



Multiscale modelling strategy for a novel wingbox structure with increased bend-twist coupling

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ABSTRACT

This paper presents a novel multiscale modelling strategy for the early stage design of novel composite components. It includes the use of a global-local simulation approach followed by training a physics guided artificial neural network to predict composite failure indices from global-level loads. As a proof of concept, a non-conventional wingbox using the Z-Beam concept, capable of providing tailored bend-twist coupling for aeroelastic tailoring is analysed. The process begins by the application of strain-based global loads on a fully parametrised Z-Beam wingbox, after which, a structural detail of interest is analysed using a global-local approach and an evolved LaRC05 composite failure criterion. A database is created based on the repetition of the previous steps and is used to train a physics guided artificial neural network. At the end, it is observed that the proposed methodology is able to accurately predict composite failure based on global loads and design variables in a swift manner, proving itself as a valuable asset for the early design stages of novel composite concepts.

1. Introduction

In order to reduce emissions, the aeronautical industry has been incorporating different technologies and solutions. Due to their excellent mechanical properties and corrosion resistance [1,2], the use of composite materials has been established, and some wide-body aircraft such as the A350 have more than half of their weight in composite materials [3]. However, the sole change of material has not given a sufficient response to the ambitions of the industry to reach carbon neutrality by 2050 [4]. High aspect ratio wings (HARW) are presented as a promising solution to reduce emissions, since they provide higher aerodynamic efficiency and, therefore, lead to a lower fuel consumption for the same mission profile [5]. However, increasing the wing span is not a straightforward task for manufacturers, as it leads to large (non-linear) displacements, increased aeroelastic effects [6] and significant increases in internal loads (bending moment), which severely penalise structural weight to the point of potentially limiting the feasibility of the entire wing or aircraft design. A lever that can help mitigate certain aeroelastic issues is the bend-twist coupling (BTC), which enables a reduction in the local angle of attack whenever bending due to lifting forces occurs [7]. There are different ways of inducing this behaviour: either by exploiting anisotropic material properties, such as the use of unbalanced laminates, or, more recently, tow-steered composites, widely studied in the literature [8–13]. Changing the geometry has

also been considered in different studies [14–16], however, to a lesser extent than the former [17]. Stodieck idealised a new structure [18], the Z-Beam concept (Fig. 1), as a potential feature to provide tailored bend-twist coupling.

This feature, also used in a recent patent by Airbus [19], is believed to be more beneficial if employed in the outer parts of the wing, increasing the ability to design a target bend-twist coupling distribution, alleviating the unwanted effects of increased span [19]. However, such structural concepts are significantly different from the conventional semimonocoque configuration. Consequently, traditional structural analysis may not be directly suitable, and a meso-scale simulation-based approach may be needed or preferable to evaluate the structure's strength and failure modes. However, a detailed analysis of some structural features can carry high computational time costs, which hinders the design stage, when many load cases, geometric variables, and quick iterations need to be analysed and evaluated. Furthermore, the increasing need of the aeronautical industry to include details in the early design stage [20,21] (to avoid later stage setbacks which carry high costs [22]) calls for the use faster and accurate tools, which Kilimtzidis et al. [23] describe as utopian, given that, generally, accuracy and computational costs are coupled.

To include the aforementioned details in an initial design stage, where larger models are typically used to drive subsequent design steps

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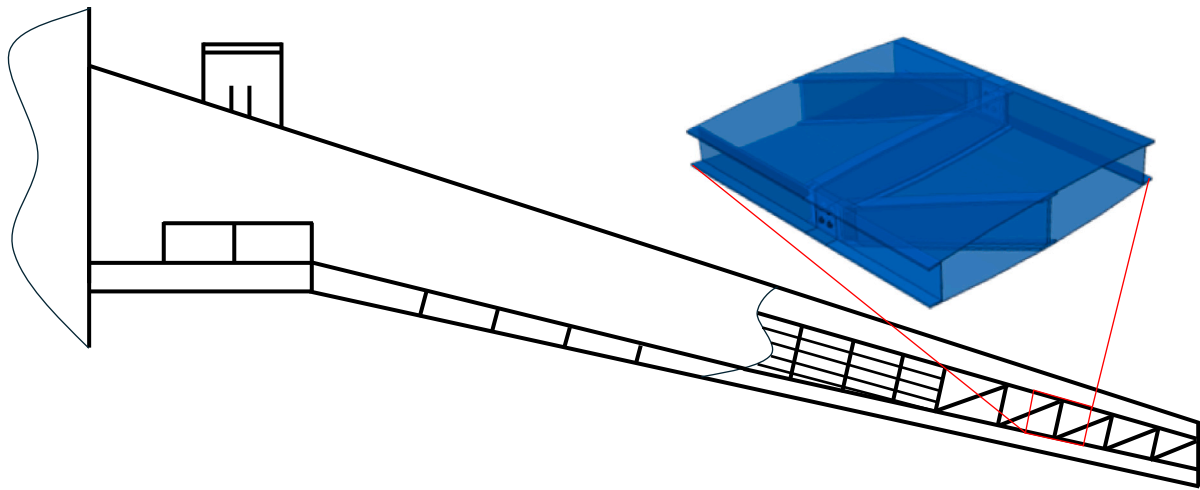


Fig. 1. Z-Beam concept applied in the outer part of a high aspect ratio wing.

rather than performing a detailed structural analysis [24–26], a global-local strategy can be employed. This strategy consists in analysing separately a complex area or detail of interest, with a more refined mesh and possibly different element types, retrieving its boundary conditions from a larger-scale finite element model [25,27]. However, a small high-fidelity model of a composite laminate can still lead to computational costs which are prohibitive for early stage design. One other way to reduce these computational costs is the use of surrogate models [28,29]. These allow one to bypass intermediate steps, approximating a specific engineering problem without explicitly determining or calculating the exact response [30], making them a valuable tool for multi-scale problems. Regarding composite materials, surrogate models are particularly useful to obtain homogenised responses [31–34] or failure envelopes [35–37] using lower scale Representative Volume Elements (RVEs). Among the various methods for creating surrogate models [38], data-driven approaches, particularly artificial neural networks (ANNs), are well established due to their ability to perform efficient “in-and-out” operations and capture complex nonlinear behaviour [39]. This makes them a valuable tool for accelerating multiscale analysis of composites [40]. Machine learning based surrogate models have been widely applied in this context [41], including numerous ANN-based approaches reviewed by Liu et al. [42] and specific applications such as predicting the effects of material defects on the response of thick laminates [29], stress states [43], failure [44], and fracture plane angles [45]. However, their use in designing large structures remains relatively limited. This is because in the majority of cases, artificially created load cases are performed at a homogenised smaller scale to create a surrogate for the behaviour of the parent structure [43], being the latter usually at the coupon [44,46,47] or element [43,48] level. Therefore, most ML-based surrogate models in literature are not compatible with early stage multidisciplinary design of large structures and are more suitable for intermediate design stages.

In this study, a methodology for multiscale analysis, including failure index calculation, is introduced to support the sizing stages of novel composite components. Simulations of a sub-component-type structure are used to predict the failure envelope of a more detailed section, which can incorporate different structural features and does not need to be periodic. One of the key novelties of this work is bridging macro-scale design variables and loads to detailed material failure indices, following an inverse trend of scales. As a proof of concept, a novel wingbox structure with increased bend-twist coupling is analysed. An ANN-based surrogate model is developed from a global-local analysis framework to accurately estimate failure indices based on global finite element model (GFEM) loads and design parameters. This enables a rapid early exploration of the design space and facilitates its integration

into optimisation procedures. The outcome of this work is expected to enable the inclusion of composite failure at the detail level in the sizing stages of novel composite components.

2. Methodology

The methodology presented herein is a two-level multiscale analysis considering global and local scales followed by machine learning. Its main objective is to quickly predict the failure mode of a specific structural feature from global level loads with a suitable degree of accuracy. The workflow begins by retrieving the loads and design variables of the feature of interest (e.g., a wingbox) from a GFEM. A global-local analysis is then performed to determine the failure indices in a hotspot or structural detail (e.g., geometric discontinuities, bolted joints, among others [22]). Two artificial neural networks (ANNs) are incorporated into the framework: the first is trained with global-local data to predict the maximum failure index from global level loads and geometry. The second predicts the effect of the design variables on the constitutive behaviour at the macro-scale (e.g., homogenised stiffness matrix). The latter is only necessary when assessing the impact of design variables on the GFEM response. An overview of the proposed framework is shown in Fig. 2.

As shown in Fig. 2, the ANN replaces the previously required time-consuming steps, leading to a significant reduction in simulation time.

3. Global model

The global finite element model is a fully parametrised (30 independent parameters) Z-beam wing box which is built using an ABAQUS oriented python script. For the sake of brevity, only general details about the global model generation are presented. The full support documentation and geometric details can be assessed in a GitHub repository (<https://github.com/swayli94/AbaqusZBeamWingBox>).

Although numerous independent parameters exist, this study will focus on only three geometric parameters: the thickness of the spars, the thickness of the Z-beam, and the Z-beam angle (Fig. 3). The range of intervals between which these variables will change is shown in Table 1.

Given that a change in thickness requires a different number of plies (herein considered to be 0.5 mm thick) a pool of candidate layouts was created following general composite design guidelines [50,51]. For each thickness, the number of required plies is approximated to the nearest even integer. Then, for a certain number of plies, several layout candidates are available, which the user can select. In this work, for

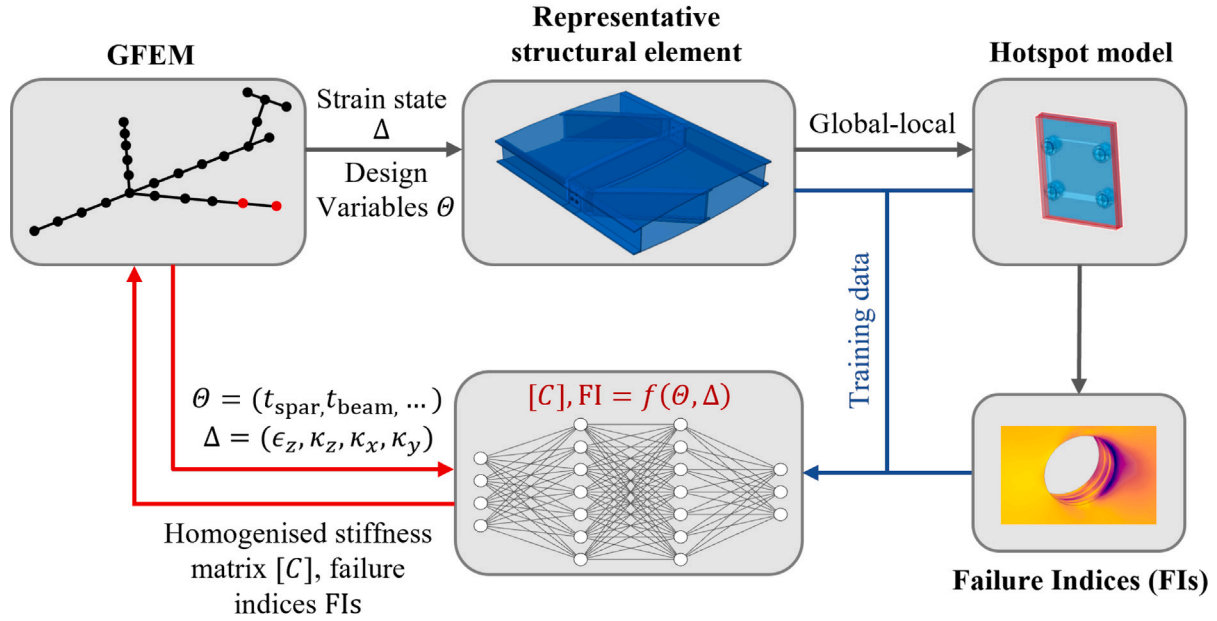


Fig. 2. Multiscale analysis sequence before (grey) and after (red) employing the proposed methodology.
Source: Based on [49].

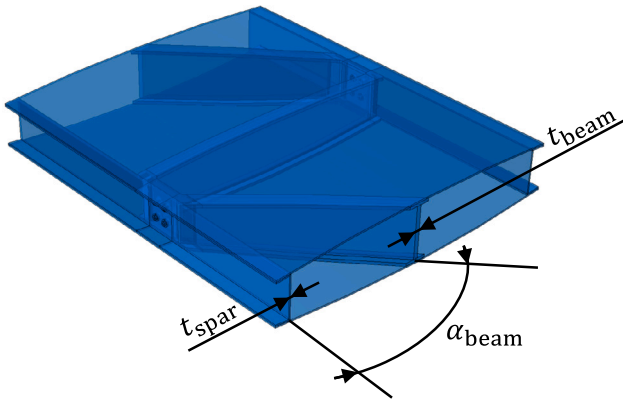


Fig. 3. Variable geometric parameters.

Table 1
Intervals of the geometric parameters.

Parameter	Value
Thickness of the spars (t_{spar})	[5, 25] mm
Thickness of the Z-Beam (t_{beam})	[10, 22] mm
Z-Beam angle (α_{beam})	[20, 60] deg

each thickness, the selected layup is the first option from the candidate list provided in the supporting documentation.

The results presented in this paper are for a wingbox with the following layups and configuration:

- The airfoil is BAC-NLF [52] with a chord of 2000 mm
- The layup of the spars is [45/−45/0/90/0]_S
- The layup of the diagonal members is [45/−45/0/90/0/0/45/−45/0/0]_S
- The layup of the chordwise member is [45/−45/0/90/0/0/45/−45/0/0]_{AS} where AS stands for anti-symmetric
- The layup of the skins is [0/45/−45/90/0]_S

Table 2
IM7/8551-7 properties [53].

Elastic properties	$E_{11} = 165$ GPa $E_{22} = E_{33} = 8.4$ GPa $\nu_{12} = \nu_{13} = 0.34$ $\nu_{23} = 0.5$ $G_{12} = G_{13} = 5.6$ GPa $G_{23} = 2.8$ GPa
Strength	$X_T = 2560$ MPa $X_C = 1590$ MPa $Y_T = 73$ MPa $Y_C = 185$ MPa $S_{12} = S_{13} = 90$ MPa $ILSS = 90$ MPa $Z_T = 63$ MPa
Other properties	$\alpha_0 = 53^\circ$ $\eta_L = 0.082$ $\eta_T = 0.287$

Table 3
Ti-6Al-4V properties [54].

Elastic properties	$E = 129$ GPa $\nu = 0.33$
Yield strength	$\sigma_y = 1085$ MPa

3.1. Materials

The materials used in this study are the IM7/8551-7 carbon/epoxy for the composite and aerospace grade titanium Ti-6Al-4V for the bolts and the properties are shown in Tables 2 and 3 respectively.

Metal plasticity was also considered, the values used for the interpolation of the true stress–strain curve are shown in Table 4.

To predict the onset of composite damage, a model [55,56] evolved from LaRC05 [57] is used. This model was chosen given its superior reliability in predicting failure modes compared to other theories [58]. It is capable of predicting 5 failure modes (4 for 2D stress states): Matrix cracking (FI_1), matrix splitting (FI_2), fibre tension (FI_3), fibre kinking (FI_4) and matrix interface (FI_5), the latter only calculated for three-dimensional stress states. Damage onset occurs whenever the value of an index reaches a unitary value ($FI_i = 1, i = 1, \dots, 5$).

Table 4
Ti-6Al-4V plastic behaviour [54].

Plastic strain	True stress [MPa]
0	1085
0.02	1093
0.04	1123
0.06	1155

Since damage onset is undesirable for primary structures, the material law only considers elastic behaviour. This means that all the indices are calculated at a specific integration point and time step, with elastic stresses, avoiding additional computational costs related to continuum damage. To this end, a UVARM user sub-routine, programmed in FORTRAN, is used. Moreover, if damage evolution was to be considered in the local model, challenges may arise in keeping comparable stiffness between the two scales, a requirement for this type of approach. In the following sections, the failure index equations used are presented.

3.1.1. Matrix cracking

This is a matrix dominated failure being the respective failure index given by:

$$FI_1 = \sqrt{\left(\frac{\tau_T}{S_T^{is} - \eta_T \sigma_N^*}\right)^2 + \left(\frac{\tau_L}{S_L^{is} - \eta_L \sigma_N^*}\right)^2 + \left(\frac{\langle \sigma_N \rangle_+}{Y_T^{is}}\right)^2} \quad (1)$$

where τ_T , τ_L and σ_N are the tractions at the matrix fracture plane [57] whose values can be determined as in Ref. [59]. The superscript $(\bullet)^{is}$ refers to the *in situ* property values, which can also be found in Ref. [59].

3.1.2. Matrix splitting and fibre kinking

These two failure mechanisms are under the same section since that fibre kinking is initiated by a matrix split, sharing the same failure equation:

$$FI_2 = FI_4 = \sqrt{\left(\frac{\tau_{23}^m}{S_T^{is} - \eta_T \sigma_2^{m*}}\right)^2 + \left(\frac{\tau_{12}^m}{S_L^{is} - \eta_L \sigma_2^{m*}}\right)^2 + \left(\frac{\langle \sigma_2^m \rangle_+}{Y_T^{is}}\right)^2} \quad (2)$$

where the superscript $(\bullet)^m$ denotes the stresses defined on a misalignment plane m [57]. The equations to determine these values are found in Ref. [59].

Since both failure modes are determined with the same failure index equation, the distinction is based on the absolute value of the axial compressive stress ($\sigma_1 < 0$):

$$\begin{cases} \text{Fibre kinking} & \text{if } \sigma_1 \leq \frac{-X_C}{2} \\ \text{Splitting} & \text{if } \frac{-X_C}{2} < \sigma_1 < 0 \end{cases} \quad (3)$$

3.1.3. Fibre tension

Fibre tensile failure occurs whenever the stress in the fibre direction is higher than the respective allowable (X_T):

$$FI_3 = \frac{\langle \sigma_1 \rangle_+}{X_T} \quad (4)$$

3.1.4. Matrix interface

Matrix interface failure occurs on a plane normal to the thickness direction due to out of plane loads ($\sigma_3 > 0$) and the failure index is given by:

$$FI_5 = \sqrt{\left(\frac{\tau_{23}}{S_{T,MI}}\right)^2 + \left(\frac{\tau_{31}}{S_{L,MI}}\right)^2 + \left(\frac{\sigma_3}{Z_T}\right)^2}, \quad (\text{valid for } \sigma_3 > 0) \quad (5)$$

where shear strengths $S_{T,MI}$ and $S_{L,MI}$ are assumed to be the same as the interlaminar shear strength (ILSS) [60].

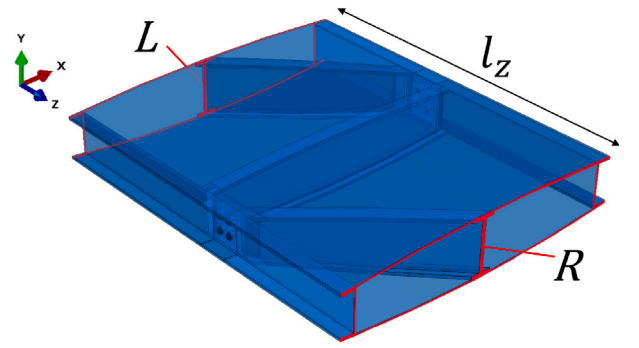


Fig. 4. Right (R) and left (L) faces of the structural element, necessary to employ the PBCs.

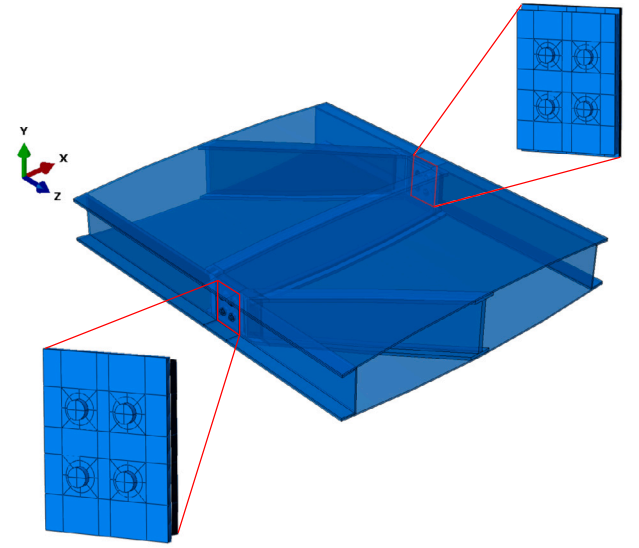


Fig. 5. Global and local finite element models.

3.2. Mesh

The laminates of the global model are modelled with a single 8-node, first-order interpolation, continuum shell with reduced integration (SC8R) [61] element through the thickness, being the respective layout assigned as a composite layout section.

3.3. Loads and boundary conditions

The loads are applied on the global model assuming Periodic Boundary Conditions (PBCs). The PBCs are enforced with constraint equations dependent of the nodes at the right and left faces (Fig. 4), denoted with $(\bullet)^R$ and $(\bullet)^L$ respectively and two master nodes, $MN_i, i = 1, 2$, which degrees of freedom control the strain to be applied in the representative structural element (global model).

The constraint equations used for the PBCs are found in Appendix A.

Although four different independent load cases can be imposed in the global model, only two will be considered for the machine learning based surrogate model: bending due to lift and torsion, since they are the main types of loads acting on a wing during flight.

4. Local model

The geometry of the local model mimics both the front and rear bolted joints of the global model, with the limits defined by the spar

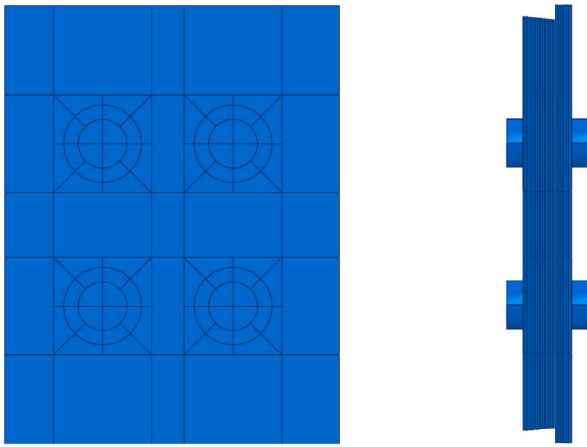


Fig. 6. Detail of the local model with partitions to allow the generation of a structured mesh.

web height and the partitions of the beam connection plate, as seen in Fig. 5.

An approximated view of one of the local model is shown in Fig. 6, where partition lines can be seen around the bolts, allowing the generation of a fully structured mesh.

4.1. Mesh

A one element per ply strategy is followed, with C3D8R elements used for both the plies and bolts. An enhanced hourglass control algorithm is used to reduce hourglass effects and the stack orientations are defined as a material orientation for each ply. Given that bolt holes can cause significant stress gradients near their boundaries, it is imperative to have a high enough mesh density around the hole to capture them. After a convergence analysis (Appendix B), the obtained mesh is as seen in Fig. 7.

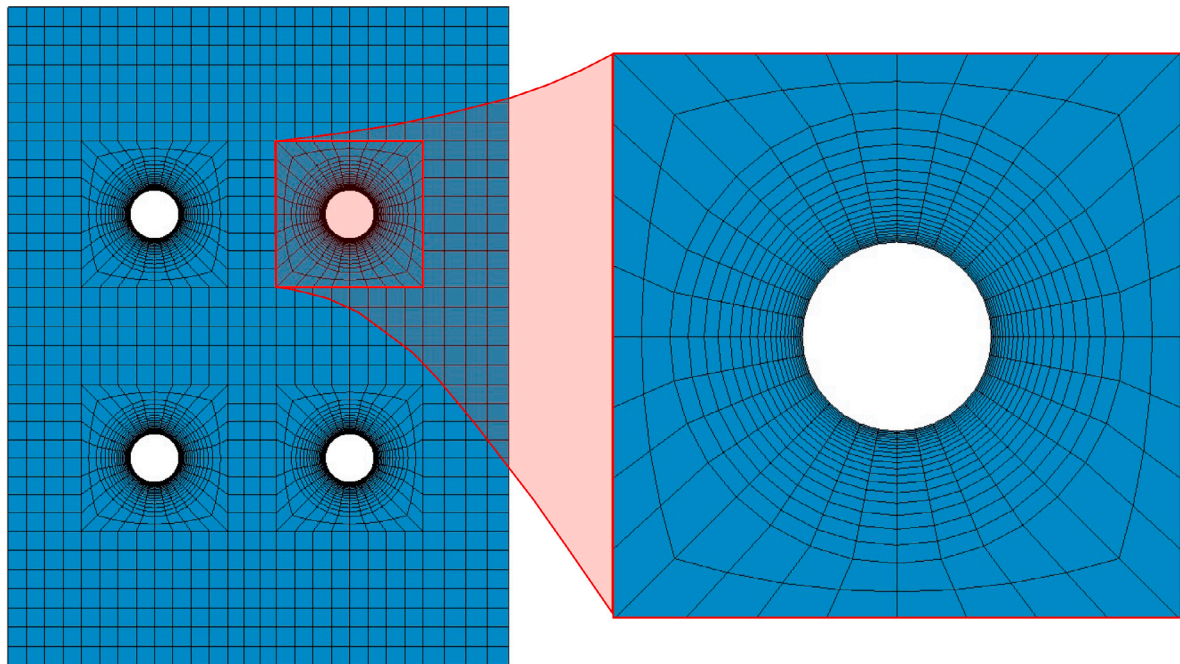


Fig. 7. Selected mesh after convergence analysis.

4.2. Boundary conditions

As aforementioned, the boundary conditions of the local model need to be interpolated from the displacements of the global. The submodelling tool offered by ABAQUS was used to perform this operation. A node based approach (i.e. nodal quantities are used for the interpolation) is used, where the displacements are the quantity of interest.

Given that continuum shell elements have a solid like nodal distribution, they are considered as solid elements for the interpolation procedure and thus, the coupling herein considered is solid-to-solid. Ensuring node proximity between the global and local models is straightforward, as they both utilise segments of the same Python scripts. However, since nodes at the shear plane of both spar and beam connection plate share the same spatial coordinate in the undeformed configuration, problems can arise if they separate during loading. As seen in Fig. 8, the node of the global spar can influence the node of the local beam, which will lead to an incorrect interpolation if the surfaces separate.

To tackle this problem, a designated driving node region within the global model is linked directly to a corresponding region in the local model. Consequently, local spar nodes are interpolated exclusively with global spar nodes, and local beam nodes with global beam nodes, thereby eliminating unwanted interferences.

5. Machine learning for failure prediction

A physics guided artificial neural network is created to bridge the global level strains and the failure indices of the local model. This section introduces the database, model architecture, training process, and performance of the proposed model. More details about the ANNs can be seen in Ref. [62,63].

5.1. Database

Since only three independent geometric parameters are considered, the database is constructed by uniformly sampling within their respective ranges, as listed in Table 1. The sampling intervals for the three

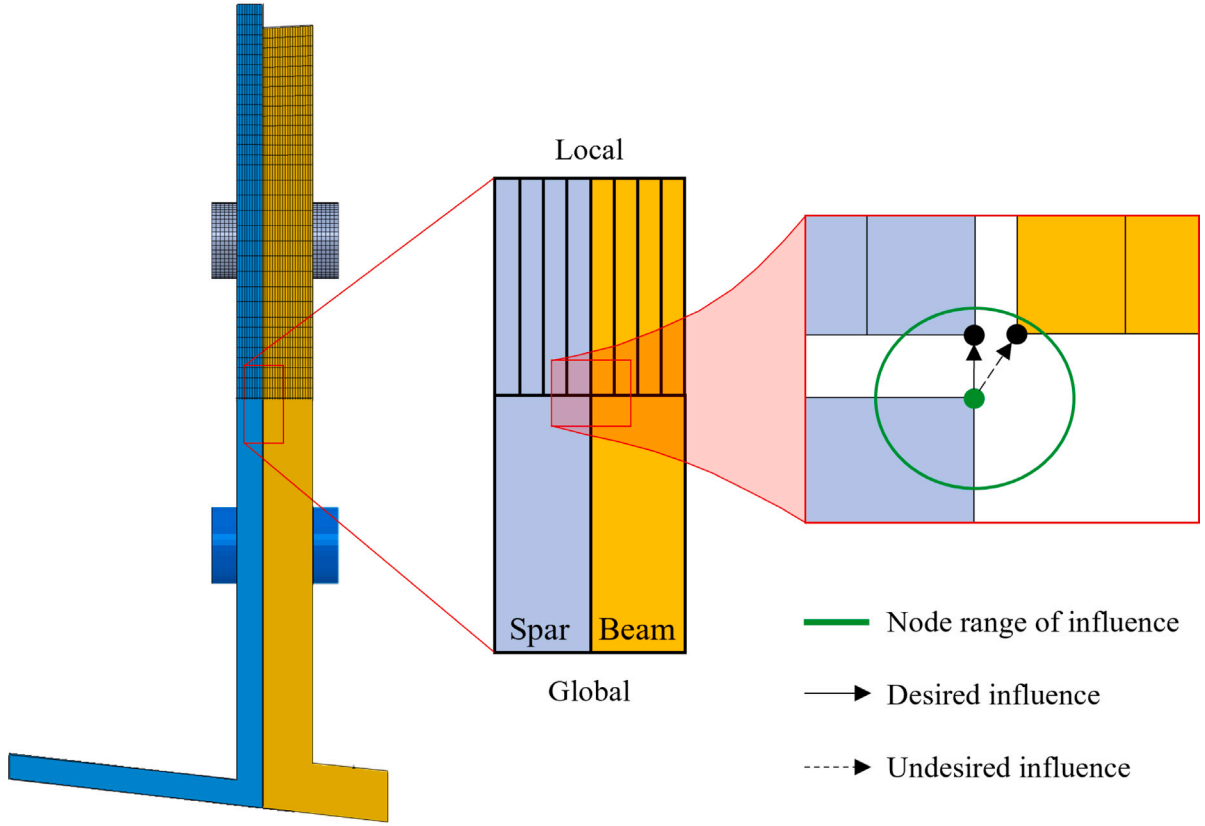


Fig. 8. Global spar node influence over local beam (local and global spars separated for visualisation purposes).

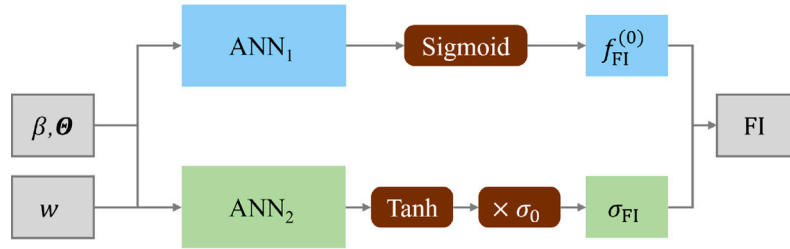


Fig. 9. Physics-guided model for failure index prediction.

parameters (t_{spar} , t_{beam} , and α_{beam}) are set to 2.0, 3.0, and 5.0, respectively. After running the simulations, 415 valid samples were obtained from an initial set of 495 candidate unit cells. Each sample contains four simulations with the four basis strain vectors, i.e., $[10^{-6}, 0, 0, 0]^T$, $[0, 10^{-6}, 0, 0]^T$, $[0, 0, 10^{-6}, 0]^T$, $[0, 0, 0, 10^{-6}]^T$. These strain vectors are scaled by a factor of 10^{-6} to ensure that the simulations remain within the elastic and linear regime in ABAQUS. The homogenised stiffness matrix $[C]$ is extracted from the global models.

Then, the refined local model is simulated using the before-mentioned global-local approach to capture the 3D stress fields at critical hotspots. The failure index field around bolt holes are extracted from the local models. In the present study, the failure due to torsion (κ_z) and bending (κ_x) is studied. The stress fields of the local model under the two basis strain vectors for pure twisting and pure bending, i.e., $[0, 10^{-6}, 0, 0]^T$, $[0, 0, 10^{-6}, 0]^T$, are used as the basis stress fields for linear superposition. In other words, given a deformation direction angle β and a scale w , the strain state is

$$\mathbf{s} = [0, w \cos(\beta) \times 10^{-6}, w \sin(\beta) \times 10^{-6}, 0]^T. \quad (6)$$

The corresponding stress field is obtained through linear superposition of the basis stress fields. Subsequently, the failure indices of the local model are calculated using LaRC05 in a post-processing approach.

5.2. Model architecture

Two machine learning models trained for the prediction of homogenised stiffness matrix $[C]$ and failure index field, respectively. A simple fully connected neural network is used to predict the homogenised stiffness matrix, its input is the geometric parameters Θ of the Z-beam unit cell. It contains three hidden layers with 256 neurons.

For predicting failure indices in the local model, the stress field is obtained by linear superposition, and the behaviour of the LaRC05 failure model exhibits limited nonlinearity. Then, the failure index of a wingbox can be expressed as:

$$\text{FI}(w, \beta, \Theta) = w \cdot f_{\text{FI}}^{(0)}(\beta, \Theta) \cdot [1 + \sigma_{\text{FI}}(w, \beta, \Theta)], \quad (7)$$

where Θ is the geometric parameters, and the strain state is $\kappa_z = w \cos(\beta) \times 10^{-6}$, $\kappa_x = w \sin(\beta) \times 10^{-6}$. Consequently, a physics-guided artificial neural network is proposed to model both the basis

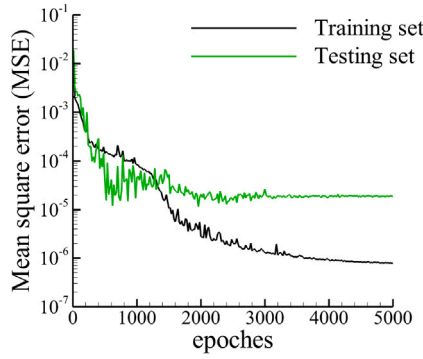


Fig. 10. Loss function history of the ANN for stiffness matrix.

failure indices and their evolution with respect to the strain scaling factor w , as shown in Fig. 9. Its architecture is designed to ensure the non-negativity of the failure indices and their monotonic relation with the scale of strain.

The $f_{FI}^{(0)}(\beta, \Theta)$ is the basis failure index when $w = 1.0$, which is modelled by ANN₁. The activation function of its output layer is a sigmoid function, so that the failure index is non-negative. The slope of failure index to w is $[1 + \sigma_{FI}(w, \beta, \Theta)]$, where $\sigma_{FI}(w, \beta, \Theta)$ is modelled by ANN₂. By the magnitude analysis of the database, it can be found out that $\sigma_{FI} \in [-0.2, 0.2]$ for the Z-beam wing boxes and current material. Therefore, the physics-guided architecture helps $FI(w, \beta, \Theta)$ to have a monotonic relationship with the scale of strain w .

5.3. Model training and performance

For both models, data is normalised for training. The loss function is the mean square error (MSE) between the predicted values and the real values. 50 samples are randomly selected for testing. The initial learning rate is 0.001, the learning rate gradually reduces during the training of 5000 epochs. Adam optimiser [64] is used for training. Figs. 10 and 11 show the training history of both machine learning models. The results indicate that the model for homogenised stiffness matrix achieves a very small root mean square error (RMSE) on both the training set (0.08%) and testing set (0.44%). As for the second model, its maximum relative prediction error of failure index field is less than 2.0% on both the training set and testing set.

6. Results

6.1. Global-local

In order to evaluate the relevance of the mesh of the local model, a specific configuration of the global model was run until failure for each

Table 5

Strains to failure of local model are at least half of the global model.

Load case	Global	Local
Tension	$\epsilon_z = 2.8 \times 10^{-3}$	$\epsilon_z = 1.2 \times 10^{-3}$ (-57%)
Bending (Lift)	$\kappa_x = 6 \times 10^{-5} \text{ mm}^{-1}$	$\kappa_x = 3 \times 10^{-5} \text{ mm}^{-1}$ (-50%)
Bending (Drag)	$\kappa_y = 6.67 \times 10^{-6} \text{ mm}^{-1}$	$\kappa_y = 2.67 \times 10^{-6} \text{ mm}^{-1}$ (-60%)
Torsion	$\kappa_z = -5.33 \times 10^{-5} \text{ mm}^{-1}$	$\kappa_z = -2 \times 10^{-5} \text{ mm}^{-1}$ (-63%)

load case separately. Then, the results were compared to those of the local model.

Referring to Table 5, using the local model results in at least a 50% decrease in strain to failure, validating its incorporation into the analysis framework. Conversely, if the global model was applied, the strain to failure would be overestimated by a factor of 2. Moreover, the critical bolt hole and respective failure mechanisms were also compared, with the results being given in Table 6.

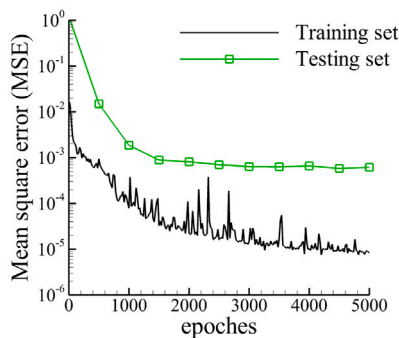
From Table 6, it is observed that the critical spots are the same for almost every case, however, the failure mechanism changed from fibre compressive nature (matrix splitting and fibre kinking due to bearing [65]) to transverse tensile dominated modes [66], such as matrix cracking. This is explained by the higher accuracy of the more refined mesh. As seen in Fig. 12, the local model mesh is refined enough to capture the high stress gradients near the hole boundary, while the global model mesh fails to do so, underestimating the stress level.

This way, the values of the shear and in-plane transverse tensile stress caused by the presence of the stress concentration, lead to matrix cracking failure in the perpendicular direction to the crushing forces exerted by the bolt. Nevertheless, these crushing forces are also the drivers of some degree of matrix splitting, caused by the compressive stresses.

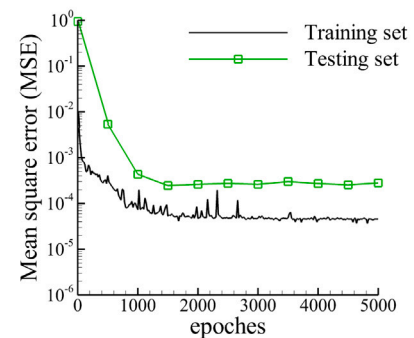
6.2. Surrogate model

After running nearly 400 different simulations, each with a different geometry or bending/torsion ratio, it was possible to create a database containing the applied strains and the respective failure indices. In Fig. 13, the failure index fields of an example wingbox representative structural element are shown. These failure index fields are obtained by extracting the maximum value of the failure index between the elements of the bolt hole boundaries for a specific combination of torsional and bending strains.

As can be seen, matrix cracking and splitting are the main failure mechanisms, for the reasons outlined in Section 6.1. Fibre tension is not an expected failure mode and fibre kinking and matrix interface failure are only predicted for extreme cases of torsion, caused by high crushing forces created by the bolt shank or increased out of plane loading. In comparison, Fig. 14 shows the failure index field prediction



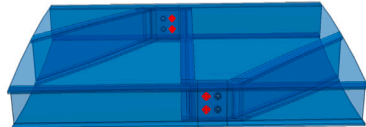
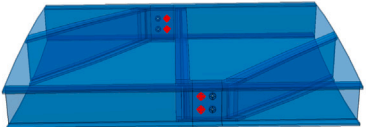
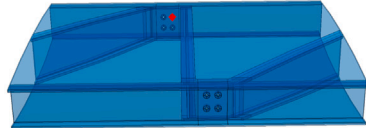
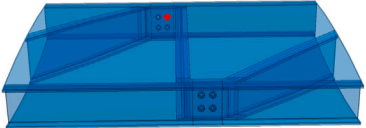
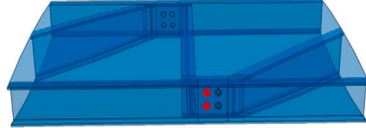
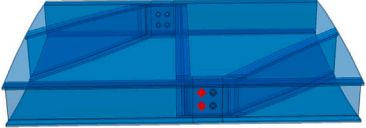
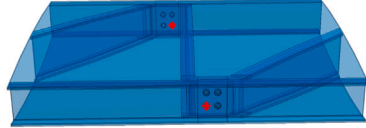
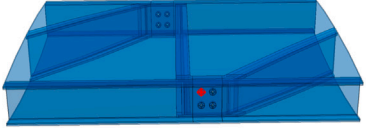
(a) ANN₁: $f_{FI}^{(0)}$



(b) ANN₂: σ_{FI}

Fig. 11. Loss function history of the physics-guided failure index prediction model.

Table 6
Hotspots and failure mechanism for each model and load case ($t_{spar} = 5$ mm, $t_{beam} = 10$ mm, $\alpha_{beam} = 45^\circ$).

Load Case	Global	Local
Tension	Splitting 	Matrix cracking and splitting 
Bending (Lift)	Splitting 	Matrix cracking 
Bending (Drag)	Splitting 	Matrix cracking and splitting 
Torsion	Fibre kinking 	Matrix cracking and splitting 

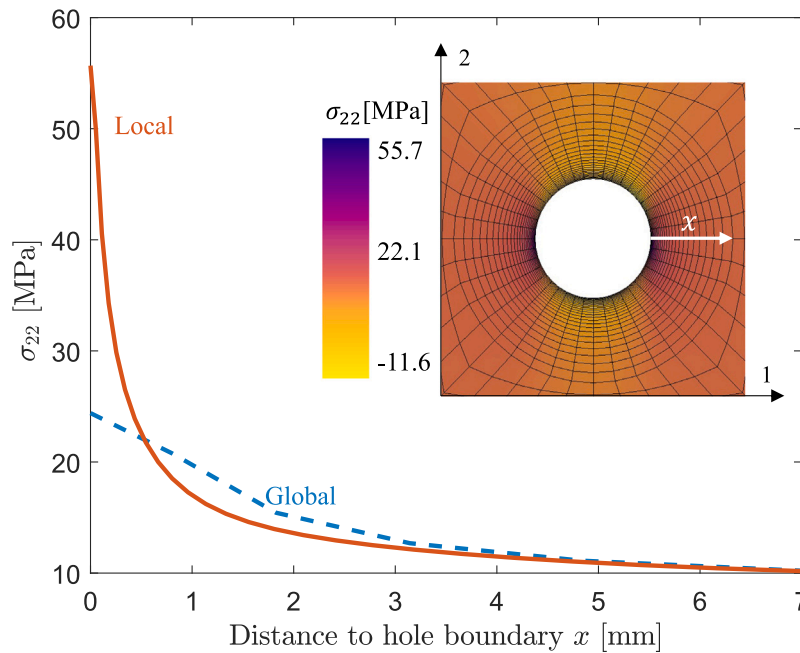


Fig. 12. Local model is able to capture higher stresses due to a better mesh refinement.

for the same model employing the artificial neural network trained on the dataset.

As observed, there is an excellent prediction of both matrix cracking and splitting failure index fields. The values of the main failure modes index were also compared for a specific geometry subject to a pure bending moment due to lift ($m_x \neq 0$), where the angle of the Z-Beam was changed. An excellent agreement between the finite element and the machine learning results was attained, as seen in Fig. 15.

7. Discussion

The total time for a conventional global local analysis, including post processing is prohibitive for the early design stages, having to be redone for each global strain values or different geometric parameters. On the other hand, following the proposed methodology, a higher initial time investment is needed to create a sufficiently large range of samples to train the machine learning model. However, it is able

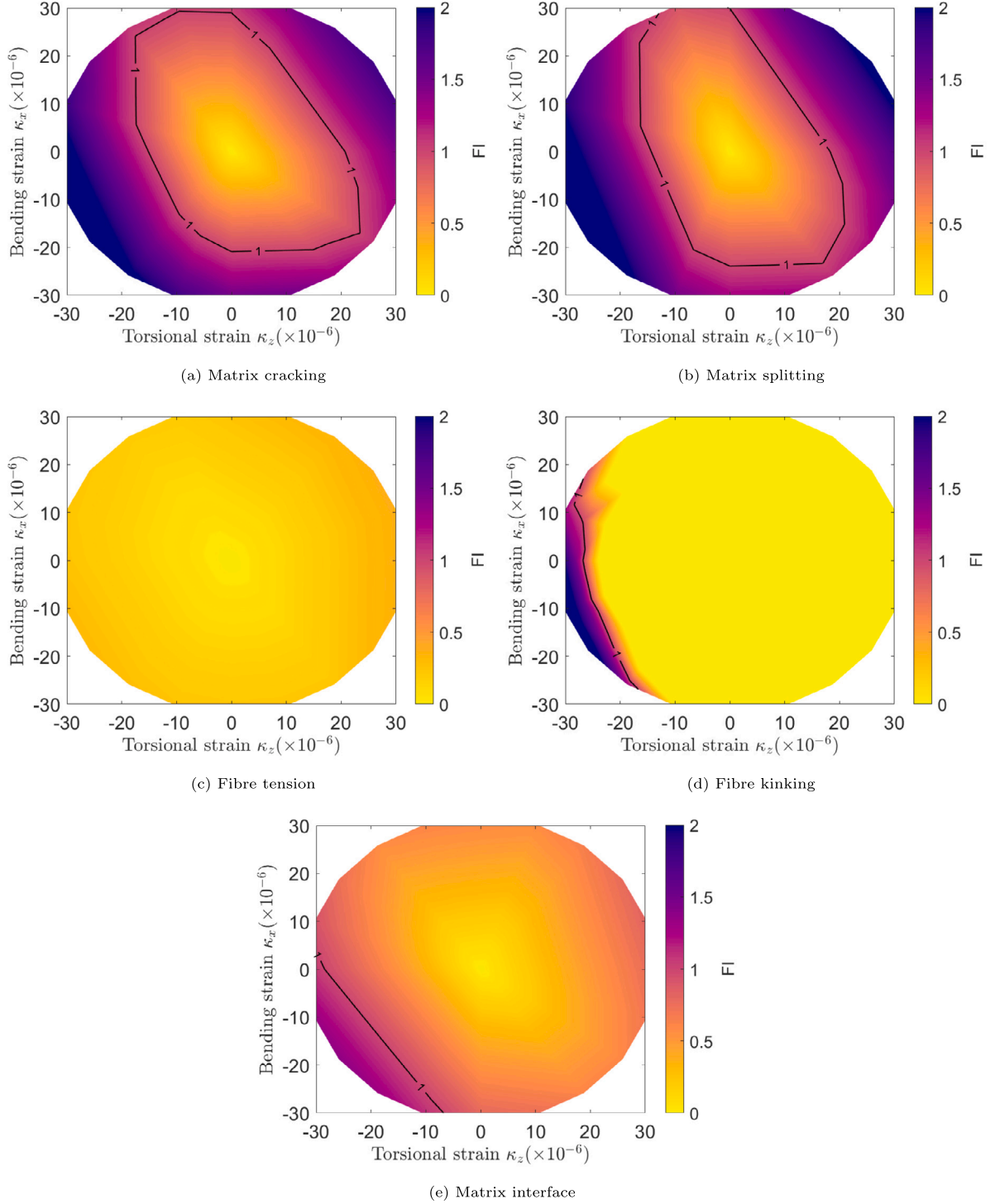


Fig. 13. Matrix cracking and matrix splitting are the main failure mechanisms as shown for an example wingbox ($t_{spar} = 5$ mm, $t_{beam} = 10$ mm, $\alpha_{beam} = 45^\circ$).

to provide failure index maps based on different global strains and geometries in a time efficient manner, and thus may be a much better option for early design stages, where the design space is wished to be kept as wide as possible. Additionally, the failure of structural details can be captured at a very preliminary stage, reducing the probability of setbacks in later design stages, resulting in additional costs.

One natural avenue of the impact of this work is to combine it with established methods for hotspot identification such as the one in Ref. [55], shown in Fig. 16. Different metrics can be used to determine

the hotspot, such as percentage of failed plies or maximum laminate failure index for each element

There are other available strategies in the literature which are compatible with the proposed methodology, such as the ones shown in Refs. [67,68]. Engineering experience can also be successful in guiding the selection of areas for which the derivation of a surrogate model would be preferred to e.g. traditional stress analysis. This is envisaged to happen primarily on structural features that are novel or do not lend themselves readily to simplified analytical solutions. The failure index

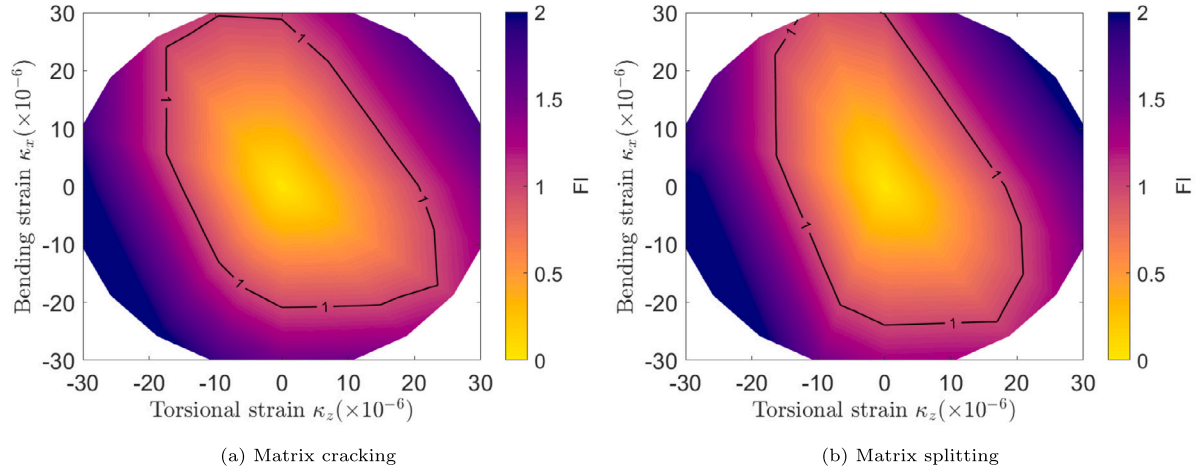


Fig. 14. Excellent predictions of the machine learning model for the main failure mechanisms, for an example wingbox ($t_{spar} = 5$ mm, $t_{beam} = 10$ mm, $\alpha_{beam} = 45^\circ$).

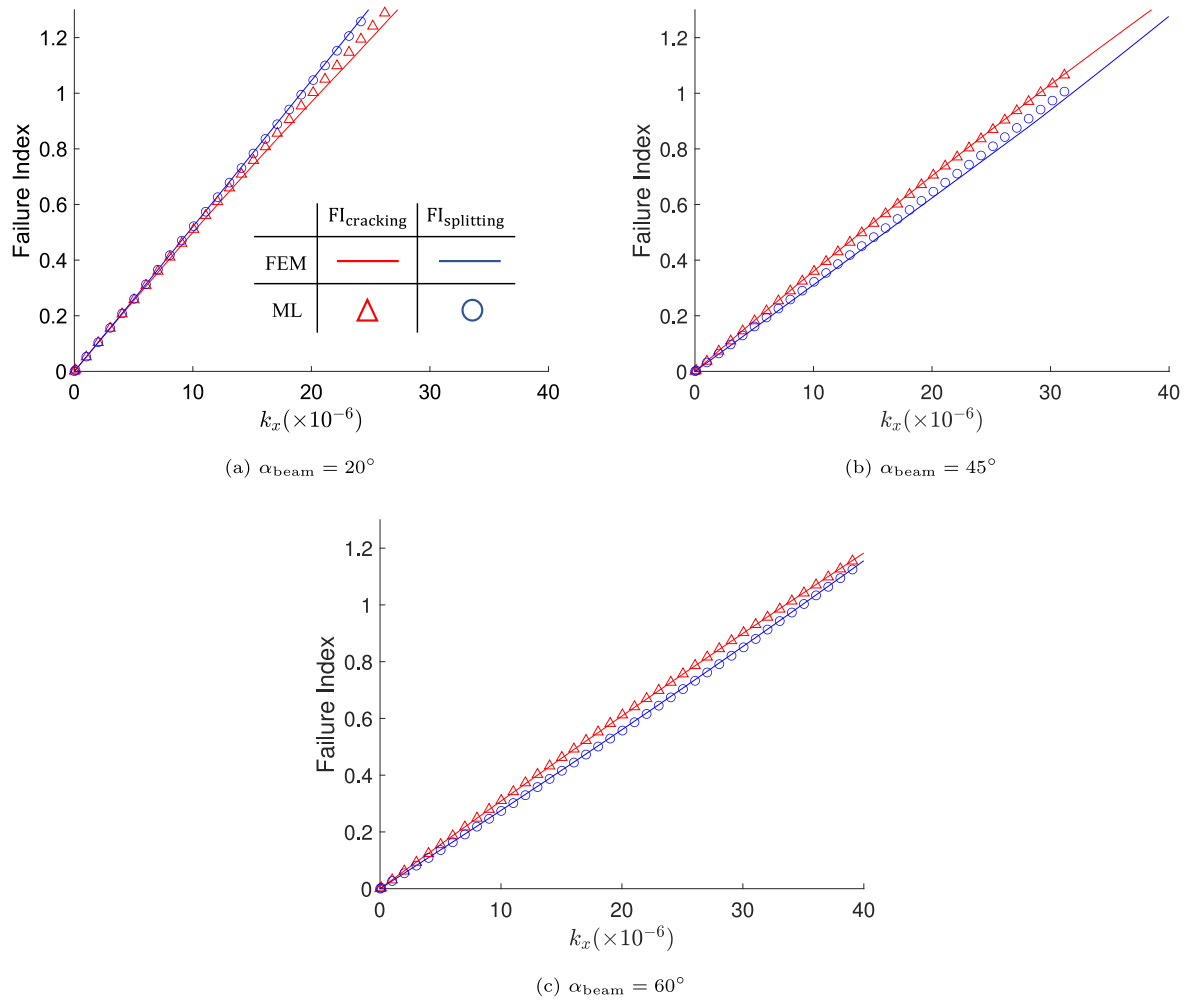


Fig. 15. Good ML predictions of the main failure indices for different Z-Beam angles ($t_{spar} = 5$ mm, $t_{beam} = 10$ mm).

fields were also obtained by considering a linear combination of the pure bending and torsion stress fields, which is an approximation of the real stress state. Nevertheless, results show that the proposed strategy is able to quickly provide excellent failure predictions of novel structural details which are of utmost interest to support the development of innovative composite components.

8. Conclusions

In the race against time for carbon neutrality, the aeronautical industry is exploring different original concepts to be applied in newer aircraft designs. However, new structural concepts bring additional challenges given the need for an exhaustive number of simulations and

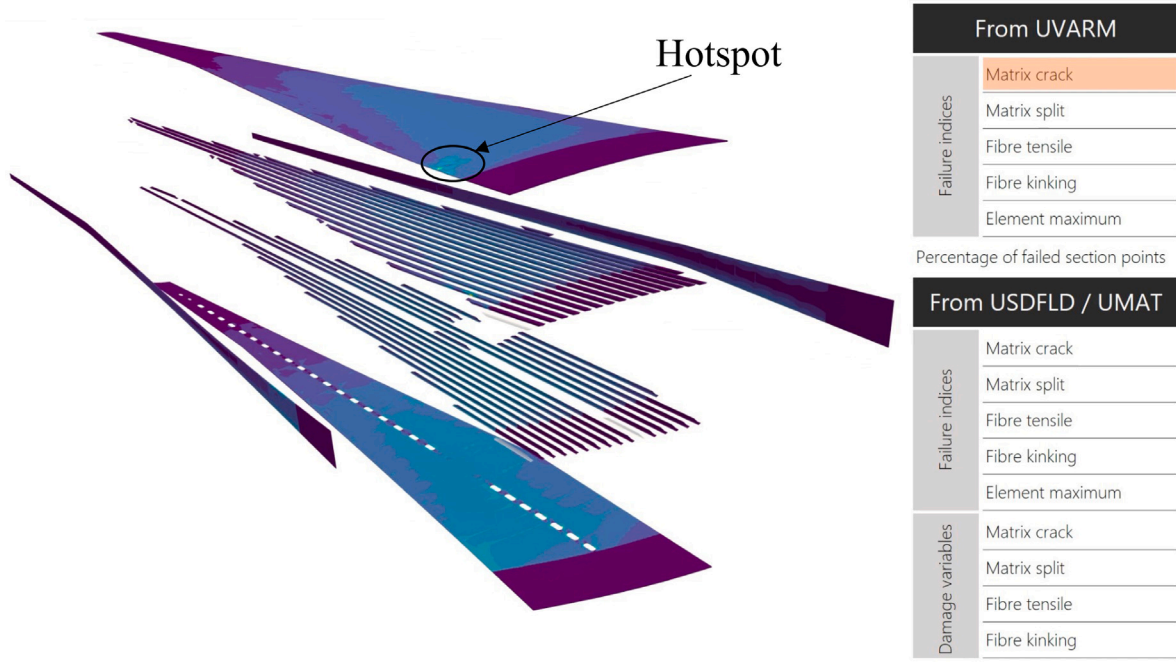


Fig. 16. Hotspot identification for a large composite component (full scale airliner wing).
Source: Adapted from [55].

tests. In this work, a multiscale modelling strategy is introduced to be used for the preliminary design of novel composite components (in this case, a Z-beam wingbox), capable of quickly predicting the failure of critical parts. Regarding the new methodology, the key points are summarised below:

- A new methodology for the early stage design of novel composite structural features is developed, including different modelling and simulation strategies such as periodic boundary conditions, a global-local approach and a physics guided artificial neural network.
- The global-local approach is observed to be crucial in the design process. Failure modes estimation appropriate for feasible designs are shown to require locally refined models. A suitable level of refinement is however not feasible for the global level due to the resulting model size and implicit long solution times.
- The obtained results have shown that the methodology is able to accurately predict failure indices (employing an evolved LaRC05 failure criteria) based on global level loads, allowing significant time cost reduction and structural details behaviour in early and exploratory phases of design of novel composite parts, diminishing the chances of late setbacks.

We consider the multiscale methodology proposed herein to be a promising strategy for the sizing of new composite structural concepts. Additionally, the fast composite failure prediction capabilities pave the way for its inclusion in optimisation frameworks.

CRedit authorship contribution statement

Mário Miranda: Writing – review & editing, Writing – original draft, Visualization, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Runze Li:** Visualization, Investigation, Formal analysis, Data curation, Conceptualization. **Lucian Iorga:** Writing – review & editing, Validation, Supervision. **Silvestre T. Pinho:** Writing – review & editing, Supervision, Resources, Project administration, Funding acquisition, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Periodic boundary conditions

The constraint equations used for the PBCs of the different load cases are explained in detail here:

Tensile

For the tensile case, the constraint equations are defined as:

$$\begin{cases} u_x^R - u_x^L = u_1^{MN_1} \\ u_y^R - u_y^L = u_2^{MN_1} \\ u_z^R - u_z^L = u_3^{MN_1} \end{cases} \quad (\text{A.1})$$

where $u_3^{MN_1}$ is the displacement to be applied in the span-wise (z) direction and both $u_1^{MN_1}$ and $u_2^{MN_1}$ are and will be left free for all the remaining load cases. The prescribed displacement can also be represented in function of strain, $u_z = \epsilon_z L_z$, where L_z is the length of the global model. Rewriting Eq. (A.1):

$$\begin{cases} u_x^R - u_x^L = u_1^{MN_1} \\ u_y^R - u_y^L = u_2^{MN_1} \\ u_z^R - u_z^L = L_z u_3^{MN_1} \end{cases} \quad (\text{A.2})$$

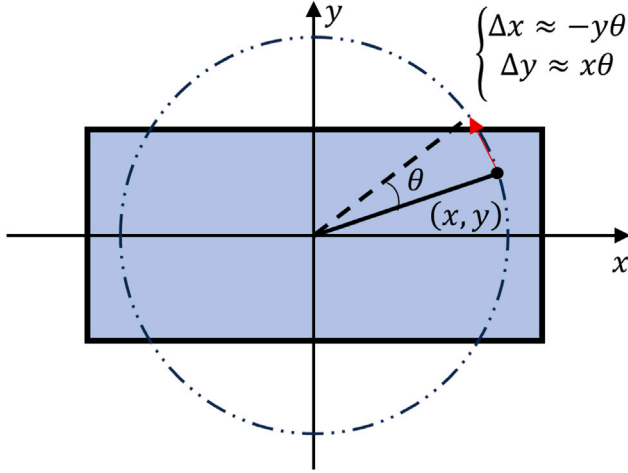


Fig. A.1. Cross sectional displacements for small angle rotations.

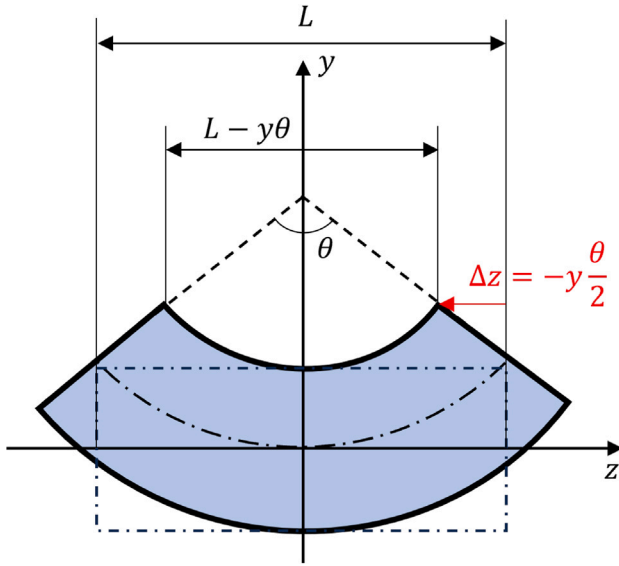


Fig. A.2. Bending displacements.

where $\tilde{u}_3^{MN_1}$ is the strain to be applied in the span-wise direction. Please note that henceforth the tilde ($\sim$) indicates that the master node components are representing values of strain/curvature instead of displacements/rotations.

Torsion

Torsion PBCs are defined assuming small rotations (Fig. A.1) and the constraints are defined as:

$$\begin{cases} u_x^R - u_x^L = u_1^{MN_1} - yL_z\tilde{u}_1^{MN_2} \\ u_y^R - u_y^L = u_2^{MN_1} + xL_z\tilde{u}_1^{MN_2} \\ u_z^R - u_z^L = u_3^{MN_1} \end{cases} \quad (\text{A.3})$$

where $\tilde{u}_1^{MN_2}$ assumes the value of rate of twist i.e. θ_z/L_z .

Bending

The bending behaviour of a representative cell can be described as seen in Fig. A.2.

The constraint equations are then defined accordingly, when bending over the x axis (lift):

$$\begin{cases} u_x^R - u_x^L = u_1^{MN_1} \\ u_y^R - u_y^L = u_2^{MN_1} \\ u_z^R - u_z^L = u_3^{MN_1} + yL_z\tilde{u}_2^{MN_2} \end{cases} \quad (\text{A.4})$$

and y axis (drag):

$$\begin{cases} u_x^R - u_x^L = u_1^{MN_1} \\ u_y^R - u_y^L = u_2^{MN_1} \\ u_z^R - u_z^L = u_3^{MN_1} - xL_z\tilde{u}_3^{MN_2} \end{cases} \quad (\text{A.5})$$

where $\tilde{u}_2^{MN_2} = \kappa_x$ and $\tilde{u}_3^{MN_2} = \kappa_y$ are the curvatures of the cell.

Homogenised stiffness

Through the use of PBCs, it is possible to obtain a homogenised stiffness matrix, C , which relates the applied strains and the reaction forces (obtained at the master nodes):

$$\begin{bmatrix} f_z \\ m_z \\ m_x \\ m_y \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} \\ C_{21} & C_{22} & C_{23} & C_{24} \\ C_{31} & C_{32} & C_{33} & C_{34} \\ C_{41} & C_{42} & C_{43} & C_{44} \end{bmatrix} \begin{bmatrix} \tilde{u}_3^{MN_1} \\ \tilde{u}_1^{MN_2} \\ \tilde{u}_2^{MN_2} \\ \tilde{u}_3^{MN_2} \end{bmatrix} \quad (\text{A.6})$$

where f_z is the reaction force in the span-wise direction and $m_i, i = \{x, y, z\}$ are the reaction moments in each direction. The homogenised stiffness matrix can be obtained through the unitary displacement method.

Appendix B. Mesh convergence analysis

To ensure the convergence of the local model predictions, a two stage mesh convergence analysis was performed. For the radial convergence analysis, six different mesh sizes were studied, being the difference between them the number of elements and bias inside the circular partition. The resulting meshes can be seen in Fig. B.1.

The six models were run, and all showed agreement on the critical spot. However, they reached damage onset at different curvature values. At the curvature where the most refined model failed, the stress values and matrix cracking failure index (FI) were extracted for the same failed element in each mesh. This was possible because the number of circumferential elements (32) remained constant. The obtained results can be seen in Fig. B.2.

As observed, the results managed to converge for both the stress and failure index values. Since the relative error of stress between the second to last and the most refined configuration is near 1% and the computational time is approximately 15% faster (5458 vs. 6386 s), the former (ID5) was chosen as it presents the best cost/accuracy ratio. A circumferential mesh refinement was also performed on the previously selected mesh. The results showed that the failure index was not significantly affected by this refinement (Fig. B.3). Therefore, the ID5 mesh was chosen for the framework.

Data availability

The data is available at <https://github.com/swayli94/AbaqusZBeamWingBox>.

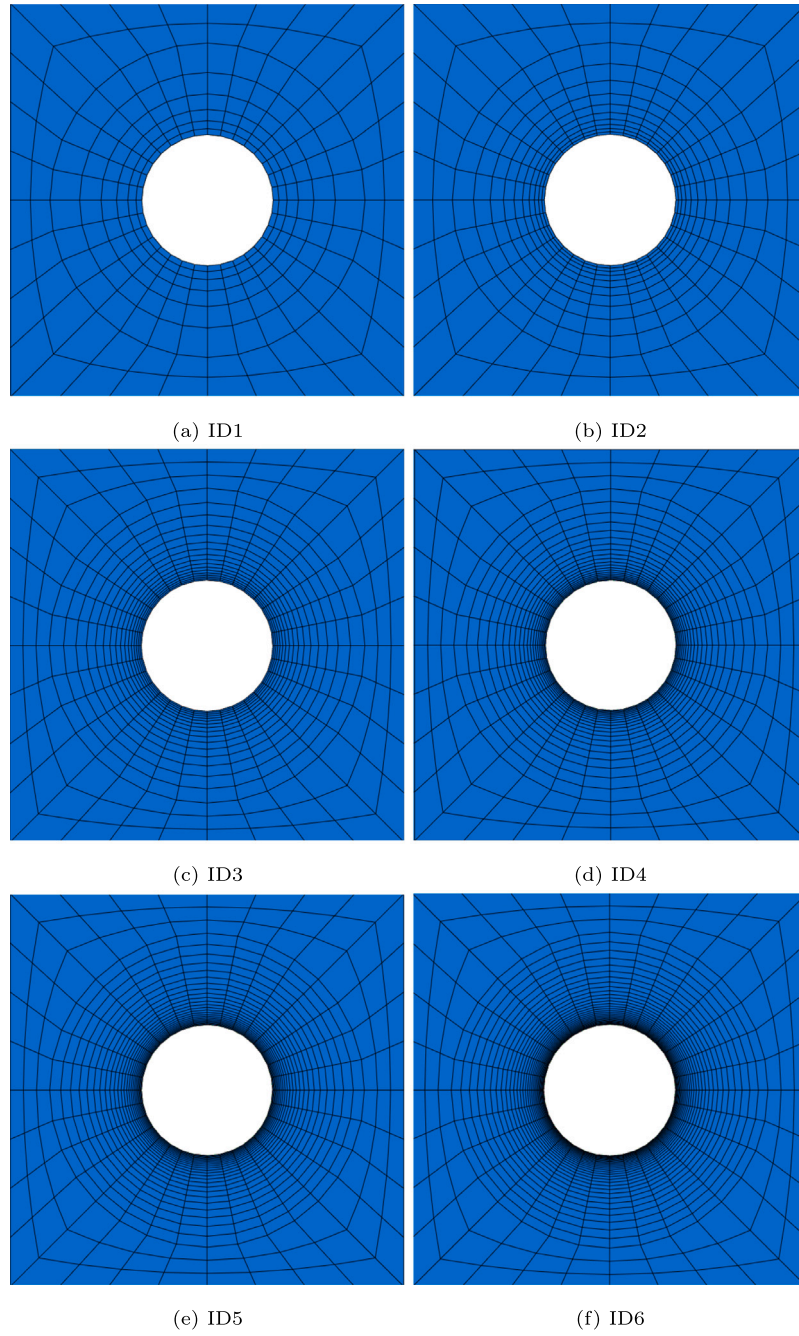


Fig. B.1. Studied radial meshes.

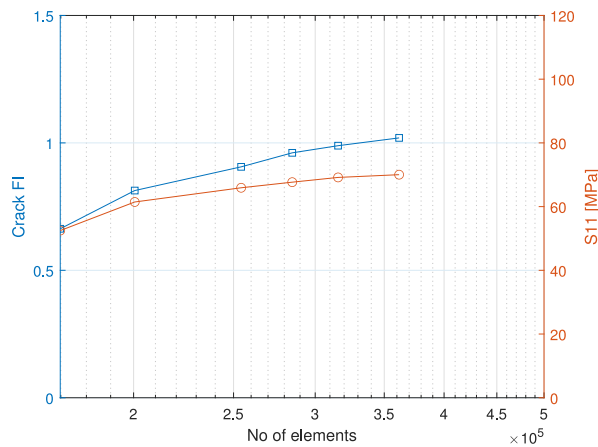


Fig. B.2. Radial convergence analysis.

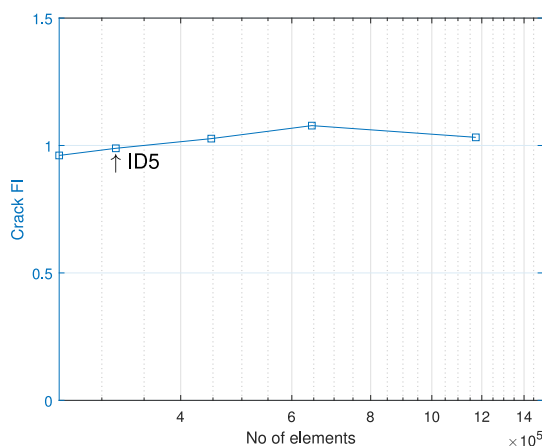


Fig. B.3. Circumferential convergence analysis.

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