NUMERICAL ESTIMATION OF MECHANICAL CHARACTERISTICS OF AN UNIDIRECTIONAL COMPOSITE PLY AND STUDY OF THE SOLUTION CONVERGENCE

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Abstract. The available micromechanics theory allows for fast estimations on certain macromechanical properties of composite structures. Despite this, the classical methods do not provide accuracy enough in the determination of all the mechanical properties of an anisotropic material (such as transverse elastic and shear moduli or Poisson coefficients).

This study presents an analysis of a generic configuration for the microstructure of a composite ply dedicated to the determination of its mechanical properties with a higher accuracy with respect to the theoretical formulation. The aim of this research is also to characterise the mechanical properties of the material further than the used theory allows. All the numerical experiments have been designed and performed with the smallest possible geometry that guarantees an acceptable precision of the solution. This optimisation has been a primary concern throughout the research. The numerical modelling had as a central piece a cubic geometry with a model of the corresponding fibre and matrix. This geometry could be easily extended in a pattern in order to study more extensive configurations. The numerical model consisted on solid elements with all boundary conditions applied as displacements. The numerical testing configurations have been designed to emulate the hypotheses assumed in the theoretical models.

In order to ensure that the obtained results were consistent several tests have been performed. In this category convergence tests have been done to ensure that the used meshing was suitable enough. Moreover, the results have been analysed together with the theoretical solutions available in the bibliography whenever possible to validate the numerical arrangement and hypotheses assumed.
1 INTRODUCTION

The study of composite laminates using finite element analysis is often performed through macroscopic mechanics. This type of analysis allows for the study of structures without having to model the behaviour of the microscopic structure that conforms the material. These analyses use the mechanical characteristics of unidirectional laminates as input parameters. To obtain this mechanical properties one can refer to the available theoretical models. The aim of this article is to prove whether these mechanical properties can be properly obtained through numerical simulation or not, and then compare them to the theoretical results to analyse any discrepancies found.

This article is divided in three main parts dividing the different activities performed during the study of the micromechanics of a laminate. The first part is a theoretical introduction to the one parameter formulation of the problem. The presented formulation is accurate enough to provide an order of magnitude of the mechanical characteristics of an unidirectional laminate. The main hypothesis considered is that the macroscopic material behaves like a homogeneous orthotropic material. This homogeneous material that exists only as a theoretical model has its mechanical properties depending on the fibre and the matrix, the fibre direction and the volume of fibres.

The second and third parts of this study focus respectively on the numerical modelling performed and the conclusions drawn when comparing the theoretical mechanical properties with the numerical simulations. The aim of this comparison is to find a correlation between the microscopic phenomenology of the material and the theoretical approach in order to determine the mechanical properties of the global material. A focus is also placed on the optimisation of the numerical configuration to obtain adequate results with the lowest possible calculation effort.

2 MICROMECHANICS THEORETICAL MODEL

The study of the behaviour of unidirectional laminates at a micromicroscopic theory is a recurrent subject in the literature on mechanical properties of composite materials. [1] [2] Such analysis is a starting point for any mechanical study in laminates due to the fact that a ply represents the constitutive element on a great variety of composite structures. The understanding of the micromechanics behaviour of a structure is crucial to understand the macroscopic mechanical properties.

Diverse theories exist to determine the macroscopic properties ranging from simple to complex and assuming different hypotheses. This study, though, focuses in a 1st order theory known as the rule of mixtures. [3] This theory considers one parameter (the volume fraction of fibre \( V_f \)) to determine the mechanical properties of an unidirectional laminate. The volume fraction of fibre is defined as follows:

\[
V_f = \frac{\text{Reinforcement volume}}{\text{Total volume}}
\]

According to this definition, the mechanical properties for the laminate can be obtained
as shown below:

\[
E_l = V_f E_f + (1 - V_f) E_m
\tag{2}
\]

\[
\frac{1}{E_t} = \frac{V_f}{E_{ft}} + \frac{1 - V_f}{E_m}
\]

\[
\nu_{lt} = V_f \nu_f + (1 - V_f) \nu_m
\]

\[
\frac{1}{G_{lt}} = \frac{V_f}{G_{ft}} + \frac{1 - V_f}{G_m}
\]

Where \(E_l\) and \(E_t\) are the elastic moduli of the laminate in the longitudinal and transverse directions respectively, \(E_f\) and \(E_m\) are the elastic moduli of the fibre and matrix, \(\nu_f\) and \(\nu_m\) the Poisson coefficients for the fibre and matrix, and \(G_{lt}, G_{flt}\) and \(G_m\) the shear moduli of the laminate, the fibre and the matrix respectively.

In this analysis, the fibre and the matrix are considered isotropic. According to the theory for isotropic materials, the shear modulus can be obtained as follows:

\[
G = \frac{E}{2(1 + \nu)}
\tag{3}
\]

In this study, the values for the mechanical properties considered have been the following: \(V_f = 0.6, E_f = 230\text{GPa}, E_m = 4.5\text{GPa}, \nu_f = 0.3\) and \(\nu_m = 0.4\). According to this values, the calculated mechanical properties for the laminate are: \(E_l = 139.8\text{GPa}, E_t = 10.9\text{GPa}, \nu_{lt} = 0.34\) and \(G_{lt} = 3.9\text{GPa}\). These values are later on compared with the results of the numerical simulations.

3 GEOMETRICAL MODEL AND MESHING

To perform the numerical simulation a geometry is required that represents a generic microstructure of an unidirectional laminate. This geometry differentiates between fibre and matrix regions in order to model each of the materials individually. The geometry is later on meshed using a mapped 3-D meshing which allows for a high degree of control over the resulting mesh and presents a lower number of elements than a free mesh for the same accuracy. The meshing is later on analysed in simple loading cases in order to ensure that no dependence exist between the number of elements used and the results obtained; the minimum number of elements for which this condition is verified is the optimal mesh for the studied problem.

3.1 Geometry analysed

The geometry to be analysed has been conceived modular given the fact that one of the focus of the study is to determine the convergence of the mechanical properties solution with the geometry. Each module has been considered as a quarter of a round fibre with its corresponding matrix (calculated from the volume fraction). This geometry can be seen in Figure 1 which shows also the meshing performed. The main advantage
of this approach is that the geometrical model can be easily escalated to generate larger geometries without having to generate a separate mesh.

The disposition of fibres in a rectangular shape as done in this study, is referred as rectangular fibre arrangement in [1] and supposes that the disposition of the fibres on the material is uniform. Other configurations exist, such as the hexagonal, to model the transverse section of the laminates. In the real material, the disposition of the fibres is random; this configuration is more complex to study numerically because a free mesh is required and the geometry is not easily scalable.

The axes defined in the geometry have been chosen $x$ parallel to the fibres, and $y$ and $z$ in the plane normal to $x$ and perpendicular each to a face of the geometry.

3.2 Meshing

The meshing of this modular geometry has been performed with solid 3-D cubic elements. The procedure has been first to mesh a geometrical module with the disposition shown in Figure 1 and then repeat the meshed geometry to complete a whole fibre with its corresponding matrix.

The analysis has been considered with the hypotheses of small deformations therefore the behaviour of the materials can be considered linear. Moreover, because the geometry does not present high curvature in any areas, elements without middle nodes can be used. This justifies the usage of 8-node elements.
3.3 Convergence analysis of the mesh

In order to determine whether the meshing performed is refined enough a short study has been performed in which the meshing has been refined from the smallest number of elements. The evolution of the results has been analysed. As expected, from a certain refinement point a convergence has been observed and the results remained almost constant.

In order to optimise the calculation time, the number of elements in the mesh has been selected the minimum in which no dependence is observed with the obtained results.

4 NUMERICAL EXPERIMENTS

Different numerical experiments have been designed and calculated to determine the mechanical properties of the studied configuration. These experiments aim to produce a response in the structure the study of which leads to a set of desired mechanical properties. In the experiments performed a set of boundary conditions have been imposed as a displacement and the study of the stresses produced in the structure led to the different mechanical properties.

4.1 Type 1: longitudinal

This configuration is designed to calculate the longitudinal elastic modulus (according to the fibre direction) of the material and the Poisson coefficients on the plane perpendicular to the longitudinal direction. A displacement is imposed in one of the faces and through the reaction force in the opposite face, the elastic modulus can be calculated. In this analysis, the transverse average deformation is also calculated. This leads to the Poisson coefficient.
4.2 Type 2: transverse

After the longitudinal mechanical properties have been calculated, the transverse ones are obtained with a similar configuration to the longitudinal one. This experiment is designed to calculate the transverse elastic modulus and the Poisson coefficients. The configurations used in types 1 and 2 can be seen in Figure 2. The only difference is the direction of the laminate fibres.

4.3 Types 3, 4 and 5: shear

The configurations used in the determination of the shear moduli are significantly different than the ones used in the previous cases. Three cases have been analysed using the configuration presented in this section for each of the axes. In this case, due to the nature of the boundary conditions required, no symmetry is presented between axes and the results for \( y \) and \( z \) are not the same. The types 3, 4 and 5 refer respectively to the axes \( x \), \( y \) and \( z \) for the following boundary condition arrangement.

A shear force has been applied to one of the faces of the structure in a direction while the opposite face has been constrained on the normal direction. The two faces perpendicular to the shear force direction present a normal force linear and proportional to the distance to the constrained face. This arrangement can be seen in Figure 3.

This set of boundary conditions imposes a pure shear force in the geometry with the same hypotheses used in the development of the elastic theory. Through the angle of deformation of the body and the reaction forces in the constrained face, the shear modulus can be obtained.

5 CRITICAL ANALYSIS

This section presents the results obtained for the different mechanical properties as a function of the geometry. In order to analyse the dependence with the geometry, the num-
The number of modelled fibres has been increased progressively starting with a 1x1 cell geometry until the 7x7 configuration. Considering that a geometry 2x3 is analogue to the 3x2 (the results for the y and z axes are inverse) a lot of configurations can be skipped during the calculations therefore reducing the calculation time.

The results have been obtained with ANSYS and later on analysed with Matlab in order to plot the different graphics. Due to the fact that not all the configurations have been calculated, a symmetry has seen performed on the graphics about the line \( y = z \). This can be seen both in Figure 4 and in Figure 5.

Figure 4 shows the stability of the solution for the longitudinal elastic modulus. This has been the most stable solution and the dependence with the geometry can only be noticed at the 5th decimal. On the other hand, the calculation of the Poisson coefficients (shown in Figure 5) has proven to converge slower. This happens due to the heterogeneous deformation of the body caused by the intense anisotropy in the transverse direction.

The comparison with the theoretical values is presented in Table 1. It is interesting to note that for some mechanical properties there is a very good correlation between the calculated and the expected results. On the other hand, other properties present substantial discrepancies. The explanation for this resides on the fact that the theoretical approach assumed a series of hypotheses that are far from reality in some cases. This limitation of the theoretical approach used is known and other, more complex, methods outside of the scope of this article exist to overcome this limitation.

The convergence of the solution has been studied for each of the mechanical properties in order to determine the minimum geometry necessary to obtain stable results. This
has been done aiming to reduce the computational effort, which is exponential with the size of the geometry. For the mechanical characteristics that presented a convergence to the theoretical values, this has been performed using the diagram shown in Figure 6 and setting an acceptable discrepancy of 5% of the theoretical value. The analysis has been later performed analogously for the properties without good correlation with the theoretical values but in this case, the reference has been taken at the convergence value for each of the mechanical properties.

**Table 1:** Comparison between theoretical and numerical results

<table>
<thead>
<tr>
<th></th>
<th>Theoretical results</th>
<th>Numerical results</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_l$</td>
<td>139.8 MPa</td>
<td>140.0 MPa</td>
</tr>
<tr>
<td>$E_t$</td>
<td>10.9 MPa</td>
<td>25.0 MPa</td>
</tr>
<tr>
<td>$\nu_{xy}$</td>
<td>0.34</td>
<td>0.33</td>
</tr>
<tr>
<td>$\nu_{yx}$</td>
<td>0.34</td>
<td>0.17</td>
</tr>
<tr>
<td>$G_{xy}$</td>
<td>N/A</td>
<td>350.0 MPa</td>
</tr>
<tr>
<td>$G_{yx}$</td>
<td>N/A</td>
<td>43.9 MPa</td>
</tr>
<tr>
<td>$G_{yz}$</td>
<td>3.90 MPa</td>
<td>3.54 MPa</td>
</tr>
</tbody>
</table>
Figure 6: Analysis of the discrepancy with the theoretical values as a function of the modelled geometry.

6 CONCLUSIONS

- Firstly, concerning the microscopical theory, a single parameter theory has been used that estimated the mechanical behaviour of the structure through one input parameter \( V_f \) and the mechanical properties of the constituents. This theory has been sufficient to analyse some of the mechanical parameters whenever the stress has been applied in the direction of the fibre. In other loading cases, the error incurred by this theory has been too large to consider any estimations acceptable. The transverse Poisson coefficients \( \nu_{yx} \) and \( \nu_{yz} \), and the shear moduli \( G_{xy} \) and \( G_{yx} \) need to be estimated using another method.

- In the cases in which it has been possible to compare the numerical and the theoretical results, the numerical analysis has closely predicted the mechanical properties when the number of modelled fibres has been large enough. The study performed concludes, though, that for each of the mechanical properties, the number of fibres that need to be modelled to achieve an acceptable accuracy in the results is different.

- It has been also possible to observe that the obtained results have been better when the number of fibres modelled in the \( y \) and \( z \) directions have been the same; this means when the geometry has been symmetric. In this situation, the relation between properties typical for transversely isotropic materials has been verified (with a sufficient number of fibres). An example of this is the value obtained for the Poisson coefficient \( \nu_{xy} \), that has been obtained equal to \( \nu_{xz} \).
- In terms of required geometry to obtain acceptable values for the mechanical properties the convergence of the different properties with the geometry change has been found a key parameter. For the most stable parameters, a single cell model is enough to provide a deviation of less than 2% in comparison with the predicted values. It is necessary, though, to study extended geometries in order to determine some of the parameters that do not present such a fast convergence in the solution. This is the case of the transverse Young modulus (2x2 geometry necessary), the \( yz \) Poisson coefficient (3x3 geometry) and the \( yz \) shear modulus (4x4 geometry required). This geometrical models provide a difference lower than 5% with their respective convergence values.

REFERENCES

