ENGINEERING TRANSACTIONS • *Engng. Trans.* • **64**, 4, 581–587, 2016
Polish Academy of Sciences • Institute of Fundamental Technological Research (IPPT PAN)
National Engineering School of Metz (ENIM) • Poznan University of Technology

On the Static Nature of Minimal Kinematic Boundary Conditions for Computational Homogenisation

Marek WOJCIECHOWSKI, Marek LEFIK

Technical University of Łódź
Chair of Geotechnics and Engineering Structures
Al. Politechniki 6, 90-924 Łódź, Poland
e-mail: mwojc@p.lodz.pl

In the paper, the concept of minimal kinematic boundary conditions (MKBC) for computational homogenisation is considered. In the presented approach, the strain averaging equation is applied to the microscopic representative volume element (RVE) via Lagrange multipliers, which are, in turn, interpreted as macroscopic stresses. It is shown that this formulation fulfil automatically Hill-Mandel macrohomogeneity condition. Also, it is demonstrated, that MKBCs are in fact static, Neumann kind boundary conditions. As a consequence the effective parameters computed with this approach are lower bounds of the true effective values. Numerical analysis illustrating these results is also provided.

Key words: RVE, minimal kinematic boundary conditions, MKBC, computational homogenisation.

1. Introduction

Computational homogenisation methods are commonly used to approximate behaviour of the microscopically complex, ordered or disordered materials like for example soils, rocks or concrete [1, 2]. These methods are shown to be especially useful when the constituents of the composite exhibit nonlinear, time-dependent behaviour which cannot be simply addressed by fraction based homogenisation methods.

Searching for effective behaviour of the composite with computational strategy assumes, that at each macroscopic integration point, a microscopic representative volume element (RVE) is defined and boundary value problem is solved. The very common approach is to use rectangular or cuboidal RVE and to apply on its faces Dirichlet or Neumann boundary conditions (BCs) representing some averaged macroscopic quantity, in order to compute another averaged macroscopic field. In the case of strain analysis, the most commonly used boundary conditions are: linear displacements BCs which impose average macroscopic strains, uniform tractions BCs which enforce macroscopic stresses and periodic displacements BCs which also impose strains, but in the periodic way.

Recently, a new concept in this area has been proposed, namely the so called *minimal kinematic boundary conditions* (MKBC) [3–6]. The idea consist in constraining the microscopic RVE directly with the averaging equation, instead of applying consistent linear, uniform or periodic boundary conditions. The only additional constraint necessary is then rigid movement prevention. It is claimed, that this approach allows for arbitrary shapes of RVE and eliminates undesirable boundary effects which can violate solution, like for example periodicity enforcement in non-periodic materials.

In this paper we investigate this kind of boundary conditions. It is assumed that the strain averaging equation is applied to RVE via Lagrange multipliers. Starting from this formulation we do show that using MKBCs ensures fulfilment of Hill-Mandel macrohomogeneity condition and we demonstrate that they are in fact static, Neumann boundary conditions. This leads to the underestimation of the effective behaviour of the material when using MKBCs as compared to the periodic or Dirichlet BCs. Numerical example illustrating these results is also provided.

2. Homogenisation framework

2.1. MKBC formulation

Let's consider microstructurally complex, solid material for which a representative volume element Ω can be defined. In the case of elastic constituents of the composite and with the assumption of small strains, the local stresses in the RVE will be given via the constitutive relation:

$$\sigma_{ij} = c_{ijkl}\varepsilon_{kl}, \tag{2.1}$$

where $\varepsilon_{kl} = \frac{1}{2}(u_{k,l} + u_{l,k})$ is the microscopic strain tensor (u_k is the displacement field) and c_{ijkl} is an elastic tensor depending on the position in RVE. Indices i, j, k, l are taken as 1, 2 for 2D and 1, 2, 3 for 3D problems. Averages of the microscopic strains and stresses over domain Ω are given by:

$$\mathcal{E}_{ij} = \frac{1}{\Omega}\int\limits_{\Omega} \varepsilon_{ij} d\Omega, \tag{2.2}$$

$$\Sigma_{ij} = \frac{1}{\Omega}\int\limits_{\Omega} \sigma_{ij} d\Omega. \tag{2.3}$$

These values are assumed to be related via the effective macroscopic tensor C_{ijkl}:

$$\Sigma_{ij} = C_{ijkl}\mathcal{E}_{kl}. \tag{2.4}$$

Homogenization problem considered here is formulated as follows: find solution u_k of the equilibrium equations $\sigma_{ij,j} = 0$ defined on Ω, subject to macroscopic strain $\mathcal{E}_{ij}$ in such a way that Eq. (2.2) is fulfilled. Equations (2.3) and (2.4) are then processed in order to obtain macroscopic stress Σ_{ij} and material tensor C_{ijkl}. The above can be viewed as the minimization of the following potential:

$$\Pi(u) = \frac{1}{2}\int_{\Omega} \varepsilon_{ij} c_{ijkl} \varepsilon_{kl} d\Omega + \lambda_{ij}\left(-\Omega\mathcal{E}_{ij} + \int_{\Omega} \varepsilon_{ij} d\Omega\right), \tag{2.5}$$

where λ_{ij} are Lagrange multipliers used to apply MKBCs. Note, that because of symmetry of macroscopic strains, also λ_{ij} is considered to be a symmetric tensor. No additional boundary conditions are necessary for homogenisation, with exception of minimal set of Dirichlet BCs for fixing rigid motion. Solution is found by equating variation $\delta\Pi(u, \delta u)$ to zero, i.e.:

$$\delta\Pi(u, \delta u) = \int_{\Omega} \delta\varepsilon_{ij}\sigma_{ij} d\Omega + \lambda_{ij}\int_{\Omega} \delta\varepsilon_{ij} d\Omega = 0, \tag{2.6}$$

where δu is an arbitrary, kinematically admissible virtual displacement and $\delta\varepsilon_{ij} = \frac{1}{2}(\delta u_{i,j} + \delta u_{j,i})$ is the virtual strain. It is immediate to see, that if $\delta\varepsilon_{ij}$ is unitary, then from Eq. (2.6) we have:

$$\lambda_{ij} = -\Sigma_{ij}. \tag{2.7}$$

Lagrange multipliers are then interpreted as the average macroscopic stresses, with minus sign. Furthermore, assuming $\delta\varepsilon_{ij} = \varepsilon_{ij}$, we obtain the equation:

$$\frac{1}{\Omega}\int_{\Omega} \varepsilon_{ij}\sigma_{ij} d\Omega - \Sigma_{ij}\mathcal{E}_{ij} = 0, \tag{2.8}$$

which is simply the well-known Hill-Mandel macrohomogeneity principle. Therefore, in the case of MKBC approach, once the solution of (2.6) is found, the Hill-Mandel condition is certainly fulfilled.

Finally, let's consider the boundary version of the variational form (2.6), which can be derived from the Green's theorem (see e.g. [7]):

$$\int_{\partial\Omega} (t_i - \Sigma_{ij} n_j)(\delta u_i - \delta\mathcal{E}_{ik} x_k) dS = 0. \tag{2.9}$$

In this equation t_i are tractions, n_j – normal vectors, x_k – coordinates and the term $\delta u_i - \delta\mathcal{E}_{ik}x_k = \delta\widetilde{u}_i$ is interpreted as the fluctuation of the virtual displacement δu_i at the external boundary $\partial\Omega$ of the RVE. $\delta\mathcal{E}_{ik} = \int_\Omega \delta\varepsilon_{ik} d\Omega$ is a virtual macroscopic strain. Equation (2.9) must be true for any fluctuation $\delta\widetilde{u}_i$ what implies, that also the condition $t_i - \Sigma_{ij}n_j = 0$ must hold. Therefore, MKBCs are in fact static, Neumann kind boundary conditions, even though the macroscopic stresses are not known a priori, but they are enforced via Lagrange multipliers.

2.2. Implementation of MKBC with finite element method

Problem of the minimization of the potential (2.5) can be rewritten in the scope of finite element method as:

$$\min_{\mathbf{u}}\left[\Pi(\mathbf{u},\boldsymbol{\lambda})\right] = \min_{\mathbf{u}}\left[\frac{1}{2}\mathbf{u}^{\mathrm{T}}\mathbf{A}\mathbf{u} + \boldsymbol{\lambda}^{\mathrm{T}}\left(-\Omega\boldsymbol{\mathcal{E}} + \mathbf{B}^{\mathrm{T}}\mathbf{u}\right)\right], \tag{2.10}$$

where $\mathbf{u}$ is a global vector of unknown displacements of the length M (M – total number of degrees of freedom), $\mathbf{A}$ is a linear operator of the size $M \times M$, $\mathbf{B}$ is a problem specific matrix of the size $M \times N$ (N – number of independent macroscopic strain components), $\boldsymbol{\lambda}$ is a vector of unknown Lagrange multipliers of the length N, and $\boldsymbol{\mathcal{E}}$ is a vector of known, macroscopic strains to be applied, also of the length N. Solution of the problem is found by differentiation of the potential defined by (2.10) with respect to unknown $\mathbf{u}$ and $\boldsymbol{\lambda}$ and equating the results to 0, i.e.:

$$\frac{\partial\Pi(\mathbf{u},\boldsymbol{\lambda})}{\partial\mathbf{u}} = \mathbf{A}\mathbf{u} + \mathbf{B}\boldsymbol{\lambda} = \mathbf{0}, \tag{2.11}$$

$$\frac{\partial\Pi(\mathbf{u},\boldsymbol{\lambda})}{\partial\boldsymbol{\lambda}} = \mathbf{B}^{\mathrm{T}}\mathbf{u} - \Omega\boldsymbol{\mathcal{E}} = \mathbf{0}. \tag{2.12}$$

This is a system of linear equations:

$$\begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{B}^{\mathrm{T}} & \mathbf{0} \end{bmatrix}\begin{bmatrix} \mathbf{u} \\ \boldsymbol{\lambda} \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ \Omega\boldsymbol{\mathcal{E}} \end{bmatrix}. \tag{2.13}$$

Macroscopic, effective material matrix can be now derived from the observation that $\boldsymbol{\lambda} = -\boldsymbol{\Sigma}$, where $\boldsymbol{\Sigma}$ is a vector of unknown macroscopic stresses. Combining Eqs. (2.11) and (2.12) results finally in the relation:

$$\boldsymbol{\Sigma} = \Omega\left(\mathbf{B}^{\mathrm{T}}\mathbf{A}^{-1}\mathbf{B}\right)^{-1}\boldsymbol{\mathcal{E}} = \mathbf{D}\boldsymbol{\mathcal{E}}. \tag{2.14}$$

Matrix $\mathbf{D}$ can be then straightforwardly transformed into elasticity tensor C_{ijkl}. One can note that derivation of $\mathbf{D}$ and $\boldsymbol{\Sigma}$ with equation (2.14) does not need the explicit solution of the system of linear equations (2.13). However, a kind of inversion of operator **A**, with LU decomposition for example, is still required for this equation.

3. Numerical analysis

In order to illustrate the properties of the MKBC approach, numerical analysis of the influence of RVE size on the homogenisation results have been performed. Custom software *fempy* was used for this purpose [8]. 2D rectangular plane strain elastic RVEs with randomly distributed circular holes and with the overall void ratio 0.25 have been used in simulations. The elastic matrix has been parameterized with the Young modulus $E = 20\,000$ kPa and the Poisson ratio $v = 0.3$. The macroscopic strain applied to the RVE is taken as $\mathcal{E}_{ij} = [[1,\ 1],\ [1,\ -1]] \cdot 10^{-4}$.

In this numerical experiment the RVE size is understood as the exponential measure of the number of holes (with base 2 – see Fig. 1). For each size of the RVE 50 different distributions of holes have been generated and the effective tensors C_{ijkl} have been computed using different boundary conditions. In the case of MKBC circular shape of RVE has been additionally used. Figure 2 shows

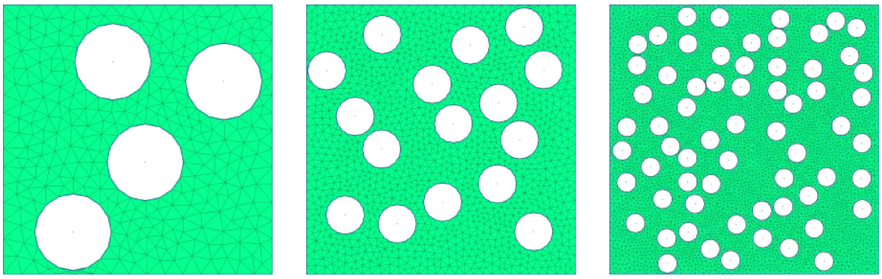

Fig. 1. Examples of the representative volume elements of the size 2, 4, 6, i.e. with 4, 16 and 64 holes, respectively. All RVEs have void ratio equal to 0.25.

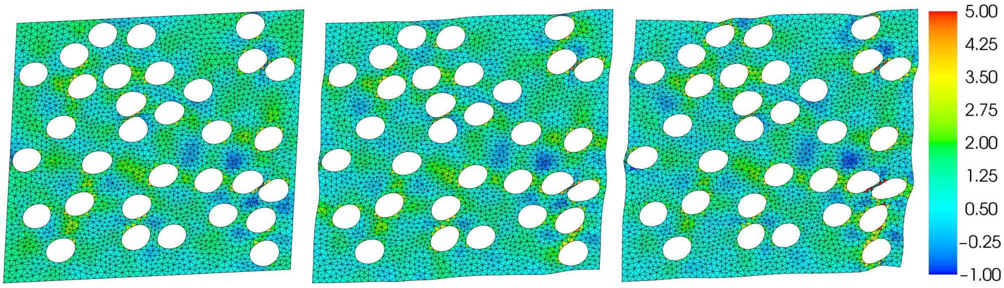

Fig. 2. Deformations (zoom 500×) and shear stresses (in kPa) for the exemplary RVE of the size 5 under different boundary conditions. From left to right: linear displacement BCs, periodic displacement BCs, minimal kinematic BCs.

deformations and shear stresses for the exemplary RVE. Mean values of the effective moduli C_{0000} and C_{0101} for each RVE size are presented in Fig. 3. Clearly the MKBCs generate *soft* response of the material and the effective moduli are approached *from the bottom*.

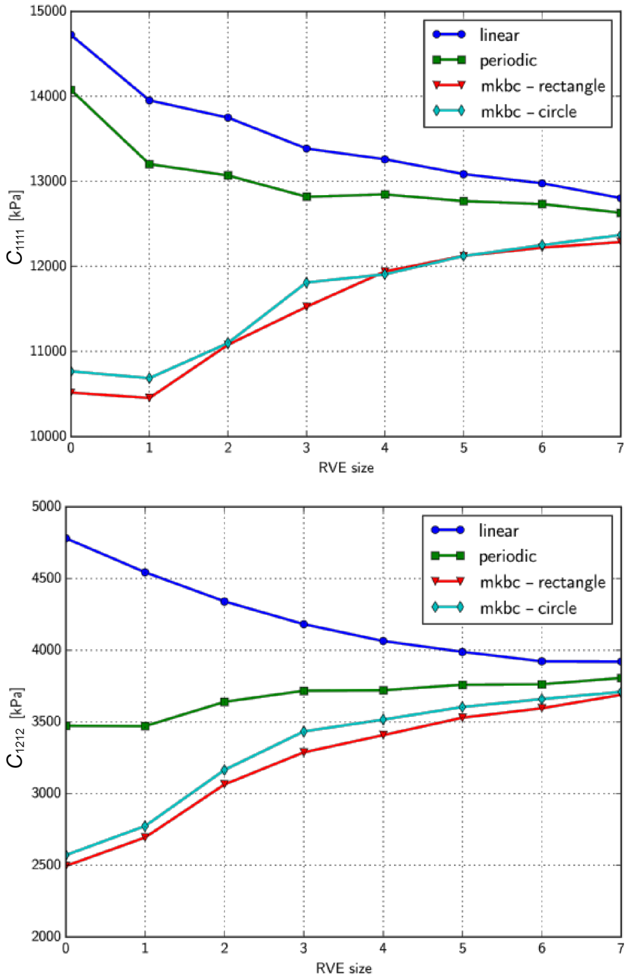

FIG. 3. Convergence of the computed elastic moduli to their effective values with increasing RVE size for different boundary conditions (C_{1111} on the top, C_{1212} on the bottom).

4. Conclusions

It has been shown in this paper, that minimal kinematic boundary conditions:

- can be easily applied to the microscopic RVE with Lagrange multipliers,
- fulfil automatically the Hill-Mandel macrohomogeneity principle,

- are Neumann kind, static boundary conditions, i.e. the effective parameters computed with MKBCs are lower bounds of the true effective values.

This last conclusion is considered to be the main contribution of the paper, since the MKBCs were presented so far as regular kinematic BCs [3, 4]. One can argue that, in the light of this, the term "minimal kinematic" is a bit misleading. However, using MKBCs ensures, that the amount of strain applied to the RVE is really constrained. This would be of great advantage when considering nonlinear microstructures with damage localization (plasticity, cracks), where classical static, uniform traction, BCs cannot be used, because of possible unlimited deformation. MKBCs could be a way to establish lower limit of the effective behavior in these cases.

References

1. Feyel F., *A multilevel finite element method (FE 2) to describe the response of highly non-linear structures using generalized continua*, Computer Methods in Applied Mechanics and Engineering, **192**(28–30): 3233–3244, 2003, doi: 10.1016/S0045-7825(03)00348-7.

2. Kousnetsova V.G., Geers M.G.D, Brekelmans W.A.M., *Computational homogenisation for non-linear heterogeneous solids*, [in:] *Multiscale Modeling in Solid Mechanics. Computational Approaches*, Galvanetto U., Ferri Aliabadi M.H. [Eds.], *Computational and Experimental Methods in Structures, Vol. 3*, Imperial College Press, London, pp. 1–42, 2009.

3. Mesarovic S.D., Padbidri J., *Minimal kinematic boundary conditions for simulations of disordered microstructures*, Philosophical Magazine, **85**(1): 65–78, 2005, doi: 10.1080/14786430412331313321.

4. Inglis H.M., Geubelle P.H., Matouš K., *Boundary condition effects on multiscale analysis of damage localization*, Philosophical Magazine, **88**(16): 2373–2397, 2008, doi: 10.1080/14786430802345645.

5. Jänicke R., Steeb H., *Minimal loading conditions for higher-order numerical homogenisation schemes*, Archive of Applied Mechanics, **82**(8): 1075–1088, 2012, doi:10.1007/s00419-012-0614-8.

6. Wojciechowski M., *Numerical homogenisation of permeability coefficient for Darcy flow in porous media*, Proceedings of 3rd Polish Congress of Mechanics & 21st Computer Methods in Mechanics, September 8–11, 2015, Gdańsk, Poland, vol. 1, pp. 101–102, 2015.

7. Nguyen V.-D., Béchet E., Geuzaine C., Noels L., *Imposing periodic boundary condition on arbitrary meshes by polynomial interpolation*, Computational Materials Science, **55**: 390–406, 2012, doi: 10.1016/j.commatsci.2011.10.017.

8. Wojciechowski M., *Fempy – finite element method in Python*, http://fempy.org, http://geotech.p.lodz.pl:5080/fempy, last access: October 2016.

Received October 16, 2016; accepted version November 11, 2016.