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Abstract

Mathematical modelling of dynamical processes often yields systems of ordinary differential equations (ODEs) or differential algebraic equations (DAEs). We investigate corresponding boundary value problems. Considering uncertainties in physical parameters of the systems, we introduce random variables. This stochastic model is resolved by the strategy of the polynomial chaos. A non-intrusive approach requires the solution of a large number of nonlinear systems with relatively small dimension. An intrusive approach yields just a single nonlinear system with a relatively high dimension. Alternatively, we present a non-intrusive method, which still exhibits a single large nonlinear system. Consequently, the convergence of only one Newton iteration has to be ensured to solve the boundary value problem, while many initial value problems of the original ODEs or DAEs are involved.

Key words: polynomial chaos, ordinary differential equations, differential algebraic equations, boundary value problem, uncertainty quantification

1. Introduction

Time-dependent systems of ordinary differential equations (ODEs) or differential algebraic equations (DAEs) result from mathematical modelling of electric circuits, mechanical systems or chemical reactions, for example. Furthermore, a space discretisation of partial differential equations often yields systems of ODEs or DAEs in time. We consider boundary value problems of

these dynamical systems. Several classes of numerical methods already exist for this type of problems, see [6, 13]. Each technique results in a nonlinear system of algebraic equations for corresponding approximations.

We assume that some physical parameters exhibit uncertainties. Consequently, we replace these parameters by random variables. For uncertainty quantification, the stochastic model can be resolved by a quasi Monte-Carlo simulation, for example. Alternatively, the generalised polynomial chaos (gPC) provides spectral methods based on an expansion with orthogonal basis polynomials, see [1, 4]. Unknown coefficient functions can be determined via an intrusive or a non-intrusive approach, respectively. The non-intrusive approach is also called stochastic collocation, see [14, 15]. Thereby, we can include numerical methods for the original dynamical systems directly. The intrusive approach, which is also called stochastic Galerkin method, applies a larger coupled system of ODEs or DAEs satisfied by the coefficient functions, cf. [8, 9].

In case of boundary value problems, the non-intrusive approach yields a large number of nonlinear systems of algebraic equations with relatively small dimension. Hence sophisticated algorithms are required to provide appropriate starting values and to ensure the convergence in each Newton iteration. In contrast, the intrusive approach involves just a single large nonlinear system of algebraic equations following from the larger coupled system of ODEs or DAEs. Thus only one Newton iteration has to be controlled. In this paper, we arrange an alternative technique, which also yields one large nonlinear system. The unknown coefficient functions do not satisfy a system of ODEs or DAEs but a projection relation. We apply transformations from the level of the original solutions to the level of the coefficients and vice versa. The technique is non-intrusive, since initial value problems of the original dynamical systems are solved. We focus on the case of ODEs, because the strategy is similar to a shooting method. The technique combines advantages from both the intrusive and the non-intrusive approach.

The paper is organised as follows. We introduce the boundary value problems of ODEs or DAEs with random parameters in Sect. 2. The gPC techniques using the intrusive approach and the non-intrusive approach are outlined in Sect. 3. We construct and analyse the combined method in Sect. 4. Finally, the results of numerical simulations of an illustrative example are presented.

2. Problem Definition

In this section, we define boundary value problems of a class of dynamical systems, which depend on parameters. A stochastic model follows from the introduction of random parameters.

2.1. Boundary value problems

We consider dynamical systems of the form

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

where the right-hand side $\mathbf{f}$ as well as the matrix $M \in \mathbb{R}^{n \times n}$ involve parameters $\mathbf{p} = (p_1, \ldots, p_q) \in Q \subseteq \mathbb{R}^q$. Thus the solution $\mathbf{x} : [a, b] \times Q \to \mathbb{R}^n$ depends on time and on the parameters. On the one hand, the system (1) consists of implicit ordinary differential equations (ODEs) in case of regular matrices $M(\mathbf{p})$. On the other hand, the system (1) results in differential algebraic equations (DAEs) for singular matrices. Although some components of the solution may be just continuous functions in case of DAEs, let $\mathbf{x}$ be smooth with respect to time in the following.

We assume that $M(\mathbf{p})$ is either regular or singular for all $\mathbf{p} \in Q$ given some relevant set $Q \subseteq \mathbb{R}^q$. The analytical and numerical behaviour of DAEs is characterised by the index of the system, where several concepts of index definitions exist, see [5], for example. For different parameters, the index of the systems (1) may vary.

Imposing an initial condition

$$\mathbf{x}(a, \mathbf{p}) = \mathbf{s}(\mathbf{p}), \tag{2}$$

we assume the existence of a unique solution for $t \in [a, b]$ provided that the initial values are consistent in case of DAEs.

We consider two-point boundary value problems

$$\mathbf{G}(\mathbf{x}(a, \mathbf{p}), \mathbf{x}(b, \mathbf{p}), \mathbf{p}) = \mathbf{0} \tag{3}$$

for each $\mathbf{p} \in Q$ with a general (nonlinear) function $\mathbf{G} : \mathbb{R}^n \times \mathbb{R}^n \times Q \to \mathbb{R}^n$. Thus the boundary conditions are allowed to be parameter-dependent. Often linear boundary conditions

$$\mathbf{G}(\mathbf{x}_a, \mathbf{x}_b, \mathbf{p}) \equiv A(\mathbf{p})\mathbf{x}_a + B(\mathbf{p})\mathbf{x}_b + \mathbf{c}(\mathbf{p}) \tag{4}$$

with matrices $A(\mathbf{p}), B(\mathbf{p}) \in \mathbb{R}^{n \times n}$ and a vector $\mathbf{c}(\mathbf{p}) \in \mathbb{R}^n$ are imposed. For example, we obtain periodic boundary value problems by the choice

$$A(\mathbf{p}) = I, \qquad B(\mathbf{p}) = -I, \qquad \mathbf{c}(\mathbf{p}) = \mathbf{0}$$

with the identity matrix $I \in \mathbb{R}^{n \times n}$. Consequently, the periodic boundary conditions do not depend explicitly on the parameters.

2.2. Numerical methods

We can solve a boundary value problem (1),(3) numerically by well-known techniques, see [6, 13]. The most important types are

- (multiple) shooting methods,

- finite difference methods,

- expansion methods (Galerkin, collocation, etc.).

Each technique yields a nonlinear system of algebraic equations, whose solution represents a numerical approximation of some data corresponding to the exact solution. Typically, the nonlinear systems are solved by a Newton iteration.

We outline the (simple) shooting method, since a similar approach will be used later to resolve the stochastic model in Sect. 4.2. Let $\mathbf{p} \in Q$ be fixed. The solution $\mathbf{x}(b, \mathbf{p})$ of (1) depends on the initial values (2). We denote this dependence by $\mathbf{x}(b, \mathbf{p}; \mathbf{s}(\mathbf{p}))$. The shooting technique consists in solving the nonlinear system

$$\mathbf{G}(\mathbf{s}(\mathbf{p}), \mathbf{x}(b, \mathbf{p}; \mathbf{s}(\mathbf{p})), \mathbf{p}) = \mathbf{0} \tag{5}$$

for the unknowns $\mathbf{s}(\mathbf{p})$. An evaluation of (5) for given values $\mathbf{s}(\mathbf{p})$ is done by solving an initial value problem (1),(2). In a Newton iteration, we require the Jacobian matrix of the nonlinear system (5) with respect to the initial values. Using a short notation, it follows

$$\frac{\partial \mathbf{G}}{\partial \mathbf{s}} = \frac{\partial \mathbf{G}}{\partial \mathbf{x}_a} + \frac{\partial \mathbf{G}}{\partial \mathbf{x}_b} \cdot \frac{\partial \mathbf{x}}{\partial \mathbf{s}}.$$

The partial derivatives of $\mathbf{G}$ can often be determined explicitly. Two approaches exist to compute the sensitivity matrices $\frac{\partial \mathbf{x}}{\partial \mathbf{s}}$ at $t = b$ in case of ODEs, cf. [12]. On the one hand, numerical differentiation can be applied, where n additional initial value problems (1),(2) are solved. On the other

hand, the sensitivity matrix represents the solution of an initial value problem of a linear matrix differential equation. The shooting technique as well as the multiple shooting can be generalised to the case of DAEs, see [2, 7], for example.

If a numerical solution of a boundary value problem (1),(3) is given for the parameters $\mathbf{p}^1 \in Q$, then we can use it as starting values for a Newton iteration corresponding to a boundary value problem for some $\mathbf{p}^2 \in Q$. However, the convergence of the iteration may fail for largely differing solutions. In this case, we apply a continuation method, see [3], based on the homotopy

$$\mathbf{p}_\lambda := (1 - \lambda)\mathbf{p}^1 + \lambda\mathbf{p}^2 \qquad \text{for } \lambda \in [0, 1].$$

The choice $\lambda = 0$ reproduces the known solution, whereas $\lambda = 1$ represents the desired state. Hence the continuation method employs variations in the scalar parameter λ.

2.3. Stochastic model

We assume that the chosen parameters exhibit some uncertainties. Consequently, we substitute the parameters by independent random variables $\mathbf{p} : \Omega \to Q$ with respect to some probability space $(\Omega, \mathcal{A}, P)$. Thereby, we apply classical random distributions like Gaussian distribution, uniform distribution, beta distribution, etc. The solution of the system (1) becomes a random process $\mathbf{x}(t, \mathbf{p}(\omega))$ for $\omega \in \Omega$. We are interested in key data of this process like the expected value and the variance or more sophisticated quantities.

Given a function $f : Q \to \mathbb{R}$ depending on the parameters, we denote the expected value (if exists) by

$$\langle f \rangle := \int_\Omega f(\mathbf{p}(\omega)) \, \mathrm{d}P(\omega) = \int_Q f(\mathbf{p})\rho(\mathbf{p}) \, \mathrm{d}\mathbf{p}. \tag{6}$$

Since we consider classical random distributions for the parameters, a corresponding probability density function $\rho : \mathbb{R}^q \to \mathbb{R}$ exists. The expected value (6) implies the inner product

$$\langle fg \rangle = \int_Q f(\mathbf{p})g(\mathbf{p})\rho(\mathbf{p}) \, \mathrm{d}\mathbf{p} \tag{7}$$

for two functions $f, g : Q \to \mathbb{R}$ depending on the parameters. Let

$$L^2(Q, \rho) := \left\{ f : Q \to \mathbb{R} : \langle f^2 \rangle < \infty \right\}.$$

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We apply the expected value (6) also to vector-valued or matrix-valued functions component-wise.

The above stochastic model can be resolved by a quasi Monte-Carlo simulation, for example. This strategy will be discussed in a more general framework within Sect. 3.2.

3. Polynomial Chaos

In this section, we introduce the approach of the generalised polynomial chaos (gPC) applied to the stochastic model, where boundary value problems are involved.

3.1. gPC expansions

Using the stochastic model from the previous section, we assume that each component of the solution of (1) exhibits finite second moments in each time point $t \in [a, b]$, i.e., $\mathbf{x}(t, \cdot) \in L^2(Q, \rho)^n$. It follows the existence of the expansion

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

point-wise for each $t \in [a, b]$, where $(\Phi_i)_{i \in \mathbb{N}}$ represents a complete set of multivariate basis polynomials $\Phi_i : \mathbb{R}^q \to \mathbb{R}$. We apply an orthonormal basis, i.e., it holds $\langle \Phi_i \Phi_j \rangle = \delta_{ij}$ with the Kronecker delta. Let $\Phi_0 \equiv 1$. Each classical random distribution implies according orthogonal polynomials. For example, the Legendre polynomials and the Hermite polynomials correspond to the uniform distribution and the Gaussian distribution, respectively. The orthonormal multivariate polynomials are just the products of the orthonormal univariate polynomials. If all random parameters exhibit Gaussian distributions, then the concept of the (homogeneous) polynomial chaos applies. In contrast, the gPC refers to non-Gaussian random distributions.

The coefficient functions $\mathbf{v}_i : [a, b] \to \mathbb{R}^n$ are unknown a priori. They satisfy the relation

$$\mathbf{v}_i(t) = \langle \mathbf{x}(t, \mathbf{p}) \Phi_i(\mathbf{p}) \rangle \tag{9}$$

for each $i \in \mathbb{N}$ and each $t \in [a, b]$. The formula (9) comprises probabilistic integrals according to (6).

We achieve a finite approximation by a truncation of the series (8), i.e.,

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

We require numerical methods to obtain approximations of the unknown coefficient functions in (10). Numerical techniques based on the gPC expansion (8) are spectral methods, since a representation involving globally defined basis functions is used. For further details on gPC expansions, we refer to [1, 4, 14, 15].

3.2. Non-intrusive techniques

Using non-intrusive methods, the unknown coefficient functions are determined via an approximative evaluation of the probabilistic integrals in (9). A sampling method yields the corresponding approximations. In case of low dimensions q, multidimensional quadrature can be applied, i.e., tensor product formulas of one-dimensional quadrature schemes. Sparse grids become advantageous for medium dimensions. In case of high dimensions q, quasi Monte-Carlo simulations have to be preferred.

In each method, we obtain a sequence of grid points $\mathbf{p}^1, \ldots, \mathbf{p}^K \in Q$. For example, we consider two independent random variables $p_1, p_2 \in [-1, +1]$ with identical beta distribution. The corresponding probability density function of each variable reads

$$\rho(p_i) = C(\alpha, \beta)(1 - p_i)^\alpha (1 + p_i)^\beta \quad \text{for} \ \ i = 1, 2 \tag{11}$$

with constants $\alpha, \beta \geq 0$. Figure 1 illustrates the behaviour of the grid points in the different methods setting $\alpha = \beta = 1$, for example.

For each grid point, a boundary value problem (1),(3) of the original system has to be solved. Hence well-known techniques yield numerical approximations as described in Sect. 2.2. Since the existing numerical methods can be used directly, the approach is called non-intrusive. The crucial part of the computational effort consists in solving the boundary value problems (1),(3). The gPC expansion of the results represents just a post-processing step. Considering the probabilistic integrals (9), the discretisation reads

$$\mathbf{v}_i(t) \doteq \sum_{k=1}^{K} w_k \, \mathbf{x}(t, \mathbf{p}^k) \Phi_i(\mathbf{p}^k) \tag{12}$$

for each $i = 0, 1, \ldots, m$ and each $t \in [a, b]$. The weights $w_k \in \mathbb{R}$ follow from the underlying sampling method. For example, it holds $w_k = 1/K$ in case of (quasi) Monte-Carlo methods.
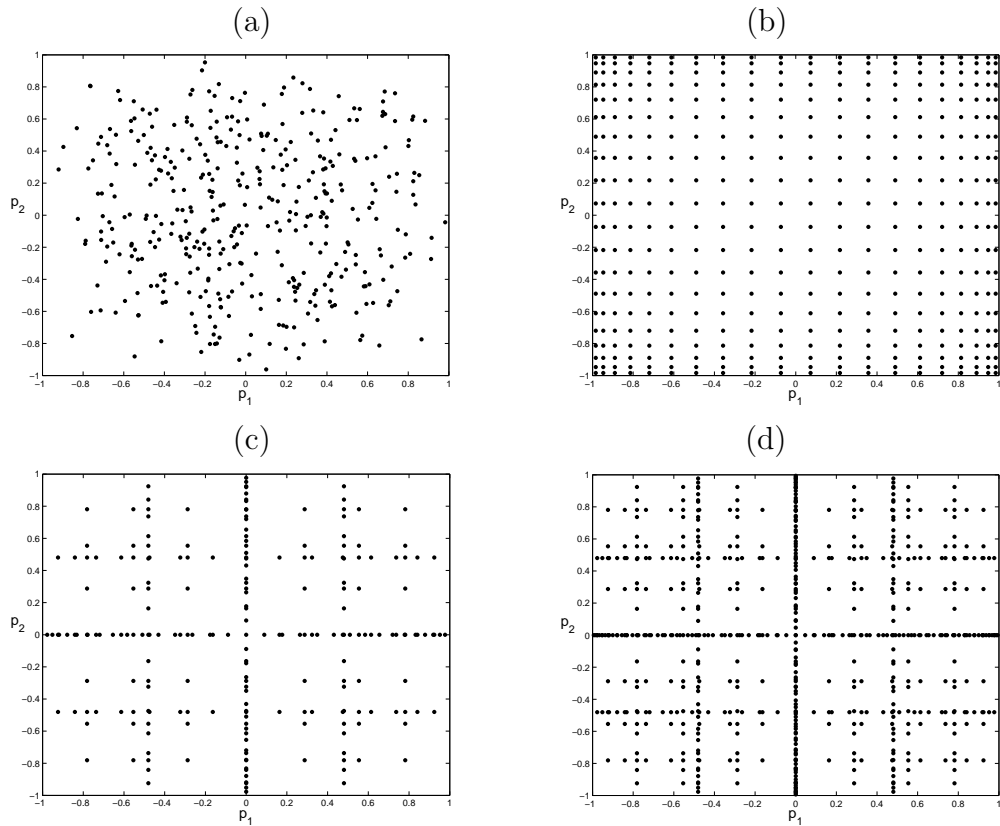
7

Figure 1: Grid points for two independent random variables with identical beta distribution: Monte-Carlo simulation with 400 points (a), Gauss-Jacobi quadrature with 400 nodes (b), sparse grid of level 4 with 223 points (c) and of level 5 with 617 points (d).

Since a numerical method implies a nonlinear system of algebraic equations, appropriate starting values are required for the Newton iteration corresponding to each grid point. We apply the numerical solution of a grid point as starting values for a neighbouring point. Thus a sophisticated ordering of the grid points is necessary to achieve an efficient technique, which means a low number of steps in each Newton iteration. The determination of such an ordering represents a non-trivial task in case of higher dimensions q, cf. Figure 1 for $q = 2$. If the convergence of an iteration fails, then we can apply the continuation method outlined in Sect. 2.2. However, this application increases the computational effort. Hence we have to control the convergence of a large number of Newton iterations by sophisticated algorithms.

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3.3. Intrusive techniques

In the intrusive method, a Galerkin approach yields a system of ODEs or DAEs, which is solved by an approximation of the unknown coefficient functions. Inserting the finite approximation (10) in the dynamical system (1), we obtain the residual

$$\mathbf{r}(t, \mathbf{p}) :\equiv M(\mathbf{p}) \left(\sum_{i=0}^{m} \mathbf{v}'_i(t) \Phi_i(\mathbf{p}) \right) - \mathbf{f} \left(t, \sum_{j=0}^{m} \mathbf{v}_j(t) \Phi_j(\mathbf{p}), \mathbf{p} \right), \qquad (13)$$

which is not identical to zero in general. The approximations $\mathbf{v}_0, \ldots, \mathbf{v}_m$ are determined such that the residual (13) becomes small in some sense. The Galerkin approach demands that the residual is orthogonal to the space of applied basis functions with respect to the inner product (7). In our case, it follows

$$\sum_{i=0}^{m} \langle M(\mathbf{p}) \Phi_i(\mathbf{p}) \Phi_l(\mathbf{p}) \rangle \mathbf{v}'_i(t) = \left\langle \mathbf{f} \left(t, \sum_{j=0}^{m} \mathbf{v}_j(t) \Phi_j(\mathbf{p}), \mathbf{p} \right) \Phi_l(\mathbf{p}) \right\rangle \qquad (14)$$

for $l = 0, 1, \ldots, m$. The equations (14) represent a coupled system of $(m+1)n$ ODEs or DAEs for the unknown coefficient functions. In case of implicit ODEs (1), mathematical modelling often results in symmetric positive definite matrices $M(\mathbf{p})$. If the matrices $M(\mathbf{p})$ are symmetric positive definite for all $\mathbf{p} \in Q$, then the coupled system (14) consists again of implicit ODEs.

We repeat the above Galerkin approach for the boundary conditions (3) and obtain the relations

$$\left\langle \mathbf{G} \left(\sum_{i=0}^{m} \mathbf{v}_i(a) \Phi_i(\mathbf{p}), \sum_{i=0}^{m} \mathbf{v}_i(b) \Phi_i(\mathbf{p}), \mathbf{p} \right) \Phi_l(\mathbf{p}) \right\rangle = \mathbf{0} \qquad (15)$$

for $l = 0, 1, \ldots, m$. Thus $(m+1)n$ boundary conditions (15) are available. In the linear case (4), the relations become

$$\begin{aligned}
\sum_{i=0}^{m} &\langle A(\mathbf{p}) \Phi_i(\mathbf{p}) \Phi_l(\mathbf{p}) \rangle \mathbf{v}_i(a) \\
+ \sum_{i=0}^{m} &\langle B(\mathbf{p}) \Phi_i(\mathbf{p}) \Phi_l(\mathbf{p}) \rangle \mathbf{v}_i(b) + \langle \mathbf{c}(\mathbf{p}) \Phi_l(\mathbf{p}) \rangle = \mathbf{0}
\end{aligned} \qquad (16)$$

for $l = 0, 1, \ldots, m$. Using the notation $\mathbf{v} := (\mathbf{v}_0^\top, \ldots, \mathbf{v}_m^\top)^\top$, the boundary conditions (16) exhibit the form

$$\tilde{A}\mathbf{v}(a) + \tilde{B}\mathbf{v}(b) + \tilde{\mathbf{c}} = \mathbf{0} \tag{17}$$

with constant matrices $\tilde{A}, \tilde{B}$ and a constant vector $\tilde{\mathbf{c}}$, i.e., we obtain a linear two-point boundary value problem again. For example, periodic boundary value problems simply demand

$$\mathbf{v}_l(a) = \mathbf{v}_l(b) \qquad \text{for all } l \tag{18}$$

due to the orthogonality of the basis polynomials.

Hence we achieve a two-point boundary value problem (14),(15) for the unknown coefficient functions. Remark that the exact solution of this boundary value problem represents just an approximation of the exact coefficients in (8). Nevertheless, we denote the functions by the same symbol for convenience. The approach is called intrusive, since a larger coupled system has to be resolved. Moreover, the probabilistic integrals in (14),(15) have to be computed analytically (if possible) or numerically.

We can use common numerical schemes to solve the two-point boundary value problem (14),(15) as outlined in Sect. 2.2. Just one large nonlinear system of algebraic equations has to be solved in this intrusive approach. Thus we have to control the convergence of only a single Newton iteration, which is more comfortable and robust.

In the intrusive approach, a continuation method can be applied if adequate starting values for the solution of the large nonlinear system are not available. Given the expected value $\bar{\mathbf{p}} := \langle \mathbf{p} \rangle$ of the parameters, we assume that the solution $\mathbf{x}(t, \bar{\mathbf{p}})$ of the boundary value problem (1),(3) is already determined. We define the random variables

$$\mathbf{p}_\lambda(\omega) = \lambda(\mathbf{p}(\omega) - \bar{\mathbf{p}}) + \bar{\mathbf{p}} \qquad \text{for } \lambda \in [0, 1].$$

In case of $\lambda = 0$, the coupled system (14) becomes deterministic and the solution of the boundary value problem reads (due to $\Phi_0 \equiv 1$)

$$\mathbf{v}_0(t) = \mathbf{x}(t, \bar{\mathbf{p}}), \qquad \mathbf{v}_i(t) = \mathbf{0} \quad \text{for } i \geq 1. \tag{19}$$

We retrieve the desired random distribution in case of $\lambda = 1$. Consequently, a continuation technique based on the parameter λ can be applied, see [3].

Stochastic models according to periodic boundary value problems (1),(4) have been solved successfully by the intrusive approach for implicit systems of ODEs in [10] and for systems of DAEs in [8, 11]. Quasiperiodic solutions of (1) have been considered via a strategy based on multirate partial differential algebraic equations in [9].

4. Combined Technique

In the intrusive method, all calculations are performed with respect to the coefficient functions using the coupled system (14). In the non-intrusive method, the original systems (1) are resolved and the results are expanded in the gPC. Now we develop an alternative technique, where the unknowns are the coefficient functions. However, just the original systems (1) are considered in this technique.

4.1. Preliminaries

For the design of the method, we introduce the following operators. Let

$$\mathcal{R} : \ell^2(\mathbb{Z})^n \to L^2(Q, \rho)^n, \quad (\mathbf{u}_i)_{i \in \mathbb{N}} \mapsto \sum_{i=0}^{\infty} \mathbf{u}_i \Phi_i(\mathbf{p}).$$

The application of $\mathcal{R}$ corresponds to a reconstruction step. The operator $\mathcal{R}$ is an isometry and thus bijective. The inverse operator reads

$$\mathcal{R}^{-1} : L^2(Q, \rho)^n \to \ell^2(\mathbb{Z})^n, \quad \mathbf{y}(\mathbf{p}) \mapsto (\langle \mathbf{y}(\mathbf{p}) \Phi_i(\mathbf{p}) \rangle)_{i \in \mathbb{N}}.$$

This operation represents a projection step into the gPC. On the one hand, the reconstruction can be applied directly to a finite set of coefficients $(\mathbf{u}_i)_{i=0}^m$. We define the restricted operator

$$\tilde{\mathcal{R}} : \mathbb{R}^{n \times (m+1)} \to L^2(Q, \rho)^n \cap C(\mathbb{R}^q)^n, \quad (\mathbf{u}_i)_{i=0}^m \mapsto \sum_{i=0}^{m} \mathbf{u}_i \Phi_i(\mathbf{p}).$$

The functions in the image of this restriction are continuous. On the other hand, we apply a truncation in the projection step and arrange the operator

$$\tilde{\mathcal{R}}^{-1} : L^2(Q, \rho)^n \to \mathbb{R}^{n \times (m+1)}, \quad \mathbf{y}(\mathbf{p}) \mapsto (\langle \mathbf{y}(\mathbf{p}) \Phi_i(\mathbf{p}) \rangle)_{i=0}^m.$$

Concerning the evolution in time, we describe the solution of the initial value problems of the system (1) by the operator

$$\mathcal{S}_{a,b} : C(Q)^n \to C(Q)^n, \quad \mathbf{s}(\mathbf{p}) = \mathbf{x}(a, \mathbf{p}) \mapsto \mathbf{x}(b, \mathbf{p}).$$

Thereby, we assume that the image of a continuous function is again a continuous function with respect to the parameters. Moreover, let the image of $\mathcal{S}_{a,b} \circ \tilde{\mathcal{R}}$ be in $L^2(Q, \rho)^n$ for some further restriction in the domain of dependence of $\tilde{\mathcal{R}}$ due to our considerations in Sect. 3.1. As an abbreviation, we define the operator

$$\mathcal{U} : G \to \mathbb{R}^{n \times (m+1)}, \quad \mathcal{U} := \tilde{\mathcal{R}}^{-1} \circ \mathcal{S}_{a,b} \circ \tilde{\mathcal{R}} \tag{20}$$

using an adequate subset $G \subseteq \mathbb{R}^{n \times (m+1)}$.

In case of DAEs (1), the image of $\tilde{\mathcal{R}}$ may include inconsistent initial values. An outcome is to restrict the domain of dependence of $\tilde{\mathcal{R}}$ further to appropriate degrees of freedom. Modifications, which are applied in solving boundary value problems of DAEs in comparison to ODEs, see [2, 7], can be used. The following method can be generalised directly to the case of semi-explicit systems of DAEs with index 1.

4.2. Shooting Method

We apply the boundary conditions (15) obtained by the Galerkin approach. Let $\mathbf{v} := (\mathbf{v}_0^\top, \ldots, \mathbf{v}_m^\top)^\top$ again. Inserting the constructed approximation $\mathbf{v}(b) \doteq \mathcal{U}(\mathbf{v}(a))$ from (20) yields

$$\left\langle \mathbf{G} \left(\sum_{i=0}^m \mathbf{v}_i(a) \Phi_i(\mathbf{p}), \sum_{i=0}^m \left(\mathcal{U}(\mathbf{v}(a)) \right)_i \Phi_i(\mathbf{p}), \mathbf{p} \right) \Phi_l(\mathbf{p}) \right\rangle = \mathbf{0} \tag{21}$$

for $l = 0, 1, \ldots, m$. Hence the method consists in solving the $(m + 1)n$ equations (21) for the unknowns $\mathbf{v}(a) \in \mathbb{R}^{n \times (m+1)}$. This approach is similar to a shooting method, since we determine the unknown initial values of the gPC representation. However, there is no system of differential equations, which the coefficient functions satisfy now.

The boundary conditions (21) can also be written in the shorter form

$$\left\langle \mathbf{G} \left(\tilde{\mathcal{R}}(\mathbf{v}(a))(\mathbf{p}), \left(\left(\mathcal{S}_{a,b} \circ \tilde{\mathcal{R}} \right)(\mathbf{v}(a)) \right)(\mathbf{p}), \mathbf{p} \right) \Phi_l(\mathbf{p}) \right\rangle = \mathbf{0} \tag{22}$$
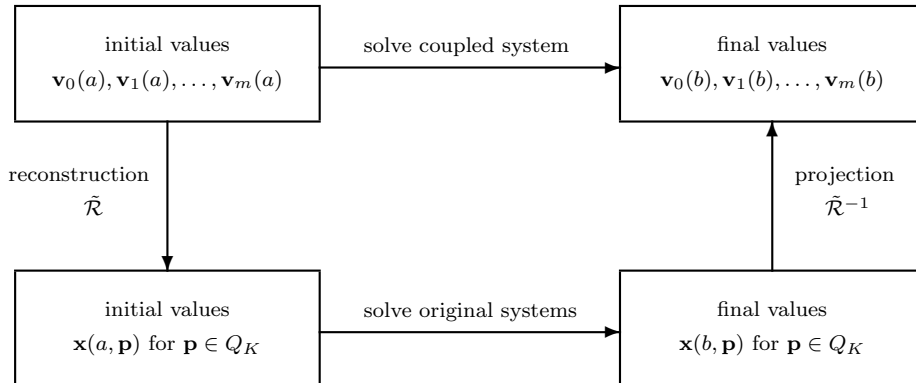
initial values
$\mathbf{v}_0(a), \mathbf{v}_1(a), \ldots, \mathbf{v}_m(a)$

solve coupled system

final values
$\mathbf{v}_0(b), \mathbf{v}_1(b), \ldots, \mathbf{v}_m(b)$

reconstruction
$\tilde{\mathcal{R}}$

projection
$\tilde{\mathcal{R}}^{-1}$

initial values
$\mathbf{x}(a, \mathbf{p})$ for $\mathbf{p} \in Q_K$

solve original systems

final values
$\mathbf{x}(b, \mathbf{p})$ for $\mathbf{p} \in Q_K$

Figure 2: Initial value problems in polynomial chaos approach.

for $l = 0, 1, \ldots, m$. If a sampling method has to be employed for evaluating (21), then the formula (22) should be used, since an additional sampling for an approximative evaluation of the operator $\tilde{\mathcal{R}}^{-1}$ is omitted.

Nevertheless, the relation (21) often allows for further manipulations. For example, the linear boundary conditions (4) imply, see (17),

$$\tilde{A}\mathbf{v}(a) + \tilde{B}\,\mathcal{U}(\mathbf{v}(a)) + \tilde{\mathbf{c}} = \mathbf{0},$$

where the result of the operator $\mathcal{U}$ is written as a long vector.

We discuss the evaluation of the operator $\mathcal{U}$ within a numerical method. Figure 2 outlines the procedure in connection to the intrusive approach from Sect. 3.3. Let $\mathbf{x}(t, \mathbf{p}; \mathbf{s}(\mathbf{p}))$ be the solution of the initial value problem (1),(2). We discretise the operator $\tilde{\mathcal{R}}^{-1}$ via a sampling method using a finite subset $Q_K \subset Q$ with K elements, i.e.,

$$(\mathcal{U}(\mathbf{v}(a)))_i \doteq \sum_{k=1}^{K} w_k \Phi_i(\mathbf{p}^k)\, \mathbf{x}\left(b, \mathbf{p}^k; \sum_{j=0}^{m} \mathbf{v}_j(a)\Phi_j(\mathbf{p}^k)\right). \tag{23}$$

Hence the reconstruction is done in the finite set of grid points $\mathbf{p}^k \in Q_K$ only to obtain the initial values. We solve the initial value problems of the dynamical system (1) via standard integrators in time. The final values of the integration are considered in the sampling method for the approximative projection.

The boundary conditions (21) represent a nonlinear system for the unknown initial values. Typically, the nonlinear systems are resolved by a

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Newton iteration. Thus we require the Jacobian matrices $\frac{\partial \mathcal{U}(\mathbf{v}(a))}{\partial \mathbf{v}(a)}$. It holds

$$\frac{\partial}{\partial \mathbf{v}_j(a)} \left(\sum_{i=0}^{m} \mathbf{v}_i(a)\Phi_i(\mathbf{p}) \right) = \sum_{i=0}^{m} \Phi_i(\mathbf{p})\frac{\partial \mathbf{v}_i(a)}{\partial \mathbf{v}_j(a)} = \Phi_j(\mathbf{p})I$$

with the identity matrix $I \in \mathbb{R}^{n \times n}$. Differentiating the discrete formulation (23) yields

$$\frac{\partial(\mathcal{U}(\mathbf{v}(a)))_i}{\partial \mathbf{v}_j(a)} = \sum_{k=1}^{K} w_k \Phi_i(\mathbf{p}^k)\Phi_j(\mathbf{p}^k) \left. \frac{\partial \mathbf{x}}{\partial \mathbf{s}} \right|_{t=b, \mathbf{p}=\mathbf{p}^k, \mathbf{s}=\mathbf{s}(\mathbf{p}^k)}$$

with $\mathbf{s}(\mathbf{p}) = \tilde{\mathcal{R}}(\mathbf{v}(a))$. Hence we achieve an approximation of the Jacobian matrix $\frac{\partial \mathcal{U}(\mathbf{v}(a))}{\partial \mathbf{v}(a)}$ by sampling the sensitivity matrices $\frac{\partial \mathbf{x}}{\partial \mathbf{s}}$. The computation of the sensitivity matrices can be done by the two approaches outlined in Sect. 2.2.

In the above approach, we have to control just a single Newton iteration like in the intrusive techniques from Sect. 3.3. Nevertheless, numerical methods for initial value problems of the original dynamical systems (1) can be used directly, which results in a non-intrusive technique. We obtain a high potential for parallelism, since an ordering of the initial value problems is not necessary for efficiency in contrast to the non-intrusive techniques from Sect. 3.2. If adequate starting values for the single nonlinear system are not available, we can apply the same continuation method as in the intrusive methods.

4.3. Multiple shooting

The generalisation of the above technique to a multiple shooting method, see [13], is straightforward. We introduce time points $a = t_0 < t_1 < \cdots < t_{r-1} < t_r = b$, where $r-1$ inner nodes occur. In each subinterval $[t_j, t_{j+1}]$, we apply an evolution according to (20), i.e.,

$$\mathbf{v}(t_{j+1}) = \left(\tilde{\mathcal{R}}^{-1} \circ \mathcal{S}_{t_j, t_{j+1}} \circ \tilde{\mathcal{R}} \right) (\mathbf{s}(t_j)) \qquad \text{for } j = 0, 1, \ldots, r-1 \qquad (24)$$

given some starting values $\mathbf{s}(t_j) \in \mathbb{R}^{n \times (m+1)}$. Thus $\mathbf{v}(t_{j+1})$ depends on $\mathbf{s}(t_j)$ only. The continuity of the coefficient functions at the inner nodes implies the conditions

$$\mathbf{v}(t_j) = \mathbf{s}(t_j) \qquad \text{for } j = 1, \ldots, r-1. \qquad (25)$$

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We arrange a nonlinear system including the continuity equations (25) and the boundary conditions (15), where $\mathbf{s}(t_0)$ is identical to $\mathbf{v}(a)$. We can solve this nonlinear system for the unknowns $\mathbf{s}(t_j)$ with $j = 0, 1, \ldots, r - 1$ by methods of Newton type again. The evaluation of these nonlinear systems and their Jacobian matrices is done as described in Sect. 4.2, since the relations (24) involve an operator of the form (20).

4.4. Finite difference methods

Finite difference schemes can be seen as a multiple shooting method with many subintervals in time, where just one integration step is done in each subinterval. The corresponding continuity conditions are used to eliminate unknowns in the nonlinear system.

To illustrate the concepts, we consider explicit ODEs, i.e., $M(\mathbf{p}) = I$ in the system (1). Let a grid of time points $a = t_0 < t_1 < \cdots < t_r = b$ be given. The explicit Euler scheme reads

$$\mathbf{x}(t_{j+1}, \mathbf{p}) = \mathbf{x}(t_j, \mathbf{p}) + (t_{j+1} - t_j)\mathbf{f}(t_j, \mathbf{x}(t_j, \mathbf{p}), \mathbf{p}). \tag{26}$$

Although the solution of the difference method represents just an approximation of the exact solution of the dynamical system (1), we apply the same symbol for convenience. At $t = t_{j+1}$, the projection step implies

$$
\begin{aligned}
\mathbf{v}_l(t_{j+1}) &= \langle \mathbf{x}(t_{j+1}, \mathbf{p})\Phi_l(\mathbf{p}) \rangle \\
&= \langle \mathbf{x}(t_j, \mathbf{p})\Phi_l(\mathbf{p}) \rangle + (t_{j+1} - t_j)\langle \mathbf{f}(t_j, \mathbf{x}(t_j, \mathbf{p}), \mathbf{p})\Phi_l(\mathbf{p}) \rangle
\end{aligned}
$$

for each $l = 0, 1, \ldots, m$. Considering the reconstruction step as well as the projection step at $t = t_j$, it follows

$$\mathbf{v}_l(t_{j+1}) = \mathbf{v}_l(t_j) + (t_{j+1} - t_j)\left\langle \mathbf{f}\left(t_j, \sum_{i=0}^{m} \mathbf{v}_i(t_j)\Phi_i(\mathbf{p}), \mathbf{p}\right)\Phi_l(\mathbf{p}) \right\rangle.$$

This numerical scheme coincides with the intrusive approach from Sect. 3.3, where the coupled system (14) is discretised by the explicit Euler method.

Alternatively, the implicit Euler scheme results in

$$\mathbf{x}(t_{j+1}, \mathbf{p}) = \mathbf{x}(t_j, \mathbf{p}) + (t_{j+1} - t_j)\mathbf{f}(t_{j+1}, \mathbf{x}(t_{j+1}, \mathbf{p}), \mathbf{p}). \tag{27}$$

If $\mathbf{x}(t_j, \mathbf{p})$ is given, then a nonlinear system has to be solved for $\mathbf{x}(t_{j+1}, \mathbf{p})$. The projection steps yield for each $l = 0, 1, \ldots, m$

$$\mathbf{v}_l(t_{j+1}) = \mathbf{v}_l(t_j) + (t_{j+1} - t_j)\langle \mathbf{f}(t_{j+1}, \mathbf{x}(t_{j+1}, \mathbf{p}), \mathbf{p})\Phi_l(\mathbf{p}) \rangle. \tag{28}$$

There are two possibilities to continue now:

1. If we replace $\mathbf{x}(t_{j+1}, \mathbf{p})$ in (28) by the reconstruction step at $t = t_{j+1}$, then it follows just the intrusive approach from Sect. 3.3, where the coupled system (14) is discretised by the implicit Euler scheme.

2. We obtain $\mathbf{x}(t_j, \mathbf{p})$ in (27) via the reconstruction step at $t = t_j$. The nonlinear systems (27) are solved for each $\mathbf{p} \in Q_K$ in a sampling method. The projection step is used at $t = t_{j+1}$. This strategy still represents a non-intrusive approach, since the scheme (27) discretises the original dynamical system (1). However many reconstruction steps as well as projection steps are required, which cause a significant amount of computational work.

Hence finite difference methods, which are used in the context of the strategy presented in this section, either coincide with an intrusive approach or become unfavourable due to a computational overhead.

5. Illustrative Example

As test example, we consider the Duffing oscillator, see [12]. The corresponding nonlinear system of ODEs of first order reads

$$\begin{aligned} x_1'(t) &= x_2(t) \\ x_2'(t) &= A\sin{(2\pi t)} - \mu x_2(t) - \nu x_1(t) - \theta x_1(t)^3, \end{aligned} \tag{29}$$

where a periodic input signal is included. We choose the constant parameters $\mu = 0.5$ and $\nu = 1$. Furthermore, we arrange the random parameters

$$A = 20(1 + 0.2p_1), \qquad \theta = 10(1 + 0.1p_2)$$

using independent random variables $p_1, p_2 \in [-1, 1]$ with identical beta distributions according to (11) for $\alpha = \beta = 1$. We consider periodic boundary conditions, since a forced oscillation satisfying (29) exists with period $T = 1$ for each tuple of parameters.

The corresponding gPC expansion (8) is based on the Jacobi polynomials. We apply two-variate polynomials up to degree 4, where $m + 1 = 15$ basis functions appear in (10). Hence 30 coefficient functions are involved. Periodic boundary conditions (18) with $a = 0$ and $b = 1$ are considered.

We determine a reference solution using the non-intrusive approach from Sect. 3.2. Thereby, a two-dimensional Gauss-Jacobi quadrature with 10×10 nodes yields the approximations (12). The boundary value problems of (29)
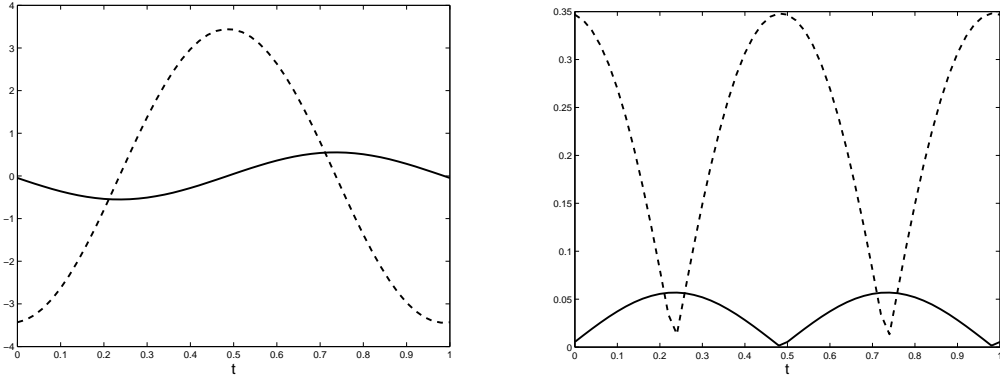
Figure 3: Expected value (left) and standard deviation (right) for stochastic solution of Duffing oscillator (x_1: solid line, x_2: dashed line).

are resolved by a shooting method. Trapezoidal rule solves the involved initial value problems, where a local error control with relative tolerance $\varepsilon_{\mathrm{r}} = 10^{-6}$ and absolute tolerance $\varepsilon_{\mathrm{a}} = 10^{-8}$ is used. Figure 3 illustrates the reconstructed expected value and standard deviation of the two random components of the Duffing oscillator (29). The expected value resembles the deterministic solution in case of $A = 20$, $\delta = 10$. Furthermore, Figure 4 depicts the coefficient functions corresponding to the first component of the Duffing oscillator. The second component exhibits a similar behaviour. We recognise that the magnitude of the coefficient functions decreases significantly for increasing polynomial degree, which indicates the convergence of the gPC expansion (8).

For comparison, we apply the three techniques: the non-intrusive method (Sect. 3.2), the intrusive method (Sect. 3.3) and the combined technique (Sect. 4.2). Involved probabilistic integrals (6) are always approximated by a two-dimensional Gauss-Jacobi quadrature with a 5×5 grid. We solve each periodic boundary value problem of ODEs by a shooting method. All time integrations are performed by trapezoidal rule with tolerances $\varepsilon_{\mathrm{r}} = 10^{-4}$, $\varepsilon_{\mathrm{a}} = 10^{-6}$. Thus we expect the same accuracy in each approach. In the non-intrusive technique, the numerical solution of a boundary value problem yields the starting values for the Newton iteration of a neighbouring boundary value problem. In the intrusive and the combined method, we apply starting values according to (19).
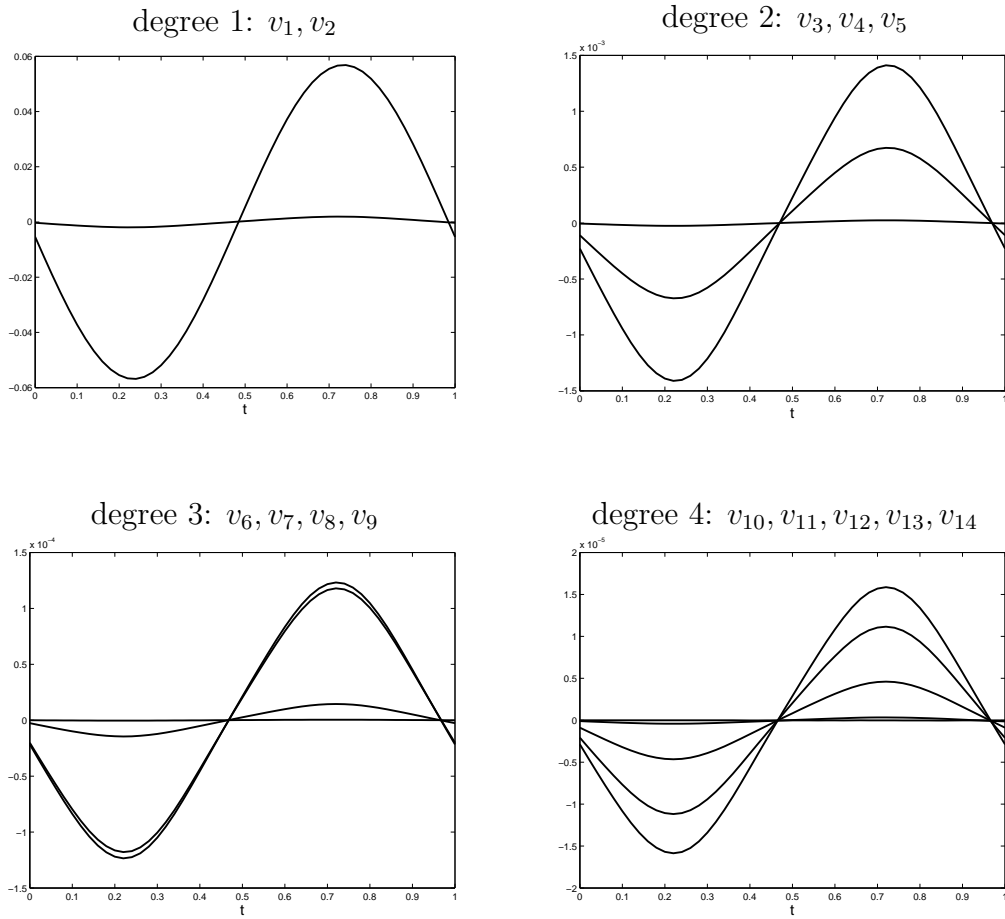
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Figure 4: Coefficient functions of gPC expansion corresponding to component x_1 of Duffing oscillator.
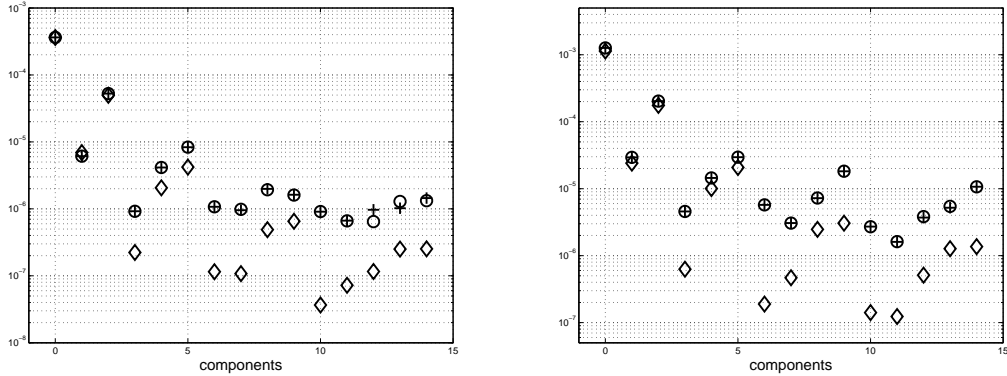
Figure 5: Maximum error in coefficient functions corresponding to x_1 (left) and x_2 (right) for different methods: non-intrusive ($\circ$), intrusive ($\diamond$) and combined technique ($+$).

Figure 5 shows the maximum error in each coefficient function. Thereby, this maximum error represents the maximum difference for $t \in [0, 1]$ with respect to the previously computed reference solution. The intrusive approach results in the highest accuracy. The non-intrusive method and the combined technique exhibit the same accuracy. The computing times for the non-intrusive method and the combined technique are nearly the same. In contrast, the intrusive approach demands five times longer computations, since many larger nonlinear systems have to be solved in the time integration.

6. Conclusions

Polynomial chaos expansions reproduce the solutions of dynamical systems with random parameters. Numerical methods can be arranged following an intrusive or a non-intrusive approach. Considering boundary value problems, a combined technique has been presented, which exhibits advantages from both approaches. On the one hand, just a single nonlinear system has to be solved, which yields a robust method. On the other hand, the dynamical systems are involved similar as in a non-intrusive approach, which provides a high potential for parallel computations. In case of ODEs, numerical results of a test example confirm that the combined technique exhibits the same accuracy as the non-intrusive method. Further investigations are necessary in the case of DAEs, since consistent initial values are required for the time integration.

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