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A 3D COMPUTATIONAL HOMOGENIZATION APPROACH FOR PREDICTING THE EFFECTIVE ELASTIC CONSTITUTIVE TENSOR OF PERIODIC POROUS MATERIALS

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1. INTRODUCTION

Porous materials have been used in a wide range of industrial and engineering applications due to their interesting physical and mechanical properties. In this sense, porous solids are suitable materials in structures designed for lightweight materials, impact energy absorption, vibration and acoustic energy damping, for instance. Cellular and lattice materials are examples of porous structures with particular characteristics, including low density and large surface area. However, the effective constitutive behavior of porous solids can be complex due to the heterogeneity created by the voids. Therefore, the design of porous media requires detailed studies to obtain the desired properties.

The study of the effective elastic properties of periodic structures can be important for the design of porous media. In particular, approaches based on computational homogenization are interesting to predict the effective elastic properties of porous materials [1]. In this context, the present work presents a computational homogenization framework for investigating the effective elastic constitutive tensor of periodic porous materials. In order to improve the accuracy of the computational approach, a strategy based on posteriori error estimation proposed by Szabó and Babuška [2] is explored to extrapolate the results from numerical simulations to estimate the components of the effective elastic constitutive tensor. The homogenization procedure is implemented in ANSYS® Mechanical-Release 18.0 using the Ansys Parametric Design Language (APDL). The consistency and applicability of the computational strategy is evaluated through the investigation of periodic porous materials. The numerical analyses are performed for RVEs composed of: (i) cubic cells with unidirectional voids of circular cross-section; (ii) cubic cells with unidirectional voids of square cross-section. The assessment of the void morphology can be of particular interest in the design of porous materials to obtain improved constitutive properties.

2. COMPUTATIONAL HOMOGENIZATION APPROACH

This section describes the 3D computational homogenization approach for predicting the effective elastic constitutive tensor of periodic porous media. The framework is implemented using the APDL language in ANSYS® Mechanical-Release 18.0. Constraint equations are explored to impose the periodic boundary condition given by

$$\boldsymbol{u} = \boldsymbol{E}^{*} \cdot \boldsymbol{x} + \tilde{\boldsymbol{u}} \quad \forall \quad \boldsymbol{x} \in \partial V \tag{1}$$

where $\boldsymbol{u}$ is the displacement vector, $\boldsymbol{E}^{*}$ is the macroscopic strain tensor imposed on the RVE contour (∂V), $\tilde{\boldsymbol{u}}$ is the portion called periodic fluctuation, and $\boldsymbol{x}$ indicates the positions.

The solution of the Boundary Value Problem is obtained by solving the linear system of equations of the RVE through 3D numerical analyses performed with the Finite Element Method. The homogenized or macroscopic fields of stress ($\boldsymbol{\Sigma}$) and strain ($\boldsymbol{E}$) are calculated by:

$$\boldsymbol{\Sigma} = \frac{1}{V}\sum_{i=1}^{nelem} \boldsymbol{\sigma}_i V_i \tag{2}$$

$$\boldsymbol{E} = \boldsymbol{E}^* \tag{3}$$

where $nelem$ is the number of finite elements; $\boldsymbol{\sigma}_i$ is the average stress on the element i calculated from the values at its integration points; V_i is the volume of the element i; V is the total initial volume of the RVE (considering the hypothesis of small displacements). The macroscopic stress and strain tensors are linearly correlated by the effective constitutive tensor ($\underline{\underline{\boldsymbol{C}}}$):

$$\boldsymbol{\Sigma} = \underline{\underline{\boldsymbol{C}}} : \boldsymbol{E} \tag{4}$$

The macroscopic constitutive behavior is assumed to be linear elastic obeying an orthotropic law. Different loading programs must be conveniently imposed on the RVE considering the homogeneous macroscopic strain tensor ($\boldsymbol{E}^*$) to determinate the components C_{ijkl}. Due to the symmetry of the problem: $C_{2222} = C_{1111}$; $C_{2233} = C_{1133}$; $C_{2323} = C_{1313}$. Therefore, the number of independent elastic components can be reduced to 6. In this context, each RVE is subject to 6 loading conditions: (1) $E_{11}^* = 1.0$; (2) $E_{22}^* = 1.0$; (3) $E_{33}^* = 1.0$; (4) $2E_{12}^* = 1.0$; (5) $2E_{23}^* = 1.0$; and (6) $2E_{13}^* = 1.0$.

The strategy proposed by Szabó and Babuška [2] is explored to estimate the effective elastic properties from the numerical results in order to improve the predictive ability of the computational approach. This strategy was initially proposed for a posteriori estimation of error in energy norm. However, the initial idea can be extended for predicting the effective properties. In this context, an effective elastic component (C_{ijkl}) can be obtained from three numerical simulations (p, $p-1$ and $p-2$) solving the following non-linear equation:

$$\frac{C_{ijkl} - C_{ijkl}^{(p)}}{C_{ijkl} - C_{ijkl}^{(p-1)}} \approx \left(\frac{C_{ijkl} - C_{ijkl}^{(p-1)}}{C_{ijkl} - C_{ijkl}^{(p-2)}} \right)^{Q} \tag{5}$$

where

$$Q = \frac{\log\left(\dfrac{N^{(p-1)}}{N^{(p)}} \right)}{\log\left(\dfrac{N^{(p-2)}}{N^{(p-1)}} \right)} \tag{6}$$

where N is the total number of degrees of freedom (D.F.) of each numerical simulation.

To illustrate the applicability of the computational framework, the influence of the void morphology on the effective elastic constitutive tensor of porous materials is assessed for cubes with unidirectional voids considering circular cross-section and square cross-section. Comparisons are performed for five porosity values: (i) $f = 0.15$; (ii) $f = 0.25$; (iii) $f = 0.35$; (iv) $f = 0.45$; (v) $f = 0.55$. Therefore, the analyses comprise a wide range of porosities. The microscopic constitutive behavior of the matrix is linear elastic, and the values for the modulus of elasticity (Y) and the Poisson coefficient (ν) are adopted according to Christoff et al. [1]: $Y_m = 70$ GPa and $\nu_m = 0.3$. Three numerical

simulations must be performed for each RVE to estimate a component of the effective elastic constitutive tensor by Eq. (1). For instance, Fig. 1 shows the simulated meshes in this paper for $f = 0.55$. The 20-node hexahedral finite element (H20) was used in numerical simulations.

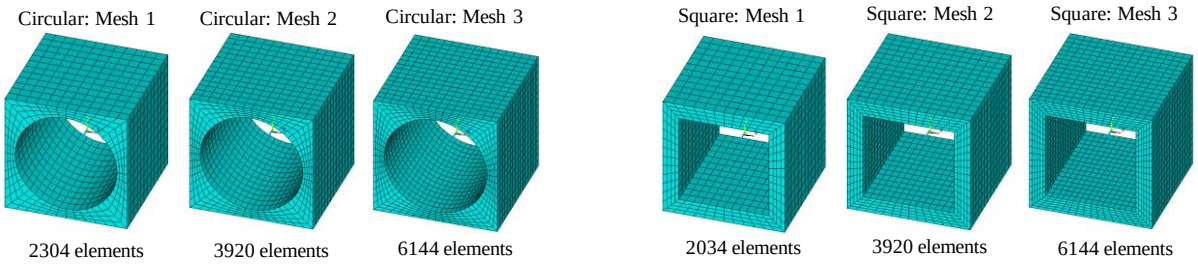

Figure 1 – RVE meshes for $f = 0.55$.

3. RESULTS AND DISCUSSION

Initially, a comparative analysis was performed to assess the accuracy of the results extrapolated by Eq. (5) when compared to the analytical solution proposed by Rodríguez-Ramos et al. [3] and the numerical results in ABAQUS® software obtained by Christoff et al. [1]. Table 1 presents the comparisons performed for the RVE with a circular cross-section void and $f = 0.55$. The effective results obtained by the computational homogenization approach are close to the compared works. The proximity of the homogenized results with the analytical solution proposed by Rodríguez-Ramos et al. [3] indicates the consistency of the computational strategy herein proposed.

Table 1 – Results of the effective elastic stiffness tensor components compared with Rodríguez-Ramos et al. [3] and Christoff et al. [1] for the RVE with a circular cross-section void and $f = 0.55$.

	Rodríguez-Ramos et al. [3]	**Christoff et al. [1]**	**Authors**	**Relative differences in module**	
Component	**(1)**	**(2)**	**(3)**	**(2) to (1)**	**(3) to (1)**
C_{1111} (GPa)	20.4986	20.5519	20.5015	0.2602%	0.0141%
C_{3333} (GPa)	35.7979	35.8392	35.7986	0.1155%	0.0020%
C_{1122} (GPa)	3.3787	3.3881	3.3783	0.2782%	0.0127%
C_{1133} (GPa)	7.1632	7.1820	7.1650	0.2627%	0.0251%
C_{1212} (GPa)	1.8088	1.8276	1.8101	1.0431%	0.0708%
C_{1313} (GPa)	7.4591	7.4795	7.4605	0.2739%	0.0182%

The extrapolated results for the components of the effective stiffness tensor considering different RVE morphologies are shown in Fig. 2. The results are presented for porosities between $f = 0.15$ and $f = 0.55$, in which 180 numerical simulations were computed for predicting the effective properties. For lower porosity values, in general, the RVE with a unidirectional void of circular cross-section provides more stiffness when compared to the RVE with a unidirectional void of square cross-section. The biggest relative differences occur for the component C_{1212}, which is directly associated with the shear modulus in plane of the void cross-section. It is also worth mentioning the differences in the case of component C_{1122}. In relation to component C_{1212}, the differences are more evident with the increase in porosity. Furthermore, the differences are also sensitive for the component C_{1133} considering lower porosity values. On the other hand, except for C_{1122} and C_{1212}, the component results are closer for high porosity values. Therefore, the void morphology and the porosity level can strongly influence the effective constitutive tensor of the porous material with periodic behavior.

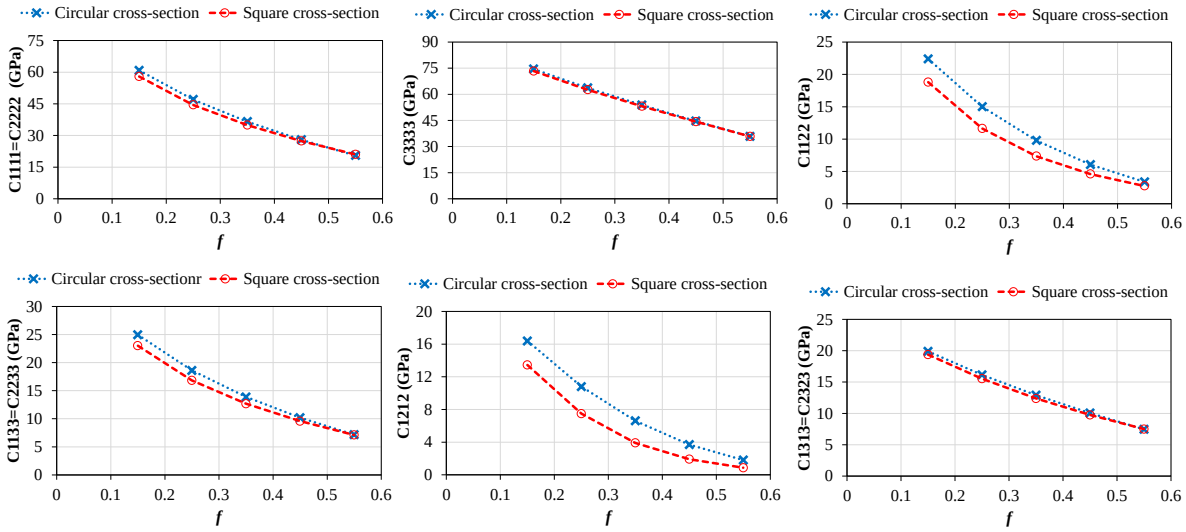

Figure 2 – Effective elastic stiffness components for the RVEs with different void morphologies and porosities.

4. CONCLUSIONS

In this paper, a computational homogenization approach was proposed for predicting with good accuracy the effective elastic constitutive tensor of periodic porous materials. In particular, an extrapolation strategy was explored to better estimate the final homogenized results from the numerical results computed by a computational homogenization procedure implemented using the APDL language in ANSYS® Mechanical, Release 18.0. The applicability of the computational strategy was investigated by a study considering the influence of the void morphology on the effective elastic constitutive tensor of porous materials with periodic structure. The study was performed for unidirectional voids of circular and square cross-sections with different porosity values.

The accuracy of the approach based on computational homogenization was assessed by means of comparisons with other works in the literature, including analytical and numerical studies. In this context, the final results showed good agreement with the compared works for unidirectional voids of circular cross-section, evidencing the consistency of the computational strategy. In particular, the effective results were very close to the results of the compared analytical approach, where the differences were minimal. The comparison between the different void morphologies showed interesting conclusions. In general, significant differences were observed for the components of the effective elastic constitutive tensor associated with the shear in the plane that cuts the void cross-section. Finally, it is worth mentioning that the computational homogenization framework herein described is an interesting strategy for the design of periodic porous materials with improved and/or specific effective properties, including applications in cellular and lattice structures.

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