Local homogenization with assessment of modeling and approximation errors

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Abstract

This paper makes use of the local homogenization with application to modeling of heterogeneous materials. Firstly, the idea of computer homogenization, method of reliable determination of heterogeneous material effective characteristics, is described briefly. Secondly, one of possible approaches, local homogenization, is presented in details. Assessment of both modeling and approximation errors is discussed. Subsequently, prospectives of hp-FEM application combined with local homogenization are discussed.

Keywords: adaptivity, composites, homogenization, multiscale problems

1. Introduction

Development of engineering sciences enables to create new materials with very good characteristics, designed for respective applications. These materials should possess much better features than conventional ones, e.g. stone, wood, steel. They should also provide greater bearing capacity and durability of the structure. Such materials are usually not homogeneous. They consist of several 'basic'components, which bound together create a new material possessing much better features than any of the components separately. Such materials are called composites. In fact, we can state that even above mentioned traditional materials exhibit heterogeneity. Their heterogeneous structure can be observed depending on the chosen scale. For respective materials some sort of sequence of observation scales can be distinguished, e.g. nanoscale, microscale, mezoscale, macroscale. That's why, usually, multiscale analysis is necessary. Implementation of any new material should be preceeded by thorough tests. The most reliable are obviously laboratory experiments or *in situ* testing. However, they are highly time consuming. The necessity for assessment of effective composite features as well as the composite structure response requires appropriate tools. Nowadays we can take advantage of numerical modeling to shorten and enhance the reliability of the whole design process. Various CAD and CAE computer programmes can be used.

2. Computer homogenization

The idea of computer homogenization is widely described in the literature, e.g. [5, 6]. It was applied to multiscale modeling succesfully, e.g. [4]. However, it was usually done by means of classical approach based on representative volume elements (RVE). Let's assume that we analyse a heterogeneous material in two separate scales: micro and macro. Both of them are circumscribed by respective *characteristic dimension*. RVEs contain 'full information 'about the microscale heterogeneities of the analysed medium. The problem is that the condition of scale separation needs to be fulfilled. Ratio of micro- *(l)* and macroscale *(L)* characteristic dimensions should be much less than 1:

$$\frac{l}{L} \ll 1.0 \tag{1}$$

It is assumed that computer homogenization in classical approach can be used if above ratio is equal to or less than 0.1.

Firstly, numerical calculations are made on every RVE (eg. one directional stretching). We can possess then in a respective way average RVE stresses and strains. Subsequently, we can calculate effective characteristics of every single RVE. If we analyze material as elastic one (according to Hooke's law), we can calculate effective Young modulus as the ratio of average stress to average strain.

In some engineering cases fulfillment of requirement (1) can be impossible. Eg. regarding asphalt layers, this condition cannot be fulfilled due to their small thickness and respective dimensions of the aggregate. In [4] this approach was applied to asphalt mix. However, it was represented by one thick layer fulfilling (1). Thus, we notice that in some cases multiscale modeling of heterogeneous materials requires different approach.

3. Local homogenization

In the classical approach FEM mesh is created on the basis of material features in respective subareas. It should consider material discontinuities. In local homogenization we do exactly the opposite. Firstly, the coarse mesh, which covers the whole analyzed region, is generated. Secondly, this mesh is h-refined inside each element to match the discontinuities. In such a way we create the fine mesh that fully considers material heterogeneities. Subsequently, homogenization is done within each element of coarse mesh. We compute effective stiffness matrices on the basis of fine mesh stiffness matrices. In this approach fulfilment of condition (1) is not required. Further analysis can be conducted using standard FEM.

Let's focus on fine scale. Let K be a symmetric stiffness matrix. Local FEM equation for $u \in R^N$ can be written as follows:

$$Ku = f \tag{2}$$

and $f \in R^N$ is a non-zero load vector. The FEM solution is equal:

$$u = K^{\dagger} f + u_0 \tag{3}$$

Where $K^{\dagger}$ denotes the Moore-Penrose pseudoinverse of K and u_0 is an arbitrary vector in the null space of K.

Let's consider the same problem in macroscale (coarse mesh). For $M \leq N$ let $\hat{K} \in R^{M\times M}$ be the effective stiffness matrix of coarse element. It is yet unknown. Load vector in coarse scale $\hat{f} \in R^{M}$ is defined as

$$\hat{f} = A^T f, \tag{4}$$

where A is a chosen interpolation operator for a respective element. The FEM coarse scale solution is equal:

$$\hat{u} = \hat{K}^{\dagger} A^T f + \hat{u}_0 \tag{5}$$

Where $\hat{K}^{\dagger}$ denotes the Moore-Penrose pseudoinverse of $\hat{K}$, and $\hat{u}_0$ is an arbitrary vector in the null space of $\hat{K}$. The difference between fine and coarse scale solution is equal then:

$$u - A\hat{u} = (K^{\dagger} - A\hat{K}^{\dagger}A^T)f + (u_0 - A\hat{u}_0) \tag{6}$$

Thus, the error, up to a constant, is equal:

$$e = (K^{\dagger} - A\hat{K}^{\dagger}AT)f \tag{7}$$

For a non-zero load vector f, known symmetric stiffness matrices for fine mesh elements K, interpolation matrix A, positive-definite symmetric matrix B, dimensionless parameter $\epsilon > 0$, we look for a symmetric matrix $\hat{K}^{\dagger}$ that minimizes E, where:

$$\mathrm{E}(\hat{K}^{\dagger}) = \frac{1}{2}\Big\|(K^{\dagger} - A\hat{K}^{\dagger}A^T)f\Big\|_B^2 + \frac{\epsilon}{2}\Big\|K^{\dagger} - A\hat{K}^{\dagger}A^T\Big\|_{F,B}^2\Big\|f\Big\|_2^2 \tag{8}$$

The first term of (8) measures the error of the local solution for a given local load and is equal:

$$\frac{1}{2}\Big\|e\Big\|_B^2 = \frac{1}{2}e^T B e \tag{9}$$

The second term is defined as:

$$\Big\|X\Big\|_{F,B}^2 = trace(X^T B X) \tag{10}$$

This is the Frobenius norm 'weighted with'B. The second term of (8) is a regularization term and is included to find a unique $\hat{K}^{\dagger}$. After obtaining matrix $\hat{K}^{\dagger}$, which minimizes (8), we can find desired matrix $\hat{K}$. Matrix $\hat{K}^{\dagger}$ is unique and symmetric [1]. Using properties of pseudoinverse matrices we can state that also $\hat{K}$is symmetric. A special case of above presented approach is $f = 0$ or is unknown. Expression (8) simplifies then to:

$$\mathrm{E}(\hat{K}^{\dagger}) = \frac{1}{2}\Big\|(K^{\dagger} - A\hat{K}^{\dagger}A^T)\Big\|_B^2 \tag{11}$$

Minimization of (11) simplifies significantly the procedure of effective stiffness matrix obtaining. For $B = I$ matrix $\hat{K}$ can be expressed as:

$$\hat{K} = \Big(A^{\dagger}K^{\dagger}(A^{\dagger})^T\Big)^{\dagger} \tag{12}$$

4. Error assessment and application of hp-adaptive FEM

After obtaining effective properties of heterogeneous material, it is numerically treated as homogeneous. Thus, hp-adaptive FEM can be used to enhance the reliability of modeling process. In respective subareas of the analyzed domain mesh can be refined and approximation order can be increased. Reference solution is obtained first (decreasing of elements dimensions and increasing of approximation order). It is compared then with solution obtained using current mesh. Automatic adaptation is done then in order to generate next mesh and change approximation order respectively [3].

The total error of the homogenized solution may be written in the following form:

$$e = u - \hat{u} \tag{13}$$

or equivalently:

$$e = u - u_0 + u_0 - \hat{u} \tag{14}$$

where u_0 denotes exact solution of the homogenized problem.

The first part of Eq.14 constitutes the modeling error:

$$e_m = u - u_0 \tag{15}$$

while the second part represents the approximation error:

$$e_a = u_0 - \hat{u} \tag{16}$$

The modeling error may be assessed by the first term of Eq.8 whenever the fine mesh is accurate enough. This assessment will be used to indicate the zones in which homogenization cannot be used due to large modeling error.

The approximation error (Eq.16) is estimated and reduced by the automatic hp-adaptive mesh refinement algorithm.

5. Conclusions

Computer homogenization is an effective tool for modeling of heterogeneous materials. One of its approaches, local homogenization, can be used in specific applications (if (1) is not fulfilled). Further improving of modeling process can be done using hp-adaptive FEM as well as approximation and modeling errors assessment

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