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Abstract

We consider periodic problems of autonomous systems of ordinary differential equations or differential algebraic equations. To quantify uncertainties of physical parameters, we introduce random variables in the systems. Phase conditions are required to compute the resulting periodic random process. It follows that the variance of the process depends on the choice of the phase condition. We derive a necessary condition for a random process with a minimal total variance by the calculus of variations. An according numerical method is constructed based on the generalised polynomial chaos. We present numerical simulations of two test examples.

Key words: ordinary differential equation, differential algebraic equation, periodic boundary value problem, oscillator, phase condition, uncertainty quantification, polynomial chaos, calculus of variations

1 Introduction

Mathematical modelling often yields systems of ordinary differential equations (ODEs) or differential algebraic equations (DAEs). We consider periodic boundary value problems of autonomous systems. Hence the corresponding periods are unknown a priori. Since a continuum of periodic solutions exists, we require phase conditions to isolate a solution.

We assume that some physical parameters of the systems exhibit uncertainties. Thus we replace the parameters by random variables with traditional distributions (uniform, Gaussian, etc.). The periodic solution of the system of ODEs

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or DAEs becomes a random process. Since different parameters imply different periods, the solutions of the systems are transformed to the unit interval. Again we need phase conditions to determine a particular random process. However, both the expected value and the variance depend on the choice of the phase condition, although each random process includes the same information. A representation of the random process in the phase space does not yield an adequate alternative.

Some phase conditions may cause a relatively large variance. We determine a random process with a minimal total variance, since this process represents an appropriate quantification of the uncertainties in case of autonomous systems. An according expected value is also specified by this strategy. In the deterministic case, Doedel [2] introduced a phase condition to minimise the distance to a predetermined periodic function. A similar constraint results in the stochastic case, where the a priori unknown expected value is involved. We use the calculus of variations to prove that this phase condition is satisfied by an optimal solution.

The system of ODEs or DAEs with random parameters has to be solved using this phase condition. We apply the generalised polynomial chaos (gPC), see [1,14], to expand the random process as well as the random period. A Galerkin method yields a larger coupled system for the unknown coefficients in the expansion. Numerical techniques based on the gPC have already been applied to forced or autonomous random oscillators in [6,7,9,10] for different tasks. In the situation at hand, the gPC is advantageous, since the expected value of the random process appears as a separate function within the expansion. Furthermore, the approach of the gPC has resolved partial differential equations with random parameters successfully in the previous works [11,12], for example.

The article is organised as follows. We introduce the deterministic model as well as the stochastic model in Sect. 2. The usage of the gPC expansions is outlined. In Sect. 3, we derive the phase condition corresponding to a random process with minimal total variance. We construct the numerical method applying the gPC. Numerical simulations with respect to a system of DAEs and an implicit system of ODEs, which represent mathematical models of electric circuits, are discussed in Sect. 4.

2 Random Oscillators

We discuss autonomous oscillators in this work. In contrast, forced oscillators involve predetermined periodic inputs, which cause a periodic solution.

2.1 Deterministic model

We consider autonomous systems of the form

$$A(\mathbf{p})\mathbf{x}'(t,\mathbf{p}) = \mathbf{f}(\mathbf{x}(t,\mathbf{p}),\mathbf{p}), \tag{1}$$

where the given matrix $A \in \mathbb{R}^{n\times n}$ as well as the right-hand side $\mathbf{f}$ include parameters $\mathbf{p} \in Q$ for some relevant set $Q \subseteq \mathbb{R}^q$. Consequently, the unknown solution $\mathbf{x} : [t_0, t_1] \times Q \to \mathbb{R}^n$ depends on these parameters. If the matrix A is regular, then the system (1) represents implicit ODEs. In contrast, a system of DAEs results in case of a singular matrix A. We assume that the matrix A is either regular or singular for all parameters $\mathbf{p} \in Q$. Moreover, let $\mathbf{x}$ depend continuously on the parameters $\mathbf{p}$.

Since the dynamical system (1) is autonomous, a particular solution $\mathbf{x}$ yields further solutions via the translations

$$\mathbf{y}(t,\mathbf{p}) := \mathbf{x}(t+c,\mathbf{p}) \qquad \text{with } \ c \in \mathbb{R}. \tag{2}$$

We analyse oscillators, i.e., periodic boundary value problems of the system (1). The periodicity condition reads

$$\mathbf{x}(t+T(\mathbf{p}),\mathbf{p}) = \mathbf{x}(t,\mathbf{p}) \tag{3}$$

for all $t \in \mathbb{R}$ and each $\mathbf{p} \in Q$ with the periods $T(\mathbf{p}) > 0$. We note that also the a priori unknown period depends on the parameters.

To achieve a uniform approach for all parameters, we transform the time intervals $[0, T(\mathbf{p})]$ to the unit interval $[0, 1]$. Let

$$\tilde{\mathbf{x}}(s,\mathbf{p}) := \mathbf{x}(sT(\mathbf{p}),\mathbf{p}). \tag{4}$$

The system (1) changes into

$$A(\mathbf{p})\tilde{\mathbf{x}}'(s,\mathbf{p}) = T(\mathbf{p})\mathbf{f}(\tilde{\mathbf{x}}(s,\mathbf{p}),\mathbf{p}). \tag{5}$$

The periodicity $\tilde{\mathbf{x}}(s+1,\mathbf{p}) = \tilde{\mathbf{x}}(s,\mathbf{p})$ for all $s \in \mathbb{R}$ implies the two-point boundary value problem

$$\tilde{\mathbf{x}}(0,\mathbf{p}) = \tilde{\mathbf{x}}(1,\mathbf{p}) \tag{6}$$

for each $\mathbf{p} \in Q$.

The boundary value problem (5),(6) is underdetermined, since the period $T(\mathbf{p})$ is unknown. Furthermore, we require an additional phase condition to identify an isolated solution within the continuum (2). Numerical techniques using phase conditions are well-known in the literature, see [13], for example. Without loss of generality, we choose the first component of the solution $\tilde{\mathbf{x}} = (\tilde{x}_1, \ldots, \tilde{x}_n)^\top$. An example of a phase condition is

$$\tilde{x}_1(0, \mathbf{p}) = \eta(\mathbf{p}) \qquad \text{for each } \mathbf{p} \in Q \tag{7}$$

using $\eta(\mathbf{p}) \in \mathbb{R}$ from the range of this component. A constant choice $\eta(\mathbf{p}) \equiv \eta_0$ is often feasible for all parameters. The constraint (7) represents an additional boundary condition. Another phase condition reads

$$\tilde{x}_1'(0, \mathbf{p}) = 0 \qquad \text{for each } \mathbf{p} \in Q, \tag{8}$$

where a local optimum or a saddle point appears at the boundary $t_0 = s_0 = 0$. If the first component corresponds to an explicit ODE ($\tilde{x}_1' = T f_1$), then the constraint (8) is equivalent to

$$f_1(\tilde{\mathbf{x}}(0, \mathbf{p}), \mathbf{p}) = 0 \qquad \text{for each } \mathbf{p} \in Q$$

due to $T(\mathbf{p}) > 0$. This condition can be added directly to the boundary conditions.

2.2 Stochastic model

Now we assume that the selected parameters $\mathbf{p} \in Q$ include some uncertainties. To achieve a quantification, we replace the parameters by independent random variables

$$\mathbf{p} : \Omega \to Q, \quad \mathbf{p} = (p_1(\omega), \ldots, p_q(\omega))^\top$$

according to a probability space $(\Omega, \mathcal{A}, \mu)$. We select some traditional distribution (Gaussian, uniform, beta, etc.) for each variable p_j. Thus it exists a joint probability density function $\rho : \mathbb{R}^q \to \mathbb{R}$. Moreover, the density function is piecewise continuous for the common distributions.

The expected value of a function $f : \mathbb{R}^q \to \mathbb{R}$, which depends on the parameters, is defined by (provided it exists)

$$\langle f(\mathbf{p}) \rangle := \int_\Omega f(\mathbf{p}(\omega)) \, \mathrm{d}\mu(\omega) = \int_{\mathbb{R}^q} f(\mathbf{p}) \rho(\mathbf{p}) \, \mathrm{d}\mathbf{p}. \tag{9}$$

The expected value yields an inner product on $L^2(\Omega)$, i.e.,

$$\langle f(\mathbf{p}) g(\mathbf{p}) \rangle = \int_{\mathbb{R}^q} f(\mathbf{p}) g(\mathbf{p}) \rho(\mathbf{p}) \, \mathrm{d}\mathbf{p} \tag{10}$$

for functions $f, g \in L^2(\Omega)$ depending on the tuple of parameters. The expected value (9) and the inner product (10) also applies component-wise to vector-valued and matrix-valued functions.

Substituting the parameters of the dynamical system (1) or (5) by random variables changes a deterministic solution into a random process

$$\mathbf{x} : [t_0, t_1] \times \Omega \to \mathbb{R}^n \quad \text{or} \quad \tilde{\mathbf{x}} : [s_0, s_1] \times \Omega \to \mathbb{R}^n,$$

respectively. In the periodic boundary value problem, the period becomes a random variable $T : \Omega \to \mathbb{R}$. For uncertainty quantification, we are interested in key data of the random process and the random period like the expected value and the variance. Nevertheless, more sophisticated quantities may be resolved.

Since the period depends on the random parameters, we transform the domain of dependence $[0, T(\mathbf{p})]$ to the unit interval $[0, 1]$. The choice of a phase condition determines the random process in the unit interval and thus also its expected value and variance. It is obvious to ask for a representation, which is independent of the phase condition. A periodic solution $\mathbf{x}(t, \mathbf{p})$ or $\tilde{\mathbf{x}}(s, \mathbf{p})$, respectively, represents a closed curve in the phase space, i.e.,

$$\Gamma(\mathbf{p}) := \{\mathbf{x}(t, \mathbf{p}) : t \in \mathbb{R}\} = \{\tilde{\mathbf{x}}(s, \mathbf{p}) : s \in \mathbb{R}\} \subset \mathbb{R}^n \quad \text{for each } \mathbf{p}.$$

The closed curve is independent of the phase condition used for the computation of the corresponding solution. The distance of two closed curves can be quantified by the Hausdorff metric, see [8]. However, we obtain only a metric space via this approach. In contrast, we like to apply a Banach space or Hilbert space. Since algebraic operations are missing in the metric space, a definition of an expected value and a variance becomes dubious in the phase space. Hence we analyse the random process within the unit interval $[0, 1]$ and make the best out of this situation by using appropriate phase conditions.

2.3 Polynomial chaos expansions

The generalised polynomial chaos (gPC) provides an expansion of a random process with finite second moments, see [1,3,14]. Since we consider the standardised system (5) with random parameters, let the involved solution $\tilde{\mathbf{x}} = (\tilde{x}_1, \ldots, \tilde{x}_n)^\top$ fulfill the demand

$$\langle \tilde{x}_l(s, \mathbf{p})^2 \rangle < \infty \quad \text{for all } l = 1, \ldots, n$$

and each $s \in \mathbb{R}$. Otherwise, the variance of the random process does not exist. The gPC expansion of the random process reads

$$\tilde{\mathbf{x}}(s, \mathbf{p}) = \sum_{i=0}^{\infty} \mathbf{v}_i(s)\Phi_i(\mathbf{p}), \tag{11}$$

where orthonormal basis polynomials $\Phi_i : \mathbb{R}^q \to \mathbb{R}$ are applied, i.e., it holds $\langle \Phi_i \Phi_j \rangle = \delta_{ij}$ with the Kronecker-delta. For example, the Hermite polynomials and the Legendre polynomials represent the orthogonal system for random parameters with Gaussian distributions and uniform distributions, respectively. The coefficient functions in (11) satisfy the relation

$$\mathbf{v}_i(s) = \langle \tilde{\mathbf{x}}(s, \mathbf{p})\Phi_i(\mathbf{p}) \rangle \quad \text{for each } \ i \in \mathbb{N}. \tag{12}$$

Since the solutions $\tilde{\mathbf{x}}$ are unknown a priori, we have to determine these coefficient functions approximatively. For fixed $s \in [0, 1]$, the gPC expansion (11) converges in $L^2(\Omega)$ due to the assumption of finite second moments.

We also apply a gPC expansion for the random period

$$T(\mathbf{p}) = \sum_{j=0}^{\infty} w_j \Phi_j(\mathbf{p}) \tag{13}$$

with coefficients $w_j \in \mathbb{R}$ and the same basis polynomials as in (11). The condition $\langle T(\mathbf{p})^2 \rangle < \infty$ guarantees the convergence of (13) in $L^2(\Omega)$.

To achieve a numerical method, the infinite sums (11) and (13) are truncated at the mth and m'th term, respectively, which implies the approximations

$$\tilde{\mathbf{x}}^m(s, \mathbf{p}) = \sum_{i=0}^{m} \mathbf{v}_i(s)\Phi_i(\mathbf{p}), \quad T^{m'}(\mathbf{p}) = \sum_{j=0}^{m'} w_j \Phi_j(\mathbf{p}). \tag{14}$$

The coefficient functions directly yield an approximation for the expected value and the variance of the random process. Let $\Phi_0 \equiv 1$ be the polynomial of degree zero. It follows

$$\langle \tilde{\mathbf{x}}^m(s, \mathbf{p}) \rangle = \mathbf{v}_0(s) \qquad \text{and} \qquad \mathrm{Var}(\tilde{x}_l^m(s, \mathbf{p})) = \sum_{i=0}^{m} v_{i,l}(s)^2,$$

since the basis polynomials are orthonormal. Corresponding approximations result for the random period.

We obtain other periodic solutions of (5) due to (2) by the transformation

$$\tilde{\mathbf{y}}(s, \mathbf{p}) := \tilde{\mathbf{x}}(s + c(\mathbf{p}), \mathbf{p}). \tag{15}$$

Let the function $c : Q \to \mathbb{R}$ be continuous. Both families $\tilde{\mathbf{x}}$ and $\tilde{\mathbf{y}}$ include the same information. Unfortunately, we cannot transform the corresponding

gPC representations. Let

$$\tilde{\mathbf{y}}(s,\mathbf{p}) = \sum_{i=0}^{\infty} \mathbf{u}_i(s)\Phi_i(\mathbf{p}).$$

The definition (12) of the coefficients shows

$$\begin{aligned}\mathbf{u}_i(s) &= \langle \tilde{\mathbf{y}}(s,\mathbf{p})\Phi_i(\mathbf{p})\rangle = \langle \tilde{\mathbf{x}}(s+c(\mathbf{p}),\mathbf{p})\Phi_i(\mathbf{p})\rangle \\ &= \left\langle \left(\sum_{l=0}^{\infty} \mathbf{v}_l(s+c(\mathbf{p}))\Phi_l(\mathbf{p})\right)\Phi_i(\mathbf{p})\right\rangle = \sum_{l=0}^{\infty}\langle \mathbf{v}_l(s+c(\mathbf{p}))\Phi_l(\mathbf{p})\Phi_i(\mathbf{p})\rangle\end{aligned}$$

provided that the summation and the integration can be interchanged. The above terms cannot be calculated further, since the coefficients $\mathbf{v}_i$ include the parameters now. In the case $c(\mathbf{p}) \equiv c_0$, it follows $\mathbf{u}_i(s) = \mathbf{v}_i(s+c_0)$ as expected.

Assume that the solutions $\tilde{\mathbf{x}}$ and $\tilde{\mathbf{y}}$ are determined by two different phase conditions, respectively. It follows that the two random processes are interconnected by a transformation (15). The function $c(\mathbf{p})$ depends on the parameters in general, even if the corresponding phase conditions do not involve the parameters explicitly (like (7) with $\eta(\mathbf{p}) \equiv \eta_0$).

2.4 Galerkin projection

We have to compute approximations of the unknown coefficients in the truncated gPC expansions (14). For this purpose, an intrusive approach (Galerkin projection) or a non-intrusive approach (stochastic collocation) can be used, see [1,15]. We apply the intrusive strategy and the reasons will be explained in Sect. 3.4.

Inserting the finite approximations (14) in the systems (5) yields the residual

$$\mathbf{r}(s,\mathbf{p}) := A(\mathbf{p})\left(\sum_{i=0}^{m}\mathbf{v}_i(s)\Phi_i(\mathbf{p})\right)' - \left(\sum_{j=0}^{m'} w_j\Phi_j(\mathbf{p})\right)\mathbf{f}\left(\sum_{i=0}^{m}\mathbf{v}_i(s)\Phi_i(\mathbf{p}),\mathbf{p}\right).$$

The Galerkin method demands $\langle \mathbf{r}(s,\mathbf{p})\Phi_l(\mathbf{p})\rangle = 0$ for all $l = 0,1,\ldots,m$ and each $s \in [0,1]$. The resulting calculations are given in [10]. It follows the coupled system

$$\sum_{i=0}^{m}\langle \Phi_l(\mathbf{p})\Phi_i(\mathbf{p})A(\mathbf{p})\rangle \mathbf{v}_i'(s) = \sum_{j=0}^{m'} w_j\left\langle \Phi_l(\mathbf{p})\Phi_j(\mathbf{p})\,\mathbf{f}\left(\sum_{i=0}^{m}\mathbf{v}_i(s)\Phi_i(\mathbf{p}),\mathbf{p}\right)\right\rangle \quad (16)$$

for $l = 0,1,\ldots,m$. Due to (12), the periodicity condition (6) implies the two-

point boundary value problem

$$\mathbf{v}_i(0) = \mathbf{v}_i(1) \qquad \text{for } \; i = 0, 1, \ldots, m. \tag{17}$$

Although a solution of the boundary value problem (16),(17) represents just an approximation of the exact coefficients in the gPC expansions, we apply the same symbols for convenience.

The problem (16),(17) is still underdetermined, since the coefficients w_j of the random period represent $m' + 1$ scalar unknowns. Phase conditions yield additional equations to determine a complete solution. We assume $m = m'$ now. Firstly, the condition (7) yields the additional relations ($\mathbf{v}_i = (v_{i,1}, \ldots, v_{i,n})^\top$)

$$v_{i,1}(0) = \langle \eta(\mathbf{p}) \Phi_i(\mathbf{p}) \rangle \qquad \text{for } \; i = 0, 1, \ldots, m. \tag{18}$$

In the special case $\eta(\mathbf{p}) \equiv \eta_0$, we obtain

$$v_{0,1}(0) = \eta_0, \qquad v_{i,1}(0) = 0 \qquad \text{for } \; i = 1, \ldots, m. \tag{19}$$

It follows that the variance of the approximation for the first component is equal to zero at $s = 0$.

Secondly, the phase condition (8) leads to the additional equations

$$\left\langle \Phi_i(\mathbf{p}) \; f_1 \left(\sum_{j=0}^{m} \mathbf{v}_j(0) \Phi_j(\mathbf{p}), \mathbf{p} \right) \right\rangle = 0 \qquad \text{for } \; i = 0, 1, \ldots, m \tag{20}$$

in case of explicit ODEs ($A(\mathbf{p}) \equiv I$). In both cases, we achieve $m + 1$ scalar boundary conditions to solve a two-point boundary value problem (16),(17).

3 Minimisation of Variance

The solution of the stochastic model depends on the used phase condition. We construct a method, which yields a random process with a minimal total variance.

3.1 Problem definition

Let $\tilde{\mathbf{x}}(s, \mathbf{p})$ be a family of periodic functions satisfying the system (5). We assume that these solutions are smooth with respect to s and continuous with respect to $\mathbf{p}$. Applying random parameters, the stochastic process exhibits an expected value and a variance. The transformation (15) yields other periodic

random processes, which own different expected values and variances in general. Nevertheless, each random process solves the system (5), i.e., it includes the same information as another solution.

Consequently, the variance depends on the chosen phase condition. Roughly speaking, the variance follows from a comparison of solutions for different parameters within the unit interval. Inappropriate phase conditions may result in a relatively large variance, which corresponds to a modelling error. Thus we determine a random process with a minimal variance, since this choice enables a fair comparison, i.e., the modelling error becomes minimal. More precisely, we minimise a total variance of the components of the random process according to the following definition.

Definition 1 *The total variance of a random process* $\tilde{\mathbf{x}}(s, \mathbf{p})$ *for* $s \in [0, 1]$ *and* $\mathbf{p} \in Q$ *is defined as*

$$V := \int_0^1 \sum_{l=1}^{n} \mathrm{Var}(\tilde{x}_l(s, \mathbf{p}))\, \mathrm{d}s \tag{21}$$

for $\tilde{\mathbf{x}} = (\tilde{x}_1, \ldots, \tilde{x}_n)^\top$.

Let σ be the standard deviation of the random process. It holds

$$V = \|\mathrm{Var}(\tilde{\mathbf{x}}(s, \mathbf{p}))\|_1 = \sum_{l=1}^{n} \mathrm{Var}(\tilde{x}_l(s, \mathbf{p})) = \sum_{l=1}^{n} \sigma(\tilde{x}_l(s, \mathbf{p}))^2 = \|\sigma(\tilde{\mathbf{x}}(s, \mathbf{p}))\|_2^2.$$

Hence the minimisation refers to the Euclidean norm of the standard deviation. Furthermore, we obtain

$$V = \int_0^1 \sum_{l=1}^{n} \langle \tilde{x}_l(s, \mathbf{p})^2 \rangle - \langle \tilde{x}_l(s, \mathbf{p}) \rangle^2 = \left\langle \int_0^1 \|\tilde{\mathbf{x}}(s, \mathbf{p}) - \langle \tilde{\mathbf{x}}(s, \mathbf{p}) \rangle\|^2 \, \mathrm{d}s \right\rangle. \tag{22}$$

In the following, we assume the existence and uniqueness of a random process with a minimal total variance (21) satisfying the system (5).

Elementary phase conditions have been introduced in Sect. 2.1. Now we assume that a smooth periodic function $\bar{\mathbf{x}}(s)$ is given for $s \in [0, 1]$. In the deterministic case, Doedel suggested a phase condition to minimise the distance of a periodic solution to the predetermined function in several publications, see [2], for example. This approach can be used efficiently in a continuation method for solving nonlinear systems via Newton iterations, since changes in the profile of the solutions are minimised. In our case, this criterion refers to the distance

$$R(\mathbf{p}) := \int_0^1 \|\tilde{\mathbf{x}}(s, \mathbf{p}) - \bar{\mathbf{x}}(s)\|_2^2 \, \mathrm{d}s \tag{23}$$

for an arbitrary $\mathbf{p} \in Q$. The corresponding phase condition reads

$$\int_0^1 \tilde{\mathbf{x}}(s, \mathbf{p})^\top \bar{\mathbf{x}}'(s) \, \mathrm{d}s = 0 \qquad \text{for arbitrary } \ \mathbf{p} \in Q, \tag{24}$$

which represents a necessary constraint for a minimum. Comparing the formulas (22) and (23), our idea is to arrange the reference function $\bar{\mathbf{x}}(s) := \langle \tilde{\mathbf{x}}(s, \mathbf{p}) \rangle$, i.e., the a priori unknown expected value. Accordingly, the phase condition (24) should yield a minimum pointwise for each $\mathbf{p} \in Q$. It follows a minimum of the total variance (22).

The above derivation is somehow heuristic. We will provide a proof in the following section.

3.2 Variational calculus

The necessary condition for a minimum of the total variance (21) is shown by the classical calculus of variations now.

Theorem 1 *Let $\tilde{\mathbf{x}}(s, \mathbf{p})$ be a periodic random process satisfying the given systems (5), which is smooth in $s \in [0, 1]$ and continuous in $\mathbf{p} \in Q$. If the corresponding total variance (21) is minimal, then the random process fulfills the condition*

$$\int_0^1 \tilde{\mathbf{x}}(s, \mathbf{p})^\top \bar{\mathbf{x}}'(s) \, \mathrm{d}s = 0 \tag{25}$$

for almost all $\mathbf{p} \in Q$ with the expected value $\bar{\mathbf{x}}(s) := \langle \tilde{\mathbf{x}}(s, \mathbf{p}) \rangle$.

Proof:

We arrange a set of competitive solutions

$$\tilde{\mathbf{x}}^\varepsilon(s, \mathbf{p}) := \tilde{\mathbf{x}}(s + \varepsilon c(\mathbf{p}), \mathbf{p})$$

with a parameter $\varepsilon \in [-1, 1]$ and an arbitrary continuous function $c : Q \to \mathbb{R}$. We assume that the support $\operatorname{supp}(c) := \overline{\{\mathbf{p} \in Q : c(\mathbf{p}) \neq 0\}}$ is a compact set. The corresponding total variance (21) reads

$$V = \sum_{l=1}^{n} \int_0^1 \int_{\mathbb{R}^q} \tilde{x}_l(s + \varepsilon c(\mathbf{p}), \mathbf{p})^2 \rho(\mathbf{p}) \, \mathrm{d}\mathbf{p} - \bar{x}_l^\varepsilon(s)^2 \, \mathrm{d}s,$$

where

$$\bar{x}_l^\varepsilon(s) := \langle \tilde{x}_l(s + \varepsilon c(\mathbf{p}), \mathbf{p}) \rangle = \int_{\mathbb{R}^q} \tilde{x}_l(s + \varepsilon c(\mathbf{p}), \mathbf{p}) \rho(\mathbf{p}) \, \mathrm{d}\mathbf{p}$$

for $l = 1, \ldots, n$. We differentiate the total variance with respect to ε. For the first part, it follows

$$
\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\int_0^1\int_{\mathbb{R}^q}\tilde{x}_l(s+\varepsilon c(\mathbf{p}),\mathbf{p})^2\rho(\mathbf{p})\,\mathrm{d}\mathbf{p}\,\mathrm{d}s\\
=&\int_0^1\int_{\mathbb{R}^q}2\tilde{x}_l(s+\varepsilon c(\mathbf{p}),\mathbf{p})\tilde{x}_l'(s+\varepsilon c(\mathbf{p}),\mathbf{p})c(\mathbf{p})\rho(\mathbf{p})\,\mathrm{d}\mathbf{p}\,\mathrm{d}s\\
=&\,2\int_{\mathbb{R}^q}\left[\int_0^1\tilde{x}_l(s+\varepsilon c(\mathbf{p}),\mathbf{p})\tilde{x}_l'(s+\varepsilon c(\mathbf{p}),\mathbf{p})\,\mathrm{d}s\right]c(\mathbf{p})\rho(\mathbf{p})\,\mathrm{d}\mathbf{p}
\end{aligned}
$$

for all $l=1,\ldots,n$, The differentiation and the integration can be interchanged, since the function c implies a compact support of the integrand. Accordingly, the succession of the two integrations is interchanged due to Fubini's theorem, because all involved functions are continuous. For the inner integral, it holds for all $l=1,\ldots,n$

$$
\int_0^1\tilde{x}_l(s+\varepsilon c(\mathbf{p}),\mathbf{p})\tilde{x}_l'(s+\varepsilon c(\mathbf{p}),\mathbf{p})\,\mathrm{d}s=0\qquad\text{for each }\ \mathbf{p},
$$

since the functions $\tilde{x}_l(\cdot+\varepsilon c(\mathbf{p}),\mathbf{p})$ are periodic for each $\mathbf{p}$ and each ε. Hence the first part vanishes. For the second part, we obtain

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\int_0^1(\bar{x}_l^\varepsilon(s))^2\,\mathrm{d}s&=\int_0^1 2\bar{x}_l^\varepsilon(s)\left(\int_{\mathbb{R}^q}\tilde{x}_l'(s+\varepsilon c(\mathbf{p}),\mathbf{p})c(\mathbf{p})\rho(\mathbf{p})\,\mathrm{d}\mathbf{p}\right)\mathrm{d}s\\
&=2\int_{\mathbb{R}^q}\left[\int_0^1\bar{x}_l^\varepsilon(s)\tilde{x}_l'(s+\varepsilon c(\mathbf{p}),\mathbf{p})\,\mathrm{d}s\right]c(\mathbf{p})\rho(\mathbf{p})\,\mathrm{d}\mathbf{p}
\end{aligned}
$$

for $l=1,\ldots,n$. The differentiation and the integrations can be interchanged due to the same reasons as for the first part.

A necessary condition for a minimum of (21) at $\varepsilon=0$ is that the derivative of V vanishes. It follows

$$
\begin{aligned}
0\ =\ \left.\frac{\mathrm{d}V}{\mathrm{d}\varepsilon}\right|_{\varepsilon=0}&=\sum_{l=1}^n 2\int_{\mathbb{R}^q}\left[\int_0^1\bar{x}_l(s)\tilde{x}_l'(s,\mathbf{p})\,\mathrm{d}s\right]c(\mathbf{p})\rho(\mathbf{p})\,\mathrm{d}\mathbf{p}\\
&=2\int_{\mathbb{R}^q}\left[\int_0^1\sum_{l=1}^n\bar{x}_l(s)\tilde{x}_l'(s,\mathbf{p})\,\mathrm{d}s\right]c(\mathbf{p})\rho(\mathbf{p})\,\mathrm{d}\mathbf{p}\\
&=2\int_{\mathbb{R}^q}\left[\int_0^1\bar{\mathbf{x}}(s)^\top\tilde{\mathbf{x}}'(s,\mathbf{p})\,\mathrm{d}s\right]c(\mathbf{p})\rho(\mathbf{p})\,\mathrm{d}\mathbf{p}.
\end{aligned}
$$

Since this relation holds for an arbitrary continuous function $c(\mathbf{p})$ with compact support, the fundamental theorem of variational calculus implies

$$
\int_0^1\bar{\mathbf{x}}(s)^\top\tilde{\mathbf{x}}'(s,\mathbf{p})\,\mathrm{d}s=0\qquad\text{for all }\ \mathbf{p}\in\operatorname{supp}(\rho)
$$

with the support of the density function $\operatorname{supp}(\rho):=\overline{\{\mathbf{p}\in Q:\rho(\mathbf{p})>0\}}$. Integration by parts yields the condition (25) due to the periodicity of the involved functions. □

The condition (25) holds necessarily for all parameters in the support of the density function. For simplicity, we can demand that this constraint is satisfied for all parameters $\mathbf{p} \in Q$. The phase condition (25) is not a boundary condition like (18) or (20), since the solution $\tilde{\mathbf{x}}(s, \mathbf{p})$ is involved for all $s \in [0, 1]$.

3.3 Scaling

The components of the solutions of the dynamical systems (1) and (5), respectively, may exhibit different physical magnitudes. To achieve a balanced contribution of the components to the total variance, a scaling is often necessary. We apply a diagonal matrix $D \in \mathbb{R}^{n \times n}$ with entries $d_1, \ldots, d_n \geq 0$. Thus the matrix D is positive semi-definite.

Definition 2 *Let a diagonal matrix D with non-negative entries $d_1, \ldots, d_n$ be given. The corresponding scaled total variance of a random process reads*

$$V_D := \int_0^1 \|D\mathrm{Var}(\tilde{\mathbf{x}}(s, \mathbf{p}))\|_1 \, \mathrm{d}s = \sum_{l=1}^{n} d_l \int_0^1 \mathrm{Var}(\tilde{x}_l(s, \mathbf{p})) \, \mathrm{d}s \tag{26}$$

with $\tilde{\mathbf{x}} = (\tilde{x}_1, \ldots, \tilde{x}_n)^\top$.

It is straightforward to generalise the result of Theorem 1 to the case of a scaled total variance (26).

Theorem 2 *Let the assumptions of Theorem 1 be fulfilled. If the periodic random process $\tilde{\mathbf{x}}(s, \mathbf{p})$ features a minimal scaled total variance (26), then the necessary condition*

$$\int_0^1 \tilde{\mathbf{x}}(s, \mathbf{p})^\top D \bar{\mathbf{x}}'(s) \, \mathrm{d}s = 0 \tag{27}$$

holds for almost all $\mathbf{p} \in Q$ with the expected value $\bar{\mathbf{x}}(s) := \langle \tilde{\mathbf{x}}(s, \mathbf{p}) \rangle$.

The proof represents a repetition of the steps done in the proof of Theorem 1. Just sums including the weights $d_1, \ldots, d_n$ have to be introduced.

Another advantage of this possibility for scaling is that we can arrange some weights equal to zero. Consequently, the minimisation is focused on the total variance of a subset of components. In particular, the choice $d_l = 0$ for all $l \neq j$ allows for optimising the variance of the component $\tilde{x}_j$ only.

3.4 Numerical method using polynomial chaos

The gPC approach is suitable for solving the above problem, since the expected value appears as the first coefficient function. The other coefficient functions yield the variance of the solution. We apply the intrusive approach

(Galerkin projection) according to Sect. 2.4, since the coupled system (16) is available for the determination of the coefficient functions. In contrast, the non-intrusive approach (stochastic collocation) requires to solve the original systems (5) repeatedly for different parameters, where a phase condition is necessary. However, the minimum condition (25) includes the a priori unknown expected value.

Inserting the gPC expansion (11) into the necessary condition (25) results in

$$\begin{aligned}\int_0^1 \left(\sum_{i=0}^{\infty} \mathbf{v}_i(s)\Phi_i(\mathbf{p})\right)^{\top} \mathbf{v}_0'(s)\,\mathrm{d}s &= \int_0^1 \sum_{i=0}^{\infty} \left[\mathbf{v}_i(s)^{\top}\mathbf{v}_0'(s)\right] \Phi_i(\mathbf{p})\,\mathrm{d}s \\ &= \sum_{i=0}^{\infty} \left[\int_0^1 \mathbf{v}_i(s)^{\top}\mathbf{v}_0'(s)\,\mathrm{d}s\right] \Phi_i(\mathbf{p}).\end{aligned}$$

We demand that this sum is identical to zero due to (25). Since the basis polynomials are linearly independent, it follows

$$\int_0^1 \mathbf{v}_i(s)^{\top}\mathbf{v}_0'(s)\,\mathrm{d}s = 0 \quad \text{for all } \; i \in \mathbb{N}_0. \tag{28}$$

In a numerical scheme, we apply the conditions for $i = 0, 1, \ldots, m$. The equivalent constraints

$$\int_0^1 \mathbf{v}_i'(s)^{\top}\mathbf{v}_0(s)\,\mathrm{d}s = 0 \quad \text{for all } \; i \in \mathbb{N}_0$$

should be avoided in a numerical method, since all derivatives of the coefficient functions for $i = 0, 1, \ldots, m$ appear. In contrast, the relation (28) involves just the derivative of $\mathbf{v}_0$. In case of explicit ODEs ($A(\mathbf{p}) \equiv I$), the condition (28) is equivalent to (recall $\Phi_0 \equiv 1$)

$$\sum_{j=0}^{m} w_j \int_0^1 \mathbf{v}_i(s)^{\top} \left\langle \Phi_j(\mathbf{p})\, \mathbf{f}\left(\sum_{k=0}^{m} \mathbf{v}_k(s)\Phi_k(\mathbf{p}), \mathbf{p}\right)\right\rangle \,\mathrm{d}s = 0 \quad \text{for all } \; i \in \mathbb{N}_0,$$

where derivatives are omitted completely.

However, the condition (28) is always satisfied for $i = 0$, since the function $\mathbf{v}_0$ is periodic. Thus we need an additional scalar condition to replace this trivial relation. According to (7), we apply the elementary condition

$$v_{0,1}(0) = \eta_0 \tag{29}$$

with some constant $\eta_0 \in \mathbb{R}$ in the (without loss of generality) first component of the expected value. The total variance (21) is invariant with respect to translations (2) due to the periodicity of the random process. Thus an additional phase condition like (29) isolates a solution from a continuum of optimal solutions.

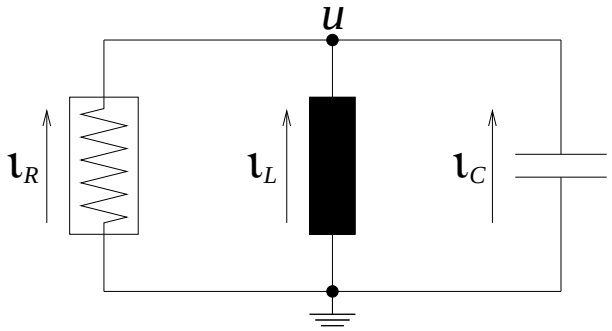

Fig. 1. Circuit of voltage controlled oscillator.

Now we can solve the periodic boundary value problem (16), (17), (28), (29) by a numerical method. This task is not a two-point boundary value problem, since the conditions (28) involve the solution for all $s \in [0, 1]$. Nevertheless, numerical schemes for periodic two-point boundary value problems of autonomous systems, see [5], can be generalised straightforward for our purpose.

4 Numerical Simulations

We apply the minimisation of the variance to two test examples, which represent mathematical models of electric circuits.

4.1 Voltage controlled oscillator

We consider a voltage controlled oscillator (VCO) with a capacitance, an inductance and a nonlinear resistor, see Fig. 1. A network approach yields a system of four DAEs

$$Cu' = \imath_C, \quad L\imath_L' = u, \quad 0 = \imath_R - g(u), \quad 0 = \imath_C + \imath_L + \imath_R \tag{30}$$

including the unknown node voltage u and the three unknown branch currents $\imath_C, \imath_L, \imath_R$. The corresponding differential index is one. The current-voltage relation of the nonlinear resistor reads

$$g(u) = (G_0 - G_\infty)U_0 \tanh(u/U_0) + G_\infty u. \tag{31}$$

In our simulations, the technical parameters are chosen as

$$C = 10^{-9}\ \text{F}, \quad L = 10^{-6}\ \text{H}, \quad U_0 = 1\ \text{V}, \quad G_0 = -0.1\ \text{A/V}, \quad G_\infty = 0.25\ \text{A/V}.$$

A modified version of this VCO with a random inductance L has been resolved successfully in another context, see [11]. Now we arrange a random parameter

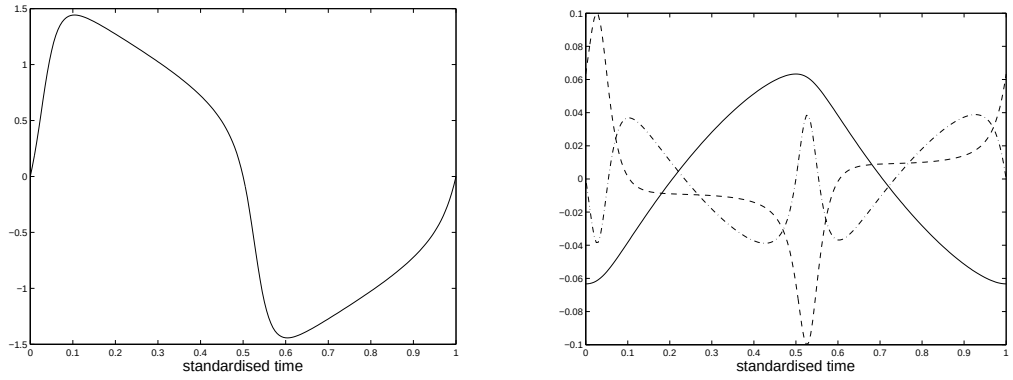

Fig. 2. Expected values of the node voltage (left) and the three branch currents (right, $\imath_L$: —, $\imath_C$: - - - , $\imath_R$: -·-·-) in VCO.

within the model (31) of the nonlinear resistor

$$G_\infty(p) = G_\infty(1 + 0.5p)$$

using a uniformly distributed random variable $p \in [-1, 1]$. Thus relatively large variations are set for demonstration. We apply the gPC expansions with the Legendre polynomials up to degree $m = 3$. If follows a coupled system (16) with 16 equations. We solve the periodic boundary value problem including the condition (28) for a minimum total variance and the additional phase condition (29) with $\eta_0 = 0$. A finite difference method yields an approximation, where asymmetric formulas (BDF) of second order are used. The resulting key data of the random period results to

$$\langle T(p) \rangle = 2.64 \cdot 10^{-7} \text{ s}, \quad \sigma(T(p)) = \sqrt{\text{Var}(T(p))} = 1.06 \cdot 10^{-8} \text{ s}.$$

Fig. 2 illustrates the expected values of the random process, i.e., the coefficient functions for degree zero. We recognise the phase condition (29) in the node voltage. Fig. 3 shows the corresponding variances, which are reconstructed by the other coefficient functions. Moreover, the coefficient functions of the node voltage are displayed in Fig. 4.

We indicate that the computed random process is optimal by a comparison to other solutions. We solve the periodic problem of the coupled system (16) with the simple phase conditions (19) using different constants η_0. Table 1 shows the corresponding values of the total variance (21) obtained by a discretisation. Furthermore, the total variances for the solutions satisfying (28) using the same values η_0 in (29) are included. As expected, these solutions exhibit a minimal total variance, whose value is independent of the constant η_0. The solution for the simple phase condition (19) with $\eta_0 = 0$ is close to the optimal solution. Thereby, $\eta_0 = 0$ can be seen as a mean value of the node voltage in $[0, 1]$. However, other choices (like $\eta_0 = -0.5$) result in a larger variance. The gPC coefficients of the random period coincide in all simulations except for numerical errors as expected.

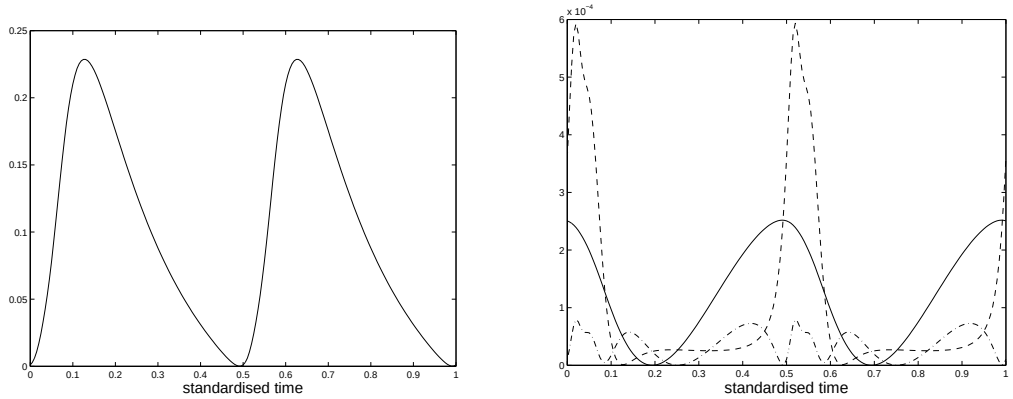

Fig. 3. Variances of the involved node voltage (left) and the three branch currents (right, $\imath_L$: —, $\imath_C$: - - - , $\imath_R$: -·-·-) in VCO.

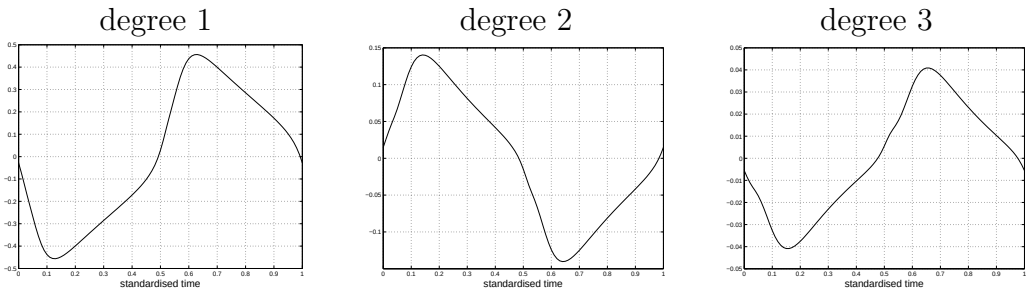

Fig. 4. Coefficient function in gPC expansion for node voltage in VCO.

Table 1
Total variance for simulations of VCO.

	$\eta_0 = -0.5$	$\eta_0 = 0$	$\eta_0 = 0.5$
optimal solution	0.1003	0.1003	0.1003
simple phase cond.	0.1236	0.1006	0.1027

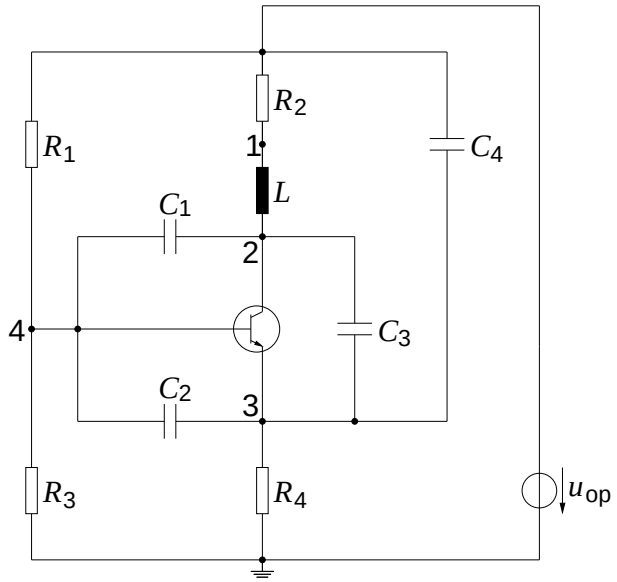

Fig. 5. Circuit of Colpitts oscillator.

4.2 Colpitts oscillator

Now we apply a Colpitts oscillator, see Fig. 5. A mathematical model introduced in [4] yields an implicit system of ODEs for the four unknown node voltages

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & C_1+C_3 & -C_3 & -C_1 \\ 0 & -C_3 & C_2+C_3+C_4 & -C_2 \\ 0 & -C_1 & -C_2 & C_1+C_2 \end{pmatrix} \begin{pmatrix} u_1' \\ u_2' \\ u_3' \\ u_4' \end{pmatrix} = \tag{32}$$

$$\begin{pmatrix} \frac{R_2}{L}(u_2-u_1) \\ \frac{1}{R_2}(u_{\mathrm{op}}-u_1)+(\imath_S+\frac{\imath_S}{b_C})g(u_4-u_2)-\imath_S g(u_4-u_3) \\ -\frac{1}{R_4}u_3+(\imath_S+\frac{\imath_S}{b_E})g(u_4-u_3)-\imath_S g(u_4-u_2) \\ -\frac{1}{R_3}u_4+\frac{1}{R_1}(u_{\mathrm{op}}-u_4)-\frac{\imath_S}{b_E}g(u_4-u_3)-\frac{\imath_S}{b_C}g(u_4-u_2) \end{pmatrix},$$

where the nonlinear function $g(u) = \exp(u/U_{\mathrm{th}}) - 1$ is involved. Although a system of ODEs appears, the behaviour of the circuit is more complex than

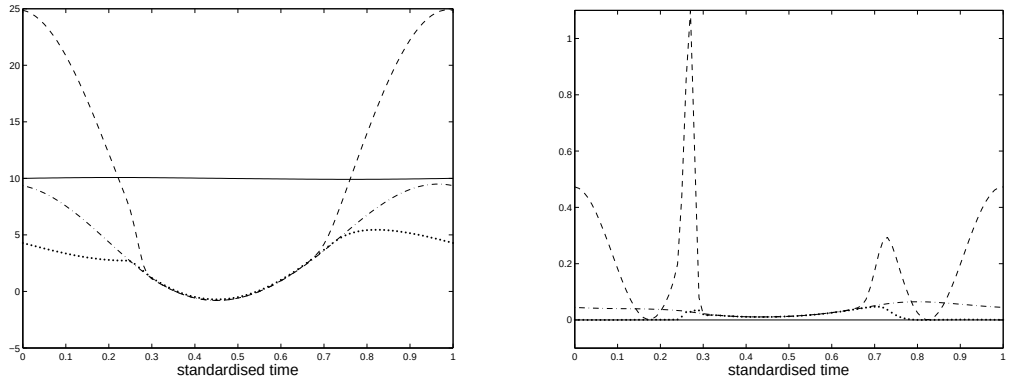

Fig. 6. Expected values (left) and variances (right) of node voltages in Colpitts oscillator (u_1: —, u_2: - - - , u_3: -·-·-, u_4: $\cdots$).

in the previous example of the VCO. The applied technical parameters are

$$C_1 = 5 \cdot 10^{-11}\ \mathrm{F}, \quad C_2 = 10^{-9}\ \mathrm{F}, \quad C_3 = 5 \cdot 10^{-8}\ \mathrm{F}, \quad C_4 = 10^{-7}\ \mathrm{F},$$
$$R_1 = 12000\ \Omega, \quad R_2 = 3\ \Omega, \quad R_3 = 8200\ \Omega, \quad R_4 = 1500\ \Omega,$$
$$L = 0.01\ \mathrm{H}, \quad u_{\mathrm{op}} = 10\ \mathrm{V}, \quad \imath_S = 10^{-3}\ \mathrm{A}, \quad b_E = 100, \quad b_C = 50,$$
$$U_{\mathrm{th}} = 2.585 \cdot 10^{-2}\ \mathrm{V}.$$

To obtain a random parameter, we replace the capacitance

$$C_3(p) = C_3(1 + 0.1p)$$

using a standardised Gaussian random variable p. In the gPC expansion, we use the Hermite polynomials up to degree $m = 3$. If follows a coupled system (16) with 16 equations. We solve the periodic boundary value problem including the condition (28) for a minimal total variance and the additional phase condition (29) with $\eta_0 = 10$. The same finite difference method as in the previous example is applied. The expected value and the standard deviation of the random period becomes

$$\langle T(p) \rangle = 1.251 \cdot 10^{-4}\ \mathrm{s}, \quad \sigma(T(p)) = \sqrt{\mathrm{Var}(T(p))} = 2.437 \cdot 10^{-6}\ \mathrm{s}.$$

The key data of the random process is illustrated in Fig. 6. All coefficient functions of the first node voltage are depicted in Fig. 7. However, the variance of the first voltage is relatively small in comparison to the other voltages.

Further simulations are done in the same form as for the previous test example. Table 2 shows the results. We recognise the same behaviour as in the first test example. Moreover, numerical simulations of the Colpitts oscillator (32) with a uniformly distributed random capacitance C_3 are presented in [10], where the elementary phase condition (19) has been applied.

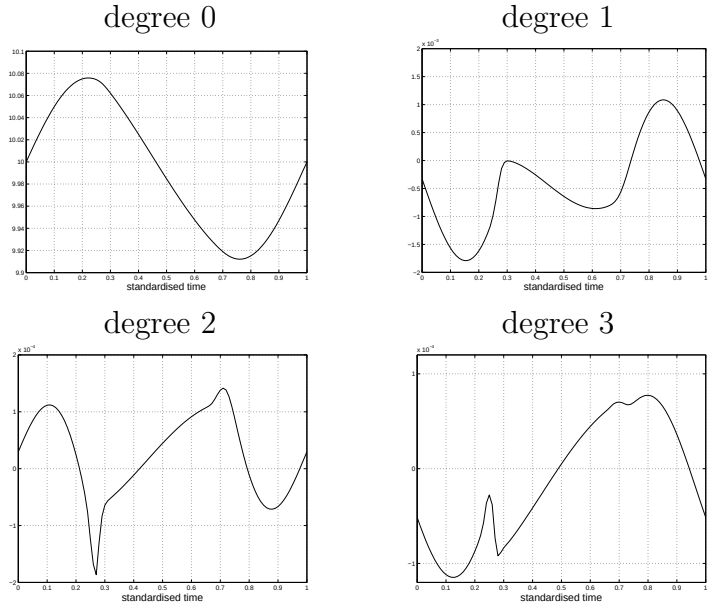

Fig. 7. Coefficient functions in gPC expansion of node voltage u_1 in Colpitts oscillator.

Table 2
Total variance for simulations of Colpitts oscillator.

	$\eta_0 = 9.95$	$\eta_0 = 10$	$\eta_0 = 10.05$
optimal solution	0.1969	0.1969	0.1969
simple phase cond.	0.2168	0.1974	0.2542

5 Conclusions

A random process corresponding to an autonomous oscillator with random parameters depends on the choice of a phase condition. An appropriate quantification of uncertainties is achieved by a random process with a minimal total variance. We have shown a necessary condition for an optimal solution using the calculus of variations. An according numerical method has been constructed based on expansions of the random process as well as the random period in the generalised polynomial chaos. A Galerkin projection yields a larger coupled system to determine an approximation of the random process and the random period. We have resolved the stochastic model successfully for two test examples, where a minimal total variance is achieved. Elementary phase conditions may result in suboptimal random processes. However, some phase conditions yield a larger variance as shown in the numerical simulations.

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