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Wang tiling aided statistical determination of the Representative Volume Element size of random heterogeneous materials

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Abstract

Wang tile based representation of a heterogeneous material facilitates fast synthesis of non-periodic microstructure realizations. In this paper, we apply the tiling approach in numerical homogenization to determine the Representative Volume Element size related to the user-defined significance level and the discrepancy between bounds on the apparent properties. First, the tiling concept is employed to efficiently generate arbitrarily large, statistically consistent realizations of investigated microstructures. Second, benefiting from the regular structure inherent to the tiling concept, the Partition theorem, and statistical sampling, we construct confidence intervals of the apparent properties related to the size of a microstructure specimen. Based on the interval width and the upper and lower bounds on the apparent properties, we adaptively generate additional microstructure realizations in order to arrive at an RVE satisfying the prescribed tolerance. The methodology is illustrated with the homogenization of thermo-mechanical properties of three two-dimensional microstructure models: a microstructure with mono-disperse elliptic inclusions, foam, and sandstone.

Keywords: Representative Volume Element size; Wang tiling; numerical homogenization

1. Introduction

The Representative Volume Element (RVE) is the key concept in modelling of heterogeneous materials. The original definition by Hill [1] requires an RVE to (i) be "structurally entirely typical of the whole mixture on average" and (ii) "contain a sufficient number of inclusions for the apparent overall moduli to be effectively independent of the surface values of traction and displacement, so long as these values are 'macroscopically uniform'." For materials with periodic microstructure, these requirements are met by any periodic part of the microstructure under periodic boundary conditions [2].

However, the majority of real-world materials display randomness in their microstructures. Sab [3] proved that microstructure ergodicity and statistical homogeneity are the essential requirements for the existence of an RVE. He also showed that the second Hill requirement is attainable only in the infinite-size limit and, thus, homogenized properties determined from any finite-size microstructure realization are biased by the adopted boundary conditions. For this reason, an error measure and its threshold have to be introduced in order to define an RVE for random heterogeneous materials (also referred to as a "computational RVE" [4] or a "numerical RVE" [5]). In practice, the RVE size is also limited from above by the requirement of separation of scales. When violated, the finite-size bounds can serve only as an input to stochastic finite element calculations [4, 6] or higher-order terms have to be introduced in a fully nested numerical homogenization [7–9, and references therein].

The RVE size depends on the type of treated physical phenomena, microstructure geometry, and contrast in microstructure constituent properties [10]. In the case of high contrast [11] or non-linear behaviour [10, 12, 13] the influence of particular geometry gets significantly pronounced, leading in turn to much larger RVE sizes or even to non-existence of an RVE [12]. Therefore, any recommendation on the RVE size, e.g., those for carbon reinforced polymers made by Trias et al. [14] or for particulate media [15, and references therein], are always highly material-specific and cannot be applied to other materials [9]. Consequently, similar procedures have to be performed for each investigated material, making the RVE determination still an open topic.

Plenty of works have been devoted to numerical studies of the RVE size; see Section 3.2 for an overview. The prevalent scheme is to (i) generate an ensemble of Statistical Volume Elements (SVEs), i.e., stochastic microstructure realizations smaller then an RVE, and (ii) compute their apparent properties under suitable boundary conditions. Then, depending on convergence criteria related to distribution of apparent properties within the ensemble, either a new ensemble of larger SVEs is produced or the generated SVEs are declared RVEs for the given threshold. The criteria typically involve fluctuations in the ap-

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