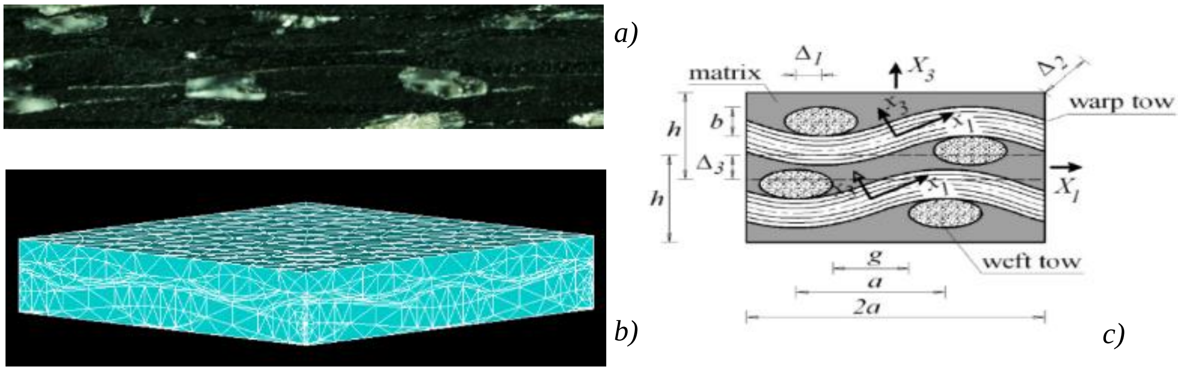

Fig. 2: a) Real microstructure; b) Discretization to finite elements; c) Two-layer SEPUC.

Tab. 1: Considered material properties.

Type of material	*Material property*								
	E_{xx}	E_{yy}	E_{zz}	G_{yz}	G_{xz}	G_{xy}	ν_{yz}	ν_{xz}	ν_{xy}
	[GPa]			[GPa]			[-]		
Basalt yarns	*53*	*6.1*	*6.2*	*2.6*	*3.6*	*3.6*	*0.3*	*0.23*	*0.23*
Matrix	*2.12*			*0.85*			*0.24*		

Tab. 2: Elements of stiffness tensor of composite system.

Homogenization procedure	*Composite with basalt reinforcement*					
	Stiffness tensor elements [GPa]					
	C_{11}	C_{22}	C_{33}	C_{44}	C_{55}	C_{66}
Feln - strain control	*13.162*	*13.168*	*0.542*	*0.328*	*0.329*	*1.758*
Feln - stress control	*13.162*	*13.168*	*0.542*	*0.328*	*0.329*	*1.758*
OOFEM - strain control	*13.540*	*13.539*	*0.704*	*0.372*	*0.372*	*1.756*
OOFEM - stress control	*13.339*	*13.342*	*0.695*	*0.371*	*0.371*	*1.753*

5. Conclusions

Four particular approaches were considered in this paper to estimate the effective elastic properties of a multi-layered textile composite reinforced with basalt fabric. The solutions performed in terms of the fluctuation (FEln) as well as total (OOFEM) displacements were examined. It is evident that both formulations deliver almost the same results regardless of the assumed loading conditions. Thus both procedures to implement the periodic boundary conditions are equally applicable.

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