Micromechanics modeling of unit cells using CUF beam models and the Mechanics of Structure Genome

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ABSTRACT

A novel approach for the micromechanics analysis of composite structures is developed using refined beam models and the mechanics of structure genome (MSG). The MSG provides a tool to obtain the complete stiffness matrix of general composite materials by asymptotically minimizing the loss of information between the original heterogeneous body and the sought homogenized body. The constitutive information is in this manner extracted from the representative volume without the need of ad-hoc assumptions and in one single loading step. The local fields are then straightforwardly recovered using the same unknowns of the original homogenization problem, with no need of additional analyses. This work proposes the use of higher-order beam models based on the Carrera unified formulation (CUF) to solve the micromechanics problem by means of MSG. The fibers, or equivalent constituents, are discretized along the longitudinal direction with beam elements and the unknown variables are expanded over the remaining two local coordinates making use of Legendre-class polynomial sets, denoted to as Hierarchical Legendre Expansions (HLE). In addition, non-local expansion domains with curved boundaries are defined to capture the exact shape of the constituents independently of the refinement of the model. In this sense, the quality of the approximation is controlled by the polynomial order of the beam model, which is introduced in the analysis as a user input, and the size of the computational problem can be reduced for many typical microstructures with no loss of accuracy.

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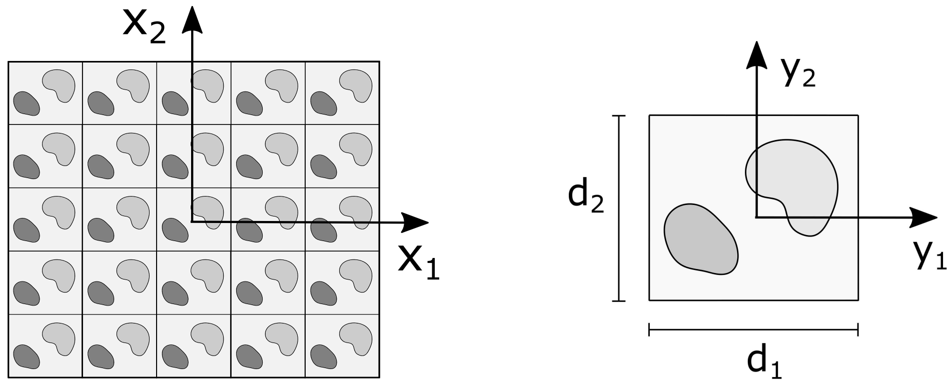
INTRODUCTION

Composite materials are constantly used nowadays in many applications such as aerospace, automotive, naval or wind energy structures, in which the ratio between the mechanical properties and the weight needs to be minimized. The inherent complexity of composites structures and the presence of different scales lead to a constant demand of new simulation techniques for the industry. Multiscale modeling techniques are required to decouple the structural analysis several steps accounting for the different length scales. In this framework, computational micromechanics methods are introduced to zoom into the microstructure level to provide accurate constitutive models and local responses for composites.

Micromechanical models are used by engineers to obtain information of the characteristics and properties of periodic heterogeneous materials and their effects on the behavior of the global structure. During the past decades, a number of micromechanical methods have been proposed and implemented in simulation tools. Most of them have in common the definition of a unit cell (hereinafter UC), that is the minimum arrangement of phases that can be ideally repeated to build the global body. Different methods can be used to solve the UC problem with the objective on obtaining the properties of the equivalent homogeneous material and the local displacements, strains and stresses within the microstructure. Some of these approaches are based on analytical formulations, such as the various rules of mixtures [1]. On the other hand, other approaches provide approximate solutions for generic cases, such as the method of cells and its developments [2] and its developments, the mathematical homogenization theories [3] or the variational asymptotic method [4]. Finally, another commonly used technique is based on the stress analysis of a rerpesentative volume element (RVE) subjected to some particular sets of boundary conditions, as in [5].

Many of the aforementioned numerical methods make use of 2D or 3D finite models to represent the geometry and materials of the UC. The focus of the present work is the demonstration of the high-fidelity capabilities of high-order beam theories to model the micromechanical problem. Refined one-dimensional models are a powerful tool to capture the complex phenomena that arises in many kinds of structures, including warping, in-plane deformations and accurate stress fields, with great advantages in terms of the computational efforts. In this framework, the Carrera Unified Formulation (CUF) [6] serves as a tool to generate theories of structure by arbitrarily refining the beam kinematics up to a desired level of accuracy, see [7, 8]. UCs that show predominant directions of the constituents, e.g. fiber reinforced composites, can be modeled by means of refined beam models in which the different phases are represented by non-local expansions of the cross-sectional coordinates. The properties of the Hierarchical Legendre Expansion (HLE) [9] are exploited to generate hierarchical models of the UC in which the exact geometry of the constituents is introduced in the model by a non-isoparametric mapping technique and the accuracy of the model is controlled by the polynomial order of the theory.

In the present paper, the mechanics of structure genome (MSG) [10] is employed to decouple the multiscale problem into global and local analysis. This approach is based on the concept of the structure genome (SG), which is defined as the smallest mathematical building block of the structure, that may be a line accounting for



(a) Periodic heterogeneous material (b) Correspondent SG

Figure 1. Reference systems of a periodic heterogeneous material and its UC.

the stacking sequence of laminates, a surface including the different phases of unidirectional materials (e.g. fiber reinforced composites), or, in general cases, the 3D volume for microstructures showing variation of the phases over all the directions. MSG has been applied to provide efficient solutions for different composite problems, such as laminated beams [11], shells [12] and micromechanics analysis [13]. In the framework of micromechanics, MSG can provide efficient solutions for:

- Computation of the effective properties of periodically heterogeneous materials, that can then be used as material inputs for the structural analysis.
- Recovering of the local fields over the SG volume from the outputs of the macroscopic analysis.

MSG is implemented in a general-purpose multiscale code called SwiftComp [14] and exploits the variational asymptotic method (VAM) [15] to minimize the loss of information between the original heterogeneous body and the sought homogenized structure. In this manner, the constitutive information is extracted from the SG without the need of introducing ad-hoc assumptions and in a single loading step. A more detailed description of the micromechanics formulation employed in the present work and how to solve the numerical problem using refined beam models is presented in the next sections. The accuracy of the proposed method to efficiently compute the effective properties and local fields is demonstrated through several benchmark examples of fiber reinforced composites.

MECHANICS OF STRUCTURE GENOME FOR THE UNIT CELL PROBLEM

In micromechanics, the composite material is idealized as an array of representative microstructures periodically repeated over the volume, as illustrated in Figure 1 (a). For the sake of clarity, a 2D sketch is considered, although a 3D frame will be consider for the formulation of the problem. It is clear that for this kind of structures, the SG of the problem is equivalent to the commonly used UC, shown in Figure 1 (b). Two coordinate systems are defined for the multiscale problem: $\boldsymbol{x} = \{x_1, x_2, x_3\}$ is selected as the global reference system, whereas $\boldsymbol{y} = \{y_1, y_2, y_3\}$ defines the local reference system of the UC. Obviously, the difference in the scales implies that $y_i = x_i/\delta$, where δ is a small parameter. In this sense, the homogenized properties obtained from the micromechanics analysis are considered intrinsic of the effective equivalent material.

Another assumption commonly employed in micromechanics is that the local solutions within the UC have a volume average which is equal to the global solution of the macroscopic problem or

$$\frac{1}{V}\int_V \phi(\boldsymbol{x}, \boldsymbol{y})\, dV = \bar{\phi}(\boldsymbol{x}) \tag{1}$$

where V is the total volume of the UC. ϕ is a generic local field that depends both on the global and the local coordinates and $\bar{\phi}_i$ are the averaged values which only depend on the global reference system.

Let the local displacements, u_i, be written as the sum of the global displacements, $\bar{u}_i$, plus the difference between both, as follows

$$u_i(\boldsymbol{x}; \boldsymbol{y}) = \bar{u}_i(\boldsymbol{x}) + \delta\chi_i(\boldsymbol{x}; \boldsymbol{y}) \tag{2}$$

where χ_i are denoted to as fluctuation functions. Performing the derivatives and discarding smaller terms according to the VAM, it is possible to write the 3D strain tensor as

$$\varepsilon_{ij}(\boldsymbol{x}; \boldsymbol{y}) = \bar{\varepsilon}_{ij}(\boldsymbol{x}) + \chi_{(i,j)}(\boldsymbol{x}; \boldsymbol{y}) \tag{3}$$

According to Eq. (1), one can write

$$\bar{u}_i = \langle u_i \rangle \qquad\qquad \bar{\varepsilon}_{ij} = \langle \varepsilon \rangle \tag{4}$$

where $\langle \bullet \rangle$ denotes the volume average $\frac{1}{V}\int_V \bullet\, dV$. This assumption, together with the definition of the local fields in Eqs. (2) and (3), implies that

$$\langle \chi_i \rangle = 0 \qquad\qquad \langle \chi_{(i,j)} \rangle = 0 \tag{5}$$

In MSG, the solution of the stationary value problem is provided by minimizing the difference between the strain energies of the heterogeneous structure and the equivalent homogeneous material. Considering the homogenized body as invariable, the problem becomes to minimize the strain energy of the heterogeneous UC, represented by the following functional:

$$\Pi_1 = \frac{1}{2}\Big\langle C_{ijkl}\left(\bar{\varepsilon}_{ij} + \chi_{(i,j)}\right)\left(\bar{\varepsilon}_{kl} + \chi_{(k,l)}\right)\Big\rangle \tag{6}$$

subjected to the constrains of Eq. (5), see [10].

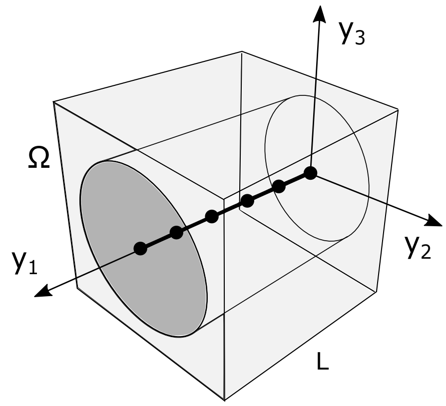


Figure 2. Reference system for the beam modeling of the UC.

REFINED BEAM MODELS BASED ON CUF

It is clear that classical beam models are not a suitable for micromechanics modeling. Classical theories, such as the Timoshenko beam model [16], are only valid for a reduced number of structures showing high slenderness ratios and homogeneous sections. These characteristics prevent its use in problems as the one shown in Figure 2, where different materials coexist, the body is short and high gradients are present in the displacement, strain and stress fields. More refined theories are needed in these cases. A solution is provided by higher-order beam theories based on CUF, which overcome the limitations of classical models by arbitrarily enriching the kinematics of the model to account for more complex phenomena.

Let a local coordinate system for the micro-scale problem be as the one shown in Figure 2, which shows a typical square pack of a fiber reinforced composite. The beam axis, y_1, falls along the fiber direction, whose total length is equal to L, whereas the cross-section, that accounts for the different phases, lays on the y_2y_3-plane, having a total surface of Ω. In the framework of CUF, the fluctuation unknowns can be expanded over the cross-section by means of arbitrary functions of the y_2 and y_3 coordinates, as follows

$$\boldsymbol{\chi}(\boldsymbol{x}; y_1, y_2, y_3) = F_\tau(y_2, y_3)\, \boldsymbol{\chi}_\tau(\boldsymbol{x}; y_1) \quad \tau = 1, 2, ..., M \tag{7}$$

where $\boldsymbol{\chi}$ is the vector of the fluctuations, F_τ are the expanding functions and $\boldsymbol{\chi}_\tau$ is the vector of the generalized fluctuations of the beam along the fiber-direction. The repeated subscript τ denotes summation and M is the total number of expansion terms assumed for the kinematic field. The choice of F_τ defines the theory of structure employed in the model. In the present work, the Hierarchical Legendre Expansion is selected due to its remarkable capabilities in capturing component-wise solutions [17].

Hierarchical Legendre Expansion

Hierarchical Legendre Expansions (hereinafter HLE) make use of hierarchical sets of Legendre-based polynomials, originally employed in the book of Szabó and

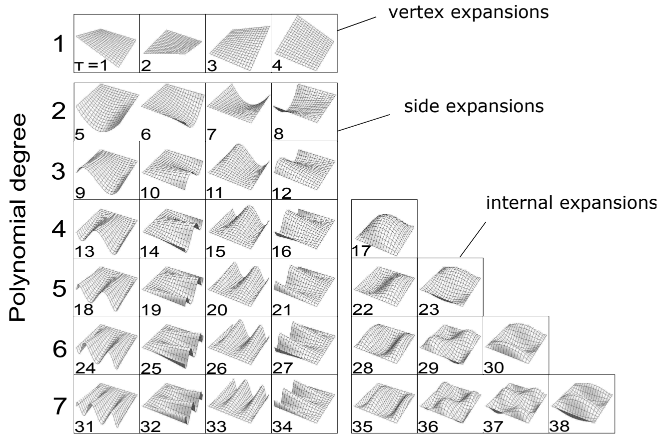


Figure 3. Set of Legendre functions employed over the cross-section.

Babuška [18], to define the arbitray functions over the cross-section, F_τ. HLE models have non-local capabilities, i.e. the different components within the cross-section are represented independently, and the accuracy of the numerical analysis relies on the polynomial order of the F_τ expansions. Figure 3 shows the set of F_τ functions employed to develop first to seventh order beam models, including vertex, side and internal expansions.

In HLE modeling, the domains of the cross-section should be kept as large as possible due to the p-refinement scheme followed. A non-isoparametric mapping technique is applied to represent the curved boundaries of the components of the microstructure, such as fibers. The blending function method, proposed by Gordon and Hall [19], is employed to introduce the exact geometry of the constituents into the mapping functions of the cross-sectional plane, see [20]. In this manner, the geometry of the model is fixed at the beginning and the accuracy of the micromechanics analysis is controlled through the polynomial order of the theory of structure.

Finite element formulation

The generalized fluctuation unknowns, $\boldsymbol{\chi}_\tau$, are interpolated along the beam axis, y_1, by means of conventional Lagrange shape functions, N_i, as

$$\boldsymbol{\chi}_\tau(\boldsymbol{x}; y_1) = N_i(y_1)\, \boldsymbol{\chi}_{\tau i}(\boldsymbol{x}) \quad i = 1, 2, ..., n \tag{8}$$

where $\boldsymbol{\chi}_{\tau i}(\boldsymbol{x})$ is the nodal unknown vector and n is the total number of beam nodes.

Substituting Eq. (8) into Eq. (7), and making use of vectorial notation, the CUF form of the functional Π_1 reads

$$\Pi_1 = \frac{1}{2}\,(\boldsymbol{\chi}_{sj}^T\, \boldsymbol{E}^{\tau sij}\, \boldsymbol{\chi}_{\tau i} + 2\, \boldsymbol{\chi}_{sj}^T\, \boldsymbol{D}_{h\varepsilon}^{sj}\, \bar{\boldsymbol{\varepsilon}} + \bar{\boldsymbol{\varepsilon}}^T\, \boldsymbol{D}_{\varepsilon\varepsilon}\, \bar{\boldsymbol{\varepsilon}}) \tag{9}$$

where $\boldsymbol{E}^{\tau sij}$ and $\boldsymbol{D}_{h\varepsilon}^{\tau i}$ are the fundamental nucleus of the UC problem, which contain all the basic information for the numerical model of the micromechanics analysis, and $\boldsymbol{\chi}_{\tau i} = \{\chi_{\tau i_1}\ \chi_{\tau i_2}\ \chi_{\tau i_3}\}^T$ is the vector of the generalized fluctuation unknowns. $\boldsymbol{D}_{\varepsilon\varepsilon}$ is the effective stiffness matrix of the material by volume average. The τ and s

subscripts refer to the loops over the cross-sectional expansions, whereas the i and j subscripts refer to the beam nodes.

Performing the variation of Π_1, one finds that the solution of the stationary problem is provided by

$$\boldsymbol{E}^{\tau sij}\,\boldsymbol{\chi}_{\tau i} = -\boldsymbol{D}_{h\varepsilon}^{sj}\,\bar{\boldsymbol{\varepsilon}} \tag{10}$$

subjected to the periodic boundary constrains over the first and last section, and also over the respective expansions falling on the sides of the UC's cross-section.

Substituting Eq.(10) into the strain energy of Eq. (9), and making the energetic equivalence, the effective stiffness matrix, C^*, can be obtained from:

$$\boldsymbol{C}^* = \frac{1}{V}\left(\boldsymbol{\chi}^T\,\boldsymbol{D}_{h\varepsilon} + \boldsymbol{D}_{\varepsilon\varepsilon}\right) \tag{11}$$

The local fields over the UC can be directly computed without solving the system again by simply introducing back the fluctuation solutions of Eq. (10) into the geometrical and constitutive definitions. Accordingly, the local strains are written as

$$\boldsymbol{\varepsilon} = \bar{\boldsymbol{\varepsilon}} + \boldsymbol{D}(F_\tau N_i\,\boldsymbol{\chi}_{\tau i}) \tag{12}$$

and the local stresses are obtained from

$$\boldsymbol{\sigma} = \boldsymbol{C}\,\boldsymbol{\varepsilon} \tag{13}$$

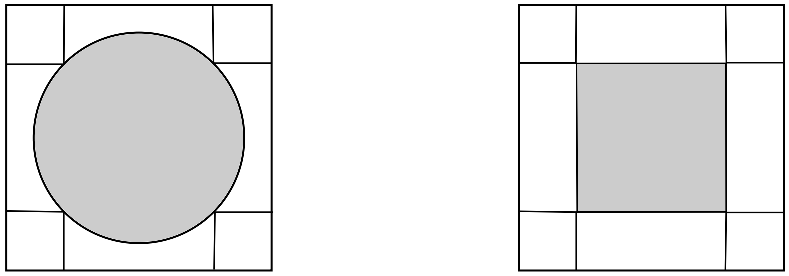
NUMERICAL EXAMPLES

Benchmark solutions of fiber reinforced and particle inclusions are addressed in this section to show the performances of the proposed modeling technique for the computation of the effective properties and the recovery of the local fields. Solutions obtained from the MSG-baseg general purpose code SwiftComp [14], is are used in all cases as references, together with others from the literature.

Homogenization

A typical micromechanics case is studied first to assess the capabilities of refined beam models for the computation of the effective properties of unidirectional fiber reinforced materials. It consists in a square pack microstructure of a graphite-epoxy composite. In fiber reinforced materials the properties along the fiber-direction do not vary, fact that can be opportunely exploited to reduce the dimension of the UC. In this sense, some approaches such as MSG make use of 2D models capturing the different phases of the heterogeneous material. Accordingly, in HLE beam modeling the computational problem is also reduced to a single cross-section by applying conveniently the periodic boundary conditions and a master-slave method.

The fiber is a transverse isotropic graphite material with $E_{11} = 235$ GPa, $E_{22} = 14$ GPa, $G_{12} = 28$ GPa, $G_{23} = 5.6$ GPa, $\nu_{12} = 0.2$ and $\nu_{23} = 0.25$. The epoxy matrix is isotropic with $E = 4.8$ GPa and $\nu = 0.34$. The fiber is circular and the fiber volume fraction is equal to 0.60. The cross-section of the beam is divided into nine sub-domains accounting for the different phases in a component-wise sense, as



(a) Circular fiber (b) Square fiber

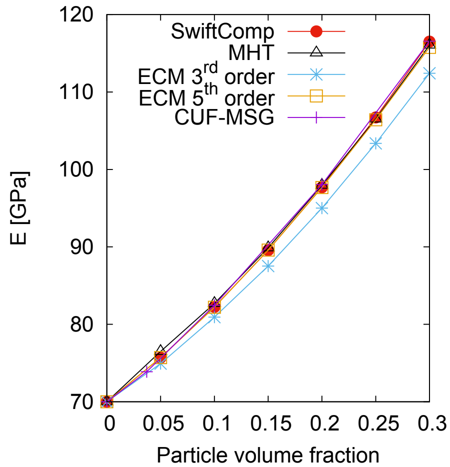
Figure 4. Distribution of expansion domains over the cross-section for fiber-reinforced composites.

TABLE I. EFFECTIVE PROPERTIES OF THE GRAPHITE-EPOXY CELL.

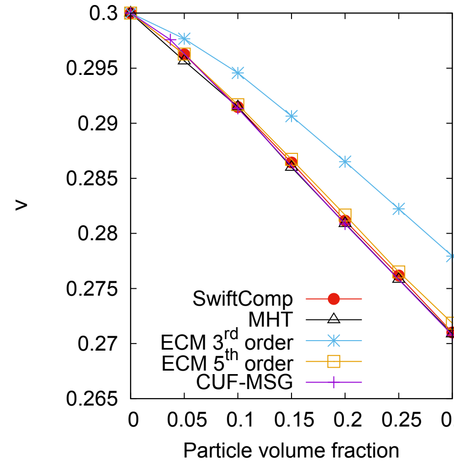
Model	E_{11} [GPa]	E_{22} [GPa]	G_{12} [GPa]	G_{23} [GPa]	ν_{12}	ν_{23}
			References			
FEM [5]	142.6	9.60	6.00	3.10	0.25	0.35
MOC [2]	143	9.6	5.47	3.08	0.25	0.35
GMC [21]	143.0	9.47	5.68	3.03	0.253	0.358
HFGMC [22]	142.9	9.61	6.09	3.10	0.252	0.350
ECM [23]	143	9.6	5.85	3.07	0.25	0.35
SwiftComp	142.9	9.61	6.10	3.12	0.252	0.350
			CUF-MSG			
HL2	143.17	9.70	6.29	3.19	0.252	0.346
HL4	143.16	9.64	6.09	3.12	0.252	0.349
HL6	143.16	9.62	6.09	3.12	0.252	0.350
HL8	143.16	9.62	6.08	3.12	0.252	0.350

shown in Figure 4 (a). The effective material properties are displayed in TABLES I for an increasing polynomial order of the theory, e.g. HL2 is the second order beam model. The results obtained from SwiftComp and several other well-known solutions are included as references.

A second case considering a particle reinforced composite is addressed now. In such microstructures the constituents vary over the three spatial directions and, consequently, 3D models are required. In the proposed modeling approach, in order to account for the different constituents along the beam axis, several 1D elements are placed along the y_1 coordinate and the material properties of the correspondent cross-section, shown in Figure 4 (b), are conveniently assigned. The UC consists in a cubic inclusion of aluminum oxide Al_2O_3 embedded in aluminum. The material properties are $E = 350$ GPa and $\nu = 0.30$ for the inclusion, and $E = 70$ GPa and $\nu = 0.3$ for the matrix. Three 4-node cubic beam elements are employed for the FEM discretization. Figures 5 (a) and (b) show the effective Young's modulus and Poisson ratio, respectively, for an increasing particle volume fraction. The reference solutions are those of a SwiftComp 3D model, ECM of 3^{rd} and 5^{th} order from Williams [24] and a mathematical homogenization approach (MHT) from Banks-Sills [25].

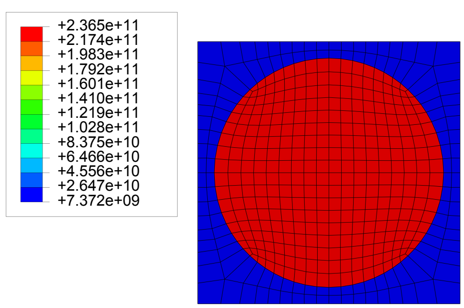


(a) Young's modulus

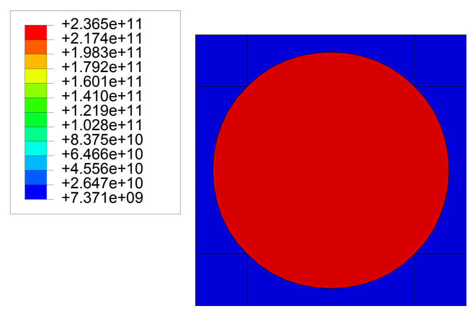


(b) Poisson ratio

Figure 5. Effective properties of the Al_2O_3/Al composite for increasing particle volume fractions.



(a) SwiftComp



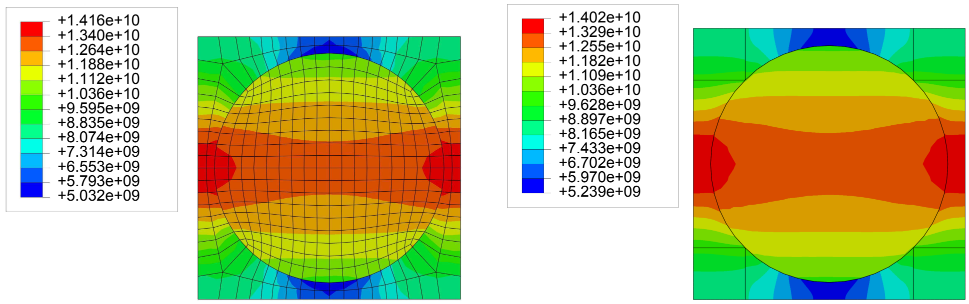
(b) HLE

Figure 6. σ_{11} under $\bar{\varepsilon}_{11}$.

Dehomogenization

More challenging for a micromechanics model is to represent accurately the local solutions within the microsctructure from the information coming from the global structural analysis. In the framework of MSG, the local fields are obtained straightforwardly from the fluctuation functions with no need of further loading steps. Indeed, this section shows the stress solutions correspondent to the graphite-epoxy analysis previously addressed for different global strain inputs. Figure 6 includes the σ_{11} component for a unitary $\bar{\varepsilon}_{11}$, Figure 7 shows σ_{22} under $\bar{\varepsilon}_{22}$ and, finally, Figure 8 shows σ_{12} under $\bar{\varepsilon}_{12}$. In all cases, the left-hand side picture corresponds to the solutions from a refined SwiftComp 2D model, whereas the right-hand side plot displays the higher-order beam solutions obtained with a HL8 model.

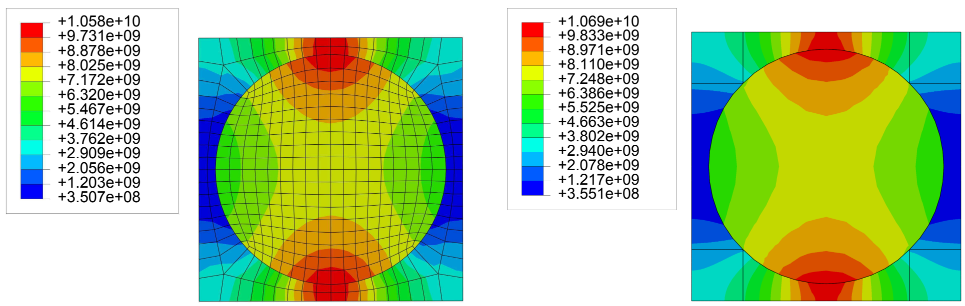
On can observe the good agreement between the proposed model and the solutions obtained from SwiftComp, both for the effective properties and the recovery of the local solutions. The high orders of the F_τ expanding functions are refined enough



(a) SwiftComp

(b) HLE

Figure 7. σ_{22} under $\bar{\varepsilon}_{22}$.



(a) SwiftComp

(b) HLE

Figure 8. σ_{12} under $\bar{\varepsilon}_{12}$.

to deal with the complex gradients of the local stress solutions within each phase of the UC, for instance within the fiber section. In addition, the component-wise distribution of the fluctuation unknowns and the use of a non-isoparametric mapping technique enable the model to provide highly accurate results independently of the complexity of the geometry.

CONCLUSIONS

A novel modeling technique based on the use of advance beam models is introduced for the multiscale analysis. The mechanics of structure genome (MSG) is employed to minimize the loss of information between the original composite and the equivalent homogeneous material and the Carrera unified formulation (CUF) is recalled to generate higher-order beam theories for the modeling and solution of the computational problem. The results obtained from the analysis of benchmark examples validate the use of the proposed model for the micromechanics analysis, both for the computation of the effective properties and the recovery of the local fields, showing the same levels of accuracy of the reference solutions.

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