Model Order Reduction and Bayesian Optimization for MDO problems

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Résumé

Cet article propose une formulation d'optimisation multidisciplinaire, en combinant l'approximation des solveurs disciplinaires par des modèles réduits disciplinaires (DPOD+I) avec l'algorithme Efficient Global Multidisciplinary Design Optimization (EGMDO). L'approximation DPOD+I permet de résoudre le problème des variables de couplage de grande dimension, en utilisant une stratégie d'entraînement basée sur la réduction de l'ordre du modèle et d'interpolation par processus Gaussien. Les méta-modèles obtenus sont ensuite enrichis tout au long de l'optimisation, pour assurer une précision donnée. Cette implémentation permet une réduction importante du nombre d'appels aux solveurs, par rapport à l'approche où aucune approximation n'est faite. La combinaison des méta-modèles DPOD+I avec l'algorithme EGMDO réduit encore le coût de calcul, en utilisant un critère d'amélioration espérée pour enrichir préférentiellement les méta-modèles dans les zones de l'espace de conception d'intérêt pour la recherche du minimum global. Sur un cas d'application aéroélastique on observe que, en combinant les deux méthodes, très peu d'enrichissements des solveurs disciplinaires sont nécessaires.

Abstract

This article proposes a framework for multidisciplinary optimization, by combining the approximation of the disciplinary solvers by Proper Orthogonal Decomposition and Interpolation (DPOD+I) models with the Efficient Global Multidisciplinary Design Optimization (EGMDO) algorithm. The DPOD+I approximation allows to address the problem of high-dimensional coupling variables, by using a surrogate training strategy based on model order reduction and Gaussian process interpolation. The obtained surrogates may then be enriched throughout the optimization, to assure a given precision. It is shown that this implementation allows for an important reduction of the number of expensive solver calls, compared to when no approximation is made. The combination of this method with the EGMDO algorithm further reduces the computational cost by using an Expected Improvement criterion to preferentially improve the surrogates in the areas of the design space found relevant for the search of the global optimum. In the context of an aeroelastic test case it is seen that, by combining the two methodologies, very few disciplinary solver enrichments are needed.

Keywords: Multidisciplinary analysis and optimization, model order reduction, surrogate models, Gaussian processes, overall aircraft design

1 Introduction

Multidisciplinary Analysis (MDA) and Optimization (MDO) are useful tools when addressing problems which involve several disciplines or subsystems. For instance, in aircraft design, the aerodynamic and structural disciplines must be taken into account in order to fully characterize the aeroelastic behaviour of a wing [1, 2]. With the aid of disciplinary solvers, it is possible to model the physical phenomena, as well as the coupling between them. These solvers then interact with one another via the coupling variables, resulting in a non-linear system of equations. To solve this coupled system, each disciplinary solver must be evaluated iteratively by a global solver until a given convergence criterion is reached. The role of MDA is thus to find the equilibrium of the system at a given design space point.

Multidisciplinary Optimization, on the other hand, may be used to iteratively change the design parameters towards a given goal. Different architectures are available for multidisciplinary optimization. The Individual Disciplinary Feasible (IDF) and Multidisciplinary Feasible (MDF) approaches attempt to find the optimal point via a single optimization problem [3, 4]. In the IDF approach, the optimization algorithm handles both the design and coupling variables, by uncoupling the disciplinary solvers and instead imposing consistency constraints. Despite the reduction in the computational cost achieved by avoiding the resolution of the coupled MDA, this formulation can become difficult to set up if the number of coupling variables is significant. Contrarily, in the MDF approach, the coupled MDA is solved via fixed point iteration, usually by means of a non-linear Gauss-Seidel solver. This formulation is easier to set up and returns a physically feasible design at every optimization iteration. Furthermore, the high cost of solving the coupled MDA may be improved if gradient information is considered, for instance, by employing Newton-based solvers.

The computational burden of solving the multidisciplinary analysis might be further reduced by constructing surrogate models of the objective and constraint functions [5, 6], thus limiting the number of whole MDA resolutions. However, without an adequate enrichment criterion, it might become necessary to have accurate surrogate models throughout the entire design space, even in areas where the local or global optima are unlikely to be. Similarly, to improve the computational time of the multidisciplinary optimization, gradient-based algorithms may be employed. Nonetheless, these are designed to converge to local minima and may require attempting different starting points in order to find a global optimum.

An alternative strategy for solving the parametrized MDA, denominated Disciplinary Proper Orthogonal Decomposition and Interpolation (DPOD+I), is proposed in [7], where the issue of using high dimensional coupling variables is addressed by uncoupling the disciplinary solvers and replacing each one by a reduced order model [8, 9]. These reduced order models are then trained using Gaussian processes, which replace the disciplinary solvers in the multidisciplinary analysis. The surrogate disciplines are enriched iteratively throughout the optimization process by means of sensitivity analysis, and according to the methodology proposed in [10]. As other surrogate-based approaches, this methodology avoids the resolution of the MDA via the potentially costly solvers, but requires enrichment of the surrogates models only when the uncertainty is high, thus resulting in a lower number of expensive solver calls. To address global optimization, the authors of [10] propose an iterative procedure denominated Efficient Global Multidisciplinary Design Optimization (EGMDO). This approach enriches the disciplinary models solely in the areas of the design space where the global optimum is more likely to be. To do so, an Expected Improvement criterion, such as the one introduced in [5], is proposed, based on the uncertainty induced by the disciplinary surrogates on the objective function. By iteratively enriching the disciplinary models in the relevant design space areas, this uncertainty is reduced and the global optimum is found.

The present article proposes to combine the replacement of the disciplinary solvers by their respective surrogates obtained by means of DPOD+I, with the use of EGMDO procedure as optimization algorithm. The proposed framework is then used to solve an aeroelastic optimization problem associated with an aircraft wing, by coupling a potential flow model with a linear elastic structural model. An inverse problem is chosen as a test case, where the goal is to retrieve the set of design parameters which results in the desired reference solution.

The present work is organized as follows. Section 2 presents the chosen test case as well as its resolution via the computationally expensive disciplinary solvers. This will serve as a reference solution against which the remaining implementations will be compared. Section 3 will address the replacement of the disciplinary solvers by their DPOD+I surrogates, while Section 4 will combine the DPOD+I with the EGMDO optimizer. Finally, some conclusions and perspectives are given.

2 Static aeroelastic optimization of an aircraft wing

We consider the aeroelastic analysis and optimization problem associated with an aircraft wing, whose coupled behaviour is described by the aerodynamic and structural disciplines. Together, these disciplines define the following non-linear system of equations:

$$\begin{cases} u_s = \mathcal{M}_s(\boldsymbol{x}, f_a) \\ f_a = \mathcal{M}_a(\boldsymbol{x}, u_s) \end{cases} \tag{1}$$

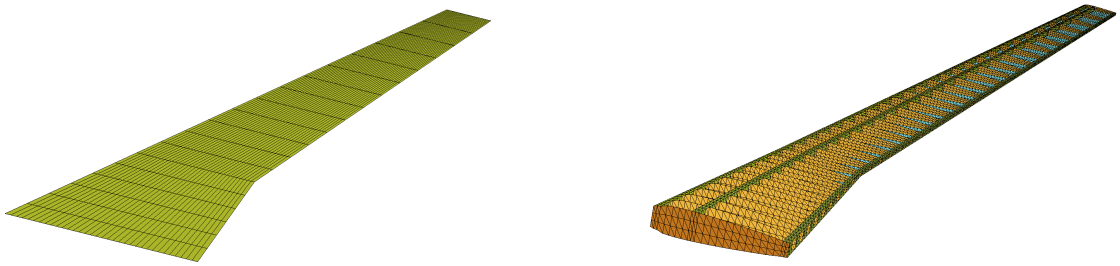
Here, u_s is the structural displacement of the wing, f_a is the vector of aerodynamic forces acting upon the wing, $\mathcal{M}_s$ and $\mathcal{M}_a$ are, respectively, the chosen structural and aerodynamics models and $\boldsymbol{x}$ is the set of the design variables. Together, u_s and f_a define the set of coupling variables considered in our problem. As will be seen in the following section, they are defined as high-dimensional vectors.

2.1 Disciplinary solvers

To solve the MDA it is necessary to model the participating disciplines. In this work, the disciplinary solvers are assumed to be black-box solvers, meaning that no intrusive methods can be used. Additionally, we assume that the derivatives of their outputs with respect to the design variables are not available.

The aerodynamics solver is then chosen as the linear, potential flow model, solved by Vortex Lattice Method (VLM) [11]. The VLM models the surface of the wing as a thin plate, neglecting both the thickness and the viscosity of the wing. If the wing geometry is discretized into a structured mesh, it is possible to compute the aerodynamic loads by modelling its surface using horseshoe vortices. Here, the considered planform geometry of the wing is that of the Common Research Model (configuration uCRM-9) [12] and the aerodynamic mesh discrezation is such that the load vector f_a is of dimension $d^a = 2100$. A representation of the aerodynamic mesh is provided in Figure 1(a).

The structural discipline is modelled via linear elastic theory, and solved by the finite element solver Code Aster [13], on which a static linear analysis is conducted to determine the wing's displacements. The finite element model is composed of the upper and lower skins, 3 spars and evenly spaced ribs, all modelled by thin plate elements. In addition, each of the skins is reinforced by 9 stiffners, modelled by beam elements. In total, the model consists of $d^s = 43416$ degrees of freedom, corresponding to the dimension of u_s. The structural mesh is presented in Figure 1(b), where the upper skin was removed to facilitate visualization.



(a) Wing aerodynamic mesh (b) Wing structural mesh

Figure 1: Wing meshes used in the disciplinary solvers.

In addition to modelling the disciplines, it is necessary to transfer the loads and displacements between the non-coincident structural and aerodynamic meshes. This is made by radial basis interpolation [14], through which an interpolation matrix $H \in \mathbb{R}^{d^a \times d^s}$ is built. This matrix allows to obtain the displacements of the aerodynamic nodes as $u_a = H u_s$ and the structural loading as $f_s = H^{\mathrm{T}} f_a$.

2.2 Problem statement

To facilitate comparison between the different implementations, an inverse problem may be defined, for which 4 parameters are chosen as design variables. Two of these parameters, namely the angle of attack α and the freestream velocity V_∞, influence only the aerodynamic analysis. Contrarily, the remaining parameters impact solely the structural model. These are the skin thicknesses t_{sk}, assumed to be the same for both lower and upper skins, and the spar thicknesses t_{sp}, considered to be the same for all three spars. The thickness of the wing ribs and stiffners is kept constant throughout the resolution of the problem. Table 1 presents the range of variation of each of the considered design variables. It is worth noting, however, that for a more practical implementation, these variables have been scaled to take values in the range $[0, 1]$.

Variable	$\alpha[^\circ]$	$V_\infty[m/s]$	$t_{sk}[m]$	$t_{sp}[m]$
	$[1, 9]$	$[220, 250]$	$[0.003, 0.01]$	$[0.01, 0.1]$

Table 1: Unscaled design variable range of variation

As previously stated, an inverse problem was chosen. This means that, throughout the optimization process, the goal is to find the set of design parameters which corresponds to a given reference solution obtained at $\boldsymbol{x} = \boldsymbol{x}_{\text{ref}}$. The objective function is then described by the sum of the relative error committed by each of the coupling variables at any evaluated design point $\boldsymbol{x}$, and the optimization problem may be written as,

$$\boldsymbol{x}^* = \arg\min_{\boldsymbol{x} \in \mathscr{X}} f_{obj}(\boldsymbol{x}) \quad \text{with} \quad f_{obj}(\boldsymbol{x}) = \frac{\|f_a(\boldsymbol{x}_{\text{ref}}) - f_a(\boldsymbol{x})\|_2}{\|f_a(\boldsymbol{x}_{\text{ref}})\|_2} + \frac{\|u_s(\boldsymbol{x}_{\text{ref}}) - u_s(\boldsymbol{x})\|_2}{\|u_s(\boldsymbol{x}_{\text{ref}})\|_2} \tag{2}$$

where $\mathscr{X} \subset \mathbb{R}^4$ is the subspace defined by the design variable bounds. For the remainder of this work, $\boldsymbol{x}_{\text{ref}}$ will be chosen as the corner of the design space for which the maximum wing tip displacement is achieved, namely, for the scaled design variables, $\boldsymbol{x}_{\text{ref}} = \{\alpha, V_\infty, t_{sk}, t_{sp}\}$, which corresponds to the

set $\{1, 1, 0, 0\}$ in scaled design variables. The wing vertical displacement field obtained at the chosen reference design point is presented in Figure 2.

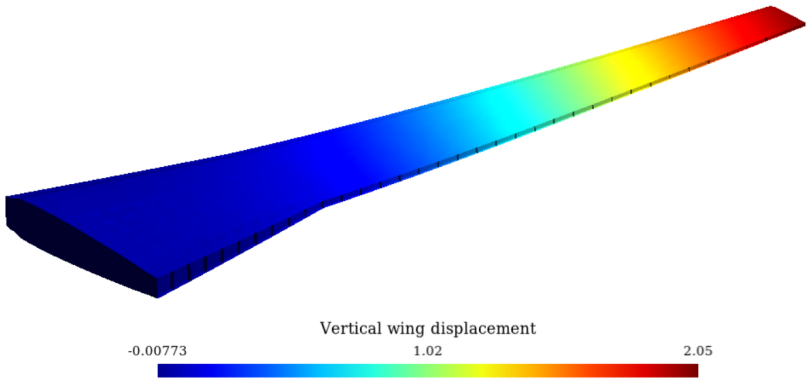


Figure 2: Wing vertical displacement field at reference solution.

As is shown, the structural displacement is maximum at the wing tip, where a vertical displacement of 2.05 meters is observed. Contrarily, and due to the imposed boundary conditions, no displacement is observed at the wing root. Although not shown here, the minimum displacement of the wing is obtained at $\boldsymbol{x} = \{0, 0, 1, 1\}$ for scaled variables, for which a vertical displacement of 0.067 meters at the wing tip is observed.

Finally, it is worth noting that, in the present work, no constraint was considered and the optimization problem is fully defined by Eq. (2).

2.3 Optimization framework

The previously defined aeroelastic problem was implemented within NASA OpenMDAO framework [15, 16], an open-source code for multidisciplinary analysis and optimization, which facilitates gradient computation. OpenMDAO allows the resolution of the non-linear MDA through the non-linear block Gauss-Seidel or Newton solvers, and makes use of SciPy optimizers to solve the MDO. OpenMDAO presents the benefit of a modular implementation, which allows for an easy reformulation of the problem. Furthermore, thanks to ONERA WhatsOpt environment [17], which generates the OpenMDAO skeleton code, the implementation of the disciplines is facilitated. Figure 3 presents the implemented optimization framework for the reference case where the real solvers are used to model the disciplines.

Some additional remarks should be made concerning the presented implementation. Firstly, to take into account the high-dimensional coupling variables, only the MDF approach could be used, hence the MDA is solved at each optimization iteration. Secondly, the resolution of the MDA is performed by the non-linear block Gauss-Seidel solver, for which the use of Aitken acceleration [18] showed to significantly reduce the number of necessary Gauss-Seidel iterations. Lastly, at the MDO level, the solver used was the gradient-based Sequential Least SQuares Programming (SLSQP) solver, which makes use of OpenMDAO capability to calculate the derivatives of the objective function with respect to the design variables via finite difference approximation. Regarding the convergence criteria, a tolerance of 10^{-8} was set for the nonlinear solver, while a tolerance of 10^{-6} was set for the optimizer.

Concerning the initial guess, the center of design space was chosen, i.e., $\boldsymbol{x}_0 = \{0.5, 0.5, 0.5, 0.5\}$. This point was kept for the DPOD+I implementation to allow for the comparison of the computational cost.

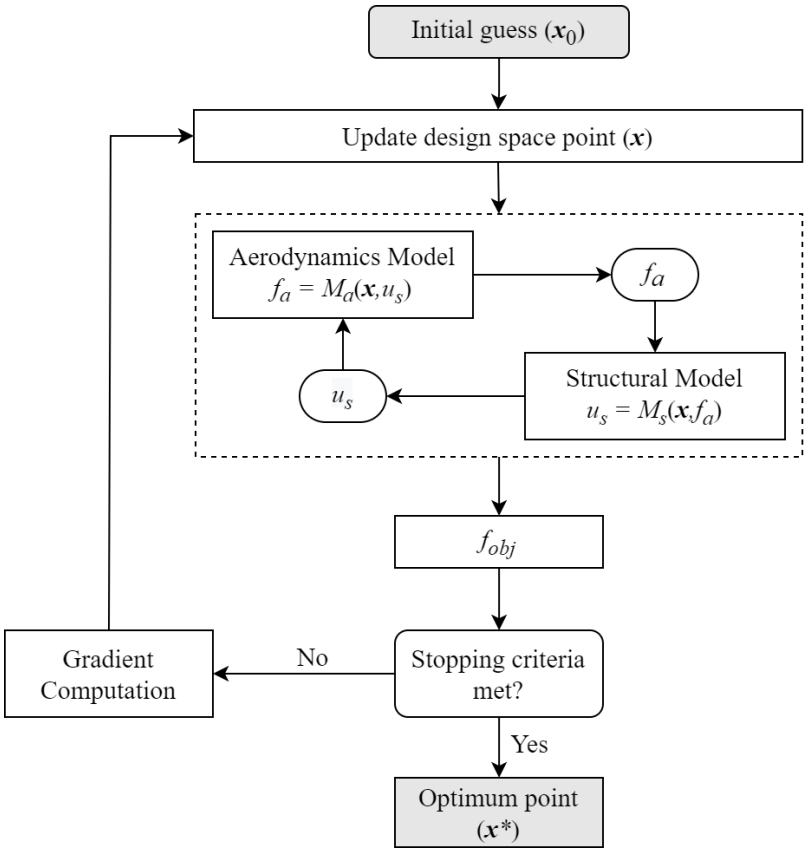


Figure 3: Reference problem optimization framework.

2.4 Reference problem solution

For the reference problem, the optimizer was able to converge to the reference solution in 17 iterations. Table 2 presents the obtained $\boldsymbol{x}^*$, the corresponding objective function value, and the number of disciplinary solver calls performed throughout the optimization. Note that while the chosen disciplinary solvers are not particularly expensive, if higher-fidelity, such as CFD, or non-linear solvers were used, their computational cost would be significantly greater.

α^*	V_∞^*	t_{sk}^*	t_{sp}^*	$f(\boldsymbol{x}^*)$	n^a	n^s
1.0	1.0	0.0	0.0	0.0	286	286

Table 2: Optimization results for the reference problem, where n^a is the number of aerodynamic solver calls and n^s is the number of structural solver calls.

As is shown, to converge exactly to the reference solution, a total of 286 solver calls to each disciplinary solver were needed. Of the 286 calls, 33.6% were made at the gradient computation step. This is an expected result, as the derivatives were calculated via finite difference approximation, which requires additional objective function evaluations.

3 DPOD+I implementation

According to the methodology proposed in [7], a surrogate model is built for each disciplinary solver. However, due to the high dimensionality of the coupling variables, a model order reduction must be

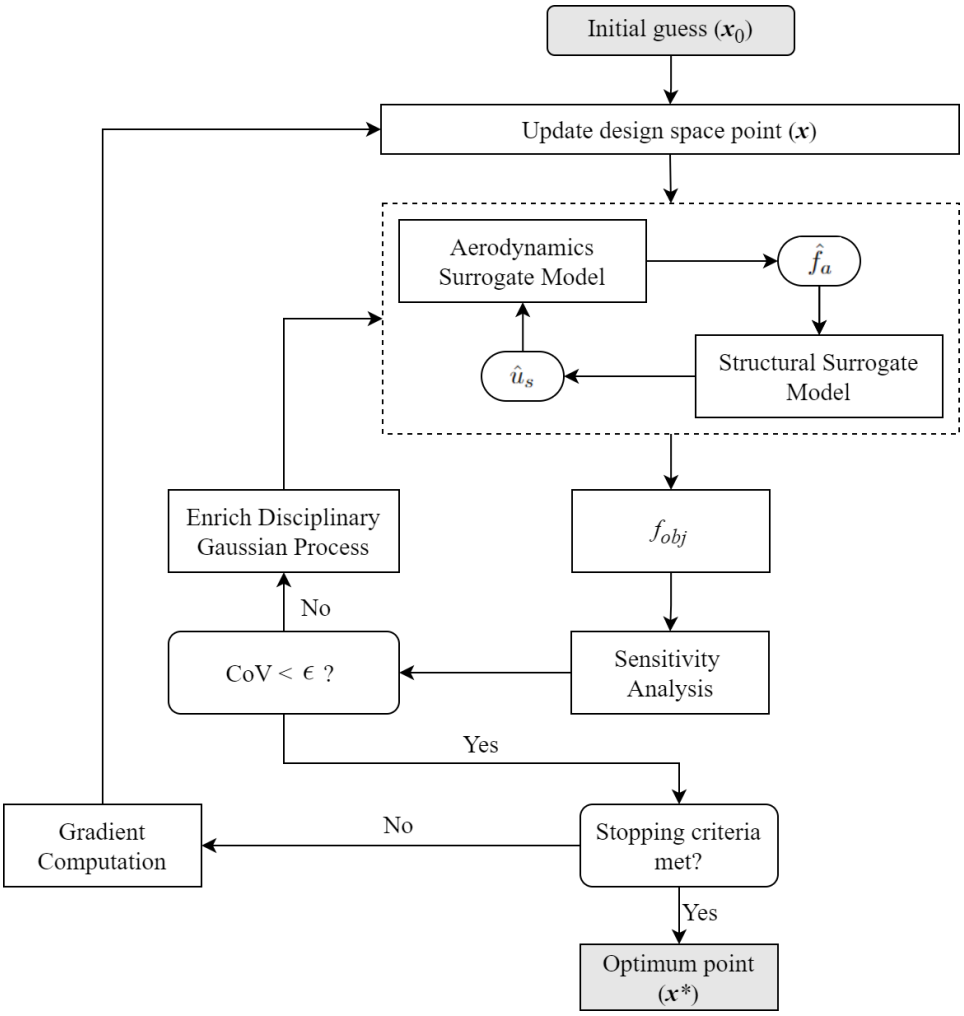


Figure 4: DPOD+I optimization framework.

performed before the surrogate interpolation. This reduction is carried out by Disciplinary Proper Orthogonal Decomposition (DPOD) and the surrogate interpolation is made by Gaussian Processes to approximate the POD coefficients. This is considered a pre-processing step which takes place before the beginning of the optimization (see [7] for details on the initial training phase).

It remains, nonetheless, possible to enrich the disciplinary surrogate models throughout the optimization. The decision of whether or not to enrich is made via sensitivity analysis, where, in the case where enrichment is deemed necessary, the less accurate discipline is identified and enriched. The adapted optimization framework is presented in Figure 4, where CoV is the coefficient of variation of the objective function and ϵ is a user defined threshold, used to decide whether or not to enrich the disciplinary surrogates. For the current implementation, a threshold of 10^{-3} was set, while the convergence criteria for the MDA and MDO were the ones defined for the reference problem. The gradient computation is made using the Gaussian process derivatives.

Lastly, it is worth noting that this implementation introduces randomness in the obtained solution. This is due to the DPOD+I training stage, where the DPOD coefficients are replaced by Gaussian processes, resulting in a corresponding random MDA (once more, readers are referred to [7] for details). For this reason, several runs must be performed so as to estimate the value of each parameter in the solution. The number of performed runs was set to 10.

3.1 DPOD+I optimization results

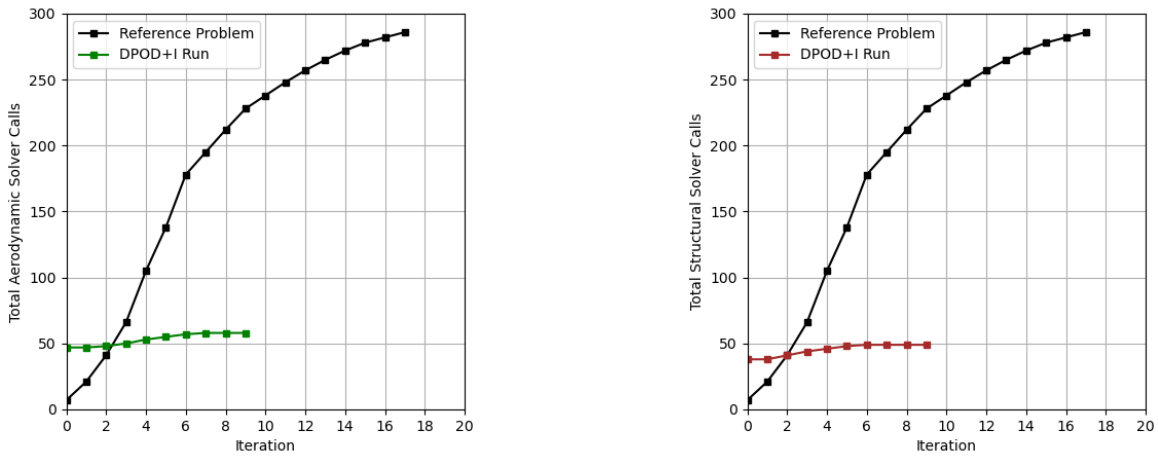
As previously stated, the construction of the disciplinary surrogates is a pre-processing step and therefore is not a part of the represented framework. Nonetheless, and to allow for a fair comparison, the associated computational cost should be taken into account. Concerning the size of the obtained POD basis, the average of the 10 performed runs resulted in a structural basis composed of 6 coefficients, while the aerodynamic basis was made of 5 coefficients.

The obtained results for the DPOD+I optimization framework are presented in Table 3, for the 10 performed runs. As is shown, the replacement of the disciplinary solvers by their DPOD+I surrogates induces a significant reduction in the overall computational cost of the optimization. Namely, for the aerodynamic discipline, an average of 60.7 solver calls were needed, of which around 52 were made in the training stage. Similarly, for the structural discipline, an average of 51.5 solvers calls were made, of which 42 corresponded to the training stage. In comparison to the reference problem this represents a reduction by a factor of 5 on the number of disciplinary solver calls. We further remark that, since the training phase is independent of the optimization, for a problem with multiple local minima where multi-start strategies are required for gradient-based solvers, the same basis may be kept regardless of the starting point. Although not explored in the present work, this is a clear advantage of the proposed DPOD+I implementation.

Finally we note that, due to the performed approximations, a small error is committed at the optimum point, both at the level of the design variables, at an order of magnitude of 10^{-4}, and of the objective function, at an order of magnitude of 10^{-2}, as is shown in table 3.

	α^*	V_∞^*	t_{sk}^*	t_{sp}^*	$f(\boldsymbol{x}^*)$	n^a	n^s
$\mathbb{E}$	1.0	1.0	3.4×10^{-4}	3.1×10^{-4}	0.0585	60.7	51.5
CoV	$\leq 10^{-12}$	$\leq 10^{-12}$	3.0	2.6346	0.1523	0.1904	0.1784

Table 3: Optimization results for the DPOD+I implementation. Average and coefficient of variation values obtained from a total of 10 runs.



(a) Aerodynamic solver calls

(b) Structural solver calls

Figure 5: History of disciplinary solver calls for the reference and DPOD+I implementations.

Figure 5 compares the number of disciplinary solver calls, as a function of the optimizer iteration, for one of the 10 performed runs of DPOD+I implementation against that of the reference problem. As is shown, the DPOD+I approach starts at a higher number of disciplinary solver calls, due to the training stage. Nonetheless, throughout the optimization not only fewer calls are made, but also a lower number of optimizer iterations is necessary, resulting in the overall lower computational cost.

4 EGMDO implementation

In addition to replacing the disciplinary solvers by their DPOD+I surrogates, we now consider the Efficient Global Multidisciplinary Design Optimization (EGMDO) algorithm proposed in [10]. Here, we depart from an initial Design of Experiments (DoE) which is used to obtain an approximation of the objective function, itself a random function. Contrarily to what is proposed in the classical Efficient Global Optimization (EGO) algorithm [5], however, in EGMDO the objective function cannot be modelled as a Gaussian Process due to the non-linearity of the MDA. Instead, its value at the DoE points is obtained by means of a Karhunen Loève expansion, and then extended to the rest of the domain via Gaussian process interpolation.

As in the previous implementation, the disciplinary surrogate models may be enriched at a given $\boldsymbol{x}^i$ point, if the coefficient of variation of the objective function is greater than a given threshold. However, in the EGMDO approach, an additional condition for enrichment is imposed – the point must have some likelihood of being the minimum, namely, $P_{\min}(\boldsymbol{x}^i) \geq \frac{1}{n_{\text{DoE}}}$. This avoids spending computational effort in areas of the design space where the global optimum is unlikely to be.

New points may also be added to the DoE. These points are determined by a modified Expected Improvement (EI) criterion, which, due to the non-Gaussian nature of the objective function, has no analytical expression and must be estimated via Monte Carlo simulation (see [10] for details on EI calculation). Regarding the stopping criterion, while in EGMDO the optimization is stopped when the change of maximum value of EI between two consecutive iterations is less than a given threshold, here we impose a maximum of 200 iterations. The computational framework of the EGMDO implementation is presented in Figure 6, where an initial DoE $\boldsymbol{x}_{\text{DoE}}$ of 20 points was considered.

Lastly, and before proceeding to the results, it is recalled that, since the combined DPOD+I and EGMDO implementation also introduces randomness in the solution, 10 runs were also performed for the present optimization.

4.1 EGMDO optimization results

As for the previous case, the training of the DPOD+I surrogates is considered as a pre-processing step and is not featured in the optimization framework. However, its computational cost is taken into account. The obtained results for the EGMDO implementation are presented in Table 4.

	α^*	V^*_∞	t^*_{sk}	t^*_{sp}	$f(\boldsymbol{x}^*)$	n^a	n^s
$\mathbb{E}$	0.999	0.987	0.006	3×10^{-7}	0.044	61	51
CoV	0.003	0.02	0.9	3.16	0.44	0.1117	0.1225

Table 4: Optimization results for the EGMDO implementation. Average and coefficient of variation values obtained from a total of 10 runs.

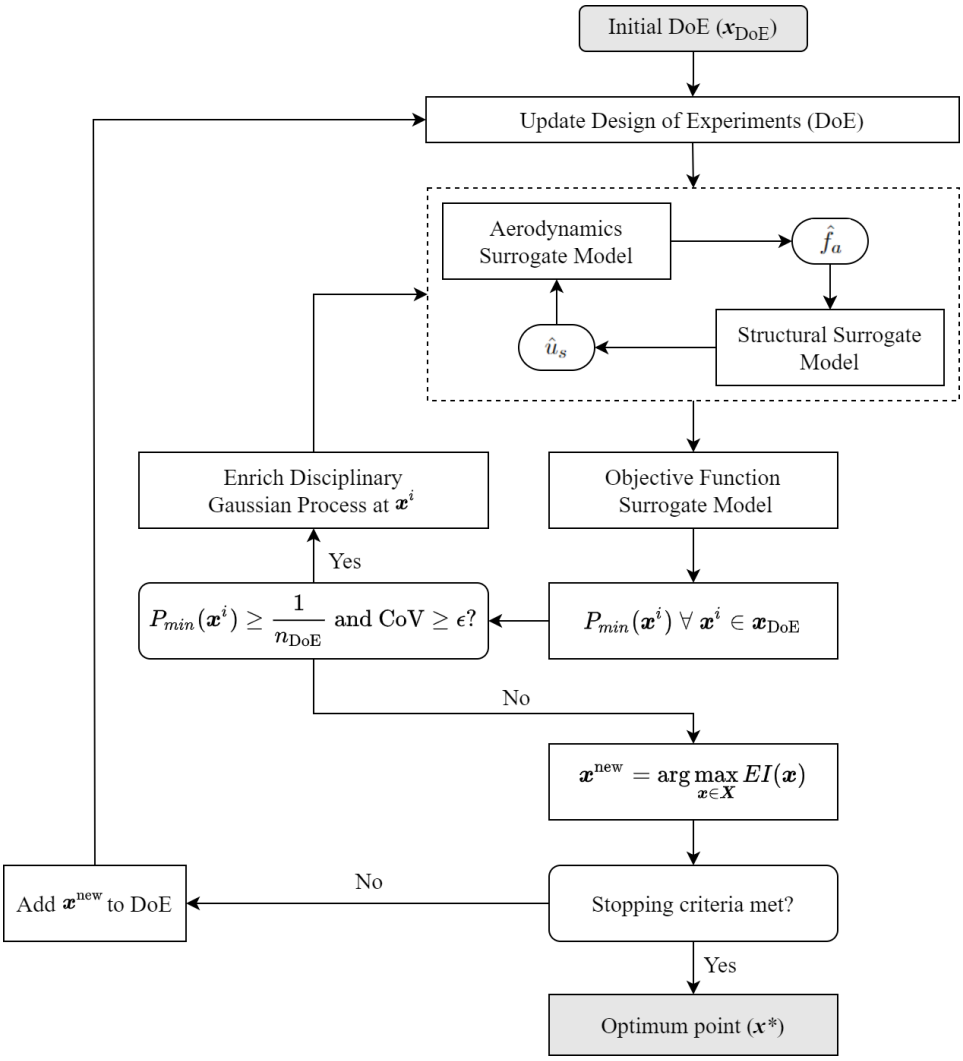


Figure 6: EGMDO optimization framework.

As is shown, an average of 61 solver calls were performed for the aerodynamics discipline, of which 59 were made during the DPOD+I surrogate training. Similarly, an average of 51 solver calls were made for the structural discipline, of which 49 corresponded to the pre-processing stage. This signifies that an average of only 2 calls were made to each disciplinary solver during the actual MDO resolution, implying that very few disciplinary solver enrichments were necessary to find the optimal point. In fact, comparing to the DPOD+I implementation, a reduction by a factor of 5 is observed in the number of disciplinary solver enrichments. A possible explanation for why very few enrichments are made is that, at the level of the DPOD+I surrogate training, a too strict convergence criterion was chosen, thus reducing the need for enrichment. For the present problem, it might be possible to further reduce the number of disciplinary solver calls if a less strict criterion was chosen. However, more complex problems will likely benefit from the well trained DPOD+I surrogates.

Finally, and as was the case for the DPOD+I implementation, due to the performed approximations, a small error, of the order of 10^{-2}, is committed both for the design variables and the objective function, as is evidenced in Table 4.

5 Conclusion and perspectives

In this work, different frameworks for multidisciplinary optimization were implemented and compared for an aeroelastic problem with two participating disciplines. The objective function was chosen as an inverse problem, where the goal was to find a known reference solution. In addition, no constraint was considered.

The initial implementation, and the most costly, consisted on modelling the disciplines by possibly expensive black-box solvers and solving the optimization by using the gradient-based SLSQP algorithm, in an MDF approach. This implementation, in addition to making several disciplinary solver calls to solve the MDA, requires gradient computation via finite difference approximation, which is itself an expensive computation.

A second implementation replaced the disciplinary solvers by their DPOD+I surrogates, according to the methodology proposed in [7]. This implementation resulted in significantly less disciplinary solver calls, as, throughout the optimization, the computationally expensive solvers were only called when the disciplinary Gaussian processes needed to be enriched. In addition, this approach eliminated the need to perform gradient computation via finite difference approximation, as the Gaussian process derivatives were used. Nonetheless, the training of the DPOD+I surrogates had an associated computational cost which could not be disregarded. As was remarked, however, in a multi-start context, the training phase would be run a single time, as it is independent of the optimization problem.

A last implementation replaced the optimizer by the EGMDO algorithm proposed in [10], in an effort to address global optimization, while keeping the DPOD+I surrogates to approximate the disciplines. This approach modelled the objective function as a non-Gaussian random field, approximated by a combination of Karhunen Loève expansion and Gaussian process interpolation, and used an adapted Expected Improvement criterion to enrich the disciplinary solvers solely where the global minimum was more likely to be. It was shown that, through this approach, very few enrichments were needed in order to find the optimum point, possibly due to the easy to find global optimum.

Having demonstrated the capabilities of the proposed framework, some perspectives are envisioned. Namely, the application of this strategy to more complex problems, such as the ones involving one or multiple non-linear disciplinary solvers, as these could prove to be a challenge for the POD approximation. Similarly, the inclusion of a greater number of design variables could raise a problem at the level of the disciplinary GP interpolation, currently done by the universal kriging model. Fortunately, some work has already been done in this field, from which we may benefit. For instance, in [19] Partial Least Squares is used for dimension reduction. Finally, it would be interesting to apply the proposed strategy to a problem with multiple local minima, which usually accompanies the aforementioned increase of complexity and dimensionality.

6 Acknowledgments

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