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EFFECTIVE AND SCALABLE UNCERTAINTY EVALUATION FOR LARGE-SCALE COMPLEX SYSTEM APPLICATIONS

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ABSTRACT

Effective uncertainty evaluation is a critical step toward real-time and robust decision-making for complex systems in uncertain environments. A Multivariate Probabilistic Collocation Method (M-PCM) was developed to effectively evaluate system uncertainty. The method smartly chooses a limited number of simulations to produce a low-order mapping, which precisely predicts the mean output of the original system mapping up to certain degrees. While the M-PCM significantly reduces the number of simulations, it does not scale with the number of uncertain parameters, making it difficult to use for large-scale applications that typically involve a large number of uncertain parameters. In this paper, we develop a method to break the curse of dimensionality. The method integrates M-PCM and Orthogonal Fractional Factorial Designs (OFFDs) to maximally reduce the number of simulations from 2^{2m} to $2^{\lceil log_2(m+1)\rceil}$ for a system mapping of m parameters. The integrated M-PCM-OFFD predicts the correct mean of the original system mapping, and is the most robust to numerical errors among all possible designs of the same number of simulations. The analysis also provides new insightful formal interpretations on the optimality of OFFDs.

1 INTRODUCTION

Modern large-scale complex systems typically involve a large number of uncertain parameters, which modulate the systems' dynamics, and which pose significant challenges for real-time system evaluation and decision-support. For instance, the management of complex information systems requires methodologies to achieve high throughput and low latency under demand uncertainties. Similarly, strategic air traffic flow management is concerned with designing management initiatives that are robust to a wide range of weather uncertainties at a long look-ahead time. As a step toward real-time management, it is critical to develop a systematic procedure to evaluate statistical system performance in the presence of uncertain parameters. This problem can be formulated as the prediction of *output* statistics subject to a set of uncertain *input* parameters. The problem has been typically addressed using the Monte Carlo simulation method (Sokolowski and Banks 2010), which simulates a *very large* set of randomly selected simulation points, and then calculates the output statistics using the simulated outputs. In large-scale complex system applications, each simulation consumes considerable computational time; as the Monte Carlo simulation method requires a very *large* number of simulations to *converge* to meaningful performance estimates, the method does not meet the requirement for real-time management. The uncertainty evaluation procedure needs to be efficient in time and also scalable with the number of uncertain input parameters.

The Multivariate Probabilistic Collocation Method (M-PCM) was developed to effectively evaluate the output statistics of a system subject to multiple uncertain input parameters, which may or may not be correlated (Zhou et al. 2014). Compared to the Monte Carlo method, the M-PCM permits using a significantly reduced number of simulations to predict to a desired precision the *correct* mean of the original system output. Specifically, the method suggests a procedure to *smartly* select a few values for each uncertain input parameter as simulation points. Simulations evaluated at these points can identify a reduced-order mapping between input parameters and the output, from which the output statistics are readily obtained. The selection procedure is based on statistical knowledge of uncertain input parameters, such as joint probabilistic distribution functions (pdfs), historical data sets, or as simple as low-order moments, e.g., the mean and the variance. The resulting accurate predictions of mean output as well as several other important statistics suggest that the reduced-order polynomial mapping approximates the original mapping well over likely ranges of parameter values. The reduced-order mapping then facilitates further studies, including parameter sensitivity analysis, optimal decision-support under uncertainties, and the application to strategic air traffic management (Zhou et al. 2012, Zhou et al. 2013, Ma et al. 2012).

Although the M-PCM significantly reduces the number of simulations required to predict the correct mean output, it is not scalable to large-scale system applications which typically involve a large number of uncertain input parameters. In particular, the number of simulations increases exponentially with the increase of the number of uncertain input parameters, and thus leads to potential computational load issues for real-time applications. In this paper, we study further reducing the number of simulations from the M-PCM designs.

Conceptually, this further reduction is possible, as the M-PCM assumes the existence of all cross-multiplication terms in system mappings. As many of these cross-terms do not exist in realistic applications, the number of mapping coefficients can be significantly reduced and thus requires a lower number of simulations to estimate. In this paper, we investigate the selection of a subset of M-PCM points to predict the correct mean output. In addition, we note a practical numerical issue on the success of M-PCM. In particular, many system simulations have constraints on the *resolutions* of input parameters, and thus require numerical truncation of selected points for simulation. Such truncation may unfortunately fail the mean output prediction. As such, we also require the selected subset to be robust to such numerical errors.

In this paper, we explore the use of an experimental design method, called the Orthogonal Fractional Factorial Design (OFFD) (J. Prinz 2013, Dey 1985, Box et al. 2005, Robert 2009) to further reduce the number of simulations from the M-PCM. Main contributions of this paper are summarized in the following.

- *An integrated design to enhance the scalability and applicability of the M-PCM for uncertainty evaluation*. By integrating M-PCM with OFFDs, the number of simulations is significantly further reduced. We focus on the case that each parameter in the original system mapping has a degree of up to 3. We show that for an m-parameter system, the integration of M-PCM and OFFDs is able to reduce the number of simulations from 2^{2m} to the range of $\left[2^{\lceil log_2(m+1)\rceil}, 2^{m-1}\right]$, where $\lceil x \rceil$ denotes the nearest integer above the number x. We prove that the integrated M-PCM and OFFDs (M-PCM-OFFD) predicts the correct mean of the original system mapping, and is the most robust to numerical errors among all designs of the same number of simulations. This study enhances M-PCM for practical uncertainty evaluation for large-scale systems.
- *A novel statistical measure and the optimality study of OFFDs*. We explore the performance of OFFDs in terms of the robustness to numerical errors for output statistics prediction, which has never been studied in the literature per knowledge of the authors. We adopt a quantitative robustness metric in the matrix theory (Dahleh et al. 2004), and show that the subset of simulations selected by OFFDs is optimal under this metric. This study provides new quantitative insights into the attributes of OFFDs, and broadens their application domains.

A related study in (Isukapalli 1999) suggested a heuristic method, called efficient collocation method (ECM), to further reduce the number of simulations. However, this method does not have a quantitative

performance analysis. We here conduct a thorough analysis on the optimality of the integrated M-PCM and OFFDs.

The remainder of this paper is organized as follows. In Section 2, fundamentals of the M-PCM and OFFDs are introduced. In Section 3, the algorithm of the integrated M-PCM-OFFD is presented, and the main results on its performance are presented from two aspects: mean output prediction and robustness to numerical errors. Section 4 includes simulation studies on an illustrative example. Finally, a brief conclusion and a discussion of future works are included in Section 5.

2 Preliminaries

We first review fundamentals of the M-PCM and motivate our approach to further reduce the number of simulations. We then review basics of the OFFDs and discuss the feasibility of integrating the two methods.

2.1 M-PCM

The M-PCM was developed to effectively evaluate uncertainty for systems with multiple uncertain input parameters. In this paper, we consider the case when these input parameters are independent; however we note that the correlated M-PCM was developed in (Zhou et al. 2014). As Theorem 1 in (Zhou et al. 2014) generally shows, for a system mapping (called response surface in the experiment design literature) of m uncertain input parameters with the degree k_i of each parameter x_i up to $2n_i-1$, a total number of $2^m\prod_{i=1}^m n_i$ simulations are needed to uniquely determine its mapping $g(x_1,x_2,...,x_m)=\sum_{k_1=0}^{2n_1-1}\sum_{k_2=0}^{2n_2-1}...\sum_{k_m=0}^{2n_m-1}\Psi_{k_1,...,k_m}\prod_{i=1}^m x_i^{k_i}$, where $\Psi_{k_1,...,k_m}\in R$ are the coefficients. The M-PCM suggests a procedure to choose n_i simulation points for each parameter, and produces a reduced mapping $g^*(x_1,x_2,...,x_m)=\sum_{k_1=0}^{n_1-1}\sum_{k_2=0}^{n_2-1}...\sum_{k_m=0}^{n_m-1}\Omega_{k_1,...,k_m}\prod_{i=1}^m x_i^{k_i}$ with the degree of each parameter up to n_i-1, where $\Omega_{k_1,...,k_m}\in R$ are the coefficients. The reduced-order mapping predicts the *correct mean output* of the original mapping.

2.1.1 Design Procedures

The three major steps of the M-PCM method are briefly summarized below. Please refer to (Zhou et al. 2014) for the details.

Step 1: Choose simulation points. For each input parameter $x_i, i=1,2,\cdots,m$, find its orthonormal polynomial $h_i^{n_i}(x_i)$ of degree n_i based on the statistics of x_i, such as the pdf, historical data, or low-order moments. The roots of $h_i^{n_i}(x_i)$ are the n_i M-PCM simulation points for x_i, denoted as $x_{i(1)},...,x_{i(n_i)}$.

Step 2: Run simulations at selected simulation points. For each simulation point identified in Step 1, run simulation and find the associated output.

Step 3: Produce the low-order mapping. Calculate the coefficients $\Omega_{k_1,...,k_m}$ in the low-order mapping $g^*(x_1,x_2,...,x_m)$ by

$$\begin{bmatrix}\Omega_{0,...,0}\\ \vdots\\ \Omega_{0,...,n_m-1}\\ \vdots\\ \Omega_{n_1-1,...,n_m-1}\end{bmatrix}=L^{-1}\begin{bmatrix}g(x_{1(1)},...,x_{m(1)})\\ g(x_{1(1)},...,x_{m(2)})\\ \vdots\\ g(x_{1(n_1)},...,x_{m(n_m)})\end{bmatrix},\ \text{where}$$

$$L=\begin{bmatrix}x_1^0(x_{1(1)})...x_m^0(x_{m(1)}) & \cdots & x_1^0(x_{1(1)})...x_m^{n_m-1}(x_{m(1)}) & \cdots & x_1^{n_1-1}(x_{1(1)})...x_m^{n_m-1}(x_{m(1)})\\ x_1^0(x_{1(1)})...x_m^0(x_{m(2)}) & \cdots & x_1^0(x_{1(1)})...x_m^{n_m-1}(x_{m(2)}) & \cdots & x_1^{n_1-1}(x_{1(1)})...x_m^{n_m-1}(x_{m(2)})\\ \vdots & \ddots & \vdots & \ddots & \vdots\\ x_1^0(x_{1(n_1)})...x_m^0(x_{m(n_m)}) & \cdots & x_1^0(x_{1(n_1)})...x_m^{n_m-1}(x_{m(n_m)}) & \cdots & x_1^{n_1-1}(x_{1(n_1)})...x_m^{n_m-1}(x_{m(n_m)})\end{bmatrix}\quad(1)$$

and $x_i^{k_i}(x_{i(j)})$ represents the k_i-th power of x_i evaluated at the simulation point $x_{i(j)}$.

Despite the significant computational load reduction enabled by the M-PCM, the method does not scale with the number of uncertain input parameters m. In particular, $\prod_{i=1}^{m} n_i$ runs are still needed to predict the correct mean output. We note that if all coefficients in the low-order mapping $g^*(x_1, x_2, ..., x_m)$ are nonzero, the full set of M-PCM points is required to uniquely determine the mapping, and in turn the mean output. In realistic applications, however, many cross-terms in the mapping do not exist or have negligible effects on the output (Box et al. 2005). Under such assumptions, only a subset of the M-PCM points is required. In this paper, we study using only a subset of the $\prod_{i=1}^{m} n_i$ simulations to predict the mean output. Next, we review the OFFDs, which we will use to achieve this further reduction.

2.2 OFFDs

Orthogonal fractional factorial designs (OFFDs) provide an approach to select a subset (from the full factorial design, that is, from the design consisting of all possible combinations of levels of all factors) of experimental combinations that best estimate the main effects of single factors (or parameters) and low-order interaction effects of multiple factors on the output. Please refer to (J. Prinz 2013, Dey 1985, Box et al. 2005, Robert 2009, Mills et al. 2011, Filliben and Simiu 2010) for the details of OFFDs.

2.2.1 Design Procedures

Consider an m-factor experiment, with each factor evaluated at P levels (or values). The full factorial design would consist of P^m runs. Such a design is statistically effective, but is also very expensive, especially when the number of parameters is large. A specific OFFD is described by $P_R^{m-\gamma}$. This design examines m parameters, but does so in a statistically balanced/optimal fashion using only $P^{m-\gamma}$ runs. The **fractionation constant**, γ, where γ is a positive integer, indicates that a fraction $P^{m-\gamma}$ of runs is selected from the full set of P^m runs (Gunst and Mason 2009, J. Prinz 2013). γ is in the range of $1 \leq \gamma \leq m - \lceil log_P(m+1) \rceil$ (Box et al. 2005), with the upper bound determined by the minimum number of runs to estimate m main effects and the mean. γ also determines the minimum number of **generators**, which decide the effects (main effects or interactions) that are confounded together (Gunst and Mason 2009, J. Prinz 2013). The length of the shortest generator is defined as the **resolution** R, which is usually represented by Roman numerical subscript (J. Prinz 2013). The procedures to generate the $P_R^{m-\gamma}$ OFFD are summarized in the following. We note that in statistical experiment design, the selections of γ and R need to balance the degree of tolerable confounding and OFFD sample sizes.

Step 1: Generate the $P^{m-\gamma}$ full factorial design for $m-\gamma$ factors. List all $P^{m-\gamma}$ combinations for $m-\gamma$ factors.

Step 2: Specify γ generators. The selection of generators is somewhat flexible. In principle, given γ and m, the highest resolution R is usually adopted to achieve the minimal aliasing for effect estimation (Box et al. 2005). We can also refer to standard designs (L.Trutna et al. 2013) to select generators.

Step 3: Determine the levels of all other γ factors for each experimental run. The generators selected in Step 2 are used to generate the levels for all other factors.

If we view all PCM points selected from the M-PCM as a full factorial design, the OFFDs provide systematic procedures to select a subset of simulation points that breaks the curse of dimensionality. In the next section, we present the integrated algorithm, and show that it produces a low-order mapping that predicts the correct mean output of the original mapping, and is the most robust to numerical errors.

3 Integrated M-PCM and OFFDs

In this section, we investigate the integrated M-PCM-OFFD that together break the curse of dimensionality for effective mean output prediction. For most of the analyses here, we assume that each input parameter in

the original system mapping $g(x_1, x_2, ..., x_m)$ is up to the degree of 3, i.e., $2n_i - 1 \leq 3$, for all $i \in \{1, 2, ..., m\}$. This assumption is placed to facilitate the use of 2-level OFFDs, which have mature design procedures (and in particular the formulation of generators). In addition, we assume that uncertain input parameters are independent. We note that the correlation among parameters, if known, can be exploited to further reduce the number of simulations (Lei et al. 2008). We leave these generalizations to the future work. We first present the integrated algorithm, and then analyze its optimality using two metrics: 1) mean output estimation, and 2) robustness to numerical errors. We note that the specific OFFD to choose is dependent on the knowledge that cross-terms have up to a certain number of parameters.

3.1 Algorithm Description

Consider an original system mapping of m input parameters, each with a degree up to 3. Mathematically,

$$g(x_1, x_2, ...x_m) = \sum_{k_1=0}^{3} \sum_{k_2=0}^{3} ... \sum_{k_m=0}^{3} \Psi_{k_1,...,k_m} \prod_{i=1}^{m} x_i^{k_i}, \tag{2}$$

where the coefficients $\Psi_{k_1,...,k_m} \in R$. Assume that the random parameters x_1, x_2, ..., x_m follow independent distributions $f_{X_1}(x_1)$, $f_{X_2}(x_2)$, ... , and $f_{X_m}(x_m)$ respectively. In addition, assume that cross-terms involve at most τ parameters, where τ is an integer in the range of $1 \leq \tau \leq m$. In other words, $\Psi_{k_1,...,k_m} = 0$ if more than τ of $k_1, ..., k_m$ are non-zero.

The following integrated algorithm constructs a low-order mapping

$$g^*(x_1, x_2, ..., x_m) = \sum_{k_1=0}^{1} \sum_{k_2=0}^{1} ... \sum_{k_m=0}^{1} \Omega_{k_1,...,k_m} \prod_{i=1}^{m} x_i^{k_i}, \tag{3}$$

where the coefficients $\Omega_{k_1,...,k_m} \in R$, and $\Omega_{k_1,...,k_m} = 0$ if more than τ of $k_1, ..., k_m$ are non-zero.

Algorithm:

Step 1: Choose 2^m M-PCM simulation points. Follow Step 1 of the M-PCM algorithm in Section 2.1.1 to select 2^m PCM points. Here $n_i = 2$ for all i. Check if $m > 2$ and $1 \leq \tau \leq \lceil \frac{m}{2} \rceil - 1$ (Lemma 2). If yes, move to Step 2; otherwise go to Step 4 as no simulations can be further reduced by OFFDs.

Step 2: Calculate γ_{max} to save $2^m - 2^{m-\gamma_{max}}$ simulations. Select $\gamma_{max} = m - \lceil log_2(\sum_{i=0}^{\tau} \binom{i}{m}) \rceil$ (Lemma 2) to save the maximum number of simulations. Here $l = \sum_{i=0}^{\tau} \binom{i}{m}$ is the number of coefficients in Equation 3.

Step 3: Select simulation subsets using the OFFD. Follow the three steps of the $2^{m-\gamma_{max}}$ OFFD algorithm in Section 2.2.1 to select $l_{offd} = 2^{m-\gamma_{max}}$ simulation points from the full set of 2^m simulations obtained in Step 1. These points constitute the M-PCM-OFFD simulation set.

Step 4: Run simulations. Run simulation at each selected simulation point.

Step 5: Produce the low-order mapping. If the number of coefficients, l, equals the number of simulation points selected using the OFFD, l_{offd}, find the coefficients in Equation 3 similar to Step 3 of the M-PCM algorithm, but with a reduced-size L matrix, denoted as the **input matrix** $L' \in R^{l \times l}$, which excludes those entries with rows representing points not selected in the reduced M-PCM-OFFD simulation set, and those columns with more than τ of $k_1, k_2, ...k_m$ being nonzero. If $l < l_{offd}$, the input matrix $L' \in R^{l_{offd} \times l}$ is not a square matrix. In this case, the coefficients can be instead found by replacing L'^{-1} with $(L'^T L')^{-1} L'^T$, according to the least square estimation (Montgomery et al. 1997).

We note that the ordering of entries in the L' matrix does not need to strictly follow that in Equation 1. They only need to match with the orderings of simulation points and the simulated outputs.

3.2 Performance of Algorithm on the Estimation of Mean Output

In this section, we show that the reduced M-PCM-OFFD simulation set in Section 3.1 estimates the correct mean output of the original system mapping with the degree of each parameter up to 3. We first present three lemmas. In Lemma 1, we show that the reduced-order mapping does not introduce additional cross-terms.

Lemma 1 Consider an original system mapping $g(x_1,x_2,...,x_m)$ that contains cross-terms of at most τ parameters (Equation 2). The low-order mapping $g^*(x_1,x_2,...,x_m)$ estimated using the M-PCM also contains cross-terms of at most τ parameters.

Proof: According to the proofs for Theorems 1 and 2 in (Zhou et al. 2014), the M-PCM recursively reduces the degree of each input parameter to produce a low-order mapping of the same mean output. As this procedure does not introduce new parameters to each cross-term, the numbers of parameters in all cross-terms in the low-order mapping do not increase. □

In Lemma 2, we study the maximum number of simulations that can be further reduced using OFFDs, given the maximum number of parameters, τ, in cross-terms of $g(x_1,x_2,...,x_m)$, or equivalently $g^*(x_1,x_2,...,x_m)$ according to Lemma 1.

Lemma 2 Consider the low-order mapping $g^*(x_1,x_2,...,x_m)$ (Equation 3) estimated using the M-PCM, which contains cross-terms of at most τ parameters. An OFFD design can further reduce the number of simulations if $1 \le \tau \le \lceil \frac{m}{2} \rceil - 1$, $m > 2$. The maximum fraction of simulations that can be reduced is $2^{-\gamma_{max}}$ using the $2^{m-\gamma_{max}}$ OFFD, where $\gamma_{max} = m - \lceil log_2(\sum_{i=0}^{\tau}\binom{i}{m}) \rceil$.

Proof: The M-PCM produces 2^m simulation points. Let us first prove that an OFFD design can further reduce the number of simulations if $1 \le \tau \le \lceil \frac{m}{2} \rceil - 1$, $m > 2$. As OFFDs reduce the number of simulations at least by half, the number of non-zero parameters $\sum_{i=0}^{\tau}\binom{i}{m}$ in $g^*(x_1,x_2,...,x_m)$ must be less than or equal to 2^{m-1} to produce the same low-order mapping $g^*(x_1,x_2,...,x_m)$. Note that $2^{m-1} = \sum_{i=0}^{\frac{m-1}{2}}\binom{i}{m}$ when m is odd and $\sum_{i=0}^{\frac{m}{2}-1}\binom{i}{m} < 2^{m-1} < \sum_{i=0}^{\frac{m}{2}}\binom{i}{m}$ when m is even. The maximum of τ thus satisfies

$$max(\tau) = \begin{cases} \frac{m-1}{2} & \text{if } m \mod 2 \equiv 1 \\ \frac{m}{2}-1 & \text{if } m \mod 2 \equiv 0 \end{cases} = \lceil \frac{m}{2} \rceil - 1. \quad (4)$$

As τ is an integer greater than or equal to 1, it needs to be in the range of $1 \le \tau \le \lceil \frac{m}{2} \rceil - 1$, such that an OFFD can further reduce simulation points without altering the low-order mapping $g^*(x_1,x_2,...,x_m)$.

Now we prove that the maximum fraction of simulations that can be reduced is achieved using the $2^{m-\gamma_{max}}$ OFFD, where $\gamma_{max} = m - \lceil log_2(\sum_{i=0}^{\tau}\binom{i}{m}) \rceil$. As the number of simulations must be larger than or equal to the number of parameters,

$$\gamma_{max} = max\{\gamma \mid 2^{m-\gamma} \ge \sum_{i=0}^{\tau}\binom{i}{m}\} = m - \lceil log_2(\sum_{i=0}^{\tau}\binom{i}{m}) \rceil. \quad (5)$$

□.

In the next lemma, we prove that the matrix L' is full column rank, i.e. $rank(L') = l$. In this process, we show the general QR decomposition expression of L'. This lemma is central to the rest of the development in this paper, as it establishes the direct relationship between the OFFD design table (captured by Q) and the input matrix L' which is used for our study of mapping construction and mean output prediction.

Lemma 3 The input matrix $L' \in R^{l_{offd} \times l}, l_{offd} \ge l$ constructed by the integrated M-PCM and OFFD is full column rank, and can be represented using the QR decomposition (Wilkinson et al. 1965) as $L' = QU$, where $Q \in R^{l_{offd} \times l}$ is an orthogonal matrix (i.e. $Q^T Q = I$) of the form:

$$Q = \begin{bmatrix} \mathbf{q}_1 & \mathbf{q}_2 & \mathbf{q}_3 & \cdots & \mathbf{q}_l \end{bmatrix} = \frac{1}{\sqrt{l_{offd}}} \begin{bmatrix} \mathbf{v}_1 & \mathbf{v}_2 & \mathbf{v}_3 & \cdots & \mathbf{v}_l \end{bmatrix}. \quad (6)$$

Here $\mathbf{q}_i \in R^{l_{offd} \times 1}$ is the orthogonal basis with $\mathbf{q}_i^T \mathbf{q}_j = 0$ if $i \neq j$ and $\|\mathbf{q}_i\|_2 = 1$, where $i, j \in \{1, 2, \cdots, l\}$. Assume that $x_{k(2)} > x_{k(1)}$ WLOG. $\mathbf{v}_i = \sqrt{l_{offd}}\mathbf{q}_i$ contains entries of ± 1, and is obtained by replacing each entry $x_{k(1)}$ in the i-th column of L' with -1 and $x_{k(2)}$ with 1, where k is the index of input parameters. Alternatively, it is obtained by replacing '-' and '+' in the OFFD design table by '-1' and '+1' respectively, and adding an all '1' vector to the left. $U \in R^{l \times l}$ is an upper triangular matrix, with the i-th diagonal entry U_{ii} expressed as

$$U_{ii} = \begin{cases} \sqrt{l_{offd}} & \text{if} \quad i = 1 \\ \frac{\sqrt{l_{offd}}}{2^{\xi_i}} \prod_{k \in S_i} \Delta x_k & \text{if} \quad i \neq 1 \end{cases} \tag{7}$$

where $\Delta x_k = x_{k(2)} - x_{k(1)}$, $S_i \subseteq \{1, 2, \cdots, m\}$ includes all the indices of input parameters in the i-th column of L', and ξ_i is the size of S_i.

Proof: The QR decomposition follows the recursive Gram-Schmidt procedure (Wilkinson et al. 1965). It is omitted due to the limited space. It is clear from the expressions of Q and R that L' is full column rank, as Q is invertible ($Q^{-1} = Q^T$) and the determinant of U is $\prod_i U_{ii} \neq 0$. □

Lemmas 1-3 and Theorems 1-2 in (Zhou et al. 2014) directly lead to the theorem on the performance of the M-PCM-OFFD in terms of the correctness of predicting the mean output of the original mapping.

Theorem 1 The low-order mapping $g^*(x_1, x_2, ..., x_m)$ (Equation 3) using the integrated M-PCM and $2^{m-\gamma_{max}}$ OFFD predicts the correct mean output of the original mapping, i.e.,

$$E[g(x_1, x_2, ..., x_m)] = E[g^*(x_1, x_2, ..., x_m)]. \tag{8}$$

The number of simulations reduces from 2^{2m} to $2^{m-\gamma_{max}}$, where $\gamma_{max} = m - \lceil log_2(\sum_{i=0}^{\tau} \binom{i}{m}) \rceil$. The maximum reduction is $2^{2m} - 2^{\lceil log_2(m+1) \rceil}$, and is achieved when $\tau = 1$.

Proof: Theorems 1-2 in (Zhou et al. 2014) suggest that the reduced-order mapping $g^*(x_1, x_2, ..., x_m)$ produced by the M-PCM predicts the correct mean output of $g(x_1, x_2, ..., x_m)$. Lemmas 1, 2 and 3 guarantee that the reduced M-PCM-OFFD simulation set produces the same mapping $g^*(x_1, x_2, ..., x_m)$. The result is then straightforward. □

3.3 Performance of the Algorithm on the Robustness to Numerical Errors

In this section, we study the robustness of the integrated design to numerical errors. We first introduce the robustness metric and formulate the problem in Section 3.3.1. We then show the optimality of the integrated design using this metric in Section 3.3.2.

3.3.1 Metric and Problem Formulation

Recall that the integrated algorithm involves the calculation of L'^{-1} or $(L'^T L')^{-1} L'^T$. This inversion is only feasible when L' is full column rank. In Lemma 3, we have shown that an OFFD guarantees that L' is full column rank. In this section, we further explore the computational feasibility by noticing that parameter resolutions of simulation software (Zhou et al. 2014) and computational limitations of computing devices (Kato 1995, Ipsen and Chandrasekaran 1991) may unfortunately *fail* this calculation. In particular, when L' is close to losing column rank, a small disturbance introduced by the aforementioned numerical errors may easily push L' to lose rank. In addition, even if such L' under a disturbance does not directly lose rank, the correctness of L'^{-1} becomes sensitive to small perturbations (Demmel 1987). In order to facilitate the inversion and minimize the impact of numerical errors, L' needs to have a *large margin to rank loss*.

Multiple metrics exist in the literature to measure the margin to invertibility, including the widely used *condition number* (the ratio between the largest eigenvalue to the smallest eigenvalue) (Boyd et al. 1994). Here we use a metric based on the perturbation theory (Kato 1995, Ipsen and Chandrasekaran 1991).

Specially, the **full-column-rank margin** for the matrix L' to rank loss, $D(L')$, is measured by the norm of the smallest perturbation matrix to make L' lose rank. Here we use the Frobenius norm ("$||\ ||_F$"), calculated by summing the squares of all its elements, and then taking a square root of the sum (Knupp 1999):

$$D(L') = min\{\|e\|_F \mid rank(L'+e) < l\} \tag{9}$$

where $e \in R^{l_{offd} \times l}$ is a perturbation matrix.

Lemma 2 suggests that all simulation subsets of size $2^{m-\gamma_{max}}$ can predict the correct mean output, provided that the input matrix of the design, L', is full column rank. We show in the next section that when $\tau = 1$, the L' matrix of the OFFD design, denoted as L'_{offd} thereafter, has the largest margin to rank loss among all designs of the size $2^{m-\gamma_{max}}$. The results can be extended to the general case ($\tau \geq 1$) through a more complicated analysis and hence is ignored here for clarity.

3.3.2 Optimal Robustness of the Integrated M-PCM-OFFD

In this section, we study the robustness of the integrated M-PCM-OFFD to numerical errors for system mappings of m uncertain input parameters and $\tau = 1$. Lemma 4 calculates the full-column-rank margin of the integrated M-PCM-OFFD. Theorem 2 shows that the OFFD produces the largest margin among all subsets of the same size.

Lemma 4 Consider an original system mapping $g(x_1, x_2, ...x_m)$ (Equation 2) with $\tau = 1$. The integrated M-PCM and $2^{m-\gamma_{max}}$ OFFD, with $\gamma_{max} = m - \lceil log_2(\sum_{i=0}^{\tau} \binom{i}{m}) \rceil$, has the following full-column-rank margin:

$$D(L'_{offd}) = \frac{\sqrt{l_{offd}}}{2} min\{\Delta x_1, \Delta x_2, \cdots, \Delta x_m\} \tag{10}$$

Proof:

According to Lemma 3, L'_{offd} is full column rank and can be expressed as a multiplication of an orthogonal matrix Q and an upper triangular matrix U. Now we find the minimum $\|e\|_F$ to make $L'+e$ lose rank, according to the definition of full-column-rank margin in Equation 9. We use $e_{x_{i(j)}}$ to represent the perturbation to $x_{i(j)}$ and $\hat{x}_{i(j)} = x_{i(j)} + e_{x_{i(j)}}$ to represent the corrupted parameter value. Similar to L'_{offd}, $L'_{offd} + e$ can also perform a QR decomposition. In particular, $L'_{offd} + e = \hat{Q}\hat{U}$, and $\hat{Q}$ is an orthogonal matrix of full column rank, and $\hat{U}$ is an upper triangular matrix with the determinant of $det(\hat{U}) = \sqrt{l_{offd}} \prod_{i=2}^{l} (\frac{\sqrt{l_{offd}}}{2^{\xi_i}} \prod_{j \in S_i} \Delta\hat{x}_j)$, where $\Delta\hat{x}_j = \hat{x}_{j(2)} - \hat{x}_{j(1)}$. Clearly, the rank of L'_{offd} is solely determined by $\hat{U}$. Therefore, $L'_{offd} + e$ loses rank if and only if at least one of $\Delta\hat{x}_i = 0, i \in \{1, 2, \cdots, m\}$. In the case of $\Delta\hat{x}_1 = 0$, we have $\Delta\hat{x}_1 = \hat{x}_{1(2)} - \hat{x}_{1(1)} = (x_{1(2)} + e_{x_{1(2)}}) - (x_{1(1)} + e_{x_{1(1)}}) = 0$ and therefore $e_{x_{1(1)}} = e_{x_{1(2)}} + x_{1(2)} - x_{1(1)} = e_{x_{1(2)}} + \Delta x_1$. As a consequence,

$$\begin{aligned} \|e\|_F &= \sqrt{(\frac{l_{offd}}{2} e^2_{x_{1(1)}} + \frac{l_{offd}}{2} e^2_{x_{1(2)}}) + (\frac{l_{offd}}{2} e^2_{x_{2(1)}} + \frac{l_{offd}}{2} e^2_{x_{2(2)}}) + \cdots + (\frac{l_{offd}}{2} e^2_{x_{m(1)}} + \frac{l_{offd}}{2} e^2_{x_{m(2)}})} \\ &\geq \sqrt{(\frac{l_{offd}}{2} e^2_{x_{1(1)}} + \frac{l_{offd}}{2} e^2_{x_{1(2)}})} = \sqrt{\frac{l_{offd}}{2}[(e_{x_{1(2)}} + \Delta x_1)^2 + e^2_{x_{1(2)}}]} \geq \frac{\sqrt{l_{offd}}}{2} \Delta x_1 \end{aligned} \tag{11}$$

The equality holds when $e_{x_{1(1)}} = \frac{1}{2}\Delta x_1$, $e_{x_{1(2)}} = -\frac{1}{2}\Delta x_1$, and $e_{x_{j(1)}} = e_{x_{j(2)}} = 0$ for all $j \neq 1$. Similarly, we obtain $\|e\|_F \geq \frac{\sqrt{l_{offd}}}{2}\Delta x_2, \cdots, \frac{\sqrt{l_{offd}}}{2}\Delta x_m$. As such, $D(L'_{offd}) = \frac{\sqrt{l_{offd}}}{2} min\{\Delta x_1, \Delta x_2, \cdots, \Delta x_m\}$, and the minimum $\frac{\sqrt{l_{offd}}}{2}\Delta x_i$ is achieved when $\Delta x_i \leq \Delta x_j$ for all $j \neq i$, $e_{x_{i(1)}} = \frac{1}{2}\Delta x_i$, $e_{x_{i(2)}} = -\frac{1}{2}\Delta x_i$, and $e_{x_{j(1)}} = e_{x_{j(2)}} = 0$ for all $j \neq i$. □

Theorem 2 Consider an original system mapping $g(x_1, x_2, ...x_m)$ (Equation 2) with $\tau = 1$. From the 2^m M-PCM simulation points, the simulation subset selected by the M-PCM-OFFD has the largest full-column-rank margin among all subsets of $2^{m-\gamma_{max}}$ simulations points, where $\gamma_{max} = m - \lceil log_2(\sum_{i=0}^{\tau} \binom{i}{m}) \rceil$. Mathematically,

$$max(D(L')) = D(L'_{offd}). \tag{12}$$

Proof:

We first construct the input matrix, L', from any subset of $2^{m-\gamma_{max}}$ simulation points selected from the 2^m M-PCM simulation points, and then show that the input matrix of the OFFD, L'_{offd}, has the largest full-column-rank margin.

Through simple row operations, the L' matrix constructed using any $2^{m-\gamma_{max}}$ M-PCM points can be transformed to an upper triangular matrix, where the first diagonal entry is 1, and the $(k+1)$-th diagonal entry is a multiple of Δx_k, i.e., $\lambda_{(k+1)(k+1)}\Delta x_k$, where $\lambda_{kk} \in Z$ and $k \in \{1, 2, \cdots, m\}$. As $\Delta x_k \neq 0$, any $\lambda_{kk} = 0$ will lead to $D(L') = 0$.

Now let us find the minimum $||e||_F$ to make $L' + e$ lose rank. The case that L' is not full rank is trivial, as e is the null matrix and $D(L') = 0$. When L' is full rank, the same procedures to calculate $D(L'_{offd})$ in the proof of Lemma 4 leads to

$$\begin{aligned} D(L') &= min\{\sqrt{[c_1 e^2_{x_{1(1)}} + (l_{offd} - c_1)e^2_{x_{1(2)}}] + \cdots + [c_m e^2_{x_{m(1)}} + (l_{offd} - c_m)e^2_{x_{m(2)}}]}\} \\ &= min\{\sqrt{\frac{c_1(l_{offd} - c_1)}{l_{offd}}}\Delta x_1, \cdots, \sqrt{\frac{c_m(l_{offd} - c_m)}{l_{offd}}}\Delta x_m\} \end{aligned} \tag{13}$$

where c_i is the number of $x_{i(1)}$ in the $(i+1)$-th column of L'. The minimum at $\sqrt{\frac{c_i(l_{offd}-c_i)}{l_{offd}}}\Delta x_i$ is achieved, when $e_{x_{i(1)}} = \frac{(l_{offd}-c_i)\Delta x_i}{l_{offd}}, e_{x_{i(2)}} = -\frac{c_i \Delta x_i}{l_{offd}}$, and for all $j \neq i, j \in \{1, 2, \cdots, m\}$, we have $\sqrt{\frac{c_i(l_{offd}-c_i)}{l_{offd}}}\Delta x_i \leq \sqrt{\frac{c_j(l_{offd}-c_j)}{l_{offd}}}\Delta x_j$, and $e_{x_{j(1)}} = e_{x_{j(2)}} = 0$.

Since $\sqrt{\frac{c_i(l_{offd}-c_i)}{l_{offd}}} = \sqrt{-\frac{1}{l_{offd}}(c_i - \frac{l_{offd}}{2})^2 + \frac{l_{offd}}{4}} \leq \frac{\sqrt{l_{offd}}}{2}$, we have $\sqrt{\frac{c_i(l_{offd}-c_i)}{l_{offd}}}\Delta x_i \leq \frac{\sqrt{l_{offd}}}{2}\Delta x_i$. Equation 13 can then be further simplified to

$$D(L') \leq \frac{\sqrt{l_{offd}}}{2} min\{\Delta x_1, \Delta x_2, \cdots, \Delta x_m\} = D(L'_{offd}) \tag{14}$$

The equality is achieved by an OFFD. □

The robustness optimality of the integrated algorithm is brought by the balance and orthogonality of OFFDs. The orthogonality (i.e., the symbolic multiplication of each pair of columns in the design table sums up to 0) guarantees the full rank of Q (as shown in in Equation 6) and thus the invertability of L'_{offd}. Moreover, the balance property (i.e., each level is evaluated the same number of times for each factor) guarantees the maximal perturbation to spoil the invertability of L'_{offd} (as shown in Equation 14).

4 Illustrative Examples

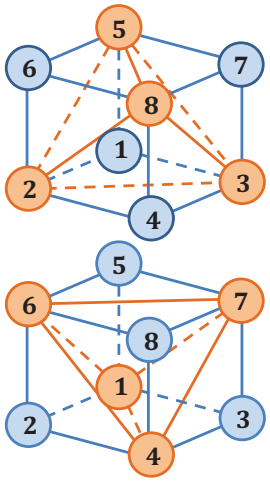
In this section, we first use a 3-parameter example to illustrate the procedures and properties of the integrated design, and then briefly discuss a large 20-parameter example to show its effectiveness.

In the first example, consider an original system mapping of the form $g(x_1, x_2, x_3) = x_1^3 + x_1^2 + x_1 + x_2^3 + x_2^2 + x_2 + x_3^3 + x_3^2 + x_3 + 1$, where x_1 follows an exponential distribution of $f_{X_1}(x_1) = 2e^{-2x_1}$, x_2 follows a uniform distribution of $f_{X_2}(x_2) = \frac{1}{15}, 5 \leq x_2 \leq 20$, and x_3 also follows a uniform distribution of $f_{X_3}(x_3) = \frac{1}{5}, 5 \leq x_3 \leq 10$. The original output mean that we aim to predict is $E[g(x_1, x_2, x_3)] =$

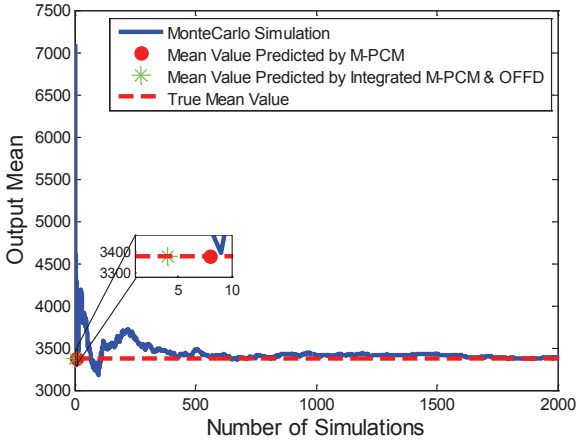
	x_1	x_2	x_3	y
1	−	−	+	y_5
2	+	−	−	y_2
3	−	+	−	y_3
4	+	+	+	y_8

	x_1	x_2	x_3	y
1	−	−	−	y_1
2	+	+	−	y_4
3	−	+	+	y_7
4	+	−	+	y_6

(a)



(b)



(c)

Figure 1: a) 2^{3-1}_{III} OFFD design table. b) 2^{3-1}_{III} OFFD with each point represented at the vertex of a 3-D cuboid. c) Comparison of the number of simulations needed to predict the correct output mean.

$\iiint g(x_1,x_2,x_3) f_{X_1}(x_1) f_{X_2}(x_2) f_{X_3}(x_3) dx_1 dx_2 dx_3 = 3381.1$. To precisely identify all coefficients in $g(x_1,x_2,x_3)$, at least $4^3 = 64$ simulations are required.

Now let us choose only 4 simulations to approximate the system mapping and predict the output mean, using the integrated M-PCM-OFFD. According to the procedures described in Section 3.1, we first choose 8 M-PCM points based upon the pdf of each parameter. The 8 simulation points are $p_1 = (x_{1(1)},x_{2(1)},x_{3(1)})$, $p_2 = (x_{1(2)},x_{2(1)},x_{3(1)})$, $p_3 = (x_{1(1)},x_{2(2)},x_{3(1)})$, $p_4 = (x_{1(2)},x_{2(2)},x_{3(1)})$, $p_5 = (x_{1(1)},x_{2(1)},x_{3(2)})$, $p_6 = (x_{1(2)},x_{2(1)},x_{3(2)})$, $p_7 = (x_{1(1)},x_{2(2)},x_{3(2)})$, and $p_8 = (x_{1(2)},x_{2(2)},x_{3(2)})$, where $x_{1(1)} = 0.2929$, $x_{1(2)} = 1.7071$, $x_{2(1)} = 8.1699$, $x_{2(2)} = 16.8301$, $x_{3(1)} = 6.0566$, and $x_{3(2)} = 8.9434$. We then use 2^{3-1}_{III} OFFD (as the design table and 3-D cube show in Figure 1a,b) to select 4 M-PCM points, which are $\{p_2,p_3,p_5,p_8\}$ or $\{p_1,p_4,p_6,p_7\}$. Here we choose to run simulations at $\{p_2,p_3,p_5,p_8\}$ and obtain the estimated low-order mapping $g^*(x_1,x_2,x_3) = -4442.2 + 6.5x_1 + 513.5x_2 + 186.8x_3$. For illustration purpose,

$$L'_{offd} = \begin{bmatrix} 1 & x_{1(1)} & x_{2(1)} & x_{3(2)} \\ 1 & x_{1(2)} & x_{2(1)} & x_{3(1)} \\ 1 & x_{1(1)} & x_{2(2)} & x_{3(1)} \\ 1 & x_{1(2)} & x_{2(2)} & x_{3(2)} \end{bmatrix} = QU = \frac{1}{2}\begin{bmatrix} 1 & -1 & -1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & 1 & 1 \end{bmatrix}\begin{bmatrix} 2 & * & * & * \\ 0 & 1.4142 & * & * \\ 0 & 0 & 8.6602 & * \\ 0 & 0 & 0 & 2.8868 \end{bmatrix}.$$

Note that Q can be directly obtained from the OFFD design table.

The output mean of $g^*(x_1,x_2,x_3)$ is $E[g^*(x_1,x_2,x_3)] = \iiint g^*(x_1,x_2,x_3) f_{X_1}(x_1) f_{X_2}(x_2) f_{X_3}(x_3) dx_1 dx_2 dx_3 = 3381.1$, precisely the same as the original output mean. For comparison, we also use the Monte Carlo simulation to find the mean output. The number of simulations and associated mean output using these three methods are compared and shown in Figure 1c.

To check the robustness of the integrated design to numerical errors, we calculate the full-column-rank margin of the input matrix $L' \in R^{4\times 4}$, and compare it with those of other designs. According to Lemma 4, we find $D(L'_{offd}) = min\{\Delta x_1, \Delta x_2, \Delta x_3\} = 1.4142$, where $\Delta x_1 = 1.4142$, $\Delta x_2 = 8.6602$ and $\Delta x_3 = 2.8868$. For all simulation subsets of the same size, the margin $D(L')$ takes one of the following three values $\{0, 0.8660, 1.4142\}$. Therefore, the OFFD design is the most robust to numerical errors.

Next, we briefly summarize a large-scale example in the limited space. Assume that a 20-parameter process involves 10 subprocesses, each with 2 uncertain input parameters. If two PCM points are chosen for each parameter, 2^{20} simulations are needed to calculate the mean of the process's output. Due to the nature of the process, each cross-term in the mapping between input parameters and the output has at most

2 parameters. With $\tau = 2$, a 2^{20-12} OFFD can be used to further reduce the number of simulations from 2^{20} to 256, saving a large amount of computations.

5 Concluding Remarks and Future Work

We developed an effective uncertainty evaluation method for large-scale complex systems with a large number of uncertain input parameters. The integrated M-PCM and OFFDs significantly reduces the number of simulations, while maintaining the statistical prediction performance of the M-PCM. Specially, for an original system mapping of m parameters with each parameter up to the degree of 3, the reduced-order mapping produced using the integrated method precisely predicts the mean output of the original system mapping, and reduces the number of simulations from 2^{2m} to $2^{\lceil log_2(m+1) \rceil}$. We also showed that the integrated design is the most robust to numerical errors, making it of practical use for simulations with constraints on parameter resolutions. The development in this paper also provided new interpretations of the optimality of OFFDs, and gave rise to broad new usage of OFFDs for system mapping estimation and uncertainty evaluation. In the future work, we will generalize the degree of uncertain input parameters by exploring multi-level OFFDs and also exploit parameter dependency to further reduce the number of simulations.

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