

Time-dependent generalized polynomial chaos

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ARTICLE INFO

Article history:

Received 11 May 2009

Received in revised form 11 June 2010

Accepted 21 July 2010

Available online 13 August 2010

Keywords:

Polynomial chaos

Monte-Carlo simulation

Stochastic differential equations

Time dependence

ABSTRACT

Generalized polynomial chaos (gPC) has non-uniform convergence and tends to break down for long-time integration. The reason is that the probability density distribution (PDF) of the solution evolves as a function of time. The set of orthogonal polynomials associated with the initial distribution will therefore not be optimal at later times, thus causing the reduced efficiency of the method for long-time integration. Adaptation of the set of orthogonal polynomials with respect to the changing PDF removes the error with respect to long-time integration. In this method new stochastic variables and orthogonal polynomials are constructed as time progresses. In the new stochastic variable the solution can be represented exactly by linear functions. This allows the method to use only low order polynomial approximations with high accuracy. The method is illustrated with a simple decay model for which an analytic solution is available and subsequently applied to the three mode Kraichnan–Orszag problem with favorable results.

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1. Introduction

To describe physical problems we often make use of deterministic mathematical models. Typical constituents of such models – material properties, initial and boundary conditions, interaction and source terms, etc. – are assigned a definite value and we seek a deterministic solution to the problem. In reality, however, a physical problem will almost always have uncertain components. Material properties, for instance, might be based on imprecise experimental data. In other words, the input to a mathematical model of a real-life problem possesses some degree of randomness. We are interested in modelling this uncertainty. To this end we look for methods to quantify the effects of stochastic inputs on the solutions of mathematical models.

The Monte-Carlo method is the most popular approach to model uncertainty. It is a ‘brute-force’ method of attack: using a sample of the stochastic inputs we calculate the corresponding realizations of the solution. From the resulting sample of solutions we then determine the desired statistical properties of the solution. In most cases we have to use a large sample size to obtain accurate estimates of these statistical properties. This makes Monte-Carlo methods very expensive from a computational point of view. Furthermore, the selection of proper (pseudo-)random number generators needed for a Monte-Carlo simulation influences the results.

Besides the statistical Monte-Carlo methods a number of nonstatistical (i.e. deterministic) approaches to modelling uncertainty have been proposed. *Polynomial chaos* is one such nonstatistical method that has been shown to be particularly effective for a number of problems, especially in low dimensions. Polynomial chaos employs orthogonal polynomial functionals to expand the solution in random space. The method is based on Wiener’s [1] homogeneous chaos theory published in 1938. This

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paper paved the path for the application of truncated expansions in terms of Hermite polynomials of Gaussianly distributed random variables to model (near-)Gaussian stochastic processes. In the 1960s these Wiener–Hermite expansions were employed in the context of turbulence modelling [2,3]. However, some serious limitations were encountered – most notably due to its non-uniform convergence – leading to a decrease of interest in the method in the years that followed.

In 1991 Ghanem and Spanos [4] pioneered the use of Wiener–Hermite expansions in combination with finite element methods and effectively modelled uncertainty for various problems encountered in solid mechanics. At this point in time the polynomial chaos method was capable of achieving an exponential convergence rate for Gaussian stochastic processes only. In 2002 Xiu and Karniadakis [5] introduced *generalized polynomial chaos* (gPC). It was recognized that the PDF of a number of common random distributions plays the same role to the weighting function in the orthogonality relations of orthogonal polynomials from the so-called Askey scheme. Xiu and Karniadakis established that, in order to achieve optimal convergence, the type of orthogonal polynomials in the chaos expansion should correspond to the properties of the stochastic process at hand, based on the association between PDF and weighting function. This gPC approach has been applied to a number of problems in fluid flow [6–11]. Although the polynomial chaos method was initially generalized to polynomials of the Askey scheme only, the extension to arbitrary random distributions soon followed. By employing the correspondence between PDF and weighting function in the orthogonality relation, we can generate optimal expansion polynomials for an arbitrary random distribution. The resulting expansion polynomials need not necessarily come from the Askey scheme. There exist various ways to calculate these optimal expansion polynomials, see for instance [12,13].

The gPC method has been shown to be effective for a number of problems resulting in exponential convergence of the solution. However, there are also situations in which gPC is not effective. A discontinuity of the solution in the random space may, for instance, lead to slow convergence or no convergence at all. In addition, problems may be encountered with long-time integration, see [11,14,15]. The statistical properties of the solution will most likely change with time. This means that the particular orthogonal polynomial basis that led to exponential convergence for earlier times may lose its effectiveness for later times resulting in a deteriorating convergence behaviour with time. Hence, for larger times unacceptable error levels may develop. These errors may become practically insensitive to an increase of the order of the polynomial expansion beyond a certain order. Part of this failure can be attributed to the global character of the approximation. Local methods seem to be less sensitive to error growth in time. Wan and Karniadakis [16] have developed a multi-element polynomial chaos method (ME-gPC). The main idea of ME-gPC is to adaptively decompose the space of random inputs into multiple elements and subsequently employ polynomial chaos expansions at element level. Pettit and Beran [17] successfully applied a Wiener–Haar approximation for single frequency oscillatory problems. This approach relies on the fact that one knows in advance that the time evolution will be oscillatory. Multi-element techniques for time-dependent stochastic for oscillatory solutions have also been applied by Witteveen and Bijl [18–20].

Despite the success of gPC methods, *unsteady dynamics* still poses a significant challenge [11,15].

The approach presented in this paper to resolve the long-time integration problems with the *global gPC method* is based on the fact that the PDF of the solution will not remain constant in time. Recognizing that the initial polynomial chaos expansion loses its optimal convergence behaviour for later times, we develop a *time-dependent* polynomial chaos (TDgPC) method. The main idea of TDgPC is to determine new, optimal polynomials for the chaos expansion at a number of discrete instants in time. These new polynomials are based on the stochastic properties of the solution *at the particular time level*. In this way optimal convergence behaviour is regained over the complete time interval. In this first paper, the method will be applied to an ordinary differential equation, namely the decay model, and a system of ordinary differential equations, the so-called Kraichnan–Orszag three-mode problem.

The outline of this paper is as follows: In Section 2 the basic idea of generalized polynomial chaos is explained. In Section 3 the breakdown of gPC is demonstrated and an explanation is given why gPC loses its optimality. In this section also the idea of time-dependent generalized polynomial chaos is introduced. In Section 4 TDgPC is applied to the Kraichnan–Orszag three-mode problem. First, one of the initial conditions is randomly distributed and subsequently the method is applied to the case in which all three initial conditions are randomly distributed. In Section 5 conclusions are drawn. Although this paper focuses on the global polynomial chaos method, the failure for long-time integration is not restricted to these methods. In the appendix some additional considerations for Probabilistic Collocation methods will be given. Although collocation methods do not rely on polynomial expansions for the evolution equation, they implicitly use polynomial representations for the calculation of the mean and variance.

2. Polynomial chaos

A second-order stochastic process can be expanded in terms of orthogonal polynomials of random variables, i.e. a polynomial chaos expansion. These polynomial chaos expansions can be used to solve stochastic problems. In this section we introduce the polynomial chaos expansion and we outline a solution method for stochastic problems based on these expansions.

2.1. The polynomial chaos expansion

Let $(\Omega, \mathcal{F}, \mathcal{P})$ be a probability space. Here Ω is the sample space, $\mathcal{F} \subset 2^\Omega$ its σ -algebra of events and $\mathcal{P}$ the associated probability measure. In addition, let $S \subset \mathbb{R}^d$ ($d = 1, 2, 3$) and $T \subset \mathbb{R}$ be certain spatial and temporal domains, respectively. In a physical context we frequently encounter stochastic processes in the form of a scalar- or vector-valued random function like

$$\mathbf{u}(\mathbf{x}, t, \omega) : S \times T \times \Omega \rightarrow \mathbb{R}^b, \quad (1)$$

where $\mathbf{x}$ denotes position, t for time, ω represents an element of the sample space Ω and $b = 1$ for scalar-valued random variables and $b > 1$ for vector-valued random variables. The probability space can often be described by a finite number of random variables

$$\xi_1, \xi_2, \dots, \xi_n : \Omega \rightarrow \mathbb{R}, \quad (2)$$

in which case the stochastic variable of (1) can be written as

$$\mathbf{u}(\mathbf{x}, t, \xi) : S \times T \times \mathbb{R}^n \rightarrow \mathbb{R}^b, \quad (3)$$

where $\xi = (\xi_1, \dots, \xi_n)$ is an n -dimensional vector of random variables. In this work we will exclusively be dealing with stochastic processes of the form (3), i.e. processes that can be characterized by a finite set of random variables.

The stochastic process (3) can be represented by the following *polynomial chaos expansion*

$$\mathbf{u}(\mathbf{x}, t, \xi(\omega)) = \sum_{i=0}^n \mathbf{u}_i(\mathbf{x}, t) \Phi_i(\xi(\omega)), \quad (4)$$

where the trial basis $\{\Phi_i(\xi)\}$ consists of orthogonal polynomials in terms of the random vector ξ .

Historically, Wiener [1] first formulated a polynomial chaos expansion in terms of Hermite polynomials of Gaussianly distributed random variables. It follows from a theorem by Cameron and Martin [21] that this Hermite-chaos expansion converges to any stochastic process $\mathbf{u}(\omega) \in L_2(\Omega, \mathcal{F}, \mathcal{P})$ in the L_2 sense. This means that a Hermite-chaos expansion can – in principle – be used to represent any stochastic process with finite variance (a requirement that is met for most physical processes). In practice, however, optimal convergence is limited to processes with Gaussian inputs. Gaussian random inputs generally result in a stochastic process that has a large Gaussian part, at least for early times. This Gaussian part is represented by the first-order terms in the Hermite-chaos expansion. Higher order terms can be thought of as non-Gaussian corrections. Hence, for Gaussian random inputs we can expect a Hermite-chaos expansion to converge rapidly.

For general, non-Gaussian random inputs, however, the rate of convergence of a Hermite-chaos expansion will most likely be worse. Although convergence is ensured by the Cameron–Martin theorem, we will generally need a large number of higher-order terms in the expansion to account for the more dominant non-Gaussian part. To obtain an optimal rate of convergence in case of general random inputs we need to tailor the expansion polynomials to the stochastic properties of the process under consideration. Although Ogura [22] had already employed Charlier-chaos expansions to describe Poisson processes, Xiu and Karniadakis [5] were the first to present a comprehensive framework to determine the optimal trial basis $\{\Phi_i\}$.

The *optimal* set of expansion polynomials forms a complete orthogonal basis in $L_2(\Omega, \mathcal{F}, \mathcal{P})$ with orthogonality relation

$$\langle \Phi_i, \Phi_j \rangle = \langle \Phi_i^2 \rangle \delta_{ij}, \quad (5)$$

where δ_{ij} is the Kronecker delta and $\langle \cdots \rangle$ denotes the ensemble average. To be more specific, the optimal set $\{\Phi_i(\xi)\}$ is an orthogonal basis in the Hilbert space with associated inner product

$$\langle G(\xi(\omega)), H(\xi(\omega)) \rangle = \int_{\Omega} G(\xi(\omega)) H(\xi(\omega)) d\mathcal{P}(\omega) = \int_{\text{supp}(\xi)} G(\xi) H(\xi) f_{\xi}(\xi) d\xi, \quad (6)$$

where $f_{\xi}(\xi)$ is the probability density function (PDF) of the random variables that make up the vector ξ . Note that the PDF acts as a weighting function in the orthogonality relation for $\{\Phi_i(\xi)\}$. So, the *type* of orthogonal expansion polynomials (determined by the weighting function in the orthogonality relation) that can best be used in a polynomial chaos expansion depends on the nature of the stochastic process at hand through the PDF of the random variables that describe the probability space. The fact that the trial basis defined in (5) and (6) is optimal hinges on the presumption that the random function $\mathbf{u}(\mathbf{x}, t, \xi(\omega))$ represented by the polynomial chaos expansion has roughly the same stochastic characteristics as the random variables in ξ , at least for early times. Hence, the higher-order terms in the expansion are expected to be small, reducing the dimensionality of the problem and resulting in rapid convergence. As a generalization of the Cameron–Martin theorem, we also expect this generalized polynomial chaos expansion (with $\{\Phi_i(\xi)\}$ being a complete basis) to converge to any stochastic process $\mathbf{u}(\omega) \in L_2(\Omega, \mathcal{F}, \mathcal{P})$ in the L_2 sense.

In [5] it was recognized that the weighting functions associated with a number of orthogonal polynomials from the so-called Askey scheme are identical to the PDFs of certain ‘standard’ random distributions. Table 1 gives some examples. The authors of [5] studied a simple test problem subject to different random inputs with ‘standard’ distributions like the ones in Table 1. Exponential error convergence was obtained for a polynomial chaos expansion with an optimal trial basis (i.e. in accordance with Table 1). Furthermore, it was shown that exponential convergence is generally not retained when the optimal trial basis is *not* used (for example, employing Hermite chaos instead of Jacobi chaos when the random input has a beta distribution).

The focus in [5] was on orthogonal polynomials from the Askey scheme and corresponding ‘standard’ random distributions. However, there is no reason to limit the members of possible trial bases to polynomials from the Askey scheme. With (5) and (6) we can determine an optimal trial basis for arbitrary, ‘nonstandard’ distributions of ξ as well. When the PDF of ξ is

Table 1

Orthogonal polynomials from the Askey scheme constitute an optimal trial basis for a number of well-known random distributions.

Distribution of ξ	Expansion polynomials $\{\Phi_i(\xi)\}$
Uniform	Legendre
Gaussian	Hermite
Beta	Jacobi
Gamma	Laguerre

known we can use various orthogonalization techniques to calculate the corresponding optimal trial basis $\{\Phi_i(\xi)\}$. In this work we will use Gram–Schmidt orthogonalization, [23,24].

Sometimes the probability space can be characterized by a single random variable, i.e. $n = 1$ in (2) and the vector ξ is reduced to the scalar ξ . In this case the index i in $\{\Phi_i(\xi)\}$ directly corresponds with the degree of the particular expansion polynomial. For example, $\Phi_3(\xi)$ is a third degree polynomial in ξ .

In the more general situation of a multidimensional probability space, $n > 1$, the correspondence between i and polynomial degree does not exist and i reduces merely to a counter. To construct the multidimensional expansion polynomials $\{\Phi_i(\xi)\}$ we first calculate the one-dimensional polynomials $\phi_p^{(\xi_j)}(\xi_j)$ for $j = 1, \dots, n$ and $p = 0, 1, 2, \dots$ using a Gram–Schmidt algorithm with orthogonality relation

$$\langle \phi_p^{(\xi_j)}, \phi_q^{(\xi_j)} \rangle = \int_{\text{supp}(\xi_j)} \phi_p^{(\xi_j)}(\xi_j) \phi_q^{(\xi_j)}(\xi_j) f_{\xi_j}(\xi_j) d\xi_j = \langle \phi_p^{(\xi_j)^2} \rangle \delta_{pq}. \quad (7)$$

For these one-dimensional polynomials p again corresponds to the polynomial degree and the superscript (ξ_j) indicates that the polynomial is orthogonal with respect to f_{ξ_j} . The *multidimensional* expansion polynomials can now be constructed from the simple tensor product

$$\Phi_i(\xi) = \phi_{p_1}^{(\xi_1)}(\xi_1) \phi_{p_2}^{(\xi_2)}(\xi_2) \cdots \phi_{p_n}^{(\xi_n)}(\xi_n) \quad (8)$$

with some mapping $(p_1, p_2, \dots, p_n) \rightarrow i$.

The procedure above assumes that $\xi_1, \dots, \xi_n$ are stochastically independent¹ which implies that

$$f_\xi(\xi) = f_{\xi_1}(\xi_1) f_{\xi_2}(\xi_2) \cdots f_{\xi_n}(\xi_n). \quad (9)$$

It can now easily be verified that the multidimensional expansion polynomials $\{\Phi_i(\xi)\}$ constructed according to (8) form an optimal orthogonal trial basis in agreement with (5) and (6).

2.2. The gPC method

In this section we outline a solution procedure for stochastic problems based on the polynomial chaos expansion given in (4). Consider the abstract problem

$$\mathcal{L}(\mathbf{x}, t, \xi(\omega); \mathbf{u}) = \mathbf{f}(\mathbf{x}, t, \xi(\omega)), \quad (10)$$

where $\mathcal{L}$ is a (not necessarily linear) differential operator and $\mathbf{f}$ some source function. The randomness, represented by the random vector ξ , can enter the problem either through $\mathcal{L}$ (e.g. random coefficients) or $\mathbf{f}$, but also through the boundary or initial conditions or some combination.

We approximate the stochastic solution function $\mathbf{u}(\mathbf{x}, t, \xi(\omega))$ by a truncated polynomial chaos expansion similar to (4). The truncation of the infinite series is necessary to keep the problem computationally feasible. In this work we will truncate the series in such a way that all expansion polynomials up to a certain maximum degree, denoted by P , are included. The number of terms $(N + 1)$ in the expansion now follows from this maximum degree P and the dimensionality n of the random vector ξ according to

$$N + 1 = \binom{P + n}{P} = \frac{(P + n)!}{P!n!}. \quad (11)$$

We continue by substituting the polynomial chaos expansion for $\mathbf{u}$ into the problem equation and execute a Galerkin projection. This means that we multiply (10) by every polynomial of the expansion basis $\{\Phi_i\}$ and take the ensemble average to obtain

¹ For the more general case, one has to employ conditional probability distributions. For the method presented in this paper this will not be necessary. Although stochastic independence will gradually be lost in the time evolution, we transform everything back to the initial distribution where all randomness is stochastically independent.

$$\left\langle \mathcal{L} \left(\mathbf{x}, t, \xi; \sum_{i=0}^N \mathbf{u}_i(\mathbf{x}, t) \Phi_i(\xi) \right), \Phi_j(\xi) \right\rangle = \langle f(\mathbf{x}, t, \xi), \Phi_j(\xi) \rangle, \quad j = 0, 1, \dots, N. \quad (12)$$

The Galerkin projection above ensures that the error we make by representing $\mathbf{u}$ by a polynomial chaos expansion is orthogonal to the function space spanned by the expansion basis $\{\Phi_i\}$ (Galerkin orthogonality). As a result of the orthogonality of the expansion polynomials, (12) can be reduced to a set of $N+1$ coupled, *deterministic* equations for the $N+1$ expansion coefficients $\mathbf{u}_i(\mathbf{x}, t)$. So, the remaining problem is stripped of all stochastic characteristics by the Galerkin projection. The remaining equations can now be solved by any conventional discretization techniques.

3. Long-time integration

In this section, we will discuss the issues of long-time integration related to polynomial chaos for a stochastic ordinary differential equation (ODE). We will use a simple differential equation, the decay model, to illustrate the inability to use gPC for long-time integration. We then explain why a standard gPC expansion is not able to describe the solution for growing time.

3.1. Stochastic ordinary differential equation

Consider the following stochastic ordinary differential equation, which can be seen as a simple model,

$$\frac{du(t)}{dt} + ku(t) = 0, \quad u(0) = 1. \quad (13)$$

The decay rate k is considered to be a random variable $k = k(\omega)$. Therefore, the solution $u(t)$ of the above equation will be a stochastic process $u(t, \omega)$. It is assumed that the stochastic processes and random variables appearing in this problem can be parameterized by a single random variable ξ . This implies that the problem modeled by (13) can be formulated as, find $u(t, \xi)$ such that it satisfies

$$\frac{du(t, \xi)}{dt} + k(\xi)u(t, \xi) = 0 \quad \text{in } \Gamma = T \times S, \quad (14)$$

and the initial condition $u(t=0) = 1$. The domain Γ consists of the product of the temporal domain $T = [0, t_{\text{end}}]$ and the domain S , being the support of the random variable ξ . In this work, we will choose k to be *uniformly* distributed in the interval $[0, 1]$, characterized by the probability density function:

$$f_k(k) = 1, \quad 0 \leq k \leq 1. \quad (15)$$

This particular distribution of the random input parameter causes the stochastic process $u(t, \omega)$ to be second-order, even for $t \rightarrow \infty$ and therefore allows a gPC expansion.

The exact solution of this equation is given by

$$u(t, \omega) = e^{-kt}, \quad (16)$$

such that both the statistical parameters of interest, the mean and the variance, can be calculated exactly. The expression for the stochastic mean $\bar{u}_{\text{exact}}(t)$ is given by

$$\bar{u}_{\text{exact}}(t) = E[u(t)] = \int_0^1 e^{-kt} f_k(k) dk = \frac{1 - e^{-t}}{t}, \quad (17)$$

and the variance $\sigma_{\text{exact}}(t)$ is given by

$$\sigma_{\text{exact}}(t) = E[(u(t) - \bar{u}(t))^2] = \int_0^1 (e^{-kt} - \bar{u})^2 f_k(k) dk = \frac{1 - e^{-2t}}{2t} - \left(\frac{1 - e^{-t}}{t} \right)^2. \quad (18)$$

From the continuous expansion we can see that the variance is bounded for all values of t so we are dealing with a second-order process.

3.2. gPC results

The first step in applying a gPC procedure to the stochastic ODE (14), is to select a proper gPC expansion. Because the input parameter k is uniformly distributed, according to the rules of gPC, we opt for a spectral expansion in terms of a uniform random variable ξ with zero mean and unit variance. This means that ξ is uniformly distributed in the interval $[-1, 1]$, yielding the following PDF:

$$f_\xi(\xi) = \frac{1}{2}, \quad -1 \leq \xi \leq 1, \quad (19)$$

such that the decay rate $k(\xi)$ is given by:

$$k(\xi) = \frac{1}{2}\xi + \frac{1}{2}. \quad (20)$$

Hence, according to Table 1, the Legendre polynomials $\{L_i\}_{i=0}^P$ should be selected as the trial basis for the spectral expansion. Using the Legendre polynomials in (12) we obtain the following system of differential equations

$$\frac{du_j(t)}{dt} = -\frac{1}{\langle L_j^2 \rangle} \sum_{i=0}^P \langle k L_i L_j \rangle u_i(t), \quad j = 0, 1, \dots, P. \quad (21)$$

Employing a gPC expansion, the approximated stochastic mean is simply equal to the first mode of the solution:

$$\bar{u}(t) = u_0(t). \quad (22)$$

The approximated variance is then given by

$$\sigma(t) = \sum_{i=0}^P (u_i(t))^2 \langle L_i^2 \rangle - (u_0(t))^2. \quad (23)$$

Fig. 1 shows the solution of the mean and variance using third-order Legendre-chaos. It can clearly be observed that the gPC solution is capable of following the solution only for early times. Especially for the variance, the gPC solution diverges after a while. The same behavior can be observed in the plot showing the evolution of the error, displayed in Fig. 2. Here, it can be seen that the error ϵ for the mean and variance, respectively defined as

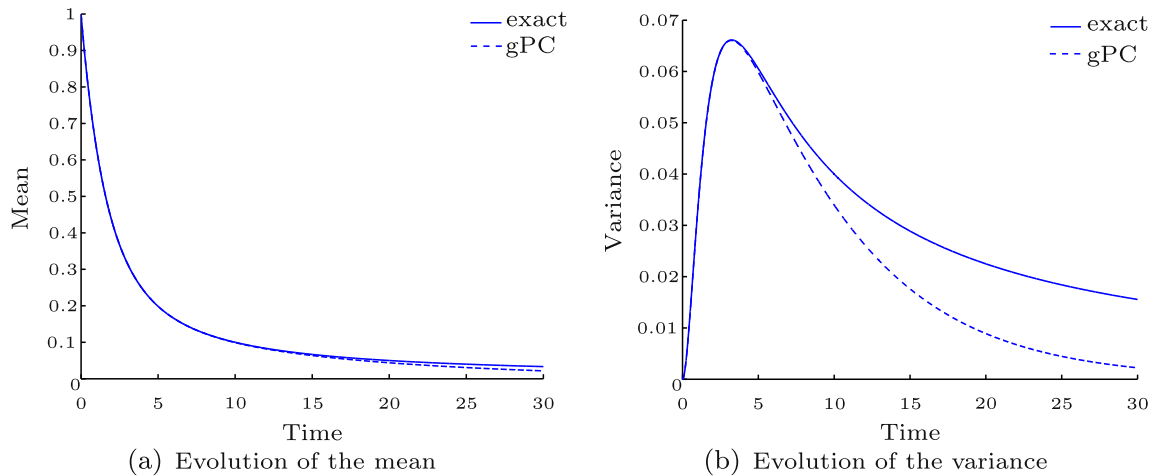


Fig. 1. Evolution of the mean and variance for third-order Legendre-chaos.

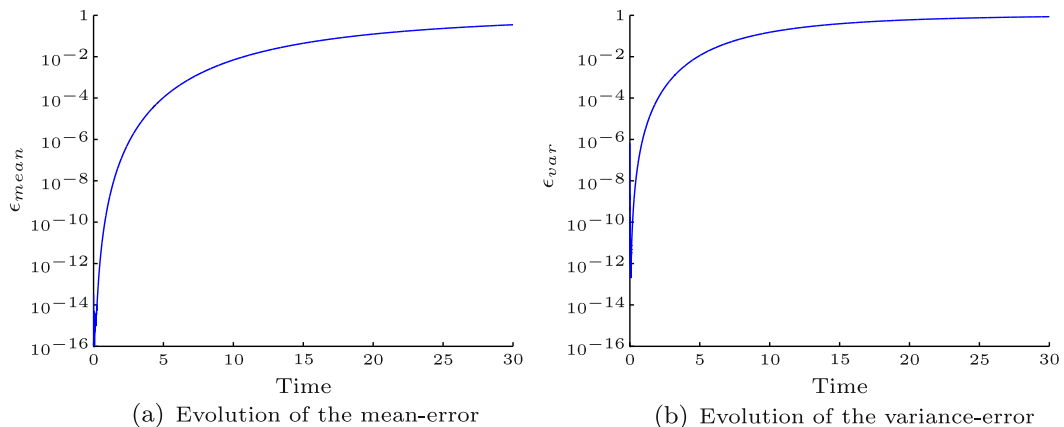


Fig. 2. Evolution of the error for third-order Legendre-chaos.

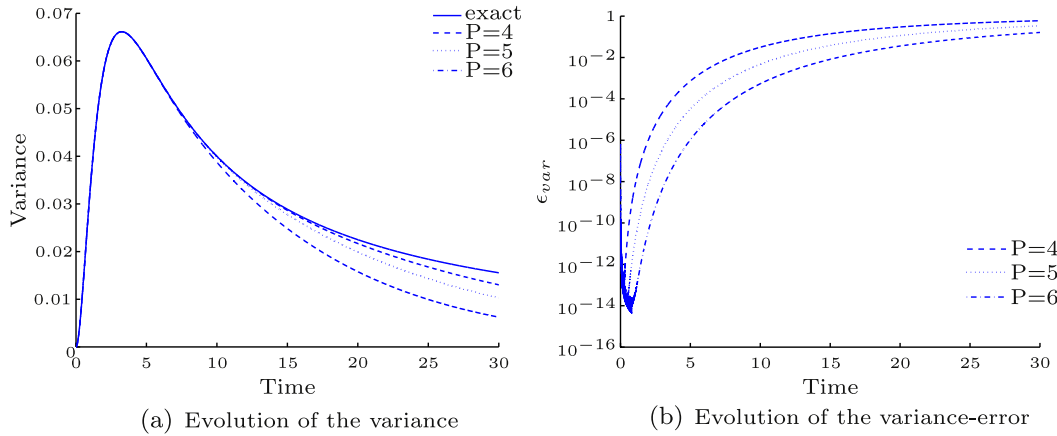


Fig. 3. Behavior of the variance for increasing order Legendre-chaos.

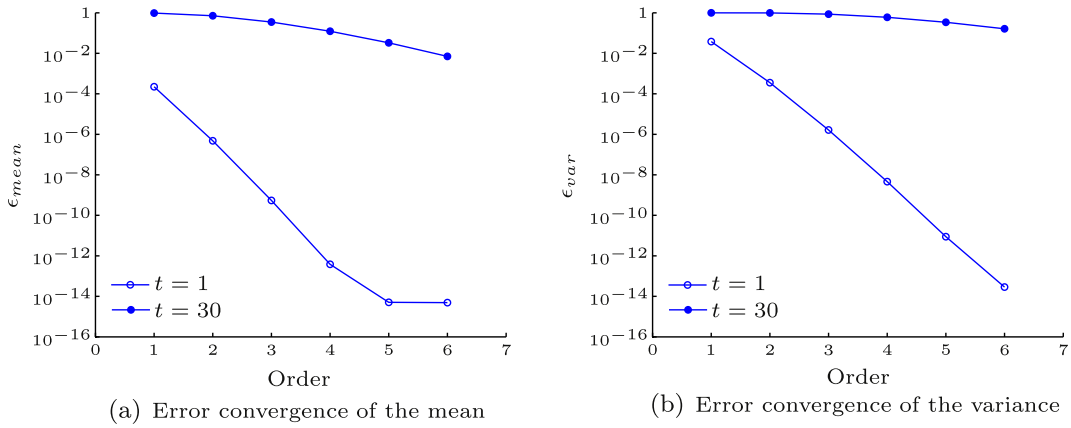


Fig. 4. Error convergence of the mean and variance.

$$\epsilon_{\text{mean}}(t) = \left| \frac{\bar{u}(t) - \bar{u}_{\text{exact}}(t)}{\bar{u}_{\text{exact}}(t)} \right|, \quad \epsilon_{\text{var}}(t) = \left| \frac{\sigma(t) - \sigma_{\text{exact}}(t)}{\sigma_{\text{exact}}(t)} \right| \quad (24)$$

is only acceptable for early times. After this, the error quickly grows to the undesired order of $O(1)$, which is unacceptable.

This rather poor behavior can be somewhat alleviated by increasing the expansion order. This is shown in Fig. 3, where it can be seen that for increasing order, the gPC solution follows the exact solution for a longer period. In Fig. 4 the convergence with polynomial enrichment is shown at $t = 1$ and $t = 30$. From this figure it is clear that p -refinement leads to exponential convergence for $t = 1$, but hardly converges for $t = 30$.

Increasing the expansion order, however, is not an effective approach. First of all, in the general case, the gPC procedure becomes quite time-consuming for high values of P . More importantly, increasing the maximal polynomial degree in fact only postpones the troubles that gPC possesses. For a fixed polynomial degree P , the error levels will become definitely unacceptable after some time. Hence, continuing to increase the end-time will require an ever-increasing polynomial degree, which is not feasible in practice.

3.3. Why gPC fails

Let us consider again the gPC expansion of the approximated solution $u(t, \xi)$:

$$u(t, \xi) = \sum_{i=0}^P u_i(t) L_i(\xi). \quad (25)$$

The best approximation to the exact solution can be achieved by minimizing the error, defined as $|u_{\text{exact}} - \sum u_i L_i|$, in a certain norm. Doing this for the $L^2(\Omega)$ norm, we end up with the Fourier–Legendre series

$$u(t, \xi) = \sum_{i=0}^P \alpha_i(t) L_i(\xi), \quad (26)$$

in which the Legendre coefficients $\alpha_i(t)$ are given by:

$$\alpha_i(t) = \frac{\langle u_{\text{exact}} L_i \rangle}{\langle L_i^2 \rangle} \quad (27)$$

with the ensemble average $\langle \cdot \rangle$ defined as in (6). More explicitly, it can be calculated that the Legendre coefficients for the stochastic ODE problem in question, are given by:

$$\alpha_i(t) = \sum_{j=0}^i \frac{1}{t^{j+1}} \frac{(i+j)!}{(i-j)!j!} ((-1)^{i+j} - e^{-t}). \quad (28)$$

The only error occurring in the finite Fourier–Legendre series approximation is due to truncation. In fact, it is the optimal P th order approximation, being the interpolant of the exact solution.

Using (28) for the coefficients, both the mean and variance of the truncated Fourier–Legendre expansion can be calculated using the (22) and (23). Because the expression to calculate the mean exactly, (17), corresponds to the first Legendre coefficient α_0 , the mean obtained by the Fourier–Legendre expansion gives the exact solution. In order to calculate the variance however, the truncation of the Fourier–Legendre series after $P+1$ terms will cause the calculated variance to be different from the exact variance, as can be seen from (23), where it can be observed that only increasing the polynomial degree will cause the variance to converge to its exact value. Plotting the evolution of the variance for different values of P , one can clearly see in Fig. 5 that even the optimal gPC expansion (optimal in the sense of minimal error) is not capable of approximating the second-order statistics accurately. Although the approximation is better than in case of the gPC procedure using a Galerkin projection, which also contains a discretization error, the error levels are still quite poor for the highest time level, and the occurrence of unacceptable error levels is just a matter of selecting a later end-time.

Because of this observation, it can be concluded that the gPC expansion itself is not suitable for the approximation of all statistics in this time-dependent stochastic ODE. As even the Fourier–Legendre polynomial chaos expansion (26) does fail for long-time integration, it does not matter what kind of gPC procedure one chooses, e.g. a collocation or a least-squares projection. The problem will not be overcome by different discretizations or time-integration methods.

The failure of gPC for long-time integration can be explained by closer examining the governing equation:

$$\frac{du(t, \xi)}{dt} + k(\xi)u(t, \xi) = 0. \quad (29)$$

At first sight, this seems a linear ODE. But due to the fact that both the input parameter k and the solution u depend on the random variable ξ , a quadratic non-linearity appears in the second term. This non-linearity in random space is responsible for the behavior of the solution. For example, it causes the deterministic solution

$$u_{\text{det}}(t) = e^{-\bar{k}t} = e^{-0.5t}, \quad (30)$$

to deviate from the mean of the stochastic solution $\bar{u}(t)$,

$$\bar{u}(t) = \frac{1 - e^{-t}}{t}, \quad (31)$$

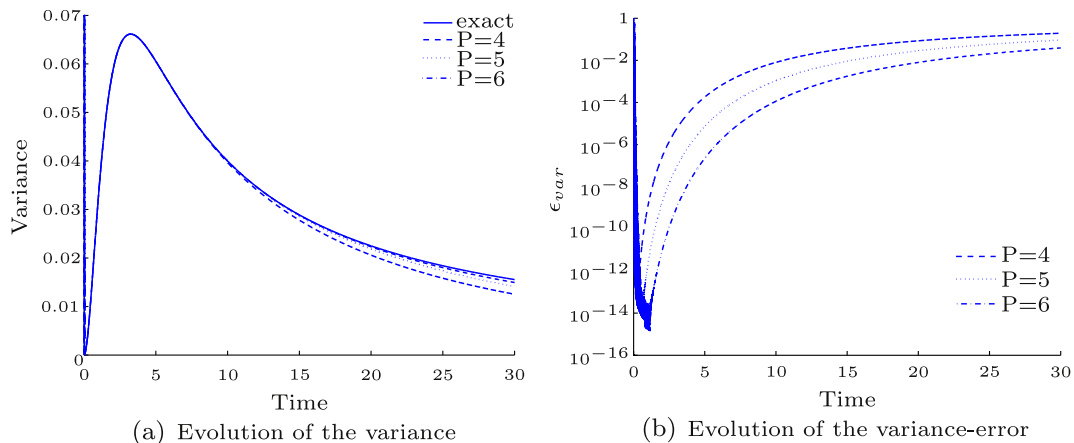


Fig. 5. Behavior of the variance using the Fourier–Legendre chaos expansion.

i.e. the deterministic solution employing the most probable value $\bar{k}$ of the input parameter k

$$\bar{k} = E[k] = \int_0^1 k f_k dk = \frac{1}{2}, \quad (32)$$

does not correspond to the mean of the stochastic solution, incorporating the range and distribution of the random parameter k . In Fig. 6, it can be clearly seen that only for early times, those values do correspond, while for increasing time, the difference grows. This behavior is known as *stochastic drift*. This implies that only for early times, the solution can be approximated as a linear continuation of the random input. For increasing time, the non-linear development becomes more and more dominant, requiring an increasing amount of terms in the polynomial chaos expansion in terms of the input expansion. A way to see this, is to consider that the solution remembers and resembles the stochastic input only for early times, while for later times, the solution starts to deviate from the distribution of the input due to the occurring quadratic non-linearity and starts to develop its own stochastic characteristics. As a result, for longer time integration, expressing the solution in terms of the input parameter requires more and more expansion terms. As for the Gaussian inputs discussed in Section 2, the appearance of the higher-order modes in the expansion indicates that the solution is drifting away from a uniformly distributed stochastic process and therefore the concept of optimal polynomial chaos as explained in [5] will no longer be applicable. The failure observed for gPC is not limited to gPC. Probabilistic Collocation methods show a similar behaviour. The behaviour of PCM and additional considerations for long-time integration are given in Appendix A.

3.4. Time-dependent Wiener–Hermite expansion

An alternative approach of expanding random variables is in terms of so-called *ideal random functions* [25]. Ideal random functions are improper functions which can be interpreted as the derivative of the Wiener random function.

The expansion in terms of ideal random functions also breaks down for time-dependent problems. In [26–28] it was proposed to make the random functions time-dependent and to set up a separate differential equation for the determination of the optimal time-dependent ideal random functions. In [27] it is stated that: “The principle idea of the method is to choose different ideal random functions at different times in such a way that the unknown random function is expressed with good approximation by the first few terms of the Wiener–Hermite expansion for long-time duration. As an example it will be shown in I that the exactly Gaussian solutions of turbulence in an incompressible inviscid fluid and the three-mode problem are expressed by the first term alone of the Wiener–Hermite expansion if we take a suitable time-dependent ideal random function as the variable.”

The assumption is that for different times t , different random functions $A(x, t) = H^{(1)}(x, t)$ should be chosen (see [25, Eq. (3.2)] for the definition of the functions $H_{i_1, \dots, i_n}^{(n)}(x)$). Assuming that the “new” random functions are not too different from the “old” random functions, they can be approximated by a rapidly converging Wiener–Hermite expansion in time, which gives the differential equation from which the new random functions can be obtained. The coefficients in the evolution equation are constrained by the fact that the new random functions should satisfy the properties of ideal random functions [25, Eqs. (2.1) and (2.2)].

In the current paper the same basic idea is employed, namely that the basis functions in which the random variable is expanded should change as a function of time, but no separate evolution equation is set up for the new basis functions. Instead, the solution at a given time t is chosen as the new random variable and the “old” basis functions are now expressed in terms of this “new” random variable.

3.5. Time-dependent polynomial chaos

In this section the basic idea, as developed by Vos [29], of time-dependent generalized polynomial chaos will be explained. This idea is easy to understand and fully reflects the notion that the PDF changes as function of time and therefore

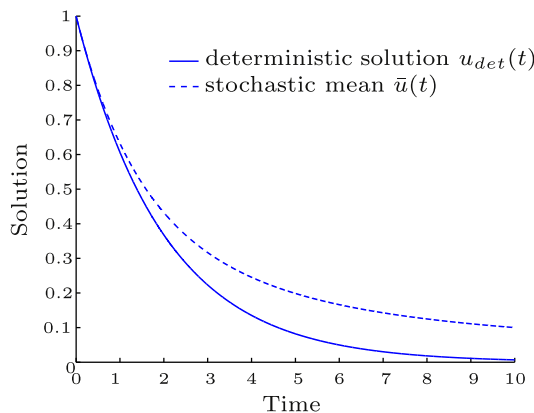


Fig. 6. Evolution of deterministic solution and the mean of the stochastic solution.

requires a different set of orthogonal polynomials. In the next section the same approach will be applied to the Kraichnan–Orszag three-mode problem and there several improvements on this basic idea will be presented.

Time-dependent polynomial chaos works as follows. Consider the same ODE problem as in Section 3.1

$$\frac{du(t, \xi)}{dt} + k(\xi)u(t, \xi) = 0. \quad (33)$$

We start with the gPC procedure using a Legendre-chaos expansion as explained in Section 3.2

$$u(t, \xi) = \sum_{i=0}^P u_i(t) L_i(\xi). \quad (34)$$

As this gPC approach works fine for early times, this is a suitable approach to start with. However, when progressing in time using an RK4 numerical integration, the results start to become worse due to the quadratic non-linearity in random space. That is why at a certain time level, the gPC procedure should be stopped, preferably before the non-linear development becomes too significant. This can be monitored by inspecting the non-linear terms in the gPC expansion of the solution. Consequently, stopping the numerical integration in time when the non-linear coefficients become too big with respect to the linear coefficient, given by the condition

$$\max(|u_2(t)|, \dots, |u_P(t)|) \geq \frac{|u_1(t)|}{\theta}, \quad (35)$$

can be used as a suitable stopping criterion.

Suppose we halt the gPC procedure at $t = t_1$. We now change the expansion by introducing a new random variable equal to the solution u at $t = t_1$, given by

$$\psi = u(t_1, \xi) = \sum_{i=0}^P u_i(t_1) L_i(\xi) = T(\xi), \quad (36)$$

where T maps ξ onto ψ . This mapping is not necessarily bijective. If the PDF of ξ is given by $f_\xi(\xi)$, then the PDF of ψ can in principle be obtained from, [30,31]

$$f_\psi(\psi) = \sum_n \frac{f_\xi(\xi_n)}{\left| \frac{dT(\xi)}{d\xi} \right|_{\xi=\xi_n}}, \quad (37)$$

where the sum is taken so as to include all the roots ξ_n , $n = 1, 2, \dots$ which are the real solutions of the equation

$$\psi = T(\xi) = 0. \quad (38)$$

The new gPC expansion should be a polynomial expansion in terms of this random variable ψ . According to the gPC rules, the polynomial basis $\{\phi_i\}$ should be chosen such that the polynomials are orthogonal with respect to a weighting function equal to the PDF of ψ . Because the random variable ψ depends on the solution, the new polynomial basis should be created *on-the-fly*. Having obtained the new PDF in terms of ψ we can set up a system of monic orthogonal polynomials with respect to the weight function $f_\psi(\psi)$. This orthogonal system is defined by

$$\begin{aligned} \phi_0(\psi) &= 1, \\ \int \phi_i(\psi) \phi_j(\psi) f_\psi(\psi) d\psi &= c_i \delta_{ij}, \quad i, j = 1, \dots, P. \end{aligned} \quad (39)$$

As mentioned before, various alternatives are feasible to create this set of polynomials numerically. In this work, we choose to create the orthogonal polynomial basis using a Gram–Schmidt orthogonalization. In this way, a new proper gPC expansion of the solution will be created. With respect to this new orthogonal system the solution u can be represented as

$$u(t, \psi) = \sum_{i=0}^P u_i(t) \phi_i(\psi). \quad (40)$$

Moreover, because it is based on the statistics of the solution, it is the optimal gPC expansion which will yield optimal convergence for early times, starting from $t = t_1$.

However, before the gPC procedure can be continued, some extra information should be updated. First of all, the solution at time level t_1 , $u(t_1, \xi) = \sum u_i(t_1) L_i(\xi)$, should be translated to new (stochastic) initial conditions for u in terms of the new random variable ψ . Due to the use of monic orthogonal polynomials in the Gram–Schmidt orthogonalization, this yields the following exact expansion

$$u(t_1, \psi) = \phi_1(\psi) - u_0(t_1) \phi_0(\psi), \quad (41)$$

in which $u_0(t_1)$ is equal to the value of $u_0(t_1)$ from the old expansion. Note that this is a linear expansion in ψ .

In practice, the new PDF (37), is not explicitly constructed, but we make use of the mapping (36)

$$\int g(\psi) f_\psi d\psi = \int g(T(\xi)) f_\xi d\xi \quad (42)$$

to convert all integrals to the original stochastic variable ξ .

This new expansion should then be employed until a next time level t_2 , at which criterion (35) is fulfilled again. Then, the algorithm should be repeated. In this way, one can march through the time domain, reinitializing the gPC expansion at certain discrete time levels. The whole idea of transforming the problem to a different random variable at those time levels is to capture the non-linearity of the problem under consideration in the PDF. The time-dependent generalized polynomial chaos can be summarized as:

Algorithm

- construct an ODE system employing gPC based on the random input
- integrate in time
- time step i : if $\max(|u_2(t_i)|, \dots, |u_P(t_i)|) \geq \frac{|u_1(t_i)|}{\theta}$
- calculate the PDF of ψ_{new}
- Gram–Schmidt orthogonalization: create a random trial basis $\{\Phi_i(\psi_{new})\}$
- generate new initial conditions: $u(t_i, \psi_{prev}) \rightarrow u(t_i, \psi_{new})$
- construct a new ODE system using (42)
- calculate mean and variance
- postprocessing

The rationale behind TDgPC is the idea that the coefficient k and the solution u need not have the same probability distribution. We assume that the solution of the decay model can be decomposed as

$$u(t, \zeta) = \sum_{i=0}^N u_i(t) \phi_i(\zeta), \quad (43)$$

where the basis functions $\phi_i(\zeta)$ are orthogonal with respect to the probability density function $f_u(t, \zeta)$ of u and **not** the probability density function $f_k(\xi)$ of the stochastically distributed decay coefficient $k(\xi)$. Then the expansion coefficients are given by

$$u_j(t) = \frac{1}{\langle \phi_j^2 \rangle} \int_{-\infty}^{\infty} u(t, \zeta) \phi_j(\zeta) f_u(t, \zeta) d\zeta, \quad (44)$$

and hence,

$$\begin{aligned} \frac{du_j}{dt} &= \frac{1}{\langle \phi_j^2 \rangle} \int_{-\infty}^{\infty} \frac{\partial u(t, \zeta)}{\partial t} \phi_j(\zeta) f_u(t, \zeta) d\zeta + \frac{1}{\langle \phi_j^2 \rangle} \int_{-\infty}^{\infty} u(t, \zeta) \phi_j(\zeta) \frac{\partial f_u(t, \zeta)}{\partial t} d\zeta \\ &= \frac{-1}{\langle \phi_j^2 \rangle} \int_{-\infty}^{\infty} k(\xi) u(t, \zeta) \phi_j(\zeta) f_u(t, \zeta) d\zeta + \frac{1}{\langle \phi_j^2 \rangle} \int_{-\infty}^{\infty} u(t, \zeta) \phi_j(\zeta) \frac{\partial f_u(t, \zeta)}{\partial t} d\zeta \\ &= \frac{-1}{\langle \phi_j^2 \rangle} \sum_{i=0}^N u_i(t) \int_{-\infty}^{\infty} k(\xi) \phi_i(\xi) \phi_j(\zeta) f_u(t, \zeta) d\zeta + \frac{1}{\langle \phi_j^2 \rangle} \sum_{i=0}^N u_i(t) \int_{-\infty}^{\infty} \phi_i(\xi) \phi_j(\zeta) \frac{\partial f_u(t, \zeta)}{\partial t} d\zeta. \end{aligned}$$

The problem with this approach is twofold

1. How is ζ related to ξ ?
2. How can we determine the time derivative $\partial f_u / \partial t$ in the second term on the right hand side?

We know that the distribution of u is related to the distribution of k . Once we fix k , we have a deterministic solution, so let us make ζ a function of ξ , i.e. $\zeta = \zeta(\xi)$, then we have for the coefficients

$$\begin{aligned} u_j(t) &= \frac{1}{\langle \phi_j^2 \rangle} \int_{-\infty}^{\infty} u(t, \zeta) \phi_j(\zeta) f_u(t, \zeta) d\zeta \\ &= \frac{1}{\langle \phi_j^2 \rangle} \int_{-\infty}^{\infty} u(t, \zeta(\xi)) \phi_j(\zeta(\xi)) f_u(t, \zeta(\xi)) \frac{d\zeta}{d\xi} d\xi \\ &= \frac{1}{\langle \phi_j^2 \rangle} \int_{-\infty}^{\infty} u(t, \zeta(\xi)) \phi_j(\zeta(\xi)) f_k(\xi) d\xi. \end{aligned}$$

If we now take the time derivative of $u_j(t)$ we obtain

$$\begin{aligned} \frac{du_j}{dt} &= \frac{1}{\langle \phi_j^2 \rangle} \int_{-\infty}^{\infty} \frac{\partial u(t, \zeta(\xi))}{\partial t} \phi_j(\zeta(\xi)) f_k(\xi) d\xi = \frac{-1}{\langle \phi_j^2 \rangle} \int_{-\infty}^{\infty} k(\xi) u(t, \zeta(\xi)) \phi_j(\zeta(\xi)) f_k(\xi) d\xi \\ &= \frac{-1}{\langle \phi_j^2 \rangle} \sum_{i=0}^N u_i(t) \int_{-\infty}^{\infty} k(\xi) \phi_i(\xi) \phi_j(\zeta(\xi)) f_k(\xi) d\xi. \end{aligned}$$

This we recognize as TDgPC, when we set $\zeta = u(t, \xi)$.

The probability density distribution for the decay problem, f_u , is given by

$$f_u(t, \zeta) = \frac{1}{\zeta t}, \quad e^{-t} \leq \zeta \leq 1. \quad (45)$$

The first two monic orthogonal polynomials for this distribution are given by

$$\phi_0(\zeta) = 1, \quad \phi_1(\zeta) = \zeta + \frac{1}{t}(e^{-t} - 1). \quad (46)$$

In terms of ξ the PDF and the orthogonal ‘polynomials’ are given by

$$f_u(t, \xi(\zeta)) \frac{d\xi}{d\zeta} = \frac{1}{2}, \quad \phi_0(\xi(\zeta)) = 1, \quad \phi_1(\xi(\zeta)) = u_0 e^{-(1+\xi)t/2} + \frac{1}{t}(e^{-t} - 1) \quad (47)$$

for $-1 \leq \xi \leq 1$. In Fig. 7 the probability density distribution of the solution $u(t, \zeta)$ is displayed for various values of t . For small t , for instance $t = 0.02$ in the figure, the probability of finding u near 1 is high. Initially the probability density function changes rapidly as a function of time. For higher values of t , for instance $t = 6.42$, the probability of finding u near 0 is highest. For $t = 0$ the solution is deterministic and the associated PDF is given by the Dirac distribution $\delta(\zeta - 1)$. For $t \rightarrow \infty$ the solution tends to the deterministic solution given by the PDF $\delta(\zeta)$. In Fig. 8 the ‘polynomial’ $\phi_1(\xi(\zeta))$ is plotted for various values of t and the polynomial $\phi_1(\xi) = \xi$ associated with the distribution of the decay coefficient k . Note that the exact solution can be represented by the two polynomials $\phi_0(\xi(\zeta))$ and $\phi_1(\xi(\zeta))$ for all t

$$u_{\text{exact}}(t, \xi) = u_0 e^{-(1+\xi)t/2} = \phi_1(\xi(\zeta)) - \frac{1}{t}(e^{-t} - 1)\phi_0(\xi(\zeta)). \quad (48)$$

3.6. Error analysis

Assuming that the time integration and the evaluation of the integrals involved are exact, we have the following error estimate:

Theorem 1. Let ϵ_M denote the error of the second-order moment of $\mathcal{P}_M u$. At time t and polynomial order M , $\epsilon_{M, \text{gPC}}$ and $\epsilon_{M, \text{TDgPC}}$ are given by

$$\epsilon_{M, \text{gPC}} = \sum_{i=M+1}^{\infty} \frac{\alpha_i^2(t)}{2i+1}, \quad (49)$$

where the $\alpha_i(t)$ are the Fourier–Legendre coefficients given by (28) and

$$\epsilon_{M, \text{TDgPC}} = 0 \quad \text{for } M \geq 1. \quad (50)$$

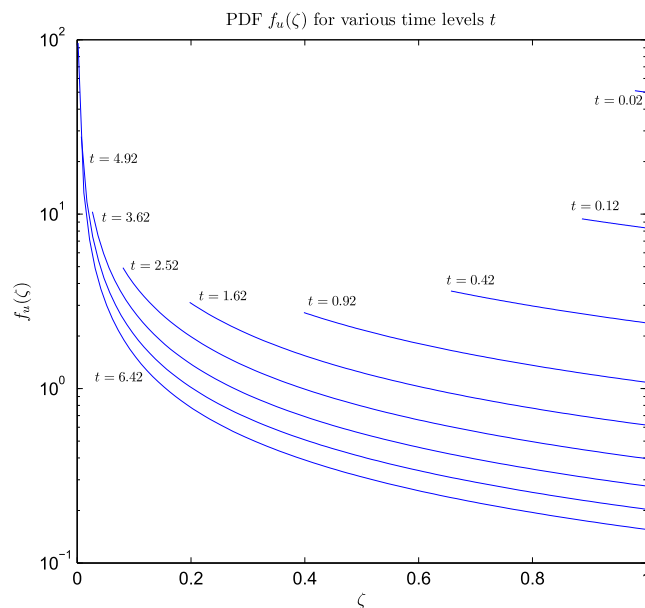


Fig. 7. The probability density distribution $f_u(t, \zeta)$ for various time levels.

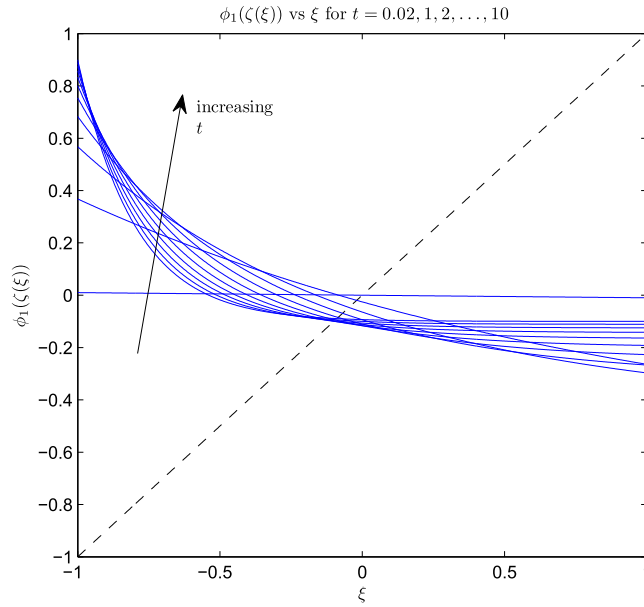


Fig. 8. The polynomials $\phi_1(\zeta(\xi))$ associated with the PDF of the solution for $t = 0.02, 1, 2, \dots, 10$ (solid lines) and the $\phi_1(\xi)$ associated with the PDF of the decay coefficient k (dashed line).

Proof. The gPC expansion is represented in terms of Legendre polynomials given by

$$u_{\text{exact}}(t, \xi) = \sum_{i=0}^{\infty} \alpha_i(t) L_i(\xi), \quad (51)$$

where the $\alpha_i(t)$ are the Fourier–Legendre coefficients given by (28)

$$\langle u^2(t, \xi) \rangle = \sum_{i=0}^{\infty} \frac{\alpha_i^2(t)}{2i+1}. \quad (52)$$

For the projection $\mathcal{P}_M u(t, \xi)$ we have

$$\mathcal{P}_M u(t, \xi) = \sum_{i=0}^M \alpha_i(t) L_i(\xi) \Rightarrow \langle (\mathcal{P}_M u)^2 \rangle = \sum_{i=0}^M \frac{\alpha_i^2(t)}{2i+1}, \quad (53)$$

and therefore

$$\epsilon_{M, \text{gPC}} = \sum_{i=M+1}^{\infty} \frac{\alpha_i^2(t)}{2i+1}. \quad (54)$$

Since in TDgPC, the new stochastic variable $\zeta = u$, we have that u can be uniquely represented in terms of linear polynomials of ζ , i.e.

$$u_{\text{exact}}(t, \zeta) = \sum_{i=0}^{\infty} \beta_i(t) \phi_i(\zeta), \quad \beta_i(t) = 0 \quad \text{for } i \geq 2 \Rightarrow u_{\text{exact}} = \mathcal{P}_M u \quad \text{for } M \geq 1. \quad \square \quad (55)$$

Wan and Karniadakis [14] have established for the multi-element version of gPC (ME-gPC), that the error for the second-order moment is given by

$$\epsilon_{M, \text{ME-gPC}} = (2N)^{-2(M+1)} \epsilon_{M, \text{gPC}}, \quad (56)$$

where N denotes the number of elements in random space and M denotes the polynomial degree, which is clearly much smaller than the error of gPC but not zero as in TDgPC.

3.7. Numerical results

If we analyze the results of this discrete time-dependent approach applied to the ODE in question, it can be observed in Fig. 9, that for a polynomial order of $P = 3$, the results indeed outperform the standard gPC approach. In order to generate the

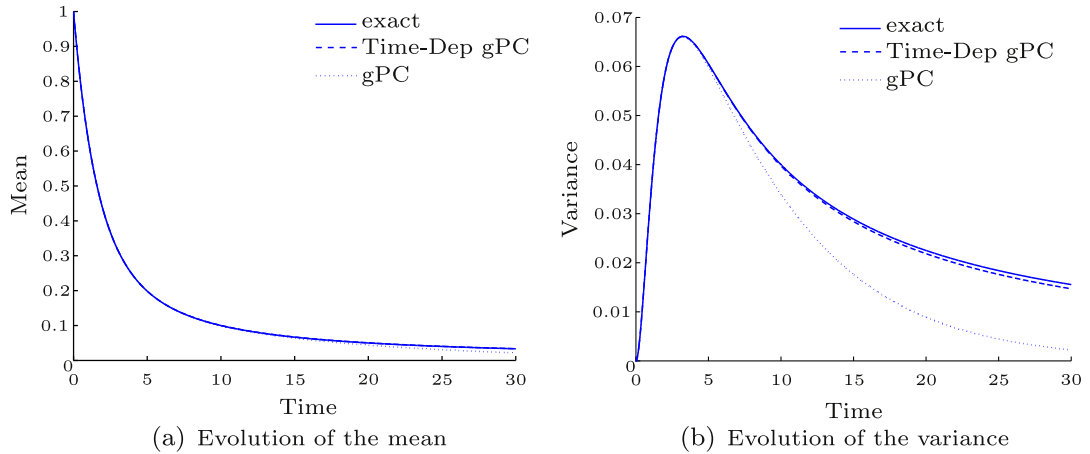


Fig. 9. Evolution of the mean and variance for third-order time-dependent gPC ($P = 3$).

results, the threshold parameter was set equal to $\theta = 6$. Especially for the second-order statistics, which were a bottleneck for the standard gPC, the improvement is significant. The same behavior can be seen from Fig. 10, displaying the evolution of the error of both the mean and variance. Although the initial error level cannot be maintained, at the end-time, we see that both the error-levels have dropped from an unacceptable order $O(1)$ to the acceptable level $O(10^{-2})$. The accuracy can be improved by increasing the polynomial degree P . As from a polynomial degree of $P = 4$, in a plot depicting the evolution the mean and variance analogous to Fig. 9, the time-dependent gPC approximation would be indistinguishable from the exact solution. In Fig. 11, the error evolution of mean and variance are depicted for different expansion orders.

Fig. 12 shows that the time-dependent TDgPC approach is more accurate than conventional gPC, but it also shows that convergence with polynomial enrichment is much slower than gPC. In fact, gPC is more accurate with respect to the mean than TDgPC for higher polynomial orders. The lack of convergence is explained by the distribution of the decay coefficient $k(\xi) = (1 + \xi)/2$ for $-1 \leq \xi \leq 1$, which in terms of ζ is given by $(-1/t) \cdot \ln \zeta$ for $\exp(-t) \leq \zeta \leq 1$. For large t this implies that we need to find a polynomial approximation in ζ to $\ln \zeta$ for $\zeta \in (0, 1]$,

$$\ln \zeta = \sum_{i=0}^{\infty} \alpha_i \zeta^i, \quad e^{-t} \leq \zeta \leq 1. \quad (57)$$

Since $\ln \zeta \notin L^2(0, 1)$ we know that this expansion does not converge in the L^2 -norm for higher values of t , see Fig. 13.

Or put differently, the transformation to the ζ -variables allows one to represent the solution at each time level exactly with linear functions in ζ , as stated by Theorem 1, but is not adequate to describe the time rate of change of the solution. We therefore expand the solution in terms of ζ and ξ as

$$u(t, \xi) = \sum_{i=0}^P \sum_{j=0}^Q \alpha_{ij}(t) \phi_i(\xi) L_j(\zeta), \quad (58)$$

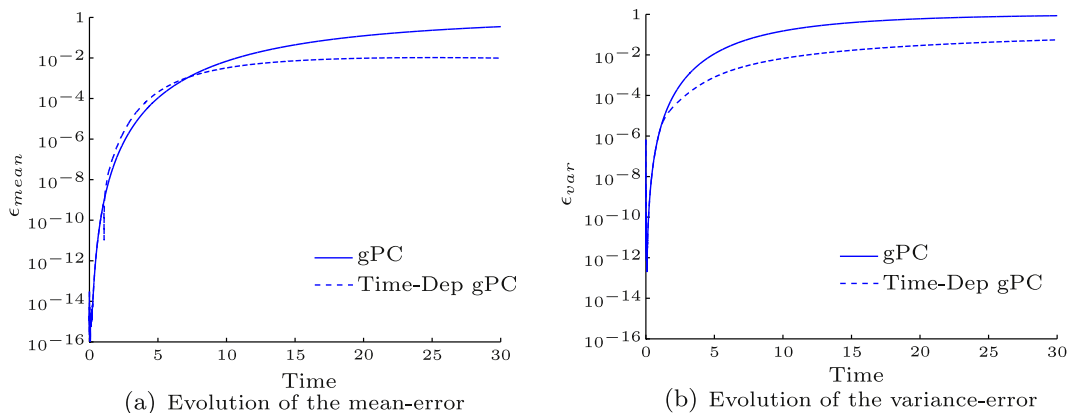


Fig. 10. Evolution of the error for third-order time-dependent gPC ($P = 3$).

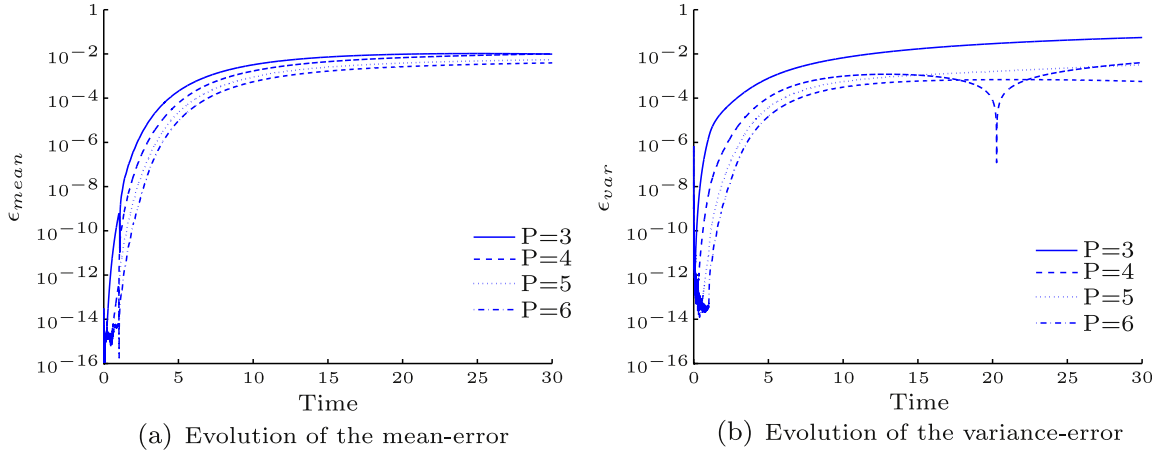


Fig. 11. Evolution of the error for polynomial order $P = 3, \dots, 6$ for time-dependent gPC.

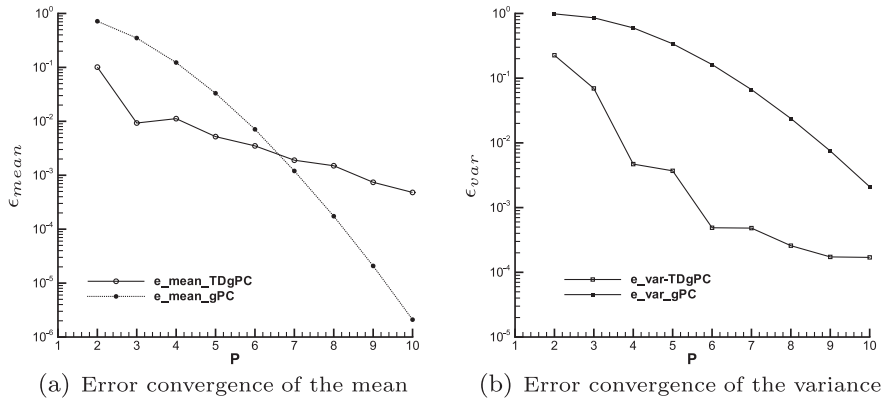


Fig. 12. Error convergence of the mean and variance at $t = 30$.

where the $\phi_i(\xi)$ constitute a set of orthogonal polynomials with respect to PDF of the solution, as discussed in this section and the $L_j(\xi)$ constitute an orthogonal set of polynomials with respect to the PDF of the decay coefficient $k(\xi)$, i.e. the Legendre polynomials. So for $P = Q = 1$, the expansion is given by

$$u(t, \xi) = \alpha_{00}(t) + \alpha_{01}(t)\xi + \alpha_{1,0}(t)\phi_1(\xi(\xi)) + \alpha_{11}(t)\xi\phi_1(\xi(\xi)). \quad (59)$$

At time $t = t^n$ the solution is given by

$$\alpha_{ij}(t^n) = \begin{cases} 1 & \text{if } i = 1 \text{ and } j = 0 \\ 0 & \text{elsewhere} \end{cases} \quad (60)$$

The time rate of change of the solution is given by

$$\frac{du}{dt} = -\frac{1}{2}(1 + \xi)u = \sum_{ij} \beta_{ij}(t)\phi_i(\xi)L_j(\xi) \Rightarrow \beta_{ij}(t^n) = \begin{cases} -1/2 & \text{if } i = 1 \text{ and } j = 0, 1 \\ 0 & \text{elsewhere} \end{cases} \quad (61)$$

So with this expansion, both the solution and the time derivative can be fully represented. The number of terms required in the expansion depends on the time-integration method employed. For Euler integration $P = 1$ and $Q = 1$ suffices and the error in the approximation is dominated by time integration, since for the Euler scheme we have:

$$u(t + \Delta t, \xi) = u(t, \xi) - \frac{\Delta t}{2}(1 + \xi)\xi(\xi) \quad (62)$$

For a fourth-order Runge–Kutta scheme a polynomial degree $P = 4$ and $Q = 1$ suffices, because for the Runge–Kutta scheme we have

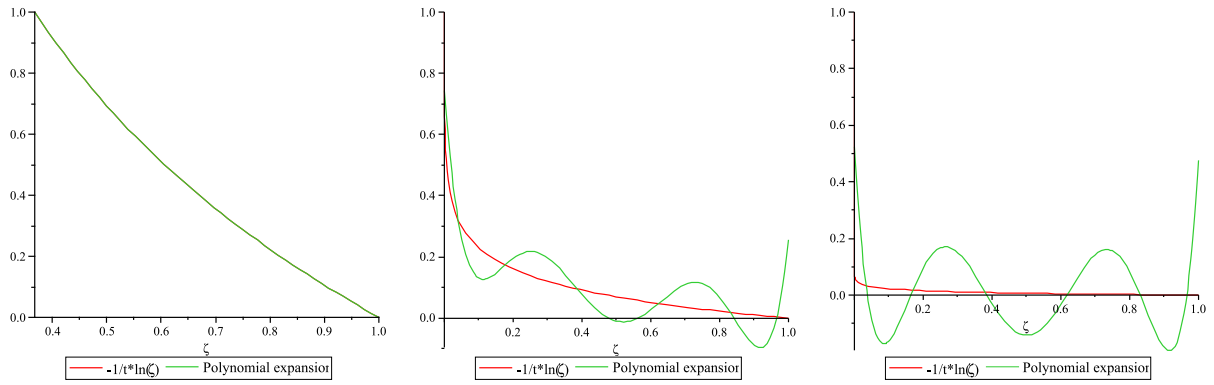
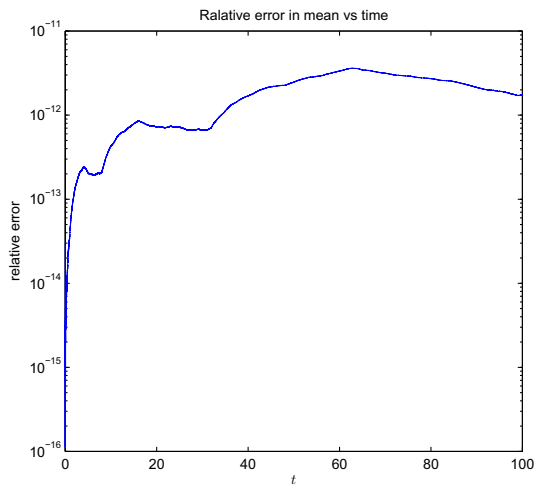
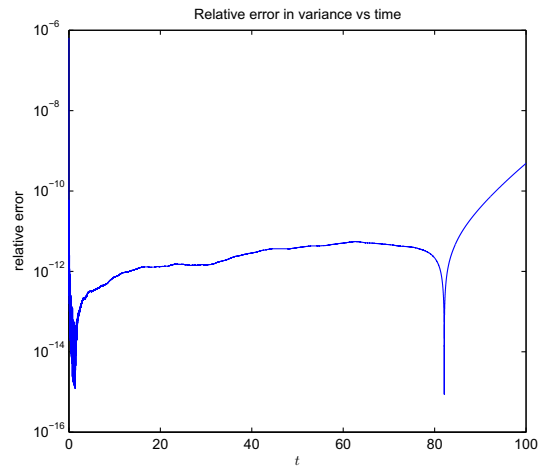


Fig. 13. Natural logarithm and its sixth order approximation for $t = 1$, $t = 10$, $t = 100$ (left to right).

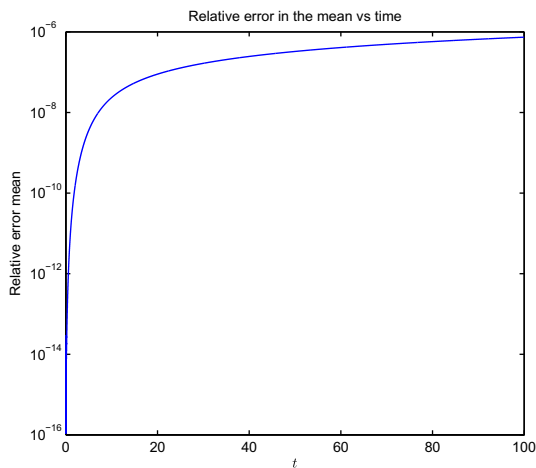


(a) Evolution of the mean-error

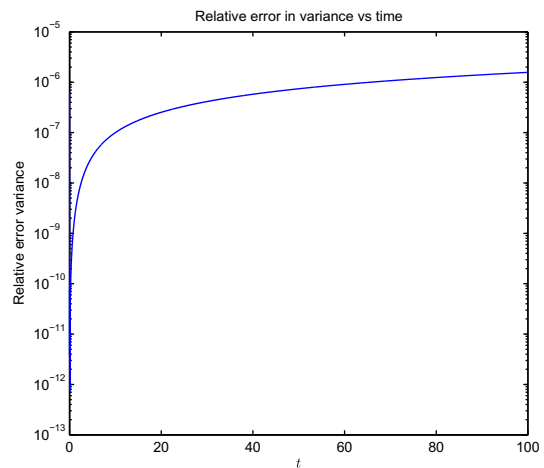


(b) Evolution of the variance-error

Fig. 14. Evolution of the error for fifth-order time-dependent gPC for $0 \leq t \leq 100$ integrated with a fourth order Runge–Kutta scheme in time, $\Delta t = 0.001$.



(a) Evolution of the mean-error



(b) Evolution of the variance-error

Fig. 15. Evolution of the error for $P = 2$ in the revised time-dependent gPC for $0 \leq t \leq 100$.

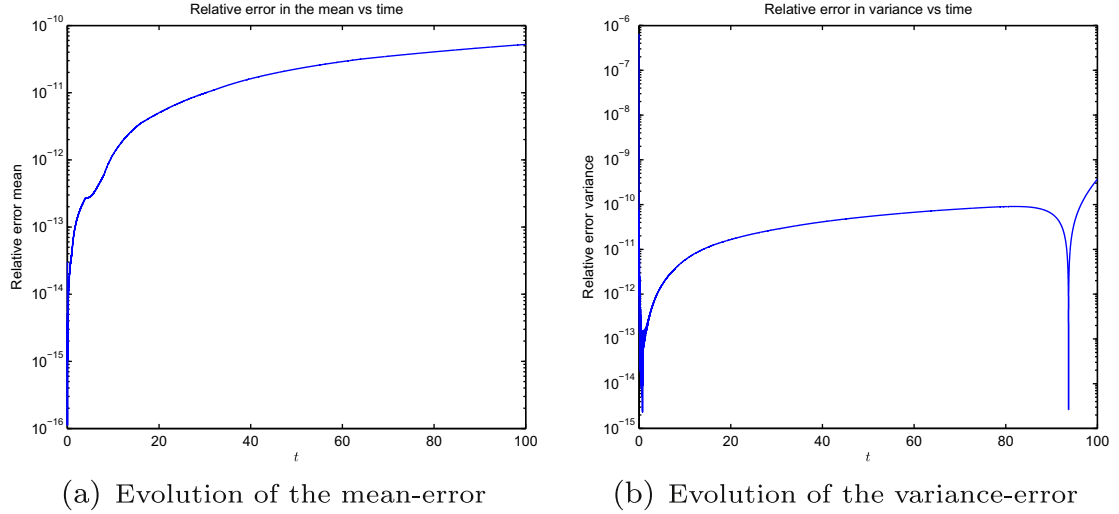


Fig. 16. Evolution of the error for $P = 3$ in the revised time-dependent gPC for $0 \leq t \leq 100$.

$$u(t + \Delta t, \xi) = u(t, \xi) - \frac{\Delta t}{2} (1 + \xi) \zeta(\xi) + \frac{\Delta t^2}{8} (1 + \xi)^2 \zeta(\xi) - \frac{\Delta t^3}{48} (1 + \xi)^3 \zeta(\xi) + \frac{\Delta t^4}{384} (1 + \xi)^4 \zeta(\xi). \quad (63)$$

Fig. 14 shows the error as a function of time for this approach.

Corollary 2. *The expansion of the random variable in orthogonal polynomials should be capable of representing the statistics at each time level (Theorem 1) and should be capable of representing the time derivative. For the decay problem we have that if P is greater or equal than the order of the time-integration scheme, the accuracy is determined by the accuracy of the time-integration scheme. If P is less than the order of the time-integration scheme the accuracy is determined by Δt^P , because in that case the higher-order terms cannot be represented by polynomials in ξ . This is illustrated numerically for the fourth-order Runge–Kutta scheme with $\Delta t = 0.001$ for $P = 2$ and $P = 3$, in Figs. 15 and 16, respectively. For $P = 2$ this yields an error in the mean and the variance of $O(10^{-6})$ and for $P = 3$ an error in the mean and the variance of $O(10^{-9})$ over the entire time interval.*

Based on these observation, we now consider the more challenging case consisting of a system of ordinary non-linear differential equations.

4. The Kraichnan–Orszag three-mode problem

The so-called Kraichnan–Orszag three-mode problem was introduced by Kraichnan [2] and studied by Orszag [3] for Gaussian distributed initial conditions.

4.1. Problem definition

The Kraichnan–Orszag problem is defined by the following system of non-linear ordinary differential equations

$$\frac{dx_1}{dt} = x_2 x_3, \quad (64a)$$

$$\frac{dx_2}{dt} = x_3 x_1, \quad (64b)$$

$$\frac{dx_3}{dt} = -2x_1 x_2. \quad (64c)$$

In this work we will consider this problem subject to stochastic initial conditions. First, we will study the 1D problem corresponding to initial conditions of the form

$$x_1(0) = \alpha + 0.01\xi, \quad x_2(0) = 1.0, \quad x_3(0) = 1.0, \quad (65)$$

where α is a constant and ξ a *uniformly* distributed random variable with unit variance (i.e. ξ is uniformly distributed on the interval $[-1, 1]$). Analysis by [16,32,33] shows that when α is in the range $(0, 0.9)$ the solution is rather insensitive to the initial conditions. However for $\alpha \in (0.9, 1)$ there is a strong dependence on the initial conditions.

In Section 4.4 we will consider the 3D case

$$x_1(0) = \alpha + 0.01\zeta_1, \quad x_2(0) = \beta + 0.01\zeta_2, \quad x_3(0) = \gamma + 0.01\zeta_3, \quad (66)$$

where α , β and γ are constants and ζ_1 , ζ_2 and ζ_3 are *uniformly* distributed random variables on the interval $[-1, 1]$, where ζ_1 , ζ_2 and ζ_3 are statistically independent.

4.2. TDgPC solution

Consider the Kraichnan–Orszag problem (64) with the initial conditions (65). We follow the procedure described in Section 3.5

$$x_i(t, \xi) = \sum_{p=0}^P x_p^{(i)}(t) L_p(\xi), \quad i = 1, 2, 3, \quad (67)$$

where L_p is the Legendre polynomial of degree p . Since ξ has a uniform distribution, the Legendre polynomials constitute an optimal trial basis for early times (see Table 1). Employing this polynomial chaos expansion of the solution and following the method outlined in Section 2.2 we arrive at a system of deterministic ordinary differential equations in time for the coefficients $x_p^{(i)}(t)$. We solve this system by standard fourth-order Runge–Kutta time integration.

From (67) we see that the approximate solutions x_i are polynomials in the random variable ξ . With time the coefficients of the solution polynomials increase in magnitude. This is an indication that the stochastic characteristics of the solution are changing. As a consequence the basis $\{L_p\}$ loses its effectiveness. When the non-linear part of the solution reaches a certain threshold level (say at $t = t_1$), we perform the transformation of the random variable from ξ to ζ_i given by

$$\zeta_i = x_i(t_1, \xi) = \sum_{p=0}^P x_p^{(i)}(t_1) L_p(\xi), \quad i = 1, 2, 3. \quad (68)$$

The three new random variables ζ_i have associated PDFs $f_{\zeta_i}(\zeta_i)$.

For each f_{ζ_i} we employ Gram–Schmidt orthogonalization to calculate a set of orthogonal polynomials $\phi_p^{(\zeta_i)}(\zeta_i)$ with $p = 0, \dots, P$. By $\phi_p^{(\zeta_i)}$ we denote the polynomial of degree p associated with f_{ζ_i} , i.e. f_{ζ_i} acts as the weighting function in the orthogonality relation. At time level $t = t_1$ these polynomials constitute an optimal trial basis again. We therefore use these newly calculated polynomials $\phi_p^{(\zeta_i)}$ and continue to obtain a numerical solution to the Kraichnan–Orszag problem in a new form given by

$$x_i(t, \zeta_1, \zeta_2, \zeta_3) = \sum_{0 \leq l+m+n \leq P} x_{lmn}^{(i)}(t) \phi_l^{(\zeta_1)}(\zeta_1) \phi_m^{(\zeta_2)}(\zeta_2) \phi_n^{(\zeta_3)}(\zeta_3), \quad t \geq t_1. \quad (69)$$

The summation in Eq. (69) is over all combinations of the integers l, m and n for which $0 \leq l + m + n \leq P$. The total number of expansion terms ($N + 1$) follows from Eq. (11) with $n = 3$ and is given by

$$N + 1 = \binom{P+3}{P} = \frac{(P+3)!}{P!3!} = \frac{1}{6}(P+3)(P+2)(P+1) \sim \frac{P^3}{6}. \quad (70)$$

Substituting (69) in (64) we once again follow the standard gPC procedure of Section 2.2. Hence, we perform a Galerkin projection to end up with a new system of ordinary differential equations for the new expansion coefficients $x_{lmn}^{(i)}(t)$.

We proceed by marching this new system forward in time again from $t = t_1$ onwards using our standard fourth-order Runge–Kutta solver. Note, however, that we need to provide ‘initial’ conditions (i.e. conditions at $t = t_1$) for all new coefficients $x_{lmn}^{(i)}$. These initial conditions follow from the requirement

$$x_i(t_1, \zeta_1, \zeta_2, \zeta_3) = \zeta_i, \quad i = 1, 2, 3. \quad (71)$$

We can arrange for the orthogonal expansion polynomials $\phi_p^{(\zeta_i)}$ to all have unity leading coefficients. Therefore, at $t = t_1$ the coefficients $x_{lmn}^{(i)}$ are given by

$$x_{lmn}^{(1)}(t_1) = \begin{cases} -\phi_0^{(\zeta_1)} & \text{if } l = m = n = 0, \\ 1 & \text{if } l = 1 \wedge m = n = 0, \\ 0 & \text{otherwise,} \end{cases}$$

$$x_{lmn}^{(2)}(t_1) = \begin{cases} -\phi_0^{(\zeta_2)} & \text{if } l = m = n = 0, \\ 1 & \text{if } m = 1 \wedge l = n = 0, \\ 0 & \text{otherwise,} \end{cases} \quad (72)$$

$$x_{lmn}^{(3)}(t_1) = \begin{cases} -\phi_0^{(\zeta_3)} & \text{if } l = m = n = 0, \\ 1 & \text{if } n = 1 \wedge l = m = 0, \\ 0 & \text{otherwise,} \end{cases}$$

where $\phi_0^{(\zeta_i)}$ denotes the zeroth-order term of the expansion polynomial of degree one associated with f_{ζ_i} .

Marching the new system of differential equations forward in time, we again monitor the non-linear part of the resulting solution. When, by some criterion, this non-linear part has become too large (say at $t = t_2$), we repeat the above procedure in order to re-establish an optimal trial basis. Hence, we start by introducing the new random variables

$$\zeta_i^{(2)} = x_i(t_2, \zeta_1^{(1)}, \zeta_2^{(1)}, \zeta_3^{(1)}), \quad i = 1, 2, 3, \quad (73)$$

and continue to calculate their PDFs from which the new optimal trial basis is calculated by Gram–Schmidt orthogonalization. Note that we have added a superscript to the random variables in (73) corresponding to the time instant at which they were introduced. Hence, we have rewritten the original variables ζ_i as $\zeta_i^{(1)}$. The process of updating the polynomial trial basis can be performed as many times as is required for the particular problem at hand. So, in general we have

$$\zeta_i^{(k+1)} = x_i(t_{k+1}, \zeta_1^{(k)}, \zeta_2^{(k)}, \zeta_3^{(k)}), \quad i = 1, 2, 3, \quad k = 1, 2, \dots, K-1 \quad (74)$$

with associated PDF $f_{\zeta_i^{(k+1)}}$ and orthogonal polynomials $\phi_p^{(\zeta_i^{(k+1)})}$ leading to a polynomial chaos expansion, similar to (69), to be used for $t_{k+1} \leq t \leq t_{k+2}$.

4.2.1. System of differential equations after a random variable transformation

Having made the transformation (68) from the single initial random variable ξ to the three new random variables ζ_i – note that we have dropped the superscript ⁽¹⁾ again for clarity – we approximate the solution to the 1D Kraichnan–Orszag problem by (69). When we substitute this expression into (64a) we obtain

$$\sum_{0 \leq i+j+k \leq P} \frac{dx_{ijk}^{(1)}}{dt} \phi_i^{(\zeta_1)} \phi_j^{(\zeta_2)} \phi_k^{(\zeta_3)} = \sum_{0 \leq p+q+r \leq P} \sum_{0 \leq u+v+w \leq P} x_{pqr}^{(2)} x_{uvw}^{(3)} \phi_p^{(\zeta_1)} \phi_q^{(\zeta_2)} \phi_r^{(\zeta_3)} \phi_u^{(\zeta_1)} \phi_v^{(\zeta_2)} \phi_w^{(\zeta_3)}. \quad (75)$$

We multiply this equation by $\phi_l^{(\zeta_1)} \phi_m^{(\zeta_2)} \phi_n^{(\zeta_3)}$ and perform a triple integration w.r.t. ζ_1, ζ_2 and ζ_3 . Taking into account the orthogonality of the basis functions, we arrive at

$$\frac{dx_{lmn}^{(1)}}{dt} = \frac{1}{\langle \phi_l^{(\zeta_1)} \rangle \langle \phi_m^{(\zeta_2)} \rangle \langle \phi_n^{(\zeta_3)} \rangle} \sum_{0 \leq p+q+r \leq P} \sum_{0 \leq u+v+w \leq P} x_{pqr}^{(2)} x_{uvw}^{(3)} \langle \phi_p^{(\zeta_1)} \phi_u^{(\zeta_1)} \phi_l^{(\zeta_1)} \rangle \langle \phi_q^{(\zeta_2)} \phi_v^{(\zeta_2)} \phi_m^{(\zeta_2)} \rangle \langle \phi_r^{(\zeta_3)} \phi_w^{(\zeta_3)} \phi_n^{(\zeta_3)} \rangle \quad (76)$$

for $l, m, n = 0, \dots, P$ with

$$\langle I(\zeta_i) \rangle = \int_{-\infty}^{\infty} I(\zeta_i) f_{\zeta_i}(\zeta_i) d\zeta_i \quad (77)$$

for some function $I(\zeta_i)$. Substituting (69) into (64b) and (64c) gives similar relations as (76) for the evolution of $x_{lmn}^{(2)}$ and $x_{lmn}^{(3)}$. Together these three equations constitute the governing *deterministic* system of differential equations in time for the expansion coefficients $x_{lmn}^{(i)}(t)$, $i = 1, 2, 3$ with $0 \leq l + m + n \leq P$.

4.2.2. Calculation of mean and variance

We are interested in the mean and variance of $x_1(t, \zeta_1, \zeta_2, \zeta_3)$, $x_2(t, \zeta_1, \zeta_2, \zeta_3)$ and $x_3(t, \zeta_1, \zeta_2, \zeta_3)$. Once we have solved for the time histories of the solution coefficients $x_{lmn}^{(i)}(t)$ (see (69)) the mean and variance of $x_i(t, \zeta_1, \zeta_2, \zeta_3)$ can be calculated as follows.

Mean The mean of x_i is defined as

$$\bar{x}_i(t) = E[x_i(t, \zeta_1, \zeta_2, \zeta_3)]. \quad (78)$$

Substituting Eq. (69) into Eq. (78) we get

$$\begin{aligned} \bar{x}_i(t) &= E \left[\sum_{0 \leq l+m+n \leq P} x_{lmn}^{(i)}(t) \phi_l^{(\zeta_1)}(\zeta_1) \phi_m^{(\zeta_2)}(\zeta_2) \phi_n^{(\zeta_3)}(\zeta_3) \right] \\ &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \sum_{0 \leq l+m+n \leq P} x_{lmn}^{(i)}(t) \phi_l^{(\zeta_1)} \phi_m^{(\zeta_2)} \phi_n^{(\zeta_3)} f_{\zeta_1, \zeta_2, \zeta_3} d\zeta_1 d\zeta_2 d\zeta_3. \end{aligned} \quad (79)$$

If ζ_1, ζ_2 and ζ_3 were statistically independent, this could be reduced to three one-dimensional integrals, using

$$f_{\zeta_1, \zeta_2, \zeta_3}(\zeta_1, \zeta_2, \zeta_3) = f_{\zeta_1}(\zeta_1) f_{\zeta_2}(\zeta_2) f_{\zeta_3}(\zeta_3). \quad (80)$$

However, this will not be the case, since the stochastic variables ζ_i are all related by various mappings to the common stochastic variables ξ .

Variance. The variance of x_i is defined as

$$\begin{aligned} \text{Var}(x_i(t)) &= E[(x_i(t, \zeta_1, \zeta_2, \zeta_3) - \bar{x}_i(t))^2] = E[x_i^2(t, \zeta_1, \zeta_2, \zeta_3) - 2x_i(t, \zeta_1, \zeta_2, \zeta_3)\bar{x}_i(t) + \bar{x}_i^2(t)] \\ &= E[x_i^2(t, \zeta_1, \zeta_2, \zeta_3)] - 2E[x_i(t, \zeta_1, \zeta_2, \zeta_3)]\bar{x}_i(t) + \bar{x}_i^2(t) = E[x_i^2(t, \zeta_1, \zeta_2, \zeta_3)] - \bar{x}_i^2(t). \end{aligned} \quad (81)$$

Substituting the numerical approximation ((69) and (79) into (81) we obtain

$$\begin{aligned}\text{Var}(x_i(t)) &= E \left[\left(\sum_{0 \leq l+m+n \leq P} x_{lmn}^{(i)}(t) \phi_l^{(\zeta_1)} \phi_m^{(\zeta_2)} \phi_n^{(\zeta_3)} \right)^2 \right] - x_{000}^{(i)2}(t) \\ &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left(\sum_{0 \leq l+m+n \leq P} x_{lmn}^{(i)}(t) \phi_l^{(\zeta_1)} \phi_m^{(\zeta_2)} \phi_n^{(\zeta_3)} \right)^2 f_{\zeta_1, \zeta_2, \zeta_3} d\zeta_1 d\zeta_2 d\zeta_3.\end{aligned}\quad (82)$$

4.2.3. Integration over the original random variable

The integrand in (82) for the variance, for instance, of x_i is a function of the transformed random variables ζ_1 , ζ_2 and ζ_3 . These transformed random variables, in turn, are all functions of the original random variable ξ : $\zeta_1 = Z_1(\xi)$, $\zeta_2 = Z_2(\xi)$ and $\zeta_3 = Z_3(\xi)$. Hence, the integrand in (82) can also be seen as a function solely dependent on ξ . To avoid the calculation of $f_{\zeta_1, \zeta_2, \zeta_3}$ we can transform the triple integral over ζ_1 , ζ_2 and ζ_3 in (82) to a single integral over ξ , based on the ideas from Van der Steen [32].

We do this by recognizing that the following relation should be valid for every realisable point $(\zeta_1^*, \zeta_2^*, \zeta_3^*)$

$$f_{\zeta_1, \zeta_2, \zeta_3}(\zeta_1^*, \zeta_2^*, \zeta_3^*) d\zeta_1 d\zeta_2 d\zeta_3 = \sum_{\xi^*} f_{\xi}(\xi^*) d\xi, \quad (83)$$

where the summation is over all points ξ^* for which $Z_1(\xi^*) = \zeta_1^*$, $Z_2(\xi^*) = \zeta_2^*$ and $Z_3(\xi^*) = \zeta_3^*$. Eq. (83) merely states that, given the transformation $\xi \rightarrow (\zeta_1, \zeta_2, \zeta_3)$, the probability that $(\zeta_1, \zeta_2, \zeta_3)$ lies within an infinitesimal volume around $(\zeta_1^*, \zeta_2^*, \zeta_3^*)$ should be equal to the probability that ξ lies within the (possibly multiple) corresponding infinitesimal interval(s) around ξ^* . It follows that the following relation should then also be valid

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \cdots f_{\zeta_1, \zeta_2, \zeta_3} d\zeta_1 d\zeta_2 d\zeta_3 = \int_{-1}^1 \cdots f_{\xi} d\xi. \quad (84)$$

Hence, with the help of (84) we can calculate the variance of x_i according to

$$\begin{aligned}\text{Var}(x_i(t)) &= E \left[\left(\sum_{0 \leq l+m+n \leq P} x_{lmn}^{(i)}(t) \phi_l^{(\zeta_1)} \phi_m^{(\zeta_2)} \phi_n^{(\zeta_3)} \right)^2 \right] - \bar{x}_i^2(t) \\ &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left(\sum_{0 \leq l+m+n \leq P} x_{lmn}^{(i)}(t) \phi_l^{(\zeta_1)} \phi_m^{(\zeta_2)} \phi_n^{(\zeta_3)} \right)^2 f_{\zeta_1, \zeta_2, \zeta_3} d\zeta_1 d\zeta_2 d\zeta_3 - \bar{x}_i^2(t) \\ &= \int_{-1}^1 \left(\sum_{0 \leq l+m+n \leq P} x_{lmn}^{(i)}(t) \phi_l^{(\zeta_1)}(Z_1(\xi)) \phi_m^{(\zeta_2)}(Z_2(\xi)) \phi_n^{(\zeta_3)}(Z_3(\xi)) \right)^2 f_{\xi}(\xi) d\xi - \bar{x}_i^2(t).\end{aligned}\quad (85)$$

Transforming an integral over the transformed random variables to an integral over the original random variable is a technique that can be used to evaluate the mean, i.e.

$$\begin{aligned}\bar{x}_i(t) &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \sum_{0 \leq l+m+n \leq P} x_{lmn}^{(i)}(t) \phi_l^{(\zeta_1)} \phi_m^{(\zeta_2)} \phi_n^{(\zeta_3)} f_{\zeta_1, \zeta_2, \zeta_3} d\zeta_1 d\zeta_2 d\zeta_3 \\ &= \sum_{0 \leq l+m+n \leq P} x_{lmn}^{(i)}(t) \int_{-1}^1 \phi_l^{(\zeta_1)}(Z_1(\xi)) \phi_m^{(\zeta_2)}(Z_2(\xi)) \phi_n^{(\zeta_3)}(Z_3(\xi)) f_{\xi}(\xi) d\xi.\end{aligned}\quad (86)$$

Furthermore, we can just as well transform a *single* integral over a transformed random variable to a single integral over the original random variable. So, similarly to (83), we also have that

$$f_{\zeta_i}(\zeta_i^*) d\zeta_i = \sum_{\xi^*} f_{\xi}(\xi^*) d\xi, \quad (87)$$

so

$$\int_{-\infty}^{\infty} \cdots f_{\zeta_i} d\zeta_i = \int_{-1}^1 \cdots f_{\xi} d\xi. \quad (88)$$

With the help of (88) we can transform all integrals needed for the determination of the governing system of differential equations ((76) and (77)) to integrals over the original random variable ξ . The integrals in the Gram–Schmidt orthogonalization algorithm (to calculate the orthogonal polynomials $\phi_p^{(\zeta_i)}(\zeta_i)$) can similarly be transformed to integrals over ξ .

To conclude, we make the following important point. Performing all integrations in ξ -space has a major advantage: there is no need to explicitly calculate the probability density functions of the transformed random variables as was done in (37).

4.3. Numerical results

Figs. 17 and 18 show results for the mean and variance for x_1 , calculated using the TDgPC solution approach where a transformation to new stochastic variables is performed every time step. Similar results are obtained for x_2 and x_3 . At approx-

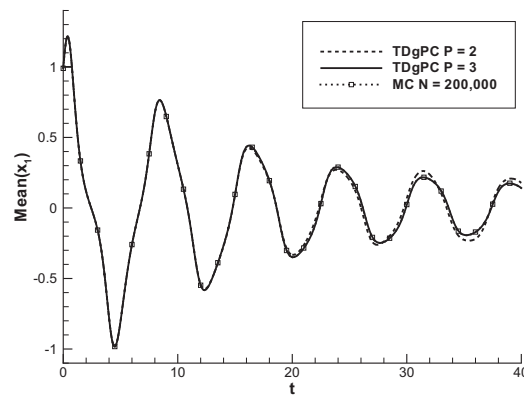


Fig. 17. Mean of x_1 vs. time for $\alpha = 0.99$: TDgPC solutions with $P = 2$ and $P = 3$ compared to Monte-Carlo analysis ($N = 200,000$).

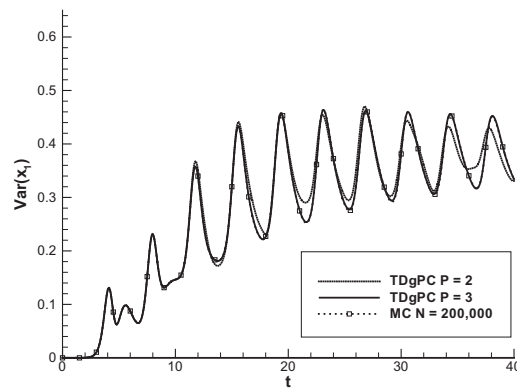


Fig. 18. The variance of x_1 vs. time for $\alpha = 0.99$: TDgPC solutions with $P = 2$ and $P = 3$ compared to Monte-Carlo analysis ($N = 200,000$).

imately $t = 13$, the results generated with the gPC solution stop to bear any resemblance to the Monte-Carlo solution. However, using a TDgPC strategy with expansion polynomials having a maximum degree of only two ($P = 2$) shows a significant improvement. The calculated solution can be seen to have the same characteristics as the results from the Monte-Carlo analysis for the entire range of t displayed. Increasing the maximum degree of the expansion polynomials to $P = 3$ leads to results with even higher accuracy. In fact, the TDgPC results with $P = 3$ are graphically indistinguishable from the Monte-Carlo results on the scale of these plots.

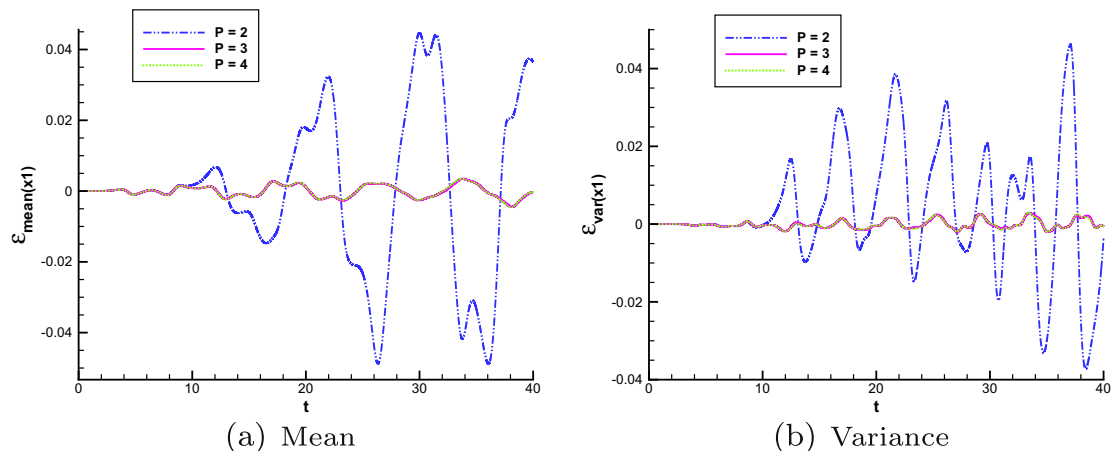


Fig. 19. Error in the mean and variance of x_1 vs. time for $\alpha = 0.99$: TDgPC solutions with $P = 2$, $P = 3$ and $P = 4$.

In Fig. 19 the time evolution of the ‘error’ in the mean and variance, respectively, of x_1 is shown for various values of P . Here ‘error’ means the difference between the TDgPC results and a Monte Carlo analysis with 200,000 samples

$$\epsilon_{x_i}(t) = \bar{x}_i^{\text{TDgPC}}(t) - \bar{x}_i^{\text{MC}}(t). \quad (89)$$

The error in the variance is calculated similarly. The error plots more clearly show the accuracy we gain by going from $P = 2$ to $P = 3$. The accuracy of a TDgPC solution with $P = 4$ can be seen to be almost identical to a solution with $P = 3$. Using Corollary 2 we can show that for $P = 2$, the method is $O(\Delta t)$, which for $\Delta t = 0.001$ is $O(10^{-3})$, for $P = 3$, the method is $O(\Delta t^2) = O(10^{-6})$ and for $P = 4$ $O(\Delta t^3) = O(10^{-9})$. If we use the expansion given by (75) we can represent the solution at each time step. For $P = 2$, we can also represent quadratic terms and therefore we can represent

$$x_1(t + \Delta, \xi) = x_1(t, \xi) + \Delta t \zeta^2 \zeta^3, \quad (90)$$

$$x_2(t + \Delta, \xi) = x_2(t, \xi) + \Delta t \zeta^3 \zeta^1, \quad (91)$$

and

$$x_3(t + \Delta, \xi) = x_3(t, \xi) - 2\Delta t \zeta^1 \zeta^2. \quad (92)$$

So for $P = 2$, we have a method that is first order in time. For $P = 3$, we can also represent all the cubic terms in ζ^1 , ζ^2 and ζ^3 multiplied by Δt^2 in the Runge–Kutta integration. So for $P = 3$ we have a second-order method in time. Analogously, we can show that for $P = 4$, we can represent all terms up to the power of 4 in ζ^i with coefficient Δt^3 . Now the difference between an error of 10^{-6} and 10^{-9} are visually undistinguishable in Fig. 19. It has been confirmed that this error cannot be attributed to

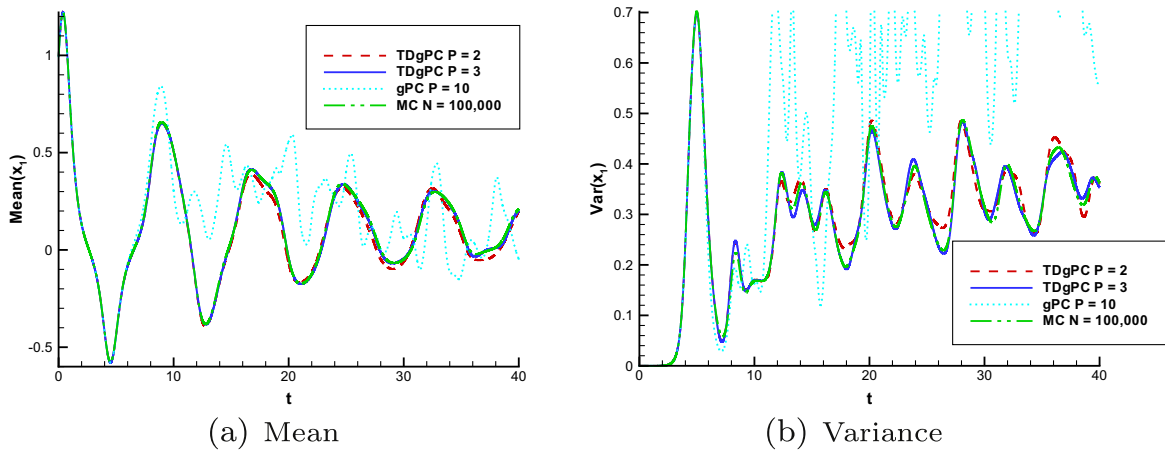


Fig. 20. Mean and variance of x_1 vs. time for $\alpha = 0.995$: TDgPC solutions with $P = 2$ and $P = 3$ compared to a gPC solution with $P = 10$ and a Monte-Carlo analysis ($N = 100,000$).

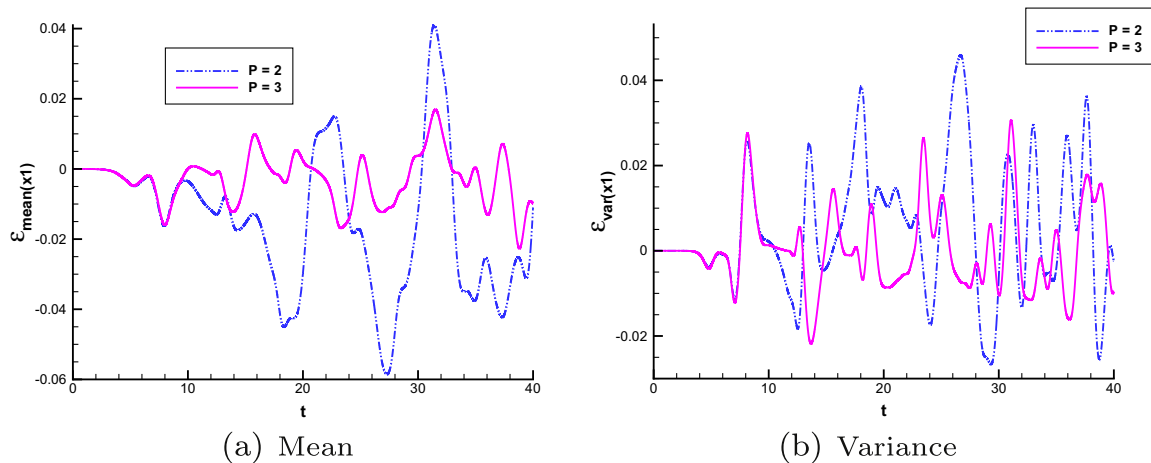


Fig. 21. Error in the mean and variance of x_1 vs. time for $\alpha = 0.995$: TDgPC solutions with $P = 2$ and $P = 3$.

the integration method and therefore the difference observed between the TDgPC results and the Monte-Carlo result must be attributed to number of samples in the Monte-Carlo simulation.

4.3.1. Results for $\alpha = 0.995$

Here we investigate the performance of TDgPC results for $\alpha = 0.995$ in (65). This is an interesting case, because for $x_1(0) < 1$ we have periodic solutions. The period becomes strongly dependent on $x_1(0) > 0.9$. When $x_1(0) > 1$ the solution curves belong to a different branch of solution trajectories than for $x_1(0) < 1$. The chance of finding an initial condition such that $x_1(0) > 1$, is $P(x_1(0) > 1) = 0.25$, so this choice of α contains two significantly different types of solutions. Furthermore, the periods T of the periodic solution near $x_1(0) = 1$ are very sensitive to the initial conditions. See, for instance [16,32], for more details on the dynamics of the Kraichnan–Orszag problem.

In Fig. 20 TDgPC results are presented for the mean (a) and variance (b) of x_1 . We again compare the TDgPC solutions with results from a Monte-Carlo simulation. Also for $\alpha = 0.995$ TDgPC remains close to the Monte-Carlo results. The accuracy of the solution with $P = 2$ is comparable to the case $\alpha = 0.99$. Again there is a significant improvement going from $P = 2$ to $P = 3$. However, the solution for $P = 3$ is not quite as accurate as in the case $\alpha = 0.99$. This is presumably due to the higher complexity of the problem with $\alpha = 0.995$. In Fig. 21 the ‘error’ in the mean and variance are plotted for x_1 , respectively, taking the Monte-Carlo simulation with $N = 100,000$ as a reference.

4.4. A three-dimensional random space

In this case we show a result where all three initial conditions are known with a given probability. These initial conditions are given by (also considered in [16])

$$x_1(0) = \alpha + 0.01\xi_1, \quad x_2(0) = \beta + 0.01\xi_2, \quad x_3(0) = \gamma + 0.01\xi_3, \quad (93)$$

where α, β and γ are constants and ξ_1, ξ_2 and ξ_3 are uniformly distributed random variables on the interval $[-1, 1]$ where ξ_1, ξ_2 and ξ_3 are statistically independent. Here we set $\alpha = 0.99, \beta = 1$ and $\gamma = 1$.

We now start with a three-dimensional expansion in terms of ξ_1, ξ_2 and ξ_3 analogous to (69). We introduce transformed random variables according to (74) and calculate new expansion polynomials similarly to the single random variable case. We also transform all integrals occurring in the solution algorithm to integrals over the original independent random variables ξ_1, ξ_2 and ξ_3 . Since we now have three original random variables instead of one (83) is rewritten as

$$f_{\xi_1, \xi_2, \xi_3}(\xi_1^*, \xi_2^*, \xi_3^*) d\xi_1 d\xi_2 d\xi_3 = \sum_{(\xi_1^*, \xi_2^*, \xi_3^*)} f_{\xi_1, \xi_2, \xi_3}(\xi_1^*, \xi_2^*, \xi_3^*) d\xi_1 d\xi_2 d\xi_3 = \sum_{(\xi_1^*, \xi_2^*, \xi_3^*)} f_{\xi_1}(\xi_1^*) f_{\xi_2}(\xi_2^*) f_{\xi_3}(\xi_3^*) d\xi_1 d\xi_2 d\xi_3 \quad (94)$$

for every realisable point $(\xi_1^*, \xi_2^*, \xi_3^*)$. The summation in (94) is over all points $(\xi_1^*, \xi_2^*, \xi_3^*)$ for which $Z_1(\xi_1^*, \xi_2^*, \xi_3^*) = \xi_1^*, Z_2(\xi_1^*, \xi_2^*, \xi_3^*) = \xi_2^*$ and $Z_3(\xi_1^*, \xi_2^*, \xi_3^*) = \xi_3^*$. Note that in (94) we have made use of the statistical independence of ξ_1, ξ_2 and ξ_3 in the initial conditions. It follows from (94) that integrals over the new random variables can be transformed according to

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \cdots f_{\xi_1, \xi_2, \xi_3} d\xi_1 d\xi_2 d\xi_3 = \int_{-1}^1 \int_{-1}^1 \int_{-1}^1 \cdots f_{\xi_1} f_{\xi_2} f_{\xi_3} d\xi_1 d\xi_2 d\xi_3. \quad (95)$$

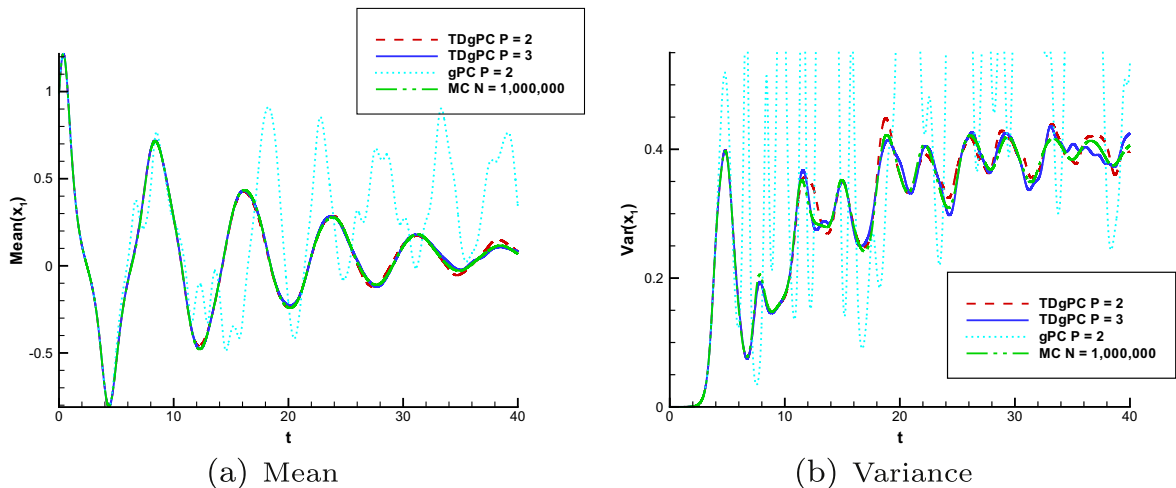


Fig. 22. Mean and variance of x_1 vs. time for $\alpha = 0.99, \beta = 1$ and $\gamma = 1$: TDgPC solutions ($P = 2$ and $P = 3$) compared to a gPC solution ($P = 2$) and a Monte-Carlo analysis ($N = 1,000,000$).

Unlike the single random variable case we still have to deal with a three-dimensional integral after transformation. We can treat this integral as a repeated one-dimensional integral, since ξ_1 , ξ_2 and ξ_3 are statistically independent.

4.4.1. Results

In Fig. 22 we compare the results from a TDgPC solution approach to gPC results and a Monte-Carlo analysis. We choose values of $P = 2$ and $P = 3$ for the two TDgPC solutions in this comparison. From approximately $t = 12$ onwards the gPC results for the mean of x_1 lose any resemblance to the correct solution. When looking at the variance of x_1 this point is already reached at $t = 4$.

The TDgPC results with $P = 2$ remain reasonably close to the Monte Carlo analysis results for the entire time interval considered, although the curves can be seen to lose some of their accuracy as time progresses. Increasing P from $P = 2$ to $P = 3$ results in an increase in accuracy: TDgPC results for the mean of x_1 are now visually indistinguishable from the Monte-Carlo results for the entire time interval displayed. The accuracy of the variance of x_1 goes up as well, but the TDgPC curve is not precisely on top of the Monte-Carlo curve as was the case for a one-dimensional random input. A comparison of TDgPC, gPC and Monte-Carlo results for x_2 and x_3 shows similar characteristics as the results for x_1 .

5. Conclusions

In this paper an adaptive gPC method in time is proposed, the time-dependent generalized polynomial chaos (TDgPC). TDgPC takes into account that the probability density function (PDF) of the solution changes as a function of time. Due to this change in PDF, orthogonal polynomials that were optimal initially, lose their optimality for increasing time and a new set of orthogonal polynomials needs to be created. The method has been applied to a simple decay model and the Kraichnan–Orszag three-mode problem. In the latter case both the situation with one random initial condition and three random initial conditions were considered. Based on computational results TDgPC ameliorates the accuracy when using long-time integration. The advantage of this approach is that the polynomial degree can be kept low ($P = 2, 3$ or 4) without introducing multiple elements (ME-gPC, [16]) in random space. This leads in the cases considered to a reduction of the number of degrees of freedom and consequently to a reduction in the number of deterministic problems that need to be solved. The additional cost is the construction of new sets of orthogonal polynomials (which for $P \approx 3$ is quite cheap) and the integral transformations in setting up the deterministic equations and the calculation of the statistical moments.

Whether gPC type methods are the preferred way of solving stochastic differential equations is beyond the scope of this paper. This generally depends on practical issues like the size of the problem, the availability of deterministic solvers, the number of stochastic variables in the problem and the required accuracy.

Current research focuses on the application of TDgPC to partial differential equations. Future directions for research include the combination of TDgPC with ME-gPC, where in each element new stochastic variables are introduced. This will lead to a very effective and efficient algorithm, especially for solutions with low regularity such as the Kraichnan–Orszag problem corresponding to $\alpha = 0.995$. Furthermore, the new polynomials associated with the PDF of the solution, introduced in this paper, may lead to improved collocation points for the multi-element probabilistic collocation method ME-PCM, [34].

Acknowledgments

The authors wish to thank Joris Oostelbos for providing some of the figures. Professor Karniadakis wishes to acknowledge the financial support from OSD/AFOSR MURI.

Appendix A. On the error development in long-time integration

In this separate part of this paper we wish to make some additional remarks on long-time integration. It is our belief that any sampling method will eventually break down for a general time-dependent random process and a given amount of samples. This statement cannot be corroborated since it would mean that we have to test all existing methods and all the methods that have yet to be developed. However, this bold statement also depends on what we mean by “long-time integration”. In order to highlight several of the pitfalls when talking about long-time integration, we will consider here a comparison between the Probabilistic Collocation method [35] and a Monte-Carlo simulation with the same amount of samples, applied to the decay problem discussed in Section 3.1.

Consider the PCM in the Gauss–Lobatto points for $P = 127$ and the Monte Carlo Method for 128 samples. The solution is advanced in time by an explicit Euler method with $\Delta t = 0.01$. The mean is calculated as

$$\mu^{PCM}(t) = \sum_{p=0}^{127} \frac{1}{2} u^n(\xi_p) \cdot w_p, \quad (96)$$

where ξ_p is the p th Gauss–Lobatto point and w_p is the associated Gauss–Lobatto weight

$$\mu^{MC}(t) = \frac{1}{128} \sum_{p=1}^{128} u(\chi_p), \quad (97)$$

where χ_p is random number from the uniform distribution $I_{[0,1]}$. And the variance is given by

$$\text{Var}^{\text{PCM}}(t) = \sum_{p=0}^{127} \frac{1}{2} (u^n(\xi_p) - \mu^{\text{PCM}}(t))^2 w_p, \quad (98)$$

and

$$\text{Var}^{\text{MC}}(t) = \frac{1}{128} \sum_{p=1}^{128} (u^n(\chi_p) - \mu^{\text{MC}}(t))^2. \quad (99)$$

The relative error in the PCM and MC solution are shown in Fig. 23. If we increase the number of degrees of freedom from 128 to 256 we obtain the results given in Fig. 24. When we compare the results in the Figs. 23 and 24, we see that there is no change in the PCM results and some change in the MC results. The change in the latter can attributed to the very small sample size, so each run will give a different result.

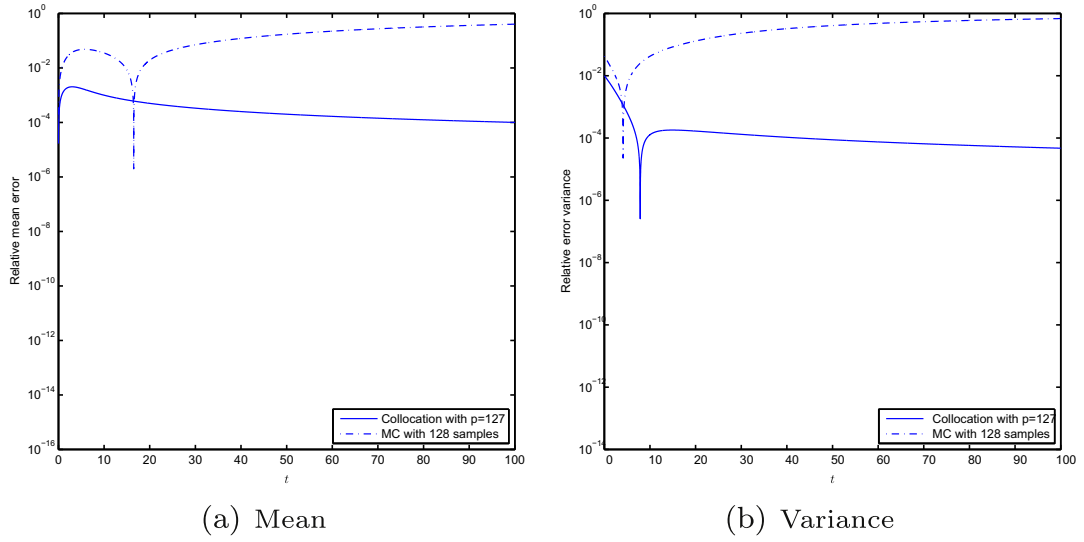


Fig. 23. Evolution of the relative error in the mean (left) and variance (right) for PCM and Monte-Carlo with 128 degrees of freedom. Explicit Euler time integration, $\Delta t = 0.01$ for $t \in [0, 100]$.

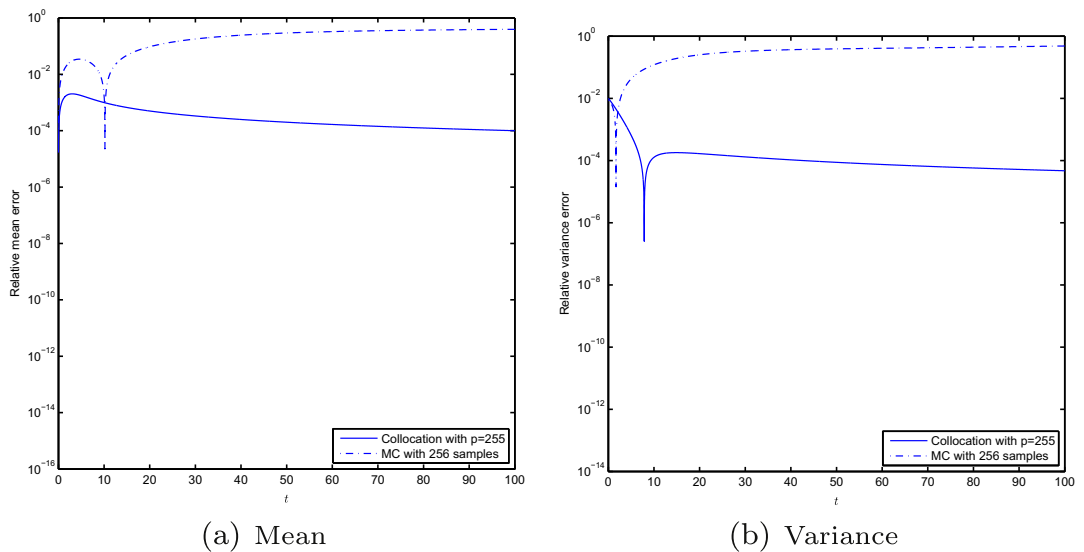


Fig. 24. Evolution of the relative error in the mean (left) and variance (right) for PCM and Monte-Carlo with 256 degrees of freedom. Explicit Euler time integration, $\Delta t = 0.01$ for $t \in [0, 100]$.

For a proper assessment of the error in time-dependent calculations we need to be able to decompose the error due to the time integration and the error due to sampling in random space. Since there is hardly any change when the sample size is doubled, it is tempting to attribute the error to the time integration. In order to investigate this, we run these two test cases again, but this time we use exact integration instead of the explicit Euler method. The results of this exercise can be found in Figs. 25 and 26.

From these figures we see that the relative error in the collocation method can be attributed to the time integration; the error drops to machine accuracy when exact integration is used instead of numerical integration. The relative error in the MC method is dominated by the error in random space; the two solutions with numerical integration and exact time integration are almost indistinguishable.

From these observations one may conclude that the collocation method provides a more accurate description in random space compared to the MC method. This conclusion is justified for *this particular problem* and *this particular time interval*.

If we run the same test case for a longer period, i.e. until $t = 5000$ instead of $t = 100$ we see that the error in random space grows and starts to dominate the relative errors in the mean and variance at $t \approx 1200$ and $t \approx 500$, respectively, as shown in

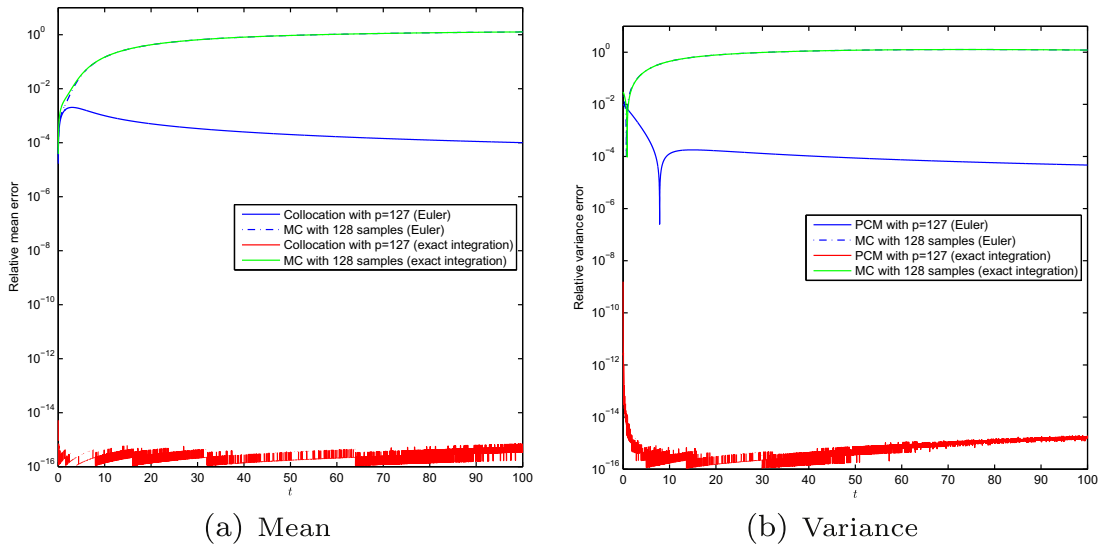


Fig. 25. Evolution of the relative error in the mean (left) and variance (right) for PCM and Monte-Carlo with 128 degrees of freedom. Explicit Euler time integration, $\Delta t = 0.01$ and exact integration in time for $t \in [0, 100]$.

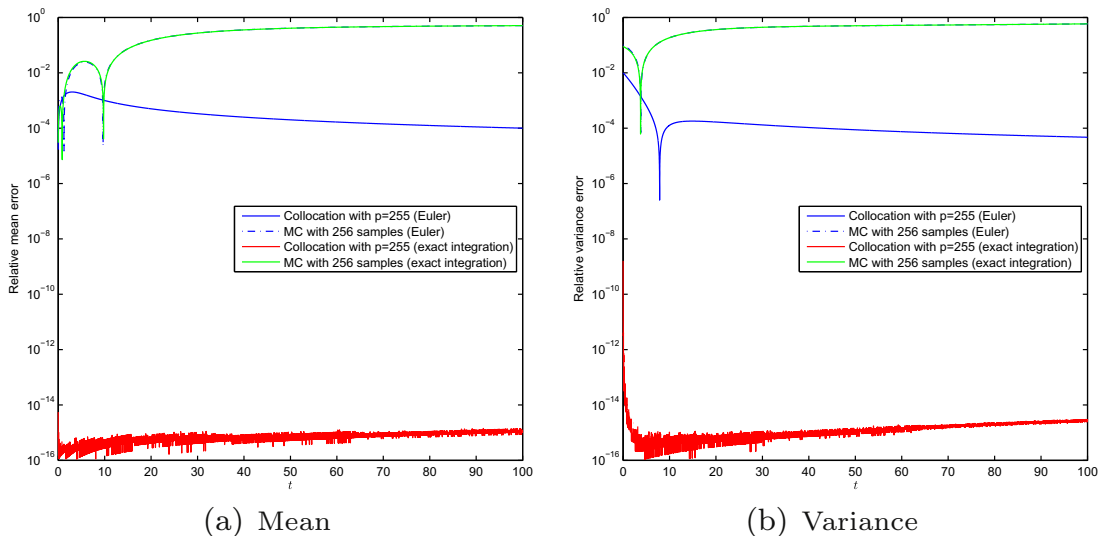


Fig. 26. Evolution of the relative error in the mean (left) and variance (right) for PCM and Monte-Carlo with 256 degrees of freedom. Explicit Euler time integration, $\Delta t = 0.01$ and exact integration in time for $t \in [0, 100]$.

Fig. 27. If we continue the simulation even longer, until $t = 10^5$, we see that the relative error in the collocation method will be larger than the relative error in the MC method as can be seen in Fig. 28. The reason that the collocation methods eventually diverges can be attributed to the location of the Gauss–Lobatto points. For the exact solution we have that $\mu(t) \rightarrow 1/t$ and $\text{Var}(t) \rightarrow 1/2t$ for $t \rightarrow \infty$. The exact solution in all Gauss–Lobatto points decays exponentially fast to zero at a rate $\exp(-0.5 \cdot (1 + \xi_p) \cdot t)$, except for the first Gauss–Lobatto point $\xi_0 = -1$, for which the solution remains 1. This means that for determination of the mean we have

$$\mu^{\text{PCM}}(t) = \sum_{p=0}^P \frac{1}{2} u^n(\xi_p) \cdot w_p \rightarrow \frac{w_0}{2}, \quad (100)$$

and for the variance

$$\text{Var}^{\text{PCM}}(t) = \sum_{p=0}^P \frac{1}{2} (u^n(\xi_p) - \mu^{\text{PCM}}(t))^2 w_p \rightarrow \frac{w_0}{2} - \frac{w_0^2}{4}, \quad (101)$$

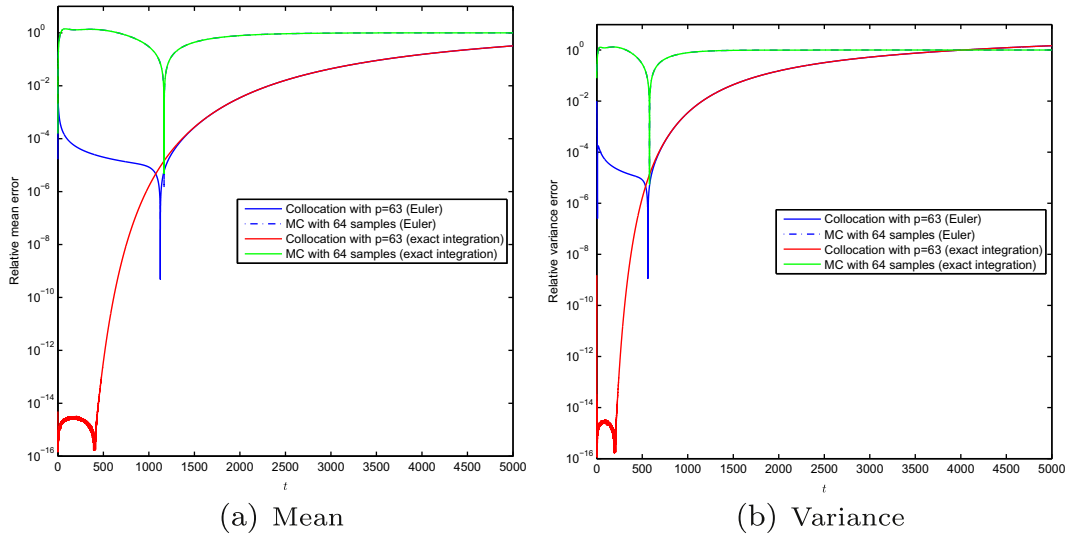


Fig. 27. Evolution of the relative error in the mean (left) and variance (right) for PCM and Monte-Carlo with 64 degrees of freedom. Explicit Euler time integration, $\Delta t = 0.01$ and exact integration in time for $t \in [0, 5000]$. Both Monte-Carlo solutions almost coincide.

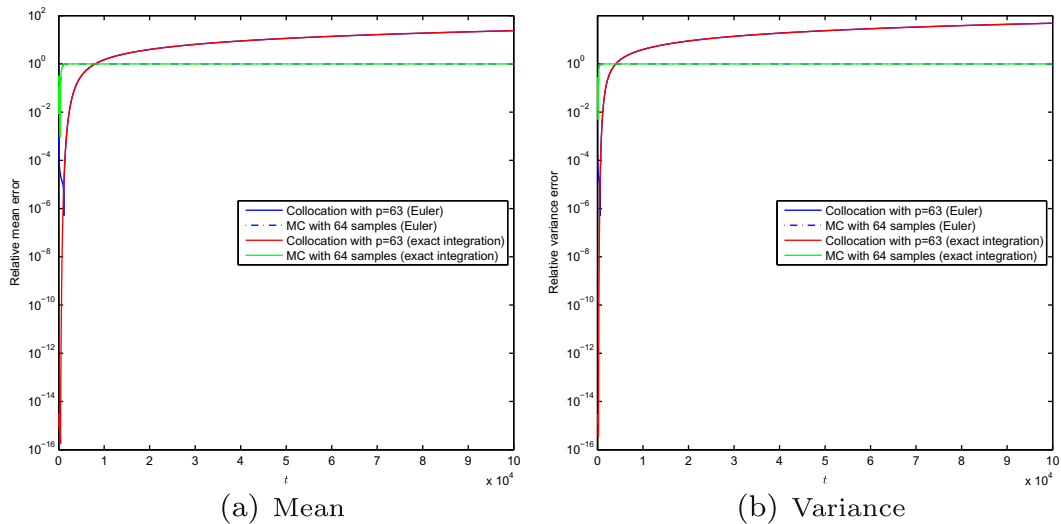


Fig. 28. Evolution of the relative error in the mean (left) and variance (right) for PCM and Monte-Carlo with 64 degrees of freedom. Explicit Euler time integration, $\Delta t = 0.01$ and exact integration in time for $t \in [0, 10^5]$.

For the relative error in mean and variance this means that

rel. mean error = $\frac{w_0}{2}t + const$ and rel. variance error = $\left(w_0 - \frac{w_0^2}{2}\right)t + const.$

(102)

This linear growth is shown in Fig. 29. In Table 2 the growth rates based on (102) are compared with the values obtained from the calculation for $P = 63$ for which $w_0 = 4.9603 \cdot 10^{-4}$. For the MC method a sample taken at the point $\zeta = -1$ has prob-

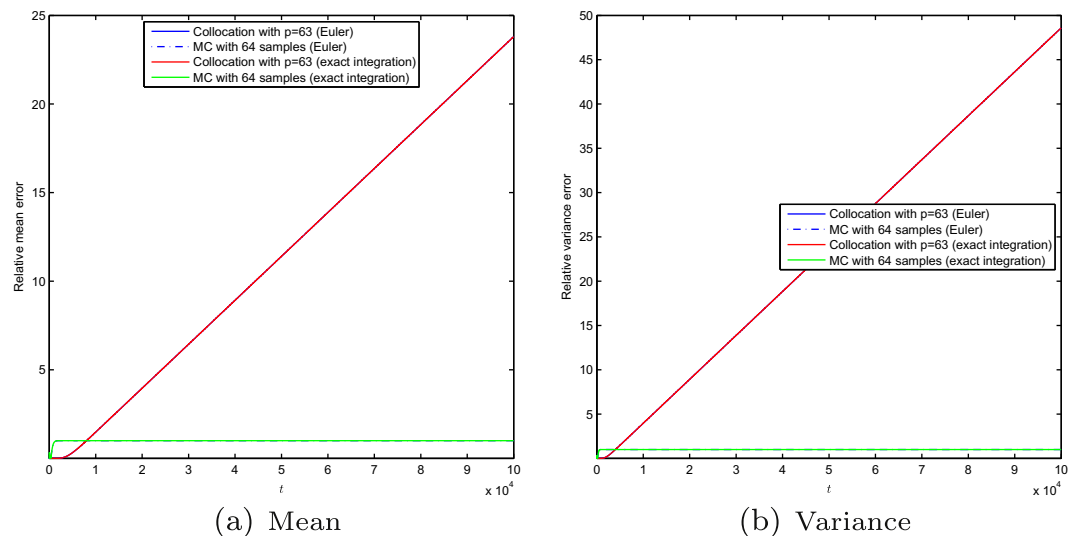


Fig. 29. Evolution of the relative error in the mean (left) and variance (right) for PCM and Monte-Carlo with 64 degrees of freedom. Exact time integration, $\Delta t = 0.01$ and exact integration in time for $t \in [0, 10^5]$.

Table 2
Theoretical and experimental growth.

	Theoretical slope	Numerical slope
Mean	$2.4802 \cdot 10^{-4}$	$2.4801 \cdot 10^{-4}$
Variance	$4.9591 \cdot 10^{-4}$	$4.9591 \cdot 10^{-4}$

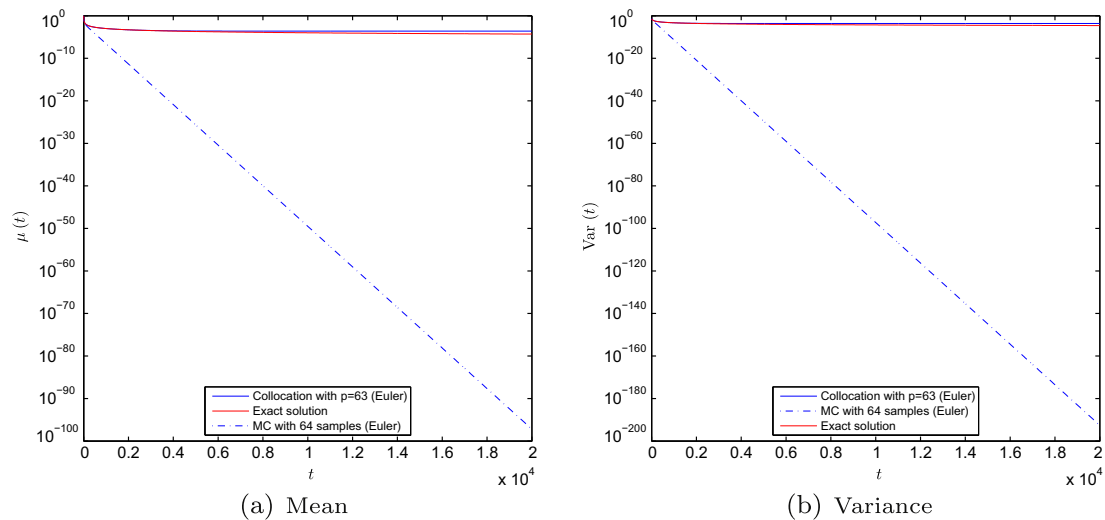


Fig. 30. Evolution of the solution of the mean (left) and variance (right) for PCM and Monte-Carlo with 64 degrees of freedom. Explicit Euler time integration, $\Delta t = 0.01$ and exact integration in time for $t \in [0, 2 \cdot 10^4]$.

ability zero, so we will not see linear growth in the relative error of the mean for the Monte-Carlo simulation. Since all solution of the samples will decay to zero exponentially fast, the relative error in the mean and the Variance of the MC method, will converge to 1, which is confirmed by the simulation. In Fig. 30 the solution of the mean and variance are plotted on a logarithmic scale. We see that the absence of the point $\chi_p = -1$ leads to solution which tend to zero too fast.

The growth is not associated with the fact that the mean and variance of the exact solution go to zero. If we solve the problem

$$\frac{du}{dt} + k(\xi)u = \frac{1}{2}, \quad (103)$$

the mean decays to a half and we see exactly the same long-time behaviour, see Fig. 31. The level of the relative mean error is lower in this figure, due to the fact for large t we divide by $1/2 + C/t$, instead of C/t , but we still observe linear growth for PCM.

If, instead of the Gauss–Lobatto nodes for the PCM method, we use the internal Gauss points and thereby exclude the detrimental node $\xi_0 = -1$, we observe that PCM and the MC method display a similar error evolution for $t \rightarrow \infty$, as can be seen in Fig. 32. So a judicious choice of integration points in the PCM method significantly affects the long-time behaviour

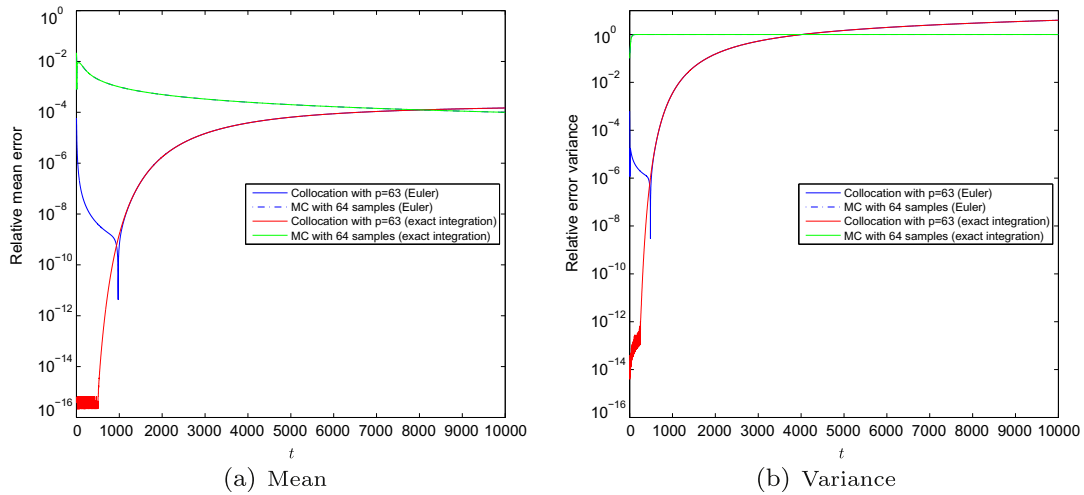


Fig. 31. Evolution of the solution of the solution of (103), mean (left) and variance (right), for PCM and Monte-Carlo with 64 degrees of freedom. Explicit Euler time integration, $\Delta t = 0.01$ and exact integration in time for $t \in [0, 10^4]$.

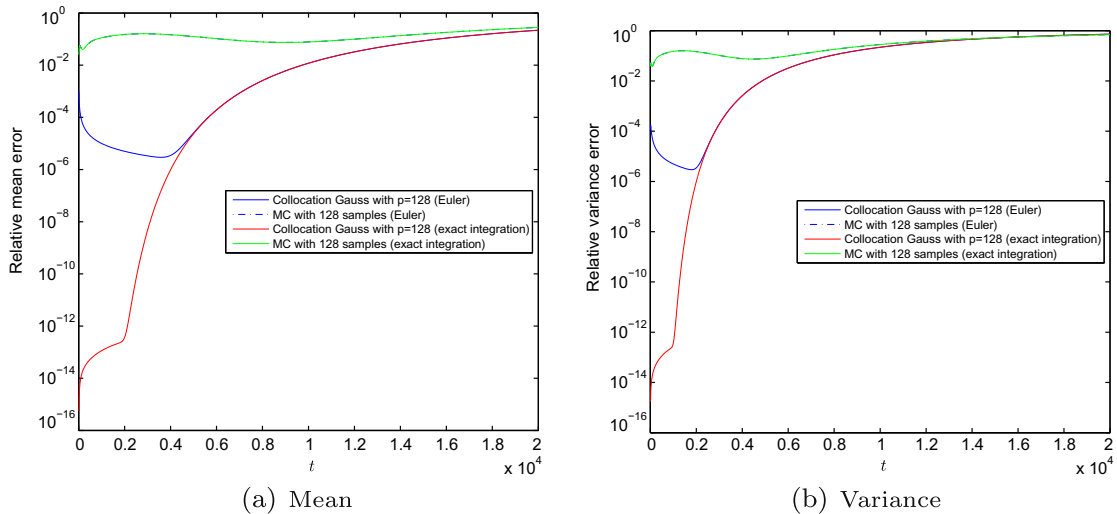


Fig. 32. Evolution of the solution of the solution of decay problem, mean (left) and variance (right), for PCM in the Gauss points and Monte-Carlo with 128 degrees of freedom. Explicit Euler time integration, $\Delta t = 0.01$ and exact integration in time for $t \in [0, 2 \cdot 10^4]$.

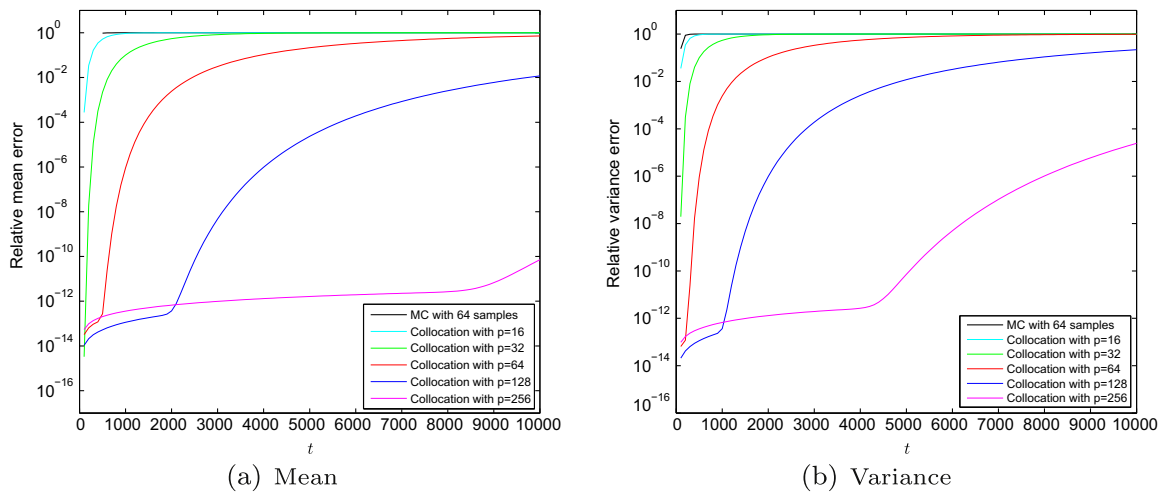


Fig. 33. Evolution of the solution of decay problem, mean (left) and variance (right), for PCM in the Gauss points for various polynomial degrees and Monte-Carlo with 64 degrees of freedom. Exact integration in time for $t \in [0, 10^4]$.

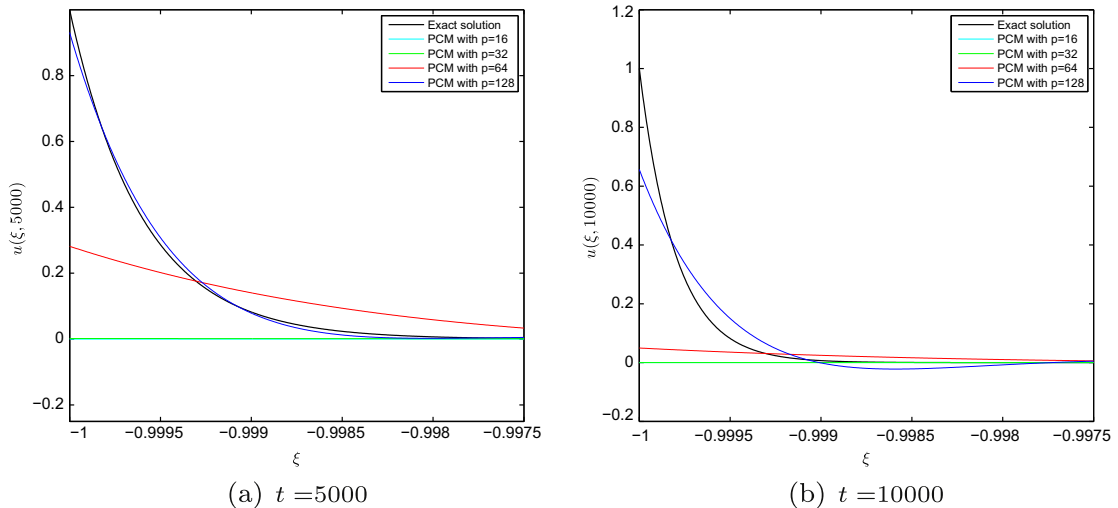


Fig. 34. PCM approximation in random space near $\xi = -1$ at $t = 5000$ (left) and $t = 10000$ (right) for various values of p .

of PCM. Although one should bear in mind that in all cases the solution is very bad and one may question the fact whether it is useful to talk about “less bad” or “worse”.

If we vary the polynomial degree in PCM (exact integration and Gauss points) all methods converge to a relative error of 1 when t tends to infinity. For higher-order approximations it takes longer for the error growth to set in. This is depicted in Fig. 33.

The main reason all sampling methods eventually depart from the exact solution for the mean and the variance even though the solution is nodally exact (in the case of exact time integration) stems from the numerical integration to evaluate the mean and the variance. Gauss or Gauss–Lobatto integration methods assume that the solution between the nodes is represented by a nodal interpolation. As long as this nodal interpolation is close to the exact solution, the corresponding integrals for the mean and the variance are close to the exact mean and variance. The exact solution for the decay problem, $\exp(-0.5 \cdot (1 + \xi)t)$, develops a boundary near $\xi = -1$ for increasing t . As long as the interpolation is able to capture this boundary layer, the relative error in the mean and the variance will be small, but as soon as the boundary layer becomes too thin to be represented by the global polynomial approximation the error starts to grow. Polynomial approximations for various p at $t = 5000$ and $t = 10,000$ are shown in Fig. 34. For all polynomial degrees, the polynomial approximation will eventually miss the boundary layer for sufficiently large t in which case the relative error in the solution tends to one. The solutions in random space shown in Fig. 34 correspond to the errors shown in Fig. 33.

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