Acceleration of Robust Experiment Design using Sobol Indices and Polynomial Chaos Expansion

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Abstract: In practice, laboratory experiments are still mostly designed by trial and error method using the expert knowledge of the material model to be calibrated. This is, however, a difficult task in the case of advanced models developed to simulate engineering problems by non-linear finite element techniques. Ruffio et al. (2012) proposed method for optimisation of model-based design of experiments using robust evolutionary algorithms. Such a method, however suffers from the high computational demands, which make their application to non-linear finite element (FE) simulations difficult. In this contribution we present a novel method introducing surrogate of FE model based on polynomial chaos expansion (PCE) and global formulation of sensitivity matrices. PCE-based surrogates bring two principal advantages. First, they allow to overcome the computational burden of many times repeated FE simulations within the process of experiment design optimisation. Second, they allow fast analytical evaluation of Sobol indices or response variances, which can be used for quantification of global sensitivity of measured quantities to identified parameters. The advantages and drawbacks of the proposed method are demonstrated on a simple problem of two-dimensional nonstationary linear heat transfer. The goal of the experiment design is to find optimal positions of three thermocouples so as to identify the volumetric thermal capacity and the conductivities in the two principal directions while considering uncertainties in the prescribed loading conditions, positions of thermocouples and measurements errors.

Keywords: robust experiment design, global sensitivity, Sobol indices, polynomial chaos, evolutionary optimisation

1. Introduction

The last decade has witnessed growing interest in the development of models that can describe materials response more realistically. This has inspired many new ideas in phenomenological model building, in which the subscale phenomena are accounted for by internal parameters. However, up to the present time, the majority of such advanced models is of a limited practical use, because they are difficult to calibrate by conventional experiments. An experiment design is often done by the trial and error method using the expert, often heuristic, knowledge on the calibrated model.

Such efforts result in a series of single-purpose tests and manual or optimisation-based fitting of measured data. In the case of complex phenomenological models, however, such an approach is often not feasible or results in excessive financial and time costs due to a high number of experiments. Thus, the model complexity brings the need for the design of new experimental procedures. Such problem goes far beyond traditional curve-fitting procedures, as the key issue is to ensure that all model parameters are correctly calibrated by activating all relevant phenomena during the experiment. In addition, the procedure must be robust with respect to inevitable experimental inaccuracies.

The topic of optimal experiment design was mostly addressed by researchers from the field of chemical engineering (Franceschini and Macchietto, 2008; Telen et al., 2012) or theoretical biology (Lindner and Hitzmann, 2006; Van Derlinden et al., 2010). The developed methods, however, suffer from two principal shortcomings:

- they aim at experiments designed for calibration of models with linear relation between the parameters and response and
- they consider inevitable errors on experimental observations, but completely neglect possible errors in parameters of the experiment arising due to its imperfect realisation.

These reasons significantly limit the use of the methods to the case of complex nonlinear material models calibrated from imprecise experiments. Therefore, our goal is to extend the existing methods towards non-linear models under consideration of all the inevitable sources of errors.

To facilitate the following discussion, we introduce a scheme of an experiment suitable for material model calibration in Figure 1. Such an experiment deals with three types of variables: (i)

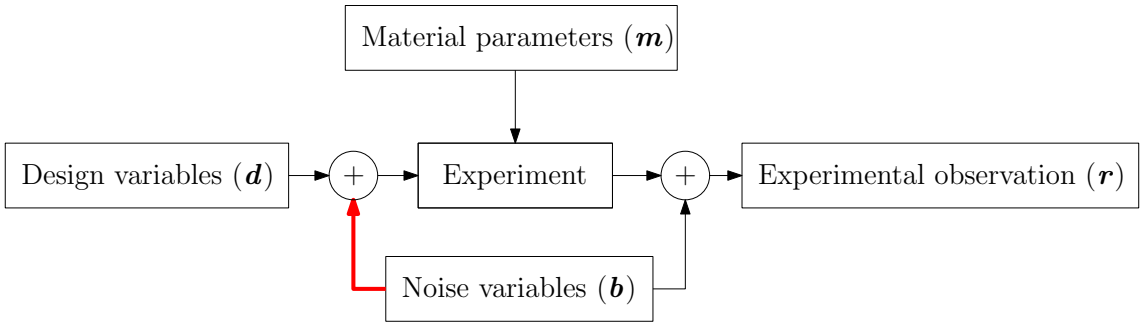


Figure 1. Experimental design problem.

material properties ($\boldsymbol{m}$) to be identified, e.g. thermal conductivity, heat capacity or water vapour resistance, (ii) design variables ($\boldsymbol{d}$) include loading types (e.g. prescribed temperature, moisture flux or heat transfer on boundary) and loading magnitude as well as positions of sensors (thermometers, hygrometers etc.) and (iii) noise ($\boldsymbol{b}$). As emphasized by red arrow, the noise variables must affect not only the experiment output characterizing measurement errors, but also the design variables so as to represent the imperfect realisation of the experiment (imprecise positioning of sensors or imperfections in prescribed loading conditions). The design variables are the only variables controlled by the experiment designer.

The goal of such a process is to find the experiment configuration defined by design variables $\boldsymbol{d}$, which (i) activates all the phenomena described by the investigated material model (i.e. is maximally sensitive to all model parameters $\boldsymbol{m}$) and (ii) reflects the technological aspects, limitations and inherent experimental errors $\boldsymbol{b}$. Hence, we speak about *model-based experiment design*, which needs to be (i) **optimal** in terms of the maximum information content on investigated parameters and (ii) **robust** to be minimally influenced by experimental errors. Both criteria – optimality and robustness – may be expressed by sensitivities of experimental observations $\boldsymbol{r}$ to given material properties and noise variables, respectively, leading to the following definition of the optimisation process:

$$\max_{\boldsymbol{d}} \ \mathbf{S}_{\boldsymbol{r},\boldsymbol{m}} \,, \tag{1}$$

$$\min_{\boldsymbol{d}} \ \mathbf{S}_{\boldsymbol{r},\boldsymbol{b}} \,, \tag{2}$$

$$\text{s.t.} \quad \boldsymbol{m} \in \mathscr{M}, \boldsymbol{b} \in \mathscr{B}, \boldsymbol{d} \in \mathscr{D} \,, \tag{3}$$

where $\mathbf{S}_{\boldsymbol{r},\boldsymbol{m}}$ and $\mathbf{S}_{\boldsymbol{r},\boldsymbol{b}}$ stand for a sensitivity measures of observations $\boldsymbol{r}$ to material properties $\boldsymbol{m}$ and noise variables $\boldsymbol{b}$, respectively. $\mathscr{M}$ is a feasible domain of material parameters typically defined by an expert on the investigated material model in terms of feasible intervals. The feasible domains of design variables $\mathscr{D}$ and noise variables $\mathscr{B}$ are supposed to be given by an expert in experimentation commonly in the form of feasible intervals for design variables and mean and variance of noise variables.

All methods reviewed in (Franceschini and Macchietto, 2008) or in many more recent articles (e.g. (Hametner et al., 2013)) completely omit the imperfections in experimental configuration and compute the sensitivities $\mathbf{S}_{\boldsymbol{r},\boldsymbol{m}}$ as local derivatives. The sensitivities are then organised into the information matrix quantifying the information content of the experiment and measurement errors enter into the information matrix simply as a scaling factors of the computed sensitivities $\mathbf{S}_{\boldsymbol{r},\boldsymbol{m}}$. Different optimality criteria are then proposed as a scalar measure of the information matrix used as an objective function for the experiment design optimisation process.

The authors in (Ruffio et al., 2012) employ the method for robust experiment design considering the uncertainties related to design variables or other known parameters of the experiment. The uncertainties are included in the modified Fisher information matrix and a new optimality criterion is proposed to quantify the information content of the experiment.

The remaining important drawback of all the presented methods consists in computing local derivatives-based sensitivities. In case of nonlinear relation between observations $\boldsymbol{r}$ and investigated parameters $\boldsymbol{m}$, the local sensitivity can be evaluated only for a given values of parameters $\boldsymbol{m}$ and thus their values can be estimated only approximately. One often employed solution is the so-called worst case or maximin approach computing the sensitivities in a set of points and optimising the experimental design so as to maximise the minimal obtained sensitivity (Asprey and Macchietto, 2002; Ruffio et al., 2012). Such a sensitivity estimate is rough, but can be quickly evaluated in case of analytically derived sensitivities. However, if a numerical computation of derivatives is inevitable, such evaluation of sensitivities becomes computationally prohibitive especially during an optimisation process requiring large number of iterations.

This limitation can be overcome by two novelties proposed in this paper. The first one consist in employment of global sensitivities quantifying the sensitivity over the whole prescribed domain of all the involved parameters. In particular, for a given set of controlled design variables $\boldsymbol{d}$, the sensitivity

is evaluated over the domains $\mathscr{B}$ and $\mathscr{M}$ defined as probability distributions (typically normal and uniform) of the respective noise and material parameters. There are different criteria measuring the global sensitivity, mostly based on the computationally expensive sampling procedure, see e.g. (Helton et al., 2006) for a thorough review. Certain time savings may be achieved by optimised sampling as presented by our team members in (Janouchová and Kučerová, 2013), but the predictions in case of high dimensional domains will be still too costly. To overcome this obstacle, the second novelty of our approach concerns the introduction of computationally cheap surrogate models, commonly used in the field of robust design optimisation of structures (Beyer and Sendhoff, 2007; Jurecka, 2007) to replace time consuming structural simulations within the optimisation process. Here we focus on polynomial chaos-based surrogates, which allow for fast analytical evaluation of Sobol indices without the need for exhaustive sampling (Blatman and Sudret, 2010). The global sensitivity measures thus come as the by-product of surrogate construction.

In this paper we follow the work of Ruffio et al. (2012) and compare our proposed global sensitivity-based strategy with their robust worst case scenario-based approach using local sensitivities. We also elaborate the same numerical example of two-dimensional nonstationary linear heat transfer. In this example, the goal of the experiment design is to find optimal positions of three thermocouples so as to identify the volumetric thermal capacity and the conductivities in the two principal directions while considering uncertainties in the prescribed loading conditions, positions of thermocouples and measurements errors.

2. Inverse Problem - Nonlinear Regression with Random Parameters

We consider a nonlinear model of an experiment resulting in multiple observations $\boldsymbol{f}(\boldsymbol{d}, \boldsymbol{b}_d, \boldsymbol{m}) = (\dots, f_i(\boldsymbol{d}, \boldsymbol{b}_d, \boldsymbol{m}), \dots)^{\mathrm{T}}$. Here $\boldsymbol{b}_d$ denotes a vector of random parameters with prescribed probability distribution quantifying our uncertainty related to experimental setting (e.g. imperfections in values of boundary conditions or loading, imperfections in sensors positioning etc.). Moreover, the experimental observations $\boldsymbol{r}(\boldsymbol{d})$ are also contaminated by measurement errors $\boldsymbol{b}_r$ and thus we write:

$$\boldsymbol{r}(\boldsymbol{d}) = \boldsymbol{f}(\boldsymbol{d}, \boldsymbol{b}_d, \boldsymbol{m}) + \boldsymbol{b}_r \,. \tag{4}$$

We suppose that the true value of material parameters $\boldsymbol{m}$ to be identified is $\boldsymbol{m}^* \in \mathscr{M}$, where $\mathscr{M}$ is some given feasible domain of material properties. The estimate $\widehat{\boldsymbol{m}}$ is generally defined as a least square solution given as

$$\widehat{\boldsymbol{m}} = \underset{\boldsymbol{m} \in \mathscr{M}}{\operatorname{argmin}} \sum_i \left(r_i - f_i(\boldsymbol{d}, \boldsymbol{b}_d, \boldsymbol{m})\right)^2 \,, \tag{5}$$

which is however nontrivial to obtain when the model $\boldsymbol{f}(\boldsymbol{d}, \boldsymbol{b}_d, \boldsymbol{m})$ is a nonlinear function of $\boldsymbol{m}$ and some robust optimisation algorithm will be necessary. Moreover, uncertainty in parameters $\boldsymbol{b}_d$ resulting in uncertainty in the obtained estimate $\widehat{\boldsymbol{m}}$ is also difficult to obtain due to the nonlinearity of the model w.r.t. random parameters $\boldsymbol{b}_d$ and generally will require some Monte Carlo-based sampling procedure.

Here we consider an approximate solution of the inverse problem based on the first order Taylor development of the model $\boldsymbol{f}(\boldsymbol{d}, \boldsymbol{b}_d, \boldsymbol{m})$ around the solution $(\widehat{\boldsymbol{m}}, \overline{\boldsymbol{b}_d})$ given as

$$\boldsymbol{f}_{\overline{\boldsymbol{b}_d}, \widehat{\boldsymbol{m}}}(\boldsymbol{d}, \boldsymbol{b}_d, \boldsymbol{m}) = \boldsymbol{f}(\boldsymbol{d}, \overline{\boldsymbol{b}_d}, \widehat{\boldsymbol{m}}) + \mathbf{S}_{\boldsymbol{b}_d}(\boldsymbol{b}_d - \overline{\boldsymbol{b}_d}) + \mathbf{S}_{\boldsymbol{m}}(\boldsymbol{m} - \widehat{\boldsymbol{m}}) \,, \tag{6}$$

where

$$\mathbf{S}_{\boldsymbol{b}_d} = \mathbf{S}_{\boldsymbol{b}_d}(\boldsymbol{d}, \overline{\boldsymbol{b}_d}, \widehat{\boldsymbol{m}}) = \begin{bmatrix} \frac{\partial f_1(\cdot)}{\partial b_{d,1}} & \frac{\partial f_1(\cdot)}{\partial b_{d,2}} & \cdots \\ \frac{\partial f_2(\cdot)}{\partial b_{d,1}} & \frac{\partial f_2(\cdot)}{\partial b_{d,2}} & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix} \quad \text{and} \quad \mathbf{S}_{\boldsymbol{m}} = \mathbf{S}_{\boldsymbol{m}}(\boldsymbol{d}, \overline{\boldsymbol{b}_d}, \widehat{\boldsymbol{m}}) = \begin{bmatrix} \frac{\partial f_1(\cdot)}{\partial m_1} & \frac{\partial f_1(\cdot)}{\partial m_2} & \cdots \\ \frac{\partial f_2(\cdot)}{\partial m_1} & \frac{\partial f_2(\cdot)}{\partial m_2} & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix} \tag{7}$$

denote the sensitivity matrices to noise parameters $\boldsymbol{b}_d$ and identified material properties $\boldsymbol{m}$, respectively.

Using this linearisation, the least square solution (Eq. (5)) can be obtained explicitly as

$$\widehat{\boldsymbol{m}}(\boldsymbol{d}, \boldsymbol{b}_d, \boldsymbol{b}_r) = \left(\mathbf{S}_{\boldsymbol{m}}^{\mathrm{T}}\mathbf{S}_{\boldsymbol{m}}\right)^{-1}\mathbf{S}_{\boldsymbol{m}}^{\mathrm{T}}\left[\boldsymbol{r}(\boldsymbol{d}) - \boldsymbol{f}(\boldsymbol{d}, \overline{\boldsymbol{b}_d}, \widehat{\boldsymbol{m}}) - \mathbf{S}_{\boldsymbol{b}_d}(\boldsymbol{b}_d - \overline{\boldsymbol{b}_d}) + \mathbf{S}_{\boldsymbol{m}}\widehat{\boldsymbol{m}}\right] \tag{8}$$

and the variance covariance matrix of $\widehat{\boldsymbol{m}}$ is then given as

$$\mathrm{cov}(\widehat{\boldsymbol{m}}) = \left(\mathbf{S}_{\boldsymbol{m}}^{\mathrm{T}}\mathbf{S}_{\boldsymbol{m}}\right)^{-1}\mathbf{S}_{\boldsymbol{m}}^{\mathrm{T}}\left[\mathrm{cov}(\boldsymbol{b}_r) + \mathbf{S}_{\boldsymbol{b}_d}\mathrm{cov}(\boldsymbol{b}_d)\mathbf{S}_{\boldsymbol{b}_d}^{\mathrm{T}}\right]\mathbf{S}_{\boldsymbol{m}}\,. \tag{9}$$

3. Robust Experiment Design

As described in previous section, the inverse problem considering the random noise parameters and nonlinear model w.r.t. to both the noise parameters $\boldsymbol{b}_d$ as well as to the identified material properties $\boldsymbol{m}$ is computationally nontrivial and generally requires some sampling procedure for evaluating the resulting uncertainty in parameter estimates. In the phase of experiment preparation, the goal is to design the experiment leading to minimal uncertainty in the parameter estimates. This generally leads to even more complex optimisation problem, where each iteration of a robust optimisation algorithm involves a solution of the underlying inverse problem.

3.1. Local sensitivity-based robust experiment design

Ruffio et al. (2012) suggest a procedure based on the linearisation described in previous section, where uncertainty in parameter estimates is expressed by variance covariance matrix obtained explicitly according to Eq. 9. The authors further propose the so-called *F-optimality* criterion, which is similar to commonly used *A-optimality* criterion given as

$$A(\boldsymbol{d}, \widehat{\boldsymbol{m}}) = \mathrm{trace}\left(\left[(\mathbf{S}_{\boldsymbol{m}}\mathrm{diag}(\widehat{\boldsymbol{m}}))^{\mathrm{T}}(\mathbf{S}_{\boldsymbol{m}}\mathrm{diag}(\widehat{\boldsymbol{m}}))\right]^{-1}\right) = \sum_i \left(\frac{\widehat{\sigma_{m_i}}}{\widehat{m_i}}\right)^2 \tag{10}$$

and which is equivalent to the sum of relative variances. The difference consists in considering the effect of the noise parameters, which is neglected by the A-optimality derived only from the sensitivity matrix $\mathbf{S}_{\boldsymbol{m}}$. The F-optimality, on the other hand, is derived from the variance covariance matrix (Eq. (9)) as

$$F(\boldsymbol{d}, \widehat{\boldsymbol{m}}, \overline{\boldsymbol{b}}) = \sqrt{\mathrm{trace}\left((\mathrm{cov}(\widehat{\boldsymbol{m}})\mathrm{diag}(\widehat{\boldsymbol{m}})^{-1})^{\mathrm{T}}(\mathrm{cov}(\widehat{\boldsymbol{m}})\mathrm{diag}(\widehat{\boldsymbol{m}})^{-1})\right)} = \sqrt{\sum_i \left(\frac{\widehat{\sigma_{m_i}}}{\widehat{m_i}}\right)^2}\,, \tag{11}$$

where variances $\widehat{\sigma_{m_i}}$ involves the effect of all noise parameters $\boldsymbol{b}$.

The F-criterion has, however, two significant drawbacks. First is the aforementioned approximative linearisation of the nonlinear model of the experiment. Second concerns the requirement of a prior guess about the values of the identified parameters $\overline{\boldsymbol{m}}$, for which the local derivatives in Eq. (7) are computed. To overcome the latter drawback, Ruffio et al. (2012) propose more robust *FR-criterion* based on the principle of worst case scenario considering for identified parameters some prescribed feasible domain. In particular, instead of evaluating the F-criterion at one single point $\overline{\boldsymbol{m}}$, they consider a set of possible solutions M given by the so-called *central star design points*, which are the points in the center of the considered feasible hypercube and in the center of all its facets, i.e. $M = \{\overline{\boldsymbol{m}}, \overline{\boldsymbol{m}} + \delta m_i \boldsymbol{e}_i, \overline{\boldsymbol{m}} - \delta m_i \boldsymbol{e}_i\}$ where vectors $\boldsymbol{e}_i$ represent canonical base in parameter domain. Figure 2 shows the set of possible solutions in case of three identified parameters.

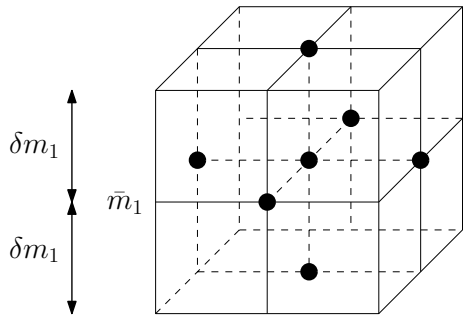


Figure 2. Set of possible solutions M considered for evaluation of robust FR criterion.

The FR-criterion is then given as maximal value of F-criterion obtained for a set of possible solutions M, i.e.

$$F_M(\boldsymbol{d}, \bar{\boldsymbol{b}}) = \max\left\{F(\overline{\boldsymbol{m}}, \bar{\boldsymbol{b}}, \boldsymbol{d}), F(\overline{\boldsymbol{m}} - \delta \boldsymbol{m}_i \boldsymbol{e}_i, \bar{\boldsymbol{b}}, \boldsymbol{d}), F(\overline{\boldsymbol{m}} + \delta \boldsymbol{m}_i \boldsymbol{e}_i, \bar{\boldsymbol{b}}, \boldsymbol{d})\right\} . \tag{12}$$

The FR-criterion increases the robustness of the obtained solution w.r.t. prior guess about the values of identified parameters, but this robustness is still limited as the central star design points M are only very rough approximation of the feasible domain for the identified parameters $\mathscr{M}$. The approximation quality can be obviously improved by increasing number of points in the set M (e.g. full factorial design points involving the corners of the hypercube), but it leads to significant increase of computational effort due to multiple evaluations of the F-criterion. Here we have to emphasize that computational complexity of F-criterion consists in evaluation of local derivatives in Eq. (7), which can be very fast if an explicit analytical expression is available. Otherwise – and very commonly in finite elements-based models – numerical and much more computationally demanding evaluation is inevitable.

3.2. Global sensitivity-based robust experiment design

In this contribution, we propose a new formulation of an optimality criterion in robust experiment design optimisation, which is derived to achieve two goals. First, we aim at increasing the robustness

of the criterion by considering whole feasible domain for identified parameters $\mathscr{M}$ and not only its rough approximation based on central star design points. Second, we focus on computational feasibility in case of complex nonlinear models of material behaviour. To that purpose, we propose a new criterion based on global sensitivity matrix consisting of Sobol indices derived analytically from coefficients of polynomial chaos-based approximation of model responses.

So as to build a polynomial chaos expansion, we consider all problem variables $(\boldsymbol{d}, \boldsymbol{b}, \boldsymbol{m})$ as random variables with prescribed probability distribution. In case of design variables and material properties, where only feasible domain is typically prescribed, we consider those variables as uniformly distributed within the feasible domain. As the noise variables are often defined as normally distributed variables, we assume that all the variables can be transformed into the standard normal variables $\boldsymbol{\xi}$ via linear (in case of normally distributed noise variables) or nonlinear (i.e. exponential in case of uniformly distributed design variables and material properties) transformation as $(\boldsymbol{d}, \boldsymbol{b}, \boldsymbol{m}) = \boldsymbol{g}(\boldsymbol{\xi} = (\boldsymbol{\xi_d}, \boldsymbol{\xi_b}, \boldsymbol{\xi_m}))$. We further assume all the problem variables $\boldsymbol{\xi}$ to be statistically independent. For an appropriate evaluation of Sobol indices, which correspond to proportional variances of model response, we need to involve all the relevant variables in our model of the experiment including measurement errors $\boldsymbol{b}_r$. Therefore we rewrite the Eq. (4) as

$$\boldsymbol{r}(\boldsymbol{d}) = \boldsymbol{f}(\boldsymbol{d}, \boldsymbol{b}, \boldsymbol{m})\,, \tag{13}$$

where vector $\boldsymbol{b} = (\boldsymbol{b}_d, \boldsymbol{b}_r)$. According to Doob-Dynkin lemma (Bobrowski, 2005), the model response $\boldsymbol{f}(\boldsymbol{d}, \boldsymbol{b}, \boldsymbol{m}) = \boldsymbol{f}(\boldsymbol{\xi})$ is a random vector which can be expressed in terms of the same random variables $\boldsymbol{\xi}$. Since $\boldsymbol{\xi}$ are independent standard Gaussian random variables, Wieners polynomial chaos expansion (PCE) based on multivariate Hermite polynomials[1] – orthogonal in the Gaussian measure – $\{H_\alpha(\boldsymbol{\xi})\}_{\alpha\in\mathcal{J}}$ is the most suitable choice for the approximation $\widetilde{\boldsymbol{f}}(\boldsymbol{\xi})$ of the model response $\boldsymbol{f}(\boldsymbol{\xi})$, see (Xiu and Karniadakis, 2002), and it can be written as

$$\widetilde{\boldsymbol{f}}(\boldsymbol{\xi}) = \sum_{\alpha\in\mathcal{J}} \boldsymbol{f}_\alpha H_\alpha(\boldsymbol{\xi})\,, \tag{14}$$

where $\boldsymbol{u}_\alpha$ is a vector of PC coefficients and the index set $\mathcal{J} \subset \mathbb{N}_0$ is a finite set of non-negative integer sequences with only finitely many non-zero terms, i.e. multi-indices, with cardinality $|\mathcal{J}| = R$. Of course, if any other type of standard random variables is more suitable (such as uniform variables), the Hermite polynomials can be replaced by other type of polynomial orthogonal w.r.t. chosen probability measure (e.g. Legendre polynomials in case of uniform variables).

Construction of PCE-based approximation is of course much more complex than construction of the first order Taylor series. Nevertheless, we recall again that the local sensitivities in Taylor development need to be recomputed for any new choice of design variables within the process of experiment optimisation. In our approach, the PCE constructions is, however, the computationally most demanding step, which needs to be done only once, before starting the experiment optimisation. Computational feasibility can be also achieved by considering low polynomial order in PCE (however with the risk of insufficient accuracy of the resulting approximation) or by employing

[1] We assume the full PCE, where number of polynomials r is fully determined by the degree of polynomials p and number of random variables s according to the well- known relation $r = \frac{(s+p)!}{(s!p!)}$.

efficient algorithms for computing PC coefficients, see e.g. (Xiu, 2009). One advantage of PCE-based model approximation is that it is well developed for nonlinear models based on finite element method. But the true beauty of PCE consists in the possibility of an analytical derivation of global sensitivity matrix based on Sobol indices, see (Blatman and Sudret, 2010), according to

$$S_{f_k,\xi_i} = \frac{\sum_{\boldsymbol{\alpha}\in\mathcal{I}_i} f_{k,\alpha}^2 \mathbb{E}[H_{\boldsymbol{\alpha}}^2(\boldsymbol{\xi})]}{\sum_{\boldsymbol{\alpha}\in\mathcal{J}\setminus\{\mathbf{0}\}} f_{k,\boldsymbol{\alpha}}^2 \mathbb{E}[H_{\boldsymbol{\alpha}}^2(\boldsymbol{\xi})]}, \tag{15}$$

where $\mathcal{I}_i$ determines the polynomials involving the terms depending only on ξ_i and polynomial degrees of other variables are null, i.e.

$$\mathcal{I}_i = \{\boldsymbol{\alpha} \in \mathbb{N}^s : 0 \leq \sum_{j=1}^{s} \alpha_j \leq p, \alpha_l = 0 \Longleftrightarrow l \notin (i), \forall l = 1, \ldots, s\}, \tag{16}$$

and

$$\mathbb{E}[H_{\boldsymbol{\alpha}}^2(\boldsymbol{\xi})] = \int H_{\boldsymbol{\alpha}}^2(\boldsymbol{\xi}) \mathrm{d}\mathbb{P}(\boldsymbol{\xi}) = \int \cdots \int_s \prod_{j=1}^{s} (H_{\alpha,j}^2(\xi_j)) \mathrm{d}\mathbb{P}(\xi_1) \cdots \mathrm{d}\mathbb{P}(\xi_s) = \prod_{j=1}^{s} p_{\alpha,j}!, \tag{17}$$

where $p_{\alpha,j}$ is a polynomial degree of variable ξ_j in the polynomial $H_{\boldsymbol{\alpha}}$.

As we aim at using the Sobol indices as components of global sensitivity matrix to be used for formulation of an optimality criteria, we introduce a simple new type of Sobol indices, so-called additive sensitivity indices (ASI), which consist of the sensitivity indices of the considered variable and a part of the sensitivity indices corresponding to the variable's combination with another variables, these indices are divided by the number of appeared variables to get their particular part. The formula for the additive sensitivity indices is

$$S_{f_k,\xi_i}^* = \frac{\sum_{\boldsymbol{\alpha}\in\mathcal{I}_i} f_{k,\boldsymbol{\alpha}}^2 \mathbb{E}[H_{\boldsymbol{\alpha}}^2(\boldsymbol{\xi})] + \sum_{\boldsymbol{\alpha}\in\mathcal{I}_i^*} {}^1\!/_{n_i^*} f_{k,\boldsymbol{\alpha}}^2 \mathbb{E}[H_{\boldsymbol{\alpha}}^2(\boldsymbol{\xi})]}{\sum_{\boldsymbol{\alpha}\in\mathcal{J}\setminus\{\mathbf{0}\}} f_{k,\boldsymbol{\alpha}}^2 \mathbb{E}[H_{\boldsymbol{\alpha}}^2(\boldsymbol{\xi})]}, \tag{18}$$

where n_i^* is a number of variables included in the polynomials from the set $\mathcal{I}_i^*$ defining all the polynomials involving ξ_i except the polynomials from $\mathcal{I}_i$, i.e.

$$\mathcal{I}_i^* = \{\boldsymbol{\alpha} \in \mathbb{N}^s : 0 \leq \sum_{j=1}^{s} \alpha_j \leq p, \boldsymbol{\alpha}_i \neq 0 \ \wedge \boldsymbol{\alpha}_l \neq 0 \Longleftrightarrow l \neq i, \forall l = 1, \ldots, s\}. \tag{19}$$

The reason is that original Sobol indices do not involve sensitivity to mixed terms involving multiple variables, which can be, however, significant and thus we do not want to neglect them. On the other hand, total sensitivity indices account for mixed terms in every index corresponding to variable present in the term. It means that sensitivity to these mixed terms will be accounted in the sensitivity matrix several times. This can lead to increased emphasis to mixed terms in comparison to terms depending uniquely on a single variable. The proposed ASI thus aim at including the sensitivity to all combinations of model variables along with their equalised significance. As a result, the sum of all ASI obtained for a chosen response component is equal to one and the indices

can be viewed as relative indices providing proportional significance of particular model variables for the response component.

In Eq. (14), the PCE is constructed also as a function of standardised design variables $\boldsymbol{\xi_d}$, but the sensitivity to those variables is of course not relevant for the experiment design. Design variables are involved only to allow an immediate analytical reconstruction of PCE as a function of only material properties and noise variables for given choice of design variables. At each step of an experiment design optimisation, the design variables $\boldsymbol{\xi_d}$ in PCE (Eq. (14)) are replaced by specific values $\boldsymbol{\xi_d^\chi}$ chosen by the governing optimisation algorithm resulting in simpler PCE given as

$$\widetilde{\boldsymbol{f}}_{\boldsymbol{\xi_d^\chi}}(\boldsymbol{\xi_m}, \boldsymbol{\xi_b}) = \widetilde{\boldsymbol{f}}(\boldsymbol{\xi})|_{\boldsymbol{\xi_d}=\boldsymbol{\xi_d^\chi}} . \tag{20}$$

Based on Eq. (20), we can define the global sensitivity matrix oppositely as a function of chosen values of design variables $\boldsymbol{\xi_d^\chi}$, which were handled as constants so far:

$$\mathbf{S}^*(\boldsymbol{\xi_d^\chi}) = \begin{bmatrix} \cdots & S^*_{f_1,\xi_{m_i}}(\boldsymbol{\xi_d^\chi}) & \cdots & S^*_{f_1,\xi_{b_i}}(\boldsymbol{\xi_d^\chi}) & \cdots \\ \cdots & S^*_{f_2,\xi_{m_i}}(\boldsymbol{\xi_d^\chi}) & \cdots & S^*_{f_2,\xi_{b_i}}(\boldsymbol{\xi_d^\chi}) & \cdots \\ & \vdots & & \vdots & \end{bmatrix} . \tag{21}$$

Here, sum of each line equals again to one and particular indices provide again the proportional significance of particular model variable (given by matrix column) to particular response component (given by matrix line). As the goal is to maximise the sensitivity to material properties and minimise the sensitivity to noise variables, from the formulation of global sensitivity matrix given in Eq. 21 it follows that maximising the sensitivity to material properties results in minimising the sensitivity to noise variables as by product. Hence, it is sufficient to evaluate only the part of sensitivity matrix corresponding to material properties given as

$$\mathbf{S}^*_{\boldsymbol{m}}(\boldsymbol{\xi_d^\chi}) = \begin{bmatrix} \cdots & S^*_{f_1,\xi_{m_i}}(\boldsymbol{\xi_d^\chi}) & \cdots \\ \cdots & S^*_{f_2,\xi_{m_i}}(\boldsymbol{\xi_d^\chi}) & \cdots \\ & \vdots & \end{bmatrix} , \tag{22}$$

where the sum of indices in each line is smaller or optimally equal to one.

As a last step we need to formulate a scaler-valued optimality criterion as some norm of the sensitivity matrix $\mathbf{S}^*_{\boldsymbol{m}}$. Since the commonly used optimality criteria such as A-optimality, D-optimality, E-optimality or others are derived for application to local sensitivity matrix obtained in linear design problem, their meaning is not fully preserved when applied to global sensitivity matrix. Therefore some further deeper research for suitable optimality criterion in case of global sensitivity matrix needs to be executed. It is, however, beyond the scope of this paper and we apply those criteria directly and only compare their behaviour on the illustrative example described in the following chapter. In particular, we implement these criteria in the following way:

$$A^*(\mathbf{S}^*_{\boldsymbol{m}}) = \operatorname{trace}\left(\left[(\mathbf{S}^*_{\boldsymbol{m}})^{\mathrm{T}}\,\mathbf{S}^*_{\boldsymbol{m}}\right]^{-1}\right) , \tag{23}$$

$$D^*(\mathbf{S}^*_{\boldsymbol{m}}) = \det\left((\mathbf{S}^*_{\boldsymbol{m}})^{\mathrm{T}}\,\mathbf{S}^*_{\boldsymbol{m}}\right) , \tag{24}$$

$$E^*(\mathbf{S}^*_{\boldsymbol{m}}) = \operatorname{cond}\left((\mathbf{S}^*_{\boldsymbol{m}})^{\mathrm{T}}\,\mathbf{S}^*_{\boldsymbol{m}}\right) , \tag{25}$$

respectively. And we emphasise that once the PCE-based approximation of model response is constructed, the criteria are defined as explicit analytical functions of design variables which make the optimisation of experiment design very computationally efficient. The criteria can of course be non-smooth or multi-modal, but any evolutionary algorithm requiring high number of iterations can be successfully applied. Here, in particular, we apply real-valued genetic algorithm GRADE extended by niching strategy CERAF allowing him to escape from local extremes (Kucerova, 2007).

4. Numerical Example

We use the example of experiment design problem elaborated in (Ruffio et al., 2012) and previously in (Sawaf et al., 1995). The example deals with two-dimensional linear nonstationary heat problem govern by energy balance equation

$$C\frac{\partial\theta}{\partial t} = \lambda_x\frac{\partial^2\theta}{\partial x^2} + \lambda_y\frac{\partial^2\theta}{\partial y^2} \tag{26}$$

on the spatial domain given as $0 \leq x \leq l_x = 5$ cm and $0 \leq y \leq l_y = 5$ cm and time domain given as $0 \leq t \leq \tau = 60$ s, see Figure 3.

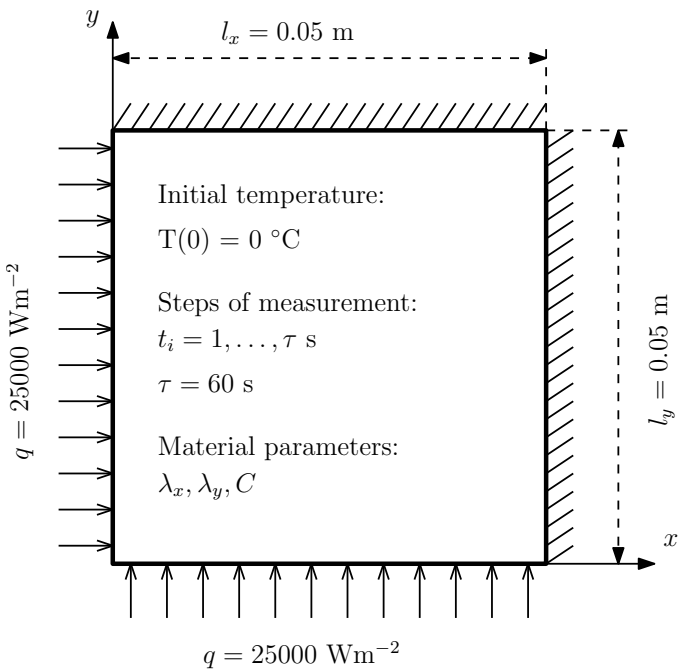


Figure 3. Experiment setup.

The boundary and initial conditions are defined by

$$-\lambda_x \frac{\partial \theta}{\partial x}(x=0) = q, \qquad -\lambda_y \frac{\partial \theta}{\partial y}(y=0) = q \tag{27}$$

$$-\lambda_x \frac{\partial \theta}{\partial x}(x=l_x) = 0, \qquad -\lambda_y \frac{\partial \theta}{\partial y}(y=l_y) = 0 \tag{28}$$

$$\theta(x,y,0) = 0\,, \tag{29}$$

where $q = 25000\mathrm{Wm}^{-2}$. The specimen consists of an orthotropic homogeneous material with three material parameters to be identified: two thermal conductivities λ_x and λ_y in principal directions and the thermal volumetric capacity C, i.e. $\boldsymbol{m} = (\lambda_x, \lambda_y, C)$. Their a priori selected feasible domains are

$$\lambda_x \in [0.3; 0.7] \quad \mathrm{Wm}^{-1}\mathrm{K}^{-1} \tag{30}$$

$$\lambda_y \in [3.0; 7.0] \quad \mathrm{Wm}^{-1}\mathrm{K}^{-1} \tag{31}$$

$$C \in [1400000; 1800000] \quad \mathrm{Jm}^{-3}\mathrm{K}^{-1} \tag{32}$$

The temperature is supposed to be measured by three sensors, each performing 60 measurements with the acquisition period $\Delta t = 1$ s. The aim of the experiment design problem is to find the optimal positions of the three sensors, i.e. $\boldsymbol{d} = (d_{x1}, d_{y1}, d_{x2}, d_{y2}, d_{x3}, d_{y3})$.

Once the experiment is realised, its parameters will not be exactly at designed values and thus we assume several parameters as random variables to account for the underlying noise. Therefore we consider following noise variables within the process of experiment design optimisation, see Figure 4:

- Heat flux density q is supposed to be constant during the measuring time period, but its mean value is perturbed by the normally distributed noise b_q with the zero mean and standard deviation $\sigma_q = 50\ \mathrm{Wm}^{-2}$.
- Temperature sensors provide results disturbed by additive Gaussian measurement noise b_r with zero mean and standard deviation $\sigma_r = 0.1°\mathrm{C}$.
- Sensors are supposed to be placed at designed positions $\boldsymbol{d}$ which are subject also to Gaussian noise $\boldsymbol{b}_x$ with zero mean and standard deviations $\sigma_{xi} = \sigma_{yi} = 0.5$ mm.

Ruffio et al. (2012) profits from the simplicity of the elaborated example consisting in possibility to derive the model response and local sensitivity matrix analytically. On the other hand, we want to present more realistic scenario, where experiment simulation involves finite elements-based discretisation. First, we transform all the involved variables into standard Gaussian variables $(\boldsymbol{\xi_m}, \boldsymbol{\xi_d}, \boldsymbol{\xi}_{b_q}, \boldsymbol{\xi}_{\boldsymbol{b}_x}, \boldsymbol{\xi}_{\boldsymbol{b}_r})$. Then we write the discretised model as

$$\mathbf{A}(\boldsymbol{\xi_m}, \boldsymbol{\xi}_{b_q})\boldsymbol{u} = \boldsymbol{q} \tag{33}$$

and we construct its PCE-based approximation in every response component as

$$\tilde{\boldsymbol{u}}(\boldsymbol{\xi_m}, \boldsymbol{\xi}_{b_q}) = \sum_{\alpha \in \mathcal{I}} \boldsymbol{\beta}_\alpha \psi_\alpha(\boldsymbol{\xi_m}, \boldsymbol{\xi}_{b_q})\,. \tag{34}$$

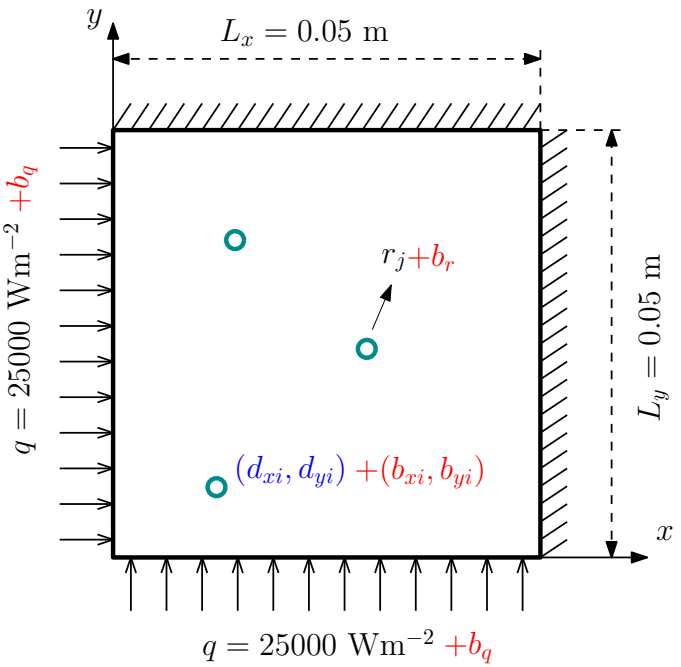


Figure 4. Design and noise variables considered in experiment design optimisation problem.

To obtain the temperature values corresponding to k-th sensor, we have to determine a specific finite element, where the sensor is located, and the polynomial expansions in its nodes

$$\tilde{\boldsymbol{u}}_k(\boldsymbol{\xi}_m) = (\tilde{u}_1(\boldsymbol{\xi}_m), \tilde{u}_2(\boldsymbol{\xi}_m), \tilde{u}_3(\boldsymbol{\xi}_m))^{\mathrm{T}}\,, \tag{35}$$

see Figure 5. By evaluating shape functions $\boldsymbol{N}_k(\boldsymbol{d}_k(\boldsymbol{\xi}_d))$ and their gradient $\mathbf{B}_k(\boldsymbol{d}_k(\boldsymbol{\xi}_d)) = \boldsymbol{\nabla}\boldsymbol{N}_k(\boldsymbol{d}_k(\boldsymbol{\xi}_d))$

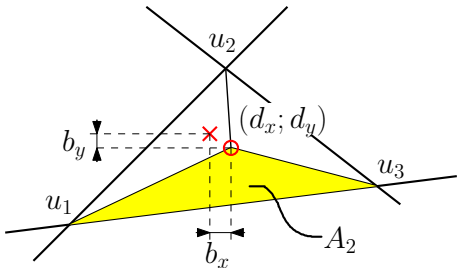


Figure 5. Scheme of a triangular finite element with the interior sensor at coordinates $(d_x + b_x, d_y + b_y)$.

(with $\boldsymbol{\nabla} = (\nabla x, \nabla y)^{\mathrm{T}}$) at the designed position of a sensor $\boldsymbol{d}_k = (d_x, d_y)$ as

$$\boldsymbol{N}_k(\boldsymbol{d}_k(\boldsymbol{\xi}_d)) = (N_1(\boldsymbol{d}_k(\boldsymbol{\xi}_d)), N_2(\boldsymbol{d}_k(\boldsymbol{\xi}_d)), N_3(\boldsymbol{d}_k(\boldsymbol{\xi}_d))) = \left(\frac{A_1(\boldsymbol{\xi}_d)}{A}, \frac{A_2(\boldsymbol{\xi}_d)}{A}, \frac{A_3(\boldsymbol{\xi}_d)}{A}\right) \tag{36}$$

we obtain an explicit function for model response component corresponding to chosen position of sensor including all relevant noise variables as

$$\begin{aligned}\widetilde{f}_k(\boldsymbol{\xi}_m, \boldsymbol{\xi}_d, \boldsymbol{\xi}_b) &= \boldsymbol{N}_k(\boldsymbol{\xi}_d)\tilde{\boldsymbol{u}}_k(\boldsymbol{\xi}_m) + \boldsymbol{b}_d(\boldsymbol{\xi}_b)\left[\mathbf{B}_k(\boldsymbol{\xi}_d)\right]\tilde{\boldsymbol{u}}_k(\boldsymbol{\xi}_m) + b_r(\xi_{b_r}) = \\ &= \left[\boldsymbol{N}_k(\boldsymbol{\xi}_d) + \boldsymbol{b}_d(\boldsymbol{\xi}_b)\left[\mathbf{B}_k(\boldsymbol{\xi}_d)\right]\right]\tilde{\boldsymbol{u}}_k(\boldsymbol{\xi}_m) + b_r(\xi_{b_r})\,, \end{aligned} \tag{37}$$

which is in fact also a polynomial expansion and can be written as

$$\widetilde{f}_k(\boldsymbol{\xi}_m, \boldsymbol{\xi}_d, \boldsymbol{\xi}_b) = \sum_{\alpha\in\mathcal{I}} \boldsymbol{\beta}_\alpha \psi_\alpha(\boldsymbol{\xi}_m, \boldsymbol{\xi}_d, \boldsymbol{\xi}_b)\,. \tag{38}$$

In this polynomial expansion, we treat the design variables as constants and get an explicit formulation for global sensitivity matrix according to Eq. (22), which can be then quickly evaluated at every iteration of the experiment design optimisation process.

5. Results

As the first numerical study we compare the performance of optimality criteria defined in Eqs. (23) – (25) and the A^*, D^* and E^*-optimal designs are plotted in the first three columns of Table I, respectively. All these designs are selected as best among the set of local optima determined by GRADE+CERAF algorithm. Last two columns are occupied by two best locally optimal solutions presented in (Ruffio et al., 2012). All experiment designs are employed in a single simulated experiment, where true values of material parameters are given according to (Ruffio et al., 2012) as

$$\begin{aligned}\lambda_x^* &= 0.6\,\mathrm{Wm^{-1}C^{-1}}\,,\\ \lambda_y^* &= 4.7\,\mathrm{Wm^{-1}C^{-1}}\,,\\ C^* &= 1700000\,\mathrm{Jm^{-3}C^{-1}}\,.\end{aligned}$$

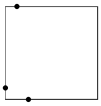
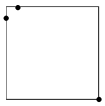
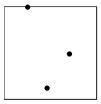
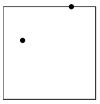
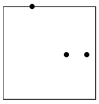
In the local sensitivity-based approach, an initial guess about the values of material properties is required for computing the local sensitivities. This guess again according to (Ruffio et al., 2012) is

$$\begin{aligned}\overline{\lambda_x} &= 0.5\,\mathrm{Wm^{-1}C^{-1}}\,,\\ \overline{\lambda_y} &= 5.0\,\mathrm{Wm^{-1}C^{-1}}\,,\\ \overline{C} &= 1600000\,\mathrm{Jm^{-3}C^{-1}}\,.\end{aligned}$$

In order to compare the quality of particular experiment designs, an inverse analysis is performed in a simplified – linearised – way as described in Section 2 and parameter estimates along with their variances are computed according to Eqs. (8) and (9). Resulting relative variances in parameter estimates obtained for particular experimental designs are written in Table I.

By comparing these results we may conclude that the applied optimality criteria do not differ too significantly. Especially A^*- and D^*-optimality provide very similar results. The E^*-optimality outperforms the others by providing almost half of the variances obtained by A^*- and D^*-optimality.

Table I. Comparison of experimental designs within a single inverse analysis.

	$A^*(\mathbf{S}^*_{\boldsymbol{m}})$	$D^*(\mathbf{S}^*_{\boldsymbol{m}})$	$E^*(\mathbf{S}^*_{\boldsymbol{m}})$	$F(\boldsymbol{d}, \widehat{\boldsymbol{m}}, \overline{\boldsymbol{b}})$:U1	$F(\boldsymbol{d}, \widehat{\boldsymbol{m}}, \overline{\boldsymbol{b}})$:U2
					
$\sigma_{\lambda_x}/\lambda_x$	19.1%	20.2%	12.1%	4.6 %	8.0 %
$\sigma_{\lambda_y}/\lambda_y$	16.2%	13.7%	5.6%	7.5 %	2.9 %
σ_C/C	10.3%	10.4%	5.1%	2.9 %	2.0 %

Nevertheless, the E^*-optimality does not outperform the results obtained by Ruffio et al. using the problem linearisation and local sensitivity matrix.

One possible explanation is that the true values of the material properties are very close the starting guess used for computation of local sensitivities. Therefore we have performed a set of 25 simulated experiments for changing values of material properties on a regular grid $5x5x5$ within the feasible domain. For each experiment, the same inverse analysis was executed as in the first example and minimal and maximal values of estimated parameter variances are listed in Table II.

Table II. Case study: min-max.

	$\sigma_{\lambda_x}/\lambda_x$	$\sigma_{\lambda_y}/\lambda_y$	σ_C/C
$F(\boldsymbol{d}, \widehat{\boldsymbol{m}}, \overline{\boldsymbol{b}})$:U2	7.9 – 31.9 %	1.7 – 6.3 %	1.53 – 4.3 %
$A^*(\mathbf{S}^*_{\boldsymbol{m}})$	17.6 – 22.0 %	15.3 – 24.2 %	8.63 – 17.3 %
$D^*(\mathbf{S}^*_{\boldsymbol{m}})$	18.5 – 25.2 %	10.5 – 20.2 %	8.55 – 16.4 %
$E^*(\mathbf{S}^*_{\boldsymbol{m}})$	10.6 – 14.4 %	2.5 – 6.2 %	3.26 – 7.2 %

Here it can be already concluded that the E^*-optimal design has a comparable quality to U2-design obtained by Ruffio et al. and it still outperforms the A^*-optimal and D^*-optimal designs.

6. Conclusions

The proposed contribution presents a new method for designing robust and optimal experiments, which is developed with regard on its practical applicability to finitThe proposed contribution presents an original method for designing robust and optimal experiments, which is developed with regard on its practical applicability to finite element-based models and its computational feasibility. The method is based on an explicit formulation of global sensitivity matrix, which constituents are defined as Sobol indices derived analytically from the polynomial chaos-based approximation of model response. Employing higher order polynomials in model surrogate allows to account for

the nonlinearity of the model as well as for the prescribed large feasible domain of the material properties to be estimated. No prior expert guess about specific parameter values is needed as it is in the case of local sensitivity-based procedure described in (Ruffio et al., 2012). Construction of the higher order polynomial surrogate is of course computationally intensive task. Nevertheless, development of efficient computational tools for polynomial chaos-based uncertainty propagation is a scientific topic still atracting the attention of many researchers pushing forward the process in this field. Moreover, the construction of the PCE-based surrogate needs to be carried out only once before the actual start of the experiment design process. During the optimisation, only very fast evaluation of Sobol indices defined explicitely from the PC coefficients is needed at each iteration of the optimisation process.

The proposed method is compared here with the local sensitivity-based method on a simple example of nonstationary linear heat transfer. It is shown that the both method provides very similar values of variances of parameter estimates. The comparison is now, however, very modest. We suspect that the model of the experiment on the feasible domain of material properties is here only mildly nonlinear and thus the robustness of the proposed method cannot be fully appreciated. Moreover the comparison is performed using the linearised inverse analysis, while full Monte Carlo-based inverse analysis would be also more appropriate to verify the quality of the obtained experimental designs. These topic will be thus next steps in our future work.

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