Multi-scale modelling and characterization of 3D woven composites using unit cells

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Abstract

Unit cells have been proven to be an effective tool for material characterisation in conjunction with the use of finite element method (FEM) to predict the effective properties of composites. A key step in the application of unit cells is to impose periodic boundary conditions to the unit cells concerned. Successful imposition of such boundary conditions requires the coordinates of nodes as well as the tessellations on each side of any pair of opposite faces to be precisely related. This requirement is difficult to satisfy in some cases without using a well-developed FE pre-processor. This is especially true for 3D textile composites, such as 3D woven composites. This paper introduces a methodology to incorporate relevant resources from different codes in a single code. This methodology was been integrated into a commercialised software, UnitCells©, which is an automated multi-scale composite analysis toolbox for characterisation of a wide range of composites, including 3D woven composites. Using this toolbox, the effective stiffness can be obtained. Under certain assumptions the strength of 3D woven composites can be evaluated, which would be at least applicable for the prediction of initial failure of such composites. Validation of the model is carried out by comparing the model predictions with the available numerical and experimental data.

1. Introduction

Because of their complex material structure, the 3D woven composites have a number of unique properties. Unlike in the conventional laminated composites, there are no interfaces hence no delamination failure mode in 3D woven composites, and this substantially improves the impact resistance of 3D woven composites in comparison with that of the laminated composites. On the other hand, because of the complicated meso scale architecture, it is almost impossible to predict the stiffness and strength of 3D woven composites analytically.

Finite element method (FEM) has been widely used for predicting the effective properties of composite materials, especially for fabric textile composites [1]. FEM is based on the analysis of the stress and strain distributions over the material model where the geometric properties and the material parameters of fibre and matrix are assumed to be known. The accuracy of stress and strain distribution calculation affects the final properties directly. Therefore, the adequate representation of the model geometry is crucial for obtaining the accurate predictions.

On a micro-scale level, yarns within 3D woven composite can be regarded as unidirectional fibre-reinforced composites. Typical idealised packing schemes of UD composites are of the hexagonal and square arrangements [2]. Both of these have a relatively simple geometry, and can be devised relatively easily. The matrix of 3D woven composite can be treated as a particulate-reinforced composite, and the particle inclusions can represent the enhancing additives or voids. There is a range of idealised packing systems for particle-reinforced composites [3].

The meso scale models of composite materials, especially those of 3D woven composites, can have very complicated yarn architectures if a detailed representation of the real composite structure is required. During the forming and curing process, the yarn cross-sections may become irregular with a non-constant area due to the interactions between the adjacent yarns [4]. The path of the yarns may also vary. This makes it a very challengeable task to represent all the geometric details of meso scale models. Because of this, a number of approximated models have been developed by different researchers.

Zeng *et. al.* [5] introduced a simplified model, where no geometric property was represented, the unit cell was discretized into a number of cubic elements, and the allocations of material properties for each integration point were determined by the position of each integration point. This kind of models can be developed relatively easily, but they are unable to describe the local stress states at the interfaces between the yarns and the matrix. Therefore, the accuracy and applicability of this kind of models is limited, e.g. they cannot be used to predict the strength properties.

There is a number of works [6,7,8], where more detailed models have been suggested. Even then, there are still simplifying assumptions made in developing these models, such as rectangular yarn cross-section, straight yarn path and constant area of the cross-section of the yarn. Such assumptions are unrealistic and will lead to the inaccurate predictions. In contrast to this approach, the models presented in this paper have the variable yarn cross sections and curved yarn paths.

Depending on the architecture of the material, the whole model can be represented either by a unit cell [1-3] or a representative volume element (RVE) [9]. The difference is that the unit cell is suitable for materials which have a periodic structure, and RVE is suitable for materials with an irregular structure. The effective material properties obtained from the unit cell and RVE should be equivalent to those of the real material. In order to obtain the effective material properties of a unit cell or RVE, appropriate boundary conditions must be assigned. The periodic boundary conditions for a unit cell require the coordinates of nodes on any pair of opposite faces to be precisely related [1-3]. This implies that the surface tessellation of the mesh for the unit cell has to be created accordingly to satisfy those boundary conditions. For the 3D woven composite models with complex architecture it is almost impossible to obtain a suitable mesh within a single piece of the conventional software, hence UnitCells© [10] software was created to achieve this objective relatively easily. The flow chart and main window of UnitCells© are given in Fig. 1 and Fig. 2, respectively.

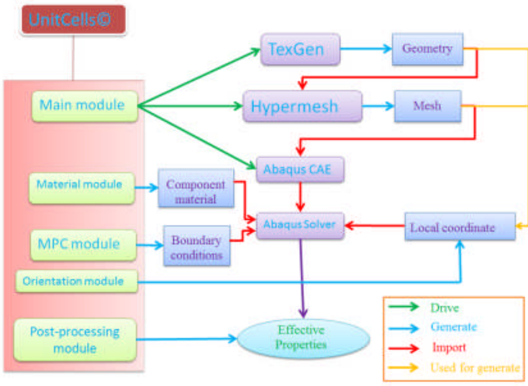


Fig.1 Flow chart of UnitCells©

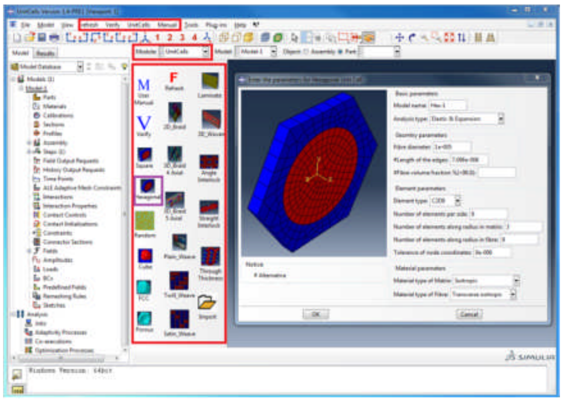


Fig.2 Main window of UnitCells©

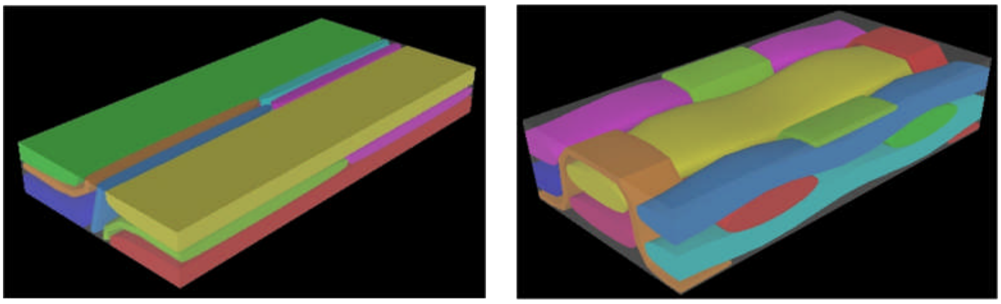
Using Abaqus [11] as a platform and its Python Script programming facility as a vehicle, UnitCells© has been established as a fully automated composites characterization tool. Moreover, it is capable of drawing relevant functions from TexGen [12], an open source code for generating textile composite architectures, to generate the desirable textile preform configurations and from Hypermesh [13], a commercial FE pre-processor, to generate the appropriate meshes. In an automated manner, correct periodic boundary conditions are imposed and precise loads are applied before a complete material characterisation simulation. The effective material properties of the composite are readily obtained from simulation using this tool. The characterisation process is also fully controllable through the visual interfaces to define relevant geometric and material parameters. It can also be used for multi-scale modelling in the sense that different phases can be characterised in a length scale below, e.g. yarns in a textile composite as UD composite and the matrix as composite of particulate inclusions, such as performance enhancing additives or voids.

In order to predict the effective strength of the 3D woven composite, failure criteria and damage evolution law for both of the yarn and matrix have been introduced to the model through the Umat subroutines. Because yarns are transversely isotropic, Hashin [14] failure criteria has been used as failure initiation criterion within the yarns. Von Mises failure criterion has been used matrix as it can be considered to be an isotropic material. Stiffness degradation is based on the approach proposed by Matzenmiller *et. al.* in [15].

This paper is aimed to demonstrate the process of using UnitCells© to predict the effective stiffness and strength of three types of 3D woven composite materials, namely, straight interlock, angle interlock and through thickness non-crimp fabric (NCF) woven composite. Finally, the validation of the results will be carried out by comparing the model predictions with the available experimental data.

2. Geometry

Because of the interaction of yarns during forming and curing process, the cross-sections of the yarns vary at different positions and the paths of the yarns become irregular. This makes it very difficult to generate the geometric model of a 3D woven composite. This issue becomes even more obvious when building a set of unit cells with different parameters. But the accurate representation of the details of model geometry is crucial for obtaining an acceptable prediction results. In order to represent more details in the geometric model, an open source software TexGen was integrated into UnitCells©. TexGen has a very powerful capability for generating geometric models of the textile composites. As a demonstration, two types of 3D woven model were created using TexGen are shown in Fig. 3.



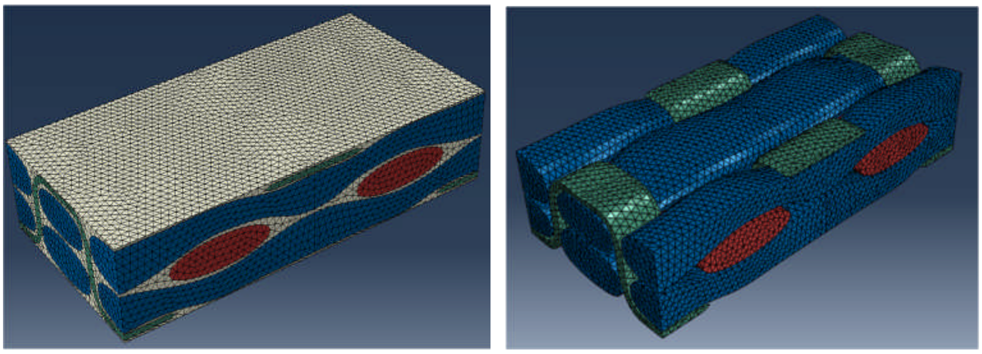
(a) Straight inter-lock (b) Through thickness (NCF)

Fig. 3 Geometry model generated with TexGen.

3. Mesh

Since the geometric model of 3D woven composite is very complex and irregular, the greatest challenge in creating unit cells of 3D woven composites is the meshing. Because of the complex yarn structures, it is quite difficult to ensure the correspondence of the nodes in a pair of opposite faces. However, due to the advanced meshing capability in Hypermesh software, yarn geometry as generated in TexGen can be imported and meshed properly using TCL script of Hypermesh. Then, the mesh can be imported into Abaqus to be used for the rest of modelling processes.

Since the yarns in a 3D woven composite model are no longer straight, and the material behaviour within the yarns is always transversely isotropic, is necessary to define the local coordinate system for the yarns at every point. The path of a yarn in a 3D woven composite is a complicated curve, hence it is not a straightforward task to define the local system for the yarns. However, TexGen can define the local coordinate system for the yarns once the geometry was created. UnitCells© call TexGen to define the local coordinate system after the mesh was generated in Hypermesh and imported into Abaqus. The periodic mesh generated by Hypermesh is shown in Fig. 4.



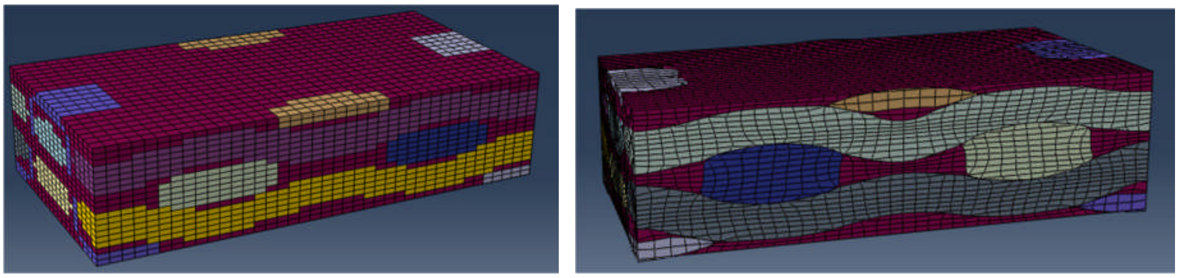
(a) Full model (b) Yarns

Fig. 4 Periodic tetrahedral mesh for NCF composite model

Because of the complicated structure of the geometric model, Hypermesh only allows to generate the mesh using the tetrahedral elements. Hexahedral elements provide higher accuracy results than the tetrahedral element. However, for the complicated 3D woven composite model, it's almost impossible to generate the hexahedral element directly, even using Hypermesh. Therefore, a smoothing methodology has been adopted to transfer the voxel mesh (exported from TexGen) to the hexahedral mesh.

The mesh smoothing algorithm used in this paper was developed based on an automatic mesh smoothing method presented by Steven et al [16]. This method was based on computationally efficient fairing technique developed for smoothing polygonal surfaces [17,18], and was extended here for volumetric FE meshes.

After performing 500 smoothing iterations, the voxel mesh exported from TexGen is transferred to a perfectly smooth hexahedral mesh, as shown in Fig. 5.



(a) Voxel mesh exported from TexGen (b) Hexahedral mesh from smooth process
Fig. 5 Periodic hexahedral mesh for NCF composite model

4. Effective stiffness prediction

With the periodic mesh, periodic boundary conditions as defined by Li *et. al.*[1-3] can be assigned to the unit cell model. This allows applying a unidirectional macro stress to the unit cell model in a straightforward manner. The strain distribution over unit cell under user-defined unidirectional stress can be calculated. From the defined stress and obtained strain, the effective stiffness of the unit cell model can be calculated. Because of the periodic boundary conditions, the effective stiffness of the unit cell model should be equal to the stiffness of the full composite model. The definition of boundary conditions, application of the unidirectional stress and the effective stiffness calculation are included in the UnitCells© and can be done automatically.

In order to demonstrate the process of using UnitCells© to predict the effective stiffness of 3D woven composites, three different types of 3D woven composite have been considered: angle interlock, straight interlock and through thickness composite. Material properties of the resin and fiber used in calculations are shown in Table 1.

Table 1 Material property of the resin and fiber used in this paper

Resin		Fibre				
E(GPa)	ν	E1(GPa)	E2(GPa)	ν12	ν23	G12(GPa)
2.89	0.3	276	90	0.25	0.3	35

As the first step, a hexagonal UD unit cell was used to calculate the effective properties of the yarns, with the fibre volume fraction being set to 90%. The effective properties of the yarns obtained by this method are given in Table 2.

Table 2 Effective properties of yarn

E1(GPa)	E2(GPa)	ν12	ν23	G12(GPa)
247.01	42.766	0.2525	0.2981	17.701

Then, three types of 3D woven unit cells were generated and set to have the same yarn volume fractions, namely, 45% in warp direction and 15% in weft direction, and the analysis has been carried out. The predicted effective stiffness values for three types of 3D woven unit cells are listed in Table 3.

Table 3 Effective properties predicted for different types of 3D woven composites

Type	E1 (GPa)	E2 (GPa)	E3 (GPa)	G12 (GPa)	G13 (GPa)	G23 (GPa)	ν12	ν13	ν23
Angle interlock	16.919	51.832	38.347	4.9312	5.0034	6.5798	0.0810	0.1285	0.0972
Straight interlock	24.654	52.193	16.105	6.6304	16.673	6.5136	0.0155	0.7772	0.1854
Through thickness	50.006	52.294	33.769	5.3411	4.5216	5.5662	0.0873	0.1117	0.1036

As a verification of the effective stiffness predictions, the effective stiffness properties obtained for two different mesh types (tetrahedral mesh and hexahedral mesh) of through thickness model were compared with the experimental data from [6]. The total yarn volume fraction was 51.1%. The yarn distribution in warp, weft and Z-fibre (binder) directions was 46.12%, 51.24% and 2.64%, respectively. The UnitCells© prediction results and the experimental data are given in Table 4.

Table 4 Effective stiffness properties of through thickness composite

	E1(GPa)	E2(GPa)	E3(GPa)
Experimental	60.0	67.0	---
Tetrahedral mesh	60.876	67.299	25.519
Hexahedral mesh	60.274	67.352	26.620

The comparison of the data in Table 4 shows that there is a good agreement between both the tetrahedral and hexahedral element model predictions and the experimental results.

5. Failure criteria and the damage evolution law

In order to obtain accurate strength predictions for the 3D woven composite, appropriate failure criteria and damage evolution law need to be included in the model. Considering the complicated composite material structure and the stress distribution, the failure mechanisms will be very complex. On the other hand, the failure in UD fibre reinforced composites is understood reasonably well, and it is commonly accepted that the failure in these materials occurs due to the fibre tension and compression, and the matrix tension and compression.

The yarn within the 3D woven composite can be treated as UD composite, hence it can be modelled as a transversely isotropic material. Therefore, the failure criteria proposed by Hashin [14] for UD composites can be applied to predict the yarn failure. The failure criteria corresponding to the four main failure modes as outlined above are as follows:

Tensile fiber mode: $\sigma_{11} > 0$

$$f_1 = \left(\frac{\sigma_{11}}{\sigma_A^+}\right)^2 + \frac{1}{\tau_A^2}(\sigma_{12}^2 + \sigma_{13}^2) \geq 1 \quad (1)$$

Compressive fibre mode: $\sigma_{11} < 0$

$$f_2 = \frac{|\sigma_{11}|}{\sigma_A^-} \geq 1 \quad (2)$$

Tensile matrix mode: $\sigma_{22} + \sigma_{33} > 0$

$$f_3 = \frac{1}{\sigma_T^{+2}}(\sigma_{22} + \sigma_{33})^2 + \frac{1}{\tau_T^2}(\sigma_{23}^2 - \sigma_{22}\sigma_{33}) + \frac{1}{\tau_A^2}(\sigma_{12}^2 + \sigma_{13}^2) \geq 1 \quad (3)$$

Compressive matrix mode: $\sigma_{22} + \sigma_{33} < 0$

$$f_4 = \frac{1}{\sigma_T^-}\left[\left(\frac{\sigma_T^-}{2\tau_T}\right)^2 - 1\right] + \frac{1}{4\tau_T^2}(\sigma_{22} + \sigma_{33})^2 + \frac{1}{\tau_T^2}(\sigma_{23}^2 - \sigma_{22}\sigma_{33}) + \frac{1}{\tau_A^2}(\sigma_{12}^2 + \sigma_{13}^2) \geq 1 \quad (4)$$

Failure is initiated when either of conditions (1)-(4) is satisfied. Here σ_{ij} is the stress components expressed in the local material coordinates of the yarn, σ_A^+ (σ_A^-) the axial tensile (compressive) strength along the longitudinal direction, σ_T^+ (σ_T^-) the axial tensile (compressive) strength along the transverse direction, τ_A and τ_T the shear strengths in the longitudinal and transverse planes, respectively.

As for the matrix of 3D woven composite, because it is can be considered isotropic, the failure of the matrix can be described using von Mises failure criterion, which is as follows:

$$(\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2 + 6(\tau_{12}^2 + \tau_{23}^2 + \tau_{31}^2) = 2\sigma_m^2 \quad (5)$$

Von Mises failure criterion involves all the stress components, hence it is suitable for failure predictions in most of the stress states. However, under hydrostatic stress conditions, the von Mises failure criterion becomes inapplicable. In the 3D woven composite, because of the complex material structure, hydrostatic tensile stress state is relatively common. To account for this, if all three principal stresses are equal, the maximum principal stress failure criterion will be used instead of von Mises failure criterion.

Once the failure in the yarns is initiated, the material still retains some of its residual stiffness before the ultimate failure occurs. Therefore, a damage evolution law is needed to estimate the value of the residual stiffness. The approach to modelling the damage evolution Matzenmiller *et. al*. [15] has been adopted, and the stiffness degradation can be represented as follows:

$$E = E_0 \cdot (1 - \omega) \quad (6)$$

$$\omega = 1 - exp\left[\frac{1-f^m}{m}\right] \quad (7)$$

Here E and E_0 are the residual and original stiffness, respectively, ω is the damage variable, f is the mode-related failure variable, and m is a material constant.

The failure criteria and damage evolution law have been coded into an Umat subroutine, which is called within the UnitCells© to predict the effective strength of 3D woven composite.

6. Effective strengths predictions

With the failure criteria and stiffness degradation expressions as given in the previous section, the effective strengths of 3D woven composites can be predicted. The periodic boundary conditions are also needed. Next, a uniaxial load (tensile, compressive and shear) has been applied to the unit cell model until the macroscopic strain reached a prescribed value (0.3 in this case). The data obtained are used to calculate an average strain-stress curve for a complete unit cell model. The effective strength in each particular load direction is defined as the maximum stress value on the average strain-stress curve calculated for this particular loading case.

A strength analysis module was integrated in UnitCells©, and it can be used to apply nine uniaxial loading cases (three tensile, three compressive and three shears) to the unit cell model one by one and create an average strain-stress curve for each. An example of nine average strain-stress curves for a unit cell model of straight interlock composite material is shown in Fig. 6. The effective strength values for all nine loading cases are obtained as the maximum stress value on the average strain-stress curves.

This approach would be applicable before localisation take place in the complete failure mechanism. This means the results before maximum stress are reasonable and acceptable. Because after this point, localise deformation will appear. This makes the model no longer periodic, therefore the periodic boundary conditions will lose their applicability.

The average strain-stress curves in Fig. 6 show that effective stiffness and strength of the model are different along different directions. This is because the effective property of straight interlock composite material is orthotropic. But the difference between shear strengths is not very obviously, this is because the effective shear strength of straight interlock composite material is dominated by matrix and matrix has isotropic property.

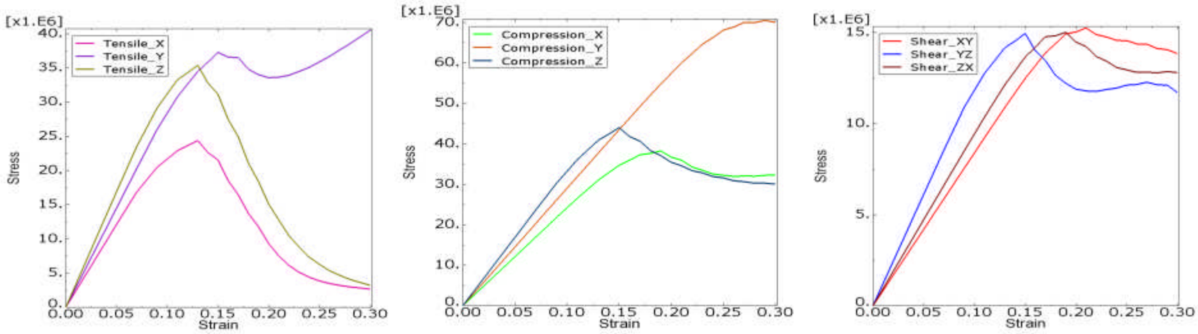


Fig. 6 Nine average strain-stress curves obtained from a unit cell model

As a demonstration, three types of 3D woven composite material were analyzed using UnitCells© to predict the effective strengths. The strength values obtained for nine loading cases are listed in Table 5.

Table 5 Strengths predicted for different types of 3D woven composite

Type	Xt (MPa)	Xc (MPa)	Yt (MPa)	Yc (MPa)	Zt (MPa)	Zc (MPa)	S12 (MPa)	S13 (MPa)	S23 (MPa)
Angle interlock	915.26	789.38	2159.9	2025.5	1652.4	1388.5	280.58	303.76	407.61
Straight interlock	871.67	858.64	2192.5	1601.9	654.03	611.88	352.16	654.43	359.86
Through thickness	2421.0	1989.0	2232.4	2013.3	1495.5	1327.6	309.63	263.38	319.30

7. Conclusions

An efficient methodology to modelling the 3D woven composite materials and predicting their effective stiffness and strength properties has been presented. Based on this method, a piece of software UnitCells© has been developed for multi scale analyses of unit cells representing composites of various architectures. It is built on the platform of ABAQUS drawing a range of facilitating functionalities from other established code including TexGen and Hypermesh for geometric model and mesh generations. A high level of automated operations has been achieved. The capabilities of UnitCells© have been demonstrated by carrying out the analysis for a range of typical 3D woven composites. The outcomes of the analysis are presented in form of effective properties of the composites considered.

Acknowledgements

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