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Tensor-based methods for numerical homogenization from high-resolution images ☆

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ABSTRACT

We present a complete numerical strategy based on tensor approximation techniques for the solution of numerical homogenization problems with geometrical data coming from high resolution images. We first introduce specific numerical treatments for the translation of image-based homogenization problems into a tensor framework. It includes the tensor approximations in suitable tensor formats of fields of material properties or indicator functions of multiple material phases recovered from segmented images. We then introduce some variants of proper generalized decomposition (PGD) methods for the construction of tensor decompositions in different tensor formats of the solution of boundary value problems. A new definition of PGD is introduced which allows the progressive construction of a Tucker decomposition of the solution. This tensor format is well adapted to the present application and improves convergence properties of tensor decompositions. Finally, we use a dual-based error estimator on quantities of interest which was recently introduced in the context of PGD. We exhibit its specificities when it is used for assessing the error on the homogenized properties of the heterogeneous material. We also provide a complete goal-oriented adaptive strategy for the progressive construction of tensor decompositions (of primal and dual solutions) yielding to predictions of homogenized quantities with a prescribed accuracy.

1. Introduction

With the development of affordable high resolution imaging techniques, such as X-ray microtomography, high resolution geometrical characterization of material microstructures is increasingly used in industry. However, the amount of informations that are available is still difficult to handle in numerical models. This is why dedicated approaches have been proposed in order to incorporate these informations for simulation purposes [57]. The most used approach in this context is the voxel-based finite element method introduced in [25,21], where each voxel of the model is transformed into a finite element. The approach is straightforward and automatic for the generation of the computational model (see [43] for a review). However, it leads to huge numerical models, as the number of elements corresponds to the number of voxels in the image (in the order of 8 billion of elements for a full resolution $2000 \times 2000 \times 2000$ voxels CT scan). In addition, the representation of the interfaces is not smooth, which induces local oscillations in the mechanical fields [9,53,40]. The size of the model can be decreased with the use of an octree coarsening away from the interfaces [40] or by decreasing the resolution of the image [42,3,38]. However, this can severely decrease the geometrical accuracy (more jagged interfaces) and increase the oscillations. In order to get rid of these oscillations, mesh smoothing techniques can be considered, e.g. [6]. Ultimately, full resolution images can still be considered, using fast Fourier transforms (FFT) algorithms [44] in the case of periodic problems.

A second class of approaches consists in extracting the material interfaces from the image and then in constructing an unstructured conforming mesh from these informations, e.g. [41,56,57]. This allows to generate smooth interfaces and adapt the mesh in order to master the size of the model. However, meshing complex geometries is still difficult and usually requires human guidance.

Finally, non-conforming approaches can be considered (see [54,13] among others): these approaches allows to avoid meshing issues. In particular, the extended finite element method (X-FEM) has been used by the authors for the treatment of 2D and 3D image-based analysis [36,35,40]. An integrated approach was proposed in order to incorporate the geometrical informations into the numerical model. It is based on the use of Level-set functions [51], for both segmentation and mechanical analysis. Thanks to the use of tailored enrichment functions, it is possible to represent the interfaces on a non-conforming mesh. The size of the numerical model is decreased thanks to the use of an octree database that enables to keep maximum geometrical accuracy near the

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interfaces. This allows to obtain a good compromise between easy mesh generation and accuracy (both geometrical and mechanical). More recently, an improvement was proposed by the use of a high-order two mesh strategy that enables high geometrical and mechanical accuracy on coarse meshes [37].

Despite of the improvements in the numerical efficiency of the methods discussed above, image-based computations are still computationally demanding, leading to time consuming studies especially for large resolution images. There is still a need for new approaches that would allow the efficient resolution of such large scale problems.

This is why an alternative path is proposed in this paper. It relies on the use of tensor approximation methods for the solution of image-based homogenization problems. The basic idea is to interpret 2 or 3-dimensional fields as 2 or 3-order tensors, and to use tensor approximation methods for the approximate solution of boundary value problems. The use of suitable tensor formats allows to drastically reduce the computational costs (time and memory storage) and therefore allows the computation on very high resolution images. This paper provides a complete tensor-based numerical methodology, going from the translation of homogenization problems into a tensor framework, to the development of a goal-oriented adaptive construction of tensor decompositions based on error estimation methods, and dedicated to the present application.

We first translate image-based homogenization problems to a tensor framework by introducing suitable tensor approximations of geometrical data. Tensor approximation methods are applied to indicator functions of material phases, which are previously smoothed in order to improve the convergence properties of their decompositions. Suitable weak formulations of boundary value problems preserving tensor format are introduced in order to handle the different types of boundary conditions that are used in classical numerical homogenization methods. Regarding the construction of tensor approximations of the solution of PDEs, we use proper generalized decomposition methods (PGD), which is a family of methods for the construction of tensor decompositions without a priori information on the solution of the PDE [10,45,46,28] (see [12] for a short review on PGD methods). Theoretical convergence properties have been recently obtained for a class of PGD algorithms [15,7,16]. Note that a basic PGD algorithm has been used in [11] for the numerical solution of PDEs with heterogeneous materials whose geometry is easily represented in a tensor format. The method has also been used for deriving efficient non-concurrent non-linear homogenization strategies [31].

Although PGD methods rely on general concepts in approximation of tensors, practical algorithms have only been provided for the approximation in canonical tensor format. However, this format is known to have bad topological properties yielding ill-posedness of best approximation problems in the set of rank-r canonical tensors for $d > 2$ and $r > 1$ [52]. Greedy constructions of canonical tensor decompositions allow to circumvent this issue but present only poor convergence properties. Here, we introduce variants of PGD algorithms for the construction of tensor decompositions in different tensor formats. In particular, we introduce a new definition of PGD which allows the progressive construction of a Tucker approximation of the solution. This tensor format is well adapted to the present application and yields to improved convergence properties of tensor decompositions. The subset of Tucker tensors with bounded rank is known to possess nice topological properties yielding well posedness and numerical stability of best approximation problems in these subsets [14]. Moreover, efficient algorithms based on SVD have been proposed for computing quasi-optimal Tucker approximations of a tensor, with controlled precision [34]. The algorithm proposed in this paper can be interpreted as an adaptive subspace-based model reduction method which consists in constructing a sequence of reduced approximation spaces extracted from successive rank-one corrections. An approximation (in Tucker format) is then obtained by a projection on the tensor product of these approximation spaces. The main drawback of the use of Tucker tensors is that it suffers from the curse of dimensionality. For dimension $d > 3$, a recent format coined "hierarchical Tucker tensors" [19] combines the advantages of the canonical and the Tucker tensors. This work is a first step toward the use of hierarchical Tucker tensors within the PGD.

We finally devise a goal-oriented error estimation strategy in order the assess the error on quantities of interest which are the homogenized properties. Error estimation methods have been first introduced in the context of PGD in [2,29]. Here, we use a classical dual-based error estimator (see [1]), which has been used in [2] in the context of PGD methods. The originality of the present contribution consists in providing a complete adaptive strategy for the progressive construction of tensor decompositions yielding to predictions of homogenized quantities with a prescribed accuracy. Note that the proposed adaptive strategy could also be used in other context for goal-oriented approximation of PDEs in tensor formats.

The outline is as follows: Section 2 presents the homogenization problems and their variational formulations. Section 3 introduces the tensor framework and notations used for separated representations. Then Section 4 presents how the solution of PDEs can be approximated under separated representations with the PGD. In particular, we detail a new algorithm for the progressive construction of a Tucker decomposition. Next, image geometry and boundary conditions are expressed in a tensor format in Section 5. First numerical examples are introduced in Section 6. Then, in section 7, we introduce a goal-oriented adaptive algorithm using error estimators on homogenized properties. Finally, the article presents an application on a cast iron image extracted from a tomography, where we use the complete goal-oriented adaptive solution method.

2. Homogenization problems and variational formulations

In this section, we introduce classical homogenization methods for a linear heat diffusion problem. Homogenization problems are boundary value problems formulated on a domain Ω which constitutes a representative volume of an heterogeneous material. The solution of these problems allows to extract effective for apparent macroscopic properties of the material depending on whether Ω is larger than the representative volume element (RVE). Note however that the prediction of the size of the representative volume is out of the scope of this paper. The reader can refer to [23,24,48,39] for methodologies to estimate the size of the representative volume. In the following, we will identify both apparent and homogenized properties.

2.1. Scale transition and localization problems

We denote by u and $\underline{q}$ the temperature and flux fields respectively. The macroscopic gradient of the field $\underline{\nabla} u^M$ and the macroscopic flux $\underline{q}^M$ are defined through a spatial averaging of the corresponding microscopic quantities $\underline{\nabla} u$ and $\underline{q}$ over the representative volume Ω:

$$\underline{\nabla} u^M = \langle \underline{\nabla} u \rangle = \frac{1}{|\Omega|} \int_\Omega \underline{\nabla} u d\Omega \tag{1}$$

$$\underline{q}^M = \langle \underline{q} \rangle = \frac{1}{|\Omega|} \int_\Omega \underline{q} d\Omega \tag{2}$$

The inverse process yielding the microscopic fields from the macroscopic ones is called localization. Given $\underline{\nabla} u^M$ or $\underline{q}^M$, microscopic