Combining polynomial chaos expansions and Kriging for solving structural reliability problems

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Keywords: Adaptive experimental designs / Kriging / Polynomial Chaos Expansions / Polynomial-Chaos-Kriging / Reliability

ABSTRACT: Nowadays advanced simulation models such as finite element models are used in every domain of science and engineering in order to predict the behaviour of systems and, in case of engineering applications, to optimize them and assess their performance. In parallel, engineers are all the more concerned with structural reliability and robust design, meaning that the quantification of uncertainties has become a key challenge.
Due to the high cost of advanced computational models (CM), classical techniques such as Monte Carlo simulation are not applicable. In this respect, meta-modelling techniques allow one to build up a surrogate model from a limited number of runs of the CM. Among many available options, Kriging and Polynomial Chaos Expansions (PCE) are two popular techniques. Kriging assumes that the computational model is a realization of a Gaussian random process whose properties (mean, autocorrelation structure) are fitted from a set of computer runs. PCE aim at approximating the CM response using a set of multivariate orthogonal polynomials in the input variables. The coefficients of a PCE are computed *e.g.* by least-square minimization.
In this paper we introduce PC-Kriging as a new non-intrusive meta-modelling technique derived from the combination of PCE and Kriging. A sparse set of orthonormal polynomials is first selected using the least angle regression algorithm as in Blatman and Sudret (2011). Then the parameters of the autocorrelation function of the underlying Gaussian field are fitted using the universal Kriging equations with the sparse PCE as a trend. Various trends and associated Kriging models are compared by cross-validation in order to eventually distinguish the best model. Based on the resulting Kriging variance, an infill criterion is used which allows one to refine the computer experiments design in an adaptive way so as to solve accurately structural reliability problems at low cost.

1 INTRODUCTION

Recently, computational simulations such as finite element analyses have become a popular tool in scientific and engineering problems. The backbone of these simulations is a computational model which imitates the behaviour of a physical system such as an engineering structure or a mechanical process. The increasing knowledge in science leads to more and more complex computational models which require increasing computational power.

At the same time, engineers are all the more concerned with (quantitative) reliability, robustness and design optimization (Rasmussen and Williams, 2006), which require quantification of uncertainties in the model. Due

to the high cost of advanced computational models, classical methods for uncertainty quantification, such as Monte Carlo simulation, become intractable. Thus, meta-modelling comes into play. *Meta-modelling* replaces the expensive-to-evaluate computational model by a simple and fast-to-evaluate meta-model. The meta-model is developed using a limited number of runs of the computational model, called the *experimental design*. Among many available options, Kriging and Polynomial Chaos Expansions (PCE) are two popular techniques. These two techniques are in the focus of this paper.

Kriging is a stochastic interpolation algorithm which assumes that the computational model is a realization of a Gaussian random process. The properties of the meta-model (*i.e.* mean and correlation structure) are fitted from a set of computer runs (Santner et al., 2003). Recent advances in Kriging are developed by *e.g.* Bachoc (2013), Ginsbourger et al. (2013), Duvenaud et al. (2012) and Dubourg (2011).

The second meta-modelling technique of interest in this paper is PCE, which approximates the computational model with a set of multivariate orthogonal polynomials in coherency with the distributions of the uncertain input quantities (Ghanem and Spanos, 2003). A sparse set of polynomials may be determined by selection algorithms such as the *least-angle regression* (Efron et al., 2004; Blatman and Sudret, 2011).

These two meta-modelling techniques have been mainly developed by different research communities. In this paper we introduce the new meta-modelling technique called *Polynomial-Chaos-Kriging* (PC-Kriging) which combines the two individual techniques. The performance of PC-Kriging is compared to that of PCE and Kriging first, in benchmark analytical problems and finally, in reliability applications.

This paper is composed as follows: Section 2 describes PCE (Section 2.1), PC-Kriging (Section 2.2) and validation tests (Section 2.3). Section 3 describes meta-modelling in the context of reliability analysis of engineering systems. In particular, Section 3.1 illustrates adaptive design algorithms and Section 3.2 applies the algorithms to a generic problem setting and a truss structure under uncertain loading.

2 META-MODELLING

Consider a computational model $\mathcal{M}$ which maps the M-dimensional input vector $\boldsymbol{x}$ to the one-dimensional scalar output y, *i.e.* $\mathcal{M} : \boldsymbol{x} \in \mathcal{D}_X \subset \mathbb{R}^M \rightarrow y \in \mathbb{R}$. Due to uncertainties in the input vector, the latter is represented by a random vector $\boldsymbol{X}$ with given probability density function (PDF) $f_{\boldsymbol{X}}$. For the sake of simplicity, the components of $\boldsymbol{X}$ are assumed independent throughout this paper. As a consequence the model response is a random variable Y obtained by propagating the input uncertainty in $\boldsymbol{X}$ through the computational model:

$$Y = \mathcal{M}(\boldsymbol{X}) \tag{1}$$

The computational model is assumed to be a black-box model, *i.e.* it provides an ouput value (supposed here scalar) for any input vector. Further, the computational model is assumed to be *deterministic* so that repeated evaluations of the model for the same input vector lead to the same output value.

In cases where the computational model is costly, repeated evaluations of $\mathcal{M}$ require large resources and reliability analyses may become intractable. Thus meta-modelling techniques have become popular recently (Sudret, 2012). They approximate the behaviour of the computational model $\mathcal{M}$ by an inexpensive-to-evaluate surrogate function, *i.e.* a *meta-model*. Two popular meta-modelling techniques are Kriging (Santner et al., 2003) and Polynomial Chaos Expansions (PCE) (Ghanem and Spanos, 2003). This section introduces PCE and in the sequence, Polynomial-Chaos-Kriging (PC-Kriging) as a modification of Kriging.

2.1 POLYNOMIAL CHAOS EXPANSIONS (PCE)

Polynomial Chaos Expansions (PCE) approximate the computational model $\mathcal{M}$ by a finite sum of orthonormal polynomials in coherency with the distributions of the input random variables:

$$Y \approx \mathcal{M}^{(PCE)}(\boldsymbol{X}) = \sum_{\boldsymbol{\alpha} \in \mathcal{A}} a_{\boldsymbol{\alpha}} \, \psi_{\boldsymbol{\alpha}}(\boldsymbol{X}) \tag{2}$$

In the above equation $\{a_{\boldsymbol{\alpha}},\ \boldsymbol{\alpha} \in \mathcal{A}\}$ are the coefficients for multi-indices $\boldsymbol{\alpha} = \{\alpha_1, \ldots, \alpha_M\}$ in the finite set $\mathcal{A}$, M is the number of independent input variables $\boldsymbol{X} = \{X_i,\ i = 1, \ldots, M\}$ and $\psi_{\boldsymbol{\alpha}}(\boldsymbol{X})$ are multivariate polynomials which are constructed as products of univariate orthonormal polynomials:

$$\psi_{\boldsymbol{\alpha}}(\boldsymbol{X}) = \prod_{i=1}^{M} \psi_{\alpha_i}^{(i)}(X_i) \tag{3}$$

where $\psi_{\alpha_i}^{(i)}(X_i)$ is a polynomial in the i-th variable of degree α_i. An *orthonormal polynomial basis* is a set of polynomials $\left\{\psi_n^{(k)}, n \in \mathbb{N}\right\}$ that are orthonormal to each other

in the following sense:

$$\langle \psi_i^{(k)}, \psi_j^{(k)} \rangle_k \overset{\text{def}}{=} \int_{\mathcal{D}_k} \psi_i(x)\, \psi_j(x)\, f_{X_k}(x) dx = \delta_{ij} \quad (4)$$

where $\psi_i(x), \psi_j(x)$ are univariate polynomials, f_{X_k} is the marginal PDF of variable X_k and δ_{ij} is the Kronecker delta, *i.e.* $\delta_{ij} = 1$ for $i = j$ and $\delta_{ij} = 0$ otherwise. For varying input marginals, different polynomial bases are available. A compilation of popular orthonormal bases can be found in *e.g.* Sudret (2012).

In practice the set of polynomials is truncated to make the computation of the coefficients tractable. Different truncation schemes have been proposed such as the *hyperbolic index sets* (Blatman and Sudret, 2011) which are defined as:

$$\mathcal{A}_q^{M,p} \equiv \{\boldsymbol{\alpha} \in \mathbb{N}^M : \|\boldsymbol{\alpha}\|_q \leq p\}, \text{ where } \|\boldsymbol{\alpha}\|_q \equiv \left(\sum_{i=1}^{M} \alpha_i^q \right)^{\frac{1}{q}} \quad (5)$$

where p is the maximum polynomial degree and $0 < q \leq 1$ is a parameter of the hyperbolic indexing technique which describes the number of interaction terms in $\mathcal{A}_q^{M,p}$. More specifically $q = 1$ corresponds to the classical truncation scheme in which all polynomials of total degree less than or equal to p are retained, whereas in the limit $q \to 0$ only additive terms are retained in the expansion.

The final step in the construction of a meta-model is the computation of the coefficients $a_{\boldsymbol{\alpha}}$ where $\boldsymbol{\alpha} \in \mathcal{A}$. Berveiller et al. (2006), Blatman (2009) and Blatman and Sudret (2010, 2011) solve this problem by casting it as a least-squares regression problem, namely:

$$\boldsymbol{a} = \underset{\boldsymbol{a} \in \mathbb{R}^{|\mathcal{A}|}}{\arg\min}\, \mathbb{E}\left[\left(Y - \sum_{\boldsymbol{\alpha} \in \mathcal{A}} a_{\boldsymbol{\alpha}}\, \psi_{\boldsymbol{\alpha}}(\boldsymbol{X}) \right)^2 \right] \quad (6)$$

PCE is based on a small set of samples of the input vector $\boldsymbol{\mathcal{X}} = \left\{ \boldsymbol{\chi}^{(1)}, \ldots, \boldsymbol{\chi}^{(N)} \right\}$, called the *experimental design*, and the corresponding response values $\mathcal{Y} = \left\{ \mathcal{Y}^{(1)}, \ldots, \mathcal{Y}^{(N)} \right\}$. Based on the experimental design, the numerical solution of Equation (6) writes:

$$\hat{\boldsymbol{a}} = (\mathbf{F}^{\mathsf{T}}\, \mathbf{F})^{-1}\, \mathbf{F}^{\mathsf{T}}\, \mathcal{Y} \quad (7)$$

where $\mathrm{F_{ij}} = \psi_{\mathrm{j}}(\boldsymbol{\chi}^{(\mathrm{i})})$ is the *information matrix* of size $N \times |\mathcal{A}|$.

This procedure is suitable for a small set of polynomials. When the size of the set of polynomials $\mathcal{A}$ increases, the efficiency of the whole procedure decreases. A typical case is when the number of dimensions M is large. To reduce the complexity of the meta-model, algorithms have recently been proposed that pick the most influential polynomials out of a candidate set of polynomials. In the context of polynomial chaos expansions Blatman and Sudret (2011) discussed the *least angle regression selection* (LARS) algorithm originally proposed by Efron et al. (2004).

After determining the set of polynomials and its coefficients, new samples of the output space can be generated straightforwardly by evaluating equation (2).

2.2 Polynomial-Chaos-Kriging (PC-Kriging)

2.2.1 Background

Kriging (a.k.a. *Gaussian process modelling*) is a stochastic interpolation technique which interprets the computational model $\mathcal{M}(\boldsymbol{x})$ as a realization of an underlying, unknown Gaussian process:

$$\mathcal{M}(\boldsymbol{x}) \approx \mathcal{M}^{(\mathsf{K})}(\boldsymbol{x}) = \boldsymbol{\beta}^{\mathsf{T}} \cdot \boldsymbol{f}(\boldsymbol{x}) + \sigma^2\, Z(\boldsymbol{x}, \omega) \quad (8)$$

where $\boldsymbol{\beta}^{\mathsf{T}} \cdot \boldsymbol{f}(\boldsymbol{x}) = \sum_{j=1}^{P} \beta_j\, f_j(\boldsymbol{x})$ is the mean value of the Gaussian process (a.k.a *trend*), P is the number of predictors, $Z(\boldsymbol{x}, \omega)$ is the zero-mean, unit-variance Gaussian process and σ^2 is the Kriging variance. ω describes outcomes of the underlying probability space with a correlation family R and its hyper-parameters $\boldsymbol{\theta}$. The autocorrelation between two samples $\boldsymbol{x}$ and $\boldsymbol{x}'$ of the input space is modelled through a parametric autocorrelation function $R(|\boldsymbol{x} - \boldsymbol{x}'|; \boldsymbol{\theta})$, such as in *e.g.* Echard (2012) and Dubourg (2011).

A Kriging model is called *ordinary Kriging* when the trend is a single parameter with unknown value. A Kriging model is called *universal Kriging* when the trend is a sum of functions as in equation (8). We introduce here a new meta-modelling technique called *Polynomial-Chaos-Kriging* (PC-Kriging) as a universal Kriging technique which models the trend by a sparse set of orthonormal polynomials (Schöbi and Sudret, 2014):

$$\mathcal{M}(\boldsymbol{x}) \approx \mathcal{M}^{(\mathsf{PCK})}(\boldsymbol{x}) = \sum_{\boldsymbol{\alpha} \in \mathcal{A}} a_{\boldsymbol{\alpha}}\, \psi_{\boldsymbol{\alpha}}(\boldsymbol{x}) + \sigma^2\, Z(\boldsymbol{x}, \omega) \quad (9)$$

where $\sum_{\boldsymbol{\alpha} \in \mathcal{A}} a_{\boldsymbol{\alpha}}\, \psi_{\boldsymbol{\alpha}}(\boldsymbol{x})$ is the trend with $|\mathcal{A}|$ polynomials, $\psi_{\boldsymbol{\alpha}}(\boldsymbol{x})$ are the polynomials indexed by $\boldsymbol{\alpha} \in \mathcal{A}$ and $a_{\boldsymbol{\alpha}}$ are their coefficients.

The parameters of the Kriging model are estimated based on a given experimental design $\boldsymbol{\mathcal{X}} = \left\{ \boldsymbol{\chi}^{(1)}, \ldots, \boldsymbol{\chi}^{(N)} \right\}$ and the corresponding response values $\mathcal{Y} = \left\{ \mathcal{Y}^{(1)}, \ldots, \mathcal{Y}^{(N)}. \right\}$. Given a specific set of polynomials $\mathcal{A}$, the algorithms of universal Kriging are applicable to calibrate the Kriging meta-model. Assuming the

shape of the autocorrelation function is known, the hyper-parameters $\boldsymbol{\theta}$ of the Gaussian process are estimated in a first step through maximum-likelihood estimate (Santner et al., 2003):

$$\widehat{\boldsymbol{\theta}} = \arg\min_{\boldsymbol{\theta}} \left[\frac{1}{N} \left(\mathcal{Y} - \mathbf{F}\,\boldsymbol{\beta}\right)^{\mathsf{T}} \mathbf{R}^{-1} \left(\mathcal{Y} - \mathbf{F}\,\boldsymbol{\beta}\right) \left(\det \mathbf{R}\right)^{1/N} \right] \tag{10}$$

Then the Kriging parameters $\left\{\boldsymbol{\beta}, \sigma_y^2\right\}$ are estimated as the generalized least-squares solution:

$$\boldsymbol{\beta}(\boldsymbol{\theta}) = \left(\mathbf{F}^{\mathsf{T}} \mathbf{R}^{-1} \mathbf{F}\right)^{-1} \mathbf{F}\, \mathbf{R}^{-1} \mathcal{Y} \tag{11}$$

$$\sigma_y^2(\boldsymbol{\theta}) = \frac{1}{N} \left(\mathcal{Y} - \mathbf{F}\,\boldsymbol{\beta}\right)^{\mathsf{T}} \mathbf{R}^{-1} \left(\mathcal{Y} - \mathbf{F}\,\boldsymbol{\beta}\right) \tag{12}$$

where $\mathbf{R}_{ij} = R(|\boldsymbol{\chi}^{(i)} - \boldsymbol{\chi}^{(j)}|; \boldsymbol{\theta})$ is the correlation matrix of the experimental design. This defines the universal Kriging model, *i.e.* the PC-Kriging model.

The prediction of new sample points $\boldsymbol{x}$ is not as straightforward as in PCE. Kriging is a stochastic meta-modelling framework which means that the prediction follows a Gaussian probability distribution with mean value $\mu_{\hat{Y}}(\boldsymbol{x})$ and variance $\sigma^2_{\hat{Y}}(\boldsymbol{x})$. These are obtained by:

$$\mu_{\hat{Y}}(\boldsymbol{x}) = \boldsymbol{f}(\boldsymbol{x})^{\mathsf{T}} \boldsymbol{\beta} + \boldsymbol{r}(\boldsymbol{x})^{\mathsf{T}} \mathbf{R}^{-1} \left(\mathcal{Y} - \mathbf{F}\,\boldsymbol{\beta}\right) \tag{13}$$

$$\sigma^2_{\hat{Y}}(\boldsymbol{x}) = \sigma_y^2 \left(1 - \langle \boldsymbol{f}(\boldsymbol{x})^{\mathsf{T}}, \boldsymbol{r}(\boldsymbol{x})^{\mathsf{T}} \rangle \begin{bmatrix} \mathbf{0} & \mathbf{F}^{\mathsf{T}} \\ \mathbf{F} & \mathbf{R} \end{bmatrix}^{-1} \begin{bmatrix} \boldsymbol{f}(\boldsymbol{x}) \\ \boldsymbol{r}(\boldsymbol{x}) \end{bmatrix} \right) \tag{14}$$

where $r_i(\boldsymbol{x}) = R(|\boldsymbol{x} - \boldsymbol{\chi}^{(i)}|; \boldsymbol{\theta})$ is the correlation between the new sample $\boldsymbol{x}$ and the experimental design points $\boldsymbol{\mathcal{X}}$.

2.2.2 PC-KRIGING IN DETAIL

The previous section 2.2.1 showed the calibration of a PC-Kriging model when the set of polynomials is given. In this section the discussion on PC-Kriging is expanded on how to obtain the optimal set of polynomials.

The PC-Kriging algorithm is summarized in Figure 1. Given are the input distributions, the experimental design and an autocorrelation structure (function). Based on the orthonormal bases (in coherency with the input distributions) LARS is used to determine the best sparse set of polynomials. LARS results in a ranked list of polynomials according to their correlation to the model response $\mathcal{Y}$, in decreasing order. Then P Kriging models are calibrated with an increasing number of polynomials. Starting point is the most correlated polynomial, *i.e.* the polynomial chosen first in the LARS algorithm. The P-th meta-model has a trend with all P polynomials in the trend. The meta-models are compared by means of *leave-one-out* (LOO) error which compares the prediction for an experimental design sample $\boldsymbol{\chi}^{(i)}$ through a meta-model based on the remaining samples in the experimental design $\boldsymbol{\mathcal{X}}^{(-i)} \overset{\text{def}}{=} \boldsymbol{\mathcal{X}} \backslash \boldsymbol{\chi}^{(i)} = \left\{\boldsymbol{\chi}^{(j)},\ j = 1, \ldots, i-1, i+1, \ldots, N\right\}$:

$$Err_{LOO} = \frac{1}{N} \sum_{i=1}^{N} \left(\mathcal{Y}^{(i)} - \mu_{\hat{Y}_{(-i)}}(\boldsymbol{\chi}^{(i)}) \right)^2 \tag{15}$$

where $\mu_{\hat{Y}_{(-i)}}(\boldsymbol{\chi}^{(i)})$ is the prediction mean at sample point $\boldsymbol{\chi}^{(i)}$ on the modified experimental design $\boldsymbol{\mathcal{X}}^{(-i)}$. Then the model with the lowest leave-one-out error is chosen as the PC-Kriging model. Note that in Schöbi and Sudret (2014) this method is called *Optimal-PC-Kriging (OPC-Kriging)*.

Dubrule (1983) derived the analytical solution for the LOO error which avoids the computation of N meta-models. The prediction mean and variance of the LOO meta-models are:

$$\mu_{\hat{Y}_{(-i)}} = \sum_{j=1, j\neq i}^{N} \frac{\mathbf{B}_{ij}}{\mathbf{B}_{ii}} \mathcal{Y}^{(j)} = \sum_{j=1}^{N} \frac{\mathbf{B}_{ij}}{\mathbf{B}_{ii}} \mathcal{Y}^{(j)} - \mathcal{Y}^{(i)} \tag{16}$$

$$\mathbf{B} = \begin{bmatrix} \sigma_y^2 \mathbf{R} & \mathbf{F} \\ \mathbf{F}^{\mathsf{T}} & \mathbf{0} \end{bmatrix}^{-1} \tag{17}$$

where $\mathbf{B}$ is a square matrix of size $(N + P)$ and σ_y^2 is the Kriging variance of the meta-model including the entire experimental design $\boldsymbol{\mathcal{X}}$.

For the prediction of new samples, equations (13) and (14) remain valid.

2.3 APPLICATION AND COMPARISON

The performance of PC-Kriging is compared to ordinary Kriging and to PCE through analytical benchmark functions which are inexpensive-to-evaluate. The goodness of fit of the meta-models is assessed through a large validation set ($n = 10^5$) using the relative generalization error:

$$\epsilon_{gen} \equiv \frac{\sum_{i=1}^{n} \left(\mathcal{M}(\boldsymbol{x}^{(i)}) - \widehat{\mathcal{M}}(\boldsymbol{x}^{(i)}) \right)^2}{\sum_{i=1}^{n} \left(\mathcal{M}(\boldsymbol{x}^{(i)}) - \mu_y \right)^2} \tag{18}$$

where $\mathcal{M}$ is the computational model (*i.e.* the exact response), $\widehat{\mathcal{M}}$ is the prediction mean value of the meta-model and μ_y is the mean value of the exact response values. This error compares the exact model response to the meta-model response and is normalized by the variance of the

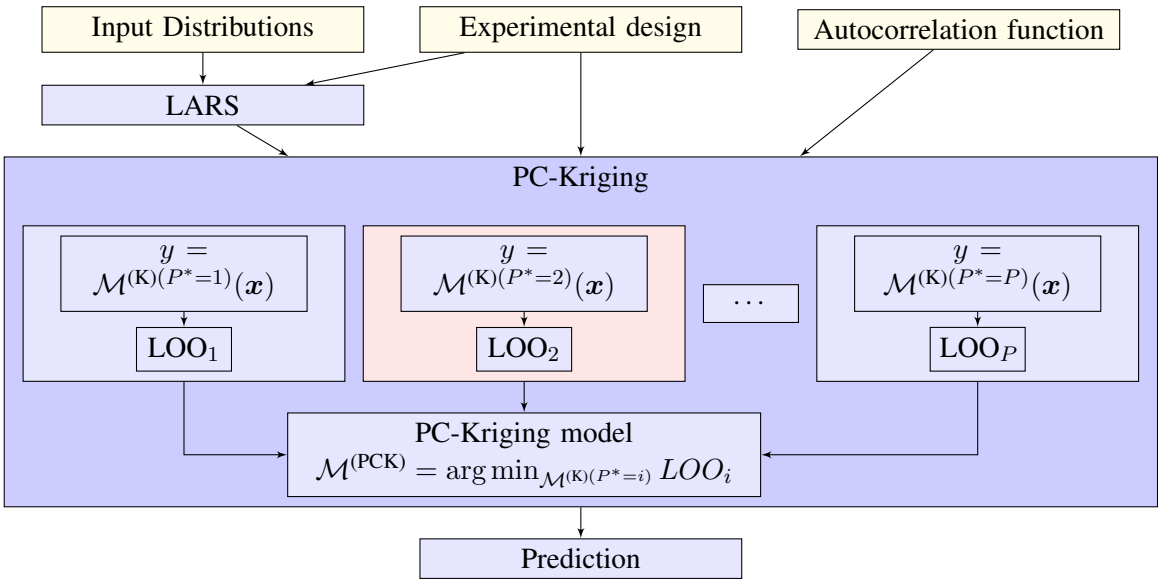


Figure 1: Flowchart PC-Kriging meta-model

exact response values. The basic settings for the comparison of the meta-models are Latin-hypercube samples and the Matérn autocorrelation function ($\nu = 5/2$).

Table 1 shows the results obtained for a selected number of benchmark analytical functions, namely the (2-dimensional) Rosenbrock (*e.g.* Eldred (2009)), Ishigami (*e.g.* Blatman (2009)), Sobol' (Sudret, 2008) and Rastrigin function. N stands for the number of samples in the experimental design and $\mu_{\epsilon_{gen}}$ is the mean of the relative generalization error of 50 replications (*i.e.* independent runs) of the full analysis using different LHS samples.

The results show that PC-Kriging performs better than the traditional techniques for the given small experimental designs. For all four functions, PC-Kriging leads (on average) to the lowest relative generalization error. In these cases PC-Kriging is preferable over PCE and Kriging.

Note that in the above example investigation the experimental designs are small. When the experimental design becomes large, PC-Kriging converges to PCE as can be seen in the last line of Table 1 for the Ishigami function. The PC-Kriging still keeps a small advantage over PCE and both of them outperform ordinary Kriging. Note that the relative generalization error of PCE and PC-Kriging is already in the order of magnitude of the precision of the numerical calculations of the computer. A comprehensive comparison of the three approaches can be found in Schöbi and Sudret (2014).

3 Reliability analysis

Reliability analysis is a framework for estimating the probability of a variable x exceeding a predefined threshold x_0. This probability is referred to as *failure probability*, *i.e.* $P_f = \mathbb{P}(X > x_0)$. The classical Monte Carlo method is a robust method to estimate the failure probability but requires a large number of model evaluations especially for small failure probabilities. Expensive-to-evaluate computational models become intractable due to the long runtime of the analysis when repeated many times and therefore, meta-modelling comes into play. Meta-modelling decreases the computational effort by approximating the model behaviour with an inexpensive surrogate function, such as PC-Kriging. The meta-model is supported by a few sample points (*i.e.* the experimental design) and is then able to predict a large Monte Carlo sample of the input random vector in order to estimate the failure probability.

3.1 Adaptive experimental designs

The experimental design has a large influence on the accuracy of the failure probability estimate, denoted by $\widehat{P}_f$. The accuracy can be increased by carefully choosing additional input points and adding them to the experimental design. Echard et al. (2011) proposed a framework incorporating ordinary Kriging and Monte Carlo simulation, called *Adaptive-Kriging-Monte-Carlo-Simulation* (AK-MCS), and Echard et al. (2013) combined ordinary Kriging and Importance Sampling. The aim is to select samples which increase the accuracy of the approximation of the limit state surface ($\mathcal{M}(\boldsymbol{x}) = 0$).

Function name	N	$\mu_{\epsilon_{gen}}$ Kriging	PCE	PC-Kriging
Rosenbrock	20	$4.63 \cdot 10^{-3}$	$1.52 \cdot 10^{-2}$	$1.48 \cdot 10^{-4}$
Ishigami	50	0.2511	0.0775	0.0430
Sobol'	64	0.1040	0.0822	0.0593
Rastrigin	128	0.1905	0.1086	0.0450
Ishigami	256	$1.381 \cdot 10^{-3}$	$1.133 \cdot 10^{-12}$	$4.147 \cdot 10^{-13}$

Table 1: Collection of the benchmark function's results

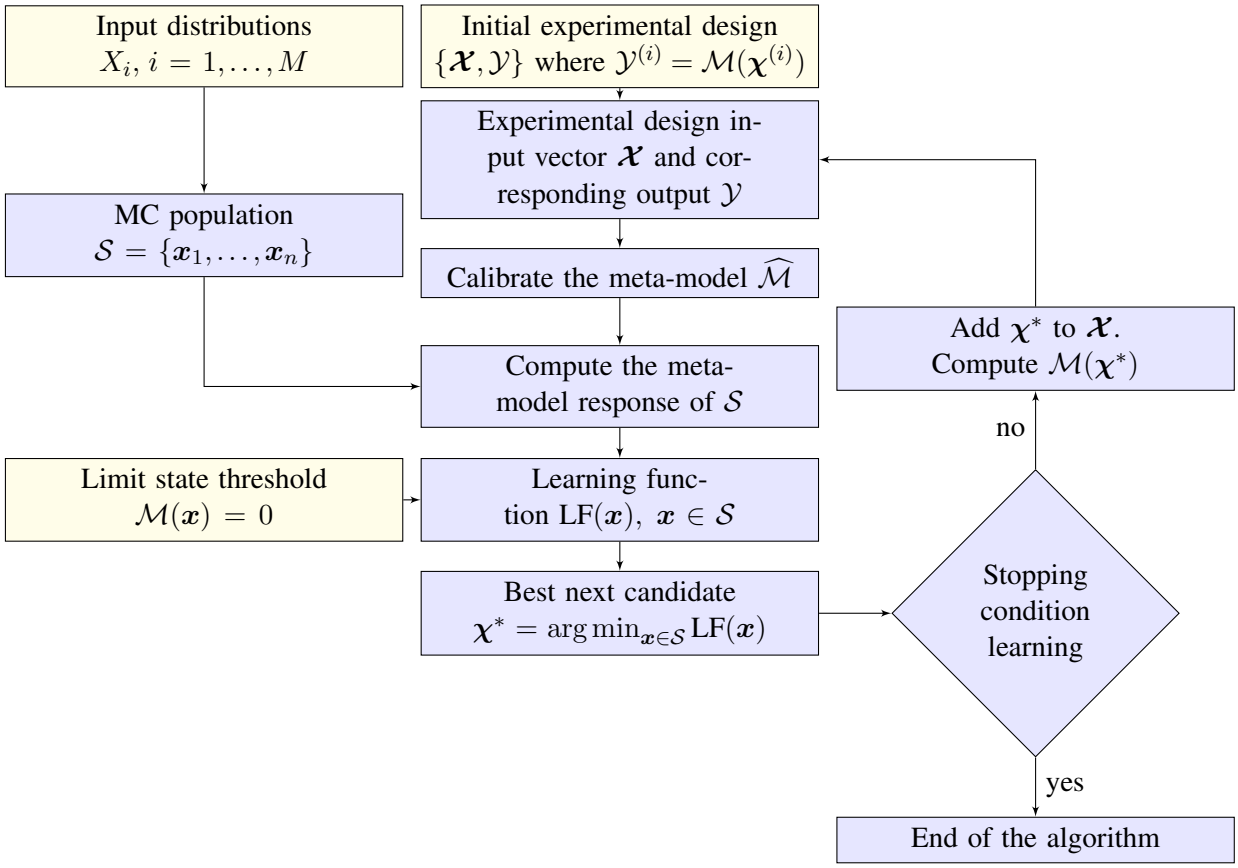


Figure 2: Flowchart of the adaptive algorithm

The two approaches are based on the same idea and are briefly summarized in this paper. A flowchart of the framework is shown in Figure 2: Starting point is a small experimental design $\boldsymbol{\mathcal{X}}$ for which the computational model response $\mathcal{Y}$ is computed. Then a Monte Carlo population $\mathcal{S}$ of the input space of n_{MC} samples is generated. The next step is to fit a Kriging (PC-Kriging) meta-model with the given experimental design and predict the model response for the population $\mathcal{S}$. A learning function assesses the best next point $\boldsymbol{\chi}^*$ which is added to the experimental design in order to increase the accuracy of the failure probability estimate. The computational model evaluates the response y^* for the chosen input sample $\boldsymbol{\chi}^*$ and adds the pair $\{\boldsymbol{\chi}^*, y^*\}$ to the experimental design $\boldsymbol{\mathcal{X}}$. Given the updated experimental design, the Kriging meta-model is updated too, *i.e.* the meta-model is recalibrated. When the meta-modelling technique is replaced by PC-Kriging, it is called *Adaptive-Polynomial-Chaos-Kriging-Monte-Carlo-Simulation* (APCK-MCS).

The core of the adaptive algorithm is the learning function which builds the basis for choosing additional samples. The performance of the adaptive algorithm depends on the selection of additional samples, *i.e.* on the learning function. A *learning function* describes the expected value of information gained (with respect to the failure probability estimate in this case) when the argument $\boldsymbol{x}$ is added to the experimental design of the meta-model. A simple

formulation is the U-function which reads:

$$U(\boldsymbol{x}) = \frac{|\mu_{\widehat{\mathcal{M}}}(\boldsymbol{x})|}{\sigma_{\widehat{\mathcal{M}}}(\boldsymbol{x})} \tag{19}$$

where $\mu_{\widehat{\mathcal{M}}}(\boldsymbol{x})$ and $\sigma_{\widehat{\mathcal{M}}}(\boldsymbol{x})$ are the Kriging mean predictor and standard deviation. The U-function favours points which are close to the failure surface ($\mu_{\widehat{\mathcal{M}}}(\boldsymbol{x}) \approx 0$) and points with a large prediction uncertainty ($\sigma_{\widehat{\mathcal{M}}}(\boldsymbol{x}) \gg 0$). The best next sample of the Monte Carlo population S is then chosen by *minimizing* the U-function:

$$\boldsymbol{\chi}^* = \underset{\boldsymbol{x}\in \mathrm{S}}{\arg\min}\, U(\boldsymbol{x}) \tag{20}$$

In the general case where the initial experimental design is small and the failure surface is complex, many additional samples are required to improve the predictability of the failure probability. The iterative procedure lasts until the algorithm converges to an accurate meta-model, *i.e.* until predefined stopping criteria are fulfilled. Echard et al. (2011) discuss stopping criteria based on the learning function. For the U-function they propose to use the stopping criterion:

$$\min_{x\in \mathrm{S}} [U(x)] \geq 2 \tag{21}$$

The adaptive algorithm stops when the prediction mean $\mu_{\widehat{\mathcal{M}}}(\boldsymbol{x})$ is at least twice the value of the prediction standard deviation $\sigma_{\widehat{\mathcal{M}}}(\boldsymbol{x})$ at each point $\boldsymbol{x} \in \mathcal{S}$. The probability of missclassification of the current point $\boldsymbol{x}$ is then defined as:

$$\gamma_f(\boldsymbol{x}) \leq \min\left[\Phi\left(\frac{\mu_{\widehat{\mathcal{M}}}(\boldsymbol{x}) - 0}{\sigma_{\widehat{\mathcal{M}}}(\boldsymbol{x})}\right), \Phi\left(\frac{0 - \mu_{\widehat{\mathcal{M}}}(\boldsymbol{x})}{\sigma_{\widehat{\mathcal{M}}}(\boldsymbol{x})}\right)\right] \tag{22}$$

It corresponds to the probability that the true response $\mathcal{M}(\boldsymbol{x})$ and the one predicted by the surrogated, namely $\mu_{\widehat{\mathcal{M}}}(\boldsymbol{x})$, have different signs (missclassification from the reliability point of view). The probability of missclassification that defines the stopping criterion Eq. (21) is then at most $\gamma_f(\boldsymbol{x}) \leq \min[\Phi(2), \Phi(-2)] = 2.3\ \%$ for $\boldsymbol{x} \in \mathcal{S}$ (note that this confidence level may be selected by the analyst).

When the adaptive algorithm stops, the failure probability is estimated through a traditional Monte Carlo simulation:

$$\widehat{P}_f = \frac{n_f}{n_{MC}} \tag{23}$$

where n_f is the number of samples in the population $\mathcal{S}$ which $\mu_{\widehat{\mathcal{M}}}(\boldsymbol{x}) \leq 0$. The theoretical coefficient of variation of the failure probability estimated by Monte Carlo sampling is:

$$\mathrm{Cov}\left[\widehat{P}_f\right] = \sqrt{\frac{1 - \widehat{P}_f}{\widehat{P}_f\, n_{\mathrm{MC}}}} \tag{24}$$

Note that the number of samples n_{MC} should be reasonably high in order to ensure a low variation of the failure probability estimate. Also note that instead of pure Monte Carlo sampling, more advanced sampling methods such as Importance Sampling are applicable too.

3.2 Applications

The adaptive algorithm is illustrated on two examples: the four-branch function and a truss structure. The four-branch function is an analytical 2-dimensional function which allows the visualization of the sample selection. The truss model is a FEM model and shows the capabilities of the adaptive design in an engineering context.

3.2.1 Four-branch function

The four-branch function describes the failure of a system with four distinct component limit states. The mathematical formulation reads:

$$f_1(\boldsymbol{x}) = \min\left\{\begin{array}{c} 3 + 0.1\,(x_1 - x_2)^2 - \frac{x_1+x_2}{\sqrt{2}} \\ 3 + 0.1\,(x_1 - x_2)^2 + \frac{x_1+x_2}{\sqrt{2}} \\ (x_1 - x_2) + \frac{6}{\sqrt{2}} \\ (x_2 - x_1) + \frac{6}{\sqrt{2}} \end{array}\right\} \tag{25}$$

where the stochastic input variables x_i are modelled by independent Gaussian random variables $X_i = \mathcal{N}(0, 1)$. The failure event is defined as $f_1(\boldsymbol{x}) \leq 0$, *i.e.* the failure probability is $P_f = \mathbb{P}(f_1(\boldsymbol{X}) \leq 0)$. Reference values of the failure probability in adaptive designs are found in *e.g.* Echard et al. (2011).

The adaptive algorithm involves an initial experimental design of 12 Latin-hypercube samples (LHS), a Monte Carlo population $\mathcal{S}$ of size $n_{MC} = 10^6$, the U-function and the stopping criterion $\min[U(\boldsymbol{x})] \geq 2$. For meta-modelling, ordinary Kriging (AK-MCS) and PC-Kriging (APCK-MCS) are compared, both with Gaussian correlation models. Table 2 shows the results of the computations and also the reference values from Echard et al. (2011). Note that the failure probability and the total number of model evaluations N_{tot} are based on 100 independent runs (replications) of the same algorithm in order to estimate the accuracy of the results in terms of the coefficient of variation (Cov). The values by Echard et al. (2011) are single run values and thus no coefficient of variation is available.

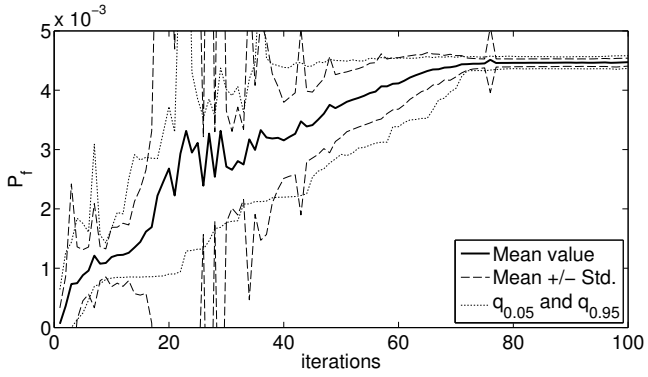
The results show that the reference value and the values computed by the authors coincide. Further notice that the total number of samples N_{tot} are higher for the APCK-MCS than for AK-MCS algorithm. The standard deviation of the number of runs (Cov $[N_{tot}]$) is also higher for APCK-MCS.

The last two lines in Table 2 show the same algorithms with a different initial design, namely k-means clustered samples. The initial design is generated as the centroids of N_0 clusters which are obtained with a standard clustering algorithm. The objective function for clustering is the distance between the samples and their centroid. The influence on the resulting meta-model after computing AK-MCS is marginal though.

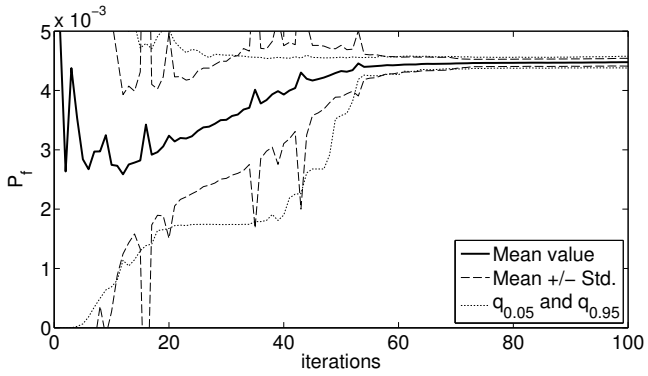
The increased number of samples N_{tot} is not intuitively understandable. This is why the convergence of the failure probability estimate is shown in Figure 3 for both adaptive algorithms: Figure 3(a) and Figure 3(b) shows the results for the AK-MCS and APCK-MCS algorithm respectively. The plots show the number of iterations on the x-axis versus the failure probability estimate on the y-axis. Results for the mean, the mean plus/minus standard deviation and the 5%- and 95%-quantiles are shown. The APCK-MCS algorithm shows a faster convergence to a stable failure probability estimate than AK-MCS. This confirms the results from the previous section about the analytical benchmark problems: PC-Kriging provides a more accurate meta-model for small experimental designs when compared to pure ordinary Kriging. On the other side there are the results in Table 2 which indicate more iterations for PC-Kriging. The total number of iterations, *i.e.* $\propto N_{tot}$, is related to the stopping criterion of the adaptive algorithm. It seems that the stopping criterion $\min[U(\boldsymbol{x})] \geq 2$ is too conservative in the case of PC-Kriging.

Figure 4 and Figure 5 display different iterations steps in the adaptive design with ordinary Kriging (AK-MCS) and PC-Kriging meta-models (APCK-MCS) respectively. The horizontal and vertical axes of each graph correspond to X_1 and X_2, respectively. The grey points represent the Monte Carlo population S, the blue squares are the initial experimental design, the blue points are the added samples in the previous iterations and the solid black line is the limit state surface of the computational model, *i.e.* $\mathcal{M}(\boldsymbol{x}) = 0$. Clearly visible are the four sections (branches) of the limit state function.

Figure 4 shows the typical behaviour of the AK-MCS algorithm for the learning function $U(\boldsymbol{x})$. The algorithm focuses on the exploitation of the identified failure surface section (Figure 4(a), 4(b)) before exploring the next branch after iteration $j = 30$ (Figure 4(c)). The remaining



(a) AK-MCS



(b) APCK-MCS

Figure 3: Convergence of the failure probability estimate for the four-branch function in AK-MCS and APCK-MCS

two branches of the limit state function of the four-branch function are then identified after iteration $j = 40$, as seen in Figure 4(d).

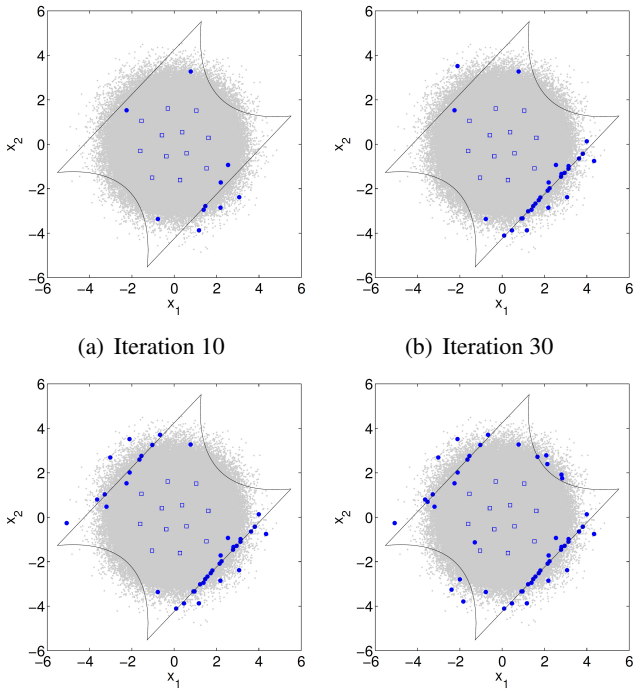
On the other side, APCK-MCS focuses more on the global search for the limit state function (Figure 5). Already after $j = 30$ iterations, the four branches of the limit state function are identified (Figure 5(b)). The remaining iterations are chosen in order to refine the limit state surface (Figure 5(c), 5(d)). The more complex trend in PC-Kriging allows for a better estimation of the limit state surface when only a few samples are chosen, *i.e.* when a few iterations are performed.

3.2.2 TRUSS MODEL

The adaptive algorithm is applied to the truss defined in Hurtado (2013). The computational model is a finite elements model of a 2-dimensional truss structure the geometry of which is shown in Figure 6. The elasticity model of all bars is $E = 100 \cdot 10^9$ Pa whereas the cross section of the bars varies: 0.00535 m^2 for the bars denoted by $\bullet$, 0.0068 m^2 for the bars denoted by $\circ$ and 0.004 m^2 for the rest of the bars. The input random variables are the

Method	Sampling	$\widehat{P}_f$	Cov $\left[\widehat{P}_f\right]$	N_{tot}	Cov $[N_{tot}]$
Monte Carlo	-	$4.460 \cdot 10^{-3}$	0.15 %	10^8	-
AK-MCS	LHS	$4.464 \cdot 10^{-3}$	1.4 %	$12 + 96 = 108$	6.7 %
APCK-MCS	LHS	$4.471 \cdot 10^{-3}$	1.4 %	$12 + 116 = 128$	24.5 %
†AK-MCS	LHS	$4.416 \cdot 10^{-3}$	-	126	-
AK-MCS	k-means	$4.466 \cdot 10^{-3}$	1.4 %	$12 + 97 = 109$	7.1 %
APCK-MCS	k-means	$4.466 \cdot 10^{-3}$	1.4 %	$12 + 120 = 132$	22.2 %

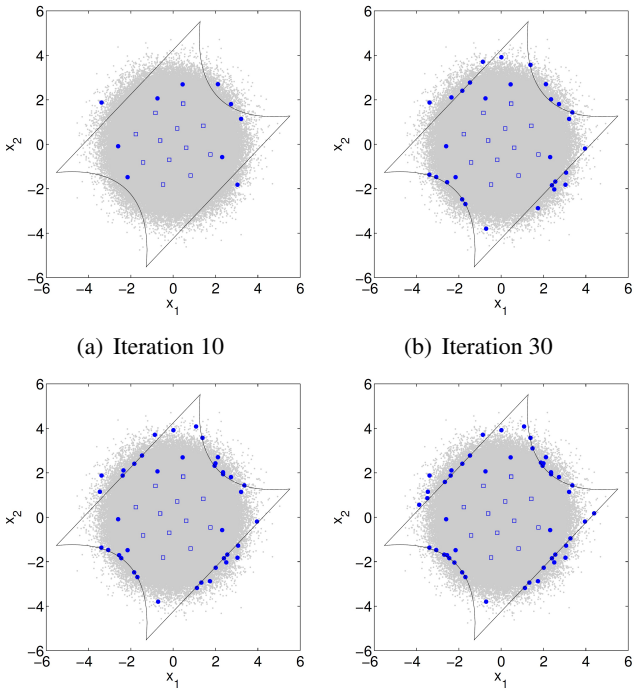
Table 2: Composition of the analysis of the four-branch function; † is a single run result by Echard et al. (2011).



(a) Iteration 10 (b) Iteration 30

(c) Iteration 40 (d) Iteration 50

Figure 4: Experimental design at different iteration steps in the AK-MCS algorithm for the four-branch function



(a) Iteration 10 (b) Iteration 30

(c) Iteration 40 (d) Iteration 50

Figure 5: Experimental design at different iteration steps in the APCK-MCS algorithm for the four-branch function

seven loads P_i which are modelled as independent lognormal variables with mean $\mu_L = 100$ kN and standard deviation $\sigma = 15$ kN.

The reliability problem is formulated in terms of the deflection at midspan (where P_4 is located). Failure is defined as a deflection larger than 29 mm, *i.e.* :

$$g(\boldsymbol{p}) = 0.029 - u_4(\boldsymbol{p}) \tag{26}$$

where u_4 is the deflection at the location of load P_4 and $\boldsymbol{p}$ is the vector of the seven input forces. Thus, the probability of failure is $P_f = \mathbb{P}(g(\boldsymbol{p}) \leq 0)$.

Consider the case of having a small initial experimental design with $N = 32$ and additional resources for another 64 runs of the computational model. For the adaptive design algorithm the following conditions are then set: an initial

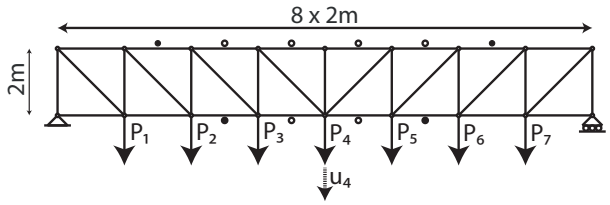


Figure 6: Two-dimensional truss model

experimental design of $N_0 = 32$ Latin-hypercube samples, resources for an additional 64 samples ($N_{tot} = 96$) and a Monte Carlo population $\mathcal{S}$ of $n_{MC} = 10^7$ samples. Remember that in AK-MCS the points of the Monte Carlo population are *not* evaluated by the computational model $\mathcal{M}$ a priori.

The algorithms are compared in terms of meta-modelling techniques, *i.e.* ordinary Kriging (AK-MCS) versus PC-Kriging (APCK-MCS).

The results are shown in Table 3. For the adaptive algorithm, 100 independent runs are carried out to get an estimate of the variance of the failure probability estimates, represented by the coefficient of variation (Cov). In the case of the reference estimate of the failure probability through Monte Carlo simulation ($N_{tot} = 10^7$), the coefficient of variation is estimated by equation (24).

In both cases, *i.e.* AK-MCS and APCK-MCS, the failure probability is accurately estimated with $N_{tot} = 96$ model runs: the mean value ($\widehat{P}_f$) is accurate and the coefficient of variation (Cov $\left[\widehat{P}_f\right]$) is small. APCK-MCS is slightly more accurate in terms of the variation of the results. Considering the case of a Monte Carlo simulation with 10^7 samples, the computational effort is not comparable to the adaptive design meta-modelling approaches.

Method	$\widehat{P}_f$	Cov $\left[\widehat{P}_f\right]$	N_{tot}
Monte Carlo	$9.573 \cdot 10^{-3}$	0.32 %	10^7
AK-MCS	$9.494 \cdot 10^{-3}$	1.5 %	96
APCK-MCS	$9.612 \cdot 10^{-3}$	1.0 %	96

Table 3: Results of the truss analysis for the total number of exact model runs $N_{tot} = 32 + 64 = 96$

4 CONCLUSIONS

This paper introduces the meta-modelling technique Polynomial-Chaos-Kriging (PC-Kriging) which is a combination of the traditional meta-modelling techniques Kriging and Polynomial Chaos Expansions (PCE). The three approaches are compared for benchmarking analytical functions and the results demonstrate that PC-Kriging leads to a more accurate meta-model in terms of relative generalization error.

In the last part of this paper, PC-Kriging is compared to Kriging in reliability problems where an adaptive experimental design algorithm is used to obtain accurate estimates of failure probabilities. PC-Kriging and Kriging perform similarly in terms of both the variance of the failure probability estimate and the number of additional samples in the experimental design.

An example application with a truss application shows the practical applicability of the adaptive design algorithm in reliability problems. When the resources (*i.e.* the number of runs of the computational model) are limited, Adaptive-PC-Kriging-Monte-Carlo-Simulation (APCK-MCS) converges to more accurate estimates of the failure probability.

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