Periodic Boundary Condition Technique on Carbon Fibre Composites

Kamarul Azhar Kamarudin*, Al Emran Ismail

Crashworthiness and Collisions Research Group, Faculty of Mechanical and Manufacturing Engineering
Universiti Tun Hussein Onn, Parit Raja, Batu Pahat, Johor.

*Corresponding author: kamarula@uthm.edu.my

Abstract. A three-dimensional finite element model of carbon fibre reinforced 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.

1. Introduction
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 Li [4], Li et al. [5], Xia et al. [6] and Tyrus et al. [7]. 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 [8] extended their research to 3D environment involving irregular geometries and local imperfection within composites. Xia et al. [6] presented unified periodic displacement boundary conditions in displacement-based FEM, which is applied into 2D multi-shaped models. Later in 2007, Tyrus et al. [7], 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 [8, 9], while few using multilayer composite [10, 11]. 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 by using ABAQUS finite element software. 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.

2. Material and composite geometry
The unidirectional laminate of epoxy resin impregnated AS4 carbon fibre was used in the study and the properties are taken from King et al. [12] as shown in Table 1. The model is illustrate in Figure 1 and has dimension of 2x2x2 that represents length a, b and c, with fibre fraction measurement of 0.6. The model was design using Abaqus software and the element chosen for meshing purposes is C3D8R.
Table 1: Properties of composite [12]

| Properties | Fibre AS4 | Matrix |
|------------|----------|--------|
| $E_1$(GPa) | 235      | 4.8    |
| $E_2$(GPa) | 14       | 4.8    |
| $G_{12}$(GPa)| 28      | 1.8    |
| $\nu_{12}$ | 0.2      | 0.34   |
| $\nu_{23}$ | 0.25     | 0.34   |

2.1 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. To implement PBC technique, 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 Figure 1) indicate the position before the translational of $x$, $y$, $z$ directions. Any parts of the given volume relatively have displacement of any point away from the existing cell tied with the number of cells $i,j,k = 0, \pm 1, \pm 2, \pm 3\ldots$, which is related with:

$$
(x_2,y_2,z_2) = (x_1 + ib,y_1 + jb,z_1 + kb)
$$

and formed as:

$$
\begin{align*}
    u_2 - u_1 &= (ib)\bar{\varepsilon}_x + (jb)\bar{\gamma}_{xy} + (kb)\bar{\gamma}_{xz} \\
    v_2 - v_1 &= (jb)\bar{\varepsilon}_y + (kb)\bar{\gamma}_{yz} \\
    w_2 - w_1 &= (kb)\bar{\varepsilon}_z \\
\end{align*}
$$

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.

![Figure 1: Illustrate of unit cell.](image-url)
In addition, the $x$-axis is constrained by the rotation of the $z$-axis. By explaining mathematically at origin, $O$:

$$x, y, z = 0, \quad \frac{\partial u}{\partial z} = \frac{\partial v}{\partial z} = \frac{\partial w}{\partial y} = 0$$  \hfill (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 and is similar as the macroscopic stress over the macroscopic strain for the volume of unit cell.

For example, if a force in the $x$-direction is applied to the degree of freedom $\varepsilon_x$ of the unit cell, while all other degrees of freedom are free from constrains, the work done by the force is taken as:

$$W = \frac{1}{2} F_x \varepsilon_x$$  \hfill (4)

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

$$E = \frac{1}{2} \int_V \sigma_x \varepsilon_x dV = \frac{1}{2} V \sigma_x \varepsilon_x$$  \hfill (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:

$$\sigma_x = \frac{F_x}{V}; \quad \sigma_y = \frac{F_y}{V}; \quad \sigma_z = \frac{F_z}{V}$$  \hfill (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 directions $E_x, E_y, E_z, G_{yz}, G_{zx}$ and $G_{xy}$ and can be obtained as in Table 2:

**Table 2: Elastic modulus**

| Direction | Apply     | Displacement formed in | To determine          |
|-----------|-----------|------------------------|-----------------------|
| $x$       | $\sigma_x$ only | $\varepsilon_x$ | $E_x = \frac{\sigma_x}{\varepsilon_x}$ |
| $y$       | $\sigma_y$ only | $\varepsilon_y$ | $E_y = \frac{\sigma_y}{\varepsilon_y}$ |
| $z$       | $\sigma_z$ only | $\varepsilon_z$ | $E_z = \frac{\sigma_z}{\varepsilon_z}$ |
| $yz$      | $\tau_{yz}$ only | $\gamma_{yz}$ | $G_{yz} = \frac{\tau_{yz}}{\gamma_{yz}}$ |
| $zx$      | $\tau_{zx}$ only | $\gamma_{zx}$ | $G_{zx} = \frac{\tau_{zx}}{\gamma_{zx}}$ |
| $xy$      | $\tau_{xy}$ only | $\gamma_{xy}$ | $G_{xy} = \frac{\tau_{xy}}{\gamma_{xy}}$ |
3. Results and discussion

3.1 Unidirectional Composite using PBC approach
Figure 2 shows 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. As mentioned earlier when the unit cell being assembled together side by side, it will form an infinite array of neighbouring unit cell as shown in Figure 3. The simulation model showed that the method were able to be used for different model geometry shapes other than single unit cell.

3.2 Bidirectional Composite using PBC approach
Applying the technique on another model, a unit cell of bidirectional fibrous composite was developed. Figure 4 shows a unit cell of fibre at cross angle of 0° and 90° respectively in its xz-plane. Using periodic method, the model was analysed and performed as illustrated in Figure 5. \( E_1 \) and \( E_3 \) produced a similar 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 also shown in Table 3. 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.

---

**Figure 2**: Stress distribution using periodic boundary condition method.
Figure 3: Shear stress images of multilayer unidirectional FRP arrangement.

Table 3: Comparison of elastic constants for Carbon Fibre Reinforced Plastic (CFRP)

| Elastic Constants | Unidirectional Composite | Bidirectional Composite |
|-------------------|--------------------------|-------------------------|
| | Sun and Vaidya [2] | Lee and Daniel [13] | Sun and Zhou [14] | Present | Elastic Constants | Kim et al. [15] |
| | | | | | $E_1 = E_3$ | $V_f=60\%$ | Present |
| $E_x$(GPa) | 142.6 | 142 | 139 | 143.94 | | 65.9/61.8 | 76.14 |
| $E_y$(GPa) | 9.60 | 10.30 | 9.85 | 9.71 | | 11.3 | 10.42 |
| $G_{xy}$(GPa) | 6.00 | 7.60 | 5.25 | 6.16 | | 6.98/7.14 | 4.96 |
| $G_{yz}$(GPa) | 3.10 | 3.8 | - | 4.48 | | 15.79 | 11.68 |
| $v_{xy}$ | 0.25 | - | 0.3 | 0.25 | | 0.46 | 0.35 |
| $v_{yz}$ | 0.35 | - | - | 0.35 | | 0.052 | 0.031 |

Figure 4: Bidirectional elliptical RUC fibre selection (left) full size (right) quarter size.

Figure 5: Stress distribution for bidirectional composite.
3.3 Weave Fibre Composite using PBC approach

One of the most common types of fabric that is used in the manufacturing of an aircraft parts is plain weave. Micromechanical FE analysis of plain weave composite can be found from many researchers [5], [16], [17]. Due to its material properties behaviour, applications for plain weave fabric are different compared to unidirectional fabric. Unidirectional has a higher strength and elastic modulus compared to plain weave by having flexibility to withstand force in different directions.

![UD elliptical lenticular fibre](image)

**Figure 6:** UD elliptical lenticular fibre

Plain weave is formed by interlacing two mutually perpendicular sets of yarns. The lengthwise threads are called warp and the crosswise threads is called fill or weft. The interlacing pattern of the warp and fill is known as the weave.

![Symmetries model of unit cell based from plain weave](image)

**Figure 7:** Symmetries model of unit cell based from plain weave.

Plain weave is formed by an orthogonal interlacing stands in a regular sequence of one over another. The mechanical behaviour of plain weave composites also depends on the fabric geometry, fibre volume fraction, weaving conditions and the type of weave and fibre interlacing.

In this model, the plain weave was made from the elliptical lenticular fibre geometry. The waviness of the lenticular throughout the model is assumed to be approximately 10 degree. Figure 6 shows the waviness degree which forms the lenticular for the single yarn. A local material orientation had been imposed to the model in the ABAQUS/Standard software.

The size of the unit cell of the plain weave as shown in Figure 7 shows one large model, can be reduced to a quarter shapes with symmetry geometry on every unit cell. Matrix dimension of 30(l) x 30(w) x 10.72(h) were used with the fibre and formed a 60% fibre volume. Table 4 shows the engineering constant results after running numerically using periodic boundary condition technique on the composite model. The plain weave composite having an orthotropic properties of $E_1 = E_3$, $E_2$, $G_{12} = G_{32}$and $G_{13}$. As expected, the properties of the plain weave composite are significantly positive correlation with Kim et al. [15]. Despite having slightly higher value, the result validates the use of periodic boundary condition method to predict elastic constant of a plain weave carbon fibre composite material. Figure 8 shows the stress distributions in three direction of plain weave carbon fibre unit cell.

| Table 4: Plain weave micromechanical unit cell properties |
|----------------------------------------------------------|
| Elastic Constants | Kim et al. [15] | Plain Weave Elliptical |

![Stress distributions in three direction of plain weave carbon fibre unit cell](image)


|                | Composite $V_f=60\%$ |
|----------------|----------------------|
| $E_x$ (GPa)    | 65.9                 |
| $E_y$ (GPa)    | 61.8                 |
| $E_y$ (GPa)    | 11.3                 |
| $G_{xy}$ (GPa) | 6.98                 |
| $G_{yz}$ (GPa) | 7.14                 |
| $G_{xz}$ (GPa) | 15.79                |
| $\nu_{xy}$    | 0.46                 |
| $\nu_{xz}$    | 0.052                |

Figure 8: Stress distribution of plain weave fibre composites.

4. 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. Periodic boundary condition method shows a similar images on each unit cell which gives good agreement between the predicted results for all models compared to experimental from other studies.

Acknowledgement
The author would like to thank Universiti Tun Hussein Onn Malaysia and the Ministry of Higher Education Malaysia for their financial support.

References
[1] R. B. Hashin Z, “The Elastic Moduli of Fiber-Reinforced Materials,” ASME, J. Appl. Mech., vol. 31, no. (2), pp. 223–232, 1964.
[2] C. T. Sun and R. S. Vaidya, “Prediction of composite properties from a representative volume element,” Compos. Sci. Technol., vol. 56, no. 2, pp. 171–179, Jan. 1996.
[3] M. B. RILEY and J. M. WHITNEY, “Elastic properties of fiber reinforced composite materials,” AIAA J., vol. 4, no. 9, pp. 1537–1542, Sep. 1966.
[4] S. Li, “General unit cells for micromechanical analyses of unidirectional composites,” Compos. Part A Appl. Sci. Manuf., vol. 32, no. 6, pp. 815–826, Jun. 2001.
[5] S. Li, C. Zhou, H. Yu, and L. Li, “Formulation of a unit cell of a reduced size for plain weave textile composites,” Comput. Mater. Sci., vol. 50, no. 5, pp. 1770–1780, Mar. 2011.
[6] Z. Xia, C. Zhou, Q. Yong, and X. Wang, “On selection of repeated unit cell model and application of unified periodic boundary conditions in micro-mechanical analysis of composites,” Int. J. Solids Struct., vol. 43, no. 2, pp. 266–278, Jan. 2006.
[7] J. M. Tyrus, M. Gosz, and E. DeSantiago, “A local finite element implementation for imposing periodic boundary conditions on composite micromechanical models,” *Int. J. Solids Struct.*, vol. 44, no. 9, pp. 2972–2989, May 2007.

[8] S. Li and A. Wongsto, “Unit cells for micromechanical analyses of particle-reinforced composites,” *Mech. Mater.*, vol. 36, no. 7, pp. 543–572, Jul. 2004.

[9] N. Abolfathi, A. Naik, G. Karami, and C. Ulven, “A micromechanical characterization of angular bidirectional fibrous composites,” *Comput. Mater. Sci.*, vol. 43, no. 4, pp. 1193–1206, Oct. 2008.

[10] A. Drago and M. Pindera, “Micro-macromechanical analysis of heterogeneous materials: Macroscopically homogeneous vs periodic microstructures,” *Compos. Sci. Technol.*, vol. 67, no. 6, pp. 1243–1263, May 2007.

[11] N. Ohno, X. Wu, and T. Matsuda, “Homogenized properties of elastic–viscoplastic composites with periodic internal structures,” *Int. J. Mech. Sci.*, vol. 42, no. 8, pp. 1519–1536, Aug. 2000.

[12] T. R. King, D. M. Blackketter, D. E. Walrath, and D. F. Adams, “Micromechanics Prediction of the Shear Strength of Carbon Fiber/Epoxy Matrix Composites: The Influence of the Matrix and Interface Strengths,” *J. Compos. Mater.*, vol. 26, no. 4, pp. 558–573, Apr. 1992.

[13] Lee JW and Daniel IM, “Progressive transverse cracking of cross ply composite laminates,” *J. Compos. Mater.*, vol. 24, pp. 1225–43, 1990.

[14] C. T. Sun and S. G. Zhou, “Failure of Quasi-Isotropic Composite Laminates with Free Edges,” *J. Reinf. Plast. Compos.*, vol. 7, no. 6, pp. 515–557, Nov. 1988.

[15] B. C. Kim, D. C. Park, B. J. Kim, and D. G. Lee, “Through-thickness compressive strength of a carbon/epoxy composite laminate,” *Compos. Struct.*, vol. 92, no. 2, pp. 480–487, Jan. 2010.

[16] I. Ivanov and A. Tabiei, “Three-dimensional computational micro-mechanical model for woven fabric composites,” *Compos. Struct.*, vol. 54, no. 4, pp. 489–496, Dec. 2001.

[17] Y. C. Zhang and J. Harding, “A numerical micromechanics analysis of the mechanical properties of a plain weave composite,” *Comput. Struct.*, vol. 36, no. 5, pp. 839–844, Jan. 1990.