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# DEVELOPMENT OF MDO FORMULATIONS BASED ON DISCIPLINARY SURROGATE MODELS BY GAUSSIAN PROCESSES

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**Abstract.** *Surrogate based optimization is now well established in the field of derivative free optimization. Among the various possible approaches, this study focuses on Bayesian optimization using Gaussian process interpolation as surrogate models. From the pioneering work on unconstrained optimization based on the expected improvement to the latest developments of enrichment criteria to deal with nonlinear constrained problems, the Bayesian framework has been extensively studied and used in many application fields. During the last few years a collaboration between the authors led to the publication of several contributions aiming at the development and the evaluation of MDO formulations based on disciplinary Gaussian process surrogate models. In these formulations each disciplinary solver is modeled by Gaussian processes that are coupled to solve the MDA. Hence, the formulation is uncoupled as only the disciplinary surrogate models are coupled and not the actual disciplinary solvers. It is proposed here to focus on two challenges raised by this formulation, to which the authors contributed in the past. The first one concerns the extension and application of the Bayesian framework to the case in which the objective function is not modelled by a Gaussian random field. To make progress with respect to this issue, an original representation of this random field using an adaptive discretization strategy has been proposed leading to the Efficient Global Multidisciplinary Optimization (EGMDO) formulation. The second one concerns the resolution of the interdisciplinary coupling in the case of large vector valued coupling variables. As an example, static aeroelasticity which couples a CFD solver and a FEM solver is studied. Some proposals, based on model order reduction (e.g. Proper Orthogonal Decomposition) and Gaussian process interpolation, have been evaluated by the authors. Objective of this paper is thus to sum up these various contributions while presenting the potential benefits and remaining challenges of these MDO formulation to the MDO researchers community.*

**Keywords:** Multidisciplinary Design and Optimization, Bayesian Optimization, Gaussian Process Interpolation, Model Order Reduction

## 1 INTRODUCTION

Multidisciplinary Design and Optimization (MDO) is an attractive approach for aeronautic industry compared to the sequential optimization of each discipline involved in the design of a complex system (such as an aircraft). Indeed, by taking into account the interactions between disciplines, MDO allows to solve both the performance optimization and the consistency constraints between disciplines. Formally, this approach deals with the optimization of complex systems involving several disciplinary solvers coupled together in a non linear system of equations called Multidisciplinary Design Analysis (MDA). On the counterpart, the main drawbacks of this approach are the difficulty to set up the disciplinary coupling (non intrusive coupling between various numerical solvers) and the numerical cost due to the resolution of the MDA's non linear system of equations. Hence many studies have been focused on the development of MDO formulations in order to ease the implementation of the MDO and to reduce its computational cost. As representative examples one can cite the Multidisciplinary Feasible approach (MDF) and the Individual Discipline Feasible approach (IDF) [1]. These two approaches solve the exact MDO problem, MDF consists in solving the MDA by a non intrusive coupling of the disciplinary solvers at each iteration of the optimization algorithm, and thus uncouples the resolution of the optimization problem and the resolution of the MDA non linear system. It offers the advantage to reach a physically relevant solution at each step of the optimization phase, but leads to an important numerical cost as the MDA has to be solved at each iteration of the optimization process. Contrarily, the IDF approach uncouples the disciplinary solvers but couples the resolution of the optimization problem and the resolution of the MDA *i.e.* the optimization algorithm handling both the design variables and the coupling variables. Several other formulations have been proposed in the literature in order to solve the MDO problem in an efficient way. A review of some of these approaches can be found in [2]. It should be noted that the majority of these approaches only solve an approximation of the original MDO formulations.

In the following we are mainly interested in derivative free optimization (DFO), thus the gradient based approaches and coupled adjoined based developments will not be discussed here. Regarding the DFO approaches this paper will focus on Bayesian approaches. Indeed, since the pioneer work of [3] leading to the Efficient Global Optimization algorithm (EGO), the Bayesian framework has been regularly used and improved in many different optimization contexts. As an example in MDO Xu et al. [4] used the EGO as optimizer in the MDF, IDF and simultaneous analysis and design (SAND) MDO formulations and compared the results with gradient based and genetic optimization algorithms. A similar approach is also applied in [5] to a mixed discrete-continuous MDO problem. Another application of Bayesian optimization to costly MDO problem is presented in [6]. However these studies use the Bayesian framework with a minimal adaptation to the MDO context and mainly substitute classical gradient based optimizers by Bayesian ones. This remark was the starting point of several developments made by the authors to further increase the coupling between MDO and the Bayesian framework in the last years. The ambition of the present paper is thus to introduce these developments and to illustrate the advantages and constraints of a Bayesian approach in a multidisciplinary context.

The starting point of Bayesian optimization is the approximation of the objective function by a stochastic process, generally a Gaussian process. Then, this approximation is sequentially enriched to increase its accuracy in promising areas for optimization. This

strategy relies on the exploitation of the stochastic character of the approximation. Several criteria have been proposed in the literature to find these promising areas, the most famous one being probably the Expected Improvement. Thus a light coupling between MDO and Bayesian optimization consists in applying the previous strategy directly to the MDO formulation. Although this approach can be efficient it does not exploit the partitioned architecture of the MDA and our motivation is to take advantage of this partitioning to further improve the efficiency of the approach in a multidisciplinary context.

As a consequence, the basic idea that drove the development of an Efficient Global Multidisciplinary Design and Optimization (EGMDO) algorithm during the last 5 years was to replace each disciplinary solver involved in the MDA by a disciplinary Gaussian process (GP) surrogate model. This simple idea is illustrated in Fig. 1 on an MDO problem involving two disciplines.

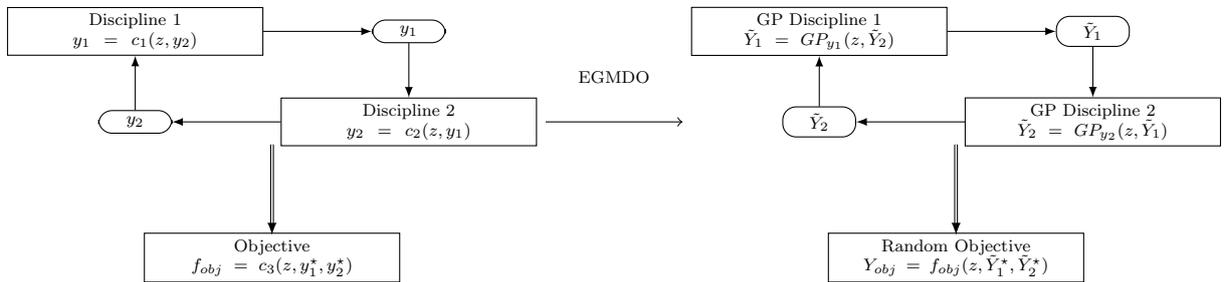


Figure 1: Illustration of an MDO problem involving two coupled disciplines and an objective function. On the left, the disciplines are given by some costly black-boxes. On the right, the disciplines have been replaced by some surrogate models (Gaussian Processes denoted by GPs).

Besides the apparent simplicity of this formulation, it raises several questions about the disciplinary surrogate model construction and their exploitation in a Bayesian framework. It is proposed here to focus on the two following topics:

1. How to sample the disciplinary surrogate models with respect to the coupling variables? In the case of scalar coupling variables this difficulty is generally solved by an expert judgement able to define appropriate variation bounds for each coupling variable. However in the case of large vector valued coupling variables, such as in the case of high fidelity aeroelastic coupling for example, this question is challenging and will be discussed in Section 3.
2. How to deal with the error introduced by the use of GP disciplinary surrogate models? Simplest answer is to construct disciplinary surrogate model *as accurate as possible* and to neglect the error introduced in the optimization process (as for example in [7], [8], [9] and [10]). Even if this approach can lead to satisfactory results it is obvious that its numerical cost can be far from optimal and that the accuracy at the minimum is hazardous.

Following the path of Bayesian optimization we proposed to sequentially enrich the disciplinary GPs with respect to their accuracy in promising areas for optimization. As a consequence the first step is to model the objective function as a stochastic process. In our context this objective function cannot be modelled by a GP as the

non linear coupling between the disciplinary GP leads to a non Gaussian model for the objective function. However this difficulty can be tackled by propagating the uncertainties introduced by the disciplinary GPs through the MDA. Section 2 described the proposed strategy to, propagate these uncertainties, model the objective function as a non Gaussian random process, and enrich the disciplinary GPs.

## 2 EFFICIENT GLOBAL MULTIDISCIPLINARY DESIGN AND OPTIMIZATION

### 2.1 Problem definition

First of all let us define the MDO problem that is of interest in the following:

Find the optimal design variables  $z^* \in \mathcal{Z}$  such that

$$z^* = \arg \min_{z \in \mathcal{Z}} f_{obj}(z, y_{c^{(obj)}}^*(z)) \quad (1)$$

where  $f_{obj}$  is the objective function to minimize which depends on the design variables  $z$  and on some (possibly all) of the converged coupling variables denoted by  $y_{c^{(obj)}}^*(z)$ . The design variables  $z$  belong to a design space  $\mathcal{Z} \subset \mathbb{R}^n$ . The converged coupling variables are denoted by  $y^*(z) = \{y_i^*(z), i = 1, \dots, n_d\}$  and  $c^{(obj)}$  is a set of indexes used to identify the coupling variables involved in the computation of the objective function. We wrote  $y^*(z)$  as the solution of the non linear system of  $n_d$  equations, called MDA,

$$y_i = f_i(z, y_{c^{(i)}}), \quad i = 1, \dots, n_d \quad \forall z \in \mathcal{Z} \quad (2)$$

where  $y_{c^{(i)}}$  is the vector of the coupling variables for the discipline  $i$  and  $n_d$  is the number of disciplines. The set of indexes denoted by  $c^{(i)}$  identifies the coupling variables *i.e.*  $\#(c^{(i)}) \leq (n_d - 1)$  and  $i \notin c^{(i)}$ . Finally,  $f_i$  is the solver of discipline  $i$ . Let us note that, with the previously introduced notations, disciplines  $i$  and  $j$  are said to have a feedback loop (or coupling) if  $i \in c^{(j)}$  and  $j \in c^{(i)}$ . In the following, it is assumed that Eq. (2) contains at least one feedback coupling. It is also assumed that Eq. (2) has a unique solution for any point of the design space.

As stand in the introduction, the idea of the proposed approach is to take advantage of the partitioned formulation of the MDA to construct disciplinary GPs. Hence the following notations are introduced to denote the disciplinary GPs. The GP that is used to approximate the disciplinary solver  $f_i$  is build from a Design of Experiments (denoted by  $\text{DoE}_{f_i}$ ) sampled over the space  $\mathcal{Z} \times C^{(i)}$  where  $C^{(i)}$  denoted the space of the coupling variables  $y_{c^{(i)}}$  for the discipline  $i$ . The idea of GP approximation is then to condition a prior GP on  $\text{DoE}_{f_i}$  and to estimate the parameters of this GP (by maximum likelihood in this work). In the following, random quantities will be denoted by upper case letters. This leads to the following stochastic approximation,

$$\tilde{Y}_i(z, y_{c^{(i)}}) = \mu_{f_i}(z, y_{c^{(i)}}) + \epsilon_i(z, y_{c^{(i)}}) \quad (3)$$

where  $\mu_{f_i}(z, y_{c^{(i)}})$  is the mean function of the GP and  $\epsilon_i(z, y_{c^{(i)}})$  is a zero mean GP whose covariance function is the one of the prior GP conditioned on  $\text{DoE}_{f_i}$ . Thus for a given couple  $(z^{(0)}, y_{c^{(i)}}^{(0)}) \in \mathbb{R}^n \times C^{(i)}$  that does not belong to  $\text{DoE}_{f_i}$ , the obtained approximation reads,

$$\tilde{Y}_i(z^{(0)}, y_{c^{(i)}}^{(0)}) = \mu_{f_i}(z^{(0)}, y_{c^{(i)}}^{(0)}) + \sigma_{f_i}(z^{(0)}, y_{c^{(i)}}^{(0)})\xi_i \quad (4)$$

where  $\mu_{f_i}(z^{(0)}, y_{c^{(i)}}^{(0)})$  is the mean value,  $\sigma_{f_i}(z^{(0)}, y_{c^{(i)}}^{(0)})$  is the standard deviation and  $\xi_i$  is a standard Gaussian random variable. It should be noted that the expressions of  $\epsilon_i$ ,  $\mu_{f_i}$  and  $\sigma_{f_i}$  are fully specified by the kind of Gaussian process approximation used. For conciseness we choose here to not detail the theory of Gaussian process interpolation and refer the reader to [11] instead.

In practice one can note that the construction of disciplinary GP assumed that it is possible to sample the disciplinary solver  $f_i$  over the space  $\mathcal{Z} \times C^{(i)}$ . If it is easy to define the range of variation for  $\mathcal{Z}$  it could be much more challenging for  $C^{(i)}$ . In this section it is assumed that an expert judgement defines the range of variation of the coupling variables.

Once each disciplinary GP has been constructed independently one can form the following stochastic non linear system of  $n_d$  equations,

$$\tilde{Y}_i(z, \tilde{Y}_{c^{(i)}}) = \mu_{f_i}(z, \tilde{Y}_{c^{(i)}}) + \epsilon_i(z, \tilde{Y}_{c^{(i)}}), \quad i = 1, \dots, n_d \quad \forall z \in \mathcal{Z} \quad (5)$$

where  $\tilde{Y}_{c^{(i)}}$  stands for the random vector of coupling variables affecting the discipline  $i$ . We define the solution of this random non linear system of equations as the joined probability distribution of the random vector of the converged coupling variables  $\tilde{Y}^*(z) = \{\tilde{Y}_i^*(z), i = 1, \dots, n_d\}$  such that,

$$\tilde{Y}_i^*(z, \tilde{Y}_{c^{(i)}}^*(z)) = \mu_{f_i}(z, \tilde{Y}_{c^{(i)}}^*(z)) + \epsilon_i(z, \tilde{Y}_{c^{(i)}}^*(z)), \quad i = 1, \dots, n_d \quad \forall z \in \mathcal{Z} \quad (6)$$

Let us underline here that the joined probability density function of  $\tilde{Y}^*(z)$  is not Gaussian as the MDA is a non linear system. However samples of  $\tilde{Y}^*(z)$  can be obtained by drawing various realizations of the GP surrogate models and solving the MDA for each draw.

Random MDA has been previously studied and several approaches have been proposed to approximate solution of such a system (see for example [12], [13], [14], and [15]). The next section details the proposed method in our context.

## 2.2 Coupling of disciplinary GPs and uncertainty propagation

Objective of this part is to solve the stochastic non linear system of equations given by Eq. (5) in order to get the probability distribution of the objective function defined by,

$$Y_{obj}(z, \tilde{Y}_{c^{(obj)}}^*(z)) = f_{obj}(z, \tilde{Y}_{c^{(obj)}}^*(z)), \quad \forall z \in \mathcal{Z} \quad (7)$$

In order to simplify this resolution we proposed in [15] to use a specific GP model for each disciplinary solver. Indeed, the GP model given by Eq. (3) involved a zero mean GP  $\epsilon_i$  with a complex correlation structure. Dealing with the simulation of such a stochastic process is not straightforward as it needs to be represented by a finite number of random variables to be exploitable (by Karhunen-Loève decomposition for example). Instead, we propose to simplify the disciplinary GP model by a perfectly dependent stochastic process that shares the same pointwise variance as the initial one and that reads,

$$\tilde{Y}_i'(z) = \mu_{f_i}(z, y_{c^{(i)}}) + \sigma_i(z, y_{c^{(i)}})\xi_i$$

where the variance is computed regarding Eq. (5) by  $\forall z, y_{c^{(i)}} \in \mathcal{Z} \times \mathbb{R}^{\#c^{(i)}}$ ,  $\sigma_i(z, y_{c^{(i)}})\xi_i = \epsilon_i(z, y_{c^{(i)}})$ , with  $\xi_i$  a standard Gaussian random variable.

The huge advantage of this approach is that each disciplinary GP is now described by a single Gaussian random variable  $\xi_i$ . As a consequence it is proposed to solve the system,

$$\tilde{Y}_i'^*(z, \tilde{Y}_{c(i)}'^*) = \mu_{f_i}(z, \tilde{Y}_{c(i)}'^*) + \sigma_i(z, \tilde{Y}_{c(i)}'^*)\xi_i, \quad i = 1, \dots, n_d \quad (8)$$

whose solution is denoted by the random vector  $\tilde{Y}'^*(z) = \{\tilde{Y}_1'^*(z), \dots, \tilde{Y}_{n_d}'^*(z)\}$ . As the variances of the simplified disciplinary GP involved in Eq. (8) and the ones of the disciplinary GP involved in Eq. (5) are equal, we assume that the probability distribution of  $\tilde{Y}'^*(z)$  is a correct approximation of the one of  $\hat{Y}^*(z)$ . It should be noted that the accuracy of this approximation has been numerically checked in [15]. Moreover, from a numerical point of view, Eq. (8) is much more simple to solve than Eq. (5) as it only involves  $n_d$  independent standard Gaussian random variables denoted by the vector  $\Xi = \{\xi_i, i = 1, \dots, n_d\}$  in the following.

Once the problem is described by  $n_d$  independent Gaussian random variables, it is easy to simulate a sample of the random vector  $\tilde{Y}'^*(z)$  by solving Eq. (8) for various draws of the simplified disciplinary GP. It should be noted that any non linear solver can be used for this task and that the numerical cost of this operation is negligible as it only involves analytical simplified GP.

Using this sample, it is straightforward to obtain a sample of  $Y_{obj}(z, \tilde{Y}_{c(obj)}^*(z))$  by evaluations of Eq. (8) and Eq. (7). At this step it is proposed to construct a representation of this random variable by a Polynomial Chaos Expansion (PCE). This choice can seem arbitrary but offers many advantages for setting up the Bayesian optimization framework presented in the next section. Hence, the objective function is approximated by

$$\hat{Y}_{obj}(z, \Xi) = \sum_{j=1}^P a_j^{(obj)}(z) H_j(\Xi) \quad \forall z \in \mathcal{Z} \quad (9)$$

where  $H_j$ ,  $j = 1, \dots, P$  are the  $n_d$ -variate Hermite polynomials,  $P$  is the number of selected polynomial terms and  $a_j^{(obj)}(z)$ ,  $j = 1, \dots, P$  are the coefficients of the expansion to be determined. The retained truncation strategy consists in keeping all the polynomials with a degree less or equal to  $d$ , thus  $P = \frac{(n_d+d)!}{n_d!d!}$ . Computation of these coefficients can be obtained by various approaches. In the following the regression approach introduced in [16] is retained. It should be noted that this method is easy to set up in the context of the study as a large number of samples of  $Y_{obj}(z, \tilde{Y}_{c(obj)}^*(z))$  can be obtained at a very low numerical cost as explained previously.

A PCE representation of  $Y_{obj}(z, \Xi)$  can thus be obtained for any point  $z \in \mathcal{Z}$  by Eq. (9). The variation of  $Y_{obj}(z, \Xi)$  is representative of the uncertainty introduced by the use of the disciplinary GPs, hence if the disciplinary GPs are not accurate for a given  $z^{(0)}$  the variation of  $Y_{obj}(z^{(0)}, \Xi)$  is expected to be important and if the disciplinary GPs are accurate for a given  $z^{(1)}$  the variation of  $Y_{obj}(z^{(1)}, \Xi)$  is expected to be low. As one is able to evaluate the variation of  $Y_{obj}(z, \Xi)$ , thanks to the PCE representation, for any point  $z \in \mathcal{Z}$ , the next step is to enrich the disciplinary GP until the variation of  $Y_{obj}(z, \Xi)$  is null at the minimum value. The difficulties are then to propose an enrichment criterion that focuses on the interesting areas and to deal with a non Gaussian representation of  $Y_{obj}(z, \Xi)$ .

### 2.3 A non Gaussian model for $Y_{obj}(z, \Xi)$ and its enrichment

The previous section introduces a *discrete* representation of the stochastic process  $Y_{obj}(z, \Xi)$  thanks to the PCE representation given by Eq. (9). This representation allows to compute approximations of  $Y_{obj}(z, \Xi)$  for different values of  $z$  by an uncertainty quantification step. In the following it is assumed that the uncertainty quantification by PCE has been performed on a DoE denoted by  $\text{DoE}_{UQ} = \{z^{(i)}, i = 1, \dots, n_{UQ}\}$ . The obtained PCE formed the following random vector

$$\hat{\mathbf{Y}}_{obj}(\Xi) = \left\{ \hat{Y}_{obj}(z^{(i)}, \Xi), i = 1, \dots, n_{UQ} \right\}$$

The random vector  $\hat{\mathbf{Y}}_{obj}$  is a discretization of the random field  $\hat{Y}_{obj}(z, \Xi)$ . As shown in [12] the Karhunen Loève expansion of this random vector can be easily obtained thanks to the coefficients of the polynomial chaos expansion and reads,

$$\hat{\mathbf{Y}}_{obj}(\Xi) = \mu_{\hat{\mathbf{Y}}_{obj}} + \sum_{k=1}^{n_{UQ}} \left( \sum_{j=2}^P \mathbf{a}_j^t \hat{\varphi}_k \phi_j(\Xi) \right) \hat{\varphi}_k \quad (10)$$

where  $\mathbf{a}_j = \left\{ a_j^{(obj)}(z^{(1)}), \dots, a_j^{(obj)}(z^{(n_{UQ})}) \right\}$ ,  $j = 2, \dots, P$ ,  $\mu_{\hat{\mathbf{Y}}_{obj}} = \mathbf{a}_1$  and  $\hat{\varphi}_k$  are the  $n_{UQ}$  eigenvectors of the covariance matrix  $\mathbf{K}_{\hat{\mathbf{Y}}} = \sum_{i=2}^P \mathbf{a}_i \mathbf{a}_i^t$ .

In order to set up a Bayesian optimization framework it is now necessary to introduce a *continuous* representation of the random field  $\hat{Y}_{obj}(z, \Xi)$ , with respect to  $z$ . For that purpose we propose in [17] to approximate the random field  $\hat{Y}_{obj}(z, \Xi)$  by Gaussian process interpolation of the mean value and of the eigenvectors based on the vectors  $\mu_{\hat{\mathbf{Y}}_{obj}}$  and  $\hat{\varphi}_k$  respectively. This leads to the following representation of the random field,

$$\hat{Y}_{obj}(z, \Xi) \approx \tilde{Y}_{obj}(z, \Xi, \eta) = \tilde{\mu}_{\hat{\mathbf{Y}}_{obj}}(z, \eta_0) + \sum_{k=1}^{n_{UQ}} \left( \sum_{j=2}^P \mathbf{a}_j^t \hat{\varphi}_k \phi_j(\Xi) \right) \tilde{\varphi}_k(z, \eta_k), \quad \forall z \in \mathcal{Z} \quad (11)$$

where  $\tilde{\mu}_{\hat{\mathbf{Y}}_{obj}}(z, \eta_0)$  and  $\tilde{\varphi}_k(z, \eta_k)$  are respectively the GP interpolation of the mean vector  $\mu_{\hat{\mathbf{Y}}_{obj}}$  and of the eigenvectors  $\hat{\varphi}_k$ . The term  $\eta = [\eta_0, \dots, \eta_k, \dots, \eta_{n_{UQ}}]^t$  is a random vector of  $n_{UQ} + 1$  independent normal random variables modeling the uncertainty associated with these GP interpolations.

Even if the representation given by Eq. (10) can look complex it is actually quiet easy to implement and, more importantly, it is a very efficient tool to set up our Bayesian optimization framework. Indeed, one can note that it contains all the uncertainties due to the proposed approximations. More precisely, the vector  $\Xi$  models the uncertainty stemming from the use of disciplinary GPs to approximate the costly disciplinary solvers and the vector  $\eta$  models the uncertainty due to the interpolation of the mean and eigenvectors of the KL decomposition used to obtain a continuous representation of the objective function random field.

Using this continuous representation it is now possible to define an enrichment criterion. The one use in this work is the classical Expected Improvement (EI) defined by,  $\forall z \in \mathcal{Z}$

$$\text{EI}(z) = \mathbb{E} \left[ \left( \hat{Y}_{min}^{(obj)}(\Xi) | z \in \text{DoE}_{UQ} - \tilde{Y}_{obj}(z, \Xi, \eta) \right) \mathbf{1}_{\tilde{Y}_{obj}(z, \Xi, \eta) \leq \hat{Y}_{min}^{(obj)}(\Xi) | z \in \text{DoE}_{UQ}} \right] \quad (12)$$

where

$$\mathbb{1}_{\tilde{Y}_{obj}(z, \Xi, \eta) \leq \hat{Y}_{min}^{(obj)}(\Xi) | z \in \text{DoE}_{UQ}} = 0 \text{ if } \tilde{Y}_{obj}(z, \Xi, \eta) > \hat{Y}_{min}^{(obj)}(\Xi) | z \in \text{DoE}_{UQ} \text{ and}$$

$$\mathbb{1}_{\tilde{Y}_{obj}(z, \Xi, \eta) \leq \hat{Y}_{min}^{(obj)}(\Xi) | z \in \text{DoE}_{UQ}} = 1 \text{ if } \tilde{Y}_{obj}(z, \Xi, \eta) \leq \hat{Y}_{min}^{(obj)}(\Xi) | z \in \text{DoE}_{UQ}.$$

One can note that  $\text{EI}(z)$  is positive for  $z \notin \text{DoE}_{UQ}$  and that  $\text{EI}(z) = 0$  if  $z \in \text{DoE}_{UQ}$ . The point  $z^{(new)}$  where the uncertainty quantification by PCE should be performed is thus solution of the optimization problem,

$$z^{(new)} = \arg \max_{z \in \mathcal{Z}} (\text{EI}(z)) \quad (13)$$

It should be noted that the EI defined by Eq. (12) is different from the one proposed in [3] in the context of optimization of black-box functions. In particular, as the approximation Eq. (11) is not a Gaussian process, the EI defined by Eq. (12) can not be computed analytically and will be estimated by MC sampling (see [17] for details about estimation and optimization of the EI).

The point  $z^{(new)} \in \mathcal{Z}$  that solves Eq. (13) is the one where the uncertainty should be reduced to improve our knowledge on the minimum of the deterministic objective function. There are two ways to reduce this uncertainty, first one is to compute the PCE representation  $\hat{Y}_{obj}(z^{(new)}, \Xi)$  which cancels the uncertainty due to the continuous representation of the random field and modelled by the random vector  $\eta$ . Second one is then to enrich the disciplinary GP in order to reduce the uncertainty modelled by the vector  $\Xi$ . As this second step is not always necessary to discriminate a candidate  $z^{(new)}$  it is proposed in [18] a two step enrichment, one at the continuous level (with respect to  $\eta$ ) and one at the discrete level (with respect to  $\Xi$ ) to further reduce the number of calls to the disciplinary solvers. The details of this enrichment strategy can be found in [18] and will not be detailed here as these technical details are not necessary for the global understanding of the proposed method. It should also be noted that two slightly different versions of the enrichment procedure are available in [19] and [18].

## 2.4 Application example

The EGMDO strategy described in the previous section has been applied to different test cases in [19] and in [18] including overall aircraft design problem.

In the following it is proposed to detail and comment an analytical example studied in [18] as this one offers a robustness study and several comparisons with other MDO algorithms. This test case is derived from the one proposed by Sellar et al. [20]. The proposed test case is unconstrained and counts one local and one global minima. It is defined by the following set of equations,

$$f_{obj}(z, y_{c^{(obj)}}^*) = z_1 + z_3^2 + y_1^* + \exp(-y_2^*) + 10 \cos(z_2)$$

where  $z = \{z_1, z_2, z_3\}$ ,  $c^{(obj)} = \{1, 2\}$  and  $y^* = \{y_1^*, y_2^*\}$  is solution of the following MDA,  $\forall z \in \mathcal{Z}$ ,

$$\begin{aligned} y_1 &= f_1(z, y_2) = z_1 + z_2^2 + z_3 - 0.2y_2 \\ y_2 &= f_2(z, y_1) = \sqrt{y_1} + z_1 + z_2 \end{aligned}$$

Design space is defined by  $\mathcal{Z} = [0, 10] \times [-10, 10] \times [0, 10]$ . Reference solution is obtained by using MDF approach with SLSQP optimization algorithm and leads to  $z^* \approx \{0, 2.634, 0\}$ ,  $f_{obj}(z^*) \approx -2.808$ . Figure 2 presents the variation of  $f_{obj}$  in the plane  $(z_2, z_3)$  with  $z_1 = 0$ .

It should be noted that the local minimum is located at  $z^{lm} \approx \{0, -2.595, 0\}$  and leads to  $f_{obj}(z^{lm}) \approx -0.809$ .

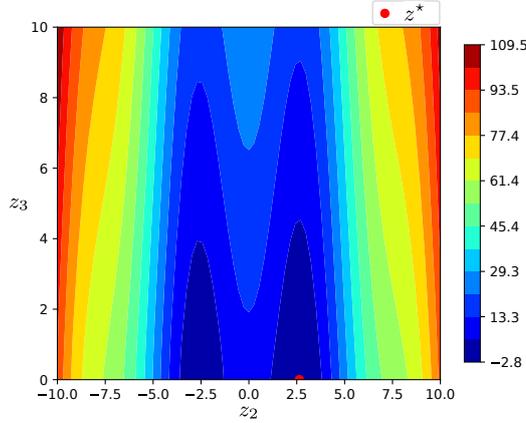


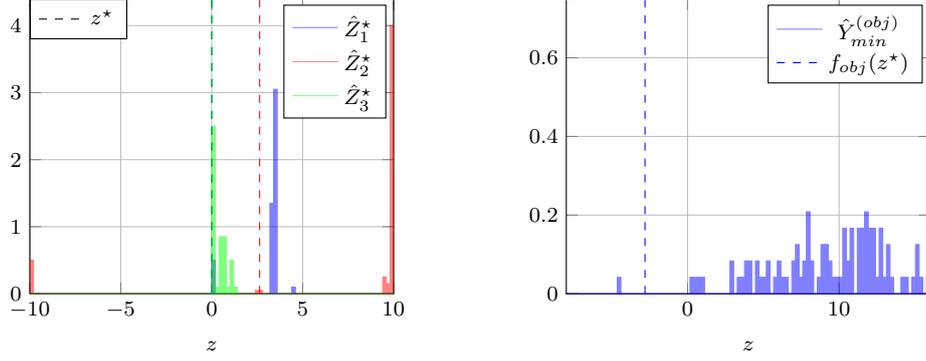
Figure 2: Application problem. Variation of  $f_{obj}$  in the plan  $(z_2, z_3)$  with  $z_1 = 0$  and location of the global minimum  $z^*$ .

In order to set up the proposed approach, the initial guesses for the coupling variables spaces are the following,  $C^{(1)} = [-5, 24]$  and  $C^{(2)} = [1, 50]$ . It should be noted that choosing the initial guesses for the coupling variables spaces is one of the drawback of the proposed approach. However, in a realistic case one can rely on expert judgment to get a first approximation and, more importantly, the proposed enrichment strategy is designed to enrich these coupling spaces in promising areas without any limitation. As a consequence the boundaries of the coupling variables spaces might evolve during the iterations of the EGMDO algorithm and thus a poor initial choice for these boundaries might lead to some extra iterations but should not be detrimental to the global convergence.

The initial disciplinary DoEs,  $\text{DoE}_{f_1}$  and  $\text{DoE}_{f_2}$ , count 5 points, respectively sampled by Latin Hypercube Sampling (LHS) over  $\mathcal{Z} \times C^{(1)}$  and  $\mathcal{Z} \times C^{(2)}$ . Initial disciplinary GPs are then constructed using these DoEs and constant mean function and Gaussian covariance function are used. According to the proposed method the objective function is represented by a random field over  $\mathcal{Z}$ . The initial  $\text{DoE}_{UQ}$ , used to discretized this random field, counts 20 points sampled by LHS over  $\mathcal{Z}$ . Hence, uncertainty propagation by PCE is carried out at 20 points, PCE of degree 3 is retained and computation of the PCE coefficients is obtained by regression over 100 points. It should be noted that the regression sample of size 100 is obtained by solving non linear systems given by Eq. (8) only involving disciplinary GPs and thus having a negligible numerical cost.

At this initial stage, the approximation given by Eq. (11) is used to compute the approximation of the random variable modeling the position of the minimum (denoted by  $\hat{Z}^*$ ) and the random variable modeling the value of the minimum (denoted by  $\hat{Y}_{min}^{(obj)}$ ). Figure 3 presents the results where histograms are obtained by 100 MC simulations using the model defined by Eq. (11).

Figure 3 shows that at initialization, the position of the global minimum (Fig. 3 i)) as well as its value (Fig. 3 ii)) are poorly predicted by the model given by Eq. (11). Indeed the mean value of the random position of the minimum  $\hat{Z}^*$  is far from the reference one and its variance is quite large and consequently the random minimum value of the objective



i) 3 components of  $\hat{Z}^*$  and the reference ones  $z^* \approx \{0, 2.634, 0\}$  ii) Objective value  $\hat{Y}_{min}^{(obj)}$  and the reference one  $f_{obj}(z^*) \approx -2.808$

Figure 3: Application example. i) Histograms of the minimum value position  $\hat{Z}^*$  ii) Histogram of the minimum value  $\hat{Y}_{min}^{(obj)}$  at initialization of the EGMDO algorithm.

function  $\hat{Y}_{min}^{(obj)}$  presents a large variation. The objective of the proposed approach is to increase the accuracy of the model given by Eq. (11) by improving the disciplinary GPs only where the minimum is likely to be.

On this example the number of enrichment steps is set to  $n_{max} = 10$ . During these 10 iterations, 6 points are added to the disciplinary GPs which leads to a number of disciplinary solver evaluations equal to  $5 + 6 = 11$ .

Figure 4 presents the evolution of the maximum value of the EI defined by Eq. (12) with respect to the enrichment steps. As expected the maximum value of the EI is globally decreasing during iterations. Hence the uncertainty about the minimum value and position of the minimum of  $f_{obj}$  is reduced by the enrichment strategy.

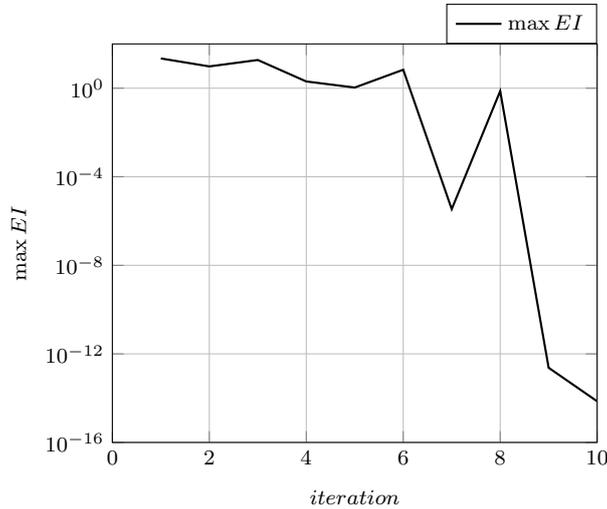
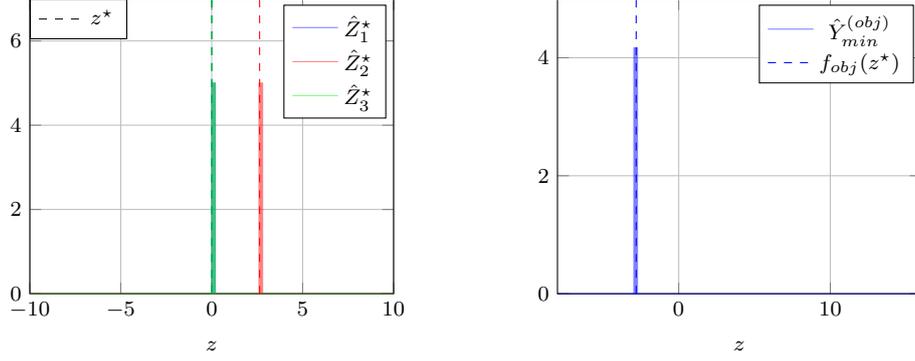


Figure 4: Application example. Evolution of the maximum value of the EI defined by Eq. (12) with respect to the number of iterations of the proposed EGMDO algorithm.

Figure 5 illustrates this uncertainty reduction and presents the histograms of  $\hat{Z}^*$  and  $\hat{Y}_{min}^{(obj)}$  obtained after the 10 enrichment steps. Histograms are still obtained by 100 MC simulations using the model defined by Eq. (11).

Compared to Fig. 3 one can note in Fig. 5 that the proposed algorithm reaches its



i) 3 components of  $\hat{Z}^*$  and the reference ones  $z^* \approx \{0, 2.634, 0\}$       ii) Objective value  $\hat{Y}_{min}^{(obj)}$  and the reference one  $f_{obj}(z^*) \approx -2.808$

Figure 5: Application example. i) Histograms of the minimum value position  $\hat{Z}^*$  ii) Histogram of the minimum value  $\hat{Y}_{min}^{(obj)}$  after 10 enrichment steps.

objective after 10 iterations as the random minimum position  $\hat{Z}^*$  is almost multi-Dirac distributed and the three modes are in perfect agreement with the reference values. Concerning the random minimum value  $\hat{Y}_{min}^{(obj)}$  the obtained probability distribution is also very close to a Dirac in perfect agreement with the reference value.

Some comparisons with classical MDO formulations are now provided. More precisely the MDF and IDF formulations are used in conjunction with the following optimization algorithm:

- A gradient based algorithm namely SLSQP Sequential Least Squares Programming [21] where gradient is estimated by finite differences,
- A gradient free algorithm namely COBYLA Constrained Optimization BY Linear Approximation [22],
- A surrogate based algorithm namely EGO Efficient Global Optimization [3] using either the Expected Improvement criterion (EI) or an alternative criterion denoted by WB2s (see [6] for the definition of WB2s criterion).

Resolution with SLSQP and COBYLA has been implemented using the python package scipy [23], resolution with EGO used an in house python implementation [6]. For each of these formulations 100 runs are performed with different starting points for SLSQP and COBYLA and different initial DoE for EGO (initial DoE of size 12 for the MDF-EGO and of size 20 for the IDF-EGO) and different  $DoE_{f_1}$ ,  $DoE_{f_2}$ ,  $DoE_{UQ}$  for EGMDO. Table 1 presents the number of runs that converged towards the global optimum (line  $n_{con}$ ) and the mean number of disciplinary solver evaluations over the  $n_{con}$  runs that converged (line  $n_{eval}$ ).

Results provided by Table 1 allow to draw several conclusions:

- As expected, the number of evaluations of the disciplinary solvers is lower using the IDF approach than the MDF approach.
- Classical local optimization algorithms (gradient based SLSQP or gradient free COBYLA) have a poor convergence rate (between 56% and 70%) using either the MDF or the IDF formulation.

	MDF-SLSQP	MDF-COBYLA	MDF-EGO-EI	MDF-EGO-WB2s	EGMDO
$n_{con}(\%)$	57	66	96	100	88
$n_{eval}$	197	638	296	212	13
	IDF-SLSQP	IDF-COBYLA	IDF-EGO-EI	IDF-EGO-WB2s	
$n_{con}(\%)$	56	70	99	100	
$n_{eval}$	68	206	63	44	

Table 1: Application example, comparative study. Results obtained with MDF and IDF formulations with 3 different optimizers (SLSQP, COBYLA, EGO with two criteria EI and WB2s). Number of converged runs and mean number of disciplinary solver evaluations are reported for each formulation over 100 runs. Results obtained by the proposed EGMDO approach are provided in the last column.

- Global surrogate based optimizer EGO reaches the best results in terms of convergence rate (between 96% and 100%). It is notable that both MDF and IDF formulations in conjunction with the WB2s criterion converge to the global optimum for every run.
- The best result is obtained using IDF formulation with EGO-WB2s as optimizer. This approach converges to the global optimum for every case with a mean number of disciplinary solver evaluations equals to 44 which is the lowest value on this comparison.
- Concerning the result obtained with the proposed EGMDO approach, one can note that the convergence rate of 88% is better than the one obtained using local optimizers but lower than the one obtained by EGO. However the mean number of disciplinary solver evaluations is only 13 for the EGMDO approach, compared to 44 for the IDF-EGO-WB2s. As a conclusion these results should be seen as promising for the new EGMDO approach as, even if it does not reach a 100% convergence rate, the benefit in terms of disciplinary solver evaluations is important.

## 2.5 Conclusions

This first section has briefly presented the EGMDO method that has been developed by the authors over the last five years. This approach can be summarized by the following few points:

- Construct disciplinary surrogate models by GP for each disciplinary solver involved in the MDA.
- Propagate the uncertainty stemming from the disciplinary GP. This step has been studied by the authors in [15] in which a PCE representation of the objective function was proposed.
- Construct a continuous representation of the non Gaussian random field modelling the objective function. Such a continuous model has been introduced by the authors in [17].
- Exploit this model to enrich the disciplinary GP until the global minimum of the objective function is reached with a given accuracy. This enrichment strategy has been proposed in [19] and in [18].

The first results obtained by this approach are promising and it is clear for the authors that many improvements can be achieved in the different steps of the proposed algorithm. However the proposed approach is dedicated to low dimensional coupling variables as each one is modelled by a disciplinary GP. In the following we proposed an extension dedicated to the large vector valued coupling variables, which opens the gate to the resolution of high fidelity MDA by a Bayesian approach as it will be presented in the last part of the next section.

### 3 HANDLING LARGE VECTOR VALUED COUPLING VARIABLES: THE EXAMPLE OF AEROELASTICITY

In the following we are interested in the partitioned resolution of non linear system of equations involving the resolution of partial differential equation by numerical methods such as the finite element method and/or the finite volume method. Compared to the previous section the new difficulty here comes from the dimension of the coupling variables. Indeed, in the *strong* coupling case, the disciplinary solvers exchange high dimensional information such as pressure or displacement fields expressed on different meshes. Sharing this high dimensional information creates some difficulties in terms of sharing information between meshes and different approaches [24] are available to set up the partitioned approach. This difficulty will not be discussed any further in the present paper and coupling will be set up using interpolation by radial basis function as presented in [25].

Even if the approach detailed in the following can be set up for any MDA involving vector valued coupling variables it is proposed to focus on static aeroelasticity of a wing. More precisely it is assumed that the structural model is linear elastic and solved by a finite element method and that the aerodynamic model is a potential fluid model solved by the vortex lattice (VLM) method. Hence this illustrative MDA problem reads:

Find the displacement field  $U(z, \Gamma)$  and the circulation vector  $\Gamma(z, U)$  over a wing that solve,

$$\begin{cases} U(z, \Gamma) = f_1(z, \Gamma) \\ \Gamma(z, U) = f_2(z, U) \end{cases} \quad (14)$$

where  $f_1$  and  $f_2$  are respectively the finite element and the VLM solvers. In Eq. (14) it is assumed that the interpolation operators discussed previously are *hidden* in  $f_1$  and  $f_2$ , thus the coupling variables of the problem are  $U \in \mathbb{R}^{n_s}$ ,  $n_s$  being the dimension of the finite element discretization (number of degrees of freedom), and  $\Gamma \in \mathbb{R}^{n_a}$ ,  $n_a$  being the size of the VLM mesh (number of panels).

As an illustration, Fig. 6 presents the type of numerical models that are used for our numerical experiments. These models, while not state of the art, are representative of the complexity of the models used in overall aircraft design MDO problems and allow to set up and assess the performance of the proposed approach efficiently. Note that we plan to increase the complexity of these models in the future.

In order to apply the EGMDO strategy developed in the previous section it is proposed to use model order reduction and interpolation by GP in different ways introduced in the following.

#### 3.1 Model order reduction of converged multidisciplinary analysis

The first idea to introduce high fidelity coupling in the EGMDO algorithm is to use reduced order model of the disciplinary solution of the MDA. Hence it is proposed to use

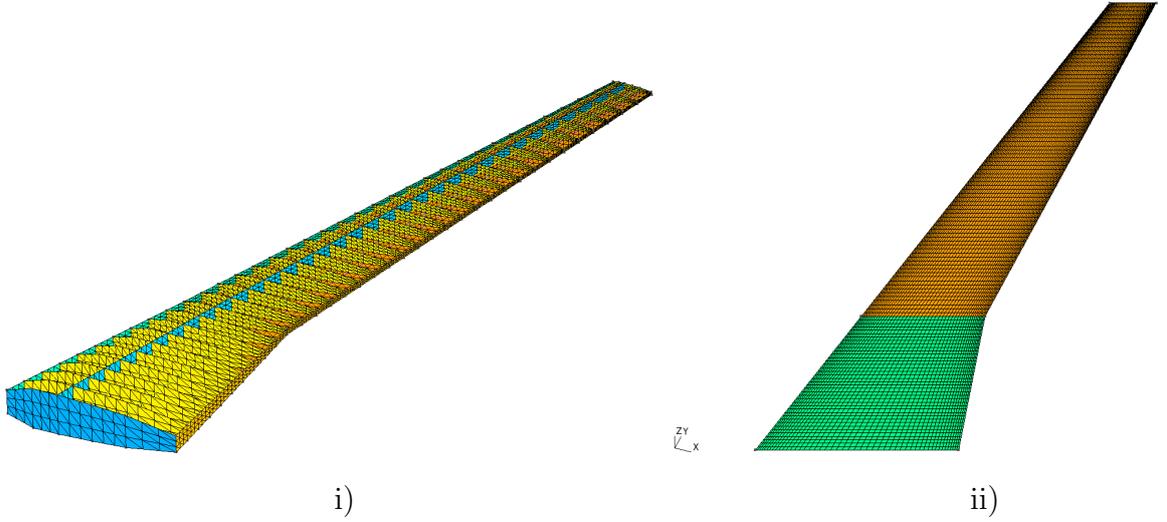


Figure 6: i) Finite element model of the structural part of the wing (skin, spars, ribs). ii) VLM mesh of the wing.

disciplinary surrogate models of the form,

$$\hat{U}(z) = \sum_{i=1}^{N_U} \hat{u}_i(z) U_i \quad (15)$$

and

$$\hat{\Gamma}(z) = \sum_{i=1}^{N_\Gamma} \hat{\gamma}_i(z) \Gamma_i \quad (16)$$

where the bases  $U_i$ ,  $i = 1, \dots, N_U$  and  $\Gamma_i$ ,  $i = 1, \dots, N_\Gamma$  are constructed by snapshot Proper Orthogonal Decomposition (POD) and  $\hat{u}_i$ ,  $i = 1, \dots, N_U$  and  $\hat{\gamma}_i$ ,  $i = 1, \dots, N_\Gamma$  are GP interpolations of the POD coefficients. These surrogates models are known as POD+I (POD+Interpolation) in the literature ([26] or [27] among others). The use of GP interpolation for the coefficients of the reduced order model, as in [28] for example, allows to quantify the uncertainty associated to the interpolation and thus to set up the EGMDO algorithm. However it should be noted that the error associated to the POD approximation is neglected. Hence, it is important to control this error, in a so called offline phase, before the use and the enrichment of the disciplinary surrogate models. In the following we present an application of this first strategy.

In this application the design space  $\mathcal{Z}$  is of dimension 6 and made by 4 thicknesses of different wingbox parts, the span and the chord. These 6 variables define the vector  $z$ . Then a DoE is created by sampling over  $\mathcal{Z}$ . In order to ensure a prescribed level of accuracy of the reduced order model built from this DoE, a greedy procedure presented in [29] is used. This construction needs the evaluation of 15 MDA using the actual disciplinary solvers. Solving this MDA using Gauss Seidel algorithm needs around 10 evaluations of each disciplinary solver to achieve convergence. Thus the number of disciplinary solver evaluations to construct the initial disciplinary surrogate models given by Eq. (15) and Eq. (16) is around  $10 \times 15 = 150$ .

Once these disciplinary surrogate models are constructed it is straightforward to set up the proposed EGMDO algorithm. Indeed, given Eq. (15) and Eq. (16), let us denote  $\mu_{\hat{u}_i(z)}$ ,

$\mu_{\hat{\gamma}_i(z)}$  and  $\sigma_{\hat{u}_i(z)}$ ,  $\sigma_{\hat{\gamma}_i(z)}$  the mean and standard deviation of the GP used to interpolate the coefficients of the reduced order model, then the disciplinary surrogate models are Gaussian random variables (by linear combination of independent Gaussian variables) whose mean and standard deviation are given by,

$$\begin{cases} \mu_{\hat{U}} = \sum_{i=1}^{N_U} \mu_{\hat{u}_i(z)} U_i \\ \sigma_{\hat{U}}^2 = \sum_{i=1}^{N_U} \sigma_{\hat{u}_i(z)}^2 U_i^2 \end{cases} \quad (17)$$

and

$$\begin{cases} \mu_{\hat{\Gamma}} = \sum_{i=1}^{N_{\Gamma}} \mu_{\hat{\gamma}_i(z)} \Gamma_i \\ \sigma_{\hat{\Gamma}}^2 = \sum_{i=1}^{N_{\Gamma}} \sigma_{\hat{\gamma}_i(z)}^2 \Gamma_i^2 \end{cases} \quad (18)$$

where  $(U_i^2)_j = ((U_i)_j)^2$ ,  $j = 1, \dots, n_s$  and  $(\Gamma_i^2)_j = ((\Gamma_i)_j)^2$ ,  $j = 1, \dots, n_a$ . These disciplinary surrogate models allow to quantify the uncertainty introduced by the interpolation on the whole solution vectors. As an example, Fig. 7 i) presents the exact displacement field for a given  $z$  as well as the mean  $\mu_{\hat{U}}$ , one can see that the approximation slightly underestimates the exact value. Figure 7 ii) presents the exact value of the displacement field and a 99% confidence interval constructed from  $\sigma_{\hat{U}}^2$ , it is interesting to note that the exact value bounded by this confidence interval meaning that the uncertainty propagation is, in that case, relevant.

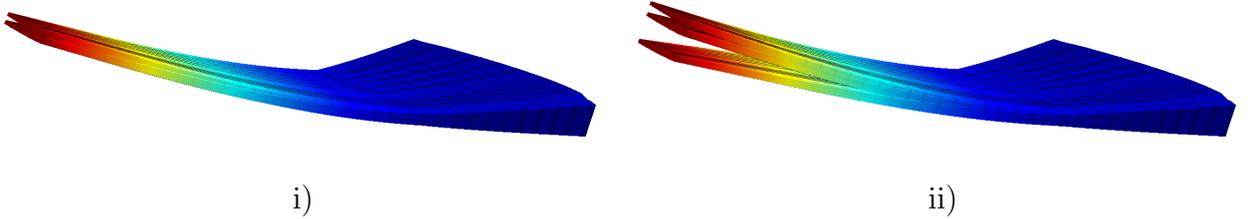


Figure 7: i) Mean value and exact value of the displacement field (the approximation slightly underestimates the exact value). ii) Exact value of the displacement field and 99% confidence interval.

It should be noted that the computation of the PCE of an objective function that depends on  $\hat{U}$  and  $\hat{\Gamma}$  is parametrized by  $N_U + N_{\Gamma}$  independent standard Gaussian variables denoted by the random vector  $\Xi$  in the previous section.

This first solution to deal with large vector valued coupling variables has the following characteristics:

- The disciplinary surrogate models only depend on the design variables  $z$  contrarily to the one introduced in the first section which depends on both the design variables and the coupling variables. This offers the advantage to be easy to implement but requires a higher computational budget as the training of these POD+I surrogate models is done on a DoE of converged MDA.
- In this approach the MDA is seen as a black box and the approximation is done on the output of this black box (the displacement field and the circulation vector that

solve Eq. (14) in that particular case). This allows to easily set up the proposed EGMDO algorithm but does not take advantage of the partitioned MDA which was our primary objective.

Hence, in order to further increase the coupling between MDO and the Bayesian framework it is proposed in the next section to extend the concept of disciplinary surrogate models that depends on both the design and the coupling variables to the case of vector valued coupling variables.

## 3.2 Coupling of disciplinary reduced order model

### 3.2.1 Proposed formulation

In order to take advantage of the partitioned MDA (i.e. the possibility to run simulations of the disciplinary solvers independently) it is proposed in this section to study the construction of POD+I disciplinary surrogate models of the form,

$$\begin{aligned}\hat{U}(z, \hat{\gamma}_j, j = 1, \dots, N_\Gamma) &= \sum_{i=1}^{N_U} \hat{u}_i(z, \hat{\gamma}_j, j = 1, \dots, N_\Gamma) U_i \\ \hat{\Gamma}(z, \hat{u}_i, i = 1, \dots, N_U) &= \sum_{j=1}^{N_\Gamma} \hat{\gamma}_j(z, \hat{u}_i, i = 1, \dots, N_U) \Gamma_j\end{aligned}\quad (19)$$

Compared to the disciplinary surrogate models given by Eq. (15) and Eq. (16) it should be noted that the ones in Eq. (19) not only depend on the design variables  $z$  but also on the coupling variables  $\hat{\gamma}_j, j = 1, \dots, N_\Gamma$  and  $\hat{u}_i, i = 1, \dots, N_U$  respectively. Hence, Eq. (19) is the *high dimensional* equivalent of the stochastic non linear system of equations given in the first section by Eq. (5). As in the first section it is proposed to model the GPs  $\hat{u}_i(z, \hat{\gamma}_j, j = 1, \dots, N_\Gamma)$  and  $\hat{\gamma}_j(z, \hat{u}_i, i = 1, \dots, N_U)$  by perfectly dependent GPs leading to a stochastic system of equations of dimension  $N_U + N_\Gamma$ . Following the notation introduced in the first section the random vector used to sample these GPs is denoted by  $\Xi = \{\Xi_U, \Xi_\Gamma\}$ , where  $\Xi_U = \{\xi_i, i = 1, \dots, N_U\}$  and  $\Xi_\Gamma = \{\xi_i, i = 1, \dots, N_\Gamma\}$  where  $\xi_i$  are  $N_U + N_\Gamma$  independent standard Gaussian variables.

This formulation relies on the capability to construct the disciplinary surrogate models. In that case, this means the construction of POD+I surrogate models over the space of the design variables and the coupling variables. Contrarily to the scalar coupling variables case, the sampling over the coupling variables space is more challenging in the large vector valued coupling variables context.

### 3.2.2 Construction of the disciplinary surrogate models and exploitation

The simplest strategy to sample over the coupling variables space and manage to construct a disciplinary surrogate model is to use the deterministic non linear solver as sampler. First, a sample of  $p$  design variables  $z_i, i = 1, \dots, p$  over the space  $\mathcal{Z}$  is generated using an appropriate DoE method, Latin Hypercube Sampling (LHS) for example. Then, the exact MDA associated to each design sample is computed using the MDA solver (or unconverged ones as proposed by [27]). For each design  $z_i$ , a certain number of iterations is needed. All those solver solutions are used as snapshots to build disciplinary POD bases  $U_i, i = 1, \dots, N_U$  and  $\Gamma_j, j = 1, \dots, N_\Gamma$ . Using these bases it is possible to obtain a sample of the POD coefficients by projection of the already computed disciplinary solver solutions.

This first strategy is relatively simple to set up and has been applied by the authors in [30] to the study of the static aeroelasticity of a wing. In this first test case the design variable is one dimensional (the angle of attack has been retained for the illustration) and the quantity of interest is the lift-to-drag ratio of the wing. Following the proposed strategy this quantity of interest is approximated by a PCE with respect to the vector  $\Xi$  (as in Eq. (9)). For this illustration the initial DoE is created by the resolution of 5 MDA (for  $z$  in  $[1, 10]$ ) leading to 50 evaluations of each disciplinary solver (Gauss Seidel algorithm is used and around 10 iterations are necessary to reach the convergence). The disciplinary surrogate models are constructed from these 50 solutions leading to  $N_U = 4$  and  $N_R = 3$  (see [30] for the numerical details of the POD implementation). Hence the stochastic dimension of the problem is 7. Figure 8 presents a sample of the lift-to-drag ratio (denoted by  $Y_{QoI}$ ) as well as its PCE approximation (denoted by  $\hat{Y}_{QoI}$ ). One can note that the PCE approximation is accurate enough to represent the uncertainty introduced by the disciplinary surrogate models. It is also notable that due the non linearity of the MDA the quantity of interest is not Gaussian.

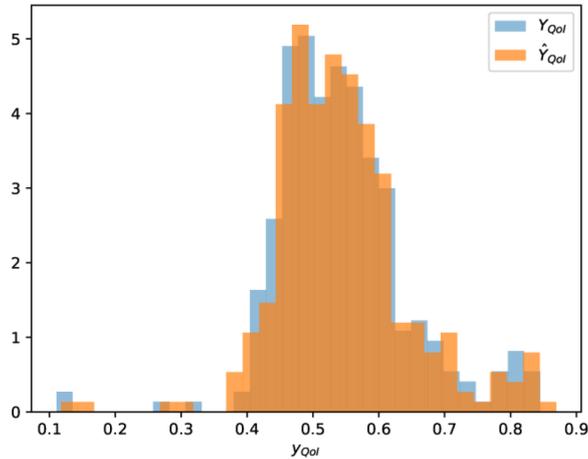


Figure 8: Illustration of the lift-to-drag ratio variation and its PCE approximation.

It is also proposed to perform a sensitivity analysis of the quantity of interest in order to decide which disciplinary solver to enrich. This PCE based sensitivity analysis approximates the Sobol indices which quantify the respective contribution of each disciplinary surrogate models to the variance of the quantity of interest. In the case study in [30] the conclusion of the sensitivity analysis was that the surrogate model  $\hat{\Gamma}$  should be enriched. It should be noted that this enrichment only involves a single resolution of the VLM solver (to be compared to the first strategy in which a whole MDA is performed at each enrichment). Figure 9 presents the results after this enrichment as well as the reference obtained by solving the MDA with the disciplinary solvers.

This figure illustrates how the uncertainty of the quantity of interest can be reduced by the enrichment of the relevant disciplinary surrogate model. One can also note that the variation of the quantity of interest is centered on the reference value. Hence it should be possible to further reduce the uncertainty of the quantity of interest by successive disciplinary enrichment. This strategy of uncertainty reduction can be seen as a Bayesian way of solving the MDA.

Even if this approach offers some interesting results it appears that it suffers from sev-

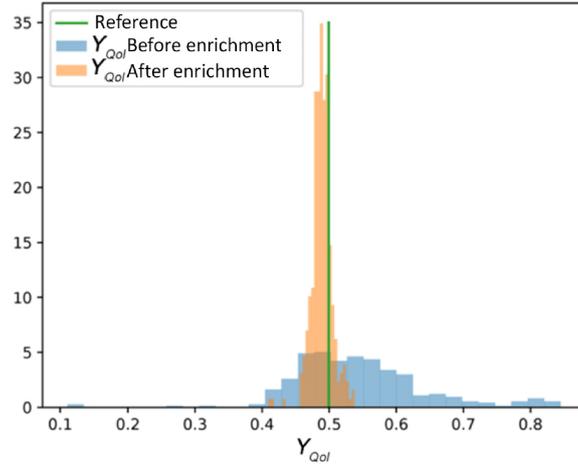


Figure 9: Illustration of the lift-to-drag ratio variation after the enrichment of the disciplinary surrogate model  $\hat{\Gamma}$ .

eral numerical issues during the creation of the initial DoE and during the enrichment step. We recall that the initial DoE is obtained by the resolution of MDA at various points of the design space, which is not efficient for the exploration of the coupling variables spaces and creates some numerical instabilities in the construction of the GPs. Indeed, during one MDA resolution, the design variables are constant (equal to  $z_i$ ) and the coupling variables follow a convergence path to the exact MDA. Hence the samples are clustered around the MDA solutions and it is well known that a cluster of points leads to numerical issues in the determination of the GP.

As a consequence we recently investigated the possibility to sample a DoE without resolving MDA. This new sampling strategy is presented in [31] and it is based on an iterative process in which some random variations in the design variables are introduced. It should be noted that this sampling problematic has been also study recently by [32] in which a sample scheme based on physical considerations is proposed. Contrarily the method we proposed assumed very little knowledge regarding the physics of the coupling variables.

Using this new sampling strategy it is possible to enrich the disciplinary surrogate models on problems of higher complexity. As an example, we present in [31] a test case based on the aerolasticity study of the previous wing (Fig. 6) that counts 8 design variables, namely the angle of attack, the speed, and 6 thicknesses of the different structural components of the wing. The initial DoE used to create the disciplinary surrogate models counts 50 solutions of the structural solver and 60 solutions of the disciplinary solvers. The POD construction leads to  $N_U = 11$  and  $N_\Gamma = 5$ .

In order to evaluate the accuracy of the proposed enrichment strategy at a point  $z$  that does not belong to the DoE it is proposed to study the dispersion of the relative error between the solution of the MDA using the mean values of the disciplinary surrogate models and the one using a sample of realisations of the disciplinary surrogate models. Figure 10 presents the evolution of this relative error (denoted by  $\hat{q}$ ) after 2 enrichment steps. According to the result of the sensitivity analysis the first model to be enriched is the structural one, followed by an enrichment of the aerodynamic surrogate model.

One can see on this figure that the proposed strategy leads to an important reduction

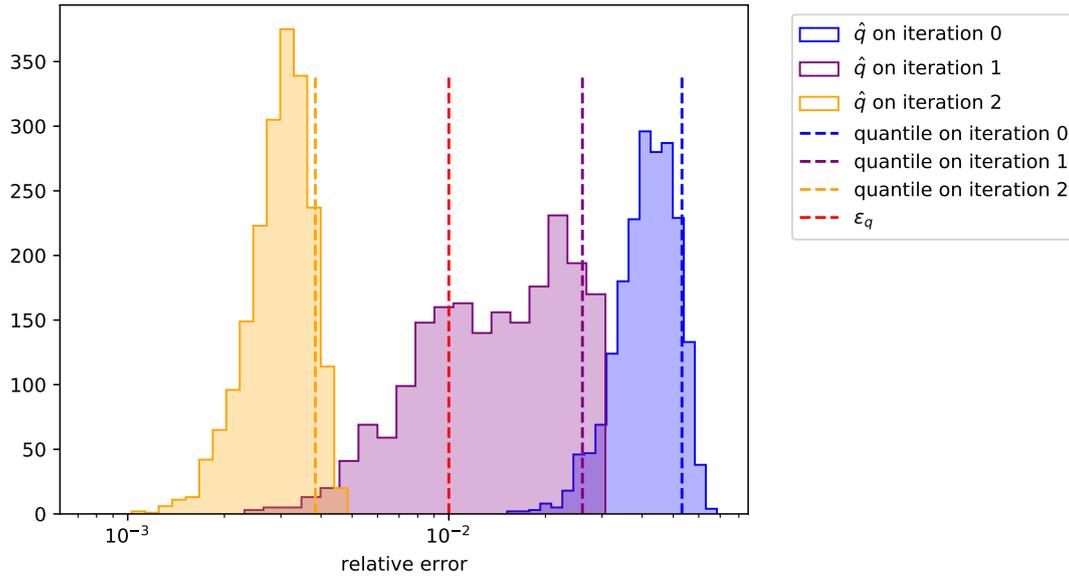


Figure 10: Evolution of the relative error of the MDA solution at a new design point after 2 enrichment steps, the 90% quantiles of the relative error distribution are also given.

of the relative error  $\hat{q}$  meaning that the dispersion of the MDA solution tends towards 0. Moreover Fig. 10 also presents the 90% quantile of the relative error distribution. It is interesting to note that this quantile is lower than 1% after the second enrichment, in practice this can be used as a criterion to stop the enrichment procedure. Details of the enrichment procedure as well as others examples and robustness study can be found in [31].

Finally it is interesting to compare the strategy based on the coupling of disciplinary GPs and successive enrichment presented in Section 3.2 with the direct approximations of converged solution presented in Section 3.1. For this comparison the previous 8 parameter test case is used and the accuracy of both approaches are evaluated. This comparison is made on a test set of 100 points randomly sampled in the design space. For both approaches the numerical cost *i.e.* the number of disciplinary solver calls, is almost equal. The direct approximations are constructed from a DoE of 30 converged MDA leading to 121 calls to the disciplinary solvers whereas the coupling of disciplinary GPs needs 128 calls to the disciplinary solvers. Figure 11 presents the relative errors on the norm of  $U$  and  $\Gamma$  between the reference results and the results obtained by the two approximation approaches.

This figure clearly illustrates that the adaptive construction of disciplinary surrogate models leads to better results than the direct approximations of converged MDA solution. It should be noted that a comparison at iso relative error level is also performed in [31] showing that the same accuracy level can be reached by the direct approximation method but a higher numerical cost. These results illustrate that by taking into account the interaction between disciplines in the disciplinary surrogate models construction it is possible to significantly reduced the numerical cost of the approximation constructions. However it should also be noted that this coupling strategy involves a higher dimension of the input spaces of the approximations which remains a problematic in surrogate model development.

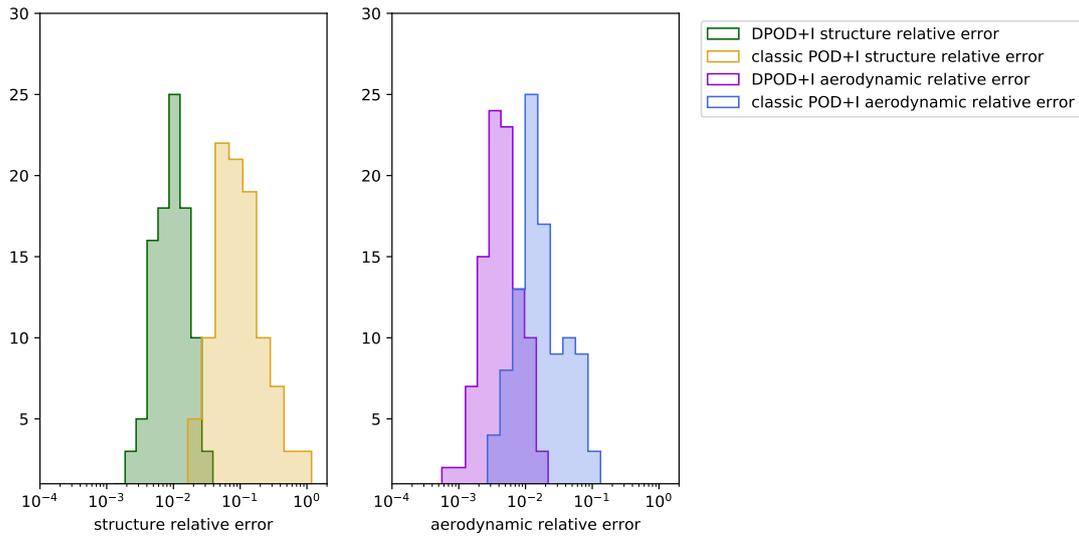


Figure 11: Comparison of the accuracy of direct approximations of converged solutions (denoted by classic POD+I) with approximations from the coupling of disciplinary GPs (denoted by DPOD+I). Relative error on a test set of 100 points.

#### 4 CONCLUSION

The objective of this study was to highlight some recent developments in the field of Multidisciplinary Design Analysis and Optimization within the Bayesian framework. With respect to this objective Section 2 presents the contribution of the authors to an Efficient Global Multidisciplinary Design and Optimization formulation. The originality of this formulation lies in the approximation of the objective function by a non Gaussian random field obtained from the uncertainty propagation of the disciplinary GPs to the objective function. This random field model of the objective function allows to follow the path of Bayesian optimization by enrichment of the disciplinary GPs based on an Expected Improvement criterion. Some promising results have been reached with this formulation with respect to the number of disciplinary solver evaluations to converge toward the global minimum of MDO problems. However many improvements with respect to the robustness of the approach and to the different approximation choices could be achieved in the future.

Section 3 focuses of the case of MDA with vector valued coupling variables and illustrates this context by the study of a high fidelity coupling for static aeroelasticity. As a first attempt to extend the concept of Bayesian framework to that case, two formulations based on model order reduction by POD and GP interpolation have been studied. Once again it is shown that a careful uncertainty propagation stemming from the randomness of the disciplinary surrogate models offers valuable information. This information can further be used to perform a sensitivity analysis and to enrich the relevant disciplinary surrogate model leading to a Bayesian way of solving the deterministic MDA. With respect to this problematic it is also clear that improvements can be obtained by working on the model order reduction method for example.

As a general conclusion on this work it appears that increasing the coupling between MDO and the Bayesian framework can help to tackle some challenges of MDO. Nevertheless, as illustrated throughout the paper, the construction and coupling of disciplinary GP brings there own new issues. Fortunately in the future we might be able to take ben-

efits of the numerous developments in both MDO and Bayesian optimization to further improved the proposed method.

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