XLI CILAMCE
XLI Ibero-Latin American Congress on Computational Methods in Engineering
16-19 November, 2020 FOZ DO IGUAÇU PARANÁ - BRAZIL

Comparative analysis in the homogenization process of heterogeneous materials using mechanics of structure genome

João F.L. Nunes[1], Francisco P.A. Almeida[1]

[1]*Technology Centre, Federal University of Alagoas*
BR-104 Cidade Universitaria, Maceió, AL 57072-900, Brazil
jfyllipy@gmail.com, patrick@lccv.ufal.br

Abstract. Concerning the mechanical properties studies of heterogeneous materials, its behaviours are obtained by ideal models. With the aim of simplify this modelling process, in other words, formulate an homogeneous model which represents the heterogeneous material (process called homogenization), as the microscopic analyses of stress and strain (process called dehomogenization), the so called Mechanics of Structure Genome method (MSG) was developed. The MSG method proposes to model a representation of a smallest particle possible that could describe the behaviour and geometry of the heterogeneous material, showing its microscopic behaviour. The method is named as so from its similarity with the gene concept in biology, standing for organic microparticles that contains all the information of a live cell. To observe the capacity and reliability of MSG compared to methods already in use among researchers and industry, this work models a stiffness matrix of an heterogeneous material, composed by a matrix of titanium and silicon carbide (SiC) fibres using SwiftComp software, available on cloud, Android and iOS, exposing the substantial reduction in computer effort and time compared to existing methods, and compares the results to the respective matrix for the same material obtained by the Zheng and Fish method, Self-Consistent Method (SCM) and Mori-Tanaka Method (MTM), discussing in the end the reliability and usage in the industry and academy of the exposed method.

Keywords: Composites, Homogenization, Structural Mechanics, MSG, Heterogeneous Materials

1 Introduction

Composites are elements made by combining two or more materials with distinct properties to obtain a new material with new properties and behaviours. Concerning the mechanical characteristics, the study of composite materials behaviour occurs with an idealization of physical-mathematical model, also called representative volume element (RVE) in three dimensional solids.

With the objective of simplify the microstructure study of these composites, in other words, formulate a homogeneous model from the union of different materials (Homogenization), as the microscopic analysis of stress and strain, the so called Mechanics of Structure Genome (MSG) [1] was idealized. Using the minimum information loss concept the need for an RVE and, as consequence, the need to apply boundary conditions, is no more required by introduction of the Structure Gene (SG) concept, which stands for the smallest particle possible that still portray the properties and geometry of the composite material (homogenization) to represent its microscopic behaviour (dehomogenization), as the gene idea in biology (from where the name of this technique came from). Using the SwiftComp software, developed by Yu and his team and with a release for iOS and Android (showing the substantial cutback in computational effort compared to already existing methods), the calculation for these models are simplified.

To observe the capacity of MSG, this work looks to the stiffness matrix obtained using the method developed by Zheng & Fish [2] for a heterogeneous composite made of a titanium matrix and silicon carbide (SiC), with a two dimensional fibre type geometry, the results of the same material using the Self Consistent Method (SCM) and Mori-Tanaka Method (MTM), and face the data against the stiffness matrix obtained using MSG for the same composite, discussing the use of this method into the academic and industrial fields.

2 Mechanics of Structure Genome

This new methodology originated from the need for the microstructural study of composite materials, that is, to model from a heterogeneous material a homogeneous idealization that retains its original mechanical properties, technique known as homogenization [1].

For that, it is considered a small structure called Structure Gene (SG), the smallest discrete possible structure for the material, that carry within all the microscopic characteristics, as the gene concept from the biology, which are small molecules that carry all the information from protein synthesis for the macroscopic being. The figure 1 shows the possible geometries for a SG for a 3D structure.

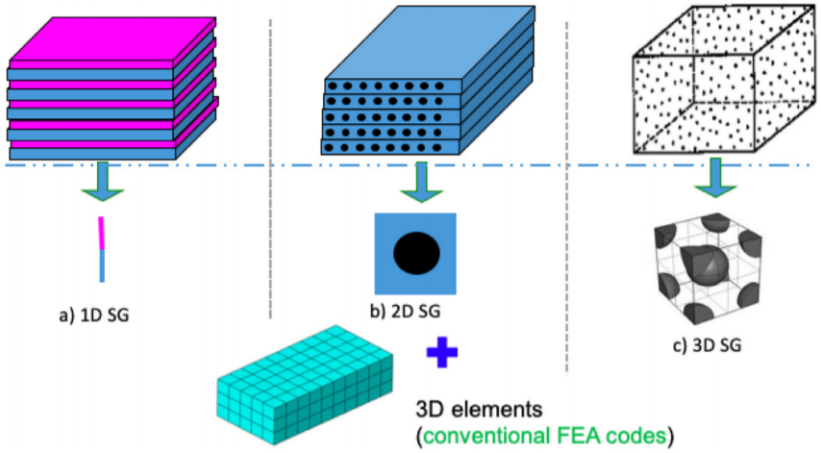

Figure 1. Geometries for a SG for a 3D structure (Yu 2016) [3]

With this technique, it is totally possible, for example, to describe a heterogeneous 3D structure, such as composites reinforced with fibres, in a 2D structure, needing for that the SG discretization as a plane. Regardless of the analysis degree it is always possible to obtain the corresponding 6x6 constitutive matrix [3]. In this fashion, we don't need to characterize an RVE, as to apply any boundary conditions for 3D elements, reducing the calculus complexity. For such, the MSG is based on the Minimum Information Loss concept, in other words, the homogenized model can be built in such a way that minimizes its differences with the original model. So, for elastic linear materials, the used information could be the strain energy density average. In short, the SG will have the smallest loss possible of this information, regarding the original structure. Almeida & Lourenço (2020) [1] presents the methodology in a simplified way as follows.

For linear elastic materials, the adopted parameter could be the strain energy density average. In this way, the MSG seeks to minimize the difference between this parameter stored on the modelled SG and in the analised structural model. The microscopic coordinates x_i e y_i relates themselves as $y_i = x_i/\delta$, where δ is a small parameter to describe the SG. The following equations subscripts rises from the matrix seen in the complete deduction on Yu (2016) [3].

The kinematics equations of the original model, from which the calculated model depends, can be written as:

$$u_i(x, y) = \overline{u}_i(x) + \delta X_i(x, y) \tag{1}$$

Where u_i is the original model's displacement field, $\overline{u}_i$ is the homogenized displacement field and X_i is the difference between these two fields, commonly called in micromechanics as fluctuating functions.

The equations for the original model displacement field is written as:

$$\epsilon_{ij}(x, y) = \overline{\epsilon}_{ij}(x) + X_{(i,j)}, \tag{2}$$

Where the subscript has the operation described as in $A_{(i,j)} = \frac{1}{2}(\frac{\partial A_i}{\partial y_j} + \frac{\partial A_j}{\partial y_i})$. The homogenized model variables that depends from the original model can be written as:

$$\overline{u}_i = \langle u_i \rangle \text{ e } \overline{\epsilon}_{ij} = \langle \epsilon_{ij} \rangle \tag{3}$$

$\langle \cdot \rangle$ is the SG average domain and involves the following requirements in the fluctuating function:

$$\langle X_i \rangle = 0 \text{ e } \langle X_{(i,j)} \rangle = 0 \tag{4}$$

The minimum information loss principle seeks to minimize the difference between the displacement energy from its original model regarding the homogenization model as follows:

$$\Pi = \langle \frac{1}{2} C_{ijkl} \epsilon_{ij} \epsilon_{kl} \rangle - \frac{1}{2} C^*_{ijkl} \overline{\epsilon}_{ij} \overline{\epsilon}_{kl}, \tag{5}$$

still submitted to the requirements of the equation 4 and other possible requirements, such as equality of X_i in the periodic boundaries.

To minimize Π, the homogenized model is considered as follows (considering that C^*_{ijkl} and $\overline{\epsilon}_{ij}$ do not change). X_i can be solved from the following variational principle:

$$\min_{X_i \in Eq.(4)} \langle \frac{1}{2} C_{ijkl} \epsilon_{ij} \epsilon_{kl} \rangle = \min_{X_i \in Eq.(4)} \langle \frac{1}{2} C_{ijkl} (\overline{\epsilon}_{ij} + X_{(i,j)})(\overline{\epsilon}_{kl} + X_{(k,l)}) \rangle. \tag{6}$$

From the variational calculus, it can be concluded that X_i needs to satisfy the Euler-Lagrange equation:

$$(C_{ijkl}(\overline{\epsilon_{kl}} + X_{(k,l)}))_{,j} = 0 \tag{7}$$

Along with what is presented in Eq. 4, X_i is obtained based on $\overline{\epsilon}_{kl}$:

$$X_k = H^{mn}_k \overline{\epsilon}_{mn} \tag{8}$$

The volumetric mean of the strain energy can then be defined as:

$$U = \langle \frac{1}{2} C_{ijkl} (\overline{\epsilon}_{ij} + H^{mn}_{(i,j)} \overline{\epsilon}_{mn})(\overline{\epsilon}_{kl} + H^{st}_{(k,l)} \overline{\epsilon}_{st}) \rangle \tag{9}$$

The effective constitutive matrix can be obtained by:

$$C^*_{ijkl} = \frac{\partial \overline{\sigma}_{ij}}{\partial \overline{\epsilon}_{kl}} = \frac{\partial^2 U}{\partial \overline{\epsilon}_{ij} \partial \overline{\epsilon}_{kl}} \tag{10}$$

$$C^*_{ijkl} = \langle C_{ijmn} + C_{ijkl} H^{mn}_{(k,l)} \tag{11}$$

For a more complete presentation and deduction of the methodology, see the article by Yu (2016) [3]

3 Zheng & Fish, Mori-Tanaka and Self Consistent Methods

In their work, the authors demonstrated how the ABAQUS software could be used for linear and nonlinear multiscale analysis of heterogeneous materials. In this work, however, we will focus on a linear analysis. The authors used a mathematical homogenization model so periodic coefficients could be decomposed. The used methodology is here described:

1. To solve a unit cell problem (a representative element), with multiples vectors under the right hand side (RHS) rule and calculate its stress.
2. To obtain a corresponding constitutive tensor.

There are two more steps described, to solve the problem for a big scale and to apply the solutions for all (or at least the most critical problem cells). These steps will not be discussed in here for being beyond the scope of this work.

In the first step, the authors introduced multiple RHS vectors, which also had thermic expansion influence take into account and with their coefficients properly defined using the ABAQUS functions. With the unit cell in hand the authors moved on to the second step, where it was introduced the boundary conditions of the representative elements. Those conditions were obtained using the surface to surface methodology. In this methodology each point on a daughter surface is linked to the nearest point on the mother surface, in such a way both have the same motion. Then they proceeded with the dehomogenization process. For more robust information about this last process their work can be reviewed [2].

The Mori-Tanaka and Self Consistent methods were also used as comparation methods by Zheng & Fish. Both are based on the Eshelby solution for elasticity, however, SCM uses the Effective Medium Theory (EMT while MTM uses the average of the nonhomogenized element internal stresses to generate the homogenized model [4][5]. Both are largely used analytical methods.

4 Numerical Results

By using all the properties shown in table 1, also used by Zheng & Fish, a 2D SG with a fibre type geometry and elastic linear behaviour was defined in SwiftComp software, using its cloud version released by Yu and his team. It is important to note the availability of this app also for iOS and Android devices for free at the time this work is being written. The elapsed calculation time exposed by the calculus log was less than 1 second. The following tables show the results obtained by Zheng & Fish on their work as to the results obtained in this work using the MSG methodology, with a percentage error table, calculated by dividing the variation between the results from each methodology with its MSG counterpart, as well.

Material	Young Module (GPa)	Poisson Coefficient	Volumetric Fraction
Titanium Matrix	68.9	0.33	0.733
SiC Fibre	379.2	0.21	0.267

Table 1. Materials properties and fractions.

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Models' Stiffness Matrix					
MSG/Zheng (SCM/MTM)					
136.2/140.3 (136.2/134.2)	59.3/57.3 (61.8/61.4)	57.3/57.7 (57.8/57.3)	0/0 (0.0/0.0)	0/0 (0.0/0.0)	0/0 (0.0/0.0)
	136.2/140.0 (131.6/134.2)	57.3/57.6 (57.8/57.3)	0/0 (0.0/0.0)	0/0 (0.0/0.0)	0/0 (0.0/0.0)
		185.1/185.6 (185.7/185.6)	0/0 (0.0/0.0)	0/0 (0.0/0.0)	0/0 (0.0/0.0)
			38.1/39.5 (40.1/38.2)	0/0 (0.0/0.0)	0/0 (0.0/0.0)
	SIM			38.1/39.4 (40.1/38.2)	0/0 (0.0/0.0)
					34.9/36.5 (37.4/36.4)

Table 2. Calculated stiffness matrix using the four methodologies

Percentage error among the four methodologies (%)					
3/0.3/1.4	3.4/4.2/3.6	0.8/0.9/0.1	0/0/0	0/0/0	0/0/0
	2.8/0.3/1.4	0.6/0.9/0.1	0/0/0	0/0/0	0/0/0
		0.3/0.3/0.3	0/0/0	0/0/0	0/0/0
			3.7/5.3/0.3	0/0/0	0/0/0
	SIM			3.5/5.3/0.3	0/0/0
					4.6/7.1/4.3

Table 3. Obtained errors among methodologies

5 Conclusion

According to the obtained results on the table 2 and percentages comparision, as the table 3 shows, it is safe to adopt with quite reasonable, the idea for the use of MSG, as stated, that the obtained error related to the analytical method used by Zheng and Fish was less than 5% in the most cases (with a peak of 7.1%), a great tolerance value in engineering and analytical field. Moreover, its simply execution, not needing fancy computers and even the possibility of modelling using a smartphone app (SwiftComp) opens a big case for usability among researchers, engineers and industries. A promising path for future researches and uses involving MSG stays open.

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References

[1] Almeida, F. P. & Lourenço, P. B., 2020. Three-dimensional elastic properties of masonry by mechanics of structure gene. *International Journal of Solids and Structures*, vol. 191, pp. 202–211.
[2] Yuan, Z. & Fish, J., 2008. Toward realization of computational homogenization in practice. *International Journal for Numerical Methods in Engineering*, vol. 73, n. 3, pp. 361–380.
[3] Yu, W., 2016. A unified theory for constitutive modeling of composites. *Journal of Mechanics of Materials and Structures*, vol. 11, n. 4, pp. 379–411.
[4] Mori, T. & Tanaka, K., 1973. Average stress in matrix and average elastic energy of materials with misfitting inclusions. *Acta metallurgica*, vol. 21, n. 5, pp. 571–574.
[5] Hill, R., 1965. A self-consistent mechanics of composite materials. *Journal of the Mechanics and Physics of Solids*, vol. 13, n. 4, pp. 213–222.