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IMPROVING THE CONVERGENCE OF BOUNDS FOR EFFECTIVE ELASTIC PARAMETERS OF HETEROGENEOUS MATERIALS

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The aim of this contribution is to improve the bounds for the effective parameters of heterogeneous materials which are calculated by computational homogenisation. Both natural and man-made materials are heterogeneous at some scale, be this the nano-, micro- or meso-scale. To model the behaviour of realistically sized structures whilst accounting explicitly for the microstructure of the material is unfeasible, but also unnecessary in practice as the effect of the heterogeneities is only "felt on average" at the macroscopic scale. Based on this observation, multiscale approaches are developed (a) to obtain the overall macro-scale material properties of materials from the knowledge of their microstructure, and (b) to get some insight into the microscopic fields without resorting to a full microscopic description of the macroscopic structure. There are several classes of multiscale approaches, including mean field theory, variational bounding techniques and computational homogenisation.

The traditional methods of mean field approaches and variational bounding aim to provide reliable, inexpensive, analytical or semi-analytical multiscale results. Mean field theory bases its predictions for the effective parameters on dilute or weakly interacting inclusions, which limits the accuracy of the result for large volume fractions (see [1] for further details). Variational bounding techniques [2, 3] provide approximate homogenised quantities with controlled, but sometimes limited accuracy. They do not offer any insight into the microscopic fields.

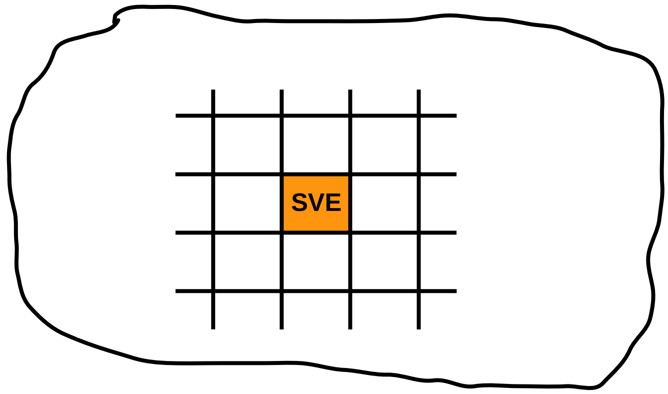
Computational homogenisation aims to address the limitations of analytical or semi-analytical homogenisation schemes by using computational power [4, 5, 6] to solve RVE problems. As RVEs for random distributions may be extremely large, the homogenisation is usually performed on smaller domains, called statistical volume elements (SVE) [7].

In order to limit the influence of the boundary conditions on the results of the SVE problems, one may employ periodic or mixed boundary conditions to represent the effect of the environment. Alternatively, using homogeneous Dirichlet and Neumann boundary conditions associated with an ensemble averaging over the SVEs leads to homogenised quantities with controlled accuracy (i.e. upper and lower bounds for the energy, which can then be used to derive lower and upper bounds for elastic constants).

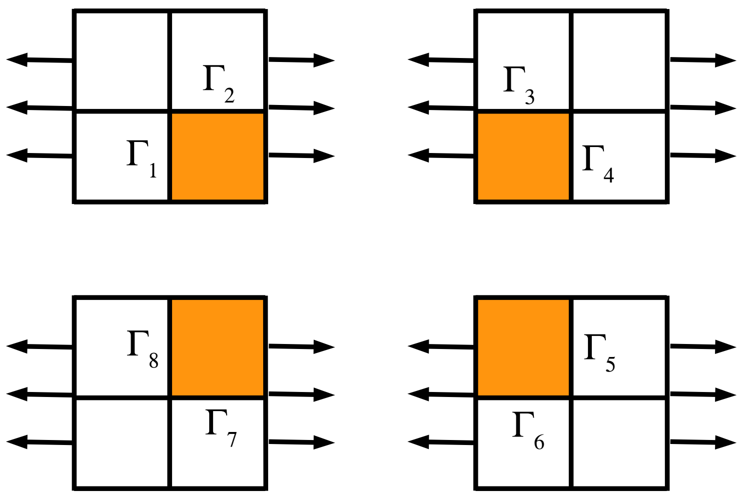
However, for these bounds to be sharp, the required size of the SVEs may be very large, leading to prohibitive computational expenses. The bounds are slow to converge because of the homogeneous boundary conditions which pollute the accuracy of the fields close to the boundary. In this contribution we propose to derive efficient non-homogeneous boundary conditions for the SVE problems in a manner that will respect the methods bounding properties.

In order to achieve our aim, we choose to apply boundary conditions to the material surrounding a statistical volume element (SVE) of the material, and not directly to the SVE. The process is summarised in Figure 1. Surrounding the SVE by eight (in 2D) similarly sized blocks of material we extract four subdomains. We apply Dirichlet boundary conditions to each of the four subdomains and solve the associated boundary-value problem. The displacement solution on the boundary of the SVE can be reconstructed from the solution of the four subdomains by using a partition of unity to weight the contributions of each subdomain to the boundary conditions of the SVE under consideration. This weighting ensures that the displacement solution is continuous over the whole RVE, which is necessary to obtain bounds on its energy. The boundary value problem on the SVE is then solved with the newly calculated (non-homogeneous) boundary conditions. The same approach is performed using Neumann boundary conditions and the results are combined to give bounds for the effective elastic parameters.

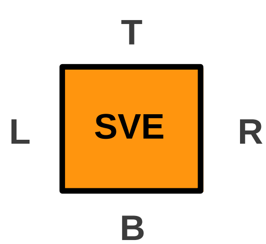
We will demonstrate the efficiency of the method by showing that the computational expense required to obtain a certain accuracy of the bounds is reduced, due to smaller SVE sizes.



(a) The material with an SVE and eight surrounding blocks of microstructure.



(b) The nine blocks of material in Figure (1a) are arranged into four subdomains, each including the SVE. Boundary conditions are applied and the problems are solved.



(c) The boundary conditions for the SVE are determined from the solutions to the four boundary value problems shown in Figure (1b). The boundary condition on T is a weighted combination of Γ_2 and Γ_3, and in a similar manner, the boundary condition on R depends on Γ_4 and Γ_5, the boundary condition on B depends on Γ_6 and Γ_7, and the boundary condition on L depends on Γ_1 and Γ_8.

Figure 1: The process of applying the boundary conditions to the material surrounding the SVE, and not to the SVE directly.

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