Model adaptivity on mean-field and full-field homogenization methods considering hierarchical unit cells

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The increasing use of heterogeneous materials like composites in the industrial praxis has made the finite element (FE) simulation using homogenization techniques a well-accepted and often even inevitable tool. For a reliable simulation, both discretization and model error need to be controlled. Aiming at a user-defined target functional called quantity of interest, error estimators are derived using duality arguments. Model adaptivity is established on the macro scale, towards an economic model distribution that exploits the advantages of mean-field and computational homogenization methods based on unit cells of increasing size. This is achieved by using the same philosophy of adaptive finite element method (FEM) for an economic mesh, which applies simultaneously to model adaptivity. A numerical example shows the effectiveness of the adaptive approach.

1 Introduction

For an error-controlled simulation at a relatively low computational cost, model adaptivity has been established for multiscale problems, e.g. by Goals algorithm [5] dealing with homogenization errors or by a coupled adaptive strategy [6] addressing micro discretization errors. A crucial step for model adaptivity is to form a model hierarchy, consisting of a series of models, from the simplest to the state-of-the-art model with an ascending hierarchical order. In [7], we developed a coupled adaptive strategy for homogenization of linear elastic heterogeneous materials, where a model hierarchy was established by means of a variational bounding theorem [2]. In this contribution, we present a novel model hierarchy consistently addressing

• the need for a computational method where an analytical (mean-field) method does not suffice for the pursued accuracy level and

• an adaptive selection of unit cell size for a further accuracy improvement of computational methods.

2 A coupled adaptive strategy

On the macro scale, we establish an adaptive scheme, which is valid for all appropriate model hierarchies. For the scheme to be goal-oriented, error estimators are directed to the quantity of interest \( Q \) depending on the macro displacement \( \bar{u} \). Following the lines of [6], we consider a residual as

\[
\bar{r}(\bar{u}_h^{(n)}, \delta \bar{u}) = F(\delta \bar{u}) - B(\bar{u}_h^{(n)}, \delta \bar{u}) = F(\delta \bar{u}) - \widehat{B}(\bar{u}_h^{(n)}, \delta \bar{u}) + \widehat{B}(\bar{u}_h^{(n)}, \delta \bar{u}) - B(\bar{u}_h^{(n)}, \delta \bar{u}), \tag{1}
\]

which defines the discretization error \( \bar{r}_h \) and the model error \( \bar{r}_m \) in an additive split manner. Here, \( F, B \) and \( \widehat{B} \) are the loading term, the exact bilinear form and the working bilinear form associated to a hierarchical order \( n \geq 0 \), respectively. Moreover, \( \bar{u}_h^{(n)} \) is the working FE solution belonging to an FE space \( V_h^{0} \), while \( \delta \bar{u} \) is a test function in an appropriate Sobolev space \( V_0^{0} \). Assuming that \( Q \) is linear w.r.t. \( \bar{u} \), by means of an auxiliary dual problem, we may express the error \( E \) of \( Q \) in terms of the dual solution \( \varpi \) as

\[
Q(\delta \bar{u}) - \widehat{B}^\ast(\varpi, \delta \varpi) = 0, \quad \forall \delta \bar{u} \in V_0^{0} \implies E(\bar{u}, \bar{u}_h^{(n)}) = Q(\bar{u}) - Q(\bar{u}_h^{(n)}) = \underbrace{E_h(\bar{u}, \bar{u}_h^{(n)})}_{:=E_h(\bar{u}, \bar{u}_h^{(n)})} + \underbrace{E_m(\bar{u}_h^{(n)}, \varpi)}_{:=E_m(\bar{u}_h^{(n)}, \varpi)}, \tag{2}
\]

where \( \widehat{B}^\ast \) is the adjoint form of \( B \) and \( \pi \varpi \in V_0^{0} \) is the projection of \( \varpi \) onto the FE space \( V_0^{0} \). For further details, we refer to [7].

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3 A model hierarchy of mean-field and full-field methods

To compute effective properties, i.e. the effective elasticity tensor $\overline{\mathcal{C}}$, for a scale transition, we consider the following two classes of homogenization methods. Mean-field methods in micromechanics are based on a mean-field formulation, which is obtained by condensing the full-field formulation merely to mean values over individual material phases. By means of analytical solutions, they are most efficient. In contrast, computational methods adopt a numerical method like FEM to solve a unit cell problem to obtain an approximation of the full-field formulation, see e.g. [4]. Hence, they are sometimes also referred to as full-field methods. Despite of a relatively large computational cost, they are very accurate.

On this basis, we establish the following model hierarchy for model adaptivity:

1. The basic model of hierarchical order $n = 0$ is chosen as a basic mean-field method (here self-consistent [1]).
2. As an accuracy improvement, a superior mean-field method (here interaction direct derivative [3]) is chosen as $n = 1$. This choice is made on an empirical basis, with an advantage to eliminate the need of a full-field method for an error estimate of the basic model $n = 0$.
3. For a further accuracy improvement, the FE-based method with an appropriately chosen boundary condition (here periodic) is adopted for $n > 1$ towards a full-field approximation. A key role is played by hierarchical unit cells with increasing sizes $n = n_s + 1 = 2, 3, \cdots$, which keep improving the obtained apparent effective properties.

4 Numerical results

As a numerical example, we consider a half model of CT specimen shown at the top of Fig.1a, which is made of a random composite material consisting of two different phases (matrix $E_1 = 70000$ MPa, $\nu_1 = 0.25$ and circular fibers with random arrangements $E_2 = 700000$ MPa, $\nu_2 = 0.25$). The random distribution of the fiber volume fraction $c_f$ is illustrated at the bottom of Fig.1a. We are interested in

$$Q(Q) := \int_{\Omega'} \sigma_{22}(\mathbf{u}) d\mathbf{v},$$

where $\sigma_{22}$ denotes the stress component in the vertical direction, while $\Omega'$ denotes the local domain marked in Fig.1a. The adaptive scheme starts with a coarse mesh assigned with the initial properties $n = \text{const.} = 0$. Fig. 1b shows the locally refined mesh and the model distribution after 14 refinement steps, respectively. In Fig. 1c, by a comparison with a reference solution, we observe a very nice convergence behavior of the adaptive scheme w.r.t. $Q$.

Fig. 1: Summary of numerical results

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