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Virtual testing of composites: Imposing periodic boundary conditions on general finite element meshes

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ABSTRACT

Predicting the effective thermo-mechanical response of heterogeneous materials such as composites, using virtual testing techniques, requires imposing periodic boundary conditions on geometric domains. However, classic methods of imposing periodic boundary conditions require identical finite element mesh constructions on corresponding regions of geometric domains. This type of mesh construction is infeasible for heterogeneous materials with complex architecture such as textile composites where arbitrary mesh constructions are commonplace. This paper discusses interpolation technique for imposing periodic boundary conditions to arbitrary finite element mesh constructions (i.e. identical or non-identical meshes on corresponding regions of geometric domains), for predicting the effective properties of complex heterogeneous materials, using a through-thickness angle interlock textile composite as a test case. Furthermore, it espouses the implementation of the proposed periodic boundary condition enforcement technique in commercial finite element solvers. Benchmark virtual tests on identical and non-identical meshes demonstrate the high fidelity of the proposed periodic boundary condition enforcement technique, in comparison to the conventional technique of imposing periodic boundary condition and experimental data.

1. Introduction

Virtual tests can reduce the cost of experimental testing in the aerospace industry by 50% [1]. Furthermore, virtual testing techniques are precluded from the physical limitations of conventional experiments such as specimen size, testing conditions etc. [2]. Thus, virtual testing is suitable for characterising the entire intrinsic mechanical response of composites. Nevertheless, the predictive fidelity of virtual testing is determined chiefly by the accuracy of the geometric domain, material models and imposed boundary condition(s) (BC) [2]. In comparison with common BCs such as Dirchlet and Neumann BCs, periodic BC is the most efficient with respect to predictive accuracy, convergence rate and geometric domain size for virtual testing of heterogeneous materials [3,4]. However, imposing periodic BC on textile geometric domains is arduous because the classic implementation method requires homologous finite element meshes at the boundaries of a geometric domain. This homologous mesh requirement is difficult to satisfy for textile composites because of their complex geometric topologies which yield non-homologous boundary mesh constructions [5,6]; therefore arbitrary mesh constructions are the norm in virtual testing of textile composites. Thus, it is desirable to develop techniques for imposing periodic BC on arbitrary mesh constructions amenable to textile composites.

Nevertheless, some authors have devised techniques to generate homologous mesh construction on boundary surfaces of textiles. For example, Lomov and associates [5] used meshed shell structures to facilitate the generation of homologous meshes. Although, this technique requires a periodic geometric structure on boundary surfaces of the textile; thus it is inapplicable to a majority of textile structures. Other authors [7,8] have adopted voxel mesh construction techniques to enforce a homologous mesh construction on boundary surfaces of textile composites. Voxel meshing, however, introduces numerical artefacts to geometric domains by virtue its discretisation process. These geometric artefacts inadvertently affect the predictive fidelity of such models. Thus, a more robust technique of imposing periodic BC to arbitrary conformal FE mesh constructions is necessary.

Jacques and co-workers [6] proposed a technique for imposing periodic BC to arbitrary textile meshes. Jacques and co-workers introduced several *reference nodes* in a Euclidean grid structure which were kinematically coupled to existing nodes on corresponding surfaces on the textile RVE. However, the use of Laplacian

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spatial averaging to determine the location of these reference nodes violates the strict enforcement of spatial 'homologousness' between boundary surface pairs, which is a pre-requisite for PCBs. Thus, numerical artefacts can ensue from this anomaly which may become apparent in finite deformation regimes. Tyrus and associates [9] imposed periodic BC to arbitrary unidirectional (UD) composite meshes in 2D using polynomial interpolation techniques. The displacement fields of fibres and matrix were interpolated using linear and cubic interpolants, respectively. Recently, Nguyen and co-workers [4] generalised the technique of Tyrus and associates [9] and extended the formalisms to 3D cases of UD and particulate composites. The authors used Lagrange and piecewise cubic Hermite polynomial interpolants to determine the displacement fields along independent boundary edges. Displacement fields on RVE surfaces were interpolated using a bi-linear Coons patch formulation.

In this communication, we describe and implement a dual-scale homogenisation model for predicting the entire effective elastic properties of textile composites, using periodic BCs amenable to arbitrary textile meshes. We extend and implement a robust variant of the periodic BC method proposed by Nguyen and co-workers [4]. Furthermore, a method for implementing this technique in commercial FE solvers using conventional MPC equations is delineated, using ABAQUS's FE solver as a case study. Section 2 recalls the essentials of downscaling and describes the proposed periodic BC technique amenable to arbitrary meshes. Section 3 describes a method for its FE implementation in commercial FE solvers. In Section 5, the proposed periodic BC method is validated. Lastly, Section 6 describes the adopted virtual testing technique used to determine the entire effective elastic properties of textile composites.

2. Periodic boundary condition (PBC)

Consider a macroscopic continuum volume, $\Omega_{\text{continuum}}$, subjected to an arbitrary loading configuration as shown in Fig. 1.

Furthermore it is assumed that a local RVE volume, Ω_{RVE}, with boundary, $\partial\Omega_{\text{RVE}}$, is sufficiently resolved at a randomly sampled macroscopic material point, $\mathbf{X} \in \Omega_{\text{continuum}}$. In order to impose PBC on Ω_{RVE} in $\mathbb{R}^N$, where N is the dimensionality of the RVE's solution space, $N, \partial\Omega_{\text{RVE}}$ must consist of at least N pairs of faces. This is achieved by decomposing the entire boundary into two distinct parts: a positive part, $\partial\Omega^+_{\text{RVE}}$, and a negative part, $\partial\Omega^-_{\text{RVE}}$. Each corresponding pair of $\partial\Omega^+_{\text{RVE}}$ and $\partial\Omega^-_{\text{RVE}}$ have material points $\boldsymbol{x}^+$ and $\boldsymbol{x}^-$, respectively, such that, $\boldsymbol{x}^+ \in \partial\Omega^+_{\text{RVE}}$ and $\boldsymbol{x}^- \in \partial\Omega^-_{\text{RVE}}$. These have unit outward normals, $\boldsymbol{n}^+ = -\boldsymbol{n}^-$, respectively. Thus, the following relationship is satisfied

$$\partial\Omega^+_{\text{RVE}} \cup \partial\Omega^-_{\text{RVE}} = \partial\Omega_{\text{RVE}} \tag{1}$$

Periodic BC is imposed on $\partial\Omega_{\text{RVE}}$ with the foregoing characteristics by enforcing periodicity of boundary fluctuation fields, $\tilde{\boldsymbol{u}}$, and anti-periodicity of boundary traction fields, $\boldsymbol{t}$, such that

$$(\forall \boldsymbol{x}^+ \in \partial\Omega^+_{\text{RVE}} \text{ and } \boldsymbol{x}^- \in \partial\Omega^-_{\text{RVE}}) \qquad \tilde{\boldsymbol{u}}(\boldsymbol{x}^+) = \tilde{\boldsymbol{u}}(\boldsymbol{x}^-) \tag{2}$$

$$(\forall \boldsymbol{x}^+ \in \partial\Omega^+_{\text{RVE}} \text{ and } \boldsymbol{x}^- \in \partial\Omega^-_{\text{RVE}}) \qquad \boldsymbol{t}(\boldsymbol{x}^+) = -\boldsymbol{t}(\boldsymbol{x}^-) \tag{3}$$

In practice two different types of FE mesh construction exists: a homologous mesh construction and a non-homologous mesh construction. Homologous FE meshes satisfy specific conditions such that

$$\#\partial\Omega^+_{\text{RVE}} = \#\partial\Omega^-_{\text{RVE}} \tag{4}$$

and

$$(\forall \boldsymbol{x}^+ \in \partial\Omega^+_{\text{RVE}} \text{ and homologous } \boldsymbol{x}^- \in \partial\Omega^-_{\text{RVE}}) \qquad \boldsymbol{n}^+ \times \boldsymbol{n}^- = \mathbf{0} \tag{5}$$

where $\#$ represents the cardinality of a set. Imposing PBC on homologous meshes is achieved by enforcing only Eq. (2) using classic methods that *kinematically tie* homologous boundary node pairs [3]. This kinematic tying is achieved using multi-point constraint equations [10]. Conversely, non-homologous FE meshes satisfy specific conditions such that

$$\#\partial\Omega^+_{\text{RVE}} \stackrel{?}{=} \#\partial\Omega^-_{\text{RVE}} \tag{6a}$$

and

$$(\exists \boldsymbol{x}^+ \in \partial\Omega^+_{\text{RVE}} \text{ and } \boldsymbol{x}^- \in \partial\Omega^-_{\text{RVE}}) \qquad \boldsymbol{n}^+ \times \boldsymbol{n}^- \neq \mathbf{0} \tag{6b}$$

The conditions described by Eq. (6b) are illustrated in Fig. 2. In these cases, the classic *kinematic tying* of node pairs is unsuitable; therefore, more robust methods such as that proposed herein should be utilised.

2.1. Imposing PBC on arbitrary FE meshes

The underlying premise of the proposed periodic BC technique hinges on the proposition that the displacement field of $\partial\Omega_{\text{RVE}}$ can be interpolated. Interpolation functions, $\mathbf{D}(\mathbf{s})$, are adopted such that Eq. (2) is satisfied. To this end, the following conditions are evoked to interpolate the displacement fields of the negative and positive parts of $\partial\Omega_{\text{RVE}}$, respectively

$$\boldsymbol{u}(\mathbf{s})^- = \mathbf{D}(\mathbf{s}) = \sum_{k=1}^{n} \mathbf{N}_k(\mathbf{s})\boldsymbol{a}_k, \tag{7}$$

and

$$\boldsymbol{u}(\mathbf{s})^+ = \mathbf{D}(\mathbf{s}) + \varepsilon(\boldsymbol{x}^+ - \boldsymbol{x}^-), \tag{8}$$

where $\mathbf{N}_k(\mathbf{s})$ for $k \in \{k = 1, 2, \ldots, n\}$ are *shape functions* which solely depend on spatial variable(s), $\mathbf{s}, \boldsymbol{a}_k$ represents *independent variables*, $\boldsymbol{\varepsilon}$ is the strain tensor imposed at the continuum scale, and $(\boldsymbol{x}^+ - \boldsymbol{x}^-)$ depends of the RVE's dimensions. Therefore the displacement field of $\partial\Omega_{\text{RVE}}$, is determined from the independent variables $\boldsymbol{a}_k$ and the applied far-field continuum scale strain $\boldsymbol{\varepsilon}$. The independent variables are selected as DOFs of specific nodes located at $\partial\Omega^-_{\text{RVE}}$: these nodes are herein called *independent nodes*.

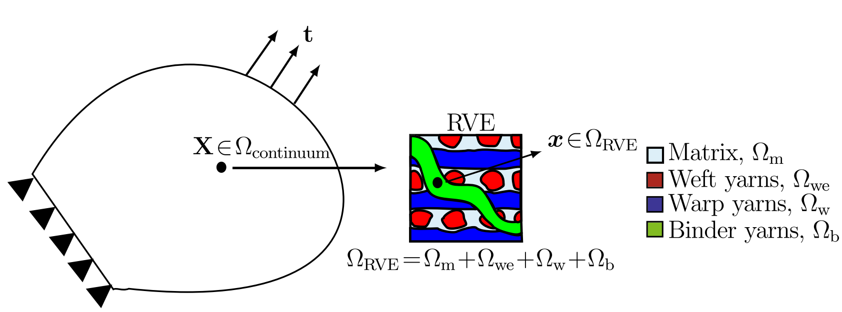

Fig. 1. Schematic of isolation of an RVE domain, Ω_{RVE}, from an arbitrarily loaded macroscopic domain, $\Omega_{\text{continuum}}$.