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On the guaranteed accuracy of Polynomial Chaos Expansions

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***Abstract*— This paper is concerned with the efficient simulation of stochastic nonlinear dynamical systems. A technique based on Polynomial Chaos Expansion (PCE) theory is used, in order to estimate the time evolution of the stochastic properties of the variables of interest. In PCE, each considered random variable is approximated by a truncated series of orthogonal polynomials, whose coefficients are identified by using the data collected in a relatively low number of numerical simulations. Then, the first and second order moments of the variables of interest, as well as an estimate of their probability density functions, can be efficiently recovered from the polynomial expansions. A least-squares identification approach is used here to identify the expansion's coefficients, and, in the framework of Set Membership identification theory, the issue of evaluating the guaranteed accuracy of the obtained PCE is tackled. As an example, the approach is tested on a nonlinear electric circuit.**

I. Introduction

The need to efficiently simulate stochastic models is common to many science and engineering problems. In these models, uncertainty and disturbances are usually taken into account by a vector of random variables $\boldsymbol{\kappa} \in \mathbb{R}^{n_\kappa}$. The typical technique employed to simulate a stochastic model is the well-known Monte Carlo (MC) approach, which basically consists in 1) drawing a large number M of samples of $\boldsymbol{\kappa}$, according to its distribution, 2) performing M simulations of the model by using the extracted values of the input random variables, 3) analyzing the statistics of the results. The MC method is able to give reliable estimates of the statistics of the variables of interest, $v \in \mathbb{R}^{n_v}(t)$, provided that the value of M is large enough. However, in some cases the use of the MC approach can be computationally prohibitive. Polynomial Chaos Expansions (PCEs) (see e.g. [1], [2], [3] [4]) can reduce significantly the computational effort required to simulate a stochastic system, by conceptually replacing the mapping between $\boldsymbol{\kappa}$ and $v(t)$ with a function $\hat{v}(t, \boldsymbol{\kappa})$, in the form of a truncated series of orthogonal polynomials. The statistical moments of $\hat{v}(t, \boldsymbol{\kappa})$ can be easily computed from the expansion's coefficients, and the evaluation time of PCEs is typically orders of magnitude shorter than integrating the system model, so that computational advantages can be obtained by using a PCE, instead of the system model, in step 2) of the above-mentioned MC procedure. PCEs have been used in a number of different areas and, more recently, also in the field of systems and control (see [4] for an overview). In one possible approach, the coefficients of the PCE are identified from the data $v(t, \tilde{\boldsymbol{\kappa}}_{(r)})$ collected through a finite number of initial simulations of the model, corresponding to some values $\tilde{\boldsymbol{\kappa}}_{(r)}$, $r = 1, \ldots, \nu$ of $\boldsymbol{\kappa}$.

In this paper, we study the use of Polynomial Chaos for the simulation of general nonlinear, continuous time stochastic models, and we use a least-squares approach to identify the PCE's coefficients. Then, we consider the issue of evaluating a guaranteed worst-case error between the obtained PCE expansion $\hat{v}(t, \boldsymbol{\kappa})$ and the actual random variable $v(t, \boldsymbol{\kappa})$. In order to tackle this problem, we derive a worst-case bound on the approximation error between the obtained PCE and the variable to be estimated, in the framework of Set Membership (SM) function identification theory. The validity of this bound is illustrated through an example related to a nonlinear electric circuit.

II. Problem Settings

A. Notation and basic definitions

Let $(\Omega, \mathcal{F}, P)$ be a probability space, where Ω is the set of elementary events, $\mathcal{F}$ is the $\sigma-$algebra of the events and P is the probability measure. The expectation (or first-order moment) of a given random variable $\kappa : \Omega \to \mathcal{K} \subseteq \mathbb{R}$ is denoted as $E[\kappa] \doteq \int_\Omega \kappa(\omega) dP(\omega) = \int_\mathcal{K} \kappa dF_\kappa$, where $F_\kappa(k) \doteq P\{\kappa < k\}$ is the probability distribution function of κ over $\mathcal{K}$. The related probability density function (p.d.f.) of κ, if it exists, is given by dF_κ/dk. The variance (or second-order moment) of κ is indicated as $\mathrm{Var}(\kappa) \doteq E\left[(\kappa - E[\kappa])^2\right] = \sigma_\kappa^2$, where σ_κ is the standard deviation of κ. The L_p norm of κ, $0 < p < \infty$, is defined as $\|\kappa\|_p \doteq E\left[|\kappa(\omega)|^p\right]^{1/p}$ and the L_∞ norm is $\|\kappa\|_\infty \doteq \operatorname{ess\,sup}_\Omega |\kappa(\omega)|$, where $|\cdot|$ denotes the absolute value. The Hilbert space $\mathcal{L}^2(\Omega, \mathcal{F}, P)$ is the space of all random variables κ such that $\|\kappa\|_2 < \infty$, and $K \subset \mathcal{L}^2(\Omega, \mathcal{F}, P)$ is a subspace that contains only centered random variables (i.e. $E[\kappa] = 0$). The covariance of two random variables κ_1, κ_2 is indicated as $\mathrm{Cov}(\kappa_1, \kappa_2) \doteq E[(\kappa_1 - E[\kappa_1])(\kappa_2 - E[\kappa_2])]$, and it defines an inner product $\langle \kappa_1, \kappa_2 \rangle \doteq \mathrm{Cov}(\kappa_1, \kappa_2)$ over K, with $\|\kappa\|_2^2 = \langle \kappa, \kappa \rangle$. A vector of n_κ random variables κ_i, $i = 1, \ldots, n_\kappa$ is indicated as $\boldsymbol{\kappa} = [\kappa_1, \ldots, \kappa_{n_\kappa}]^T$, where ^{T} is the vector transpose operation. The n_κ-dimensional multi-index of order l, $\boldsymbol{\alpha}_{n_\kappa}^l$, is the

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set of all possible vectors of integers $\boldsymbol{\alpha}_{n_\kappa} = [\alpha_1, \ldots, \alpha_{n_\kappa}]$ defined as $\boldsymbol{\alpha}^l_{n_\kappa} \doteq \left\{ \boldsymbol{\alpha}_{n_\kappa} : \sum_{i=1}^{n_\kappa} \alpha_i = l \right\}$. Given a basis of mono-variate polynomials $\Phi^{(q)}(\kappa)$ of degree $q = 0, \ldots, \infty$, a vector $\boldsymbol{\kappa}$ of random variables and a vector of indices $\boldsymbol{\alpha}_{n_\kappa} \in \boldsymbol{\alpha}^l_{n_\kappa}$, the corresponding multi-variate polynomial $\Phi_{\boldsymbol{\alpha}_{n_\kappa}}$ is defined as $\Phi_{\boldsymbol{\alpha}_{n_\kappa}} \doteq \prod_{i=1}^{n_\kappa} \Phi^{(\alpha_i)}(\kappa_i)$.

B. Polynomial chaos expansions and probabilistic collocation

Consider a time-invariant system in state-space form:

$$\begin{aligned} \dot{x}(t) &= f\left(x(t), u(t), w(t), \theta\right) \\ v(t) &= h\left(x(t), u(t), w(t), \theta\right) \end{aligned} \tag{1}$$

where $t \in \mathbb{R}$ is the time variable, $x(t) \in \mathbb{R}^{n_x}$ is the system state, $u(t) \in \mathbb{R}^{n_u}$ is a known input, $w(t) \in \mathbb{R}^{n_w}$ is an unknown external input, $\theta \in \mathbb{R}^{n_\theta}$ is an unknown parameter vector, finally $v(t) \in \mathbb{R}^{n_v}$ is a variable of interest. $w(t)$ and θ are assumed to have stochastic nature, in a sense that will be better detailed afterwards. The aim of this paper is to devise a computationally efficient technique to approximate the first and second order moments and the p.d.f. of $v(t)$ at a finite number $N+1$ of time instants t_i, $i = 0, \ldots, N$ in the interval between an initial time $t_0 = 0$ and a finite time $t_N = T$, starting from (possibly random) initial conditions $x(t_0, \theta)$, by using the model (1). We consider the following assumptions:

Assumption 1: (Stochastic model and input random variables) The parameter θ and the unknown input $w(t)$, $t \in [t_0, t_N]$ in (1) can be expressed as functions of a n_κ-dimensional vector $\boldsymbol{\kappa} \in K^{n_\kappa}$ of independent random variables κ_i such that $\kappa_i \in K \subset \mathcal{L}^2(\Omega, \mathcal{F}, P)$, $i = 1, \ldots, n_\kappa$, all with the same probability distribution F_κ, which is known. The variables $\boldsymbol{\kappa}$ are named "input random variables". ■

Assumption 2: (Existence and computation of the solutions) It is assumed that functions $f : \mathbb{R}^{n_x} \times \mathbb{R}^{n_u} \times \mathbb{R}^{n_w} \times \mathbb{R}^{n_\theta} \to \mathbb{R}^{n_x}$, $h : \mathbb{R}^{n_x} \times \mathbb{R}^{n_u} \times \mathbb{R}^{n_w} \times \mathbb{R}^{n_\theta} \to \mathbb{R}^{n_v}$, the random variables $\theta(\boldsymbol{\kappa})$, $w(t, \boldsymbol{\kappa})$, $t \in [t_0, t_N]$ and the time interval $[t_0, t_N]$ are such that a solution of the dynamical equations (1) exists, it is finite and unique for any admissible value of $\boldsymbol{\kappa}$, and it can be numerically or analytically computed. ■

Clearly, under Assumptions 1-2, at each time instant $t_i, i = 0, \ldots, N$, each one of the variables of interest $v_j(t_i)$, $j = 1, \ldots, n_v$ is a random variable $v_j(t_i, \boldsymbol{\kappa})$. We consider also the following assumption:

Assumption 3: (Finiteness of variance of $v(t_i, \boldsymbol{\kappa})$) The model equations (1) are such that, for all of the considered time instants $t_0, \ldots, t_N$, each one of the variables of interest has finite variance:

$$v_j(t_i, \boldsymbol{\kappa}) \in \mathcal{L}^2(\Omega, \mathcal{F}, P),\ \forall j = 1, \ldots, n_v,\ \forall i = 0, \ldots, N \tag{2}$$

■

Assumptions 1-3 are typically satisfied in practical applications.

The problem of simulating a stochastic system may be very complex and the main technique employed so far in engineering applications is the well-known Monte Carlo (MC) approach. MC simulations are used for many problems, however the required computational times may be prohibitive in some cases, e.g. when the system's model is complex and its simulation requires a significant amount of time. Polynomial Chaos Expansion techniques (see e.g. [1],[2],[3],[5]) are able to significantly reduce such a computational load, by replacing the simulation of the dynamical model with the evaluation of a static function. For a given random variable $\kappa \in K \subset \mathcal{L}^2(\Omega, \mathcal{F}, P)$, with probability distribution F_κ, consider a set of multi-variate polynomials $\Phi_{\boldsymbol{\alpha}_{n_\kappa}}(\boldsymbol{\kappa})$, which are orthogonal with respect to the inner product in K, i.e. for any two vectors of indices $\boldsymbol{\alpha}_{n_\kappa,k}$, $\boldsymbol{\alpha}_{n_\kappa,j}$ it holds:

$$\langle \Phi_{\boldsymbol{\alpha}_{n_\kappa,k}}, \Phi_{\boldsymbol{\alpha}_{n_\kappa,j}} \rangle = E\left[\Phi^2_{\boldsymbol{\alpha}_{n_\kappa,k}}\right] \delta_{kj}, \tag{3}$$

where $\delta_{kj} = 1$ if $k = j$ and 0 in any other case. For a given vector of indices $\boldsymbol{\alpha}_{n_\kappa,k} \doteq [\alpha_{k,1}, \ldots \alpha_{k,n_\kappa}]^T$, the corresponding orthogonal multi-variate polynomial $\Phi_{\boldsymbol{\alpha}_{n_\kappa,k}}(\boldsymbol{\kappa})$ can be constructed, as recalled in Section II-A, by starting from a basis of mono-variate polynomials $\Phi^{(q)}(\kappa)$, $\Phi^{(q)} : \mathbb{R} \to \mathbb{R}$ of degree $q = 0, \ldots, \infty$. Now, let Assumptions 1-3 hold, and consider a random variable $v_j(t_i, \boldsymbol{\kappa}) \in \mathbb{R}$, which is a function of the underlying vector $\boldsymbol{\kappa}$ of input random variables. Then, we have that [2]:

$$v_j(t_i, \boldsymbol{\kappa}) = \sum_{k=0}^{\infty} a_{j,i,k} \Phi_{\boldsymbol{\alpha}_{n_\kappa,k}}(\boldsymbol{\kappa}). \tag{4}$$

In (4), all of the multi-variate polynomials computed by considering $\forall \boldsymbol{\alpha}_{n_\kappa} \in \boldsymbol{\alpha}^l_{n_\kappa}$, $\forall l \in \mathbb{N}$ are used. The series (4) has been shown to converge exponentially as the order l of the polynomial basis increases [3]. For practical reasons, the series is truncated by tolerating some approximation error:

$$\hat{v}_j(t_i, \boldsymbol{\kappa}) \doteq \sum_{k=0}^{L-1} a_{j,i,k} \Phi_{\boldsymbol{\alpha}_{n_\kappa,k}}(\boldsymbol{\kappa}) = \boldsymbol{a}^T_{j,i} \boldsymbol{\Phi}(\boldsymbol{\kappa}), \tag{5}$$

where $\boldsymbol{a}_{j,i} = [a_{j,i,0}, \ldots, a_{j,i,L-1}]^T$ and $\boldsymbol{\Phi}(\boldsymbol{\kappa}) = [\Phi_{\boldsymbol{\alpha}_{n_\kappa,0}}(\boldsymbol{\kappa}), \ldots, \Phi_{\boldsymbol{\alpha}_{n_\kappa,L-1}}(\boldsymbol{\kappa})]^T$ are, respectively, the vectors of the PCE's coefficients and of the bases computed at $\boldsymbol{\kappa}$. The function $\hat{v}_j(t_i, \boldsymbol{\kappa}) \approx v_j(t_i, \boldsymbol{\kappa})$ is the PCE of the variable $v_j(t_i, \boldsymbol{\kappa})$. For given number n_κ of input random variables and given maximal order l of the multi-variate polynomials, the total number L of terms is computed as:

$$L = \frac{(n_\kappa + l)!}{n_\kappa!\, l!} \tag{6}$$

An example of the multi-variate polynomials corresponding to $l = 2$, $n_\kappa = 3$ is shown in Table I. It can be clearly noted that the number of terms in the series (5) grows rapidly with n_κ and l. The term polynomial chaos for the expansion (4) was introduced in [1], where $\boldsymbol{\kappa}$ was assumed to be Gaussian and the corresponding polynomials are the

TABLE I

EXAMPLE OF MULTI-VARIATE POLYNOMIALS USED IN POLYNOMIAL CHAOS, CORRESPONDING TO $l = 2$, $n_\kappa = 3$.

Order	Multi-index	Multi-variate Polynomial
0	$\boldsymbol{\alpha}_{n_\kappa,0} = [0,0,0]$	$\Phi_{\boldsymbol{\alpha}_{n_\kappa,0}}(\boldsymbol{\kappa}) = 1$
1	$\boldsymbol{\alpha}_{n_\kappa,1} = [1,0,0]$	$\Phi_{\boldsymbol{\alpha}_{n_\kappa,1}}(\boldsymbol{\kappa}) = \Phi^{(1)}(\kappa_1)$
1	$\boldsymbol{\alpha}_{n_\kappa,2} = [0,1,0]$	$\Phi_{\boldsymbol{\alpha}_{n_\kappa,2}}(\boldsymbol{\kappa}) = \Phi^{(1)}(\kappa_2)$
1	$\boldsymbol{\alpha}_{n_\kappa,3} = [0,0,1]$	$\Phi_{\boldsymbol{\alpha}_{n_\kappa,3}}(\boldsymbol{\kappa}) = \Phi^{(1)}(\kappa_3)$
2	$\boldsymbol{\alpha}_{n_\kappa,4} = [2,0,0]$	$\Phi_{\boldsymbol{\alpha}_{n_\kappa,4}}(\boldsymbol{\kappa}) = \Phi^{(2)}(\kappa_1)$
2	$\boldsymbol{\alpha}_{n_\kappa,5} = [0,2,0]$	$\Phi_{\boldsymbol{\alpha}_{n_\kappa,5}}(\boldsymbol{\kappa}) = \Phi^{(2)}(\kappa_2)$
2	$\boldsymbol{\alpha}_{n_\kappa,6} = [0,0,2]$	$\Phi_{\boldsymbol{\alpha}_{n_\kappa,6}}(\boldsymbol{\kappa}) = \Phi^{(2)}(\kappa_3)$
2	$\boldsymbol{\alpha}_{n_\kappa,7} = [1,1,0]$	$\Phi_{\boldsymbol{\alpha}_{n_\kappa,7}}(\boldsymbol{\kappa}) = \Phi^{(1)}(\kappa_1)\Phi^{(1)}(\kappa_2)$
2	$\boldsymbol{\alpha}_{n_\kappa,8} = [1,0,1]$	$\Phi_{\boldsymbol{\alpha}_{n_\kappa,8}}(\boldsymbol{\kappa}) = \Phi^{(1)}(\kappa_1)\Phi^{(1)}(\kappa_3)$
2	$\boldsymbol{\alpha}_{n_\kappa,9} = [0,1,1]$	$\Phi_{\boldsymbol{\alpha}_{n_\kappa,9}}(\boldsymbol{\kappa}) = \Phi^{(1)}(\kappa_2)\Phi^{(1)}(\kappa_3)$

Hermite ones. Generalization to other types of continuous and discrete distributions can be achieved via the Askey scheme [5], leading to the so-called generalized polynomial chaos. Table II shows the suitable orthogonal polynomials for different kinds of input random variables. By applying

TABLE II

ORTHOGONAL POLYNOMIALS FOR DIFFERENT KINDS OF PROBABILITY MEASURE.

Random variable	Polynomial basis
Gaussian	Hermite
Uniform	Legendre
Gamma	Laguerre
Beta	Jacobi

the orthogonality property (3), it is easy to show that the first and second order moments of the random variable $\hat{v}_j(t_i, \boldsymbol{\kappa})$ can be computed directly from the coefficients of its PCE, as follows:

$$E\left[\hat{v}_j(t_i, \boldsymbol{\kappa})\right] = a_{j,i,0} \tag{7}$$

$$\mathrm{Var}\left(\hat{v}_j(t_i, \boldsymbol{\kappa})\right) = \sum_{k=1}^{L-1} a_{j,i,k}^2 E\left[\Phi_{\boldsymbol{\alpha}_{n_\kappa,k}}(\boldsymbol{\kappa})^2\right] \tag{8}$$

where $a_{j,i,0}$ is the coefficient of the polynomial of order $l = 0$ (i.e. $\Phi_{\boldsymbol{\alpha}_{n_\kappa,0}} = 1$) in the PCE. Indeed, if the approximation error $v_j(t_i, \boldsymbol{\kappa}) - \hat{v}_j(t_i, \boldsymbol{\kappa})$ is small, equations (7)-(8) provide an estimate of the first and second order moments of $v_j(t_i, \boldsymbol{\kappa})$ with small error, too. Moreover, a Monte Carlo approach can be used to estimate the p.d.f. of $\hat{v}_j(t_i, \boldsymbol{\kappa})$ (and, hence, of $v_j(t_i, \boldsymbol{\kappa})$) once the coefficients of its PCE are known, according to the following algorithm:

Algorithm 1: (Polynomial Chaos Monte Carlo simulations)

1) extract M samples $\tilde{\boldsymbol{\kappa}}_{(r)}$, $r = 1, \ldots, M$ of $\boldsymbol{\kappa}$;
2) for each sample, compute the corresponding values of $\hat{v}_j(t_i, \boldsymbol{\kappa}_{(r)})$, $i = 0, \ldots, N$, $j = 1, \ldots, n_v$, $r = 1, \ldots, M$ by evaluating the PCEs (5);
3) analyze the statistics of the collected data.

■

A critical point in the use of PCE for the simulation of stochastic systems is the computation of the expansion's coefficients. A possible approach is known as Probabilistic Collocation Method (PCM, see e.g. [4]) and it basically relies on the identification of the PCEs' coefficients from a finite number of simulation data. In this paper, we consider the PCM for the computation of the PCEs' coefficients, since it appears to be a viable approach for large-scale, complex dynamical systems, and we focus our attention on the particular issue of the evaluation of the accuracy of the PCEs $\hat{v}_j(t_i, \boldsymbol{\kappa})$ (5) with respect to the actual (unknown) functions $v_j(t_i, \boldsymbol{\kappa})$. In the next Section, in order to cope with this problem, we consider a least-square approach to identify the PCEs' parameters, and we present a procedure to derive a guaranteed worst case bound on the error between each one of functions $v_j(t_i, \boldsymbol{\kappa})$ and the corresponding PCE. Such an accuracy bound is derived in the framework of Set Membership function identification theory.

III. A BOUND ON THE GUARANTEED ACCURACY OF POLYNOMIAL CHAOS EXPANSIONS

A. Identification algorithm

The algorithm we consider to identify the PCEs' coefficients is:

Algorithm 2: (PCE identification via least-squares)

1) select a finite number ν of values of the input random variables $\tilde{\boldsymbol{\kappa}}_{(r)}$, $r = 1, \ldots, \nu$;
2) carry out ν simulations of the system (1), each one corresponding to one of the selected samples $\tilde{\boldsymbol{\kappa}}_{(r)}$;
3) collect the obtained values of the variables of interest, indicated as $v_j(t_i, \tilde{\boldsymbol{\kappa}}_{(r)})$, $j = 1, \ldots, n_v$, $i = 0, \ldots, N$, $r = 1, \ldots, \nu$;
4) for each one of the variables of interest $v_j(t_i, \boldsymbol{\kappa})$, select a (high) maximal order l for the respective PCE $\hat{v}_j(t_i, \boldsymbol{\kappa})$ (5) and compute the corresponding values of $\boldsymbol{\Phi}(\tilde{\boldsymbol{\kappa}}_{(r)})$, $r = 1, \ldots, \nu$. Then, solve the following least-squares problem to compute the coefficients $\boldsymbol{a}_{j,i}^*$ of $\hat{v}_j(t_i, \boldsymbol{\kappa})$:

$$\left(\boldsymbol{a}_{j,i}^*, \mu_{j,i}^*\right) = \arg \min_{\boldsymbol{a} \in \mathbb{R}^L,\, \mu \in \mathbb{R}} \mu \tag{9a}$$

subject to

$$\left(\sum_{r=1}^{\nu} \left| v_j(t_i, \tilde{\boldsymbol{\kappa}}_{(r)}) - \boldsymbol{a}^T \boldsymbol{\Phi}(\tilde{\boldsymbol{\kappa}}_{(r)}) \right|^2\right) - \mu \leq 0 \tag{9b}$$

■

We denote with $\hat{v}_j^*(t_i, \boldsymbol{\kappa})$ the PCE obtained by using the optimal coefficients $\boldsymbol{a}_{j,i}^*$ computed at step 4) of Algorithm 2.

Remark 1: The choice of the values $\tilde{\boldsymbol{\kappa}}_{(r)}$ in step 1) of Algorithm 2 is an important aspect. Typically, the value $\boldsymbol{\kappa} = E[\boldsymbol{\kappa}]$ should be included among the chosen values of $\tilde{\boldsymbol{\kappa}}_{(\boldsymbol{r})}$. As regards the other $\nu - 1$ values, good choices are a uniform gridding in a bounded subset of the support of $\tilde{\boldsymbol{\kappa}}$, in which $\boldsymbol{\kappa}$ lies with reasonably high probability (e.g. the interval $\pm 3\sigma$ in the case of centered Gaussian input variable $\tilde{\boldsymbol{\kappa}}$), or also sampling of $\tilde{\boldsymbol{\kappa}}$ according to its probability measure. ■

B. Analysis of PCEs' accuracy: a Set Membership approach

The issue of evaluating the accuracy achieved by an approximating function $\hat{v}_j^*(t_i, \boldsymbol{\kappa}) \approx v_j(t_i, \boldsymbol{\kappa})$ is clearly of high importance. Indeed, Algorithm 2 guarantees that the error between the PCE $\hat{v}_j^*(t_i, \cdot)$ and the actual value of $v_j(t_i, \cdot)$ is bounded by some finite quantity when the data $\tilde{\boldsymbol{\kappa}}_{(r)}$ used for the identification procedure are considered, but it does not give by itself any guarantee on the accuracy *for all possible values* of $\boldsymbol{\kappa}$ (i.e. the value $\mu_{j,i}^*$ is just a lower bound of the largest approximation error that can occur). Here, we propose a worst-case accuracy analysis, based on SM identification theory, which allows us to estimate a worst-case bound $\zeta_{j,i}$, $j = 1, \ldots, n_v$, $i = 0, \ldots, N$ on the error $\Delta_j^*(t_i, \boldsymbol{\kappa})$, defined as:

$$\Delta_j^*(t_i, \boldsymbol{\kappa}) \doteq v_j(t_i, \boldsymbol{\kappa}) - \hat{v}_j^*(t_i, \boldsymbol{\kappa}). \tag{10}$$

Thus, we look for a (possibly tight) bound $\zeta_{j,i}$ such that:

$$\left|\Delta_j^*(t_i, \boldsymbol{\kappa})\right| \leq \zeta_{j,i}, \forall \boldsymbol{\kappa}.$$

In order to derive a finite value for the bound $\zeta_{j,i}$, we restrict our analysis to values of $\boldsymbol{\kappa}$ belonging to a compact set $\mathbb{K} \subset \mathbb{R}^{n_\kappa}$. If $\boldsymbol{\kappa}$ already lies in a bounded or compact set (e.g. for uniformly distributed variables in the interval $[-1, 1]$), then such a set can be considered as the set $\mathbb{K}$. If $\boldsymbol{\kappa}$ belongs to an unbounded domain (e.g. if its components κ_i are centered Gaussian random variables), then the set $\mathbb{K}$ can be chosen as an arbitrarily large compact set, leaving out values of $\boldsymbol{\kappa}$ that can occur with arbitrarily low probability. Furthermore, let us consider the following assumption:

Assumption 4: For each value of $j = 1, \ldots, n_v$ and for each t_i, $i = 0, \ldots, N$, the function $v_j(t_i, \boldsymbol{\kappa})$ is Lipschitz continuous over $\mathbb{K}$. ■

The SM accuracy analysis is based on the prior information on the unknown function $v_j(t_i, \boldsymbol{\kappa})$, which include the knowledge of the exact values of $v_j(t_i, \tilde{\boldsymbol{\kappa}}_{(r)})$, used in Algorithm 2 to identify the coefficients of the PCE $\hat{v}_j^*(t_i, \boldsymbol{\kappa})$, as well as some knowledge on the approximation error $\Delta_j^*(t_i, \boldsymbol{\kappa})$. In particular, the following Proposition establishes the regularity properties of $\Delta_j^*(t_i, \boldsymbol{\kappa})$:

Proposition 1: (Lipschitz continuity of the error function) Let Assumptions 2 and 4 hold. Then for each value of $j = 1, \ldots, n_v$ and for each t_i, $i = 0, \ldots, N$, the approximation error function $\Delta_j^*(t_i, \boldsymbol{\kappa})$ (10) belongs to the set $\mathcal{A}_{j,i}$ of Lipschitz continuous functions over $\mathbb{K}$, with constant $L_{j,i}$:

$$\begin{gathered}\Delta_j^*(t_i, \boldsymbol{\kappa}) \in \mathcal{A}_{j,i} \\ \doteq \{\Delta(\boldsymbol{\kappa}) : |\Delta(\boldsymbol{\kappa}_{(1)}) - \Delta(\boldsymbol{\kappa}_{(2)})| \leq L_{j,i}\|\boldsymbol{\kappa}_{(1)} - \boldsymbol{\kappa}_{(2)}\|_2, \\ \forall \boldsymbol{\kappa}_{(1)}, \boldsymbol{\kappa}_{(2)} \in \mathbb{K}\}\end{gathered} \tag{11}$$

Proof: Due to Assumptions 2 and 4, function $v_j(t_i, \boldsymbol{\kappa})$ is finite and Lipschitz continuous over $\mathbb{K}$. The PCE $\hat{v}_j^*(t_i, \boldsymbol{\kappa})$, being a sum of polynomials, is finite, continuous and differentiable over the compact $\mathbb{K}$. Thus, function $\Delta_j^*(t_i, \boldsymbol{\kappa})$ (10) is finite and continuous over the compact set $\mathbb{K}$, hence Lipschitz continuous over $\mathbb{K}$. ■

The Euclidean norm $\|\cdot\|_2$ has been used in (11) without loss of generality, since the Lipschitz condition holds for any norm, with a suitable finite Lipschitz constant. The Lipschitz constant $L_{j,i}$ can be estimated from data as:

$$\begin{aligned}\hat{L}_{j,i} = \min\{L : |\Delta_j^*(t_i, \tilde{\boldsymbol{\kappa}}_{(a)}) - \Delta_j^*(t_i, \tilde{\boldsymbol{\kappa}}_{(b)}))| \leq \\ L\|\tilde{\boldsymbol{\kappa}}_{(a)} - \tilde{\boldsymbol{\kappa}}_{(b)}\|_2, \forall a, b \in [1, \nu]\}\end{aligned}$$

It can be easily shown that $\lim_{\nu \to \infty} \hat{L}_{j,i} = L_{j,i}$ (see e.g. Theorem 1 in [6]).

By collecting the information given by (11) and by the available values of $\Delta_j^*(t_i, \tilde{\boldsymbol{\kappa}}_{(r)})$, $r = 1, \ldots, \nu$, we can define the Feasible Function Set for the j-th component of $v(t)$ at time t_i:

$$\begin{gathered}FFS_{j,i} \doteq \{\tilde{v}_j(t_i, \boldsymbol{\kappa}) : \tilde{v}_j(t_i, \boldsymbol{\kappa}) = \hat{v}_j^*(t_i, \boldsymbol{\kappa}) + \Delta_j(t_i, \boldsymbol{\kappa}), \\ \Delta_j(t_i, \boldsymbol{\kappa}) \in \mathcal{A}_{j,i}, \Delta_j(t_i, \tilde{\boldsymbol{\kappa}}_{(r)}) = \Delta_j^*(t_i, \tilde{\boldsymbol{\kappa}}_{(r)}), \forall r \in [1, \nu]\}\end{gathered} \tag{12}$$

In practice, $FFS_{j,i}$ is the set of all functions $\tilde{v}_j(t_i, \boldsymbol{\kappa})$ consistent with the available prior information and data related to $v_j(t_i, \boldsymbol{\kappa})$. Such a prior information is considered validated if at least an estimate consistent with it exists, i.e. if $FFS_{j,i}$ is not empty, see also [7]. The following result shows that, by using Algorithm 2, the set $FFS_{j,i}$ is always non-empty.

Proposition 2: (Non-emptiness of the FFS) Let Assumptions 2 and 4 hold, let Algorithm 2 be used and let $\boldsymbol{a}_{j,i}^*$, $\mu_{j,i}^*$ be a solution to problem (9). Then, $FFS_{j,i} \neq \varnothing$. ■

Proof: The least-square problem (9) is obviously always feasible, meaning that there is always a coefficient vector $\boldsymbol{a}_{j,i}^*$ defining the resulting optimal PCE $\hat{v}_j^*(t_i, \boldsymbol{\kappa})$. Then, by construction the exact function $v_j(t_i, \boldsymbol{\kappa})$ is equal to $\hat{v}_j^*(t_i, \boldsymbol{\kappa}) + \Delta_j^*(t_i, \boldsymbol{\kappa})$ and, according to Proposition 1, $\Delta_j^*(t_i, \boldsymbol{\kappa})$ belongs to $\mathcal{A}_{j,i}$, moreover its values at the points $\tilde{\boldsymbol{\kappa}}_{(r)}$ are equal to $\Delta_j^*(t_i, \tilde{\boldsymbol{\kappa}}_{(r)})$, $r = 1, \ldots, \nu$. Thus, the unknown function $v_j(t_i, \boldsymbol{\kappa})$ belongs to $FFS_{j,i}$, which results to be non-empty. ■

Now, thanks to the fact that $v_j(t_i, \boldsymbol{\kappa})$ belongs to $FFS_{j,i}$, an expression for the bound $\zeta_{j,i}$ can be obtained. Let us define the following functions:

$$\begin{aligned}\overline{\Delta}_{j,i}(\boldsymbol{\kappa}) &\doteq \min_{r=1,\ldots,\nu} \left(\Delta_j^*(t_i, \tilde{\boldsymbol{\kappa}}_{(r)}) + L_{j,i}\|\boldsymbol{\kappa} - \tilde{\boldsymbol{\kappa}}_{(r)}\|_2\right) \\ \underline{\Delta}_{j,i}(\boldsymbol{\kappa}) &\doteq \max_{k=1,\ldots,\nu} \left(\Delta_j^*(t_i, \tilde{\boldsymbol{\kappa}}_{(r)}) - L_{j,i}\|\boldsymbol{\kappa} - \tilde{\boldsymbol{\kappa}}_{(r)}\|_2\right)\end{aligned}. \tag{13}$$

which have been shown to be tightest upper and lower bounds, respectively, of the absolute value of the error $\Delta_j^*(t_i, \boldsymbol{\kappa})$ (see e.g. [8]). Then, the following result hold.

Theorem 1: Let Assumptions 1-4 hold, let Algorithm 2 be used and let $\boldsymbol{a}_{j,i}^*$, $\mu_{j,i}^*$ be a solution to problem (9). Then,

the approximation error of the resulting PCE is bounded as:

$$\begin{array}{l} \forall \boldsymbol{\kappa} \in \mathbb{K},\, \forall j \in [1, n_v],\, \forall i \in [0, N] \\ |\Delta_j^*(t_i, \boldsymbol{\kappa})| \leq \zeta_{j,i} \\ \zeta_{j,i} \doteq \sup_{\boldsymbol{\kappa} \in \mathbb{K}} \max\{\left|\overline{\Delta}_{j,i}(\boldsymbol{\kappa})\right|,\, \left|\underline{\Delta}_{j,i}(\boldsymbol{\kappa})\right|\}. \end{array} \tag{14}$$

Proof: See [9]. ■

The bound $\zeta_{j,i}$ given by (14) can be numerically estimated to have an indication on the worst-case error between the PCE $\hat{v}_j^*(t_i, \boldsymbol{\kappa})$ and the exact function $v_j(t_i, \boldsymbol{\kappa})$ (see [10]).

Remark 2: We considered a least-squares approach to identify the PCEs' coefficients just for simplicity. The Set Membership procedure to compute the guaranteed accuracy bounds is general and it does not depend on how the coefficients have been derived. The use of more sophisticated ways to derive the PCEs' coefficients is actually part of future research. ■

IV. Simulation example

We consider an electric LRC circuit, and we are interested in simulating the courses of the output voltage $v_C(t)$ and of the current $i_L(t)$ when a step input voltage $u(t) = 5\,10^{-3}$ V is applied to the circuit, starting from the initial conditions $v_C(0) = i_L(0) = 0$, i.e. $v(t) = [v_1(t),\, v_2(t)]^T = [i_L(t),\, v_C(t)]^T$. The time instants t_i, $i = 0, \ldots, 99$ are chosen as $t_i = i\,T_s$ s, where $T_s = 1.21\,10^{-4}$ s. The system equations are

$$\begin{array}{rcl} \dot{i}_L(t) & = & -\dfrac{1}{L} v_C(t) - \dfrac{R}{L} i_L(t) + \dfrac{1}{L} u(t) \\ \dot{v}_C(t) & = & \dfrac{1}{C} i_L(t). \end{array} \tag{15}$$

The resistance R is assumed to be a random variable $R = R_0(1 + 0.3\,\kappa_1)$, where $R_0 = 3.5\,\Omega$ and κ_1 is a random variable with uniform distribution over $[-1, 1]$. The inductance L and the capacitance C are nonlinear functions of the current $i_L(t)$ and voltage $v_C(t)$, respectively:

$$\begin{array}{l} L(i_L(t)) = 0.5\,\overline{L}\,(1 + \exp(a_1\, i_L(t)^2)) \\ C(v_C(t)) = 0.5\,\overline{C}\,(1 + \exp(a_2\, v_C(t)^2)), \end{array}$$

where $a_1 = -0.5\,10^8$, $a_2 = -0.5\,10^6$. Moreover, the maximal values $\overline{L}$ and $\overline{C}$, achieved when $v_C(t) = i_L(t) = 0$, are equal to $\overline{L} = L_0(1 + 0.2\,\kappa_2)$, $\overline{C} = C_0(1 + 0.2\,\kappa_3)$, where κ_2, κ_3 are also random variables with uniform distribution over $[-1, 1]$. κ_1, κ_2, κ_3 are assumed to be independent. Clearly, the input random variable is $\boldsymbol{\kappa} = [\kappa_1,\, \kappa_2,\, \kappa_3]^T$. According to Table II, the PCE is carried out by using Legendre polynomial. Algorithm 2 has been applied to identify a PCE for the values of $v_C(t_i, \boldsymbol{\kappa})$ and $i_L(t_i, \boldsymbol{\kappa})$ at all the considered time instants. The values of $\tilde{\boldsymbol{\kappa}}_{(r)}$ have been chosen by extracting eight values for each random variable over the interval $[-1, 1]$ according to their probability measure (i.e. uniform) and taking all possible combinations, thus resulting in $\nu = 512$ total values. A maximal order $l = 5$ has been chosen in step 4) of Algorithm 2 for all of the variables of interest, thus resulting in $L = 56$ maximal number of terms in the expansions. The obtained PCEs $\hat{v}_1^*(t_i, \boldsymbol{\kappa}) \approx i_L(t_i, \boldsymbol{\kappa})$ and $\hat{v}_2^*(t_i, \boldsymbol{\kappa}) \approx v_C(t_i, \boldsymbol{\kappa})$ result to be very accurate, as it is shown for example in Fig. 1, where the first-order moments $E[\hat{v}_1^*(t_i, \boldsymbol{\kappa})]$, computed according to (7) (i.e. by simply taking, for each t_i, the coefficients of the polynomial of degree 0 in the PCEs) are compared with the first-order moments computed numerically by averaging over 27000 MC simulations of the model (15). It can be noted that an almost perfect matching exists between the two estimates at all of the considered time instants.

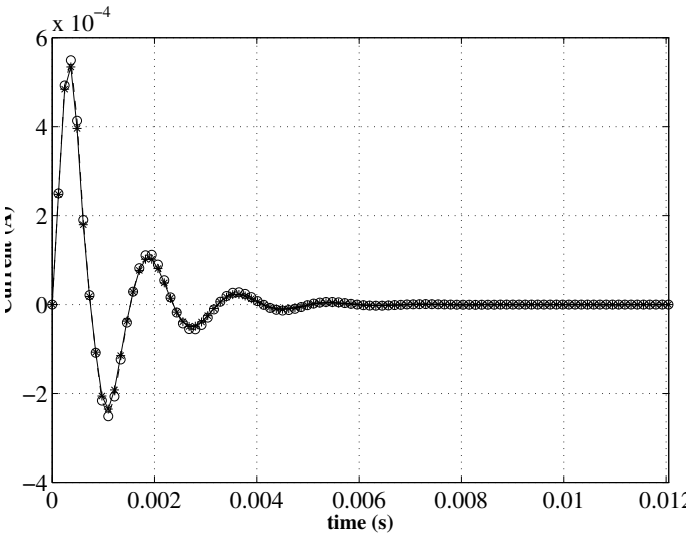

Fig. 1. Simulation example. Mean values at $t = t_i$, $i = 0, \ldots, 99$ of the current $i_L(t)$, obtained either with MC simulations of the model (dashed line with '$\circ$') or with the coefficients of the term of degree 0 in their respective PCEs $\hat{v}_1^*(t_i, \boldsymbol{\kappa})$ (solid line with '$*$').

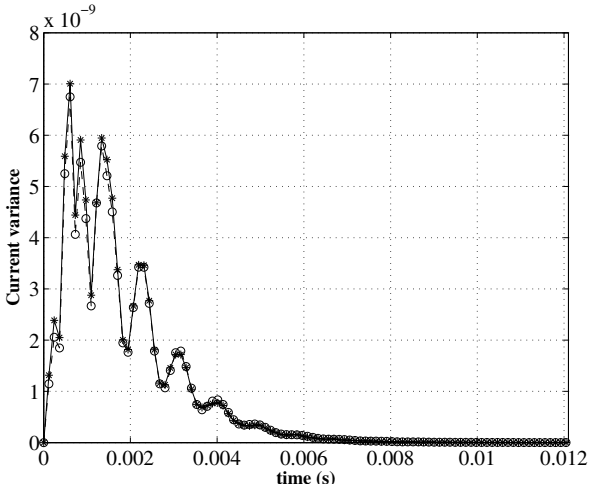

Fig. 2. Simulation example. Variances at $t = t_i$, $i = 0, \ldots, 99$ of the current $i_L(t)$, obtained either with MC simulations of the model (dashed line with '$\circ$') or on the basis of the coefficients of the PCEs $\hat{v}_1^*(t_i, \boldsymbol{\kappa})$ (solid line with '$*$').

A similar good accuracy is achieved with the second order moments (see Fig. 2), again computed either with the relationship (8) or with MC simulations of the system model. Fig. 3 shows the comparison between the p.d.f. of the voltage $v_C(t_{21}, \boldsymbol{\kappa})$ computed with 27000 MC simulations

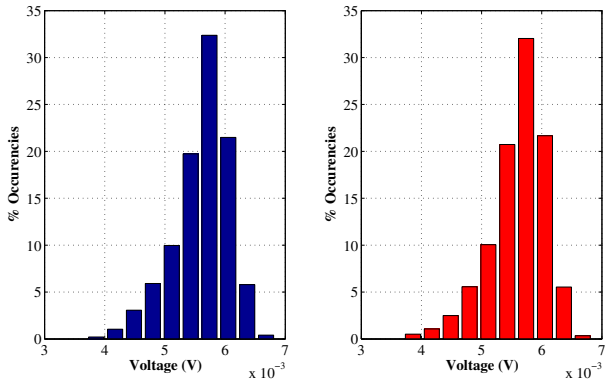

Fig. 3. Simulation example. Comparison between the p.d.f. of variable $v_C(t_{21}, \boldsymbol{\kappa})$ either with 27000 MC simulation with the system model (left) or with 27000 MC evaluations of the PCE $\hat{v}_2^*(t_{21}, \boldsymbol{\kappa})$ (right).

by using either the dynamical model (15) or the related PCE $\hat{v}_2^*(t_{21}, \boldsymbol{\kappa})$. It can be seen that, also for the p.d.f., a good matching is achieved (and the same results have been obtained for all of the considered variables of interest at all time instants), however while the MC simulations with the model equations require about 377 s, the MC simulations with PCE take only 2.7 s (both on a Intel® Core™ 2 Duo processor with 4 GB RAM and MatLab® 2009).

Finally, the guaranteed error bound $\zeta_{1,9}$ has been evaluated, as an example, for the variable $\hat{v}_1^*(t_9, \boldsymbol{\kappa}) \approx i_L(t_9, \boldsymbol{\kappa})$. In particular, a value $\mu_{1,9}^* = 4.08\,10^{-6}$ is obtained and a Lipschitz constant $L_{1,9} = 2.2\,10^{-5}$ has been estimated from data. The resulting estimate of $\zeta_{1,9}$ (14), computed with a dense uniform gridding over $\mathbb{K} = [-1, 1] \times [-1, 1] \times [-1, 1]$, is equal to $1.55\,10^{-5}$. Fig. 4 depicts the errors $\Delta_1^*(t_9, \boldsymbol{\kappa})$ (10)

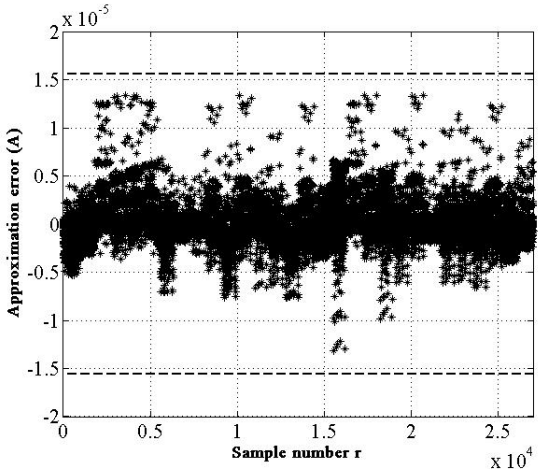

Fig. 4. Simulation example. Approximation errors $\Delta_1^*(t_9, \boldsymbol{\kappa})$ ('$*$') and worst-case bounds $\pm\zeta_{2,9}$ (dashed lines).

obtained in the performed 27000 MC simulations together with the obtained bound $\pm\zeta_{1,9}$, which result to be quite tight.

V. Conclusions

In this paper, we considered a least-squares approach to indentify the coefficients of Polynomial Chaos Expansions (PCEs), starting from a finite number of simulation data. We carried out an analysis of the worst-case error between the PCEs and the corresponding random variables of interest, resulting in guaranteed error bounds that can be used to evaluate the accuracy of the obtained PCE. The features of the proposed approach have been shown on an example concerning a nonlinear electric circuit.

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