

Prediction of Elastic Properties for Unidirectional Carbon Composites: Periodic Boundary Condition Approach

Kamarul Azhar Kamarudin^{a*}, Al Emran Ismail^b

Faculty of Mechanical and Manufacturing Engineering, Universiti Tun Hussein Onn Malaysia, Batu Pahat, 86400 Johor, Malaysia

^akamarula@uthm.edu.my, ^bemran@uthm.edu.my

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Abstract. A three-dimensional finite element model of unidirectional fibre reinforced composites has been investigated numerically using periodic boundary condition method. This method was used to predict the elastic mechanical behaviour of a unit cell of such composites. Periodic boundary condition was used due to its capability to represent a single unit cell similar to the neighbouring unit cells with continuous physical elements. It is assumed that the paired nodes displaced continuously without separating or interrupting other nodes during the deformation step. From the study, it was revealed that the elastic modulus agreed well with the experimental results, indicating that the present model could be used effectively.

Introduction

The past decades have seen rapid development in micromechanics elastic modulus prediction such as the use of energy variation principles [1], energy balance approach [2] and mechanics approach [3]. Another technique known as periodic boundary condition (PBC) method has been studied extensively by [4-6]. The early development of PBC used a 2D model to solve the problem. Li [4] developed a general packing approach that is able to accommodate unidirectional fibre of irregular cross sections. Later, Li and Wongsto [7] extended their research to 3D environment involving irregular geometries and local imperfection within composites. Xia *et al.* [5] presented unified periodic displacement boundary conditions in displacement-based FEM, which is applied into 2D multi-shaped models. Later in 2007, Tyrus *et al.* [6] demonstrated the study on 2D triangular and square shapes which focused on the effectiveness of computational speed.

In many publications, the analysis using periodic boundary condition is modelled to a single unit cell [7,8] while few using multilayer composite [9,10]. This paper attempts to reveal the elastic properties results from PBC in comparison with the experimental study, as well as the elastic prediction on unidirectional micromechanics of a single unit cell. In addition, the final results try to examine the application of periodic boundary condition method in a multi-layer unidirectional and bidirectional composite in three-dimensional model analysis.

Material Properties and Composite geometry

The unidirectional laminate of epoxy resin impregnated AS4 carbon fibre was used in the study and the properties are taken from [11] as shown in Table 1.

Table 1: Properties of composite [11]

Properties (GPa)	Fibre AS4	Resin
E ₁	235	4.8
E ₂	14	4.8
G ₁₂	28	1.8
ν ₁₂	0.2	0.34
ν ₂₃	0.25	0.34

The model of matrix and fibre in Table 1 has the dimension of 2x2x2 that represents a, b and c, with fibre fraction measurement of 0.6. By keeping the fibre length constant, the fibre diameter is 0.87 in radius. Due to expression for transverse isotropic to the material, only four different loading conditions will be determined i.e. E_1 , E_2 , G_{12} and G_{23} . An element chosen for meshing purposes in ABAQUS was C3D8R.

Periodic Boundary Conditions for Repeating Unit Cells (RUCs)

Periodic methods are composed of fundamental building blocks called repeating unit cells (RUCs) which when assembled together side by side will form an infinite array. The displacement of each unit cell must be continuous, which means that the neighbouring RUC cannot be separated from each other after the deformation. In addition, traction distribution should also be similar at the opposite parallel boundaries of a RUC. This means that the element in forming macroscopic structure will produce the individual RUC, which can thus be assembled as a physically continuous body. Internal microstructure within the RUC is not important but only within the outer surface of the whole structure is considered.

To generalise the model into a cubic unit cell, subscripts 1 and 2 (in Fig. 1) indicate the position before and after the translational of x , y , z three-dimensional directions. Any parts of the given volume relatively have displacement of any point away from the existing cell tied with the number of cells $i, j, k = 0, \pm 1, \pm 2, \pm 3 \dots$, which is related with:

$$(x_2, y_2, z_2) = (x_1 + ib, y_1 + jb, z_1 + kb) \quad (\text{Eq. 1})$$

and formed as:

$$\begin{aligned} u_2 - u_1 &= (ib)\bar{\epsilon}_x + (jb)\bar{\gamma}_{xy} + (kb)\bar{\gamma}_{xz} \\ v_2 - v_1 &= (jb)\bar{\epsilon}_y + (kb)\bar{\gamma}_{yz} \\ w_2 - w_1 &= (kb)\bar{\epsilon}_z \end{aligned} \quad (\text{Eq. 2})$$

The equations established above are related with the displacement boundary condition that can be prescribed by macroscopic strains as loads, which can be treated as an independent degree of freedom to the system. With regards to the displacement of boundary conditions, positions x , y and z at origin O are constrained from displacements in all respective directions. In addition, the x -axis is constrained by the rotation of the z -axis. By explaining mathematically at origin, O :

$$x, y, z = 0, \quad \frac{\partial u}{\partial z} = \frac{\partial v}{\partial z} = \frac{\partial w}{\partial y} = 0 \quad (\text{Eq. 3})$$

Concentrated forces related forms are expressed as strains rather than displacements and are applied for the key degree of freedom. It is also equivalent to the key nodal forces. Macroscopic stresses that are related to the concentrated forces are applied on this key degree of freedom. These manners are similar when considering simple energy equivalent as the work done by concentrated forces over the macroscopic strain is similar as the macroscopic stress over the macroscopic strain for the volume of unit cell. For instance, if a force in the x -direction is applied to the degree of freedom ϵ_x of the unit cell, while all other degrees of freedom are free from constraints, the work done by the force is taken as:

$$W = \frac{1}{2} F_x \epsilon_x \quad (\text{Eq. 4})$$

Meanwhile, the strain energy stored in the unit cell can be expressed in macroscopic stress and strains as:

$$E = \frac{1}{2} \int_V \sigma_x \varepsilon_x dV = \frac{1}{2} V \sigma_x \varepsilon_x \quad (\text{Eq. 5})$$

where V is the volume of unit cell and work done W is equal to the strain energy. Equalizing both strain energy and work done on the unit cell gives simple stress relations obtained as:

$$\sigma_x = \frac{F_x}{V}; \quad \sigma_y = \frac{F_y}{V}; \quad \sigma_z = \frac{F_z}{V}; \quad (\text{Eq. 6})$$

where x , y , and z are the directions of forces acting on the volume V of the unit cell. To make it simpler, it can be said that the magnitude of the concentrated load (F) is equal to the volume of the unit cell (V) times the stress it will generate macroscopically. In this study, the macroscopic stress is taken as 1 MPa. The effective material properties on the 'key nodes' for Young's modulus parallel to the fibre direction E_x , E_y , E_z , G_{yz} , G_{xz} and G_{xy} and can be obtained as:

Direction	Apply	Displacement formed in	To determine	(Eq. 7)
x	σ_x only	ε_x	$E_x = \frac{\sigma_x}{\varepsilon_x}$	
y	σ_y only	ε_y	$E_y = \frac{\sigma_y}{\varepsilon_y}$	
z	σ_z only	ε_z	$E_z = \frac{\sigma_z}{\varepsilon_z}$	
yz	τ_{yz} only	γ_{yz}	$G_{yz} = \frac{\tau_{yz}}{\gamma_{yz}}$	
zx	τ_{zx} only	γ_{zx}	$G_{zx} = \frac{\tau_{zx}}{\gamma_{zx}}$	
xy	τ_{xy} only	γ_{xy}	$G_{xy} = \frac{\tau_{xy}}{\gamma_{xy}}$	

Results and Discussions

Unidirectional Composite using PBC approach. Fig. 1 illustrates stress distribution of periodic boundary condition with regards to elastic constant. This scenario of boundary condition for PBC showed a continuous deformation along its boundaries. The simulation model also showed a convincing method to be used for different model geometry shapes.

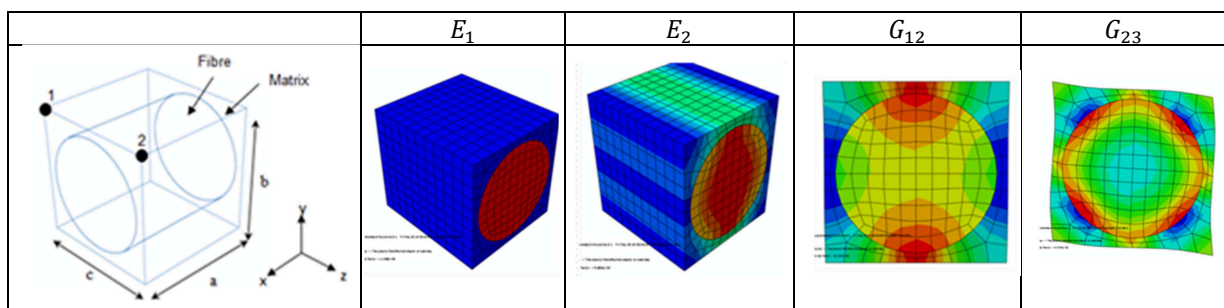


Fig. 1: Stress distribution using periodic boundary condition method.

Table 2: Comparison of elastic constants for CFRP

Unidirectional Composite					Bidirectional Composite		
Elastic Constants (GPa)	[12]	[13]	[14]	Present	Elastic Constants (GPa)	[15] $V_f=60\%$	Present
E_1	142.6	142	139	143.94	$E_1 = E_3$	65.9/61.8	76.14
E_2	9.60	10.30	9.85	9.71	E_2	11.3	10.42
G_{12}	6.00	7.60	5.25	6.16	$G_{12} = G_{32}$	6.98/7.14	4.96
G_{23}	3.10	3.8	-	4.48	G_{13}	15.79	11.68
ν_{12}	0.25	-	0.3	0.25	ν_{12}	0.46	0.35
ν_{23}	0.35	-	-	0.35	ν_{13}	0.052	0.031

Bidirectional Composite using PBC approach. To extend the technique on another model, a unit cell of bidirectional fibrous composite was developed. Fig. 2 shows a RUC of fibre at cross angle of 0° and 90° respectively in its xz -plane.

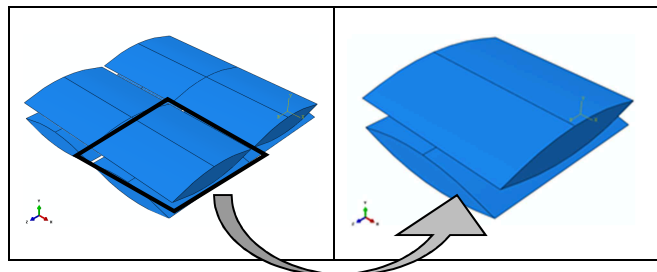


Fig. 2: Bidirectional elliptical RUC fibre selection (left) full size (right) quarter size.

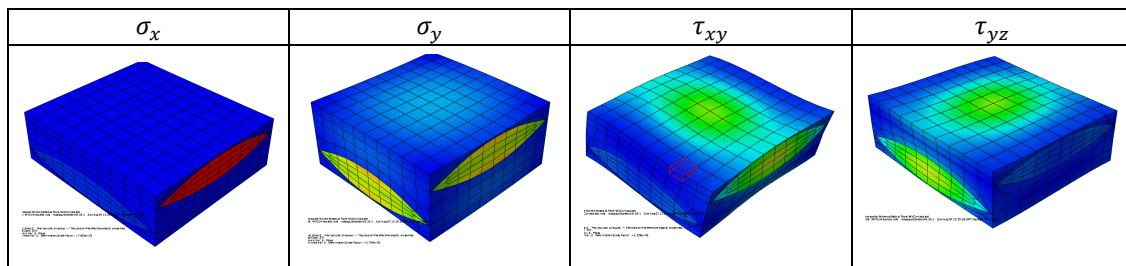


Fig. 3: Stress distribution for bidirectional composite.

Using periodic method, the model was analysed and performed as illustrated in Fig. 3. σ_1 and σ_3 produced the same elastic value due to the symmetric fibre orientation while E_2 will approximately be 10% of the E_1 and E_3 values. The results of the 60% fibre volume bidirectional CFRP analysis are shown in Table 2. There are numbers of similarities of the elastic properties which resulted from the PBC methods against experimental result by other researchers. The accuracy of the PBC method for elastic constants prediction against the existing results is tested.

Conclusion

The focus of this paper is to compare elastic properties for reinforced composite fibre using periodic boundary condition method. The method was introduced on micromechanical unit cells with sets of boundary conditions applied. The translation of displacement along the boundary condition at the surrounding unit cell was symmetrical, including translations, reflections and rotations. Good agreement was obtained between the predicted and test results for all models.

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