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New boundary conditions for the computation of the apparent stiffness of statistical volume elements

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ABSTRACT

We present a new auxiliary problem for the determination of the apparent stiffness of a Statistical Volume Element (SVE). The SVE is embedded in an infinite, homogeneous reference medium, subjected to a uniform strain at infinity, while tractions are applied to the boundary of the SVE to ensure that the imposed strain at infinity coincides with the average strain over the SVE. The main asset of this new auxiliary problem resides in the fact that the associated Lippmann–Schwinger equation involves without approximation the Green operator for strains of the infinite body, which is translation-invariant and has very simple, closed-form expressions. Besides, an energy principle of the Hashin and Shtrikman type can be derived from this modified Lippmann–Schwinger equation, allowing for the computation of rigorous bounds on the apparent stiffness. The new auxiliary problem requires a cautious mathematical analysis, because it is formulated in an unbounded domain. Observing that the displacement is irrelevant for homogenization purposes, we show that selecting the strain as main unknown greatly eases this analysis. Finally, it is shown that the apparent stiffness defined through these new boundary conditions "interpolates" between the apparent stiffnesses defined through static and kinematic uniform boundary conditions, which casts a new light on these two types of boundary conditions.

1. Introduction

The determination of the macroscopic properties of heterogeneous materials can be carried out by means of micromechanical models such as the model of Mori and Tanaka (1973) (see also Benveniste, 1987; Ponte Castañeda and Willis, 1995), the model of Maxwell (McCartney and Kelly, 2008; McCartney, 2010), the self-consistent model (Walpole, 1969; Kröner, 1977) or the generalized self-consistent model (Christensen and Lo, 1979; Hervé and Zaoui, 1993). These are invaluable tools, which provide semi-analytical (or even closed-form) estimates; besides, material non-linearities can be accommodated (Suquet, 1997). However, it is well-known that they fail to account for the finest details of the microstructure. This is due to the fact that most of them are based on the elementary solution to the problem of one single inhomogeneity, embedded in an infinite, homogeneous matrix (Eshelby, 1957). Since the inhomogeneity under consideration in this auxiliary problem is isolated, microstructural correlations can only be approximately incorporated. In cases where a more faithful representation of the microstructure is needed, it is therefore essential to resort to numerical homogenization, which provides accurate estimates derived from full-field computations.

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Within the framework of numerical homogenization, the effective stiffness of heterogeneous materials is usually estimated as the limit of the apparent stiffness of Statistical Volume Elements (SVEs, using the terminology introduced by Ostoja-Starzewski, 2006) of growing size (Sab, 1992). In turn, the apparent stiffness is derived from the solution to an auxiliary boundary value problem which states the elastic equilibrium of the SVE. The present paper is devoted to the issue of selecting appropriate boundary conditions for this auxiliary problem. Three types of boundary conditions are frequently adopted, namely static and kinematic uniform boundary conditions (Hill, 1963, 1967; Mandel, 1972), and periodic boundary conditions (Gusev, 1997, among others).

In the case of linear elasticity and kinematic uniform boundary conditions, the Lippmann–Schwinger equation is an alternative (equivalent) formulation of the auxiliary problem (Zeller and Dederichs, 1973). Upon introduction of a so-called reference medium, the classical boundary value problem of elasticity with the *displacement* as main unknown is replaced with a unique integral equation with the *polarization* as main unknown.

In comparison with the initial boundary value problem, the equivalent integral equation has a number of assets, both in periodic and random homogenization. In periodic homogenization, for example, the structure of the equation lends itself to efficient numerical treatments in the Fourier space (Moulinec and Suquet, 1994, 1998; Brisard and Dormieux, 2010, 2012). The resulting schemes can be extended to non-linear problems (Michel et al., 2001). In the present paper, periodic boundary conditions are not adopted, and discretization of the Lippmann–Schwinger equation can no longer benefit from formulations in the Fourier space. However, discretization of this equation in the real space can still be carried out in an efficient way under certain circumstances. This is true of e.g. random matrix–inclusions composites. Indeed, the polarization in the matrix vanishes if the latter is selected as reference medium. Then, the polarization needs only to be approximated in the inclusions (by e.g. piecewise polynomials), which results in a significant reduction of the number of degrees of freedom. This is the basis of the Equivalent Inclusion Method (Moschovidis and Mura, 1975), a variational version of which will be proposed by the authors in a future publication.

Solving numerically the auxiliary problem with kinematic uniform boundary conditions would require the discretization of a Lippmann–Schwinger equation involving the Green operator for strains of a *bounded* domain. Such an approach has two shortcomings. First, this operator is known for very specific shapes of the bounded domain only. Second, it is not translation-invariant; as a consequence, the influence pseudo-tensors, which characterize the interaction between two inclusions, would depend on the *position* of both inclusions. This would result in a costly assembly of the linear system resulting from the discretization of the Lippmann–Schwinger equation.

To overcome these shortcomings, it is necessary to substitute the Green operator of the infinite domain (whole space) to the Green operator of finite domains. This substitution effectively amounts to embedding the SVE in an infinite medium, with imposed strain at infinity (see Fig. 3). The Equivalent Inclusion Method is in fact formulated in this spirit. Since the Green operator of the infinite domain is translation-invariant, the influence pseudo-tensors of two inclusions depend on their *relative position* only, thus easing assembly of the underlying linear system.

However, the resulting Lippmann–Schwinger equation is not well-suited to numerical homogenization, as the corresponding boundary conditions do not allow for the specification of neither the macroscopic strain nor the macroscopic stress. Although it is still possible to define the apparent stiffness associated with these boundary conditions (see Fond et al., 2002 and Section 3.2 in the present paper), the resulting estimates cannot be regarded as bounds, as the principle of Hashin and Shtrikman is lost.

In the present paper, we introduce a new auxiliary problem, with mixed boundary conditions, and the associated modified Lippmann–Schwinger equation, which involves the Green operator of the infinite domain. As previously suggested by Willis (1977), this operator is applied to the *fluctuations* of the polarization. However, Willis regarded the resulting integral equation as an *approximation* of the Lippmann–Schwinger equation associated to kinematic uniform boundary conditions for infinitely large SVEs. By contrast, in this paper, we regard this equation as the *exact* Lippmann–Schwinger equation associated to the new, mixed boundary conditions, combining imposed strain at infinity and imposed tractions at the boundary of the finite-size SVE (see Fig. 2).

This new auxiliary problem with mixed boundary conditions has a number of assets. First, the loading parameter is the macroscopic strain (unlike the problem depicted in Fig. 3). This results in a direct definition of the corresponding apparent stiffness; it differs from the apparent stiffness based on static or kinematic uniform boundary conditions. Second, minimum potential and complementary energy principles can be derived, which in turn allow for the mathematical analysis of the well-posedness of the new auxiliary problem, as well as the elementary properties of the apparent stiffness. Third, an energy principle of the Hashin and Shtrikman (1962a) type can be derived; under classical restrictions on the stiffness of the reference medium, it is therefore possible to exhibit bounds on the apparent stiffness. As the underlying Green operator is translation-invariant, this energy principle lends itself to direct discretization in a numerical setting. Finally, the new definition of the apparent stiffness "interpolates" between the two classical definitions based on static and kinematic uniform boundary conditions. Indeed, when the reference (embedding) medium becomes infinitely soft (resp. stiff), the apparent stiffness associated with static (resp. kinematic) uniform boundary conditions is recovered. For finite stiffness reference media, the apparent stiffness associated with mixed boundary conditions is bounded by these two limit apparent stiffnesses.

The remainder of this paper is organized as follows. In Section 2, the definitions of static and kinematic uniform boundary conditions are first recalled. Then, the new, mixed boundary conditions are introduced. The mathematical properties of the resulting auxiliary problem, and the associated apparent stiffness are stated without proof. The essential