OPTIMAL BOUNDARY CONDITIONS AND RVE OF ARBITRARY SHAPE FOR COMPUTATIONAL HOMOGENIZATION OF DISORDERED MEDIA

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1. Introduction

Many engineering materials exhibit random internal structure. This includes (but is not limited to) soils, rocks and concrete. In order to determine the macroscopic response of such materials with accurate account for microstructural characteristics and evolution, computational homogenization strategy can be exploited [1]. Looking for effective behavior of composite with this strategy assumes, that at each macroscopic integration point, a microscopic representative volume element (RVE) is defined and boundary value problem (BVP) is solved. The very common approach in the literature of the subject is to use square (or cubic) shape of the RVE and to apply Dirichlet or Neumann boundary conditions (BCs) on its faces in order to simulate some averaged macroscopic behavior. In this paper we will apply the BCs without constraining the shape of RVE [2][3][4]. Approach being used is a kind of Dirichlet boundary conditions, but the BCs are applied via Lagrange multipliers. This is done in such a way that the macroscopic averaging equation of the homogenized quantity is fulfilled exactly and no undesirable "boundary effects" are present. In elasticity, this approach is known under the term of minimal kinematic boundary conditions. One can show that no additional energy is generated by applying such BCs. In this paper we will use the name *optimal boundary conditions* (OBCs) since the concept is general and it can be used in many engineering fields.

Once the arbitrary shape of RVE is allowed, one can adapt the "boundary cut" of the RVE to the microstructure of macroscopic body. Along with the mentioned optimality of the BCs this leads to smaller sizes of RVEs necessary to obtain satisfactory accuracy of homogenization. In this paper we will show comparisons of the results of homogenization of elasticity and Darcy flow parameters for different shapes of the RVEs and different types of BCs (homogeneous, periodic, optimal). We will conclude that irregular shape of RVE with optimal boundary conditions is the best choice for disordered media.

2. Optimal boundary conditions

Let's consider a microstructurally complex solid material for which a representative volume element (RVE) Ω can be defined. In 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:

(1) $$\sigma_{ij} = c_{ijkl}\varepsilon_{kl}$$

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

(2) $$\mathcal{E}_{ij} = \frac{1}{\Omega}\int_{\Omega} \varepsilon_{ij} d\Omega$$

(3) $$\Sigma_{ij} = \frac{1}{\Omega}\int_{\Omega} \sigma_{ij} d\Omega$$

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

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

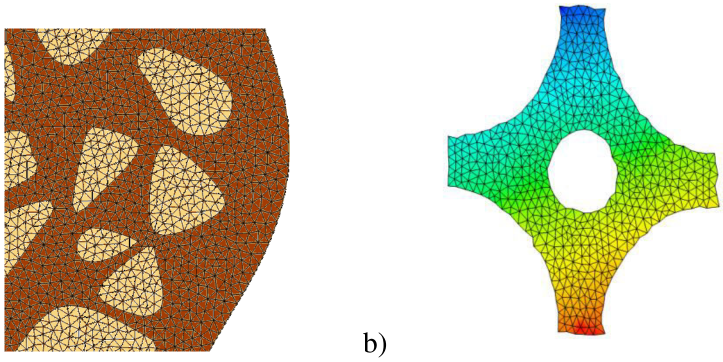
Homogenization problem considered here is formulated as follows: find solution u_k of equations (1) defined on Ω, subject to some macroscopic strain $\mathcal{E}_{ij}$ in such a way that equation (2) is fulfilled. Equation (3) is then fulfilled automatically and C_{ijkl} from equation (4) can be derived. The above can be viewed as a problem of minimization of total potential energy [3] with additional averaging constraint:

(5) $$\min_u \left[\int_\Omega \varepsilon_{ij} c_{ijkl} \varepsilon_{kl} \, \mathrm{d}\Omega + \lambda_{mn}(-\Omega \mathcal{E}_{mn} + \int_\Omega \varepsilon_{mn} \mathrm{d}\Omega)\right]$$

where λ_{mn} are Lagrange multipliers interpreted as macroscopic stresses. No additional boundary conditions are necessary for homogenization (with exception of minimal set of Dirichlet BCs for fixing the rigid body motion). The fundamental Hill-Mandel macrohomogeneity condition is also fulfilled here. Equation (5) is then solved with finite element method.

3. Numerical examples

Figure 1 shows the examples of representative volume elements being used in numerical simulations [5]. The shapes of RVEs result from the internal structure of the considered media and the homogenization is performed by solving (5). Smaller RVEs are necessary for the same accuracy in comparison to RVEs with straight and plane boundaries.



a) b)

Figure 1. RVEs used in numerical simulations: a) part of the RVE used in Darcy flow simulation, b) deformation of a small RVE used in homogenization of elastic media.

6. References

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