Proper Generalized Decomposition solutions of composite laminates parameterized with fibre orientations for fast computations

PhD thesis defense

Karim M. El-Ghamrawy

Advisors: Prof. Ferdinando Auricchio & Prof. Pedro Díez
Co-Advisor & Programme coordinator: Dr. Sergio Zlotnik

Dipartimento di Ingegneria Civile ed Architettura (DiCAr), Università di Pavia

Department d'Enginyeria Civil i Ambiental, Universitat Politècnica de Catalunya

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Background and Motivation

Existence through time:

- Composite materials have been used since Mesopotemia and the Pharaonic civilisations
- Reinforced construction components for enhanced mechanical properties $\Rightarrow$ brick and straw, reinforced concrete, etc...

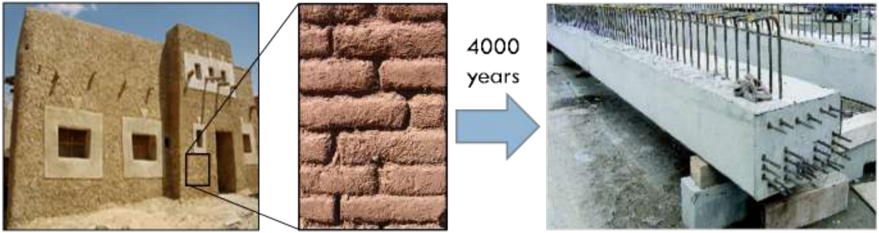
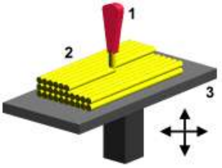


Figure: Typical ancient house in south of Egypt and a modern reinforced beam

Background and Motivation

Industrial needs:

- Enhanced mechanical properties ⇒ stiffness, load-carrying capacity, increased strength to weight ratio, etc...
- Numerical analyses for complex shapes and designs
- Ability to manufacture optimized complex designs
- Additive manufacturing deposits thermoplastic molten filament layer by layer.
- **3D printing steps:**
  CAD based 3D model ⇒ STL file ⇒ sliced layers ⇒ 3D printing ⇒ part finishing.



What are the different types of structural optimization?

Structural optimization

- **Topology optimization:** how to remove material
- **Shape optimization:** how to change the shape of the boundaries
- **Size optimization:** how to change the thicknesses of components
- **Material optimization:** how to orient material

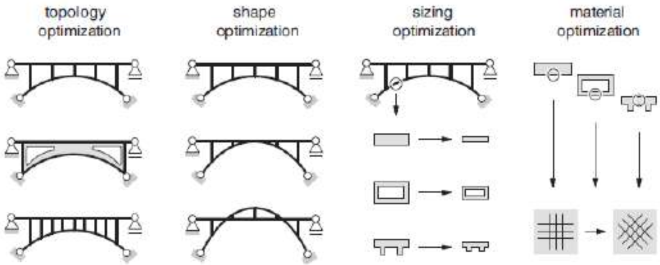
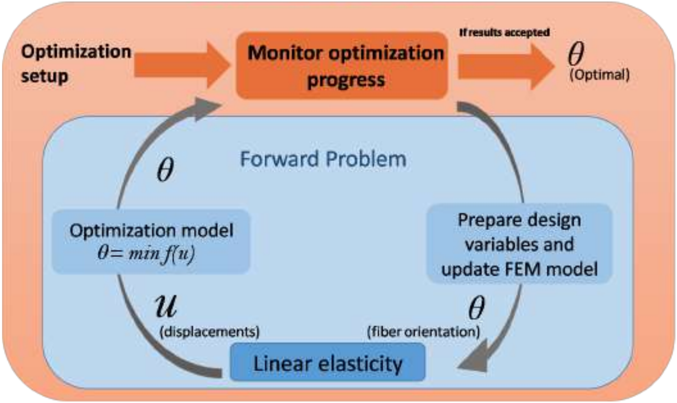


Figure: Four levels of structural optimization. Figure adapted from Ramm et al. (1998)

Optimization Problem



Optimization problem
Requires solving a large number of 3D forward models corresponding to different values of the parameters (orientation of material)

Proper Generalized Decomposition (PGD) framework

Steps of PGD

Obtain pre-computed solutions in the form of a *computational vademecum* by

1. Considering the parameters as extra-coordinates in the problem
2. Making use of a separated representation of the solution to overcome the *curse of dimensionality*

Offline phase

- Important computational resources only once
- Results in a generalized solution

Online phase

- Very fast browsing of solutions
- Availability of the solution for any value in the parametric space

Objectives

Present a new computational tool for the 3D numerical analysis of fibrous composite laminates with the goal of optimizing the orientation of fibers for 3D printing applications

Main goals

1. Apply a set of newly in-house developed tools known as *encapsulated* PGD [Díez et al. (2018, 2019)]
2. Implement a post-process algortihm to solve the optimization problem
3. Apply the methodology to a couple of numerical examples to assess the capabilities of the model
4. Enhance the model by implementing and applying a data analysis algorithm

Governing Equations: Linear Elasticity

Strong form (Voigt's notation)

- Given a 3D domain $\Omega \in \mathbb{R}^3$, find the displacement $\boldsymbol{u}(\boldsymbol{x})$ satisfying the following:

$$
\begin{aligned}
\nabla_{\mathrm{S}}^{\mathsf{T}} \boldsymbol{\sigma} + \boldsymbol{b} &= 0 && \text{in } \Omega && \text{(equilibrium)} \\
\boldsymbol{u} &= \boldsymbol{u}_D && \text{on } \Gamma_D && \text{(Dirichlet BC)} \\
\boldsymbol{n}^{\mathsf{T}} \boldsymbol{\sigma} &= \boldsymbol{t}_N && \text{on } \Gamma_N && \text{(Neumann BC)} \\
\boldsymbol{\sigma} &= \boldsymbol{\mathcal{C}} \boldsymbol{\varepsilon} && && \text{(Constitutive law)} \\
\boldsymbol{\varepsilon} &= \nabla_{\mathrm{S}} \boldsymbol{u} && &&
\end{aligned}
$$

Weak form

- The weak form is as follows, find $\boldsymbol{u} \in U$ such that

$$
\int_{\Omega} (\boldsymbol{\nabla}_{\mathrm{S}} \boldsymbol{w})^{\mathsf{T}} \boldsymbol{\mathcal{C}} \boldsymbol{\nabla}_{\mathrm{S}} \boldsymbol{u} \, d\Omega = \int_{\Gamma_N} \boldsymbol{w}^{\mathsf{T}} \boldsymbol{t} d\Gamma + \int_{\Omega} \boldsymbol{w}^{\mathsf{T}} \boldsymbol{b} d\Omega \qquad \forall \boldsymbol{w} \in U_o
$$

Governing Equations: Linear Elasticity

Finite dimensional

- The integration over the whole domain could be a sum of integrals over the elements Ω_e.

$$\sum_{e=1}^{\mathtt{n_{el}}} \left\{ \int_{\Omega^e} (\boldsymbol{\nabla}_{\mathrm{S}} \boldsymbol{w}_{\boldsymbol{h}}^{\boldsymbol{e}})^{\mathsf{T}} \boldsymbol{\mathcal{C}} \boldsymbol{\nabla}_{\mathrm{S}} \boldsymbol{u}_{\boldsymbol{h}}^{\boldsymbol{e}} \, d\Omega - \int_{\Gamma_N^e} \boldsymbol{w}_h^{e\mathsf{T}} \boldsymbol{t} \, d\Gamma - \int_{\Omega^e} \boldsymbol{w}_h^{e\mathsf{T}} \boldsymbol{b} \, d\Omega \right\} = 0$$

- After derivations, the element stiffness matrix and force vector read:

$$\boldsymbol{K}^e = \int_{\Omega^e} \boldsymbol{B}^{e\mathsf{T}} \boldsymbol{\mathcal{C}} \boldsymbol{B}^e \, d\Omega \qquad \boldsymbol{f}^e = \int_{\Omega^e} \boldsymbol{N}^{e\mathsf{T}} \boldsymbol{b} \, d\Omega + \int_{\Gamma_N \bigcap \bar{\Omega}^e} \boldsymbol{N}^{e\mathsf{T}} \boldsymbol{t} \, d\Gamma$$

- Applying assembly operators, the global stiffness matrix and force vector read:

$$\boldsymbol{K} := \sum_{e=1}^{\mathtt{n_{el}}} \boldsymbol{L}^{e\mathsf{T}} \boldsymbol{K}^e \boldsymbol{L}^e \text{ and } \boldsymbol{f} := \sum_{e=1}^{\mathtt{n_{el}}} \boldsymbol{L}^{e\mathsf{T}} \boldsymbol{f}^e \quad \text{yielding: } \boxed{\boldsymbol{K}\boldsymbol{d} = \boldsymbol{f}}$$

Material Parameterization

- The material properties are described by $\mathcal{C}_0$ and its orientation is described by the angle θ.
- The oriented material is described as follow:

$$\boxed{\mathcal{C}(\theta) = \boldsymbol{T}^{-1}(\theta)\mathcal{C}_0\boldsymbol{T}^{-\mathsf{T}}(\theta)}$$

- Each parameter θ_i is assigned to a sub-domain Ω_i, $\Omega_i \subset \Omega$, and many $\Omega^e \subset \Omega_i$.
- The element stiffness:

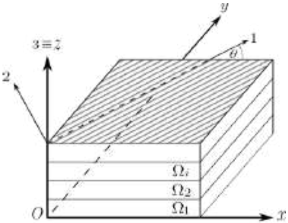
$$\boxed{\boldsymbol{K}^e(\theta_i) = \int_{\Omega^e} \boldsymbol{B}^{e\mathsf{T}}\mathcal{C}(\theta_i)\boldsymbol{B}^e d\Omega}$$

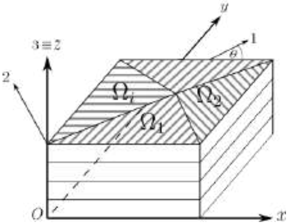
.

- The parametric linear system of equations:

$$\boxed{\boldsymbol{K}(\boldsymbol{\theta})\boldsymbol{d}(\boldsymbol{\theta}) = \boldsymbol{f}}$$

- The $\mathtt{n_p}$ parameters are gathered in vector $\boldsymbol{\theta} = [\theta_1, \theta_2, ..., \theta_{\mathtt{n_p}}]^{\mathsf{T}}$.





Tsai-Wu Failure Criterion

- The Tsai-Wu failure index:

$$\boxed{\mathcal{I}_\mathrm{f}\left(\boldsymbol{\sigma}\right) = \boldsymbol{\sigma}^\mathsf{T}\boldsymbol{\mathcal{F}}\boldsymbol{\sigma} + \boldsymbol{\sigma}^\mathsf{T}\boldsymbol{F}}$$

- $\mathcal{I}_\mathrm{f}(\boldsymbol{\sigma}) \leq 1 \Rightarrow$ Material is safe.
- Alternative expression of the failure criterion:

$$\boxed{\mathcal{I}_\mathrm{f}\left(\bar{\boldsymbol{\sigma}}\right) = \mathcal{I}_\mathrm{f}\left(\lambda\boldsymbol{\sigma}\right) = \lambda^2\boldsymbol{\sigma}^\mathsf{T}\boldsymbol{\mathcal{F}}\boldsymbol{\sigma} + \lambda\boldsymbol{\sigma}^\mathsf{T}\boldsymbol{F}}$$

- The critical value of λ corresponds to the onset of failure $\mathcal{I}_\mathrm{f}\left(\bar{\boldsymbol{\sigma}}\right) = 1$.
- Assuming that $\boldsymbol{\mathcal{F}}$ is symmetric positive definite, $\boldsymbol{\sigma}^\mathsf{T}\boldsymbol{\mathcal{F}}\boldsymbol{\sigma} \geq 0$, there is a unique positive root of the equation $\mathcal{I}_\mathrm{f}\left(\bar{\boldsymbol{\sigma}}\right) = 1$.

$$\boxed{\lambda_s = \frac{1}{2\boldsymbol{\sigma}^\mathsf{T}\boldsymbol{\mathcal{F}}\boldsymbol{\sigma}}\left(\sqrt{(\boldsymbol{\sigma}^\mathsf{T}\boldsymbol{F})^2 + 4\,\boldsymbol{\sigma}^\mathsf{T}\boldsymbol{\mathcal{F}}\boldsymbol{\sigma}} - \boldsymbol{\sigma}^\mathsf{T}\boldsymbol{F}\right)}$$

- The smallest positive root, denoted as λ_s, is the safety factor

Tsai-Wu Failure Criterion

- **Our goal** is to obtain expressions $\mathcal{I}_{\mathfrak{f}}(\boldsymbol{\theta})$ and $\lambda_s(\boldsymbol{\theta})$ that could be evaluated very fast
- Expressions of $\boldsymbol{\mathcal{F}}$ and $\boldsymbol{F}$ with respect to the global axes are obtained using the transformation matrices:

$$\boxed{\begin{aligned} \boldsymbol{\mathcal{F}}(\theta_i) &= \boldsymbol{T}^{\mathsf{T}}(\theta_i)\boldsymbol{\mathcal{F}}_0\boldsymbol{T}(\theta_i) \\ \boldsymbol{F}(\theta_i) &= \boldsymbol{T}^{\mathsf{T}}(\theta_i)\boldsymbol{F}_0 \end{aligned}}$$

- Marking explicitly the parametric dependence, for $\boldsymbol{x} \in \Omega_i$, the failure index $\mathcal{I}_{\mathfrak{f}}$ and the safety factor λ_s are rewritten as:

$$\boxed{\begin{aligned} \mathcal{I}_{\mathfrak{f}}\big(\boldsymbol{\sigma}(\boldsymbol{x},\boldsymbol{\theta})\big) &= \boldsymbol{\sigma}(\boldsymbol{x},\boldsymbol{\theta})^{\mathsf{T}}\boldsymbol{\mathcal{F}}(\theta_i)\boldsymbol{\sigma}(\boldsymbol{x},\boldsymbol{\theta}) + \boldsymbol{\sigma}(\boldsymbol{x},\boldsymbol{\theta})^{\mathsf{T}}\boldsymbol{F}(\theta_i) \\ \lambda_s\big(\boldsymbol{\sigma}(\boldsymbol{x},\boldsymbol{\theta})\big) &= \frac{\sqrt{(\boldsymbol{\sigma}(\boldsymbol{x},\boldsymbol{\theta})^{\mathsf{T}}\boldsymbol{F}(\theta_i))^2 + 4\,\boldsymbol{\sigma}(\boldsymbol{x},\boldsymbol{\theta})^{\mathsf{T}}\boldsymbol{\mathcal{F}}(\theta_i)\boldsymbol{\sigma}(\boldsymbol{x},\boldsymbol{\theta})} - \boldsymbol{\sigma}(\boldsymbol{x},\boldsymbol{\theta})^{\mathsf{T}}\boldsymbol{F}(\theta_i)}{2\boldsymbol{\sigma}(\boldsymbol{x},\boldsymbol{\theta})^{\mathsf{T}}\boldsymbol{\mathcal{F}}(\theta_i)\boldsymbol{\sigma}(\boldsymbol{x},\boldsymbol{\theta})} \end{aligned}}$$

- The failure index $\mathcal{I}_{\mathfrak{f}}$ and the safety factor λ_s are our objective functions for the optimization problem.

Optimization problem

- The first choice is to find $\boldsymbol{\theta}$ that minimizes the maximum value of $\mathcal{I}_{\mathtt{f}}\big(\boldsymbol{\sigma}(\boldsymbol{x},\boldsymbol{\theta})\big)$ evaluated at all points $\boldsymbol{x}$ in Ω.

$$\boxed{\boldsymbol{\theta}_{\mathtt{f}}^{\mathtt{Opt}} = \arg\min_{\boldsymbol{\theta}} \;\max_{\boldsymbol{x}} \mathcal{I}_{\mathtt{f}}\big(\boldsymbol{\sigma}(\boldsymbol{x},\boldsymbol{\theta})\big)}$$

- The second choice is to find $\boldsymbol{\theta}$ that maximizes the minimum value of $\lambda_s(\boldsymbol{x},\boldsymbol{\theta})$ evaluated at all points $\boldsymbol{x}$ in Ω.

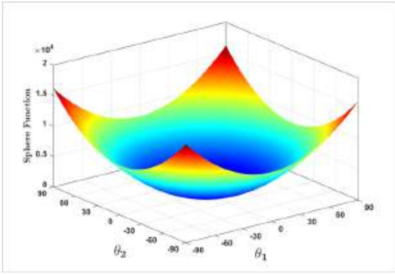
$$\boxed{\boldsymbol{\theta}_{\mathtt{s}}^{\mathtt{Opt}} = \arg\max_{\boldsymbol{\theta}} \;\min_{\boldsymbol{x}} \lambda_s(\boldsymbol{x},\boldsymbol{\theta})}$$

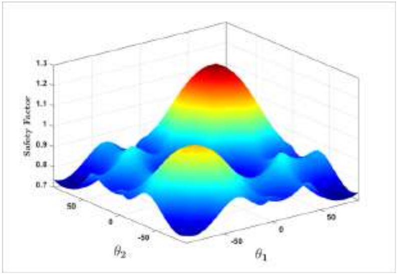
- The objective functions are not necessarily smooth and they are non convex-concave which might lead to being stuck in local minima/maxima

Optimization Algorithms

Types of algorithms

- The optimization algorithms are classified into deterministic and stochastic algorithms.
- Gradient-based methods (Newton method) converge fast but are easily stuck in local minima/maxima.
- Evolutionary methods (Genetic Algorithm) converge slow but yield a global optimal in complex problems.





PGD at a glance

1. The parameters are taken as extra coordinates stating the problem in a multidimensional framework; finding an approximation to $\boldsymbol{d}(\boldsymbol{\theta})$ in $\mathbb{R}^{\mathtt{n_d}} \times \boldsymbol{I_\theta}$.

2. The solution is sought in a separable format reducing the order of the problem

$$\mathtt{n_{full}} = \mathtt{n_d} \prod_{i=1}^{\mathtt{n_p}} n_D, i \quad \rightarrow \quad \mathtt{n_{PGD}} = \mathtt{n_d} + \sum_{i=1}^{\mathtt{n_p}} n_{D,i} \qquad \text{with } \mathtt{n_{PGD}} << \mathtt{n_{full}}$$

.

3. The PGD solver is based on a greedy strategy (computing one rank-one term at a time) and an alternating directions method to solve the nonlinear rank-one problems.

Encapsulated PGD

Separated global stiffness matrix is needed for the PGD solver!

- **Input:** the global separated stiffness matrix $\boldsymbol{K}(\boldsymbol{\theta})$.

$$\boldsymbol{K}(\boldsymbol{\theta}) \approx \boldsymbol{K}^{\mathrm{sep}}(\boldsymbol{\theta}) = \sum_{k=1}^{\mathtt{n_k}} \boldsymbol{K}^k \prod_{j=1}^{\mathtt{n_p}} \varphi_j^k(\theta_j)$$

- **Output:** the unknown vector of displacements $\boldsymbol{d}(\boldsymbol{\theta})$.

$$\boldsymbol{d}(\boldsymbol{\theta}) \approx \boldsymbol{d}_{\mathtt{PGD}}^{n}(\boldsymbol{\theta}) = \sum_{m=1}^{n} \beta^m \boldsymbol{d}^m \prod_{j=1}^{\mathtt{n_p}} G_j^m(\theta_j)$$

- *Encapsulated PGD* provides tools that directly produce computational vademecums for the high-dimensional tensor data.
- The toolbox[1] permits the performance of operations such as: solving linear system of equations, compression, addition, multiplication, division, etc...

[1] Publicly available at `https://git.lacan.upc.edu/zlotnik/algebraicPGDtools`

PGD compression

- The goal is to remove excess terms associated with redundant information from the PGD solution and increase othogonality between terms
- Least-squares projection of the PGD solution into the same approximation space:
  find a PGD-type approximation $\boldsymbol{d}_{\mathtt{com}}^{\mathtt{n_c}}$ minimizing

$$\boxed{\|\boldsymbol{d}_{\mathtt{com}}^{\mathtt{n_c}} - \boldsymbol{d}_{\mathtt{PGD}}^{n}\|_{L^2(I_{\boldsymbol{\theta}})} = \int_{I_1} \cdots \int_{I_{\mathtt{n_p}}} \left(\boldsymbol{d}_{\mathtt{com}}^{\mathtt{n_c}} - \boldsymbol{d}_{\mathtt{PGD}}^{n}\right)^2 d\theta_{\mathtt{n_p}} \ldots d\theta_1}$$

- The number of terms $\mathtt{n_c}$ in the compressed solution $\boldsymbol{d}_{\mathtt{com}}^{\mathtt{n_c}}$ is significantly lower than the original one ($\mathtt{n_c} \ll n$)

Separation of input for PGD solver

- The separated representation of $\boldsymbol{\mathcal{C}}(\boldsymbol{\theta})$:

$$\boldsymbol{\mathcal{C}}(\theta_i) = \sum_{\ell=1}^{\mathtt{n_t}} \boldsymbol{\mathcal{C}}^{\ell} \prod_{j=1}^{\mathtt{n_p}} \phi_j^{\ell,i}(\theta_j) \qquad \phi_j^{\ell,i}(\theta_j) \equiv 1 \text{ for } j \neq i$$

- The element stiffness, $\Omega_e \in \Omega_i$, yields:

$$\boldsymbol{K}^e(\theta_i) = \sum_{\ell=1}^{\mathtt{n_t}} \Big[\int_{\Omega_e} \boldsymbol{B}^{e\mathsf{T}} \boldsymbol{\mathcal{C}}^{\ell} \boldsymbol{B}^e d\Omega \Big] \prod_{j=1}^{\mathtt{n_p}} \phi_j^{\ell,i}(\theta_j)$$

- Assembling the global stiffness matrix yields:

$$\begin{aligned} \boldsymbol{K}(\theta_1, \theta_2, ..., \theta_{\mathtt{n_p}}) &= \sum_{e=1}^{\mathtt{n_{el}}} \boldsymbol{L}^{e\mathsf{T}} \boldsymbol{K}^e(\theta_i) \boldsymbol{L}^e \\ &= \sum_{e=1}^{\mathtt{n_{el}}} \sum_{\ell=1}^{\mathtt{n_t}} \Big[\int_{\Omega_e} \boldsymbol{L}^{e\mathsf{T}} \boldsymbol{B}^{e\mathsf{T}} \boldsymbol{\mathcal{C}}^{\ell} \boldsymbol{B}^e \boldsymbol{L}^e \, d\Omega \Big] \prod_{j=1}^{\mathtt{n_p}} \phi_j^{\ell,i}(\theta_j) \end{aligned}$$

Post-process and Sensitivities

- PGD gives the displacement $\boldsymbol{d}(\boldsymbol{\theta}) = \sum_{m=1}^{n} \beta^m \boldsymbol{d}^m \prod_{j=1}^{\mathtt{n_p}} G_j^m(\theta_j)$
- The parametric strain tensor is a linear output of the overall displacements $\boldsymbol{d}$
- The parametric stress tensor $\Rightarrow \boldsymbol{\sigma}_g(\boldsymbol{\theta}) = \boldsymbol{\mathcal{C}}(\theta_i)\boldsymbol{\varepsilon}_g(\boldsymbol{\theta})$ with $\boldsymbol{\varepsilon}_g^m = \boldsymbol{B}_g^e \boldsymbol{L}^e \boldsymbol{d}^m$

$$\boxed{\boldsymbol{\sigma}_g(\boldsymbol{\theta}) = \sum_{m=1}^{n} \sum_{\ell=1}^{\mathtt{n_t}} \beta^m \boldsymbol{C}^\ell \boldsymbol{\varepsilon}_g^m \prod_{j=1}^{\mathtt{n_p}} \phi_j^{\ell,i}(\theta_j) G_j^m(\theta_j)}$$

- Using the parametric stress tensor and the transformed strength tensors, the failure index could be reconstructed:

$$\boxed{\mathcal{I}_{\mathtt{L}}\big(\boldsymbol{\sigma}_g(\boldsymbol{\theta})\big) = \boldsymbol{\sigma}_g^{\mathsf{T}} \boldsymbol{F}(\theta_i) \text{ and } \mathcal{I}_{\mathtt{Q}}\big(\boldsymbol{\sigma}_g(\boldsymbol{\theta})\big) = \boldsymbol{\sigma}_g^{\mathsf{T}} \boldsymbol{\mathcal{F}}(\theta_i) \boldsymbol{\sigma}_g}$$

Failure Vademecums

- The expressions for the quadratic and linear terms:

$$\mathcal{I}_{\mathtt{Q}}\left(\boldsymbol{\sigma}_g(\boldsymbol{\theta})\right) = \sum_{b=1}^{\mathtt{n_Q}} \tilde{\gamma}^b \tilde{A}_g^b \prod_{j=1}^{\mathtt{n_p}} \tilde{H}_j^{b,i}(\theta_j) \text{ and } \mathcal{I}_{\mathtt{L}}\left(\boldsymbol{\sigma}_g(\boldsymbol{\theta})\right) = \sum_{v=1}^{\mathtt{n_L}} \hat{\gamma}^v \hat{A}_g^v \prod_{j=1}^{\mathtt{n_p}} \hat{H}_j^{v,i}(\theta_j)$$

- The final expression for the failure index $\mathcal{I}_{\mathtt{f}}$ is readily recovered by summing up $\mathcal{I}_{\mathtt{Q}}$ and $\mathcal{I}_{\mathtt{L}}$

$$\mathcal{I}_{\mathtt{f}}\left(\boldsymbol{\sigma}_g(\boldsymbol{\theta})\right) = \mathcal{I}_{\mathtt{Q}}\left(\boldsymbol{\sigma}_g(\boldsymbol{\theta})\right) + \mathcal{I}_{\mathtt{L}}\left(\boldsymbol{\sigma}_g(\boldsymbol{\theta})\right) = \sum_{f=1}^{\mathtt{n_Q}+\mathtt{n_L}} \gamma^f A_g^f \prod_{j=1}^{\mathtt{n_p}} H_j^{f,i}(\theta_j)$$

- The quantities γ^f, A_g^f and $H_j^{f,i}(\theta_j)$ depend on the index f

$$\gamma^f,\, A_g^f,\, H_g^f = \begin{cases} \tilde{\gamma}^f, \tilde{A}_g^f, \tilde{H}_g^f & \text{if} f \leq \mathtt{n_Q} \\ \hat{\gamma}^{f-\mathtt{n_Q}}, \hat{A}_g^{f-\mathtt{n_Q}}, \hat{H}_g^{f-\mathtt{n_Q}} & \text{if } f > \mathtt{n_Q} \end{cases}$$

Failure Index $\mathcal{I}_{\mathtt{f}}$ Sensitivities

- The gradient of the failure index $\nabla_\theta \mathcal{I}_{\mathtt{f}}(\boldsymbol{\theta})$:

$$\frac{\partial \mathcal{I}_{\mathtt{f}}(\boldsymbol{\theta})}{\partial \theta_k} = \sum_{f=1}^{\mathtt{n_Q}+\mathtt{n_L}} \gamma^f A_g^f \left[\frac{dH_k^{f,i}}{d\theta_k}(\theta_k) \right] \prod_{j \neq k}^{\mathtt{n_P}} H_j^{f,i}(\theta_j)$$

- For optimization methods requiring the Hessian matrix, for $k \neq \tilde{k}$

$$\frac{\partial^2 \mathcal{I}_{\mathtt{f}}(\boldsymbol{\theta})}{\partial \theta_k \partial \theta_{\tilde{k}}} = \sum_{f=1}^{\mathtt{n_Q}+\mathtt{n_L}} \gamma^f A_g^f \left[\frac{dH_k^{f,i}}{d\theta_k}(\theta_k) \frac{dH_{\tilde{k}}^{f,i}}{d\theta_{\tilde{k}}}(\theta_{\tilde{k}}) \right] \prod_{j \neq k, \tilde{k}}^{\mathtt{n_P}} H_j^{f,i}(\theta_j)$$

- And for the diagonal terms

$$\frac{\partial^2 \mathcal{I}_{\mathtt{f}}(\boldsymbol{\theta})}{\partial {\theta_k}^2} = \sum_{f=1}^{\mathtt{n_Q}+\mathtt{n_L}} \gamma^f A_g^f \left[\frac{d^2 H_k^{f,i}}{d{\theta_k}^2}(\theta_k) \right] \prod_{j \neq k}^{\mathtt{n_P}} H_j^{f,i}(\theta_j)$$

Safety Factor λ_s Sensitivities

- The gradient of the safety factor $\nabla_\theta \lambda_s(\boldsymbol{\theta})$:

$$\frac{\partial \mathcal{I}_{\mathtt{Q}}(\boldsymbol{\theta})}{\partial \theta_k} = \sum_{b=1}^{\mathtt{n_Q}} \tilde{\gamma}^b \tilde{A}_g^f \left[\frac{d\tilde{H}_k^{b,i}}{d\theta_k}(\theta_k) \right] \prod_{j \neq k}^{\mathtt{n_P}} \tilde{H}_j^{b,i}(\theta_j)$$

$$\frac{\partial \mathcal{I}_{\mathtt{L}}(\boldsymbol{\theta})}{\partial \theta_k} = \sum_{v=1}^{\mathtt{n_L}} \hat{\gamma}^v \hat{A}_g^f \left[\frac{d\hat{H}_k^{v,i}}{d\theta_k}(\theta_k) \right] \prod_{j \neq k}^{\mathtt{n_P}} \hat{H}_j^{v,i}(\theta_j)$$

- Recalling the safety factor expression, and applying the quotient rule for derivatives of divisions

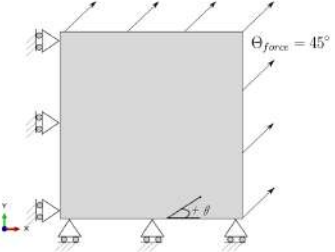
$$\lambda_s\big(\boldsymbol{\sigma}(\boldsymbol{x},\boldsymbol{\theta})\big) = \frac{-\mathcal{I}_{\mathtt{L}} + \sqrt{\mathcal{I}_{\mathtt{L}}^2 + 4\,\mathcal{I}_{\mathtt{Q}}}}{2\mathcal{I}_{\mathtt{Q}}}$$

$$\frac{\partial \lambda_s(\boldsymbol{\theta})}{\partial \theta_k} =$$

$$\frac{\mathcal{I}_{\mathtt{Q}} \left[-\frac{\partial \mathcal{I}_{\mathtt{L}}(\boldsymbol{\theta})}{\partial \theta_k} + 0.5(\mathcal{I}_{\mathtt{L}}^2 + 4\mathcal{I}_{\mathtt{Q}})^{-1/2} \cdot \left(2\mathcal{I}_{\mathtt{L}} \frac{\partial \mathcal{I}_{\mathtt{L}}(\boldsymbol{\theta})}{\partial \theta_k} + 4 \frac{\partial \mathcal{I}_{\mathtt{Q}}(\boldsymbol{\theta})}{\partial \theta_k} \right) \right] - \frac{\partial \mathcal{I}_{\mathtt{Q}}(\boldsymbol{\theta})}{\partial \theta_k} \left[-\mathcal{I}_{\mathtt{L}} + \sqrt{\mathcal{I}_{\mathtt{L}}^2 + 4\mathcal{I}_{\mathtt{Q}}} \right]}{2\mathcal{I}_{\mathtt{Q}}^2}$$

Plate under tensile load: Description

- **Plate dimensions:** $60 \times 60 \times 6\ \mathrm{mm}^3$.
- **Type and number of elements:** Serendipity 800 elements.
- **Parameters range:** $\theta_1 \in I_1 = [-90°, 90°]$ $\theta_2 \in I_2 = [-90°, 90°]$.
- **Parametric mesh:** 181 nodes.
- **Material:** Carbon Fibre ABS.



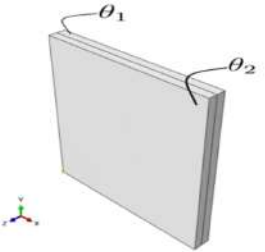
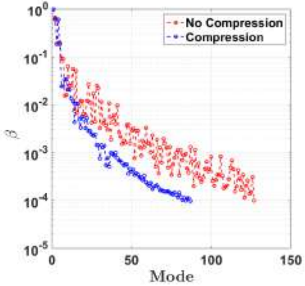


Plate under tensile load: PGD performance

- The stopping criterion for computing terms is controlled by $\xi = \frac{\beta^m}{\beta^1}$.
- The number of modes is reduced by 31.5% in the compressed solution.
- The reltive error between FE and PGD is 0.1%

$$\varepsilon_{glob} = \frac{\|\boldsymbol{d}_{\text{PGD}} - \boldsymbol{d}_{\text{FE}}\|_{\Omega \times I_1 \times \ldots \times I_{\text{n}_\text{p}}}}{\|\boldsymbol{d}_{\text{FE}}\|_{\Omega \times I_1 \times \ldots \times I_{\text{n}_\text{p}}}}$$



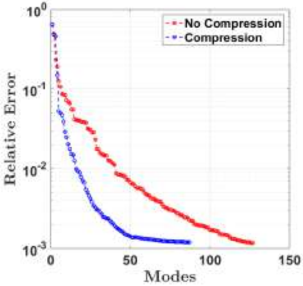
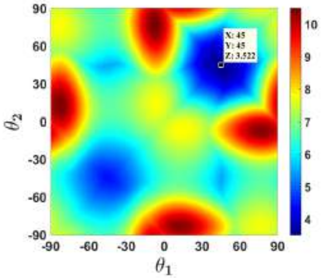
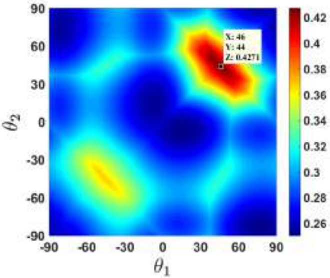


Plate under tensile load: Optimization output

- Maps represent the objective functions in the parametric space.
- The optimal $(\theta_1, \theta_2) = (45°, 45°)$.



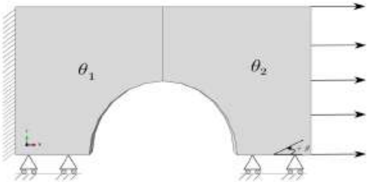


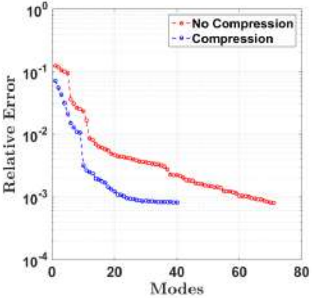
CPU time

- The CPU time for the FE whole solution is $\sim \mathbf{6.5}$ days with 32761 FE solves.
- The CPU time for the offline PGD solution is $\sim \mathbf{2.5}$ hours and the online browsing is in seconds.

Plate with circular hole under tensile load: Two parameters

- No more symmetry in the optimal solution due to patches of elements.
- The optimal solution is ambiguous due to the hole existence.
- The compression yields a reduction in the number of modes 43.5%.





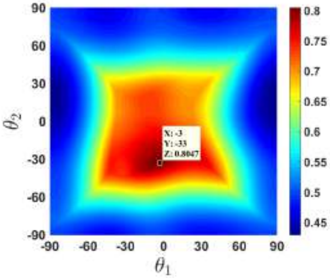
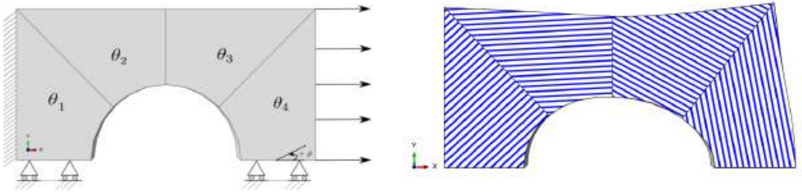


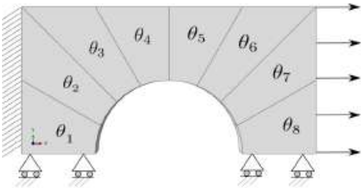
Plate with circular hole under tensile load: Four parameters

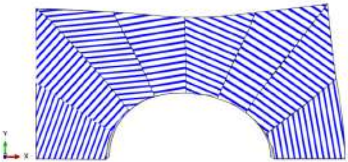


Optimal Angles		
	ga function	`fmincon` function
θ_1	$42°$	$42.062°$
θ_2	$3°$	$2.9944°$
θ_3	$-22°$	$-22.4586°$
θ_4	$-83°$	$-84.1544°$
Index value	$\max(\min \lambda_s) = 0.8254$	$\max(\min \lambda_s) = 0.8255$
CPU time	~ 40 min	~ 1 min

Table: Optimized angles for square plate with circular hole using the safety factor as objective function.

Plate with circular hole under tensile load: Eight parameters



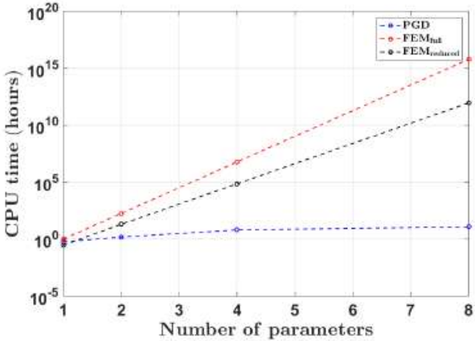


Optimized angles of the safety factor using GA				
# of GA evaluations	1000	10,000	100,000	1,000,000
θ_1	$81°$	$86°$	$70°$	$84°$
θ_2	$42°$	$43°$	$42°$	$41°$
θ_3	$5°$	$6°$	$6°$	$4°$
θ_4	$-6°$	$8°$	$8°$	$-20°$
θ_5	$-20°$	$-21°$	$-23°$	$17°$
θ_6	$-24°$	$-25°$	$-26°$	$-51°$
θ_7	$-26°$	$-25°$	$-30°$	$-61°$
θ_8	$45°$	$-86°$	$-85°$	$-82°$
$\max(\lambda_s)$	0.8249	0.8803	0.879	0.8501
CPU time	$\sim$ 1.2 min	$\sim$ 12 min	$\sim$ 120 min	$\sim$ 1300 min

Table: Different number of evaluations yielding different GA precision

Plate with circular hole under tensile load: Computational cost

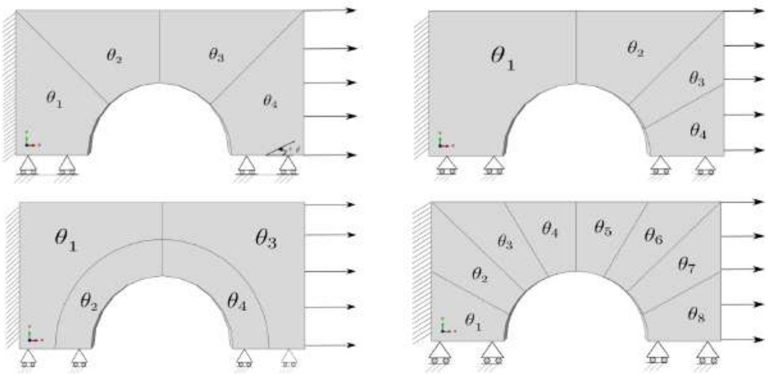
- **Four parameters:** PGD provides a solution in ~ 30 hours while computing the standard FE solution at every parametric point would take $\sim 10^6$ hours.
- **Eight parameters:** PGD provides a solution in ~ 42 hours while computing the standard FE solution at every parametric point would take $\sim 10^{16}$ hours.



The computational cost is drastically reduced when using PGD!

Domain decomposition strategy: Introduction

- Changing the partitioning patterns and increasing the number of partitions affects the optimal fibre orientation results.
- Increasing the number of subdomains does not guarantee fast convergence



We need to find a smarter partitioning strategy!!!

Domain decomposition strategy: Clustering algorithm steps

- Clustering techniques are unsupervised learning techniques such as: K-means, hierarchical clustering.
- Clustering aims to group elements having similar features in a data set into coherent groups.
- The clustering strategy is applied as a preprocess before solving the mechanical problem using PGD.

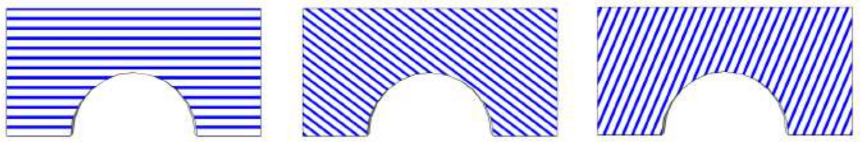
Clustering techniques for efficient partitioning of the domain

1. **Preanalyses:** snapshots of the system at each finite element for different orientations are taken and stored.
2. **Principal Component Analysis:** responsible for the data transformation from correlated fields to uncorrelated new components.
3. **Clustering of factors and their intersection:** the clustering techniques are applied to the factors (components) obtained from PCA.
4. **Error computation and clustering optimization:** clustering optimization in order to find the best clusters representing the data.

Domain decomposition strategy: Clustering algorithm steps

Preanalyses

- Collecting as much data as possible.
- The data represents a quantity of interest taken at different fibres configurations in each FE.
- More data $\Rightarrow$ accurate results.
- We assume a unidirectional laminate in each single snapshot.
- The quantity of interest is the safety factor at each element.
- The data is stored, in the $\mathtt{n_{el}} \times \mathtt{N_c}$ matrix $\tilde{\boldsymbol{\lambda}}_s$, to be manipulated and analyzed.



Domain decomposition strategy: Clustering algorithm steps

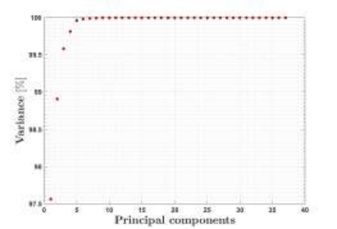
Principal Component Analysis (PCA)

- PCA reduces the dimensionality of the data while maintaining its variance as high as possible.
- First we find the covariance matrix

$$\boxed{\boldsymbol{\Sigma} = \frac{1}{\mathtt{n_{el}}} \tilde{\boldsymbol{\lambda}}_s{}^{\mathsf{T}} \tilde{\boldsymbol{\lambda}}_s}$$

- We then solve for the eigenvalues λ_i and the eigenvectors $\boldsymbol{v}^i$
- The factors or principal components are defined

$$\boxed{\mathbf{f}^i = \tilde{\boldsymbol{\lambda}}_s \boldsymbol{v}^i}$$

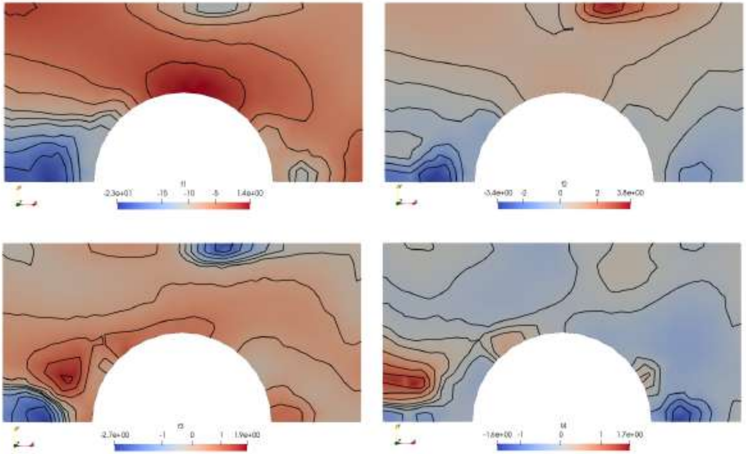


- The eigenvalues expressed in terms of the obtained factors

$$\boxed{\lambda_i = \frac{1}{\mathtt{n_{el}}} \sum_{j=1}^{\mathtt{n_{el}}} (\mathrm{f}_j^i - \hat{\mathrm{f}}^i)^2 \qquad \text{with } \lambda_1 > \lambda_2 > \ldots, > \lambda_{\mathtt{N_c}}}$$

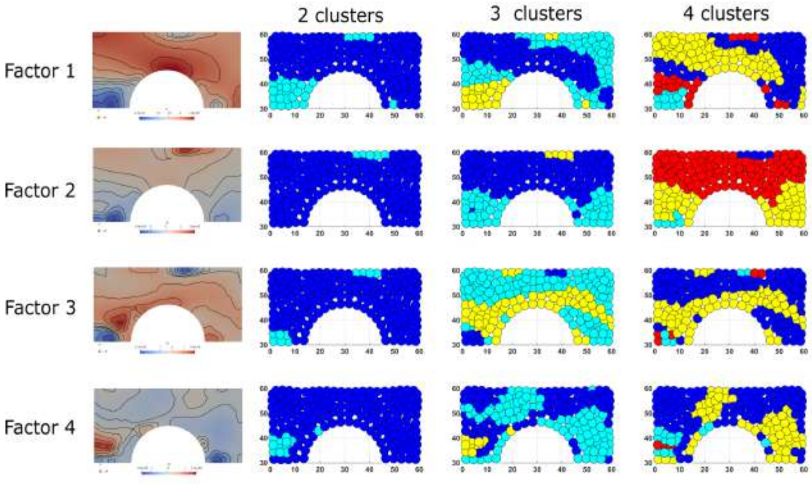
Domain decomposition strategy: Clustering algorithm steps

First four factors from PCA:
Factors based on the safety factor data $\tilde{\lambda}_s$ that will be clustered using the K-means algorithm



Domain decomposition strategy: Clustering of factors

K-means clustering of four factors



Domain decomposition strategy: Error computation

- **Our goal**: find the best partition $\mathcal{P}$
- The optimization objective is to minimize the error measure called Sum of Squares Error (SSE) [Alaimo et al. (2019)].
- SSE is a measure of discrepancy between the data of an element and the average of the data in the cluster where the element belongs.

$$E(\mathcal{P}) = \sum_{s=1}^{\mathtt{N_c}} E^s(\mathcal{P}) = \frac{1}{E_{max}} \sum_{s=1}^{\mathtt{N_c}} \sum_{\ell=1}^{\mathtt{n_s}} \sum_{i=1}^{n_\ell(\mathcal{P})} (\omega_i^s - \overline{\omega_{,\ell}^s})^2$$

$$E_{max} = \sum_{s=1}^{\mathtt{N_c}} \sum_{i=1}^{\mathtt{n_{el}}} (\omega_i^s - \overline{\omega^s})^2$$

- Each finite element is a cluster on its own $\mathtt{n_s} = \mathtt{n_{el}} \Rightarrow E(\mathcal{P}) = 0\%$
- Partition $\mathcal{P}$ consists of only one cluster $\mathtt{n_s} = 1 \Rightarrow E(\mathcal{P}) = 100\%$

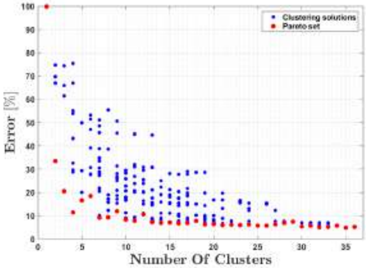
Domain decomposition strategy: Clustering optimization

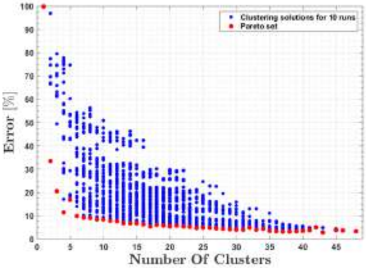
- The clustering multi-objective problem is defined as

$$\mathcal{P}^{\mathtt{Opt}} = \arg\min_{\mathcal{P}} \ \{E(\mathcal{P}), \mathtt{n}_{\mathtt{s}}(\mathcal{P})\} \quad \text{s.t.} \quad \mathcal{P} \in \mathbb{P}$$

- There exists a *Pareto optimality situation*.
- A *Pareto set* has optimization solutions that are superior to the rest of the solutions in the search space $\mathbb{P}$.
- The solutions among the set do not dominate each other.
- A partition $\mathcal{P}_1$ is said to dominate another partition $\mathcal{P}_2$ only when the following inequalities hold

$$\begin{array}{ccc} E(\mathcal{P}_1) \leq E(\mathcal{P}_2) & \text{and} & \mathtt{n}_{\mathtt{s}}(\mathcal{P}_1) \leq \mathtt{n}_{\mathtt{s}}(\mathcal{P}_2) \\ E(\mathcal{P}_1) < E(\mathcal{P}_2) & \text{or} & \mathtt{n}_{\mathtt{s}}(\mathcal{P}_1) < \mathtt{n}_{\mathtt{s}}(\mathcal{P}_2) \end{array}$$



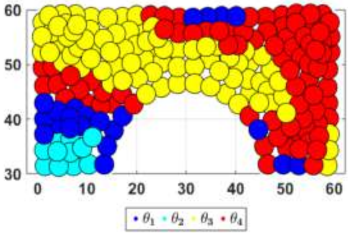


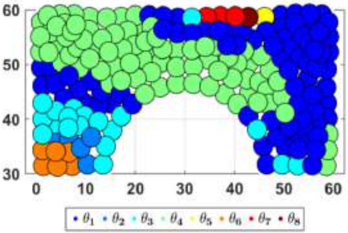
Pareto set error comparison				
	Stress based clusters		Safety factor based clusters	
	4 clusters	8 clusters	4 clusters	8 clusters
K-means single run	38%	29%	11.5%	9.5%
K-means 10 runs	37%	29%	11.2%	9.1%
Ward's method	41%	26%	11.9%	9.3%

Table: Pareto set error comparison between K-means with a single run, K-means with 10 runs, and Ward's method

Domain decomposition strategy: Clustered domains

Optimal domain decomposition obtained from the clustering algorithm





	Domain with 4 parameters	Domain with 8 parameters
Stress based clustering with K-means	0.7863	0.8788
Stress based clustering with Ward's	0.8653	0.9037
Transformed safety factor clustering with K-means	**1.013**	**0.9934**
Transformed safety factor clustering with Ward's	0.7973	0.8244
Based on intuition	0.8254	0.879

Table: Safety factor index λ_s obtained from PGD based on different domain parameterization

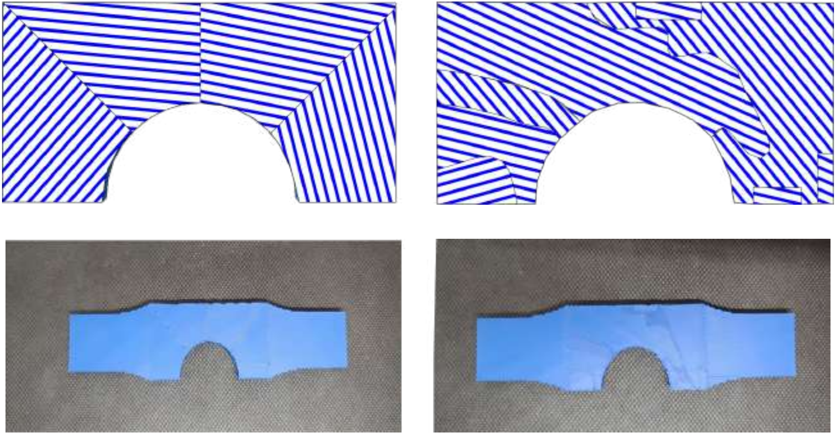
Domain decomposition strategy: Experimental testing

Experimental testing for the validation of the model using 3D printing

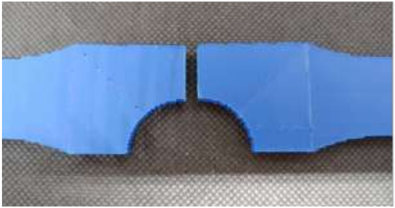
1. **Simulation and analysis:** Run the model to obtain optimal fibre orientation in different domains.
2. **Specimen preparation and 3D printing:** The preparation of the STL files of the components to be printed and slicing the part for the G-Code generation.
3. **Tensile test and monitor results:** Perform traction on the part until failure occurs and then record the corresponding load for comparison.

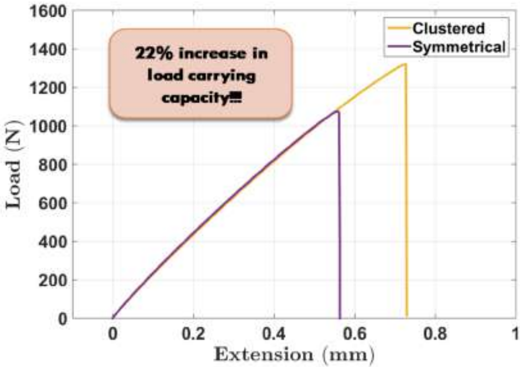
Domain decomposition strategy: Experimental tests

Optimal fibre orientation in optimized partitions in the domain



Domain decomposition strategy: Experimental tests





Conclusions

- PGD reduces the computational cost significantly.
- Applying the encapsulated PGD concept facilitates the manipulation of high-dimensional data.
- Using PGD in optimization problems is extremely efficient since we have the whole space of solutions available.
- Applying clustering techniques as a pre-process leads to better optimization results.
- The whole methodology opens the door for customized mechanical components.
- Experimental tests show the improvement in the load carrying capacity of the optimized 3D printed components
- The clustering techniques approach reduces the CPU time for the PGD.

Future work

- **Enhancement of the model:**
  From the PGD point of view, it is important to enhance the vademecum by including geometrical parameterization, load location parameter, and boundary conditions parameterization.
- **Programming languages:**
  From the programming point of view, the PGD package could be implemented using high-efficiency languages such as C/C++ and/or FORTRAN. Moreover, modern simulation applications on smartphones could be developed to make use of the fast response of the PGD vademecums.
- **Error estimation:**
  Obtaining an error estimator of a quantity of interest to be able to accurately choose the stopping criterion for the greedy algorithm in the PGD.
- **Additive manufacturing:**
  The need to explore the possibility of printing continuous fibres with the aim of enhancing the mechanical properties of 3D printed components by avoiding jumps between partitions.

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