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On the convergence of the iterative self-consistent embedded cell model

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ABSTRACT

The convergence behavior of the recently developed iterative self-consistent embedded cell method for the determination of the effective properties of composite materials has not been analyzed in detail up to now. In this contribution, we prove it to be unconditionally stable and to converge to the effective macroscopic value ± small error. This error is found to be inherent to the method and is attributed to the presence of the direct interface between the micro- and macro-world in the same model. Furthermore, we derive a lower bound of the amount of iterations till convergence and show it to be insensitive to the above error.

1. Introduction

Presently, there are ever increasing number of approaches to numerical analysis of materials' properties. For an excellent introduction into the topic one can consult Zohdi and Wriggers [1]. These approaches differ from each other mainly due to differences in the available data and the purpose of the analysis. For example, a microstructural data obtained as a three-dimensional image (like MRI, ultrasound or X-ray computer tomography), may lead to a voxel-based approach [2,3]. On the other hand a well defined, a priori known microstructure may be analyzed with a unit cell model of an idealized segment [3–5]. To investigate the possible damage development mechanism one may need to include cohesive zone elements [6–8] or any other appropriate technique.

However regardless of the data-purpose combination, all these methods share one common requirement – the analyzed property must be recovered as a relationship between the applied load (tractions, stresses, temperatures, etc.) and the obtained reactions (displacements, strains, etc.). In other words a boundary value problem must be solved. This task is commonly accomplished with the aid of the finite-element method. Unfortunately, the obtained results may depend on the applied boundary conditions. In particular, there exists a strict hierarchy, which can symbolically be expressed as $\mathbb{C}_{KUBC} > \mathbb{C}_{SUBC}$. Here $\mathbb{C}$ denotes a resulting stiffness tensor and the subscripts stand for 'Kinematic Uniform Boundary Conditions' (i.e. prescribed uniform displacements) and 'Static Uniform Boundary Conditions' (i.e. prescribed uniform tractions). Extensive studies on the boundary conditions effects, the proof of the described hierarchy and sub-hierarchies of mixed boundary conditions can be found in [9–11].

To reduce the interaction between the boundary conditions and the analyzed microstructure, Dietrich et al. [12] have developed the embedded cell model for microstructures which are periodic in loading direction. The model was subsequently extended to non-periodic two-dimensional [13–15] and three-dimensional composites [14]. In this model, the analyzed specimen (the cell) is surrounded by a layer of 'equivalent' material. The properties of the equivalent material are determined in an iterative self-consistent manner and as soon as these converge, the properties of the inner cell are obtained by averaging the stresses and strains in the cell.

Dong and Schmauder observe later that "If the dimension of the embedding composite is sufficiently large compared to the embedded cell, the external geometry boundary conditions introduced around the embedding composite are almost without influence on the composite behavior of the inner embedded cell" and also "It has been found from systematic studies over a wide parameter range that convergence to the final stress strain curve of the composite is independent on the initial mechanical behavior of the embedding composite" [16]. In other words, the method should be insensitive, neither to the initial guess, nor to the boundary conditions. The above observation seems to be never proven analytically. The present work aims to fill this gap.

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It shall be noted that recently a different implementation of the iterative self-consistent homogenization was developed [17], which is based on two separate finite-element models – a fine heterogeneous and a coarse homogeneous. The properties of the coarse model are iteratively improved to match the response of the fine heterogeneous. However since the models are separate, the method is not a typical self-consistent one. Moreover, since the boundary conditions must be applied directly to both models, the method is not immune from the associated boundary effects.

2. A formal proof of convergence

Without limiting the generality of the foregoing, we assume that the required property is the stiffness tensor $\mathbb{C}^*$ of some composite material. Let us also assume that the microstructure can be represented as a unit cell (not necessarily periodic). Surrounding this cell with a layer of some homogeneous material we obtain the embedded cell model, Fig. 1.

To compute the stiffness of a unit cell one applies a series of six prescribed displacement boundary conditions. The resulting responses fill the corresponding six columns of the stiffness tensor. Note that the boundary conditions in our case are applied to the added outer layer and not to the original unit cell. It can be expected that in case the stiffness tensor of the wrapping material $\mathbb{C}^W$ is exactly the same as the effective stiffness of the original composite $\mathbb{C}^C$, the wrapping material will not affect the overall behavior. In reality, the stiffness of the added phase differs, since the effective stiffness of the original composite is not known a priori. However, the resulting total effective stiffness (original + added) $\mathbb{C}^E$ will be always closer to $\mathbb{C}^C$ than $\mathbb{C}^W$ to $\mathbb{C}^C$ i.e.

$$\|\mathbb{C}^W - \mathbb{C}^C\| > \|\mathbb{C}^E - \mathbb{C}^C\| \tag{1}$$

For the purpose of measuring the 'distance' between the matrices (here tensors in matrix form) we use the Frobenius norm [18], defined as

$$\|A\| = \sqrt{\mathrm{tr}(AA^T)} \tag{2}$$

Consequently, each subsequent iteration improves the initial guess by substituting the result of the previous step into the guess of the next one. The iterative procedure can be outlined as:

Algorithm 1. Iterative homogenization procedure

Step 1: guess the initial stiffness tensor for the added phase ($\mathbb{C}_0^W$)
Step 2: find the effective stiffness of the resulting composite ($\mathbb{C}_i^E$)
Step 3: if the stopping criterion is fulfilled – stop. Else,
Step 4: update the guess ($\mathbb{C}_i^W = \mathbb{C}_{i-1}^E$)
Step 5: repeat steps 2–4 until the stopping criterion is fulfilled.

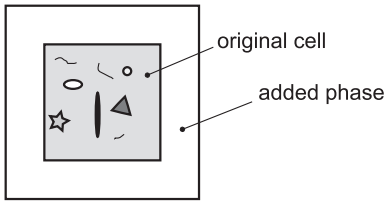

Fig. 1. A unit cell surrounded by an additional phase.

The first three iterations are illustrated in Fig. 2 for the case $\|\mathbb{C}^C\| > \|\mathbb{C}^W\|$.

Since Voigt and Reuss bounds, depicted as continuous lines in Fig. 2, are absolute bounds for both analytical homogenization and numerical alike, any homogenization result must lie within these bounds. Clearly, the closer the results of each iteration to the 'target' value, the faster and the easier the convergence. It follows that the most unfavorable (conservative) situation is when the iteration results stay always on one of the bounds. Thus, to prove that these iterations converge, we need to show that (i) iterations, resulting in values on Voigt bound and (ii) iterations, resulting in values on Reuss bound, both converge. Finally it is necessary to show that both (i) and (ii) converge to exactly the same result.

Let us start with the (i) – the Voigt bound. The first iteration is given by

$$\mathbb{C}_1^E = v^C\mathbb{C}^C + v^W\mathbb{C}_0^W \tag{3}$$

where the zero index denotes the initial guess for the equivalent phase, and $0 < v < 1$ is the volume fraction, defined as the ratio between the volume of the phase and the total volume of the sample. Consequently,

$$v^C + v^W = 1 \tag{4}$$

Volume fractions of the phases do not change during the iterations. The kth iteration is then

$$\mathbb{C}_k^E = v^C\mathbb{C}^C + v^W\mathbb{C}_{k-1}^W \tag{5}$$

By substitution of the $k-1$ first iterations into the kth iteration, (5) can be written as

$$\mathbb{C}_k^E = v^C\mathbb{C}^C\sum_{n=0}^{k-1}(v^W)^n + (v^W)^k\mathbb{C}_0^W \tag{6}$$

where a lowercase upper index denotes power. To complete the proof we find $\mathbb{C}_\infty^E$:

$$\lim_{k\to\infty}\mathbb{C}_k^E = v^C\mathbb{C}^C\lim_{k\to\infty}\left(\sum_{n=0}^{k-1}(v^W)^n\right) + \mathbb{C}_0^W\lim_{k\to\infty}(v^W)^k \tag{7}$$

However, since $\forall v \in [0,1)$, $\lim_{k\to\infty} v^k = 0$ and $\lim_{k\to\infty}\left(\sum_{n=0}^{k} v^n\right) = \frac{1}{1-v}$, Eq. (7) simplifies to

$$\lim_{k\to\infty}\mathbb{C}_k^E = \frac{v^C\mathbb{C}^C}{1-v^W} \tag{8}$$

Recalling that $1 - v^W = v^C$, we complete the first part of the proof:

$$\lim_{k\to\infty}\mathbb{C}_k^E = \mathbb{C}^C \tag{9}$$

A proof for the (ii) – the Reuss bound, is identical, if one uses compliance instead of stiffness. Since

$$\mathbb{C}^{-1} \equiv \mathbb{S} \tag{10}$$

the Reuss bound for the first iteration can be written as

$$\mathbb{S}_1^E = v^C\mathbb{S}^C + v^W\mathbb{S}_0^W \tag{11}$$

and the rest of the proof follows Eqs. (5)–(8). For this reason, we show only the end result:

$$\lim_{m\to\infty}\mathbb{S}_m^E = \mathbb{S}^C \tag{12}$$

Note that we have made no assumptions regarding the nature of the initial guess. It means the convergence is guaranteed for any guess no matter whether it is isotropic or anisotropic and no matter how 'far' it is from the final value. Note also that there are also no restrictions on the amount of the added wrapping layer.