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WebinarsAEMAC N°63

Simulation and design of composite structures across the scales
using physical and data-driven models.



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Simulation and design of composite materials and structures across the scales using physical and data-driven models

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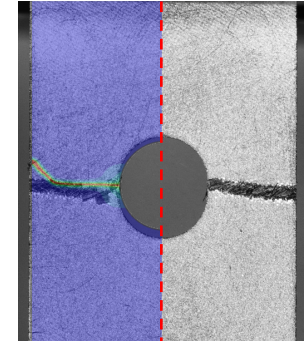
Carolina Furtado, Albertino Arteiro, Federico Danzi, José Reinoso, Miguel Bessa, Rodrigo Tavares,
Giuseppe Catalanotti, Fermin Otero, Martim Salgado, Anatoli Mitrou

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1. Introduction.
2. Analytical framework to predict notched strength.
3. Design of experiments and computational analysis.
4. Generation B-basis allowables using machine learning.
5. Conclusions.

Important innovation drivers in the aerospace industry

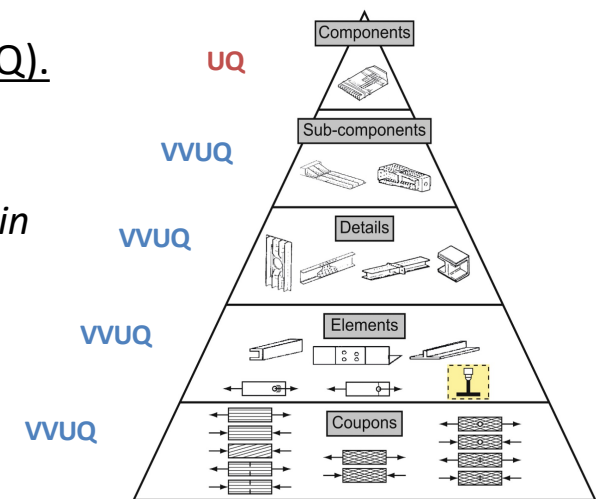
- Digitalization of processes/digital transformation, leading to reductions in cost and lead time. 50% reduction of certification costs by 2050 (ACARE vision for 2050). End-to-end simulation, including design, manufacturing and certification.



- Model verification, validation and uncertainty quantification (VVUQ).

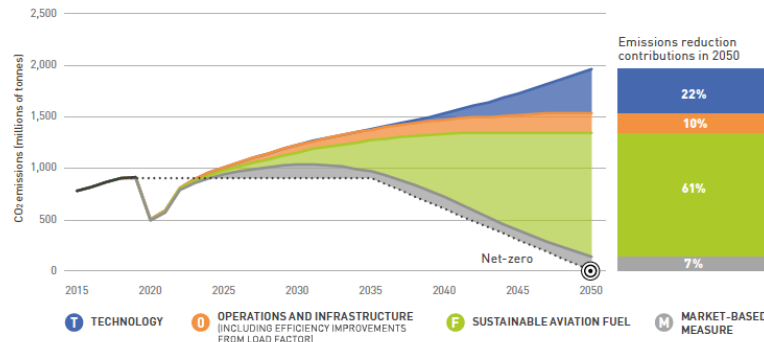
“VVUQ are the primary methods for quantifying and building credibility in computational models”.

(J. Fatemi, Airbus NL, Porto, 2023)

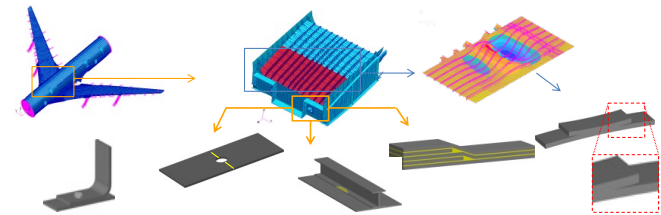


Important innovation drivers in the aerospace industry

- Highly optimized composite structures & non-conventional composite materials, requiring simulation across the scales.

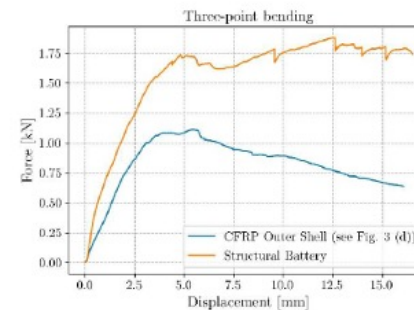
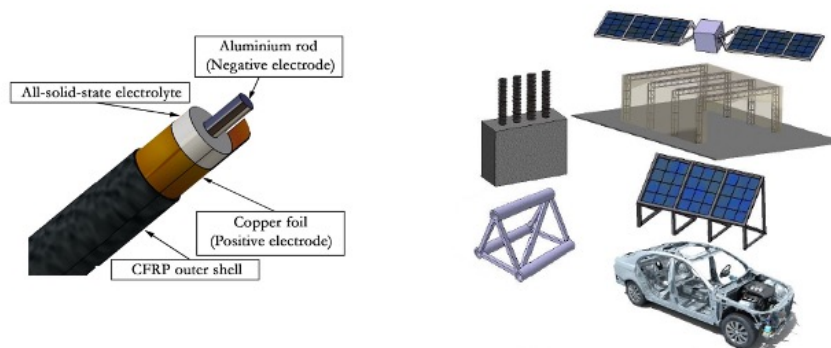


(Waypoint 2050, Air Transport Action Group, 2nd ed., Sept. 2021).

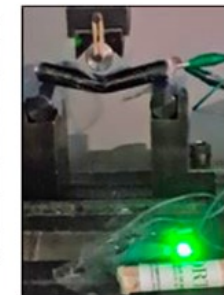


(Picture courtesy of Dr. Stéphane Mahdi, Airbus).

- Multifunctional composites (electrification, SHM).



(a)

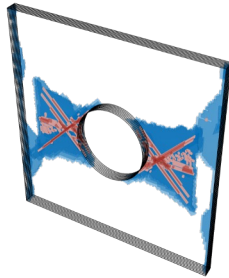


(b)

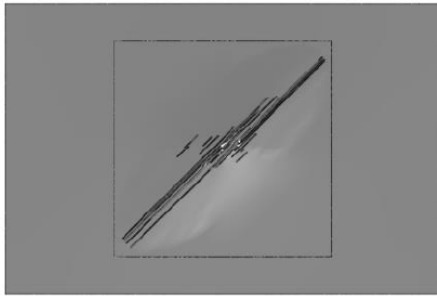
(F. Danzi, H. Braga, P.P. Camanho, Coaxial energy harvesting and storage, patent EP4324008)

Finite Element models

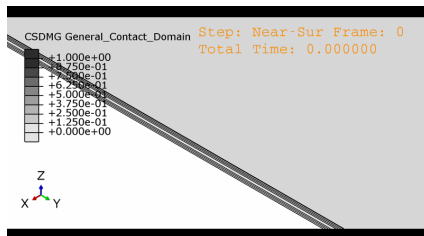
Open-hole
tension/compression



Low-velocity
impact and
CAI



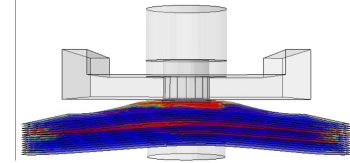
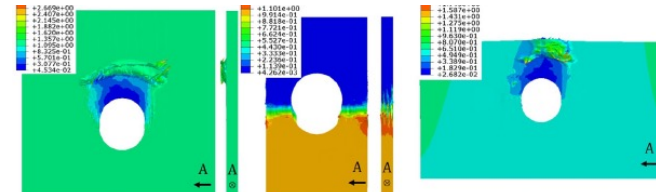
Lightning strike



Computing times (16 CPUs) - between 1h and 80h; expert users required.



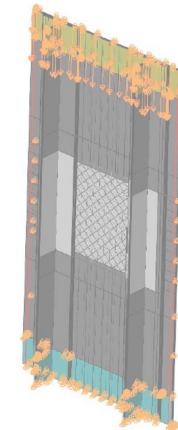
Bolted joint
(in-plane and
pull-through)



Low-velocity edge
impact and CAEI



CAI of stiffened panels



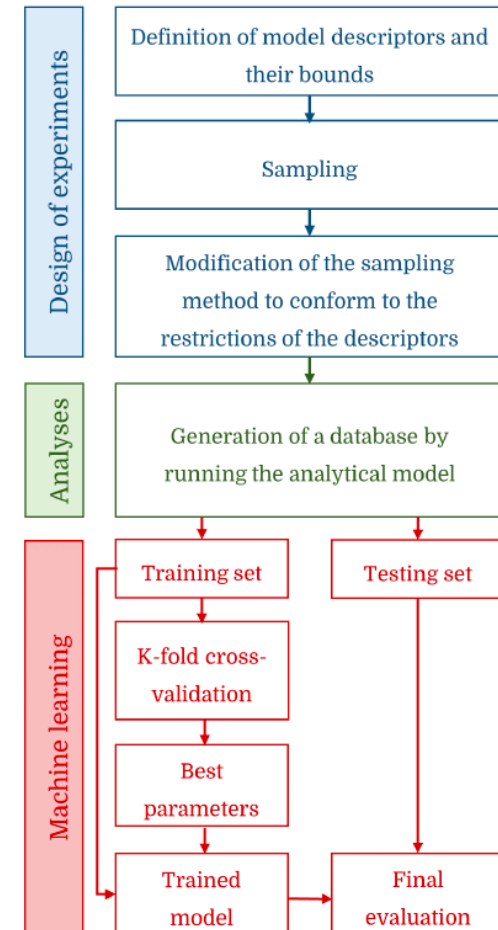
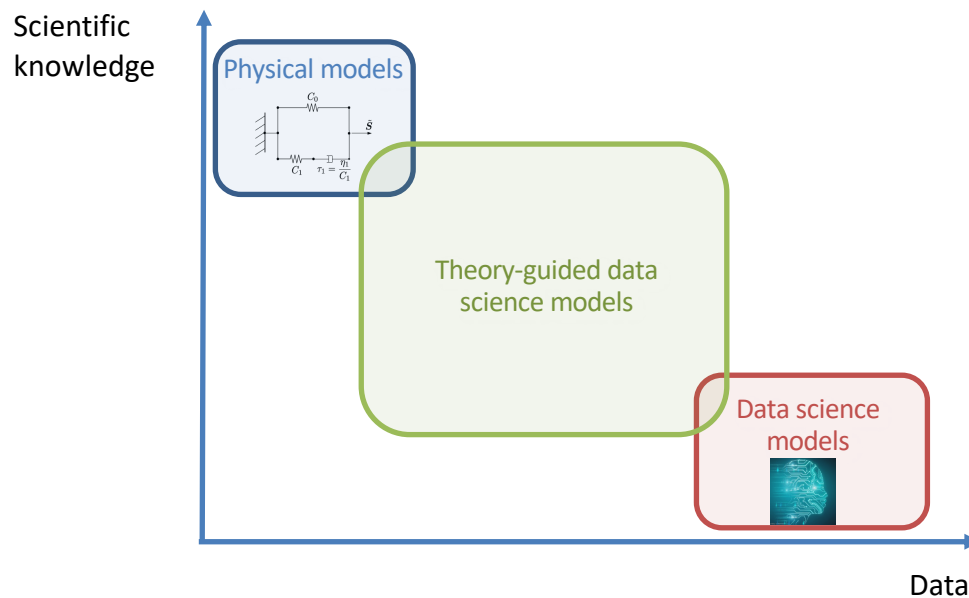
High computational costs may limit the use of the FE models.

Questions to be addressed:

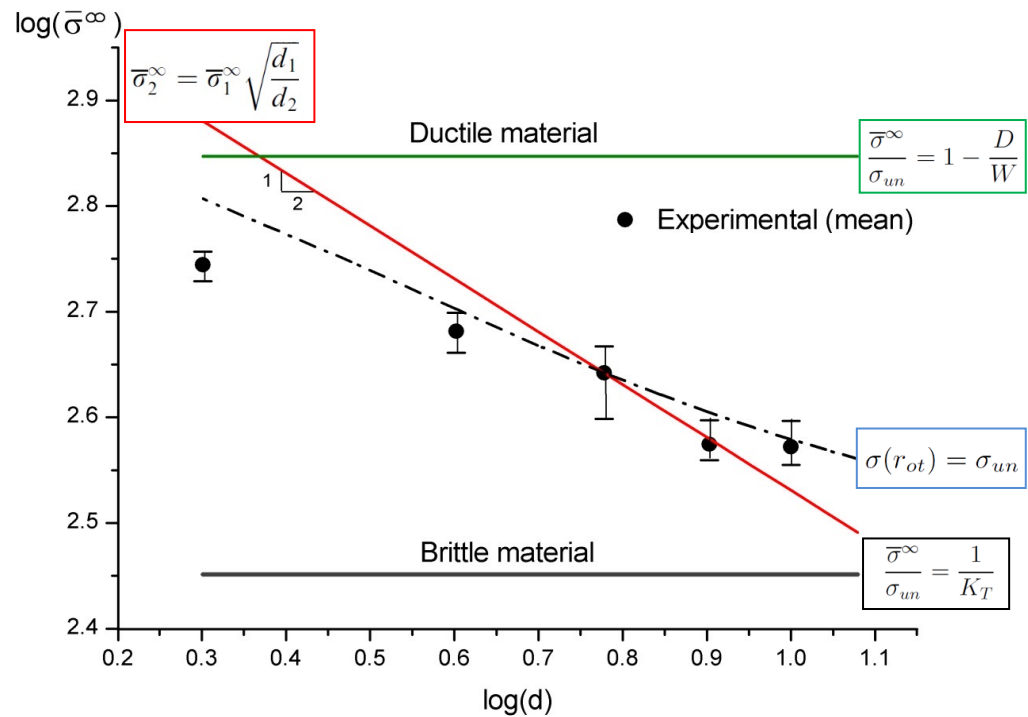
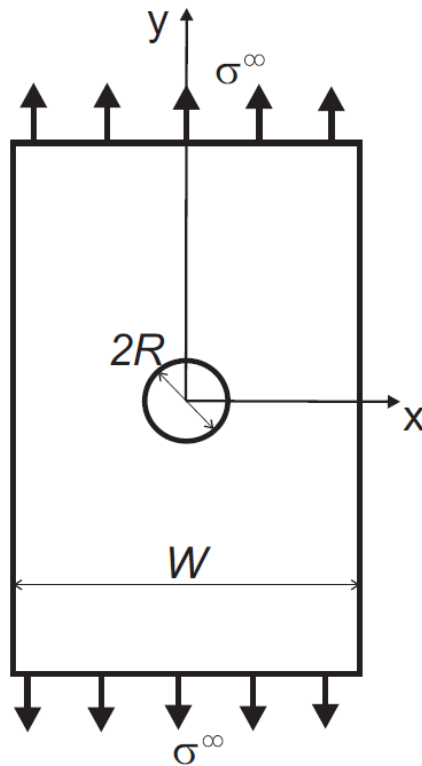
- How to define a machine learning-based approach to predict composite design allowables?
- What is the best machine learning algorithm to predict composite design allowables?

Proposed approach:

Theory guided machine learning for the generation of surrogate models:



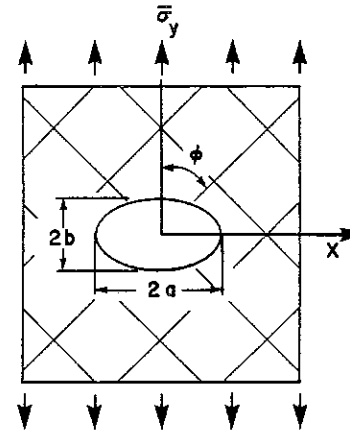
Analytical framework to predict the notched strength of composite laminates



IM7-8552 CFRP, [90/0/±45]_s

Analytical framework to predict the notched strength of composite laminates

$$\begin{cases} \frac{1}{l} \int_a^{a+l} \sigma_{yy}(x) dx = X_T^L \\ \int_a^{a+l} \mathcal{K}_I^2(a) da = \int_0^l \mathcal{K}_C^2(\Delta a) d(\Delta a) \end{cases}$$



$$\gamma = x/a$$

$$\lambda = b/a$$

$$\sigma_{yy}(x, 0) = \sigma^\infty \mathcal{S}(\lambda, \gamma, K_T^\infty) \frac{K_T}{K_T^\infty}$$

Complex Variable Theory
(Lekhnitskii)

Finite width correction
factor

$$\mathcal{K}_I = \frac{1}{\sqrt{1 - \left(\frac{2a}{w}\right)^2}} \sigma^\infty \sqrt{\pi a} \quad , \lambda \rightarrow 0$$

$$\mathcal{K}_I = \sigma^\infty F_h F_w \sqrt{\pi a} \quad , \lambda = 1$$

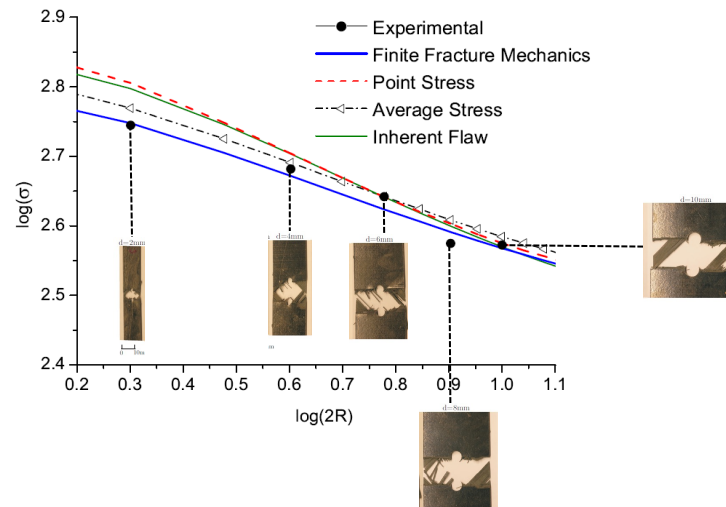
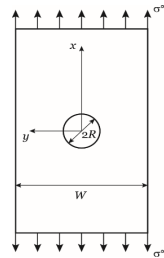
(Camanho et al., **Composites Part A**, 2012).

New development required for the implementation of the proposed approach: stress intensity factor for non-quasi-isotropic laminates.

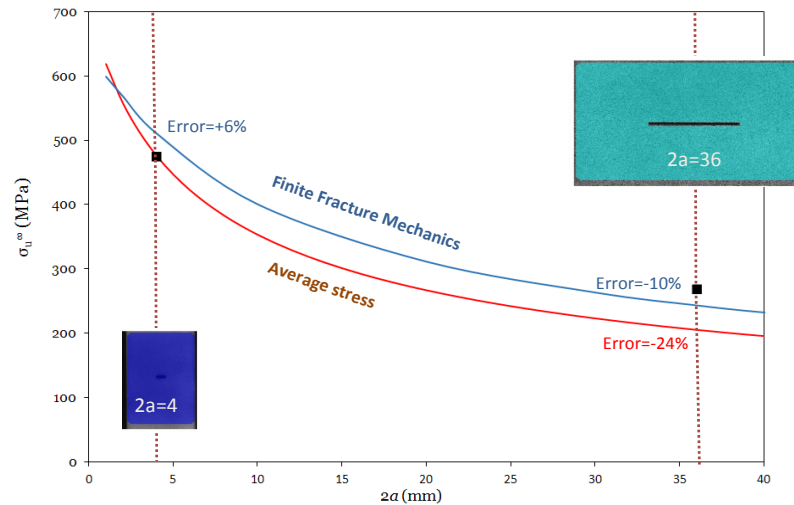
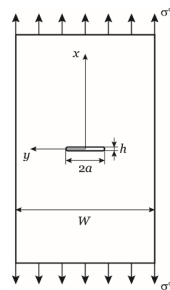
(Catalanotti, Salgado, Camanho, **Engineering Fracture Mechanics**, 2021).

Analytical framework to predict the notched strength of composite laminates

$\lambda=1$



$\lambda \rightarrow 0$



Good accuracy, but the model relies on laminate properties.

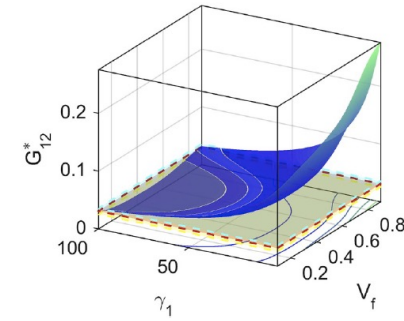
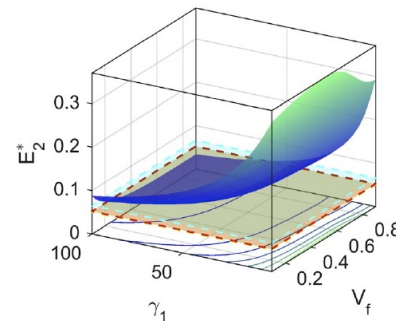
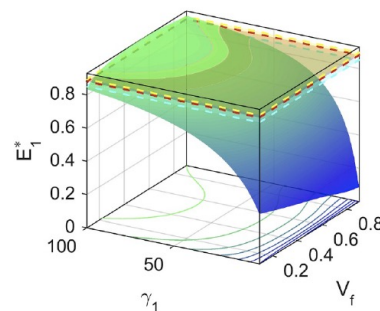
$$\begin{cases} \frac{1}{l} \int_a^{a+l} \sigma_{yy}(x) dx = X_T^L \\ \int_a^{a+l} \mathcal{K}_I^2(a) da = \int_0^l \mathcal{K}_C^2(\Delta a) d(\Delta a) \end{cases}$$

Laminate property
Laminate property

A_{ij} (4 ply elastic properties)

Laminate elastic properties

$$\mathbf{Q} = \begin{bmatrix} Q_{11} & Q_{12} & 0 \\ Q_{21} & Q_{22} & 0 \\ 0 & 0 & 2Q_{66} \end{bmatrix} = \begin{bmatrix} \frac{E_1}{1-\nu_{12}\nu_{21}} & \frac{\nu_{12}E_2}{1-\nu_{12}\nu_{21}} & 0 \\ \frac{\nu_{21}E_1}{1-\nu_{12}\nu_{21}} & \frac{E_2}{1-\nu_{12}\nu_{21}} & 0 \\ 0 & 0 & 2G_{12} \end{bmatrix}$$



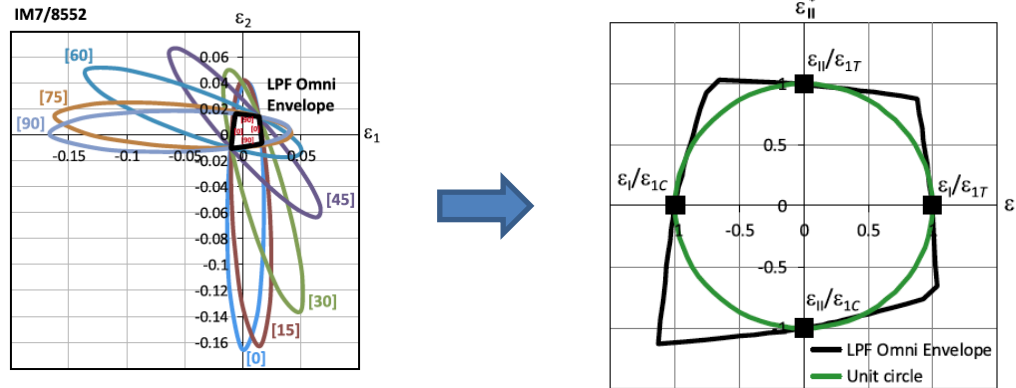
$$\gamma_1 \gtrsim 50$$

$$0.5 < V_f < 0.7$$

Master Ply	E_1^*	E_2^*	G_{12}^*
[0]	0.880	0.052	0.031

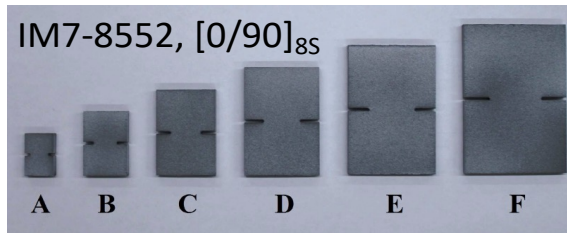
$$\text{Tr}(\mathbf{Q}) = \frac{E_1}{E_1^*}$$

Laminate strength

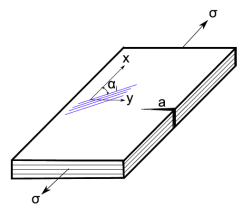
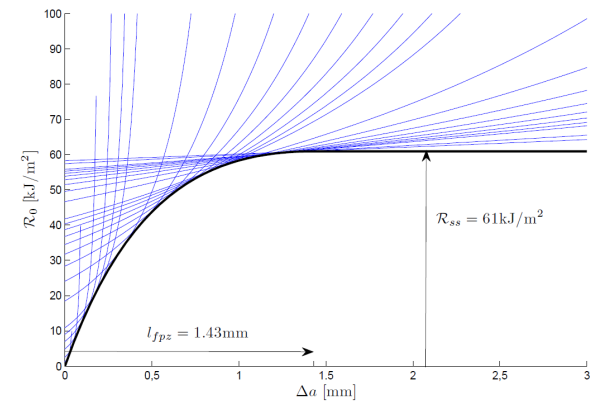


Laminate fracture toughness

$$\mathcal{G}_{Ic}^0$$



(Catalanotti, Xavier, Camanho, **Composites – A**, 56, 2014).

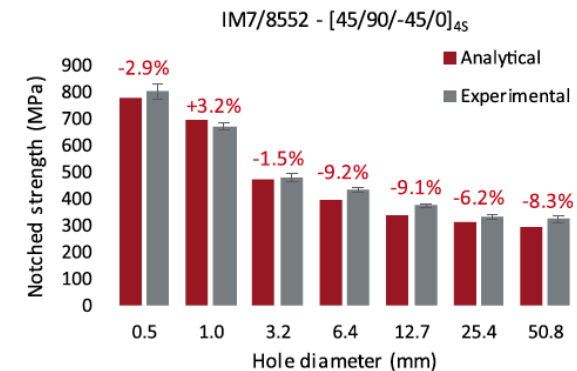
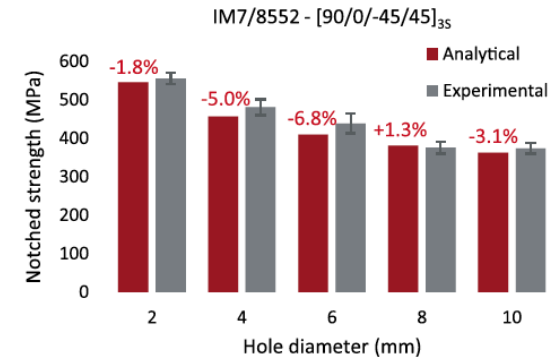
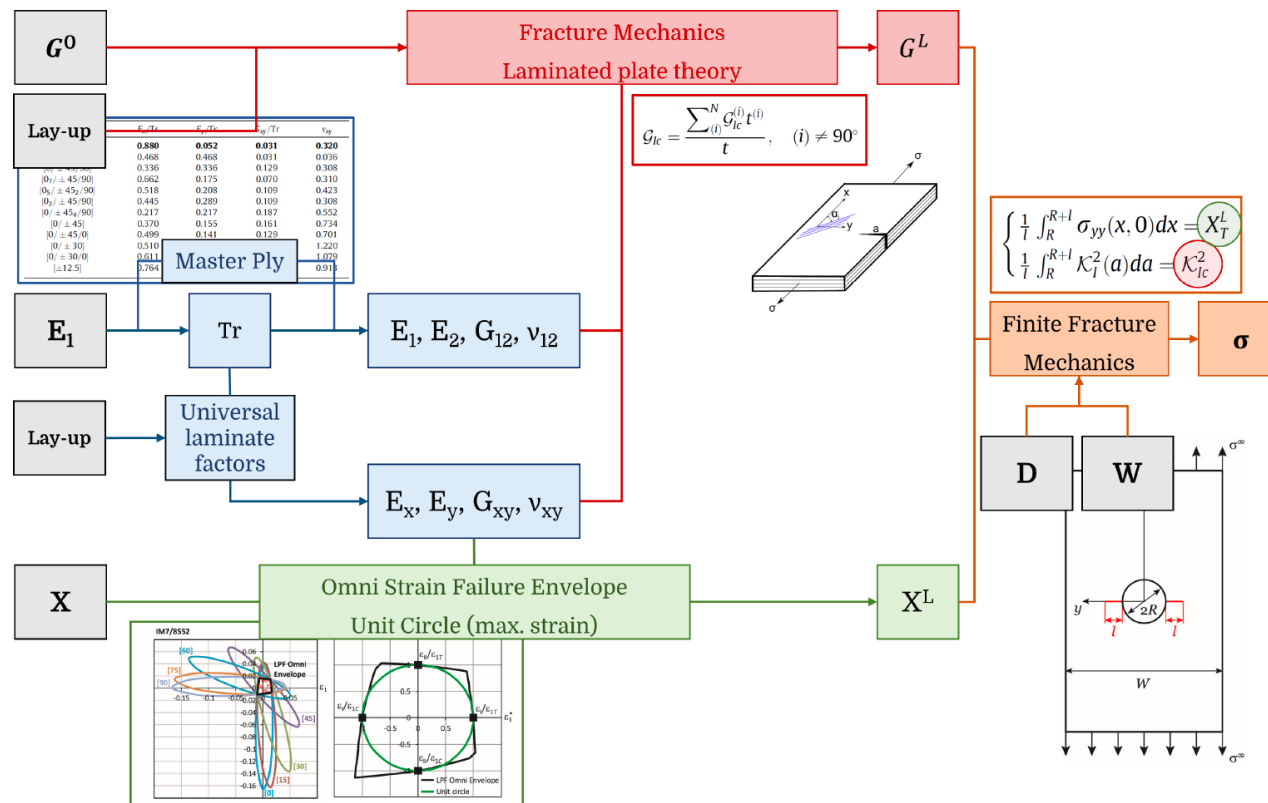


$$\Omega_0^{(i)} = \frac{\bar{\sigma}^{(i)}}{\bar{\sigma}^0} \rightarrow \begin{aligned} \bar{\sigma}^{(i)} &= \frac{\mathcal{K}_{Ic}^{(i)}}{\chi^{(i)} Y \sqrt{\pi a}} \\ \bar{\sigma}^0 &= \frac{\mathcal{K}_{Ic}^0}{\chi^0 Y \sqrt{\pi a}} \end{aligned}$$

$$\mathcal{K}_{Ic}^{(i)} = \frac{\chi^{(i)} \Omega_0^{(i)}}{\chi^0} \mathcal{K}_{Ic}^0 \rightarrow \mathcal{G}_{Ic}^{(i)} = \frac{[\mathcal{K}_{Ic}^{(i)}]^2}{E_{eq}^{(i)}} \quad \mathcal{G}_{Ic}^L = \frac{\sum_{(i)}^N \mathcal{G}_{Ic}^{(i)} t^{(i)}}{t^L}, \quad (i) \neq 90^\circ$$

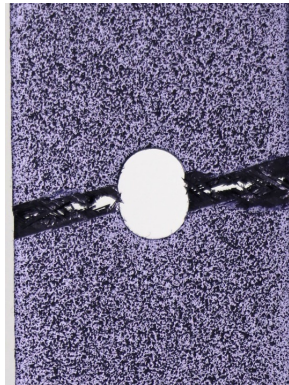
(Camanho, Catalanotti, **Engineering Fracture Mechanics**, 78, 2011).

Analytical framework to predict the notched strength of composite laminates

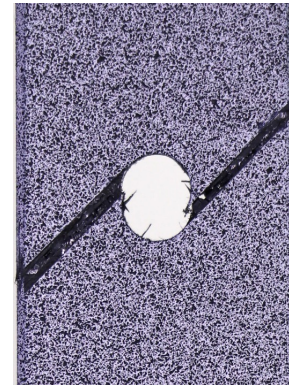


(Furtado, Arteiro, Camanho et al., **Composites Part A**, 2017).

15° off-axis



45° off-axis



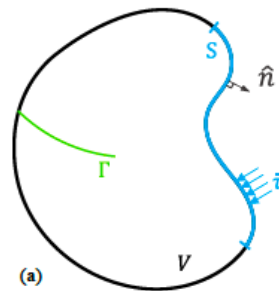
60° off-axis



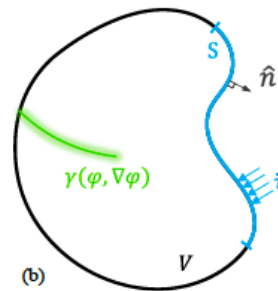
T700/M21 75gsm
[90/±45/90/±45/90/0]_{4s}

Phase-field methods for fracture: variational form of the Griffith thermodynamic balance

Sharp crack



Approximated diffuse crack band –
phase field



$$\Pi(\mathbf{u}) = \int_{\Omega} \psi_0(\mathbf{u}) d\Omega + \int_{\Gamma} G_c dS + W_{ext}(\mathbf{u}) \quad \int_{\Gamma} G_c dS \approx \int_{\Omega} G_c \gamma(\phi; \nabla \phi) d\Omega$$

$$\Pi(\mathbf{u}) \approx \Pi(\mathbf{u}, \phi) = \int_{\Omega} \psi(\mathbf{u}, \phi) d\Omega + \int_{\Omega} G_c \gamma(\phi; \nabla \phi) d\Omega + W_{ext}(\mathbf{u})$$

Analytical framework to predict the notched strength of composite laminates

Modeling a thin-ply laminate at the macroscale, in an **equivalent single layer form**, requires proper consideration of:

- Elastic Anisotropy
- **Fracture energy anisotropy**

*structural tensor
that defines
preferred fracture
directions*

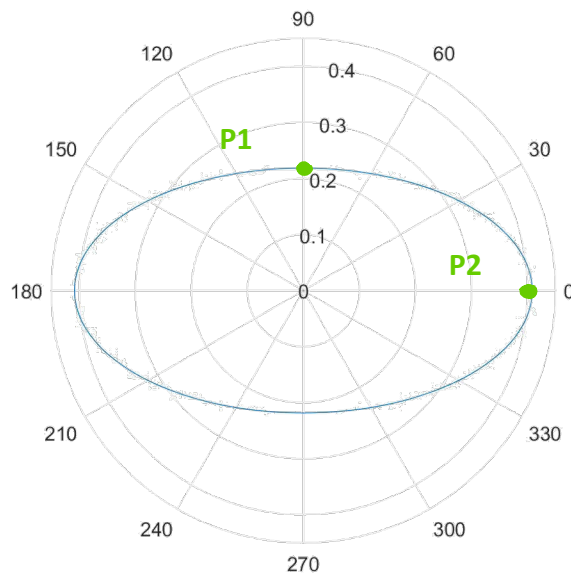
The crack surface density function:

$$G_c(\theta) = g_c \sqrt{1 + a_1 \sin^2(\theta) + a_2 \cos^2(\theta)}$$

$$\gamma(\varphi, \nabla\varphi) = \frac{1}{2l} \left(\varphi^2 + \frac{l}{2} \nabla\varphi \cdot \mathbf{A} \cdot \nabla\varphi \right)$$

$$\mathbf{A} = 1 + a_1 \mathbf{a}_1 \otimes \mathbf{a}_1 + a_2 \mathbf{a}_2 \otimes \mathbf{a}_2$$

scaling constants

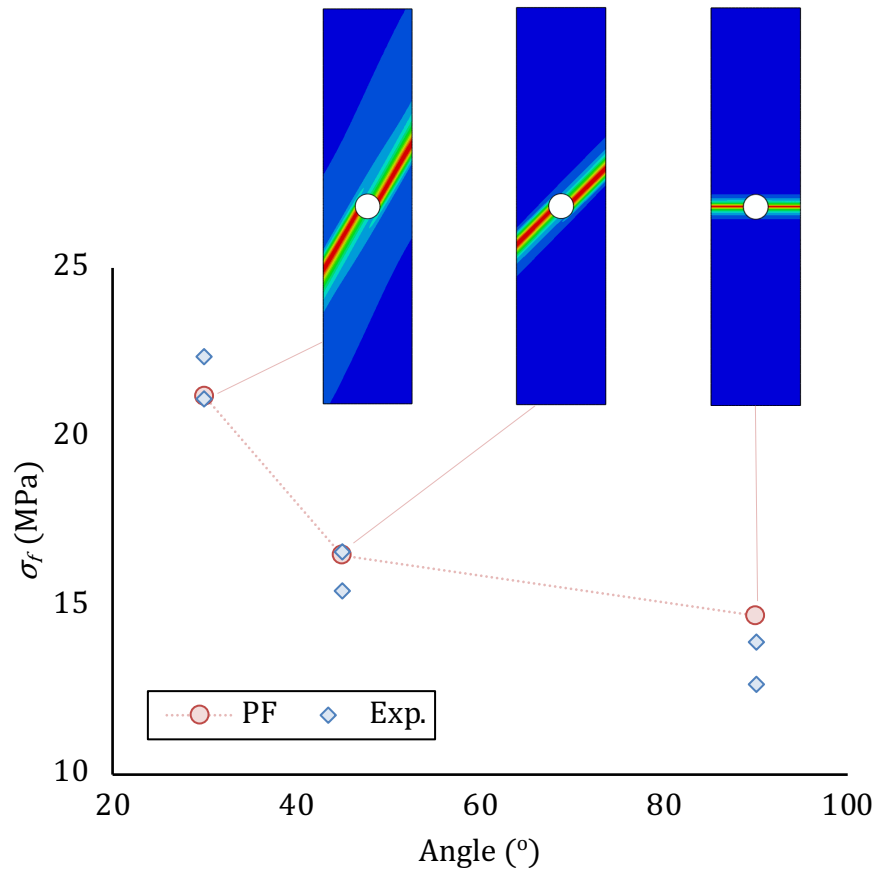


Known Points **P1, P2**

$$a_1 = \left(\frac{G_c(90^\circ)}{g_c} \right)^2 - 1 \quad a_2 = \left(\frac{G_c(0^\circ)}{g_c} \right)^2 - 1$$

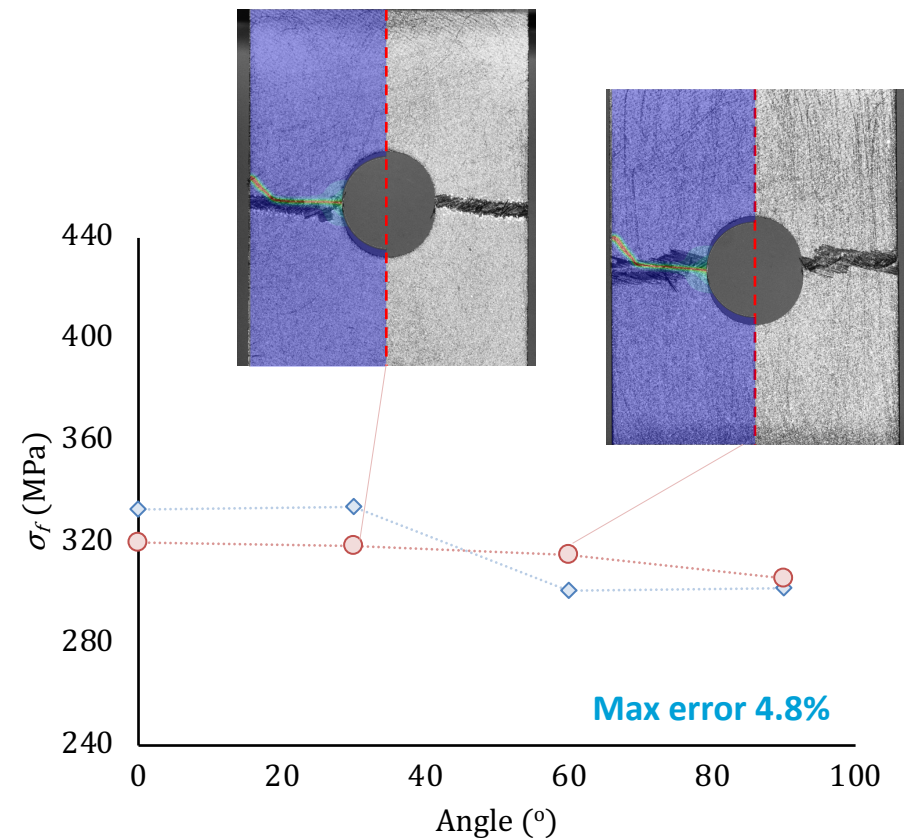
The scaling constants typically used as numerical inputs are **a material input** and represent the full fracture toughness of the laminate

UD off-axis response is seamlessly captured:



Off-axis predictions:

$[45/-45/0/45/-45/90/0/45/-45/90/0]_s$



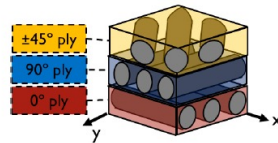
Design of experiments and computational analysis

Laminate definition

Considering each ply orientation of a given stacking sequence as an input parameter yields a highly dimensional space that is unsuitable for machine learning.

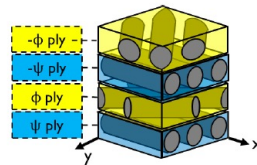
Two classes of laminates considered: **Legacy Quads (LQ)** and **Double-Double (DD)**.

Legacy Quads

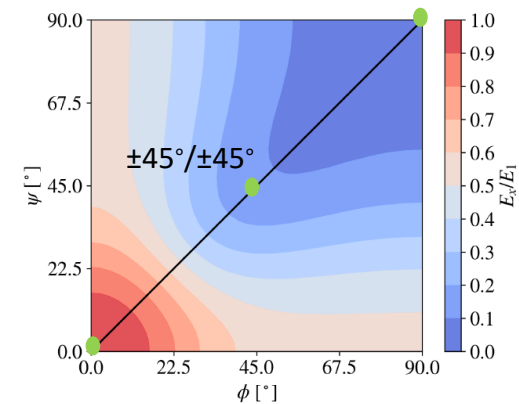
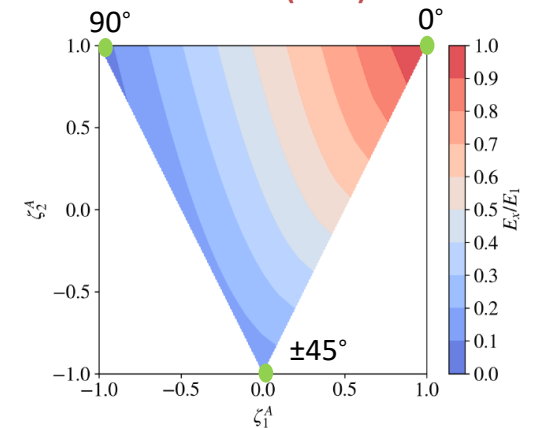


Two lamination parameters: $\zeta_{\{1,2,3,4\}}^A = \frac{1}{h} \sum_{i=1}^N \begin{Bmatrix} \cos(2\theta_i) \\ \cos(4\theta_i) \\ \sin(2\theta_i) \\ \sin(4\theta_i) \end{Bmatrix} (z_i - z_{i-1})$

Double-Double



Two fibre orientation angles: $[\pm\phi / \pm\psi]_n$



Definition of dimensionless parameters

$$\sigma = f_1(E_1, X_T, \mathcal{G}_0, D, W/D, \text{lay-up}) \quad \text{lay-up} = f_2(\alpha, \beta)$$

$$\left\{ \begin{array}{l} \text{Legacy Quads} \\ \text{Double-Double} \end{array} \right\} \left\{ \begin{array}{l} \alpha = \zeta_1^A \\ \beta = \zeta_2^A \\ \alpha = \phi \\ \beta = \psi \end{array} \right.$$

Reduction of input parameters - Buckingham's Π theorem:

$$\frac{\sigma}{X_T} = f\left(\frac{\mathcal{G}_0 E_1}{D X_T^2}, W/D, \alpha, \beta\right)$$

Design of experiments

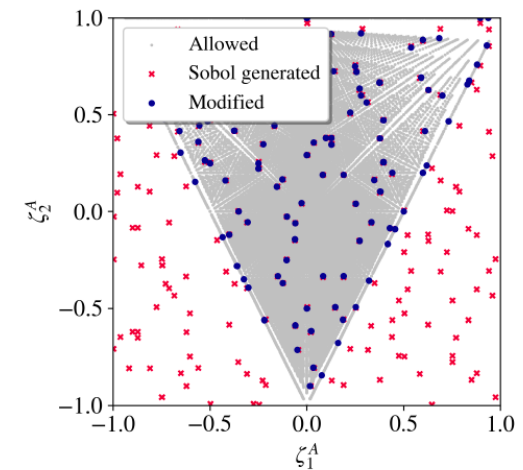
Sobol sequence using SALib Python library; material, geometric and laminate bounds:

	Legacy Quad	Double-Double
Material Property	$E_1 \in [150, 200] \text{ GPa}$	$E_1 \in [150, 200] \text{ GPa}$
	$X_T \in [2000, 2500] \text{ MPa}$	$X_T \in [2000, 2500] \text{ MPa}$
	$\mathcal{G}_0 \in [150, 250] \text{ N/mm}$	$\mathcal{G}_0 \in [150, 250] \text{ N/mm}$
Geometric	$D \in [1, 12] \text{ mm}$	$D \in [1, 12] \text{ mm}$
	$W/D \in [3, 8]$	$W/D \in [3, 8]$
Layup	$\zeta_1^A \in [-1, 1]$	$\phi \in [0, 90]^\circ$
	$\zeta_2^A \in [-1, 1]$	$\psi \in [0, 90]^\circ$

Legacy Quads

Requires the solution of an inverse problem: from the lamination parameters to the lay-up.

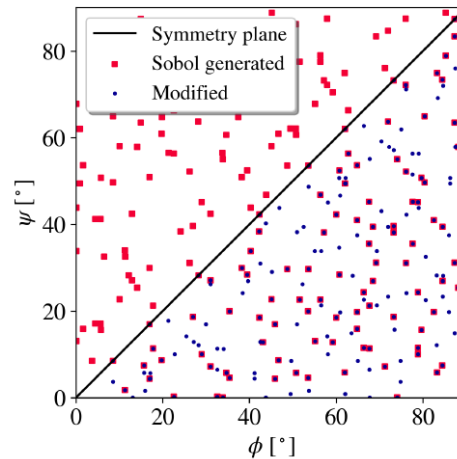
A database relating all possible ζ_1^A/ζ_2^A combinations to the corresponding lay-up was created with the following restrictions: up to 32 plies and balanced laminates.



Input data point: $x_i = [E_1, X_T, G_0, D, W/D, \zeta_1^A, \zeta_2^A]_i$

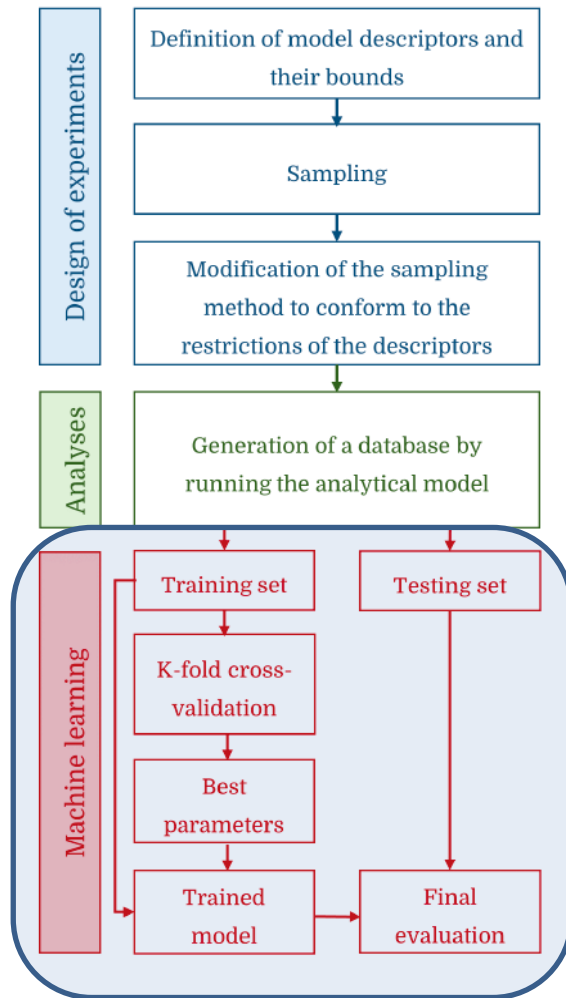
1. The laminate parameters (ζ_1^A and ζ_2^A) are converted into a lay-up by accessing the database.
2. Computation of the notched strength σ and normalized σ/X_T notched strength.
3. Conversion of the 7D space into a 4D space: $x_i^* = [\frac{G_0 E_1}{D X_T^2}, W/D, \zeta_1^A, \zeta_2^A]_i$

Double-Double



Input data point: $x_i = [E_1, X_T, \mathcal{G}_0, D, W/D, \phi, \psi]_i$

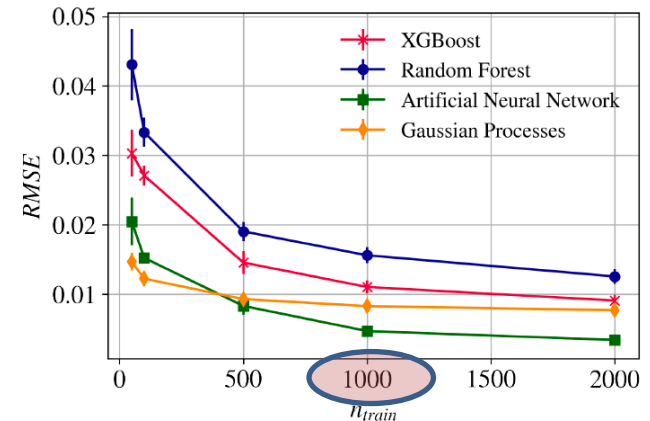
1. The laminate parameters (ϕ and ψ) are converted into a lay-up $[\pm\phi/\pm\psi]$.
2. Computation of the notched strength σ and normalized σ/X_T notched strength.
3. Conversion of the 7D space into a 4D space: $x_i^* = [\frac{\mathcal{G}_0 E_1}{D X_T^2}, W/D, \phi, \psi]_i$



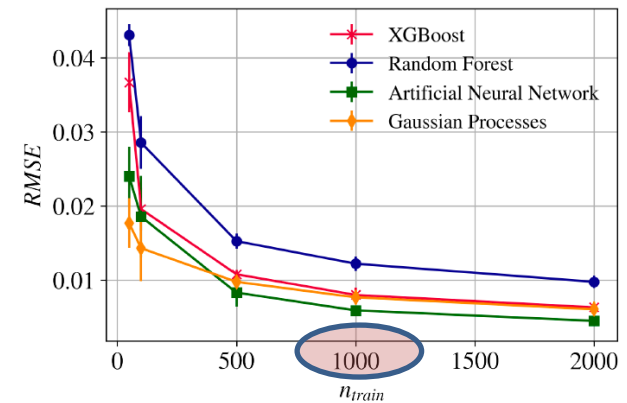
Algorithms used:

- Gaussian Processes.
- Artificial Neural Networks
- Random Forests.
- XGBoost.

Legacy Quads



Double-Double

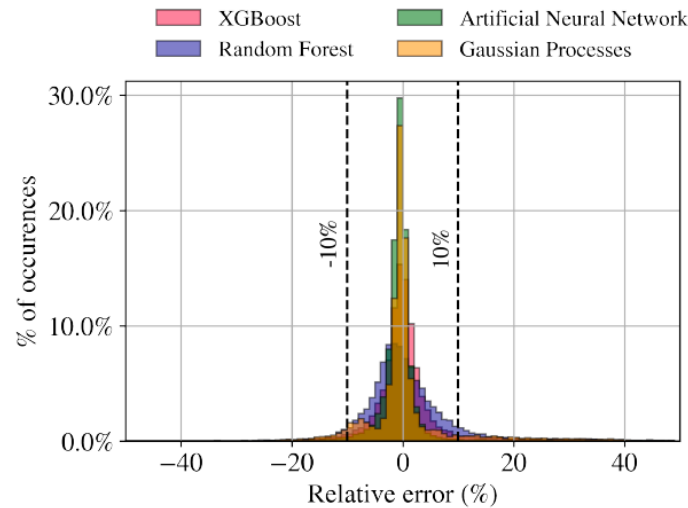


Generation of B-basis allowables using machine learning

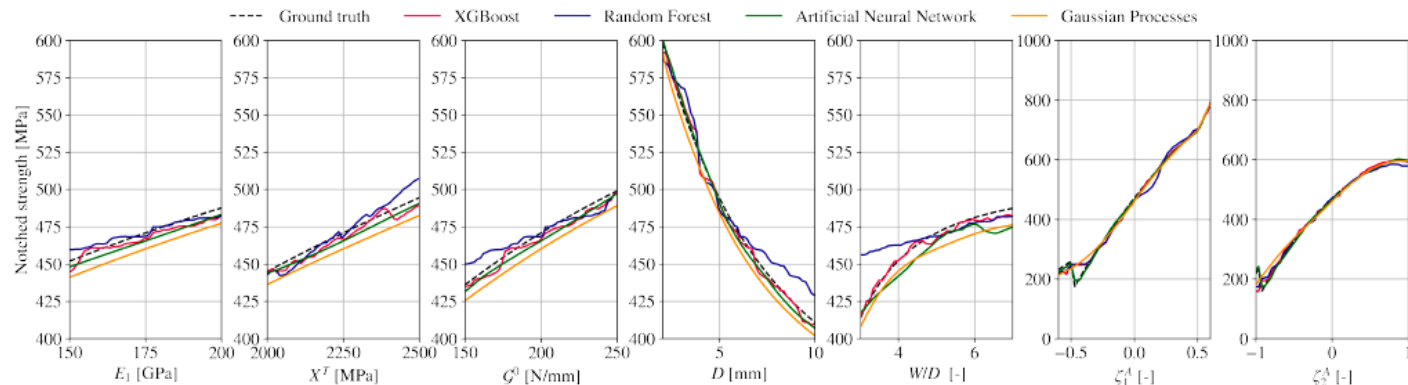
Representation of the design space – 1,000 training points and 9,000 testing points

Legacy Quads

Relative error



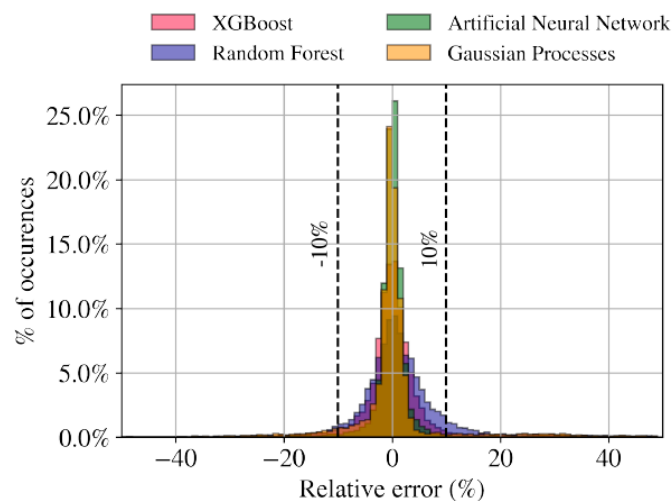
Sensitivity analysis



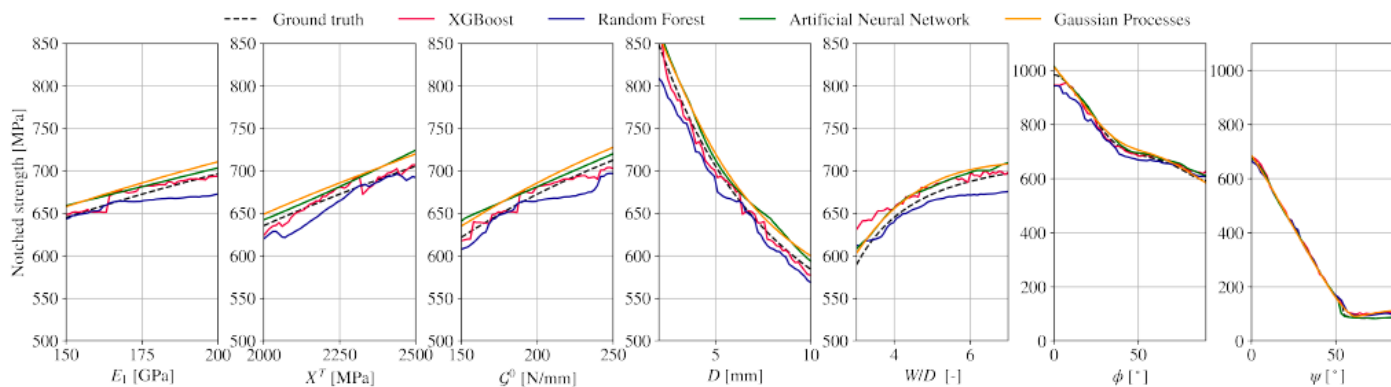
Generation of B-basis allowables using machine learning

Double-Double

Relative error



Sensitivity analysis



Generation of B-basis allowables using machine learning

B-basis – 95% lower confidence bound on the tenth percentile of a specified population; it accounts for geometric and material variabilities.

Monte Carlo-based approach used:

1. 10,000 material (E_1 , X^L , G_0) and geometric (D and W) parameters are generated following a given statistical distribution.
2. The distribution of the notched strength is calculated using the analytical model and the trained machine learning algorithms.
3. The 10th percentile of the distribution on the notched strength is obtained and taken as the B-basis value.

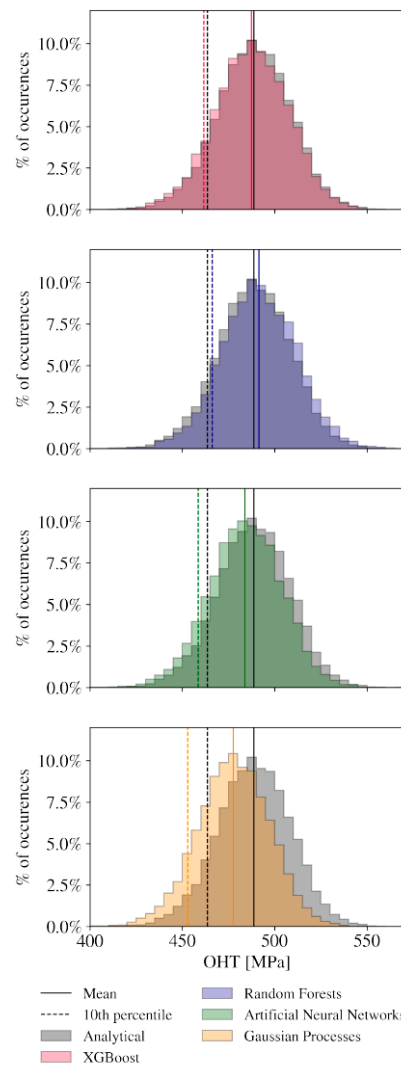
IM7/8552, $3 < W/D < 8$, $D=2, 4, 6, 8$ and 10mm

Legacy Quad: (90/0/-45/45)_{3s}

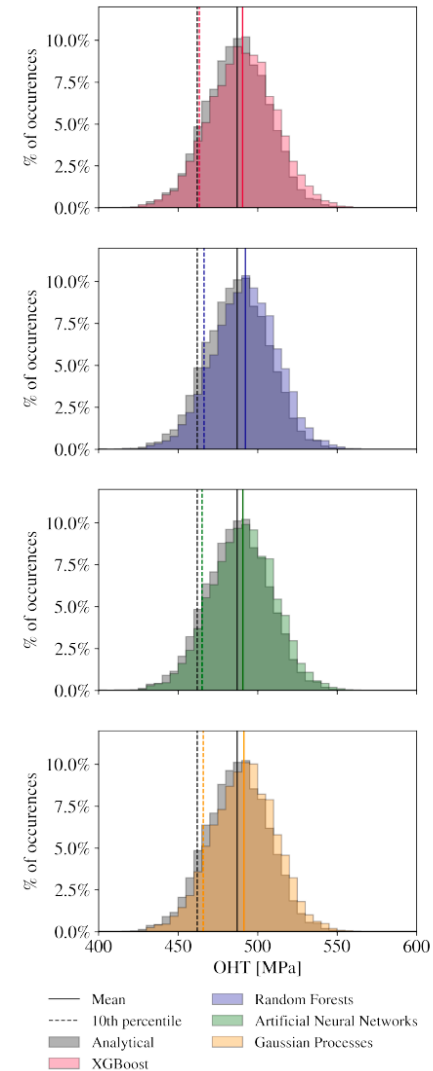
Double-Double: (45/-45/20/-20)

Distribution of the notched strength, B-basis and mean value of the notched strength. D=6mm, W=36mm

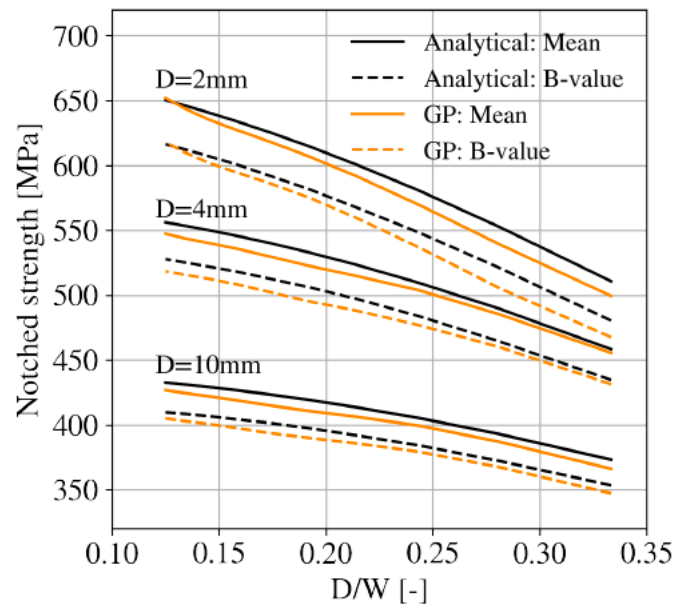
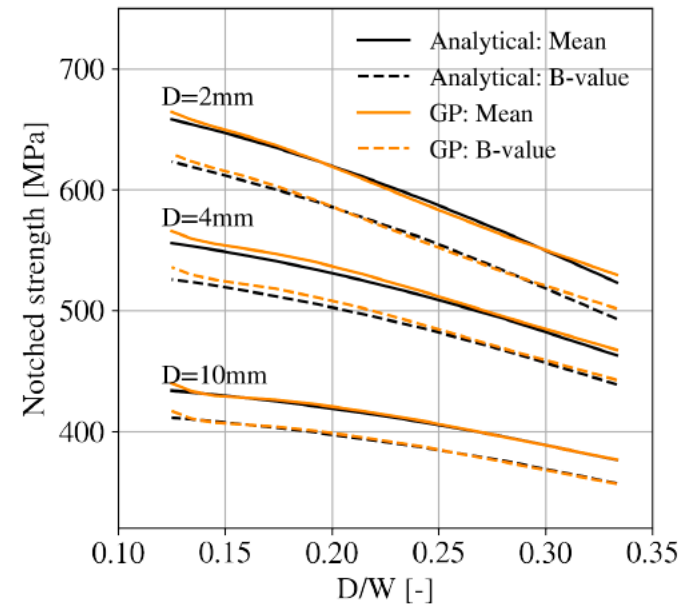
Legacy Quad



Double-Double



Design charts

Legacy QuadDouble-Double

Conclusions

- ✓ Using analysis models and restrictions in the definition of lay-ups it is possible to define machine learning models to predict the notched strength of composite laminates.
- ✓ Gaussian Processes achieved the best performance for a small number of data points.
- ✓ Artificial Neural Networks outperformed all other algorithms for larger data sets.
- ✓ All machine-learning models provided good estimations of B-basis design allowables.
- ✓ Gaussian processes is the preferred machine learning model taking into account:
 - ✓ Continuous and accurate representation of design space.
 - ✓ Low errors of the predictions.
 - ✓ Fast learning process.
 - ✓ Low number of hyperparameters to optimize.
 - ✓ Better performance for small training sets.

More information: Carolina Furtado et al., *A methodology to generate design allowables of composite laminates using machine learning*, **International Journal of Solids and Structures**.

Acknowledgements

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Funded by the European Commission under the Marie Skłodowska-Curie Actions
Grant Agreement n° 861061

