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Title:	**D2.2 Intermediate Report on Parametrized MOR techniques for sub-problems and associated error bounds**
	Summary: The report gives an overview of existing PMOR methods and where they have been applied to UQ problems. The planned applications in nanoCOPS are also shown.
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D2.2 Intermediate Report on Parametrized MOR techniques for sub-problems and associated error bounds

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Contents

1 Introduction to Parametrized Model Order Reduction

Systems of large order appear in many applications. For an efficient simulation it is necessary to reduce the system dimension by a reliable Model Order Reduction (MOR) method. Nowadays, it is often required that the systems include physical parameters to allow more flexibility in the simulation. These parameters should be preserved in the reduced-order system: a task that motivated the development of new methods for MOR, called parametric, or parameterized, model order reduction (PMOR). Larger parts of Section 1 are taken from [6]. For further informatio,n see [8].

1.1 System Description

Consider a parameterized dynamical system of order n with parameter-dependent system matrices $E(p)$, $A(p) \in \mathbb{R}^{n\times n}$, $B(p) \in \mathbb{R}^{n\times m}$, $C(p) \in \mathbb{R}^{\ell\times n}$:

$$\begin{aligned} E(p)\,\dot{x}(t;p) &= A(p)\,x(t;p) + B(p)\,u(t), \\ y(t;p) &= C(p)\,x(t;p). \end{aligned} \tag{1}$$

The parameter p can be a scalar or a vector. We assume that, for all considered parameter values, $E(p)$ is invertible and the system is stable, i.e., the eigenvalues of $E^{-1}(p)A(p)$ lie in the open left half of the complex plane[1]. In the following, the parameter dependency of the state x and of the output y is (often) omitted in notation for a simplified presentation. We define a parameterized transfer function accordingly (where $s \in i\mathbb{R}$),

$$G(s,p) = C(p)(sE(p) - A(p))^{-1}B(p). \tag{2}$$

PMOR, based on projection, seeks (full column rank) matrices V, $W \in \mathbb{R}^{n\times r}$ with $r \ll n$ such that the output error, $y(t) - \hat{y}(t)$, between the original and the reduced-order system

$$\begin{aligned} W^TE(p)V\,\dot{\hat{x}}(t) &= W^TA(p)V\,\hat{x}(t) + W^TB(p)\,u(t), \\ \hat{y}(t) &= C(p)V\,\hat{x}(t), \end{aligned} \tag{3}$$

is small and the computational time for the simulation of (1) and (2) is decreased significantly by using (3) instead. The reduced-order transfer function is obtained analogously,

$$\hat{G}(s,p) = C(p)V(sW^TE(p)V - W^TA(p)V)^{-1}W^TB(p). \tag{4}$$

1.2 Existing PMOR Techniques

The reduction is especially of value (w. r. t. reduced computational complexity) if the parameter dependency in (1) is affine in the system matrices [3], i.e., we have the following matrix representations

$$\begin{aligned} E(p) &= E_0 + e_1(p)E_1 + \ldots + e_{P_E}(p)E_{P_E}, \\ A(p) &= A_0 + f_1(p)A_1 + \ldots + f_{P_A}(p)A_{P_A}, \\ B(p) &= B_0 + g_1(p)B_1 + \ldots + g_{P_B}(p)B_{P_B}, \\ C(p) &= C_0 + h_1(p)C_1 + \ldots + h_{P_C}(p)C_{P_C}, \end{aligned}$$

[1] Usually single, free-running, oscillators are not that large in size. Hence, for the moment, we neglect them.

leading to reduced-order matrices

$$\begin{array}{rcrcrcl} \hat{E}(p) & := & W^T E(p) V & = & W^T E_0 V & + & \sum_{i=1}^{P_E} e_i(p) W^T E_i V, \\ \hat{A}(p) & := & W^T A(p) V & = & W^T A_0 V & + & \sum_{i=1}^{P_A} f_i(p) W^T A_i V, \\ \hat{B}(p) & := & W^T B(p) & = & W^T B_0 & + & \sum_{i=1}^{P_B} g_i(p) W^T B_i, \\ \hat{C}(p) & := & C(p) V & = & C_0 V & + & \sum_{i=1}^{P_C} h_i(p) C_i V. \end{array} \tag{5}$$

It is assumed that the number of summands P_E, P_A, P_B, P_C is moderate. The parameter dependency in the functions e_i, f_i, g_i, h_i might be linear or nonlinear. The reduced parameter-independent matrices $W^T E_i V$, $W^T A_i V \in \mathbb{R}^{r \times r}$, $W^T B_i \in \mathbb{R}^{r \times m}$ and $C_i V \in \mathbb{R}^{\ell \times r}$ can be pre-computed (i.e., off-line). The computation of the projection matrices V and W is of main interest in PMOR and differs very much along the presented approaches.

1.2.1 POD and POD-Greedy

The POD (Proper Orthogonal Decomposition) [50] method, or also called PCA (Principal Component Analysis), is based on the singular value decomposition (SVD).
In the PMOR setting, the system is solved for a number of state vectors corresponding to various parameter configurations $p_1, p_2, \ldots, p_{N_{SVD}}$, and these state vectors form the snapshot matrix $X_{SVD} \in \mathbb{R}^{n \times N_{SVD}}$. Here, N_{SVD} is the number of state vectors given to the snapshot matrix.
The SVD produces a diagonal matrix S_{SVD} of the same dimension as X_{SVD} and with nonnegative diagonal elements and unitary matrices U_{SVD} and V_{SVD} so that

$$X_{SVD} = U_{SVD} S_{SVD} V_{SVD}^T.$$

The first columns of U_{SVD} are chosen as projection matrices for both V, W, i.e. the singular vectors corresponding to the largest singular values.The singular vectors form the projection matrices V and W as used in (5), typically with $W = V$.
In a time-dependent PMOR setting the POD is often used in a POD-Greedy algorithm. The POD-Greedy algorithm [23, 51] meanwhile is standard in Reduced Basis (RB) Methods.
In short, the POD-Greedy algorithm uses the SVD to condense trajectories corresponding to certain parameter configurations, which were chosen by finding the maximum of an error estimator $\Delta(p)$ over a set of samples of the parameter domain. The error estimator gives bounds to the approximation error and stops the MOR algorithm once a predefined tolerance is satisfied, see [15, 24, 26]. In general, the RB Methods require an affine decomposition as (5).
Let Ξ denote a finite sample of the parametric domain and set $S_1 = \{p^1\}$ and $X_1 = [x(p^1)]$ and $N = 2$. Let $\Xi_1 = \Xi \backslash \{p^1\}$. The steps of the Greedy sampling process are:
1) find $p^N = \arg\max_{p \in \Xi_1} \Delta_{N-1}(p)$,
2) Set $S_N = S_{N-1} \cup p^N, \quad \Xi_N = \Xi_{N-1} \backslash \{p^N\} \quad X_N = [X_{N-1} \;\; x(p^N)]$,
3) While ($\max_{p \in \Xi} \Delta_{N-1}(p) >$ tolerance and $\Xi_N \neq \emptyset$, N:=N+1, goto 1).such that the Greedy algorithm finds a set of parameter values S_N and a corresponding snapshot matrix X_N.

1.2.2 Interpolatory methods for PMOR

A short description of several interpolatory methods for PMOR follows.

A) (Multi)parameter moment matching
A generalization of moment matching MOR, called *(multi)parameter moment matching*, was first considered in [14]. This method is based on a multivariate Taylor expansion with expansion points in frequency and parameter space. We denote the parameter points by $p_1, \ldots, p_K$ and the frequency expansion points by $s_1, \ldots, s_L$ in the following. The number of matched moments is q. The approach ensures the following moment matching,

$$\frac{\partial^k}{\partial s^k}\frac{\partial^\ell}{\partial p^\ell}G(s_i, p_j) = \frac{\partial^k}{\partial s^k}\frac{\partial^\ell}{\partial p^\ell}\hat{G}(s_i, p_j),$$

for $i = 1, \ldots, L$, $j = 1, \ldots, K$, $k = 0, \ldots, q$, $\ell = 0, \ldots, q$. Improvements, which avoid explicitly moment matching can be found in [17, 18, 30].

B) Transfer function interpolation
Another approach for parameter-preserving MOR is based on a combination of balanced truncation (BT) at certain distinct parameter values (the interpolation points) $p_1, \ldots, p_K$ with interpolation. The approach, which is called *transfer function interpolation*, was originally proposed in [4] using polynomial interpolation. It leads to a reduced-order transfer function

$$\hat{G}(s, p) = \sum_{j=1}^{K} L_j(p)\hat{C}_j(s\hat{E}_j - \hat{A}_j)^{-1}\hat{B}_j, \tag{6}$$

where $L_j(p)$ are the Lagrange basis polynomials. The locally reduced matrices $\hat{E}_j$, $\hat{A}_j$, $\hat{B}_j$, $\hat{C}_j$ (of possibly different reduced order r_j) are obtained by applying K-times BT on $G(s, p_j)$ with $j = 1, \ldots, K$. This PMOR approach can simply be extended to a hybrid approach of BT, by applying different kinds of interpolation, as demonstrated in [5] for rational interpolation. However, in contrast to polynomial interpolation, other interpolation techniques will not necessarily preserve the structure of the original system in the reduced-order representation. PMOR by transfer function interpolation benefits from the system theoretical properties of BT, such that we can guarantee stability for the reduced-order system and an error bound can be derived, see Subsection 1.3.

C) Piecewise $\mathcal{H}_2$ tangential interpolation
A structure-preserving MOR method called *piecewise $\mathcal{H}_2$ tangential interpolation* (with $\mathcal{H}_2$ optimal frequency points) was introduced in [3]. Local projection matrices are computed by applying the Iterative Rational Krylov Algorithm (IRKA) [22] on $G(s, p_j)$ and concatenated

$$V = [V_1,\ V_2, \cdots, V_K], \quad W = [W_1,\ W_2, \cdots, W_K],$$

to obtain (4). Thus, the dimension of the reduced-order system is $K \cdot r$. Note that the number of columns $K \cdot r$ of V and W can further be reduced by an SVD or a rank-revealing QR factorization to ensure that V and W have full rank. IRKA computes optimal (frequency) shifts s_i and corresponding tangential directions b_{ij} and c_{ij} such that (4) matches the p-gradient and p-Hessian of the original system response (2) with respect to the parameters:

$$\nabla_p c_{ij}^T G(s_i, p_j)b_{ij} = \nabla_p c_{ij}^T \hat{G}(s_i, p_j)b_{ij}, \quad \nabla_p^2 c_{ij}^T G(s_i, p_j)b_{ij} = \nabla_p^2 c_{ij}^T \hat{G}(s_i, p_j)b_{ij},$$

for $i = 1, \ldots, r,\ j = 1, \ldots K$. Additionally, the usual tangential interpolation properties hold

$$G(s_i, p_j)b_{ij} = \hat{G}(s_i, p_j)b_{ij}, \quad c_{ij}^T G(s_i, p_j) = c_{ij}^T \hat{G}(s_i, p_j).$$

D) PMOR by matrix interpolation

PMOR by matrix interpolation [39] computes a parameterized reduced-order system by interpolation of locally reduced system matrices. A parameterized reduced-order system (3) is obtained by interpolation of the locally reduced system matrices $\hat{E}_j$, $\hat{A}_j$, $\hat{B}_j$, $\hat{C}_j$, where

$$\begin{array}{rclcrcl} \hat{E}(p) & = & \sum_{j=1}^K \omega_j(p) M_j \hat{E}_j T_j^{-1}, & & \hat{A}(p) & = & \sum_{j=1}^K \omega_j(p) M_j \hat{A}_j T_j^{-1}, \\ \hat{B}(p) & = & \sum_{j=1}^K \omega_j(p) M_j \hat{B}_j, & & \hat{C}(p) & = & \sum_{j=1}^K \omega_j(p) \hat{C}_j T_j^{-1}, \end{array}$$

with properly chosen transformation matrices $M_j,\ T_j \in \mathbb{R}^{r \times r}$ and weights ω_j. The transformation matrices are chosen so as to give a common physical meaning to all reduced state vectors: $M_j = (W_j^T R)^{-1}$, $T_j = R^T V_j$ with $R \in \mathbb{R}^{n \times r}$ obtained from a thin SVD of $[\omega_1(p)V_1, \omega_2(p)V_2, \ldots, \omega_K(p)V_K]$. Note that one R is used to compute the transformation matrices M_j, T_j for $j = 1, \ldots, K$.

E) Generalized Loewner matrix $\mathbb{L}$ approach

Two-variable rational interpolation for MOR of single parameter systems is proposed in [1]. In this work, a generalized Loewner matrix $\mathbb{L}$ is constructed from measurements such that a (two-variable) reduced system is given by the null space of $\mathbb{L}$ in barycentric formula.

Conclusion

All interpolatory approaches can be applied for PMOR of linear parametric systems. The parameter-dependence in the matrices may be linear or nonlinear, but is assumed to be smooth enough to allow for approximation by interpolation. An affine parameter dependency is not required for PMOR by transfer function or by matrix interpolation.

1.3 Error Bounds

For PMOR by transfer function interpolation as described in Section 1.2.2 B), a global error bound can be derived by a combination of the BT $\mathcal{H}_\infty$ error bound at the interpolation points p_j and an error estimate for the interpolation error [4]. We obtain an error bound for $\|G(s,p) - \hat{G}(s,p)\|$, exemplarily described for (6), using the BT error bound (for the locally reduced systems by a given error tolerance *tol*)

$$\|G(s, p_j) - \hat{G}(s, p_j)\|_{\mathcal{H}_\infty} \leq 2 \left(\sum_{i=r_j+1}^{n} \sigma_i \right) < \textit{tol}. \tag{7}$$

The error over the whole parameter interval $\mathcal{I}$ is bounded by

$$\sup_{\substack{s \in \mathbf{C}^+ \\ p \in \mathcal{I}}} \|G(s,p) - \hat{G}(s,p)\| \overset{(7)}{\leq} \sup_{\substack{s \in \mathbf{C}^+ \\ p \in \mathcal{I}}} \|R_k(G,s,p)\| + \textit{tol} \sup_{p \in \mathcal{I}} |\sum_{j=0}^{k} L_j(p)|,$$

with a remainder $R_k(G, s, p)$ which depends on the applied interpolation technique.
For parametrized linear time invariant systems, an a posteriori error bound for the transfer function of the reduced model is proposed in [19]. The error bound is independent of the discretization method (finite difference, finite element, finite volume) applied to the original PDEs. Furthermore, the error bound can be directly used in the discretized vector space, without going back to the PDEs, and especially to the weak formulation associated with the finite element discretization, which must be known a priori for deriving the error bound for the RB method. This is typically useful when only discretized systems of ODEs/DAEs are available, for example the system of DAEs established based on modified nodal analysis in circuit simulation.
Technically, the error bound enables automatic generation of the reduced models computed by parametric model reduction methods based on interpolation of the transfer function, e.g. Krylov subspace based methods [7], which is desired in design automation for circuits and MEMS. The error bound, depending on the residuals of the primal and the dual system, is valid for systems of the form (1), where the transfer function (2) fulfills

$$\inf_{\substack{w\in\mathbb{C}^n\\ w\neq 0}} \sup_{\substack{v\in\mathbb{C}^n\\ v\neq 0}} \frac{w^* G(s,p) v}{||w||_2 ||v||_2} =: \beta(p) > 0.$$

2 PMOR for Uncertainty Quantification

In the last years, the discussed PMOR techniques have been used for several Uncertainty Quantification (UQ) methods like, e. g. Monte Carlo (MC), Stochastic Collocation (SC), and Stochastic Galerkin (SG).
One of the first publications in this field was [31], where a projection based MOR method for RLC interconnect circuits is presented including variational analysis to capture manufacturing variations.
The SG approach yields a coupled deterministic system to which non-parametric MOR methods can be applied. This is done, e. g., in [35, 54].
In [41], the SG method is considered for linear dynamical systems with random parameters. On the one hand, the original systems are reduced in the state space and the SG scheme is applied to the reduced systems. On the other hand, the SG method changes the original systems into a huge linear dynamical system, where MOR is used in the state space of this Galerkin system.
In the first approach, PMOR is examined for the original systems. The used PMOR strategy collects local bases for the reduction of systems for different samples of the parameters and an SVD is employed to construct a global basis for a reduced system, cf. [3].
In [42, 43], a variance-based sensitivity analysis is applied to the transfer function. Typically, just a few random parameters are relevant for the variations of the output. Thus unessential random parameters are identified by the sensitivity analysis. An MOR of the random space is achieved by restoring the insignificant random variables to constants. In Section 2.1 this is described in some more detail.
Passive electromagnetic devices under random input conditions are considered in [47]. The authors propose a Krylov-based PMOR in combination with sparse grid SC and apply it to a coaxial cable.
In [9] a POD-reduced model is used for SC and MC simulation of the time-harmonic Maxwell's equations with uncertain material parameters. The speedup is much higher

for the MC but also visible for SC and the relative errors for the output voltage are of order 10^{-6} and 10^{-12} for SC and MC, respectively.
A combination of RB and SC is in [16] applied to stochastic versions of the diffusion equation and the incompressible Navier-Stokes equations.
In [21] a non-linear PMOR method for large-scale statistical inverse problems in a Bayesian inference setting is applied to a combustion problem governed by an advection-diffusion-reaction partial differential equation. The reduced order model (ROM) is then used for the Markov chain MC sampling employed by the Bayesian inference approach.

2.1 Uncertainty Quantification

[2]We consider UQ by expanding the solution in so-called generalized Polynomial Chaos expansions. In these expansions the solution is decomposed into a series with orthogonal polynomials in which the parameter dependency becomes an argument of the orthogonal polynomial basis functions. The time and space dependency remains in the coefficients. In UQ two main approaches are in use: SC and SG. In SC the coefficients in the expansion are approximated by quadrature and thus lead to a large series of deterministic simulations for several parameters. In SG one assumes a finite sum of the expansion as approximation to the solution and requires that the vector of residuals is orthogonal to all basis functions used in the finite expansion (using an inner product in parameter space), which leads to one big, but coupled, system. Also here quadrature can be applied but this does not automatically lead to decoupling as happens for SC.

We will denote parameters by $\mathbf{p} = (p_1, \ldots, p_P)^T$ again and assume a probability space $(\Omega, \mathcal{A}, \mathcal{P})$ given where $\mathcal{A}$ represents a σ-algebra, $\mathcal{P} : \mathcal{A} \rightarrow \mathbb{R}$ is a measure and $\mathbf{p} = \mathbf{p}(\omega) : \Omega \rightarrow B \subseteq \mathbb{R}^P$. Here we will assume that the p_i are independent.
For a function $f : B \rightarrow \mathbb{R}$, the mean or expected value is defined by

$$\mathbf{E}_p[f(\mathbf{p})] =< f >= \int_\Omega f(\mathbf{p}(\omega)) \mathrm{d}\mathcal{P}(\omega) = \int_B f(\mathbf{p})\ \rho(\mathbf{p}) \mathrm{d}\mathbf{p}.$$

The specific probability distribution density is defined by the function $\rho(\mathbf{p})$. A bilinear form $< f, g >$ (with associated norm L^2_ρ) is defined by

$$< f, g >= \int_B f(\mathbf{p})\ g(\mathbf{p})\ \rho(\mathbf{p}) \mathrm{d}\mathbf{p} =< f\ g > .$$

We assume a complete orthonormal basis of polynomials $(\phi_i)_{i \in \mathbb{N}}$, $\phi_i : B \rightarrow \mathbb{R}$, given with $< \phi_i, \phi_j >= \delta_{ij}$ $(i, j, \geq 0)$. When $P = 1$, ϕ_i has degree i. To treat a uniform distribution (i.e., for studying effects caused by robust variations) Legendre polynomials are optimal in some sense; for a Gaussian distribution one can use Hermite polynomials [34, 52]. A polynomial ϕ_i on $\mathbb{R}^P$ can be defined from one-dimensional polynomials: $\phi_i(\mathbf{p}) = \prod_{d=1}^P \phi_{i_d}(p_d)$. Actually i orders a vector $\mathbf{i} = (i_1, \ldots, i_P)^T$.
A solution $\mathbf{x}(t, \mathbf{p}) = (x_1(t, \mathbf{p}), \ldots, x_n(t, \mathbf{p}))^T$ of a dynamical system (which we do not further specify) becomes a random process. We assume that second moments are finite: $< x_j^2(t, \mathbf{p}) > < \infty$, for all $t \in [t_0, t_1]$ and $j = 1, \ldots, n$. We express $\mathbf{x}(t, \mathbf{p})$ in a

[2]This section is taken from Section 5 in [10].

Polynomial Chaos expansion

$$\mathbf{x}(t,\mathbf{p}) = \sum_{i=0}^{\infty} \mathbf{v}_i(t)\ \phi_i(\mathbf{p}), \tag{8}$$

where the coefficient functions $\mathbf{v}_i(t)$ are defined by

$$\mathbf{v}_i(t) =< \mathbf{x}(t,\mathbf{p}), \phi_i(\mathbf{p}) > . \tag{9}$$

Here the inner product is considered component wise. A finite approximation $\mathbf{x}^m(t,\mathbf{p})$ to $\mathbf{x}(t,\mathbf{p})$ is defined by

$$\mathbf{x}^m(t,\mathbf{p}) = \sum_{i=0}^{m} \mathbf{v}_i(t)\ \phi_i(\mathbf{p}). \tag{10}$$

When exploiting SC, the integrals (9) are computed by (quasi) MC, or by multi-dimensional quadrature. We assume quadrature grid points $\mathbf{p}^k$ and quadrature weights w_k, $0 \leq k \leq K$, such that

$$\mathbf{v}_i(t) =< \mathbf{x}(t,\mathbf{p}), \phi_i(\mathbf{p}) > \approx \sum_{k=0}^{K} w_k\ \mathbf{x}(t,\mathbf{p}^k)\ \phi_i(\mathbf{p}^k). \tag{11}$$

Typically, for low numbers of random parameters, Gaussian quadrature is used with corresponding weights. We solve the dynamical system for $\mathbf{x}(t,\mathbf{p}^k)$, $k = 0,\ldots,K$ ($K+1$ deterministic simulations). By post-processing we determine the $\mathbf{v}_i(t)$ in (11).
As alternative to SC, SG can be used. One puts the approximation (10) in the equations of the dynamical system and makes the residuals orthogonal to each basis function used. The result is a big system that involves all coefficients $\mathbf{v}_i(t)$, $0 \leq i \leq m$, as unknowns. For linear dynamical systems one can determine all integrals over B exactly, in advance. For nonlinear systems one may approximate these again by quadrature, similar as done for SC.
After determining the approximation (10) by SC or by SG, the expansion provides a response surface facility from which the solution can be determined for any values of t and $\mathbf{p}$. It also provides (fast) information about mean, variance and sensitivity. In [2, 49, 38] efficient methods are described to determine the coefficients by SC. In [49, 42, 41] also the combination with (parameterized) MOR was studied.
In Fig. 1 at the top-left MC Sampling and Importance Sampling generate a list of samples of $\mathbf{p}$ for which the dynamical system has to be solved, after which statistical analysis can be done. At the top-right the alternative path by UQ is indicated. Stochastic Collocation provides a list of deterministic values $\mathbf{p}$ for which the dynamical system has to be solved. In both cases parameterized MOR (pMOR) can be of help to faster provide approximations. The path via Stochastic Galerkin results in a huge system that involves all coefficients. The system is independent of $\mathbf{p}$, due to averaging. Here normal MOR can be of use - it may be even necessary to reduce the huge system to be able to obtain approximative solutions.
In [29, 49, 40] (response surface) approximations or the combination between them and more accurate solutions was studied for Failure Analysis. In [37] the method can shift the (probability density) weighting function in the inner product to the area of interest (shifted Hermite chaos). One also can use a windowed Hermite chaos. The shift is tuned by some optimization procedure. The windowed Hermite chaos looks to be the most accurate alternative. In [38] various multi-dimensional integration methods have been studied for the purpose of efficient reliability analysis.

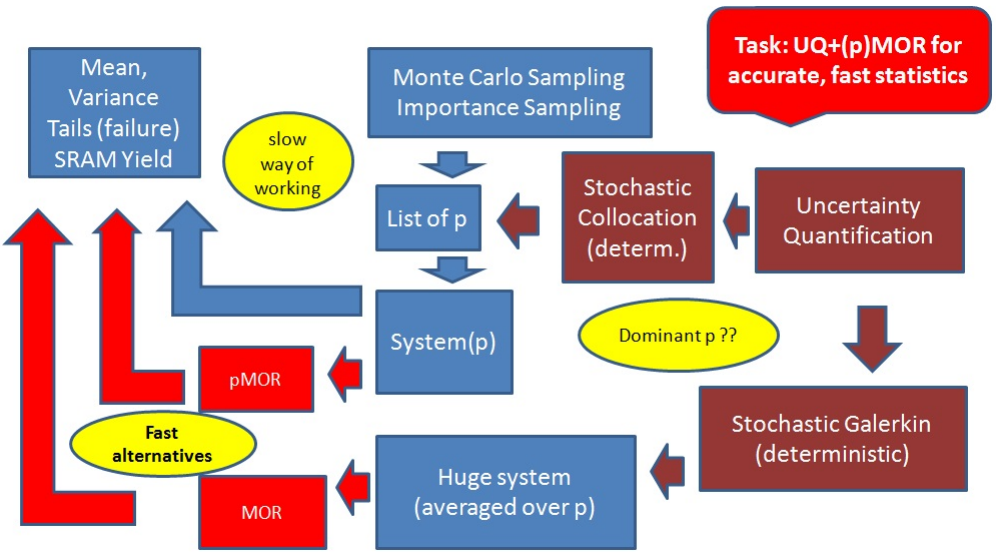

Figure 1: The various ways to obtain statistic information.

Central in Fig. 1 is the question on dominant parameters. In [42, 43] the sensitivity coefficients of parameters to the variance of the solution have been studied via a Sobol decomposition [44] and using uniform distributions. Assuming a scalar solution x in (8), the variance of x (at time t) reads as

$$\mathrm{Var}_x(t) = \sum_{i=1}^{\infty} v_i^2(t).$$

The total normalized sensitivity of the j-th random parameter can be written as

$$S_j := \frac{V_j}{\mathrm{Var}_x}, \quad \text{with} \quad V_j := \sum_{i \in \mathcal{I}_j} v_i^2, \quad \text{for} \quad j = 1, \ldots, P.$$

Here $i \in \mathcal{I}_j$ if and only if ϕ_i varies with respect to the random variable p_j , i.e., ϕ_i includes a non-constant univariate polynomial in p_j . Clearly the bounds $0 \leq S_j \leq 1$ apply for each j. One obtains approximations of these total normalized sensitivities by a truncated expansion

$$V_j^D := \sum_{i \in \mathcal{I}_j^D} v_i^2, , \quad \text{with} \quad \mathcal{I}_j^D := \{i \in \mathcal{I}_j \ : \ \mathrm{degree}(\phi_i) \leq D\}.$$

Although the bounds $1 \leq S_1 + \cdots + S_P \leq P$ hold, the sum of the total normalized sensitivities is often close to the lower bound. In view of this variability of the sum of sensitivities, we further normalize

$$S_j^* := S_j \Big(\sum_{l=1}^{P} S_l \Big)^{-1}, \quad j = 1, \ldots, P.$$

We now have $S_1^* + \cdots + S_P^* = 1$. This facilitates to compare the S_j^*. After determining the dominant S_j^* [42] we only deal with the S_j. Note that Var_x and the S_j vary with

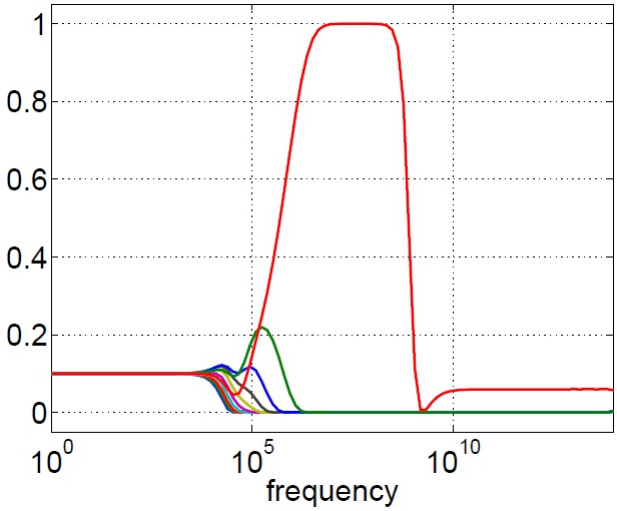

Figure 2: Normalized variation sensitivities of $H(s, \mathbf{p})$ for conductances as random parameters [42].

t. If we assume a partitioning (possibly after re-ordering) $\mathbf{p} = (\mathbf{q}, \mathbf{r})$, where $\mathbf{q}$ are $P_{\rm red}$ parameters that will be allowed to vary, while $\mathbf{r}$ are the parameters set to a fixed value $\mathbf{r}_0$, we obtain, for the error $\delta(t, \mathbf{r}_0)$ in doing this, the estimate in the following theorem [42, 43].

Theorem (Scaled approx. error after fixing parameters)

$$\begin{aligned} \delta^2(t, \mathbf{r}_0) &= \frac{< \Big(x(t, \mathbf{q}, \mathbf{r}) - x(t, \mathbf{q}, \mathbf{r}_0) \Big)^2 >}{\mathrm{Var}_x(t)}, \\ &\leq (1 + \varepsilon^{-1}) \sum_{j=P_{\rm red}+1}^{P} S_j(t). \end{aligned} \tag{12}$$

In (12), ε is a confidence parameter, and $\mathbf{q} \in \mathbb{R}^{P_{\rm red}}$ and $\mathbf{r}_0 \in B_\varepsilon$ with $\mathcal{P}(\mathbf{p}^{-1}(\mathbb{R}^{P_{\rm red}} \times B_\varepsilon)) \geq 1 - \varepsilon$ (here $\mathbf{p}^{-1}$ is the inverse mapping in the sense of $\mathbf{p}^{-1}(C) := \{\omega \in \Omega : \mathbf{p}(\omega) \in C\}$). Note that $\delta^2(t, \mathbf{r}_0)$ is scaled by Var_x. It assumes that $\mathrm{Var}_x(t)$ is bounded away from 0. Clearly, if $\mathrm{Var}_x(t)$ is bounded, small S_j, corresponding to the parameters $\mathbf{r}$ set to $\mathbf{r}_0$, lead to an upper bound for the mean of the squared approximation error. In [42] the parameter reduction is considered for the transfer function $H(s, \mathbf{p})$ where $s \in i\mathbb{R}$ on the imaginary axis. Now, first an approach similar to (12) is applied to the transfer function $H(s, (\mathbf{q}, \mathbf{r}_0))$ after splitting $\mathbf{p}$, resulting in an error estimate for $\delta_H^2(s, \mathbf{r}_0)$ and leading to a mean squared error $< |H(s, \mathbf{q}, \mathbf{r}) - H(s, \mathbf{q}, \mathbf{r}_0)|^2 >$. From this an upper bound for $\max_{t>0} < x(t, \mathbf{q}, \mathbf{r}) - x(t, \mathbf{q}, \mathbf{r}_0) >$, for the solution $x(t, \mathbf{p})$ in the time domain, can be derived. For an RLC-circuit, Fig. 2 shows a typical outcome for the variation sensitivities of $H(s, \mathbf{p})$ of various conductances as random parameters. Similar results can be shown for capacitances and for inductances. By this we obtain error estimates for the coefficients in the generalized polynomial chaos expansion by which we can provide error plots of the mean and of the variance (as functions of time).
Next, parameterized MOR on $H(s, (\mathbf{q}, \mathbf{r}_0))$ can be applied, which leads to an additional error. In [42] a typical Krylov-subspace MOR-technique was used after first applying

SG. As alternative, BT MOR techniques could be applied, which provide error estimation. This type of MOR-technique leads to an L_2-norm estimate (in time). In [41] the authors did focus on SG and considered first reducing the original system by parameterized MOR, followed by SG, versus first applying SG on the original system, followed by a (global) MOR.
The sensitivity technique described in this section can lead to variation-aware MOR approaches. Clearly, MOR should not lead to reduced models that do not preserve the main statistical characteristics of the full model.

2.2 Reduced Basis Method for Uncertainty Quantification

We shortly describe RB for UQ. The beginning is very similar to Section 2.1. Let $(\Omega, \mathcal{F}, \mathcal{P})$ denote a probability space. Given is a square integrable random parameter variable $P : \Omega \to \Gamma \subset \mathbb{R}$ (with realization $p = p(\omega) \in \Gamma$), with probability density function ρ and a function $s : \mathbb{R}^n \times \Gamma \to \mathbb{R}^d$, corresponding to a mapping of realizations of a random variable to the output of the electromagnetic system. The state vector $x \in \mathbb{R}^n$ depends implicitly on the realization of the random variable.
In statistical analysis, the expectation and variance of quantities of interest like the response surface of the output functional s w.r.t. uncertain parameters is computed.
SC computes statistical quantities like the mean by a quadrature rule

$$\mathbb{E}(s)(x) = \int_\Gamma s(x;p)\rho(p)dp \approx \sum_{i=1}^{n_{sample}} s(x;\xi_i)w_i,$$

where the realizations ξ_i are the sample points, n_{sample} denotes the sample size and the weights w_i are determined using the probability density function ρ. See [13] for more details.
To enhance the computation speed of statistical quantities, RB MOR can be applied to generate a ROM for the domain of interest, which will greatly increase the speed to perform the MC simulation or SC. Under the assumption of bounded variations, the RB error estimators can also be used to certify the accuracy of the computed statistics. See [25] for more details.

3 Outlook: Scope for nanoCOPS

Section 2.1 shows that UQ can deal with material parameters for nonlinear problems. The described MOR techniques in the Sections 1 and 2 show confidence that PMOR can be of help to reduce the size in case of linear problems. Also, implementations can be made to work for UQ purposes.
Clearly, also two additional steps will have to be made: generalization to parameterized, nonlinear problems, as well as provisions in being able to deal with *geometrical* parameters. Apart from that parameterized MOR for coupled problems will have to be considered, together with Work Package WP1.

- MOR for nonlinear problems. POD, as described in Section 1.2.1, is one of the methods that can be used. POD is also an essential ingredient in a regression-based method, like DEIM (Discrete Empirical Interpolation Method) [12]. Modifications to DEIM are needed to guarantee that after reduction a passive model remains passive [11]. In this area we will have to make further research.

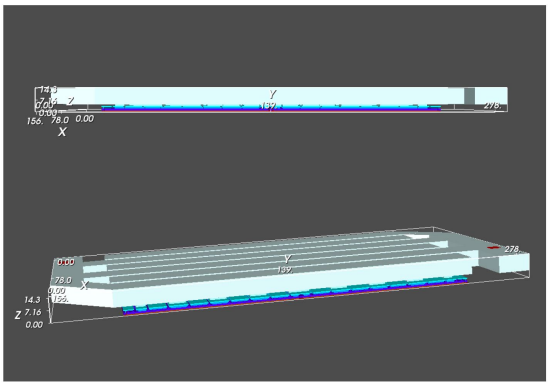

Figure 3: Cross section and three dimensional model of device [33].

- Varying geometry. This is not directly a problem of circuits, which usually are fixed networks. However, in the modeling for the electromagnetics and/or heat small displacements already can result in a different discretization, which can influence the dimension of the unknowns [46, 45].

The geometry aspect we describe a bit further.
Since in many applications, used in power electronic systems, the physical domain cannot be determined precisely, the problem with the *uncertain geometry* has been formulated as the first attempt to cope with a more general problem called *Use Case I: Power-MOS - electro-thermal-stress coupling*. Such variations result from the imperfections in manufacturing processes, including, for example, sub-wavelength lithography, lens aberration, and chemical-mechanical polishing [36]. The problem under consideration comes from the automotive industry, where there is a need to handle the demanding electro-thermal operational constraints to design both components and systems. Therefore, a similar structure to the one proposed in the USE Case I has been considered as a case study. The geometrical finger structure of a device design has been shown on Figure 3. The source and drain contacts are located at the top of the design. The current to drains and away from the sources of the individual channels is ultimately transported by series of metal stripes and via patterns. In our experiment, the height of the metal3 layer and, as a result, also the z-th coordinate of the source and drain contacts, located at the top of design, are assumed to be uncertain. The uncertainty associated with geometry is modeled by the uniform distribution. This topological uncertainty (the domain with rough boundaries), in consequence, has impact on all the device characteristics including the total resistance, the interconnect resistance, resistance in particular layers, for example. In general, the computational methods used to model uncertainties can be divided into two major categories: these based on a statistic approach like the MC method and its variants, and methods based on a non-statistical approach such as SG and SC. Thus, to deal with this problem, the following methods have been considered and proposed:

- the crude MC simulation [20], in order to investigate the effect of uncertain geometry on relevant quantities such as the total and interconnect resistance,
- the pseudo-spectral approach (SC), where the application of a stochastic mapping that transforms the deterministic/ stochastic problem of a random domain into a stochastic problem in a deterministic (fixed) domain, has been applied [27, 48, 53],

- the pseudo-spectral approach (SC), where the geometric uncertainties [32] can be modeled by the spatially varying threshold, for example in the Heaviside projection [28].

4 Planning

Between M6-M12 implemenation will start. Here choices will have to be made on best methods to be chosen. As indicated above, also new methods may have to be developed, and existing methods may have to be improved during implementation (which is a natural step in industrializing a particular method). We deal with

- PMOR for (linear) electromagnetics, or heat or circuit parts. Here several methods are available.
- MOR and PMOR for linear, coupled problems. Here some first steps are known in literature. All methods are candidate for improvement.
- PMOR for nonlinear problems. Here bilinear approximatoins will be considered more closely. A method like DEIM [12] still has to be extended to parameterized problem, albeit that some steps (like generating an overall basis) may be similar to the case for linear problems.
- Geometrical variations. For the moment this will be the second stage type of variations, see also Section 5.

We will prepare the above topics for discussion at our 2nd nanoCOPS Workshop, on Oct. 6-7, 2014 (M12), at HUB, Berlin.

5 Risks

First experiments with topology optimization learned us impact on FEM/Finite Volume/FIT discretizations. This can even make UQ by SC much less trivial than expected: the method can become intrusive - which, clearly, will become a point of attention by our industrial partner MAG.

References

[1] A. C. Antoulas, A. C. Ionita, and S. Lefteriu. On two variable rational interpolation. *Linear Algebra Appl.*, 436(8):2889–2915, 2012.

[2] F. Augustin, A. Gilg, M. Paffrath, P. Rentrop, and U. Wever. Polynomial chaos for the approximation of uncertainties: Chances and limits. *Euro. J. of Appl. Math.*, 19:149–190, 2008.

[3] U. Baur, C. A. Beattie, P. Benner, and S. Gugercin. Interpolatory projection methods for parameterized model reduction. *SIAM J. Sci. Comput.*, 33(5):2489–2518, 2011.

[4] U. Baur and P. Benner. Modellreduktion für parametrisierte Systeme durch balanciertes Abschneiden und Interpolation (Model reduction for parametric systems using balanced truncation and interpolation). *at-Automatisierungstechnik*, 57(8):411–420, 2009.

[5] U. Baur, P. Benner, A. Greiner, J. G. Korvink, J. Lienemann, and C. Moosmann. Parameter preserving model reduction for MEMS applications. *Mathematical and Computational Modelling of Dynamical Systems*, 17(4):297–317, 2011.

[6] U. Baur, P. Benner, B. Haasdonk, C. Himpe, and M. Ohlberger. Comparison of methods for parametric model order reduction of dynamical systems. In P. Benner, A. Cohen, M. Ohlberger, and K. Willcox, editors, *Model Reduction and Approximation for Complex Systems*, chapter 10. in preparation.

[7] P. Benner and L. Feng. A robust algorithm for parametric model order reduction based on implicit moment matching. In A. Quarteroni and G. Rozza, editors, *Reduced Order Methods for modeling and computational reduction*, MS & A series. Springer, 2014.

[8] P. Benner, S. Gugercin, and K. Willcox. A survey of model reduction methods for parametric systems. MPI Magdeburg Preprint MPIMD/13-14, August 2013. Available from `http://www.mpi-magdeburg.mpg.de/preprints/`.

[9] P. Benner and J. Schneider. Uncertainty quantification for Maxwell's equations using stochastic collocation and model order reduction. Max Planck Institute Magdeburg Preprint MPIMD/13–19, October 2013. Available from `http://www.mpi-magdeburg.mpg.de/preprints/`.

[10] A. Di Buccianico, J. ter Maten, R. Pulch, R. Janssen, J. Niehof, M. Hanssen, and S. Kapora. Robust and efficient uncertainty quantification and validation of RFIC isolation. *Radioengineering*, 23(1):308–318, 2014. Online: `http://www.radioeng.cz/fulltexts/2014/14_01_0308_0318.pdf`.

[11] S. Chaturantabut, C. Beattie, and S. Gugercin. Structure-preserving model reduction for nonlinear port-Hamiltonian systems, 2013. Presented at MODRED 2013, Max Planck Institute Magdeburg, Germany, `http://www2.mpi-magdeburg.mpg.de/mpcsc/events/ModRed/2013/`.

[12] S. Chaturantabut and D. S. Sorensen. Nonlinear model reduction via discrete empirical interpolation. *SIAM J. Sci. Comput.,*, 32(5):2737–2764, 2010.

[13] P. Chen, A. Quarteroni, and G. Rozza. Comparison between reduced basis and stochastic collocation methods for elliptic problems. *Journal of Scientific Computing*, 59:187–216, 2014.

[14] L. Daniel, O. C. Siong, L. S. Chay, K. H. Lee, and J. White. A multiparameter moment-matching model-reduction approach for generating geometrically parameterized interconnect performance models. *IEEE Trans. Comput.-Aided Des. Integr. Circuits Syst.*, 23(5):678–693, May 2004.

[15] J. L. Eftang, D. J. Knezevic, and A. T. Patera. An hp certified reduced basis method for parametrized parabolic partial differential equations. *MCMDS, Mathematical and Computer Modelling of Dynamical Systems*, 17(4):395–422, 2011.

[16] H. C. Elma and Q. Liao. Reduced basis collocation methods for partial differential equations with random coefficients. *SIAM/ASA J. Uncertainty Quantification*, 1(1):192–217, 2013.

[17] O. Farle, V. Hill, P. Ingelström, and R. Dyczij-Edlinger. Multi-parameter polynomial order reduction of linear finite element models. *Math. Comput. Model. Dyn. Syst.*, 14(5):421–434, 2008.

[18] L. Feng and P. Benner. A robust algorithm for parametric model order reduction based on implicit moment matching. *PAMM Proc. Appl. Math. Mech.*, 7:1021501–1021502, 2008.

[19] L. Feng, P. Benner, and A. C. Antoulas. An a posteriori error bound for reduced order modeling of micro- and nano-electrical (-mechanical) systems. SCEE 2014, abstract accepted, 2014.

[20] G. S. Fishman. *Monte Carlo: Concepts, Algorithms and Applications*. Springer Series in Operations Research and Financial. Springer, 1996.

[21] D. Galbally, K. Fidkowski, K. Willcox, and O. Ghattas. Non-linear model reduction for uncertainty quantification in large-scale inverse problems. *Int. J. Numer. Meth. Engng*, 81(12):1581–1608, 2010.

[22] S. Gugercin, A. C. Antoulas, and C. Beattie. $\mathcal{H}_2$ model reduction for large-scale dynamical systems. *SIAM J. Matrix Anal. Appl.*, 30(2):609–638, 2008.

[23] B. Haasdonk and M. Ohlberger. Reduced basis method for finite volume approximations of parametrized linear evolution equations. *M2AN, Math. Model. Numer. Anal.*, 42(2):277–302, 2008.

[24] B. Haasdonk and M. Ohlberger. Efficient reduced models and a-posteriori error estimation for parametrized dynamical systems by offline/online decomposition. *MCMDS, Mathematical and Computer Modelling of Dynamical Systems*, 17(2):145–161, 2011.

[25] B. Haasdonk, K. Urban, and Wieland B. Reduced basis methods for parametrized partial differential equations with stochastic influences using the Karhunen-Loève expansion. *SIAM Journal on Uncertainty Quantification*, 1:79–105, 2013.

[26] D. J. Knezevic and A. T. Patera. A certified reduced basis method for the Fokker-Planck equation of dilute polymeric fluids: FENE dumbbells in extensional flow. *SIAM Journal of Scientific Computing*, 32(2):793–817, 2010.

[27] Y. N. Lazarev, P. V. Petrov, and D. M. Tartakovsky. Interface dynamics in randomly heterogeneous porous media. *Advances in Water Resources*, 28(4), 2005.

[28] B. S. Lazarov, M. Schevenels, and O. Sigmund. Topology optimization considering material and geometric uncertainties using stochastic collocation methods. *Structural and Multidisciplinary Optimization*, 46(4):597–612, 2012.

[29] J. Li and D. Xiu. Evaluation of failure probability via surrogate models. *J. Comput. Physics*, 229:8966–8980, 2010.

[30] Y. T. Li, Z. Bai, Y. Su, and X. Zeng. Parameterized model order reduction via a two-directional Arnoldi process. In *Proceedings of the 2007 IEEE/ACM international conference on Computer-aided design*, pages 868–873. IEEE Press Piscataway, NJ, USA, 2007.

[31] Y. Liu, L. Pileggi, and A. Strojwas. Model order reduction of RC(L) interconnect including variational analysis. In *Proc. Design Automation Conference*, pages 201–206, 1999.

[32] A. Loeven and H. Bijl. Airfoil analysis with uncertain geometry using the probabilistic collocation method. In *PAPERS- AMERICAN INSTITUTE OF AERONAUTICS AND ASTRONAUTICS*, volume 7, pages 4412–4422, 2008.

[33] `http://www.magwel.com/`.

[34] O. P. Le Maître and O. M. Knio. *Spectral methods for uncertainty quantification, with applications to computational fluid dynamics*. Springer Science+Business Media B.V., Dordrecht (NL), 2010.

[35] N. Mi, S. X.-D. Tan, P. Liu, J.Cui, Y. Cai, and X. Hong. Stochastic extended Krylov subspace method for variational analysis of on-chip power grid networks. In *Proceedings of the 2007 IEEE/ACM International Conference on Computer-aided Design*, ICCAD '07, pages 48–53. IEEE Press, 2007.

[36] S. P. Mohanty and E. Kougianos. Incorporating manufacturing process variation awareness in fast design optimization of nanoscale CMOS VCOs. *IEEE Trans. on Semiconductor. Manuf.*, 27(1):22–31, 2014.

[37] M. Paffrath and U. Wever. Adapted polynomial chaos expansion for failure detection. *J. of Comput. Physics*, 226:263–281, 2007.

[38] M. Paffrath and U. Wever. Stochastic integration methods: comparison and application to reliability analysis. In *Proceedings of ASME Turbo Expo 2012, Copenhagen (Denmark)*, 2012.

[39] H. Panzer, J. Mohring, R. Eid, and B. Lohmann. Parametric model order reduction by matrix interpolation. *at-Automatisierungstechnik*, 58(8):475–484, 2010.

[40] R. Pulch. Polynomial chaos for the computation of failure probabilities in periodic problems. In J. Roos and L. Costa, editors, *Scientific Computing in Electrical Engineering SCEE 2008*, volume 14 of *Mathematics in Industry*, pages 191–198. Springer, 2010.

[41] R. Pulch and J. ter Maten. Stochastic Galerkin methods and model order reduction for linear dynamical systems. Preprint AMNA 28, Bergische Universität Wuppertal, 2013.

[42] R. Pulch, J. ter Maten, and F. Augustin. Sensitivity analysis and model order reduction for random linear dynamical systems. CASA-Report 15, Eindhoven University of Technology, 2013.

[43] R. Pulch, J. ter Maten, and F. Augustin. Sensitivity analysis of linear dynamical systems in uncertainty quantification. *PAMM Proc. Appl. Math. Mech.*, 13:507–508, 2013.

[44] M. Sobol´. Sensitivity analysis for nonlinear mathematical models. *Matem. Modelirovanie*, 2-1:112–118 (in Russian), 1990. MMCE - Mathematical Modeling and Computational Experiment, 1993, vol. 1-4, p. 407–414 (in English).

[45] K. K. Stavrakakis. *Model order reduction methods for parameterized systems in electromagnetic field simulations*. PhD thesis, TU Darmstadt, Germany, 2012.

[46] K. K. Stavrakakis, T. Wittig, W. Ackermann, and T. Weiland. Parametric model order reduction by neighbouring subspaces. In B. Michielsen and J.-R. Poirier, editors, *Scientific Computing in Electrical Engineering SCEE 2010*, volume 16 of *Mathematics in Industry*, pages 443–451. Springer, 2012.

[47] P. S. Sumant, H. Wu, A. C. Cangellaris, and N. R. Aluru. A sparse grid based collocation method for model order reduction of finite element approximations of passive electromagnetic devices under uncertainty. In *Microwave Symposium Digest (MTT), 2010 IEEE MTT-S International*, pages 1652–1655. IEEE, 2010.

[48] D. M. Tartakovsky and D. Xiu. Stochastic analysis of transport in tubes with rough walls. *J. of Comp. Phys.*, 217(1):248–259, 2006.

[49] E. J. W. ter Maten, R. Pulch, W. H. A. Schilders, and H. H. J. M. Janssen. Efficient calculation of uncertainty quantification. In M. Fontes, M. Günther, and N. Marheineke, editors, *Progress in Industrial Mathematics at ECMI 2012*, volume 19 of *Mathematics in Industry*, pages 361–370. Springer, 2014.

[50] S. Volkwein. *Proper Orthogonal Decomposition: Theory and Reduced-Order Modelling. Lecture Notes. Universitat Konstanz*, 2013.

[51] S. Waldherr and B. Haasdonk. Efficient parametric analysis of the chemical master equation through model order reduction. *BMC Systems Biology*, 6:81, 2012.

[52] D. Xiu. *Numerical methods for stochastic computations - A spectral method approach*. Princeton Univ. Press, 2010.

[53] D. Xiu and D. M. Tartakovsky. Numerical methods for differential equations in random domains. *SIAM J. Sci. Comput.*, 28(3):1167–1185, 2006.

[54] Y. Zou, Y. Cai, Q. Zhou, X. Hong, S. X.-D. Tan, and L. Kang. Practical implementation of stochastic parameterized model order reduction via Hermite polynomial chaos. In *Proceedings of the 2007 Asia and South Pacific Design Automation Conference*, ASP-DAC '07, pages 367–372. IEEE Computer Society, 2007.