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An Efficient Sampling Method for Regression-Based Polynomial Chaos Expansion

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Abstract. The polynomial chaos expansion (PCE) is an efficient numerical method for performing a reliability analysis. It relates the output of a nonlinear system with the uncertainty in its input parameters using a multidimensional polynomial approximation (the so-called PCE). Numerically, such an approximation can be obtained by using a regression method with a suitable design of experiments. The cost of this approximation depends on the size of the design of experiments. If the design of experiments is large and the system is modeled with a computationally expensive FEA (Finite Element Analysis) model, the PCE approximation becomes unfeasible. The aim of this work is to propose an algorithm that generates efficiently a design of experiments of a size defined by the user, in order to make the PCE approximation computationally feasible. It is an optimization algorithm that seeks to find the best design of experiments in the D-optimal sense for the PCE. This algorithm is a coupling between genetic algorithms and the Fedorov exchange algorithm. The efficiency of our approach in terms of accuracy and computational time reduction is compared with other existing methods in the case of analytical functions and finite element based functions.

AMS subject classifications: 60H15, 62K20, 62K05

Key words: Polynomial chaos expansion, regression, D-optimal design, Fedorov Algorithm, genetic algorithms.

1 Introduction

In the recent years, there has been an increasing interest in the simulation of systems with uncertainties. Due to the uncertainties in the input parameters, the response of the mechanical system has a deterministic component and a random component; this random

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component is often ignored in traditional engineering practice. The reliability analysis consists in defining the probability density functions (pdf) of the uncertain input parameters and then propagating them through the mathematical model of the mechanical system in order to characterize the random component of the output.

The polynomial chaos expansion (PCE) method builds a multidimensional polynomial function that approximates the output of the system around its nominal value with respect to the uncertainty of the input parameters. There are two non-intrusive methods to construct the PCE approximation: the projection method and the regression method (see [22] and [23]). Both of them are black box methods that require a set of independent simulations for different values of the input parameters.

The total computational time depends on three factors: the computer resources, the computational time of one finite element analysis (FEA) and the number of simulations needed to build PCE approximation. Usually, the industrial applications require expensive finite element analysis. Hence, if the number of analyses for building the PCE is large, the total computational time becomes unfeasible. Reducing the total computational time by tuning the first two factors is not an easy task. The computer resources are usually limited and reducing the computational time of one FEA means reducing its accuracy. Therefore, one has to reduce the third factor, the number of analyses for the PCE, in order to be able to carry out a reliability analysis of an expensive FEA-based application.

Recently, some new methods have been introduced to reduce the number of independent simulations. The projection method requires running a set of simulations defined over a sparse grid of nodes following some quadrature rules. In [16–19], the reduction of the size of sparse grid is based on the anisotropy of the problem and the contribution of each node of the sparse grid in the overall accuracy of the numerical evaluation.

The regression method requires the definition of a design of experiments depending on the PCE polynomial function. In [1,20,21], a model reduction approach is considered where some terms of the PCE approximation are discarded according to their pertinence in the model. This leads to a reduction of the size of the design of experiments.

The preceding methods prescribe their number simulations without providing to the user a direct control over the total number of simulations to perform the PCE approximation. The contribution of this paper is to propose a sampling algorithm for the regression method where the user can choose the number simulations depending on the available computer resources, the computational time of one FEA and the desired total computational time. The proposed algorithm gives the possibility to carry out a PCE approximation with the fewest number of simulations which is equal to the number of terms in the PCE. Therefore, with this approach it is always possible to carry out a reliability analysis based on an expensive FEA model and a large number of uncertain parameters.

The accuracy of the PCE approximation given by the regression method is proportional to the determinant of the regression matrix. The approach proposed in this paper consists in maximizing this determinant for a given number of samples. This leads to a small sized design of experiments that covers efficiently all the space of the uncertain-

ties. The proposed algorithm for maximizing the determinant of the regression matrix is a coupling between genetic algorithms and the Fedorov exchange algorithm. The motivation for this choice is discussed in Section 4. The efficiency of our approach in terms of accuracy and computational time reduction is compared with other existing methods (the projection method) for analytical and industrial cases.

2 Probability space and random variables

Computing the output of a mechanical system with uncertain parameters is considered as a random experiment and can be studied using the PCE. In order to give a mathematical framework of the PCE, a brief review of some definitions regarding probability space and random variables is introduced in the sequel.

A probability space is a mathematical entity which models the uncertainty in the input and the output of the mechanical system. Three ingredients $(\Omega,\mathcal{F},P)$ are necessary to define a probability space, where Ω is the set of all possible outcomes, $\mathcal{F}$ is a σ-algebra over Ω, containing all possible events and P is a function $\mathcal{F}\to\mathbb{R}$ which gives a probability measure for each random event. A random variable X is a function $X:(\Omega,\mathcal{F},P)\to\mathbb{R}$.

Using the preceding definitions, one can also define the expectation and the variance of a random variable:

$$\bar{X}=\mathrm{E}[X]=\int X dP, \tag{2.1}$$

$$var(X)=\mathrm{E}[(X-\bar{X})^2]=\int (X-\bar{X})^2 dP. \tag{2.2}$$

We call $<X,Y>=\int XY dP$ the inner product of two random variables on the probability space and $\mathcal{L}^2(\Omega,\mathcal{F},P)$ the set of random variables having a finite variance.

Before introducing the PCE, one must also have a look at the Hermite polynomials. These polynomials are defined in a recursive way as follows:

$$H_0=1, \tag{2.3}$$

$$H_{n+1}(x)=xH_n(x)-(n)H_{n-1}(x), \tag{2.4}$$

and they have the property of being orthogonal with respect to the Gaussian measure. If H_i and H_j are two Hermite polynomials of degrees i and j respectively, we have:

$$\int H_i(x)H_j(x)e^{-x^2/2}dx=i!\delta_{ij}. \tag{2.5}$$

Thus, if ξ is a Gaussian random variable, the two random variables $H_i(\xi)$ and $H_j(\xi)$ are orthogonal with respect to the above inner product and the Gaussian measure. This orthogonality property constitutes the basis of the PCE.

Note that, if ξ is a uniform random variable, the Hermite polynomials must be replaced by the Legendre polynomials and the density function $e^{-x^2/2}$ by 1.

3 The polynomial chaos expansion (PCE)

In the following, the basis of the regression method and the D-optimal criterion are given. More details can be found in [7].

The PCE method consists in considering a set of orthogonal multivariate polynomials with respect to some inner product. Let M be the number of uncertain parameters in the mechanical system and $\{\xi_i(\omega)\}_{i=1}^M$ be a set of M independent Gaussian random variables. Each random variable is associated to an uncertain parameter and represents its perturbation. Consider Γ_p the space of multivariate polynomials of degree less or equal to p and $\tilde{\Gamma}_p$ the space of polynomials of degree equal to p and orthogonal to Γ_{p-1}. We have $\Gamma_p = \oplus_{i=1}^p \tilde{\Gamma}_i$. If the inner product is considered with the Gaussian measure, $\tilde{\Gamma}_p$ is spanned with the multivariate Hermite polynomials $\{\psi_\alpha(\xi)\}$ of degree p, where $\alpha \in \mathbb{N}^M$ and $|\alpha| = \sum_{i=1}^M \alpha_i = p$. These multivariate Hermite polynomials $\{\psi_\alpha(\xi)\}$ are defined as the product of M univariate Hermite polynomials of degree α_i:

$$\psi_\alpha(\xi) = \prod_{i=1}^M H_{\alpha_i}(\xi_i). \tag{3.1}$$

If S denotes the random output of the mechanical system and has a finite variance, it can be expressed as an infinite series of multivariate Hermite polynomials (see [14]):

$$S = \sum_{|\alpha|=0}^{|\alpha|=\infty} S_\alpha^{pce} \psi_\alpha(\xi) = \sum_{i=0}^{\infty} S_i^{pce} \psi_i(\xi). \tag{3.2}$$

Here, the multi-index α of ψ is replaced by an index i given the univocal relationship between these two notations. S_i^{pce} are the deterministic coefficients of the PCE.

One of the advantages of such a representation of the random output S is that computing the expectation and variance of S is straightforward. From the orthogonality property of ψ_i, one can deduce that:

$$\bar{S} = S_0^{pce}, \tag{3.3}$$

$$var(S) = \sum_{i=1}^{\infty} (S_i^{pce})^2. \tag{3.4}$$

For computational reasons, this infinite series must be truncated to degree p and S is replaced by $\tilde{S}$ with:

$$\tilde{S} = \sum_{i=0}^{N} S_i^{pce} \psi_i(\xi), \tag{3.5}$$

where $N = \frac{(M+p)!}{M!p!} - 1$ is the number of terms involved in $\tilde{S}$.

In this paper, we consider the regression method to compute the coefficients S_i^{pce} of the PCE. This method consists in defining a design of experiments, $\Xi = \{\xi_i^j\}^{j=1,\cdots,Q}$, which

is a set of Q different perturbations of the input parameters and then computing (by simulation) the output of S for each value ξ^j of the design of experiment. These output values are gathered in a vector $S^{sim} \in \mathbb{R}^Q$. The coefficients S_i^{pce} are then computed by solving the following linear least squares problem:

$$\min_{S^{pce}} R = \frac{1}{2}\sum_{j=1}^{Q}\left(S_j^{sim} - \sum_{i=0}^{N} S_i^{pce}\psi_i(\xi^j)\right)^2, \tag{3.6}$$

where R is the squared residual between the simulated and the approximated output values.

The solution of this optimization problem is derived in the following. Writing the derivative of R with respect to S_k^{pce} equal to zero leads to:

$$\sum_{j=1}^{Q}\psi_k(\xi^j)\left(S_j^{sim} - \sum_{i=0}^{N} S_i^{pce}\psi_i(\xi^j)\right) = 0 \quad \forall k = 1,\cdots,N. \tag{3.7}$$

The above equation can be rearranged in the following form (called the normal equations):

$$\sum_{j=1}^{Q}\sum_{i=0}^{N}\psi_k(\xi^j)\psi_i(\xi^j)S_i^{pce} = \sum_{j=1}^{Q}\psi_k(\xi^j)S_j^{sim} \quad \forall k = 1,\cdots,N. \tag{3.8}$$

Let $\Psi_{ji} = \psi_i(\xi^j)$ be a rectangular matrix in $\mathbb{R}^{Q,N}$. Each row j of this matrix is the set of all ψ_i's computed for the experiment ξ^j. Hence, the matrix representation is deduced from the above equations:

$$S^{pce} = (\Psi^t\Psi)^{-1}\Psi^t S^{sim}. \tag{3.9}$$

$\Psi^t\Psi$ is called the information matrix [7].

3.1 D-optimal design

In this section, it is shown how the choice of the DOE $\Xi = \{\xi^j\}^{j=1,\cdots,Q}$ affects the accuracy of the estimation of S^{pce}. We recall that the output of the mechanical system is expressed as a series of multivariate Hermite polynomial truncated at degree p (Eq. 3.5):

$$S^{sim} = \sum_{i=0}^{N} S_i^{pce}\psi_i(\xi) + \varepsilon, \tag{3.10}$$

where ε is the truncation error between the PCE and S^{sim} and is a random variable. The presence of this random truncation error induces a random error in the estimation of S^{pce}. The variance of S^{pce} is derived as follows:

$$\begin{aligned}\mathrm{var}(S^{pce}) &= \mathrm{var}((\Psi^t\Psi)^{-1}\Psi^t S^{sim}) \\ &= (\Psi^t\Psi)^{-1}\Psi^t\mathrm{var}(S^{sim})((\Psi^t\Psi)^{-1}\Psi^t)^t.\end{aligned} \tag{3.11}$$

Assuming that $\text{var}(S^{sim}) = I\sigma^2$ meaning that the truncation errors in each simulation are independent and have a constant variance equal to σ, we obtain:

$$\text{var}(S^{pce}) = (\Psi^t\Psi)^{-1}\sigma. \tag{3.12}$$

From Eqs. (3.9) and (3.12), one can deduce the relationship between Ξ and $\text{var}(S^{pce})$. Each S_i^{pce} is a linear combination of the terms of S^{sim}. Using the central limit theorem, S^{pce} is a vector of Gaussian variables of variance $(\Psi^t\Psi)^{-1}\sigma$. It is known that its confidence region is a hyper-ellipsoid of volume proportional to the determinant of $(\Psi^t\Psi)^{-1}$. In order to reduce $\text{var}(S^{pce})$, the error in the estimation of S^{pce}, one needs to reduce the confidence region. A D-optimal design is a design that gives an estimation of S^{pce} with the smallest confidence region. It is the solution of the following optimization problem:

$$\max_{\Xi} \det(\Psi^t\Psi). \tag{3.13}$$

This optimization problem constitutes the main task of our work: finding the D-optimal design in the case of the regression based PCE. Several methods based on Fedorov exchange formula or heuristic optimization have been proposed to solve this particular optimization problem. In the following section, we give a review of these methods and we introduce our coupling optimization algorithm adapted to the case of regression based PCE as was discussed in Section 1.

4 Optimization algorithms

We recall that the purpose of this optimization algorithm is to generate a design of experiments for the PCE approximation, as much accurate as possible, given a user defined number of experiments.

Each uncertainty of each parameter is discretized such that it takes a finite number of values, depending on the degree of the PCE. The combination of the discrete values of all the parameters constitutes a grid of nodes where each node is an experiment candidate. The design of experiments is a set of experiments chosen from this grid of nodes. One can see that the size of the grid increases exponentially with the number of uncertain parameters and the degree of the PCE.

A common criterion for selecting a DOE is the D-optimality one by maximizing the determinant of the information matrix. This criterion can be computed using the Fedorov algorithm (see [4]), which belongs to the family of "exchange algorithms". It is detailed in Section 4.1. The underlying idea is to find the best DOE from a grid of nodes. At each iteration, an experiment of the DOE is compared with all the experiments candidates of the grid by applying the Fedorov exchange formula and it is exchanged with the best one. The algorithm can handle efficiently a DOE of large size but it can become expensive in computations when the size of the grid is large. Moreover, it can be trapped into a local optimum.

Two different approaches have been proposed to optimize the determinant of the information matrix without scanning all the experiments candidates. In [2, 3] a genetic algorithm is used to optimize the D-optimality criterion and in [5, 6] a heuristic search is preferred. These algorithms are global methods and they can be a good choice over the Fedorov method because they do not scan the whole set of candidates at each iteration. However, the crossover operator presents two major drawbacks. First, it can be expensive when DOEs have a large size because it requires the computation of the determinant of the information matrix. Second, it has been observed in the numerical examples in Section 5 that the crossover operator fails to optimize the determinant when the set of experiments candidates is also large.

For this reason, an algorithm is proposed that couples the Fedorov exchange algorithm with the genetic algorithms to overcome this difficulty. The use of the genetic algorithms allows to avoid scanning all the experiments candidates. A cheap crossover can be defined using the Fedorov exchange formula which avoids computing the determinant of the information matrix. Some numerical experiments are carried out to show the performances of this coupling with large DOEs.

4.1 The Fedorov algorithm

We start by showing how the determinant of $\Psi^t\Psi$ changes when an experiment of the DOE is exchanged with a new one.

The matrix $\Psi^t\Psi$ can be written as $\sum_{j=1}^{Q}\psi(\xi^j)\psi(\xi^j)^t$ where $\psi(\xi^j)=\{\psi_i(\xi^j)\}_{i=1,\cdots,N}$ is the row of the matrix Ψ corresponding to experiment j. $\Psi^t\Psi$ is a sum of outer products over the experiments of the DOE. When a new ξ^{Q+1} experiment is added to the DOE, the new information matrix $\Psi_{new}^t\Psi_{new}$ becomes $\sum_{j=1}^{Q+1}\psi(\xi^j)\psi(\xi^j)^t$. From the matrix determinant lemma, the determinant of $\Psi_{new}^t\Psi_{new}$ can be updated from the one of $\Psi^t\Psi$ as follows:

$$\begin{aligned}\det(\Psi_{new}^t\Psi_{new}) &= \det(\Psi^t\Psi+\psi(\xi^k)\psi(\xi^k)^t)\\ &= \det(\Psi^t\Psi)\times\Big(1+\psi(\xi^k)^t(\Psi^t\Psi)^{-1}\psi(\xi^k)\Big).\end{aligned} \tag{4.1}$$

If an experiment k is removed from the DOE, the update formula is the same as above but the sign $+$ is replaced with a $-$. Now, when an experiment l from the DOE is exchanged with an experiment k, the determinant of the new information matrix $\Psi_{new}^t\Psi_{new}$ can be obtained by applying the above formula twice:

$$\det(\Psi_{new}^t\Psi_{new}) = \det(\Psi^t\Psi)\times\Big(1+\Delta(\xi^k,\xi^l)\Big), \tag{4.2}$$

where

$$\Delta(\xi^k,\xi^l) = d(\xi^k,\xi^k)-d(\xi^k,\xi^k)+d^2(\xi^k,\xi^l)-d(\xi^k,\xi^k)d(\xi^l,\xi^l), \tag{4.3}$$

$$d(\xi^k,\xi^l) = \psi(\xi^k)^t(\Psi^t\Psi)^{-1}\psi(\xi^l). \tag{4.4}$$

When two experiments are exchanged, the determinant of the information matrix changes with rate Δ.

The Fedorov algorithm for maximizing $\det(\Psi^t\Psi)$ is based on the above formula. Consider a set $\mathcal{C}$ of experiment candidates (a grid of nodes) and $\Xi \subset \mathcal{C}$ a random DOE of Q experiments. The idea of the algorithm is that for each experiment $\xi^l \in \Xi$ we compute the values of the function $\Delta(\xi^k,\xi^l)$ for all $\xi^k \in \mathcal{C}\backslash\Xi$ and exchange ξ^l with the ξ^k that gives the maximal value of Δ. It can be summarized in Algorithm 4.1. One can see that this algorithm is efficient in the sense that it uses the update formula to compute the determinant at each iteration which is not an expensive operation. However, it can still be quite expensive when the size of $\mathcal{C}$ becomes large.

It is important to note that the initial DOE has to be nonsingular, otherwise the determinant of the matrix will stay equal to zero during all the execution of the algorithm.

Algorithm 4.1: The Fedorov Algorithm

```
Generate a random Ξ ⊂ C
Compute the determinant of Ξ
for all ξ^j ∈ Ξ do
  set Δ_max = 0
  for all ξ^l ∈ C\Ξ do
    Compute Δ(ξ^k, ξ^l)
    if Δ(ξ^k, ξ^l) > Δ_max then
      Set Δ_max = Δ(ξ^k, ξ^l)
      Exchange ξ^l with ξ^k
      Update the determinant of Ξ
    end if
  end for
end for
```

4.2 Generating a nonsingular random DOE

If a DOE is generated by randomly selecting some experiments from a set of candidates and the size of the DOE is small, there is a high probability to get a singular DOE. In this case, the Fedorov exchange algorithm is not applicable because the determinant will remain zero during the whole procedure. In the following, a method is proposed which ensures that it always generates a nonsingular DOE.

We suppose that each parameter uncertainty can take $p+1$ distinct values, $\{r_0,r_1,\cdots,r_p\}$, indexed from 0 to p. An experiment is a node of the grid $\{r_0,r_1,\cdots,r_p\}^M$ and each experiment is identified by an multi-index $\alpha \in \mathbb{N}^M$. The set of experiments such that $|\alpha| \leq p$ guarantees to have a nonsingular DOE. Taking a DOE with these nodes and following the Fedorov exchange formula, each experiment of this DOE can be exchanged with a randomly selected one from the grid if the determinant of the DOE increases. Some highlights of the proof are given:

- We recall that the PCE approximation is expressed in a Hermite basis. The terms of the approximation can be developed in the canonical basis which leads to a polynomial expression:

$$\tilde{S} = \sum_{|\alpha|=0}^{|\alpha|=p} S_\alpha^{pce} \psi_\alpha(\xi) = \sum_{|\alpha|=0}^{|\alpha|=p} S_\alpha^{can} \phi_\alpha(\xi), \tag{4.5}$$

  where the $\phi_\alpha(\xi)$ are the canonical monomials, S_α^{can} are the coefficients in this basis and α is a multi-index in $\mathbb{N}^M$. This notation with the multi-index is equivalent to the one in (3.5). The change of basis is defined in a matrix form, $S^{pce} = C.S^{can}$ where C is a nonsingular matrix. This implies that one can directly get the S_α^{pce} from the S_α^{can}.

- If the PCE is of degree p, it is easy to see that the S_α^{can} associated to the monomials of degree p are equal to $\frac{\partial^{|\alpha|}\tilde{S}}{\partial\xi^\alpha} / \prod_{i=1}^M \alpha_i!$.

- the α-derivative of a polynomial function of degree p with $|\alpha|=p$ is equal to its finite difference approximation because the finite difference approximation of order α is derived from the Taylor expansion of the function and the Taylor expansion of order α of a polynomial function is equal itself.

- Thus, one can choose the experiments of the DOE such that they correspond to a finite differences scheme and directly compute the coefficients S_α^{can} with $|\alpha| = p$. Once these coefficients are evaluated, this operation can be repeated iteratively for the degrees from $p-1$ to 0 and hence all the coefficients are computed.

- Given that the set of nodes with $|\alpha| \leq p$ contains all the finite differences schemes needed for computing all the PCE coefficients, a DOE containing these nodes is nonsingular.

4.3 The coupled Fedorov-genetic algorithm

In [2, 3, 12], genetic algorithms have been used for finding D-optimal designs. They are based on the definition of a random population which in this case is a set of DOE candidates. These individuals will interact with each other in order to evolve toward the optimal solution. This evolution process can be summarized in the following steps. First, the population of DOEs is initialized by generating randomly a certain number of DOEs. Next and at each iteration, the determinant of each DOE of the population is computed. A random procedure, called crossover, is applied to select the parents according to their determinant and obtain the new DOEs offspring of the new population. For more information on genetic algorithms see [11, 15].

During the optimization procedure, all the DOEs are nonsingular. This is guaranteed by coupling the Fedorov exchange formula with the genetic algorithms.

In the initialization step, the random and nonsingular DOEs are generated like in the previous section. In the crossover step, the two parents DOEs exchange some of their

experiments without producing new singular DOEs. Let the two parents DOEs be Ξ_1 and Ξ_2 and N_c be the number of crossover points which is the number experiments to be exchanged between them. An experiment is randomly selected in Ξ_1 and it is exchanged with another one in Ξ_2 such that according to the Fedorov exchange formula the determinant of both DOEs does not decrease. This operation is repeated N_c times to generate new offsprings.

Algorithm 4.2: The GA-Fedorov Algorithm

Initialize a random population $\{\Xi_i\}$ of DOEs
for $k=1$ to number of iterations **do**
  Compute all the determinants of the population $\{\Xi_i\}$
  for $l=1$ to population size **do**
    Select two parents randomly according to their determinants
    Reproduce an offspring using the Fedorov algorithm:
    for $m=1$ to number of crossover points **do**
      Choose randomly an experiment ξ_i of the offspring
      Compute $\Delta(\xi_i,\xi_j)$ for all ξ_j in the second parent
      Replace ξ_i with the ξ_j that has a maximal Δ
    end for
  end for
  Replace the parents population $\{\Xi_i\}$ with the offspring population
end for

5 Numerical results

In this section, we show the efficiency of the coupling algorithm in generating accurate and small-sized DOE for the regression based PCE. Three sets of tests are performed: a comparison with the standard GA algorithm, a comparison with the closest to the origin sampling method proposed in [1] and finally a comparison with the projection method.

5.1 Comparison with the Standard GA Algorithm

We start by comparing the standard genetic algorithm with the Fedorov-GA algorithm. The set $\mathcal{C}$ of experiment candidates is taken the same as the one in [1]. It is the grid of nodes $\{r_0,r_1,\cdots,r_p\}^M$ where r_i are the roots of the Hermite polynomials of degree $p+1$. The number of experiments in each DOE is taken as twice the number of coefficients in the PCE. We compare the efficiency of our Fedorov based crossover with the standard one. The PCE is of degree 4 and has 6 variables. The number of experiments in the DOEs is 420. In Figs. 1 and 2, it is shown how the standard crossover is not able to improve the determinant of the DOE unlike the Fedorov based crossover of our algorithm. In the first case the determinant decreases during the iterations, while in the case of the

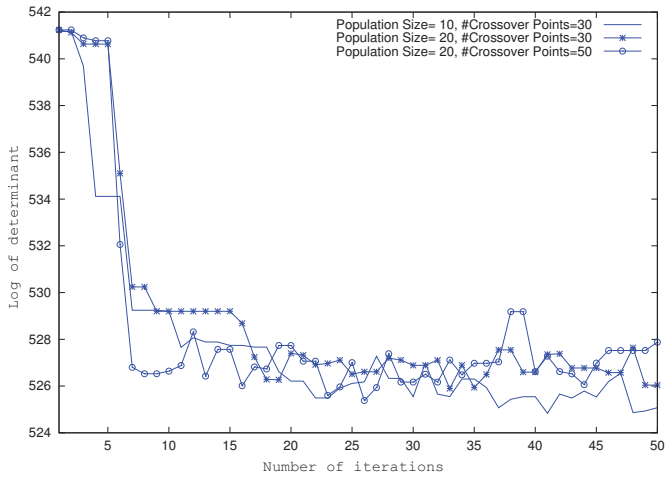

Figure 1: Standard genetic algorithm: case of Hermite polynomial of degree $p=4$, with $M=6$ variables and $N=420$ experiments.

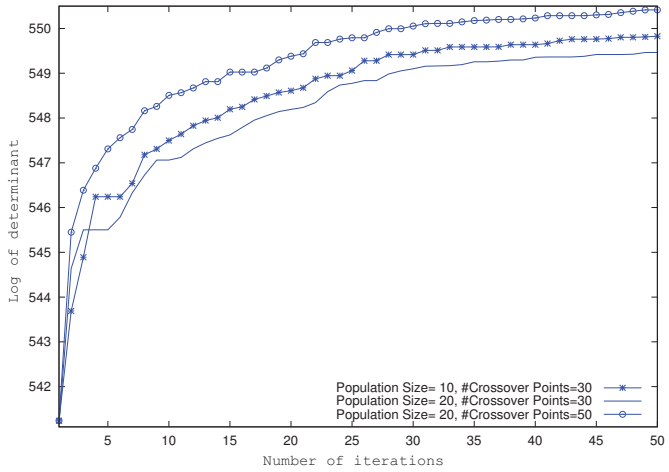

Figure 2: Coupled Fedorov genetic algorithm: case of Hermite polynomial of degree $p=4$, with $M=6$ variables and $N=420$ experiments.

coupled algorithm the determinant increases. The optimization experiments are repeated for several population sizes (10 and 20 individuals) and several number of crossover points ($N_c=30$ and 50).

5.2 Comparison with the closest to the origin sampling method

In the second experiment, we compare the sampling method of DOE proposed in [1] with our coupling method. The DOE in the quoted paper is made of the N closest points to the origin in $\mathcal{C}$. This method, as it is mentioned in the paper, has the drawback of requiring

Table 1: Comparing the minimal size of the DOE required by the closest to origin method and the Fedorov-GA method.

$p\times M$	# of experiments /$\det(\Psi^t\Psi)$ (closest to origin)	N+1/$\det(\Psi^t\Psi)$ (Fedorov-GA)	$2\times N$/$\det(\Psi^t\Psi)$ (Fedorov-GA)
3×4	87/29	36/35	70 /51
3×5	247/72	57/71	112/95
3×6	747/145	85/120	168/160
4×4	175/22	71/112	140/141
4×5	1125/270	127/240	252/293
4×6	4180/550	211/447	420/551

a large number of experiments in order to have a nonsingular DOE. Table 1 shows the smallest DOE sizes that both methods can generate and it compares their accuracies by computing their respective determinants. The minimal number of experiments required for the coupling algorithm is always equal to the number of terms in the PCE. It can be seen that the closest to origin method requires much more experiments than Fedorov-GA. This can be very expensive in computations. The determinant of the DOE with the closest to origin method is in the same range of values as the one obtained with the Fedorov-GA. In conclusion, the coupled Fedorov-GA is more efficient because it gives DOE with the same accuracy and much less samples.

5.3 Comparison with the projection method

In this third set of tests, the coupling algorithm is compared to the projection method in terms of cost and accuracy. Three tests are based on analytical functions and one on a finite elements model. The exact standard deviations of the analytical functions are known in advance. By comparing it to the computed standard deviation, this gives the accuracy of the PCE approximations by both methods.

- Test one: $f(x)=\sum_{i=1}^{3}\sin(x_i)$, $x_i\in[-\pi,\pi]$ and the variance of f is equal to 1.5.
- Test two: $g(x)=\sin(x_1)+a.\sin^2(x_2)+b.x_3^4\sin(x_1)$, $x_i\in[-\pi,\pi]$ and the variance of g is equal to $\frac{a^2}{8}+b\frac{\pi^4}{5}+b^2\frac{\pi^8}{18}+\frac{1}{2}$. In this example, $a=7$ and $b=0.1$.
- Test three: $h(x)=\prod_{i=1}^{3}\frac{|4x_i-2|+a_i}{1+a_i}$, with $a=(1,2,5)$ and $x_i\in[0,1]$; the variance is equal to 0.1336.

Table 2 gives the results corresponding to the analytical functions. It also shows the relative errors of the two methods in computing the standard deviations of the three analytical functions. One can see that both methods are able to compute accurately the standard deviations of these functions: the highest relative error is only 1.23% with the Fedorov-GA method for test 2. This method is also 2.5 to 3 times faster than the projec-

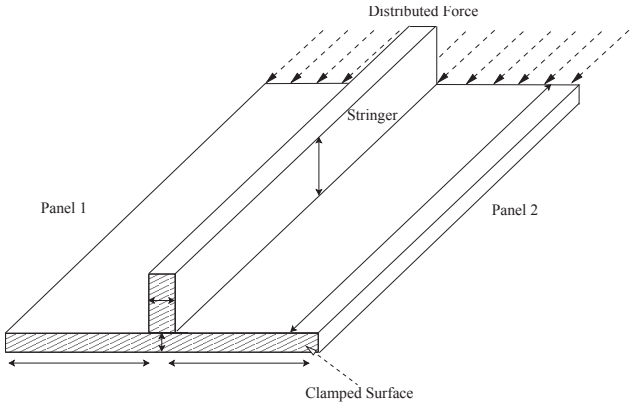

Figure 3: Description of the finite element based test: the solid arrows are the uncertain variables.

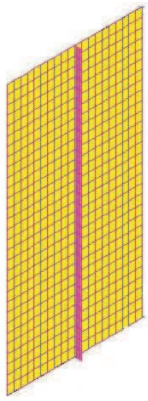

Figure 4: The finite element model of the structure: two panels and one stringer.

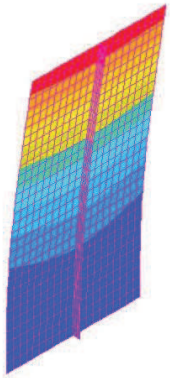

Figure 5: The first buckling mode of the structure.

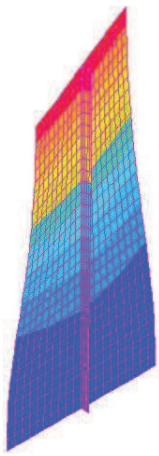

Figure 6: The second buckling mode of the structure.

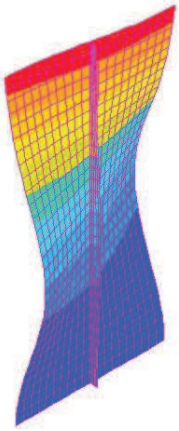

Figure 7: The third buckling mode of the structure.

Table 2: Comparison of the results obtained by the projection method and the coupled Fedorov-GA method for the analytical functions.

	Projection Method			Fedorov-GA Method		
	# samples	StD	Rel. Err.	# samples	StD	Rel. Err.
$f(x)$	135	1.2243	0.03%	57	1.2235	0.1%
$g(x)$	495	3.720	0%	168	3.675	1.23%
$h(x)$	495	0.141	2.9%	168	0.148	5.4%

Table 3: Comparison of the means and the standard deviations obtained with the projection method and the coupled Fedorov-GA method for the finite element test case.

	Projection Method		Fedorov-GA Method		Rel. Diff.	
	Mean	StD	Mean	StD	Mean	StD
	Degree=2 (78 samples)		Degree=2 (30 samples)			
Weight	73100	3.73×10^{3}	72000	3.75×10^{3}	1.3%	0.7%
Mode 1	0.529	5.47×10^{-2}	0.568	5.13×10^{-2}	7.3%	6.1%
Mode 2	0.903	8.79×10^{-2}	0.910	8.55×10^{-2}	0.7%	2.7%
Mode 3	1.315	1.32×10^{-1}	1.33	1.27×10^{-1}	1.6%	3.5%
	Degree=3 (257 samples)		Degree=3 (84 samples)			
Weight	83900	3.39×10^{3}	84900	3.37×10^{3}	1.1%	1.1%
Mode 1	0.539	5.56×10^{-2}	0.503	5.92×10^{-2}	6.7%	6.4%
Mode 2	1.04	8.13×10^{-2}	1.00	8.12×10^{-2}	3.29%	0%
Mode 3	1.514	1.2×10^{-1}	1.45	1.23×10^{-1}	3.9%	1.1%

tion method. This result shows that the Fedorov-GA method is able to generate a PCE approximation that accurately approximates these functions and with a low cost.

Table 3 gives the results corresponding to the finite element based functions. Here, the exact means and standard deviations are not known in advance. Hence, the relative difference between the standard deviations of both methods is compared. One can see that both methods give close results because the highest relative difference is about 7% and it is in the case of mode 1 with degree two. On can see that the Fedorov-GA method gives comparable results to the projection method with a computational cost 2.5 to 3 times lower. This concludes that these finite element based functions are accurately approximated with the PCE generated by the Fedorov-GA method.

6 Conclusion

In this paper an optimization algorithm is proposed for generating small sized DOEs for regression based polynomial chaos expansion. This method has the advantage of not prescribing the number of samples but it gives the possibility to the user to define the number of samples. For example, one can choose to take the fewest number of samples which is the number of terms involved in the PCE. The optimization algorithm is a ge-

netic algorithm with a crossover operator based on the Fedorov algorithm. It is used to maximize the D-optimal criterion of the DOE. We show the efficiency of this coupled algorithm by comparing it with the standard GA, the closest to origin sampling method and the projection method. Some analytical and finite element based tests are considered. The efficiency of the proposed algorithm is shown in terms of cost reduction and accuracy in all the preceding cases.

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