Surrogate Based Optimization of Functionally Graded Plates

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Abstract. This work presents an efficient methodology for the optimization of functionally graded plates based on the use of surrogates. These models are an alternative to reduce the computational cost of optimization, efficiently approximating the results of numerical simulations. The surrogate was incorporated into an optimization methodology known as Sequential Approximate Optimization, where the surrogate is continuously updated and improved by the insertion of new points, enhancing the model approximation. This approach is applied to the design optimization of a functionally graded plate, maximizing the critical buckling load. The performance is evaluated in terms of accuracy and computational efficiency.

Keywords: Optimization, Functionally Graded Plates, Surrogate Models.

1 Introduction

Functionally Graded Materials (FGM) are advanced composites, usually made of ceramic and metal, in which the volume fraction of their constituents varies smoothly along chosen directions. These materials were initially proposed as a solution for structures subjected to high temperatures, but now your applications are both diverse and numerous [1]. The variation in composition results in a gradual change in their properties, improving the performance of structures subjected to thermal and mechanical loads, but making structural analysis more complex.

Seeking better performance of functionally graded structures, it is necessary to select both the materials and their gradation. After defining the materials, optimization techniques are used to explore the design space to find the optimal material gradation based on the results of computational methods that simulate the behavior of these structures. Many optimization techniques can be used to solve the optimization problem. Kou et al. [2] used Particle Swarm Optimization (PSO) to minimize the thermal stresses of different functionally graded structures. A hybrid PSO algorithm was used by Barroso et al. [3] to maximize the load factor and minimize the weight of laminated structures. Kim et al. [4] used a Differential Evolution (DE) algorithm to maximize the first three natural frequencies of a functionally graded beam.

However, the high computational cost of the analyses can be a limiting factor in the optimization process. The use of these bio-inspired algorithms requires a large number of analyses to find the optimal design. Therefore, an alternative to reduce the computational cost of optimizing complex structures is to use surrogate models capable of efficiently approximating the results of numerical simulations. This work uses the Kriging surrogate model, which was incorporated into an optimization methodology known as Sequential Approximate Optimization (SAO), where the surrogate is continuously updated and improved by the insertion of new points, refining the model approximation.

2 Functionally Graded Plates

Plates are three-dimensional flat structures whose thickness is much smaller than their two other dimensions. Various theories have been proposed to analyze this type of structure, such as the Classical Plate Theory and the First-Order Shear Deformation Theory. The theory used in this work was Redyy's theory, also known as Third Order Shear Deformation Theory (TSDT). It was chosen for its ability to more accurately represent the distribution of shear deformations along the thickness of plates without a correction factors, unlike the previously mentioned theories. However, the displacement field it describes requires C^1 continuity and is a challenge for traditional isoparametric elements. Therefore, alongside TSDT, the analysis method chosen was Isogeometric Analysis (IGA) based on Non-Uniform Rational B-Splines (NURBS), which ensures elements with high continuity.

Gradation in functionally graded plates occurs based on the variation of volume fractions throughout the thickness of the plate. This variation can be described in various ways, and in this work, it is represented by B-Splines [5]. Using this type of function is justified because it allows greater flexibility, or rather, greater control over the effective properties of the constituents of the structure, providing a broader design space. While the elastic properties are calculated using the Mori-Tanaka micromechanical model [6].

3 Sequential Approximate Optimization

The optimization method used in this work is PSO, a very popular meta-heuristic algorithm. The technique, based on the behavior of bird flock in search for food, aims to optimize nonlinear continuous functions. The algorithm starts by generating an initial swarm of random particles N_p each particle j is assigned a position $\mathbf{x}_j^{(0)}$ and a velocity $\mathbf{v}_j^{(0)}$, at each iteration (i) the particles move in the design space according to their velocity:

$$\boldsymbol{x}_j^{i+1} = \boldsymbol{x}_j^{i} + \boldsymbol{v}_j^{i+1} \tag{1}$$

where:

$$\boldsymbol{v}_j^{i+1} = w\boldsymbol{v}_j^{i} + c_1 r_1\left(\boldsymbol{x}_{p,j}^{i} - \boldsymbol{x}_j^{i}\right) + c_2 r_2\left(\boldsymbol{x}_{g,j}^{i} - \boldsymbol{x}_j^{i}\right) \tag{2}$$

where w is inertia, c_1 is the cognitive factor, c_2 is the social factor, r_1 and r_2 are uniformly distributed random numbers between 0 and 1, $\mathbf{x}_{p,j}^{(i)}$ is the best position that particle j obtained during optimization and $\mathbf{x}_{g,j}^{(i)}$ is the best position of the particles in the neighborhood of particle j obtained during optimization [3]. The main steps for the PSO optimization procedure are described in Fig. 1.

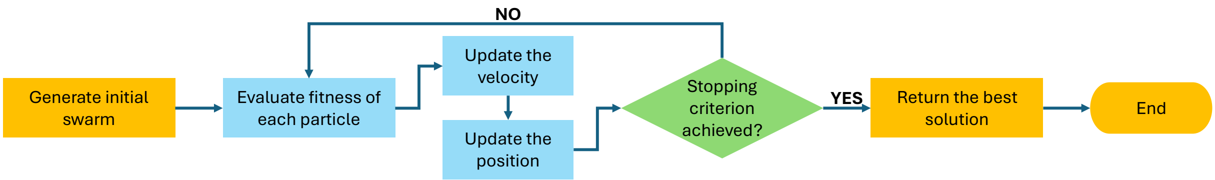


Figure 1. Flowchart of PSO.

The surrogate model adopted in this study was the Kriging model, first developed by mining engineer Danie Krige and introduced into engineering design by Sacks et al. [7], who applied the method to the approximation of computer experiments. It is a non-parametric interpolation method, implying that the training points are used in determining the unknown parameters. The model exactly interpolates the known values at the sampling points. Kriging has several variants, and its general form can be described as:

$$\hat{f}(\boldsymbol{x}) = g(\boldsymbol{x}) + Z(\boldsymbol{x}) \tag{3}$$

where $\hat{f}(\mathbf{x})$ is the Kriging prediction, $g(\mathbf{x})$ is the global trend and $Z(\mathbf{x})$ are its localized correlated deviations. This work adopts the Ordinary Kriging, where it is assumed that the global trend is unknown and constant, adopting the average (μ).

The construction of the model begins with a sample dataset $\mathbf{x}$ with observed responses $\mathbf{y}$. The random variables are correlated with each other using the expression of the base function [8]:

$$cor\left[Y\left(\boldsymbol{x}^{(i)}\right), Y\left(\boldsymbol{x}^{(l)}\right)\right] = exp\left(-\sum_{j=1}^{k} \theta_j \left|x_j^{(i)} - x_j^{(l)}\right|^{p_j}\right) \tag{4}$$

These correlations depend on the absolute distance between the sample points $\left|x_j^{(i)} - x_j^{(l)}\right|$ and the parameters $\mathbf{p}$ and $\boldsymbol{\theta}$. Knowing these correlations, the Maximum Likelihood Estimator (MLE) method was used to determine the parameters, aiming to choose $\boldsymbol{\theta}$ and $\mathbf{p}$ to maximize the likelihood of $\boldsymbol{y}$. Ultimately, we hope this minimizes the model's generalization error [8]. The PSO algorithm was used in this work to find the values of these parameters that maximize the likelihood function.

The surrogate model was incorporated into Sequential Approximate Optimization (SAO), an approach proposed by Schmit and Farshi [9], where the surrogate is continuously updated and improved by adding new points primarily in promising regions, enhancing the model approximation. This formulation adopted a trust region approach, where the regions in which subproblems should be built and solved are continuously updated [9].

However, in this work, a SAO approach based on adaptive sampling is used, which leverages the global response surface throughout the process. To generate the initial sampling of the planning space, the Latin Hypercube Sampling (LHS) algorithm is used, where a number of sampling plans are generated, and the one that provides the best uniformity is selected to construct the initial surrogate [8]. The responses of the planning space were evaluated with IGA.

When implementing this strategy, it is important to adopt a criterion to add new sampling points. Thus, to improve the model's accuracy, the selection of new sampling points was done using Expected Improvement (EI), which calculates the amount of improvement we expect given the mean and variance [8]. This approach seeks to balance exploitation (local search) and exploration (global search), including points near the current optimum and points where the model error is large. The steps of this optimization procedure in which the SAO methodology is used are described in Fig. 2.

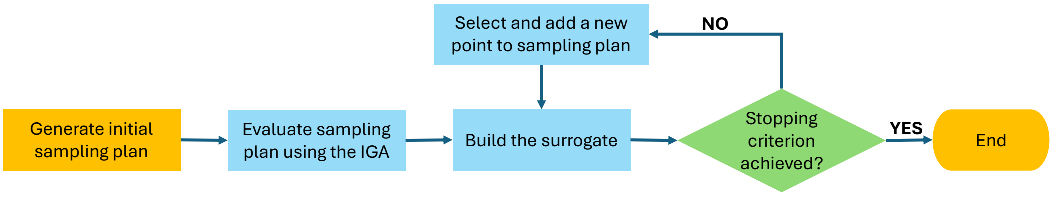


Figure 2. Flowchart of SAO using Kriging.

4 Numerical Example

In this section, the SAO approach discussed earlier is used to optimize a functionally graded plate, and its results are compared with a high-fidelity model (HFM) and results from the literature. The mechanical properties of the materials used are shown in Tab. 1.

Table 1. Material properties.

Material	E (GPa)	ν	ρ (kg/m³)
Al	70.00	0.3	2707
Al_2O_3	380.00	0.3	3800

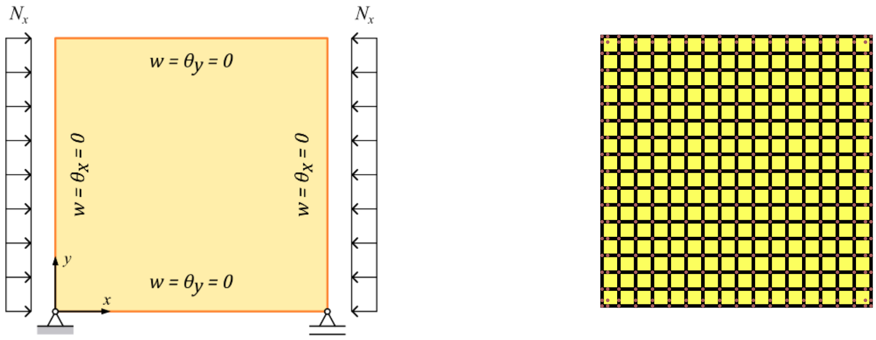
For the construction of the initial surrogate model, only $n = 5m$ sampling points are generated using the LHS approach. The surrogate is improved by adding new points until the maximum number of generations $N_{gen} =$ 100 is reached or after 15 iterations of the SAO algorithm without solution improvement $\left(Stall_{gen}\right)$. The Square topology is considered in the PSO, and the optimization parameters are $Stall_{gen} = 15$, $N_{gen} = 100$, $N_p = 30$, $\omega = 0.72$, $c_1 = 1.5$ and $c_2 = 1.5$.

For the optimization problem, $N_r = 10$ runs were performed, and the metrics to characterize the approach are the average number of high-fidelity evaluations $(\bar{n}_p)$ and the Relative Difference (RD) to assess accuracy:

$$RD = \frac{|y_{min} - y_{opt}|}{y_{opt}} \tag{5}$$

where y_{min} is the best result found and y_{opt} is the best result from the HFM. All simulations were carried out on a computer running on an Intel i5-9400 CPU @ 2.90GHz, 6 cores, and 8 GB RAM. No parallelization procedure was adopted.

The objective is maximize the buckling load of a simply supported square plate made of Al/Al_2O_3, with $a/h = 10$, subjected to a uniform uniaxial compressive loading N_x, as illustrated in Fig. 3a. A 16 × 16 cubic NURBS mesh, shown in Fig. 3b, used in the structural analysis.



(a) Simply support FGM plate. (b) 16 × 16 cubic NURBS mesh.

Figure 3. Simply support FGM plate and mesh used for the maximization of the buckling load.

The gradation is defined by 9 control points along the thickness, symmetric with respect to the midplane. Thus, this problem has 5 design variables. A maximum percentage constraint of ceramic material is considered:

$$g(\boldsymbol{x}) = \bar{V}_c(\boldsymbol{x}) - \bar{V}_{c,max} \leq 0, where\ \bar{V}_c(\boldsymbol{x}) = \frac{1}{h}\int_{-\frac{h}{2}}^{\frac{h}{2}} V_c\, dz \tag{6}$$

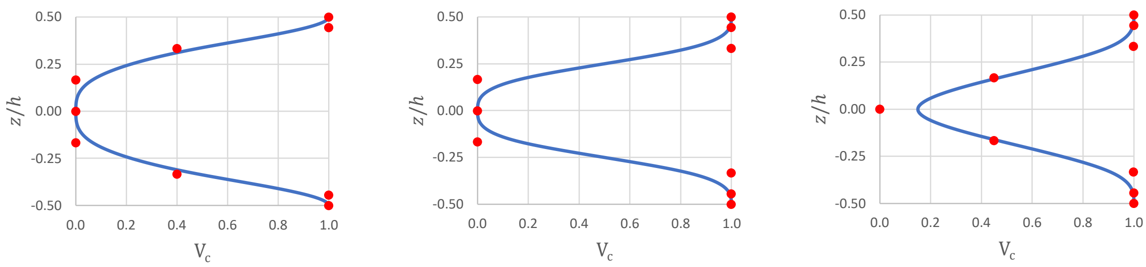
The optimization problem is given by:

$$\begin{cases} maximize & N_{cr}(\boldsymbol{x}) \\ subjected\ to & g(\boldsymbol{x}) \leq 0 \\ with & 0 \leq \boldsymbol{x} \leq 1 \end{cases} \tag{7}$$

where N_{cr} is the critical buckling load. The problem was proposed by Do et al. [5], where a Deep Neural Network (DNN) was used as a surrogate model. Ten thousand sampling points were evaluated, with 80% used for training and 20% for validation. The authors considered three different cases, with $\bar{V}_{c,max}$ equal to 35%, 50%, and 65%.

Table 2 presents the optimal designs found using the SAO approach and conventional optimization (PSO + IGA), while Fig. 4 shows the optimal gradations across the thickness for the three cases found by SAO. These results are compared with the best design found by the DNN [5]. The non-dimensional buckling load is given by:

$$\lambda_{norm} = N_{cr}a/D_m\ , where\ \ D_m = E_m h^3/12(1 - \nu_m^2) \tag{8}$$



(a) $\bar{V}_{c,max} = 35\%$. (b) $\bar{V}_{c,max} = 50\%$. (c) $\bar{V}_{c,max} = 65\%$.

Figure 4. Optimal gradation.

Table 2. Optimal design.

Design variable	$\bar{V}_{c,max} = 35\%$			$\bar{V}_{c,max} = 50\%$			$\bar{V}_{c,max} = 65\%$		
	Do et al. [5]	HFM	SAO	Do et al. [5]	HFM	SAO	Do et al. [5]	HFM	SAO
1	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
2	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
3	0.3920	0.3999	0.3999	0.9880	0.9999	0.9999	1.0000	1.0000	1.0000
4	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4420	0.4500	0.4500
5	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
λ_{norm}	11.185	11.213	11.213	14.603	14.709	14.709	16.193	16.231	16.231
RD	0.25%	-	0.00%	0.73%	-	0.00%	0.23%	-	0.00%
$\bar{n}_p$		1821	44		2223	48		1719	45

The results obtained demonstrate that the surrogate model successfully reduced the computational cost of the optimization, decreasing the number of high fidelity evaluations when compared to evaluations performed in HFM and DNN. The surrogate also accurately predicted the buckling load, returning values very close to those of the HFM.

5 Conclusion

This work the use of Kriging as a surrogate model to reduce the computational cost of the optimization process for functionally graded plates. The surrogate model proved to be accurate and efficient for designs with functionally graded materials. Its application in the optimization of real structures can be quite advantageous, presenting great potential as a resource to reduce the high computational cost in designs of complex structures, making the optimization of these structures more feasible.

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