Multi-Scale Characterisation for Micro-Architectures

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Résumé :

Les microarchitectures naturelles et artificielles (mousses, os etc.) suscitent un intérêt considérable dans les applications nécessitant la création de propriétés de matériaux sur mesure. La méthode développée par les auteurs permet d'obtenir une homogénéisation de larges domaines inhomogènes et les caractéristiques obtenues par ce procédé peuvent aussi être visualisées afin de mettre en valeur les variations de ces propriétés. En découpant le problème en sous-volumes indépendants, il est possible de paralléliser cette méthode de caractérisation et de réduire son utilisation mémoire considérablement.

Abstract :

Synthetic and natural micro-architectures (e.g. foams, bone, etc.) are becoming increasingly popular for applications requiring tailored material properties. The method developed by the authors enables the bulk response of large inhomogeneous domains with two distinct length-scales to be obtained through characterisation. The characteristics obtained from the process can also be visualised to highlight the variation of properties. By considering independent sub-volumes the characterisation technique provides a high degree of parallelism and considerably reduced memory requirements.

Mots clefs : micro-architectures, homogenization, characterization

1 Introduction

When dealing with micro-architectures one issue likely to eventually arise is the analysis of the mechanical properties of macroscopically inhomogeneous multi-scale structures. Structures of this class may be naturally occurring, such as bone, or computationally generated. The generated micro-architectures are an obvious target for numerical optimization due to their flexibility. The optimization of these structures will inevitably introduce macroscopic inhomogeneities at some stage in the process. The bulk response of these structures can be determined by performing 'full' finite element analysis that is with the entire geometry discretized at a resolution high enough to ensure mesh independence. However, these full models may easily exceed hundreds of millions, potentially billions, of degrees of freedom. A problem only exacerbated by the fact that the number of degrees of freedom grows with the cube of the resolution. Solving problems of this magnitude is possible with the use of supercomputing facilities, although they will likely require hundreds of hours of CPU time. For a very limited number of simulations this may be an acceptable solution, with the added advantage of also capturing localized effects. However, in an iterative optimization process where the 'performance' of the structure may be evaluated thousands of times the use of full FEA simulations becomes highly impractical. When the performance of a structure is evaluated in an optimization process typically only some aspect of the bulk response, such as deflection, is considered. For such properties full FEA simulations model the problem in an excessive amount of detail. Thus, there is a need for a method to approximate the models in order to reduce the time required to evaluate the structure.

The approach taken for this work will be to treat sub-volumes of the structure as actual elements and, through a series of tests, infer appropriate effective material properties.

2 2D Problems

To demonstrate the proposed homogenization technique we first concentrate on developing it for 2D problems. While there may not be such demand for producing 2D approximate models, as very large 2D linear problems can be solved with modest hardware requirements, the simplicity of 2D problems provides a good starting point for explaining the proposed technique.

2.1 Constitutive Matrix Recovery from a 3 Noded Triangle Element

To highlight the basic principle of the proposed homogenization method this section will demonstrate how the material properties of a simple 3-node element can be recovered by way of virtual testing. This in itself has little to no direct practical use, but the principle is fundamental to the proposed homogenization method. The Constant Strain Triangle (CST) element is chosen due to its simplicity.

We know that the material matrix and element geometry determine the behavior of the element. This is clear from how the element's stiffness matrix is formed:

$$[K] = tA[B]^T [D][B] \tag{1}$$

where A is the area of the triangle, $[D]$ the constitutive (or stress/strain) matrix and t the thickness of the element (assumed to be equal to 1 hereon in). The $[B]$ matrix is constructed from the element's shape functions, a set of linear displacement functions.

In this problem we have a triangle element of known geometry consisting of an unknown (assumed) homogeneous material. As previously stated, the aim of this exercise is to demonstrate that the material properties of the element can be recovered using a series of virtual tests. The only tests which can be performed using the finite element method in this instance involve either applying displacements or forces to nodes.

We know that applying a displacement to one of the element's nodes will result in a force, as described by Hooke's Law. As this is more straightforward than applying forces to nodes ($[K]^{-1}$ need not be computed) the virtual tests will described in terms of nodal displacement. With a known displacement vector the only values which remain unknown are those in the constitutive matrix $[D]$, as expected. Thus, it is possible to express the nodal forces in terms of $[D]$. These forces must be equal to those measured by way of virtual testing:

$$F_n([D], \{U\}_n) = \{\mathcal{F}_n(\{U\}_n)\} \tag{2}$$

where $\{\mathcal{F}_n(\{U\}_n)\}$ is the vector of measured forces for the displacements $\{U\}_n$ and $F_n([D], \{U\}_n)$ is the force in terms of $[D]$. It is known that, in 2D, three tests must be performed to recover all unknowns. For simplicity we choose single node, single DOF tests, which can be shown to be more than sufficient. The choice of test is important though. Depending on the macro element's geometry certain combinations of tests can results in linear dependent equations being created.

To find the actual values of the constitutive matrix the following system must be solved:

$$[M] \cdot \{d\} = \{\mathcal{F}\} \tag{3}$$

where $[M]$ is the coefficient matrix, $\{d\}$ the vector of unknowns (i.e. $D_{1,1},\ldots,D_{3,3}$) and $\{\mathcal{F}\}$ the vector of measured forces. As the system is over-determined (i.e. contains more equations than unknowns) the coefficient matrix is non-square and hence the value of $\{d\}$ cannot be computed by $\{d\} = [M]^{-1} \cdot \{\mathcal{F}\}$. To solve this system it is possible to use the method of least squares. Thus we have:

$$d = ([M]^T [M])^{-1}[M]^T \{\mathcal{F}\} \tag{4}$$

2.2 Multi-Scale Triangle Elements

We have previously demonstrated how the constitutive matrix of a 3-node triangle element can be recovered by way of virtual testing. In each of these virtual tests a single node is displaced along one axis. The resulting forces are then equated to the nodal forces in terms of the effective constitutive matrix in order to find the matrix values. As has been noted, this in itself has little direct practical use since the constitutive matrix to be recovered must first be known.

For practical applications we aim to recover an effective constitutive matrix from a sub-volume bounded by a triangle (now referred to as the macro element). This macro element will contain smaller triangles used to discretize the sub-volume, which we shall refer to as micro elements. To adapt the method described in the previous section we must impose appropriate boundary conditions on the micro mesh such that it is constrained to the displacement of the macro element.

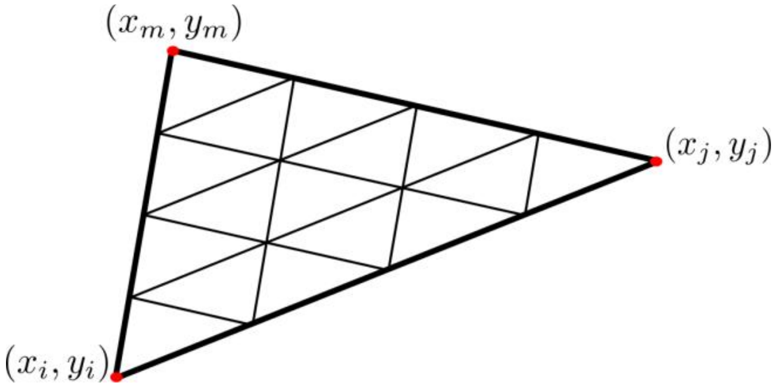


FIG. 1 – Macro triangle (bold) discretized using micro triangles

Given the displacement functions of the macro element and a macro displacement vector (which defines the virtual test) the displacement of the external micro nodes can be calculated.

To follow the same methodology as with the single homogeneous triangle element we must also calculate the forces on the macro triangle, for each test. We achieve this using weighted summation of the micro forces, again using the element's shape functions. This then provides sufficient information to recover the effective homogeneous properties as in the previous section.

3 3D Problems

The previous sections presented the principle of the homogenization technique in 2D. We also extended the method to 3D and the recovery of effective material properties of inhomogeneous sub-volumes. In the previous section the multi-scale example given had been manually constructed for a fictitious domain conforming exactly to the macro element. However, in real-world applications where the geometry to be homogenized has been acquired (or generated) using an imaging technique it is unlikely to conform exactly to the chosen macro element. To address this, a method for 'cutting' image volumes to accurately fit macro elements will also be developed. As with the 2D case we choose use a simple element to use as the macro element for the homogenization, the 4 node linear tetrahedron.

3.1 Multi-Scale Triangle Elements

For practical applications of the homogenization the sub-volume within the macro element will likely be a multi-phase structure, such as a solid/void micro-architecture. The geometry of which can be specified using image data, either generated or acquired using one of the various imaging modalities (e.g. MRI, or CT). Traditionally, for any characterization or homogenization, the sub-volume of interest is cropped to fit either a cubic or cuboidal domain. For image data, where the domain is aligned with the primary axes, the cropping process is trivial - voxels inside the domain are simply extracted. However, when the domain is not aligned with the image data, or as in this case is non-cuboidal, simply extracting the voxels considered inside leads to a surface which conforms very poorly to the macro element. A distance function based algorithm is used to improve this. Fig. 2 shows an example micro-architecture cropped to fit a tetrahedral macro element.

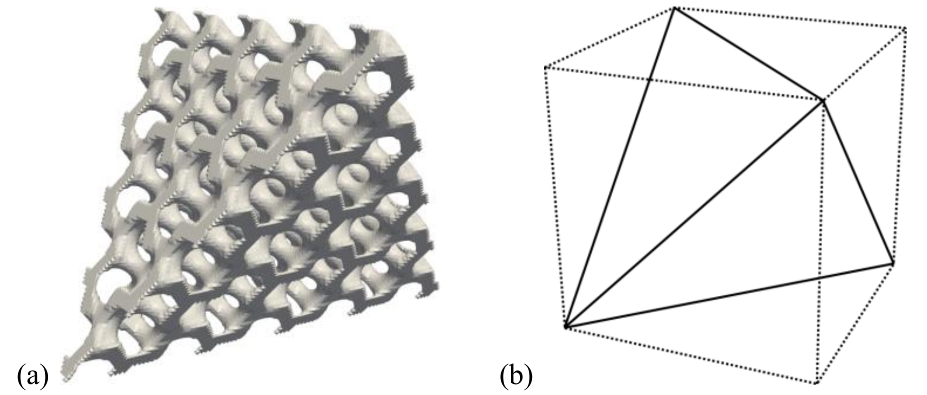


FIG. 2 – (a) Example micro-architecture conforming to (b) a tetrahedral macro element

After the sub-volume has been extracted a volume mesh must be generated to act as the micro mesh in the homogenization. The sub-volume is meshed using Simpleware's ScanIP+FE. To ensure the mesh consists of good quality elements the "off surface" option is used which allows nodes to deviate from the iso-surface for the purpose of improving element quality. Consequently, when locating nodes which lie on the macro element's surface a small tolerance must be used. A tolerance of appropriately 1 unit spacing appears suitable.

Following the creation of an appropriate micro mesh, the same methods presented in Section 2 can be directly extended to 3D with the linear tetrahedral element.

4 Validation

In order to validate the developed homogenization method we compare it to the often used *kinematic uniform boundary conditions* (KUBC). Further details of how these boundary conditions are applied can be found in [1]. The structure chosen for this validation is a periodic micro-architecture known as the Schoen Gyroid. A sample equivalent to 8 x 8 x 8 unit cells is tested at a number of volume fractions. Results are presented in Fig. 3. The Voigt and Hashin-Shtrikman (HS+) bounds are also included.

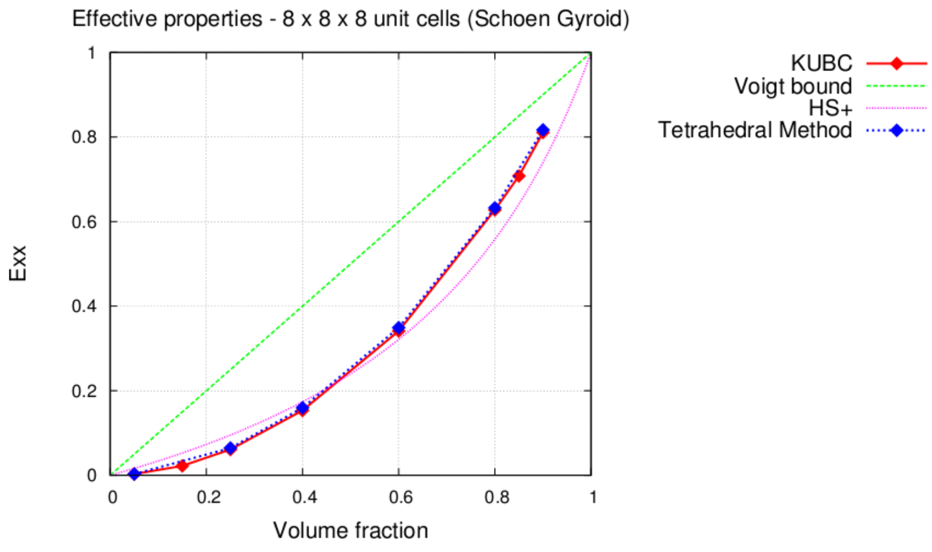
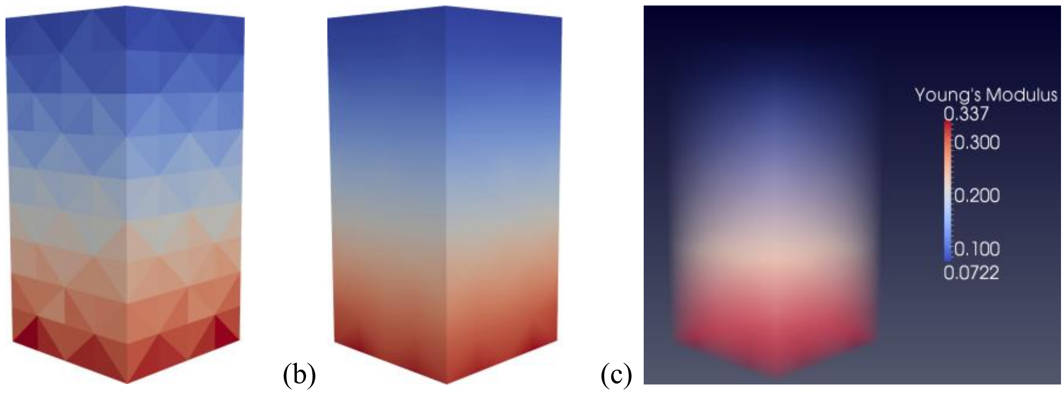


FIG. 3 – The effective properties of the Schoen Gyroid unit cell at various volume fractions

It can be seen, in Figure 3, that the results obtained using the developed methods are in good agreement with those obtained using KUBC. The results for both techniques also appear to 'overtake' the Hashin-Shtrikman bounds beyond a volume fraction of 0.5. This is likely due to the Hashin-Shtrikman bounds providing an upper limit for an *isotropic distribution* of phases, whereas the Schoen Gyroid may no longer be considered as such in this range.

5 Approximate Models

With the ability to determine an effective constitutive matrix for an arbitrary tetrahedral sub-volume we can now address the issue of multi-scale problems. Of particular interest are the set of problems having an irregular (i.e. non-cuboidal) domain. While problems of a more regular nature may be addressed with more conventional methods of determining effective constitutive matrices, they are never the less addressable using the methods developed in this paper. Fig. 4 shows the results of characterizing a large functionally graded structure using the methods described in this paper.



(a) (b) (c)

FIG. 4 – Visualizing the variation of Young's modulus over a functionally graded structure: (a) original, (b) interpolated and (c) volumetric

These approximate models may then be exported directly to a finite element package, such as Abaqus, where macroscopic simulations on the domain can be performed.

6 Conclusions

This paper has presented a novel approach to large multi-scale characterization problems in irregular domains. By dividing the domain of interest into smaller sub-volumes, based on a coarse macroscopic mesh, large problems can be processed efficiently either in parallel or series. The processing of problems using this method in series has the advantage that hardware requirements can be considerably reduced as they need only be sufficient for the largest sub-volume to be homogenized. In comparison to more classical approaches, the developed method is well-suited for multi-scale problems in which macroscopic inhomogeneities prevent a single, suitable, representative volume element from being established. Such problems often occur in natural structures. For instance, a single RVE cannot be used to model the cancellous bone in the femoral head as homogeneous. However, the drawback to this is the requirement that each macro element must itself be sufficiently large to be considered an RVE. This in-turn tends to lead to macroscopic meshes consisting of a small number of large elements and therefore an over-stiffening of the macroscopic model. An issue addressed by introducing additional degrees of freedom to the model. Approximate models produced using this technique are exportable to existing finite element packages for macroscopic simulations. They may also be used with existing visualization packages where a number of techniques may be used to visualize the distribution of effective properties over the domain and hence the influence of any macroscopic inhomogeneities, as shown in Section 5.

The homogenization method itself has been shown to yield effective properties comparable to those achieved when using KUBC. The potential application of this approach to additional properties, such as permeability, permittivity, thermal, etc... is to be investigated in future work.

References

[1] Kanit T, Forest S, Galliet I, Mounoury V, Jeulin D. Determination of the size of the representative volume element for random composites: statistical and numerical approach. International Journal of Solids and Structures.2003;40;3647-3679.