Statically perturbed kinematic boundary conditions for computational homogenisation of unstructured composites

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Abstract

In this short paper the idea of statically perturbed kinematic boundary conditions for computational homogenisation is introduced and explained. Instead of being periodic, the perturbation of the displacement field at the RVE boundary is taken from the constant traction BCs solution, which have to be obtained first. This primary solution is established with the so called *minimal kinematic boundary conditions* method. It is shown that this approach provides better homogenisation results, in statistical sense, than other BCs commonly used in this context.

Keywords: computational homogenisation, RVE size, boundary conditions

1. Introduction

The results of the computational homogenisation of the geometrically irregular composites depend strongly on the quality of the so called representative volume element (RVE). The error rate of the estimated effective properties is then often used to determine the necessary size and shape of the RVE (see e.g. [1]). It is important to notice that one of the the main sources of discrepancies between the estimated and true effective properties of the composite are the boundary conditions (BCs) used to load the microscopic RVE with the average macroscopic quantities. In case of unstructured media, the answer of the surrounding of the RVE always includes an unknown random perturbation. This perturbation obviously cannot be deduced from the material structure like in case of periodic media. However, many authors [1, 2] propose at this point to assume the so called *local periodicity* (not the whole body is periodic, but the closest surrounding of the RVE only) and to use periodic boundary conditions. It is shown that this approach provides better homogenisation results than other common choices for RVE boundary conditions, i.e. linear displacements BCs and uniform tractions BCs.

In this paper we propose new approach for establishing boundary conditions in computational homogenisation of random media. Instead of being periodic, the perturbation of the displacement field at the RVE boundary is taken from the compatibile uniform traction BCs solution, which have to be obtained first. As it is shown in [3] this primary solution can be established with the so called *minimal kinematic* boundary conditions method. This approach provides better homogenisation results, in statistical sense, than other BCs used in this context.

2. Homogenisation framework

Let's consider a composite material for which a representative volume element Ω with the external boundary $\partial\Omega$ 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:

$$\sigma_{ij} = c_{ijkl}\varepsilon_{kl}, \tag{1}$$

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. Averages of the microscopic strains and stresses over domain Ω are given by:

$$\mathcal{E}_{ij} = \frac{1}{\Omega}\int_{\Omega}\varepsilon_{ij}d\Omega = \frac{1}{\Omega}\oint_{\partial\Omega}(u_i n_j + u_j n_i)dS, \tag{2}$$

$$\Sigma_{ij} = \frac{1}{\Omega}\int_{\Omega}\sigma_{ij}d\Omega = \frac{1}{\Omega}\oint_{\partial\Omega}t_i x_j dS. \tag{3}$$

In the above, the Gauss theorem is used to represent the volume averages with boundary integrals and also n_i are the boundary normals, t_i are the boundary tractions and x_j are boundary coordinates. It is assumed, that the average values are related via the effective macroscopic tensor C_{ijkl}:

$$\Sigma_{ij} = C_{ijkl}\mathcal{E}_{kl} \tag{4}$$

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 equation (2) is fulfilled.

3. RVE boundary conditions

Let's assume, without loss of generality, that the displacement field at the RVE can be decomposed as follows:

$$u_i = \mathcal{E}_{ij}x_j + \tilde{u}_i \tag{5}$$

where $\mathcal{E}_{ij}x_j$ is interpreted as the mean displacement and $\tilde{u}_i$ is the perturbation part. We define also the perturbation strain as $\tilde{\varepsilon}_{ij} = \frac{1}{2}(\tilde{u}_{i,j} + \tilde{u}_{j,i})$. The total strain is then given via:

$$\varepsilon_{ij} = \mathcal{E}_{ij} + \tilde{\varepsilon}_{ij} \tag{6}$$

From equations (2), (5) and (6) it is immediately deduced that the integral of strain perturbation over the RVE must vanish, i.e.:

$$\int_{\Omega}\tilde{\varepsilon}_{ij}d\Omega = \oint_{\partial\Omega}(\tilde{u}_i n_j + \tilde{u}_j n_i)dS = 0. \tag{7}$$

The boundary conditions used in homogenisation process must then assure the condition (7) is fulfilled.

3.1. Linear displacements BCs

Linear displacements BCs are defined by assuming $\tilde{u}_i = 0$ at the RVE boundary. This is realized by applying $u_i = \mathcal{E}_{ij}x_j$ at $\partial\Omega$. Let's denote the solution of such defined boundary value problem, as:

$$u_i^k = \mathcal{E}_{ij}x_j + \tilde{u}_i^k, \tag{8}$$

From this solution also ε_{ij}^k, σ_{ij}^k, Σ_{ij}^k and C_{ijkl}^k can be computed. Because of the kinematic nature of these BCs they lead to the overestimated components of the effective tensor C_{ijkl}^k.

3.2. Uniform tractions BCs

Uniform tractions BCs are defined by assuming $t_i = \Sigma_{ij}n_j$ at RVE boundary. In order to generate uniform tractions which are compatible with the given macroscopic strain tensor $\mathcal{E}_{ij}$, the *minimal kinematic* BCs approach can be used [3]. In this method the RVE is constrained directly with the averaging equation (2) by means of the Lagrange multipliers. The solution is found by searching of the minimum of the following potential:

$$\Pi(u_i) = \int_\Omega \varepsilon_{ij}\sigma_{ij}d\Omega + \lambda_{ij}\left(-\Omega\mathcal{E}_{ij} + \int_\Omega \varepsilon_{ij}d\Omega\right) \tag{9}$$

Lagrange multipliers λ_{ij} are interpreted here as the average macroscopic stresses Σ_{ij}, with minus sign. Let's denote the solution of such defined boundary value problem, as:

$$u_i^s = \mathcal{E}_{ij}x_j + \tilde{u}_i^s, \tag{10}$$

from which also ε_{ij}^s, σ_{ij}^s, Σ_{ij}^s and C_{ijkl}^s can be computed. Because of the static nature of these BCs they lead to the underestimated components of the effective tensor C_{ijkl}^s. Obviously in this solution perturbation of the displacement field $\tilde{u}_i^s$ at boundary is non-zero (although it vanishes in the integral sense).

3.3. Statically perturbed kinematic BCs

In the current research we propose to apply at the RVE boundary $\partial\Omega$ the kinematic BCs which do include the perturbation computed previously with uniform traction approach, namely:

$$u_i^\alpha = \mathcal{E}_{ij}x_j + \alpha\tilde{u}_i^s, \tag{11}$$

where $\alpha \in \langle 0, 1\rangle$. In case of linear elastic constituents of the composite and under the small strain regime it can be shown, that the solution of such defined boundary value problem can be represented as the linear combination of the previously defined solutions. Namely, we have at Ω:

$$u_i^\alpha = (1-\alpha)u_i^k + \alpha u_i^s \tag{12}$$

from which also ε_{ij}^α, σ_{ij}^α, Σ_{ij}^α and C_{ijkl}^α can be computed subsequently. Depending on the parameter α some intermediate effective tensors C_{ijkl}^α are obtained with this method.

4. Numerical verification

Two-dimensional, plane strain elastic body with randomly distributed, constant radius, circular holes, and with the overall void ratio 0.25, has been investigated numerically. Custom software *fempy* was used for this purpose [4]. The elastic matrix has been parametrized with the Young modulus $E = 20000$ kPa and the Poisson ratio v=0.3. The macroscopic strain applied to the investigated RVEs is taken as $\mathcal{E}_{ij} = [[1,1],[1,-1]]\cdot[10]^{-4}$. For each size of the RVE (the size is understood here as the exponential measure of the number of holes contained in RVE, with base 2) 50 different distributions of holes have been generated and the effective tensors C_{ijkl} have been computed using the linear displacements, minimal kinematic and statically perturbed kinematic boundary conditions. Additionally the periodic BCs have been used for comparison purposes.

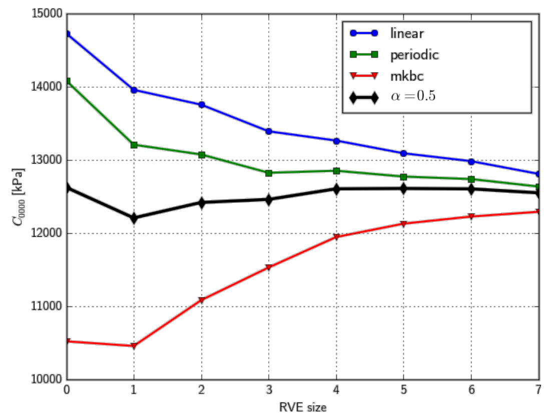

Figure 1: Mean values of the C_{0000} elastic modulus obtained for different boundary conditions.

As it is shown in the figure 1 the mean value of the elastic modulus C_{0000} (computed from 50 homogenisation results for each RVE size) tend to some true effective value when the RVE size is increasing. Clearly, the statically perturbed kinematic boundary conditions with $\alpha = 0.5$ provide best homogenisation result for all RVE sizes and it is always close to the true effective value, even if the RVE is very poor (size 0 signifies one hole only). The similar results are obtained also for the remaining components of the elastic tensor.

5. Conclusions

The statically perturbed kinematic boundary conditions provide better homogenisation results, in statistical sense, than any other BCs commonly used in this context. The key ingredient of the proposed method is the computation of the perturbation of the boundary displacements with the minimal kinematic boundary conditions investigated in detail in [3]. In case of linear elastic problems the resulting effective parameters can be computed as linear combinations of linear displacements and minimal kinematic BCs predictions. For non-linear problems the new solution have to be independently found. The possible drawback of the method is the necessity for solving two BVPs during homogenisation process. However, this can be compensated by the smaller required RVE size.

References

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