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Exploiting symmetries in solid-to-shell homogenization, with application to periodic pin-reinforced sandwich structures

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Abstract

In this paper, a novel set of Periodic Boundary Conditions named Multiscale Periodic Boundary Conditions (MPBCs) that apply to *reduced* Unit Cells (rUCs) and enable the two-scale (solid-to-shell) numerical homogenization of periodic structures, including their bending and twisting response, is presented and implemented in an FE code. Reduced Unit Cells are domains smaller than the Unit Cells (UCs), obtained by exploiting the internal symmetries of the UCs. When applied to the solid-to-shell homogenization of a sandwich structure with unequal skins, the MPBCs enable the computation of all terms of the fully-populated **ABD** matrix with negligible error, of the order of machine precision. Furthermore, using the MPBCs it is possible to correctly simulate the mechanical response of periodic structures using rUCs (retrieving the same results as if conventional UCs were used), thus enabling a significant reduction of both modelling/meshing and analysis CPU times. The results of these analyses demonstrate the relevance of the proposed approach for an efficient multiscale modelling of periodic materials and structures.

Keywords: Multiscale modelling, Periodic structures, Numerical homogenization, Symmetries, PBCs, Sandwich

1. Introduction

For a faster structural design of large composite components, the numerical analysis of their mechanical response requires different parts of the structure to be modelled at multiple length/time-scales [1]. In addition, due to the heterogeneous microstructure of composite materials, the applicability of conventional FE analyses based on 3D (solid) models is limited to small components; 2D (shell) FE models with equivalent homogenised properties are preferable for larger components.

Within this framework, numerical homogenization of periodic structures and materials represents a powerful numerical tool. The latter commonly involves the analysis of Unit Cell (UC)

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models in which the structure is explicitly resolved at the lowest length-scale; several studies on the existence and size of suitable UCs are available in literature [2, 3]. Furthermore, numerous works concerning the correct application of Periodic Boundary Conditions (PBCs) to representative UCs can be found, e.g. [4–7] and references therein.

However, for several practical cases, e.g. textile composites and pin-reinforced composite sandwich structures, the topological complexity of the representative UCs may lead to unaffordable modelling/meshing and analysis CPU times. Therefore, the internal symmetries of the UCs should, whenever they exist, be exploited to reduce the analysis domain, thus enabling a reduction of both the modelling/meshing and analysis CPU times.

Domains smaller than the UCs, obtained by exploiting the internal symmetries of the latter, are referred to as *reduced* Unit Cells (rUCs). Several works can be found discussing the determination of suitable rUCs (and corresponding appropriate PBCs) for UD composites [8], particle-reinforced composites [9] and textile composites [10–12].

The PBCs proposed in these studies allow the determination of the homogenised 3D elasticity tensor of the investigated structure. Nevertheless, for the numerical analysis of large components using equivalent shell models, it is of interest to determine the homogenised shell constitutive response of the structure using high-fidelity three-dimensional UCs or, preferably, rUCs.

To address this, we present a novel set of PBCs named Multiscale Periodic Boundary Conditions (MPBCs), that represents the first set of PBCs that apply to rUCs and enable the direct two-scale (solid-to-shell) numerical homogenization of periodic structures, including their bending and twisting response.

The proposed MPBCs are formulated in Section 2.2 while their complete derivation is provided in Appendix A. Details on their use within the context of a solid-to-shell homogenization and on their FE implementation are provided in Section 2.3 and Section 3, respectively. The MPBCs are applied to the solid-to-shell homogenization of a sandwich structure with unequal skins in Section 4.1 and to the analysis of the mechanical response of a periodic sandwich structure with unequal skins and pin-reinforced core in Section 4.2. Conclusions are drawn in Section 5.

2. Theory

2.1. Problem formulation

Consider a three-dimensional deformable body $\mathcal{B}_3$ occupying the domain $\mathcal{D}_3 \in \mathbb{R}^3$, as shown in Figure 1, and assume that one of the dimensions of $\mathcal{D}_3$, designated as the thickness (denoted as h), is much smaller than the other two. Furthermore, let $\mathcal{D}_3$ be periodic in the plane normal to the thickness direction. For reasons of numerical efficiency, the macroscopic mechanical response of $\mathcal{B}_3$ is more conveniently simulated by means of an equivalent shell model with homogenized properties contained in $\mathcal{D}_2 \in \mathbb{R}^2$. The corresponding shell constitutive response can be expressed by the relation $\mathbf{R} = \mathbf{K}\boldsymbol{\xi}_o$, where $\mathbf{R}$ is the vector of resultant forces/moments per unit-length

Figure 1: Problem formulation. The macroscopic response of the periodic domain $\mathfrak{D}_3$ can be simulated by means of an equivalent shell model, provided the equivalent 2D constitutive response of a representative three-dimensional UC/rUC (subdomain $\mathfrak{s}$) is correctly determined.

acting on the structure, $\boldsymbol{\xi}_o$ is the resultant mid-surface membrane strains/curvatures vector and the $\mathbf{K}$ matrix (referred to, in lamination theory, as the **ABD** matrix) contains the equivalent shell stiffness terms.

Therefore, the accurate determination of the entire $\mathbf{K}$ matrix, including all bending and twisting terms, as well as the shear-extension, bending-extension and bending-twisting coupling terms, is of paramount importance for the use of equivalent shell models of large composite components.

2.2. Multiscale Periodic Boundary Conditions (MPBCs)

The homogenized 2D response of a three-dimensional periodic structure can be evaluated through the analysis of three-dimensional UCs/rUCs modelled at the meso-scale, provided the appropriate PBCs are applied to its boundaries. These PBCs, referred to in the following as Multiscale PBCs (MPBCs), are prescribed such that the three-dimensional UC/rUC behaves as it were contained in an infinite body $\mathcal{B}_3$ (in domain $\mathfrak{D}_3$) whose macroscopic response can be analysed using shell theory (in domain $\mathfrak{D}_2$).

Assume that domain $\mathfrak{D}_3$ can be reconstructed from the tessellation of repeating UCs, as schematically shown in Figure 2; in addition, let these UCs have internal symmetries, which if exploited lead to the definition of rUCs (see Figure 2). Moreover, let $\mathfrak{s} \in \mathfrak{D}_3$ and $\hat{\mathfrak{s}} \in \mathfrak{D}_3$ be two adjacent subdomains satisfying both the physical and loading equivalence (Equations A.1 and A.2) and let $\mathfrak{s}$ be a suitable rUC as defined in Appendix A.2. Furthermore, denote with $[O, \mathbf{e}_i]_{\mathfrak{s}}$ and $[\hat{O}, \hat{\mathbf{e}}_i]_{\hat{\mathfrak{s}}}$ the Local Coordinate Systems (LCSs) of subdomains $\mathfrak{s}$ and $\hat{\mathfrak{s}}$, respectively, and define the two-dimensional symmetry transformation matrix between $[O, \mathbf{e}_i]_{\mathfrak{s}}$ and $[\hat{O}, \hat{\mathbf{e}}_i]_{\hat{\mathfrak{s}}}$ as $\mathbf{T} = \{T_{ij}\}$ where $T_{ii} = \frac{\partial \mathbf{e}_i}{\partial \hat{\mathbf{e}}_i}$ with $i \in \{1, 2\}$ and $T_{ij} = 0$ if $i \neq j$. In the following, the coordinate values along the direction $\mathbf{e}_i$ are indicated as x_i . Consider now two equivalent points $A \in \mathfrak{s}$ and $\hat{A} \in \hat{\mathfrak{s}}$ (see Equation A.1); if A is at the boundary of $\mathfrak{s}$, i.e. $A \in \partial \mathfrak{s}$, then also $\hat{A} \in \partial \hat{\mathfrak{s}}$ (see Figure 2). Under these premises, the proposed MPBCs can be expressed as

$$\begin{aligned} \mathbf{u}(A) - \gamma \mathbf{T} \mathbf{u}(\hat{A}) &= \left[\langle \nabla \mathbf{u}_o \rangle - (T_{33} x_3^{\hat{A}}) \langle \nabla \nabla w_o \rangle \right] \mathbf{T} \left[(O\hat{A})_o - (O\hat{O})_o \right] + [\mathbf{I} - \gamma \mathbf{T}] \mathbf{u}(O) + \\ &- \gamma \mathbf{T} \left[\langle \nabla \mathbf{u}_o \rangle - x_3^{\hat{A}} \langle \nabla \nabla w_o \rangle \right] (O\hat{A})_o \end{aligned} \quad \forall x_3^{\hat{A}} \in \left[-\frac{h}{2}, \frac{h}{2} \right], \quad (1)$$

$$\begin{aligned} w(A) - \gamma T_{33} w(\hat{A}) &= \left[(O\hat{A})_o - (O\hat{O})_o \right]^t \mathbf{T} \left[\frac{\langle \nabla \nabla w_o \rangle}{2} \right] \mathbf{T} \left[(O\hat{A})_o - (O\hat{O})_o \right] + [1 - \gamma T_{33}] w(O) + \\ &- \gamma T_{33} (O\hat{A})_o^t \left[\frac{\langle \nabla \nabla w_o \rangle}{2} \right] (O\hat{A})_o \end{aligned} \quad \forall x_3^{\hat{A}} \in \left[-\frac{h}{2}, \frac{h}{2} \right], \quad (2)$$

where $\mathbf{u} = \{u, v\}^t$ is the in-plane displacement vector, w the out-of-plane displacement, $\gamma = \pm 1$ the load reversal factor (see Equation A.5), $\mathbf{I}$ the 2×2 identity matrix and $x_3^{\hat{A}}$ the out-of-plane

Figure 2: The periodic domain $\mathfrak{D}_3$ can be reconstructed by tessellation of repeating Unit Cells (UCs): UC's internal symmetries, if they exist, can be exploited for defining reduced Unit Cells.

coordinate of point $\hat{A}$. In Equations 1-2, the superscript t indicates the transpose of a tensor, the subscript $\circ$ denotes quantities evaluated at the mid-surface of the UC/rUC and $\langle \bullet \rangle = \frac{1}{V_s} \int_{V_s} (\bullet) dV$ denotes the volume average operator over domain $\mathfrak{s}$. The membrane deformation tensor $\nabla \mathbf{u}_\circ$ and the curvature tensor $\nabla \nabla w_\circ$ are defined, respectively, as

$$\nabla \mathbf{u}_\circ = \begin{bmatrix} \frac{\partial u_\circ}{\partial x_1} & \frac{\partial u_\circ}{\partial x_2} \\ \frac{\partial v_\circ}{\partial x_1} & \frac{\partial v_\circ}{\partial x_2} \end{bmatrix} \quad \text{and} \quad \nabla \nabla w_\circ = \begin{bmatrix} \frac{\partial^2 w_\circ}{\partial x_1^2} & \frac{\partial^2 w_\circ}{\partial x_1 \partial x_2} \\ \frac{\partial^2 w_\circ}{\partial x_1 \partial x_2} & \frac{\partial^2 w_\circ}{\partial x_2^2} \end{bmatrix}. \quad (3)$$

For the derivation Equations 1 and 2, the reader is referred to Appendix A. At this point, the following aspects of the proposed MPBCs can be highlighted:

- the proposed formulation is valid for both conventional UCs and, more relevantly, for rUCs. Secondly, no limitations on the undeformed shape of the UC/rUC are assumed, therefore, complex UC/rUC geometries can be considered;
- no limitations on the deformed shape of the UC/rUC were hypothesized. Hence, the *plane-remains-plane* boundary conditions [13, 14], which have been proven to be over-constraining [4], as well as to violate the stress-strain periodicity condition [5], are avoided;
- since no periodicity exists in the thickness direction, the MPBCs are applied only on the lateral faces of the UC/rUC; in addition, as a result of the plane-stress assumption of shell theory, the upper and lower faces of the UC/rUC are traction-free;

- the MPBCs are expressed in terms of the relative displacement between equivalent points belonging to the boundary of the UC/rUC. This approach is supported by the results presented in [7] which demonstrate that imposing equilibrium and/or compatibility equations as part of the boundary conditions, see e.g. [15], is not only unnecessary but it also violates the minimum total potential energy principle;
- no *a priori* restrictions to the nonlinear behaviour at the lowest length-scale were made (provided there is no localization [16]);
- The presented MPBCs can be used for the two-scale (3D-2D) homogenization of any microstructure, regardless of its complexity, and all loading components can be prescribed to the UC/rUC, including bending and twisting.

2.3. Two-scale (solid-to-shell) homogenisation of periodic structures

Provided the MPBCs are applied to all points on the lateral boundary of the three-dimensional UC/rUC, the 2D constitutive response, i.e. all terms of the equivalent shell stiffness matrix $\mathbf{K}$, can be determined by sequentially subjecting the UC/rUC to the six conventional loadings of shell theory, i.e. membrane stretching, membrane shearing, bending and twisting, see Figure 3. These are applied by specifying the components of $\langle \nabla \mathbf{u}_o \rangle$ for the macroscopic membrane deformations, and of $\langle \nabla \nabla w_o \rangle$ for the bending and twisting curvatures. In the remaining, all quantities are evaluated in the LCS of the UC/rUC; the corresponding subscripts and superscripts will be omitted hereafter for convenience.

The components of $\langle \nabla \mathbf{u}_o \rangle$ and of $\langle \nabla \nabla w_o \rangle$ can be related to the membrane strains and curvatures adopted in shell theory as follows:

$$\begin{aligned} \varepsilon_o^1 &=: \left\langle \frac{\partial u_o}{\partial x_1} \right\rangle, & \varepsilon_o^2 &=: \left\langle \frac{\partial v_o}{\partial x_2} \right\rangle, & \gamma_o^{12} &=: \left\langle \frac{\partial u_o}{\partial x_2} \right\rangle + \left\langle \frac{\partial v_o}{\partial x_1} \right\rangle \\ \kappa_o^1 &=: \left\langle \frac{\partial^2 w_o}{\partial x_1^2} \right\rangle, & \kappa_o^2 &=: \left\langle \frac{\partial^2 w_o}{\partial x_2^2} \right\rangle, & \kappa_o^{12} &=: 2 \left\langle \frac{\partial^2 w_o}{\partial x_1 \partial x_2} \right\rangle \end{aligned} \quad (4)$$

where ε_o^1 and ε_o^2 are the membrane direct strains, γ_o^{12} is the membrane shear strain, κ_o^1 and κ_o^2 are the bending curvatures and κ_o^{12} is the twisting curvature.

The 2D equivalent strains/curvatures vector $\boldsymbol{\xi}_o = [\varepsilon_o^1, \varepsilon_o^2, \gamma_o^{12}, \kappa_o^1, \kappa_o^2, \kappa_o^{12}]^t$ can be related to the vector of the equivalent forces/moments per unit length $\mathbf{R} = [N_1, N_2, N_{12}, M_1, M_2, M_{12}]^t$,

Figure 3: The six loading cases in shell theory.

through the tensor equation $\mathbf{R} = \mathbf{K}\boldsymbol{\xi}_o$ or, in its expanded form:

$$\begin{bmatrix} N_1 \\ N_2 \\ N_{12} \\ \text{---} \\ M_1 \\ M_2 \\ M_{12} \end{bmatrix} = \begin{bmatrix} A_{11} & A_{12} & A_{16} & | & B_{11} & B_{12} & B_{16} \\ & A_{22} & A_{26} & | & & B_{22} & B_{16} \\ & \text{sym} & A_{66} & | & \text{sym} & & B_{66} \\ \text{---} & \text{---} & \text{---} & \text{---} & \text{---} & \text{---} & \text{---} \\ & & & | & D_{11} & D_{12} & D_{16} \\ & \text{sym} & & | & & D_{22} & D_{16} \\ & & & | & \text{sym} & & D_{66} \end{bmatrix} \begin{bmatrix} \varepsilon_1^o \\ \varepsilon_2^o \\ \gamma_{12}^o \\ \text{---} \\ \kappa_1^o \\ \kappa_2^o \\ \kappa_{12}^o \end{bmatrix} \quad (5)$$

The $\mathbf{K}$ matrix can be determined according to either of the two procedures:

Procedure A- by prescribing a non-zero value to the i -th term of $\boldsymbol{\xi}_o$ (while fixing the remaining terms to zero), all terms of $\mathbf{R}$ are, in the most general case, non-zero. Therefore, from Equation 5 the i -th column of the $\mathbf{K}$ matrix is proportional to the vector of generalized forces that is obtained from the solution of the FE problem. Repeating the same procedure for all six components of $\boldsymbol{\varepsilon}^o$, the entire $\mathbf{K}$ matrix can be computed;

(a) FE discretization of a generic heterogeneous UC/rUC. (b) Equivalent nodes at the boundary of the UC/rUC.

Figure 4: FE implementation of the MPBCs. The DOFs of equivalent nodes on the boundary of the UC/rUC are coupled using constraint equations; the external loading are specified through the DOFs of the master node $\mathcal{M}$ which does not belong to the mesh of the UC/rUC.

Procedure B- by prescribing a non-zero value to the i -th term of ξ_o (while letting the remaining terms unconstrained), all terms but the i -th of $\mathbf{R}$ are equal to zero. Hence, the i -th column of the compliance matrix $\mathbf{C} = \mathbf{K}^{-1}$ ($\xi_o = \mathbf{C}\mathbf{R}$) is proportional to the vector of generalized displacements that is obtained from the solution of the FE problem. Repeating the same procedure for all six components of ξ_o , the entire $\mathbf{C}$ matrix can be computed, and by inverting the latter, the $\mathbf{K}$ matrix can be determined.

3. FE implementation

Concerning the FE implementation of the proposed MPBCs, let us consider a discretized UC/rUC as the one shown in Figure 4a. The MPBCs, expressed for the continuum case in the form of Equations 1 -2, are enforced through constraint equations (CEs) acting on equivalent nodes on the boundary of the UC/rUC (see e.g. nodes $\mathcal{A}$ and $\hat{\mathcal{A}}$ in Figure 4b). Since they are based on a node-to-node coupling, the application of the MPBCs is ideally suited for a periodic discretization along the boundary of the UC/rUC.

The terms of ξ_o are prescribed by specifying the degrees of freedom (DOFs) of master nodes that do not belong to the mesh of the UC/rUC. In principle, a single master node $\mathcal{M}$ with at least six DOFs is sufficient for this purpose. Regarding the terms of the generalized forces vector $\mathbf{R}$, these simply correspond to the reaction forces/moments at node $\mathcal{M}$. Therefore, assuming

that the i -th component of ξ_o is associated to the j -th DOF of node $\mathcal{M}$, the i -th term of $\mathbf{R}$ corresponds to the j -th reaction force/moment at node $\mathcal{M}$.

The MPBCs have been implemented in the Finite Element (FE) package Abaqus (6.12) [17] through the in-built Python scripting facilities [18]. The simulations have been performed using Abaqus/Standard, and linear geometric behaviour was used in the examples that follow.

4. Numerical Examples

4.1. Validation

4.1.1. Description

The aim of this validation example is to demonstrate that the current formulation can predict the fully-populated shell stiffness matrix $\mathbf{K}$, in a situation for which the exact analytical solution is known, even if there are no real in-plane symmetries. To do so, we consider a composite sandwich structure with unequal skins, for which the values of the corresponding fully-populated $\mathbf{K}$ matrix can be analytically computed by means of Classical Lamination Theory (CLT) [19].

The considered sandwich structure can be ideally subdivided in UCs, as schematically shown in Figure 5; however, given the structure's homogeneity at the ply-level, such subdivision is a purely mathematical abstraction rather than a result of periodicity. Furthermore, let the selected UC (see Figure 5) be subdivided into rUCs which, in the most general case, have different LCSs. As for the definition of the UCs, for this specific example, the existence of rUCs results from the definition of their LCSs rather than from the exploitation of UC's internal symmetries. Nonetheless, albeit the solid-to-shell homogenization of the considered sandwich structure requires neither the analysis of UCs nor of rUCs, this example is useful to validate the proposed MPBCs for a problem whose exact solution is known analytically.

The facesheets material is composed of multiple layers of Saertex triaxial weave with Toho Tenax HTS carbon fibres and a polyester knitting yarn, infused with RTM6 epoxy resin [20]. The layup of the individual Non-Crimp Fabric (NCF) weaves is $[45^\circ/0^\circ/-45^\circ]$ and their material properties are listed in Table 1 along with their thickness h_w . The core material is the closed-cell polymetacrylimide foam Rohacell HERO 150 [21], whose elastic properties and density are provided in Table 2.

The thicknesses of the individual layers of the sandwich structure, along with the layups for the top and bottom facesheets are provided in Table 3. Here, h_f^t and h_f^b are, respectively, the thickness of the top and bottom facesheet, and h_c is the thickness of the foam core (see

Table 1: Elastic properties, density and thickness of the NCF triaxial weave [22].

E_{11}	$E_{22} = E_{33}$	$G_{12} = G_{13} = G_{23}$	ρ
54.7 GPa	9.0 GPa	23.3 GPa	1600 kg/m ³
ν_{12}	ν_{13}	ν_{23}	h_w
0.73	0.26	0.45	0.375 mm

Figure 5: Schematic of the sandwich structure with unequal skins considered. The latter can be subdivided into UCs, which in turn can be further subdivided into rUCs. For the solid-to-shell homogenization of this structure we considered as rUC the subdomain denoted as $\mathfrak{s}$ (in green). The LCSs of the rUC and of the surrounding subdomains are also shown.

Table 2: Elastic properties and density of the HERO G3 150 foam [21].

E_f	ν_f	ρ_f
127.5 MPa	0.33	150 kg/m ³

Table 3: Sandwich layers' thicknesses and facesheets layups.

h_f^t	h_f^b	h_c	Top skin Layup	Bottom skin Layup
3.0 mm	3.0 mm	10.5 mm	$[0^\circ/30^\circ/60^\circ, 90^\circ]_s$	$[15^\circ/45^\circ/75^\circ, -15^\circ]_s$

Figure 5); furthermore, the individual NCF weave orientations are defined relatively to their 0° -plies.

The solid-to-shell homogenization was performed using the rUC schematically shown in Figure 5 (denoted as subdomain $\mathfrak{s}$), along with its surrounding subdomains. The latter are assumed to have LCSs differing from the one of the modelled rUC, such that the corresponding transformation matrices are not equal to the unity matrix, i.e. $\mathbf{T}_i \neq \mathbf{I}$.

The facesheets and the core were discretized using eight-noded reduced integration solid elements (C3D8R) with enhanced hourglass control, and a constant element size $\ell_s = 0.375$ mm

was adopted; the interfaces between different plies and between the facesheets and the core were not explicitly modelled, i.e. they share nodes. A size-sensitivity analysis was performed by considering rUCs with different in-plane area $A_{\text{rUC}} = \ell_1 \ell_2$, while maintaining a constant aspect ratio $\frac{\ell_1}{\ell_2} = 1$. The number of elements in the laminate plane was varied from 1 to 1600.

4.1.2. Results and discussion

For the sandwich structure considered, all components of its equivalent shell stiffness matrix $\mathbf{K}$ are non-zero. The terms of the latter, computed with the two-scale homogenization approach described in Section 2.3, are compared against the reference values obtained using CLT, i.e.

$$\mathbf{K} = \begin{bmatrix} 250258.93 & 20681.60 & 33423.69 & | & 121762.28 & -11954.09 & 5993.59 \\ & 217723.17 & 27288.85 & | & & -97854.09 & -35416.61 \\ \text{sym} & & 117280.58 & | & \text{sym} & & -11954.09 \\ - & - & - & - & - & - & - \\ & & & | & 11582015.04 & 940158.09 & 1544715.91 \\ & \text{sym} & & | & & 9978361.94 & 1276987.46 \\ & & & | & \text{sym} & & 5413619.71 \end{bmatrix}, \quad (6)$$

where the dimensions of the A_{ij} , B_{ij} and D_{ij} terms (see Equation 5) are, respectively, N/mm, N and N·mm.

The relative percentage error for all terms of the $\mathbf{K}$ matrix are plotted in Figure 6 as function of the number of nodes in the laminate plane indicated with n_{nodes} . All terms of the $\mathbf{K}$ matrix, including the bending and twisting terms, as well as the shear-extension, bending-extension and bending-twisting coupling terms, are computed with negligible error, of the order of machine precision. Furthermore, this error exhibits, for all terms, a satisfactory convergence trend as the size of the rUC increases.

4.2. Application

4.2.1. Description

The aim of this application example is to demonstrate that the current formulation enables to correctly simulate the mechanical response of periodic structures using rUCs (retrieving the same results as if conventional UCs were used but at a fraction of the CPU time). To this purpose, the MPBCs have been applied for the analysis of the mechanical response of a periodic composite sandwich structure with unequal skins and pin-reinforced core.

The unreinforced sandwich configuration corresponds to that described in Section 4.1.1. The reinforcements consist of CFRP pins made of dry intermediate modulus (IM7 12K) [23] carbon fibres infiltrated with RTM6 epoxy resin during the manufacturing of the sandwich panel [24]; the resulting elastic modulus in the fibre direction is $E_{\text{pin}} = 126$ GPa.

The pins are inserted through the foam core (without going through or penetrating the facesheets) in a periodic pattern, see the UC in Figure 7. As shown in the latter, the UC

Figure 6: Homogenisation of a composite sandwich structure with unequal skins. The computed terms of the $\mathbf{K}$ matrix are compared to the analytical values obtained with CLT, for different rUCs sizes (n_{nodes} is the the number of nodes in the laminate plane of the rUC).

Table 4: Geometrical parameters defining the rUC of the periodic sandwich structure with unequal skins and pin-reinforced core.

$\ell_1 = \ell_2$	ϕ	φ	β
10.125 mm	1.0 mm	60°	45°

can be reconstructed by tessellation of smaller subdomains (rUCs), by exploiting its internal symmetries; in this example, the analysis is performed using the rUC highlighted in green in Figure 7. The geometrical parameters of the rUC are provided in Table 4. Here, φ and β are, respectively, the through-the-thickness and in-plane stitching angles (see Figure 7); ℓ_1 and ℓ_2 are the in-plane dimensions of the rUC and ϕ is the diameter of the pin-reinforcements.

The pin-reinforcements were discretized with two-noded linear beam elements (B31); to simplify the meshing of the pin-reinforced core, the pins' finite elements were embedded within the foam core exploiting the Embedded Element Method (EEM) available in Abaqus. This method has been already used for modelling pin-reinforced cores [25] and textile composites [26]. The optimal ratio between the embedded beam elements' size ℓ_e and the hosting elements' size ℓ_h , i.e $\alpha = \frac{\ell_e}{\ell_h}$ was determined so to avoid the characteristic artificial stiffness [27] resulting from the EEM implementation. In this example, the value of $\alpha = 1$ was adopted.

The sandwich structure was subjected to a twisting loading, i.e. $\kappa_o^{12} = 10^{-3}$ rad/mm and the reference solution for this problem was obtained using the entire UC (see Figure 7). It is worth-noting that, when using the latter, the MPBCs reduce to the standard PBCs already used

Figure 7: Schematic of the UC and rUC considered for the analysis of the mechanical response of a periodic sandwich structure with unequal skins and pin-reinforced core. The UC's internal symmetries are exploited for the definition of the rUC (in green). The red dotted line A-B indicates the path along which the membrane strains distribution, computed with the UC and the rUC models, have been compared.

by other authors [28, 29].

4.2.2. Results and discussion

The in-plane strains (e_{11}, e_{22}, e_{12}) evaluated along the path shown in Figure 7 (red dotted line A-B passing through the center of the UC), computed with the rUC and the UC models are compared, respectively, in Figures 8a, 8b and 8c. These strain values are extracted at each element's integration point.

The total CPU time t associated to the analyses using the rUC and the UC models are compared in Figure 9a. In addition, results are provided in terms of both the modelling/meshing CPU time t_m needed for the Python script to create the FE model and apply the suitable MPBCs (Figure 9b), and the analysis CPU time t_A needed to perform the FE analyses

(a) Membrane direct strain e_{11} .

(b) Membrane direct strain e_{22} .

(c) Membrane shear strain e_{12} .

Figure 8: Membrane strains distributions in the UC and rUC models along the path A-B shown in Figure 7 under twisting load. Since the discretizations of the UC and rUC models are the same, the strains distributions computed with the UC and the rUC models are, as expected, identical.

Figure 9: The MPCs enable the use of rUCs for the analysis of the mechanical response of periodic structures. This translates into a reduction of the total CPU time required **(a)**, as a result of the reduction of both the modelling/meshing CPU time t_M needed to create the FE model and apply the suitable MPBCs **(b)** and the analysis CPU time t_A necessary to run the FE analysis **(c)**.

(Figure 9c). The CPU times provided in Figure 9 have been normalized with respect to the values associated with the analysis performed using the UC model, respectively, t^{UC} , t_M^{UC} and t_A^{UC} .

Since the discretizations of the UC and rUC models are the same, as expected, the membrane strains distributions computed with these models are identical; this demonstrate that, through the correct application of the proposed MPBCs, the mechanical response of periodic structures can be analysed using domains smaller than the Unit Cell, while maintaining the same level of accuracy.

Compared to the UC model, the rUC model has, approximately, 25% of the degrees of freedom (DOFs) and 50% of the constraint equations (CEs). These attributes lead to a reduction of the total CPU time of about 87% (see Figure 9a); the latter results from the reduction of both the modelling/meshing CPU time ($\approx -85\%$) and the analysis CPU time ($\approx -89\%$), as shown in Figures 9b and 9c, respectively.

Although these specific values are, admittedly, dependent on the model's size and on the specific analysis performed, they confirm the capabilities of the approach proposed in this paper.

5. Conclusions

In this paper, a novel set of Multiscale Periodic Boundary Conditions (MPBCs) enabling the direct two-scale (solid-to-shell) numerical homogenization of periodic structures, including their bending and twisting response, using domains smaller than the Unit Cells (UCs), named reduced Unit Cells (rUCs), is presented.

Firstly, the validity of proposed MPBCs is demonstrated through the solid-to-shell homogenization of a composite sandwich structure with unequal skins: all terms of the equivalent shell stiffness matrix $\mathbf{K}$ are computed with a negligible error, of the order of machine precision. Secondly, the MPCs are applied to the analysis of the mechanical response of a periodic composite sandwich structure with unequal skins and pin-reinforced core, using a rUC. The results show that the use of the proposed MPBCs allows to correctly simulate the mechanical response of periodic structures using rUCs, retrieving the same results as if conventional UCs were adopted.

When compared to MPBCs which do not exploit symmetries, the MPBCs presented in this paper are shown to achieve a significant reduction in analysis CPU time (approximately 89%), as well as modelling/meshing CPU time (over 85%). These results demonstrate the relevance of the proposed approach for an efficient multiscale modelling of periodic materials and structures.

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Appendix A. Multiscale Periodic Boundary Conditions (MPBCs)

The formulation of the MPBCs is derived following the equivalence framework proposed by de Carvalho et al. [11, 12].

Appendix A.1. Physical equivalence and Periodicity

Consider a deformable body $\mathcal{B}_3$ occupying the domain $\mathcal{D}_3 \in \mathbb{R}^3$ and let $\mathfrak{s}, \hat{\mathfrak{s}} \subseteq \mathcal{D}_3$ be two generic subdomains within $\mathcal{D}$ as shown in Figure A.1. Let subdomains $\mathfrak{s}$ and $\hat{\mathfrak{s}}$ have, respectively, Local Coordinate Systems (LCSs) $[O, \mathbf{e}_i]_{\mathfrak{s}}$ and $[\hat{O}, \hat{\mathbf{e}}_i]_{\hat{\mathfrak{s}}}$, where O and $\hat{O}$ are the origins of the LCSs, while $\mathbf{e}_i$ and $\hat{\mathbf{e}}_i$ indicate the bases defining the LCSs, with $i = \{1, 2, 3\}$. Furthermore, assume a generic spatial distribution of n physical properties $\mathbf{\Pi}^j$ with $j \in \{1, \dots, n\}$ and let each of these to be expressed as tensors $\mathbf{\Pi}_{\mathfrak{s}}^j$ and $\mathbf{\Pi}_{\hat{\mathfrak{s}}}^j$, respectively in $[O, \mathbf{e}_i]_{\mathfrak{s}}$ and $[\hat{O}, \hat{\mathbf{e}}_i]_{\hat{\mathfrak{s}}}$.

Definition 1. Two subdomains $\mathfrak{s}$ and $\hat{\mathfrak{s}}$ are physically equivalent, i.e. $\mathfrak{s} \hat{=} \hat{\mathfrak{s}}$, if

$$\forall A \in \mathfrak{s} \Rightarrow \exists \hat{A} \in \hat{\mathfrak{s}} \left| (OA)_{\mathfrak{s}} \equiv (\hat{O}\hat{A})_{\hat{\mathfrak{s}}} \wedge \mathbf{\Pi}_{\mathfrak{s}}^j(A) \equiv \mathbf{\Pi}_{\hat{\mathfrak{s}}}^j(\hat{A}). \quad (\text{A.1}) \right.$$

In Equation A.1, as well as in the remaining of this work, the subscripts refer to the LCS in which the vectors and tensors are expressed, when it is required to do so.

Figure A.1: Physical equivalence.

Definition 2. A domain $\mathcal{D}_3 \in \mathbb{R}^3$ is periodic if it can be reconstructed by tessellation of non-overlapping physically equivalent (see Equation A.1) subdomains with parallel LCSs as shown in Figure A.2, i.e. if

$$\mathfrak{s}_k \stackrel{\wedge}{=} \mathfrak{s}_l \quad \wedge \quad [O, \mathbf{e}_i]_{\mathfrak{s}_k} \parallel [O, \mathbf{e}_i]_{\mathfrak{s}_l}, \quad \forall k \neq l. \quad (\text{A.2})$$

The smallest subdomain verifying Equation A.2 is referred to as Unit Cell (UC).

Appendix A.2. Subdomain admissibility

Let $[O, \mathbf{e}_i]_{\mathfrak{s}}$ and $[\hat{O}, \hat{\mathbf{e}}_i]_{\hat{\mathfrak{s}}}$ be, respectively, the LCS of subdomains $\mathfrak{s}$ and $\hat{\mathfrak{s}}$, as shown in Figure A.3. Let $\mathbb{T} = \{T_{ij}\}$ be the transformation matrix between $[\mathbf{e}_i]_{\mathfrak{s}}$ and $[\hat{\mathbf{e}}_i]_{\hat{\mathfrak{s}}}$, where $T_{ii} = \frac{\partial \mathbf{e}_i}{\partial \hat{\mathbf{e}}_i}$ with $i \in \{1, 2, 3\}$ and $T_{ij} = 0$ if $i \neq j$; furthermore, denote the corresponding projection in the 1,2 plane as $\mathbf{T}$, i.e. $\mathbf{T} = \{T_{ij}\}$ with $i, j \in \{1, 2\}$.

From Figure A.3, the position of two equivalent points $A \in \mathfrak{s}$ and $\hat{A} \in \hat{\mathfrak{s}}$ can be related by

$$(O\hat{A}) = (O\hat{O}) + \mathbb{T}(OA). \quad (\text{A.3})$$

In the remaining of this work, we will indicate the three-dimensional displacement vector as $\mathbf{u} = \{u, v, w\}^t$ and the corresponding projection in the 1,2 plane as $\mathbf{u} = \{u, v\}^t$. The displacement gradient at the point $A \in \mathfrak{s}$ can be decomposed as

$$\nabla \mathbf{u}(A) = {}^s \langle \nabla \mathbf{u} \rangle + {}^s \widehat{\nabla \mathbf{u}}(A), \quad (\text{A.4})$$

Figure A.2: Periodicity condition and Unit Cell (UC).

Figure A.3: Geometrical relation between equivalent points.

where $\mathfrak{s}\langle \bullet \rangle = \frac{1}{V_s} \int_{V_s} (\bullet) dV$ denotes the volume average operator while, $\mathfrak{s}\tilde{\bullet} = \bullet - \mathfrak{s}\langle \bullet \rangle$ represents the first-order fluctuation term over subdomain $\mathfrak{s}$. Equation A.4 is valid only if the displacement vector and the gradient operator are expressed in the LCS of the domain where the volume average is taken and the displacement fluctuation term is evaluated.

Definition 3. A generic subdomain $\mathfrak{s}$ is defined as admissible for the analysis of a periodic structure under a given loading $\mathfrak{s}\langle \nabla \mathbf{u} \rangle$ if for any other subdomain $\hat{\mathfrak{s}}$, with transformation matrix $\mathbb{T}_k$, there is a $\gamma_k = \pm 1$ such that

$$\mathfrak{s}\langle \nabla \mathbf{u} \rangle = \gamma_k \mathbb{T}_k \left[\hat{\mathfrak{s}}_k \langle \nabla \mathbf{u} \rangle \right] \mathbb{T}_k \quad \forall k, \quad (\text{A.5})$$

where $\gamma_k = \pm 1$ is the loading reversal factor (correspondent to subdomain $\hat{\mathbf{s}}_k$) used to enforce the equivalence between the stress/strain fields of physically equivalent subdomains [11]. The subdomain, smaller than the UC, verifying the condition expressed in Equation A.5 is referred to as reduced Unit Cell (rUC), see Figure A.2.

Appendix A.3. Derivation of the MPBCs

Within subdomain $\mathfrak{s}$, the displacement field $\mathbf{u}(A)$ can be expressed in the form of a truncated Taylor series as

$$\mathbf{u}(A) = \mathbf{u}(O) + {}^{\mathfrak{s}}\langle \nabla \mathbf{u} \rangle (OA) + {}^{\mathfrak{s}}\tilde{\mathbf{u}}(A), \quad (\text{A.6})$$

where $\mathbf{u}(O)$ is the displacement at the origin of the LCS of $\mathfrak{s}$ while ${}^{\mathfrak{s}}\tilde{\mathbf{u}}$ indicates the higher-order (2nd and higher) fluctuation components of the field $\bullet$ over subdomain $\mathfrak{s}$.

Let $\mathfrak{s}$ and $\hat{\mathfrak{s}}$ be two adjacent subdomains satisfying both the physical and loading equivalence (Equations A.1 and A.2) and consider two equivalent points $A \in \mathfrak{s}$ and $\hat{A} \in \hat{\mathfrak{s}}$. If A is at the boundary of $\mathfrak{s}$, i.e. $A \in \partial \mathfrak{s}$, then also $\hat{A} \in \partial \hat{\mathfrak{s}}$ (see Figure A.2); therefore, according to Equation A.6, the displacement at these two points is

$$\mathbf{u}(A) = \mathbf{u}(O) + {}^{\mathfrak{s}}\langle \nabla \mathbf{u} \rangle (OA) + {}^{\mathfrak{s}}\tilde{\mathbf{u}}(A), \quad (\text{A.7})$$

$$\mathbf{u}(\hat{A}) = \mathbf{u}(O) + {}^{\mathfrak{s}}\langle \nabla \mathbf{u} \rangle (O\hat{A}) + {}^{\mathfrak{s}}\tilde{\mathbf{u}}(\hat{A}). \quad (\text{A.8})$$

The fluctuation components of the displacement field at two equivalent points are related, as derived by de Carvalho et al. [11, 12], by the expression

$${}^{\mathfrak{s}}\tilde{\mathbf{u}}(A) = \gamma \mathbb{T} \left[{}^{\mathfrak{s}}\tilde{\mathbf{u}}(\hat{A}) \right]. \quad (\text{A.9})$$

Thus, if Equation A.8 is pre-multiplied by $\gamma \mathbb{T}$ and subtracted to Equation A.7, we obtain the equation to apply PBCs for the analysis of a generic subdomain (the superscript $\mathfrak{s}$ for the volume average operator is omitted for readability):

$$\mathbf{u}(A) - \gamma \mathbb{T} \mathbf{u}(\hat{A}) = [\mathbb{I} - \gamma \mathbb{T}] \mathbf{u}(O) - \langle \nabla \mathbf{u} \rangle \mathbb{T} (O\hat{O}) + [\langle \nabla \mathbf{u} \rangle \mathbb{T} - \gamma \mathbb{T} \langle \nabla \mathbf{u} \rangle] (O\hat{A}), \quad (\text{A.10})$$

where $\mathbb{I}$ is the 3×3 identity matrix. Therefore, Equation A.10 is applied to all points belonging to the boundary of subdomain $\mathfrak{s}$ and the external loading can be applied by prescribing the terms of $\langle \nabla \mathbf{u} \rangle$.

At this point, let one of the dimensions of $\mathfrak{D}_3$, designated as the thickness and denoted as h , be much smaller than the other two, and assume that $\mathfrak{D}_3$ is periodic in the plane normal to the thickness direction. Under these assumptions, the thickness of subdomain $\mathfrak{s} \in \mathfrak{D}_3$ is also equal to h . The displacement field at the point $A \in \mathfrak{s}$, i.e. $\mathbf{u}(A) = \{u(A), v(A), w(A)\}^t$, can be decomposed into an in-plane component $\mathbf{u}(A) = \{u(A), v(A)\}^t$ and an out-of-plane displacement

term $w(A)$, i.e.

$$\mathbf{u}(A) - {}^s\tilde{\mathbf{u}}(A) = \mathbf{u}_o(A) - x_3^A \nabla w_o(A) \quad \forall x_3^A \in \left[-\frac{h}{2}, \frac{h}{2}\right], \quad (\text{A.11})$$

$$w(A) - {}^s\tilde{w}(A) = w_o(A), \quad (\text{A.12})$$

where x_3^A is the out-of-plane coordinate of point A and the subscript o denotes the quantities evaluated at the mid-surface of subdomain s . Within such framework, Equation A.10 can be reformulated for the in-plane and out-of-plane displacement, respectively as

$$\mathbf{u}(A) - \gamma \mathbf{T} \mathbf{u}(\hat{A}) = \left[\langle \nabla \mathbf{u}_o \rangle - (T_{33} x_3^{\hat{A}}) \langle \nabla \nabla w_o \rangle \right] \mathbf{T} \left[(O\hat{A})_o - (O\hat{O})_o \right] + [\mathbf{I} - \gamma \mathbf{T}] \mathbf{u}(O) + \quad (\text{A.13})$$

$$- \gamma \mathbf{T} \left[{}^s \langle \nabla \mathbf{u}_o \rangle - x_3^{\hat{A}} \langle \nabla \nabla w_o \rangle \right] (O\hat{A})_o \quad \forall x_3^{\hat{A}} \in \left[-\frac{h}{2}, \frac{h}{2}\right],$$

$$w(A) - \gamma T_{33} w(\hat{A}) = \left[(O\hat{A})_o - (O\hat{O})_o \right]^t \mathbf{T} \left[\frac{\langle \nabla \nabla w_o \rangle}{2} \right] \mathbf{T} \left[(O\hat{A})_o - (O\hat{O})_o \right] + [1 - \gamma T_{33}] w(O) + \quad (\text{A.14})$$

$$- \gamma T_{33} (O\hat{A})_o^t \left[\frac{\langle \nabla \nabla w_o \rangle}{2} \right] (O\hat{A})_o \quad \forall x_3^{\hat{A}} \in \left[-\frac{h}{2}, \frac{h}{2}\right],$$

where $\mathbf{I}$ is the 2×2 identity matrix and $x_3^{\hat{A}}$ is the out-of-plane coordinate of point $\hat{A}$.

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