Time-Dependent Polynomial Chaos

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The undersigned hereby certify that they have read and recommend to the Faculty of Aerospace Engineering for acceptance the thesis entitled **"Time-Dependent Polynomial Chaos"** by **Peter Vos** in fulfillment of the requirements for the degree of **Master of Science**.

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TIME-DEPENDENT POLYNOMIAL CHAOS

Peter Vos

Key words: uncertainty, stochastic ODE, polynomial chaos, long-term integration

Abstract. *Generalized polynomial chaos is known to fail for long-term integration, loosing its optimal convergence behavior and developing unacceptable error-levels. In this work, we present a time-dependent alternative of polynomial chaos in order to overcome these issues. This technique exists out of an on-the-fly reinitialization of the polynomial chaos expansion at different discrete time-levels. At those time-levels, the new polynomial chaos expansion will be created in terms of the stochastic solution. This time-dependent approach is applied on a stochastic ODE of which the results are compared with a standard gPC solution.*

1 INTRODUCTION

In most engineering applications, one aims to solve physical problems by converting it into a deterministic mathematical model. This is a rough approximation of reality, as many physical input parameters describing the problem are fixed through this conversion. In reality however, these parameters, like material properties or boundary conditions for example, show some randomness which definitely influence the behavior of the solution. This randomness is not incorporated in the deterministic model.

In order to include this uncertainty in the mathematical model, probabilistic methods have been developed. Next to statistical approaches, which use a large sample of (pseudo-) random numbers and therefore can turn out to be very costly (e.g. Monte Carlo simulation), extensive research has been done on nonstatistical (deterministic) approaches. Recently, a new nonstatistical approach, called *polynomial chaos*, has been developed [1]. This approach, based on Wiener's concept of homogeneous chaos [2], has proved to be efficient in engineering applications [1]. Here, the term *chaos*, as coined by Wiener, refers to randomness (as, for example, in physics observed in the statistical theory of a gas or a liquid) and it should not be confused with the concept of chaos theory related to non-linear dynamical systems, in which the term chaos was first used by Yorke [3] only 37 years later. The theoretical basis of the polynomial chaos approach is based on Cameron and Martin's [4] findings, that a polynomial chaos expansion does converge to any L^2 functional in the L^2 sense. In the context of stochastic processes, this implies that every stochastic process with finite second-order moment can be represented by an (infinite) polynomial chaos expansion. The original form of polynomial chaos is a spectral expansion based on the orthogonal Hermite polynomials in terms of Gaussian random variables and using deterministic coefficients. However, using this original form, optimal convergence is only achieved when dealing with Gaussian stochastic processes.

In order to obtain optimal convergence for more general stochastic processes, Karniadakis and co-workers extended this approach into a broader framework called *generalized Polynomial Chaos* (gPC) [5]. Within this framework, the close connection between the probability functions of certain random variables and the weighting function in the orthogonality relationship of certain orthogonal polynomials is used to represent non-Gaussian processes. More precisely, it has been realized that spectral expansions based on the orthogonal polynomials of the Askey-scheme [6] in terms of the corresponding random variable, chosen according to the weighting function of the polynomials, can be efficiently employed to represent a broad range of ”standard” distributions such as the uniform distribution, the Gamma and Beta distribution (see for instance [7]), yielding optimal convergence.

Although gPC, in its plain form, has been successfully applied in different cases showing an exponential convergence in approximating the solution [5, 8], it is known to perform inadequate for problems concerning discontinuities induced by random inputs. For the Kraichnan-Orszag problem, Wan [9] showed that the solution's discontinuous dependence (fixed point versus limit cycle) of the random initial conditions causes gPC to fail, and he successfully proposed a Multi-Element gPC approach to alleviate this problem.
Furthermore, also for long-term integration, gPC in its plain form turns out to be inefficient, even for a simple (stochastic) ordinary differential equation (ODE). Although in the previous mentioned work of Xiu [5], gPC has been successfully applied in approximating the solution of a stochastic ODE, showing an exponential convergence, one should notice that those optimal results only hold for early times. More than that, for long term integration, not only the convergence behavior will deteriorate, also the approximation of the solution for a fixed polynomial order P will start to fail, resulting in unacceptable error levels. Also here, Wan's Multi-Element gPC Method is capable of overcome this problem.

In this work, we present another form of polynomial chaos, suitable to deal with the problems concerning long-term integration. We develop a time-dependent polynomial chaos that reinitializes itself at some discrete time-levels based on the solution at those time-levels, in order maintain an optimal polynomial chaos expansion when progressing in time.

This paper is organized as follows: In Section 2, the standard gPC technique will be introduced and reviewed. In Section 3, the performance of these techniques for long-term integration will be discussed and analyzed. Next, in Section 4, the time-dependent polynomial chaos technique is presented and by means of numerical results, it is shown to display a proper long-term behavior. Finally, conclusions are drawn, and some possible applications for future work are recommended in Section 5. It should be noted that starting from section 3, all explanations are made on the basis of a stochastic ODE modeling exponential growth, which will be used as the example throughout this work.

2 GENERALIZED POLYNOMIAL CHAOS

In this section, we first explain how a stochastic process can be represented by a polynomial chaos expansion. We then introduce the general procedure of applying the generalized polynomial chaos expansion in order to solve stochastic differential equations.

2.1 The Chaos Expansion

Generalized polynomial chaos (gPC) is employed to represent stochastic processes. Stochastic processes can be seen as a process involving some randomness. They can be represented by a stochastic mathematical model, often expressed in terms of stochastic differential equations. Stochastic mathematical models are based on a probability space $(\Omega, \mathcal{F}, \mathcal{P})$ where Ω is the sample space, $\mathcal{F} \subset 2^{\Omega}$ its σ-algebra of events, and $\mathcal{P}$ its probability measure. In addition considering some physical domain $D \subset \mathbb{R}^d \times T$ $(d = 1, 2, 3)$, which can be a combination of spatial and temporal dimensions, a stochastic process can be seen as a scalar- or vector-valued function $\mathbf{u}(\mathbf{x}, t, \omega) : D \times \Omega \rightarrow \mathbb{R}^b$ where $\mathbf{x}$ is an element of the physical space, t denotes the time and ω is a point in the sample space Ω. Furthermore, because of the infinite-dimensional nature of the probability space, we discretize this space by characterizing it by a finite number of random variables $\{\xi_j(\omega)\}_{j=1}^{N}$, $N \in \mathbb{N}$. This can be seen as assigning a finite number of coordinates $\{\xi_j\}_{j=1}^{N}$ to the probability space reducing it to a finite dimensional space $\Lambda \subset \mathbb{R}^N$. Consequently, the stochastic process $\mathbf{u}$ becomes a mapping $\mathbf{u}(\mathbf{x}, t, \boldsymbol{\xi}) : D \times \Lambda \rightarrow \mathbb{R}^b$. It is important to note that in this work, we assume that the occurring stochastic processes are already characterized by a known set of random variables.

Wiener was the first to represent stochastic processes by orthogonal polynomial expansions [2]. To accomplish this, he used Hermite polynomials in terms of Gaussian random variables to represent Gaussian processes, which is referred to as homogeneous chaos. In this way, the stochastic process is represented in the form:

$$\mathbf{u}(\mathbf{x}, t, \boldsymbol{\xi}(\omega)) = \sum_{i=0}^{\infty} \mathbf{u}_i(\mathbf{x}, t) H_i(\boldsymbol{\xi}(\omega)) \tag{1}$$

in which H_i are Hermite polynomials and $\boldsymbol{\xi}$ is a vector of Gaussian random variables with zero mean and unit variance. It is a spectral expansion in the random dimensions employing deterministic coefficients. According to the Cameron-Martin theorem [4], for a fixed value of $\mathbf{x}$ and t, this expansion converges to any $L^2(\Omega)$ functional in the $L^2(\Omega)$ sense. This implies that the application of polynomial chaos is restricted to those stochastic processes yielding

$$\int_{\omega\in\Omega} |\mathbf{u}(\mathbf{x}, t, \omega)|^2 d\mathcal{P}(\omega) < \infty \tag{2}$$

As a result, polynomial chaos is restricted to second-order stochastic processes, i.e. processes with finite second-order moments. These are processes with finite variance, and this applies to most physical processes.

Although Wiener's original polynomial chaos expansion converge to any second-order stochastic process, it is most suitable to represent Gaussian processes, due to the random variable's Gaussian nature, yielding a fast convergence. In order to deal with a broader range of stochastic processes, the Wiener-Hermite chaos has been generalized to the generalized polynomial chaos [5], also referred to as Wiener-Askey polynomial chaos. Analogously, gPC is a means of representing second-order stochastic processes through the expansion:

$$\mathbf{u}(\mathbf{x}, t, \boldsymbol{\xi}(\omega)) = \sum_{i=0}^{\infty} \mathbf{u}_i(\mathbf{x}, t)\Phi_i(\boldsymbol{\xi}(\omega)) \tag{3}$$

Here the random trial base $\{\Phi_i(\boldsymbol{\xi}(\omega))\}$ exists out of orthogonal polynomials from the Askey-scheme, of which the Hermite polynomials are a subset, in terms of a random vector $\boldsymbol{\xi} = \{\xi_j(\omega)\}_{j=1}^{N}$. The combination of random vector and polynomials is carefully selected based on the distribution of the random input. It seems that for certain random variables, their probability distribution function (PDF) uniquely corresponds to one of the weighting functions $w(\boldsymbol{\xi})$ in the orthogonality relation of the different orthogonal polynomials of the Askey-scheme. An overview of this correspondence is shown in table (1). Choosing the corresponding combination leads to a proper gPC expansion. Since

Table 1: The correspondence of the type of Wiener-Askey polynomial chaos and their underlying random variables

Random variables $\boldsymbol{\xi}$	Wiener-Askey chaos $\{\Phi_j(\boldsymbol{\xi})\}$
Gaussian	Hermite-chaos
Gamma	Laguerre-chaos
Beta	Jacobi-chaos
Uniform	Legendre-chaos

each of the polynomials of the Askey-scheme forms a complete basis in the Hilbert space determined by their corresponding support, it is expected, according to Xiu et al. [5], that each type of Wiener-Askey expansion converges to any $L^2(\Omega)$ functional in the $L^2(\Omega)$ sense in the corresponding Hilbert functional space as a generalized result of Cameron-Martin theorem.

This generalized polynomial chaos has later been further generalized for arbitrary random inputs [10, 11]. In this way, gPC is not restricted anymore to random inputs of standard types. In order to expand the solution in a polynomial chaos expansion in terms of this arbitrary random variables, a proper random trial base $\{\Phi_j(\boldsymbol{\xi})\}$ should be created, and this according to the gPC rules. This means that a set of orthogonal polynomials is created in such a way that they are orthogonal with respect to a weighting function which equals the probability density function of the random input. Different algorithms can be employed for this orthogonalization, among others the Stieltjes procedure, the Lanczos algorithm [10] or the Gram-Schmidt orthogonalization [11]. Taking this further generalization into account, one can truly speak of generalized polynomial chaos.

The polynomials of the gPC's random trial base satisfy following orthogonality relation

$$\langle \Phi_i \Phi_j \rangle = \langle \Phi_i^2 \rangle \delta_{ij} \tag{4}$$

where δ_{ij} is the Kronecker delta and $\langle \cdot, \cdot \rangle$ denotes the ensemble average. The inner product in (4) is in the Hilbert space determined by the measure of the random variables

$$\langle f(\boldsymbol{\xi}) g(\boldsymbol{\xi}) \rangle = \int_{\omega \in \Omega} f(\boldsymbol{\xi}) g(\boldsymbol{\xi}) d\mathcal{P}(\omega) = \int f(\boldsymbol{\xi}) g(\boldsymbol{\xi}) w(\boldsymbol{\xi}) d\boldsymbol{\xi} \tag{5}$$

with $w(\boldsymbol{\xi})$ the corresponding weighting function and with integration in the last integral taken over the support of $\boldsymbol{\xi}$.

With the introduction of the gPC, optimal performance can now be achieved for a broader range of stochastic processes. In order to accomplish this, it is important to choose the appropriate type of chaos depending on the stochastic process' nature. Although every type of chaos converges to any second-order process, choosing the appropriate Wiener-Askey polynomial chaos leads to an optimal solution. This has been presented in [5], where it is computationally shown that exponential convergence is achieved when applying the optimal gPC through a Galerkin projection in random space on a stochastic ordinary differential equation.

2.2 The General Procedure

The gPC expansion for stochastic processes, as defined in the previous section, can be employed to solve stochastic differential equations. Stochastic differential equations are a way of modeling a stochastic process through a (set of) stochastic differential equation(s). The randomness enters the system through some uncertain initial or boundary condition or through some uncertain parameter appearing in the equations. Solving this set of differential equations results in the sought stochastic process. This problem can be formulated as: find the stochastic process $u(\boldsymbol{x}, t, \boldsymbol{\xi}(\omega))$, which solves the stochastic differential equation:

$$\mathcal{L}(\boldsymbol{x}, t, \boldsymbol{\xi}(\omega); u) = f(\boldsymbol{x}, t, \boldsymbol{\xi}(\omega)) \tag{6}$$

where $f(\boldsymbol{x}, t, \boldsymbol{\xi}(\omega))$ is a source term and $\mathcal{L}$ is a differential operator involving differentiation in space and/or time, which can be nonlinear.

The first step in the procedure is to expand the solution in a proper gPC expansion:

$$\mathbf{u}(\mathbf{x}, t, \omega) = \sum_{i=0}^{Q} \mathbf{u}_i(\mathbf{x}, t)\Phi_i(\boldsymbol{\xi}(\omega)) \tag{7}$$

Notice that here, in order to be computationally relevant, the stochastic solution is represented by a finite order gPC expansion. Because of this truncation, the resulting solution will be an approximation of the actual exact solution. The total number of expansion terms $(Q + 1)$ is determined by the dimension N of random the random vector $\boldsymbol{\xi}$ and the highest order P of the Askey polynomials $\{\Phi_k\}$

$$(Q + 1) = \frac{(N + 1)!}{N!P!} \tag{8}$$

In the spectral expansion (7) of the solution, in which the trial basis $\{\Phi_i\}$ has been chosen in correspondence with the type of random vector $\boldsymbol{\xi}$ according to the rules of gPC, the unknown deterministic coefficients $\mathbf{u}_i(\mathbf{x}, t)$, which represent the different modes of the solution, need to be determined. To accomplish this, start with substituting the expansion for the solution (7) into the governing equation (6)

$$\mathcal{L}\left(\boldsymbol{x}, t, \boldsymbol{\xi}; \sum_{i=0}^{Q} \mathbf{u}_k\Phi_i\right) = f(\boldsymbol{x}, t, \boldsymbol{\xi}) \tag{9}$$

Next, successively multiplying this equation by the different orthogonal polynomials of the finite expansion, and taking the statistical average

$$\left\langle \mathcal{L}\left(\boldsymbol{x}, t, \boldsymbol{\xi}; \sum_{i=0}^{Q} \bar{\mathbf{u}}_i\Phi_i\right), \Phi_j \right\rangle = \left\langle f(\boldsymbol{x}, t, \boldsymbol{\xi}), \Phi_j \right\rangle \qquad j = 0, 1, ..., Q \tag{10}$$

results in a set of $(Q + 1)$ coupled equations for the different random modes $\mathbf{u}_i(\mathbf{x}, t)$. Notice that this last step corresponds to a Galerkin projection in random space ensuring that the residual is orthogonal to the functional space spanned by the finite-dimensional basis $\{\Phi_i\}$. Next to the error induced by the truncation of the infinite expansion, this Galerkin projection does produce another additional error. Because of the averaging in the projection, the randomness does not explicitly appear in the resulting system anymore. As a result, the governing set of equations for the expansion coefficients $\mathbf{u}_k(\mathbf{x}, t)$ is completely deterministic. This system should further be solved in space and time using other preferred (numerical) methods.

3 LONG-TERM INTEGRATION

In this section, we will discuss the issues of long-term integration related to polynomial chaos for a stochastic ordinary differential equation (ODE). We will start with introducing this ODE, which will be the equation we will be studying in the remainder of this work. We then analyze its performance for long-term integration and finally we 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, representing exponential population growth

$$\frac{du(t)}{dt} + ku(t) = 0, \qquad u(0) = 1 \tag{11}$$

The reproduction 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 equation (11) can be formulated as, find $u(t, \xi)$ such that it satisfies

$$\frac{du(t,\xi)}{dt} + k(\xi)u(t,\xi) = 0 \qquad \text{in} \quad \Gamma = T \times S \tag{12}$$

and the initial condition $u(t = 0) = 1$. The domain Γ consists of the product of the temporal domain $T = [0, t_{end}]$ 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:

$$f_k(k) = 1, \qquad 0 \leq k \leq 1 \tag{13}$$

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

The exact solution of this equation is known and given by

$$u(t, \omega) = e^{-kt} \tag{14}$$

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

$$\bar{u}_{exact}(t) = E[u(t)] = \int_0^1 e^{-kt} f_k dk = \frac{1 - e^{-t}}{t} \tag{15}$$

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

$$\sigma_{exact}(t) = E[(u(t) - \bar{u}(t))^2] = \int_0^1 (e^{-kt} - \bar{u})^2 f_k dk = \frac{1 - e^{-2t}}{2t} - \left(\frac{1 - e^{-t}}{t}\right)^2 \tag{16}$$

Here, it can indeed be seen that the variance is bounded for all values of t such that we are dealing with a second-order process.

3.2 gPC Results

We first briefly repeat the gPC procedure, this time applied to the ODE. We then present the numerical results focusing on the long-term behavior of the approximated solution.

3.2.1 gPC Procedure

The first step in applying a gPC procedure to the stochastic ODE (12), 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:

$$f_\xi(\xi) = \frac{1}{2}, \qquad -1 \leq \xi \leq 1 \tag{17}$$

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

$$k(\xi) = \frac{1}{2}\xi + \frac{1}{2} \tag{18}$$

Hence, according to table (1), the Legendre polynomials $\{L_i\}_{i=0}^{P}$ should be selected as the trial basis for the spectral expansion. Summarized, for a proper gPC expansion, one should use Legendre polynomials in terms of a uniform random variable.

Next, the solution $u(t, \xi)$ should be expanded in a P-th order Legendre chaos expansion. This takes the form

$$u(t, \xi) = \sum_{i=0}^{P} u_i(t) L_i(\xi) \tag{19}$$

in which the time-dependent coefficients $u_i(t)$ are the unknowns to be determined.
In order to do so, substitute the gPC expansions in the governing equation (12), obtaining

$$\sum_{i=0}^{P} \frac{du_i(t)}{dt} L_i(\xi) = -\sum_{i=0}^{P} u_i(t) k(\xi) L_i(\xi) \tag{20}$$

Then, apply a Galerkin projection on the random space spanned by the polynomial basis $\{L_i\}_{i=0}^{P}$ and use the orthogonality of the Legendre polynomials in order to obtain the following set of ordinary differential equations for the unknown coefficients $u_m(t)$:

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

Consequently, the time-evolution of the coefficients can be calculated by employing a standard ODE solver to solve the resulting system in time. For this purpose, we used the standard fourth-order Runge-Kutta scheme in this work.

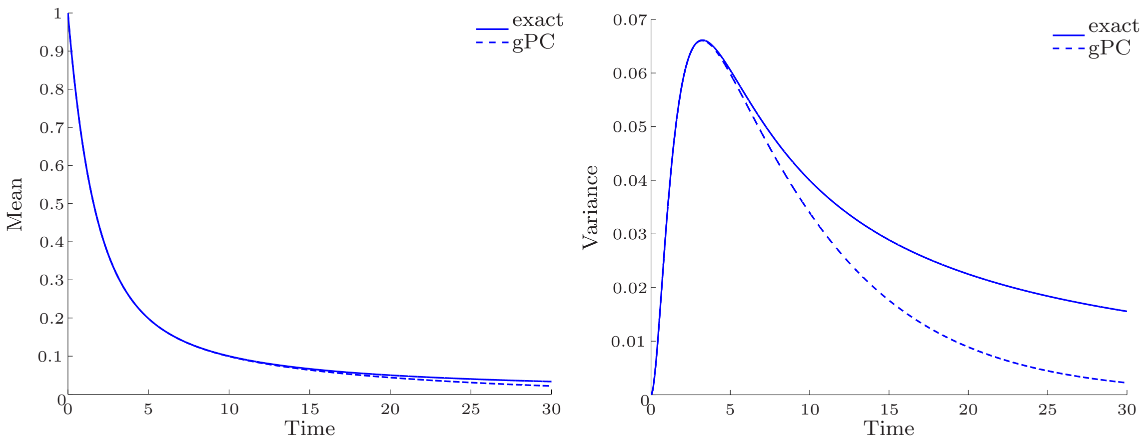
3.2.2 Numerical Results

Using the coefficients of the solution, found by solving system (21), it is possible to calculate the approximated mean and variance. Employing a gPC expansion, the approximated stochastic mean is simply equal to the first mode of the solution:

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

Thanks to the orthogonality of the Legendre polynomials, also the approximated variance has a rather straightforward expression in terms of the calculated coefficients:

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



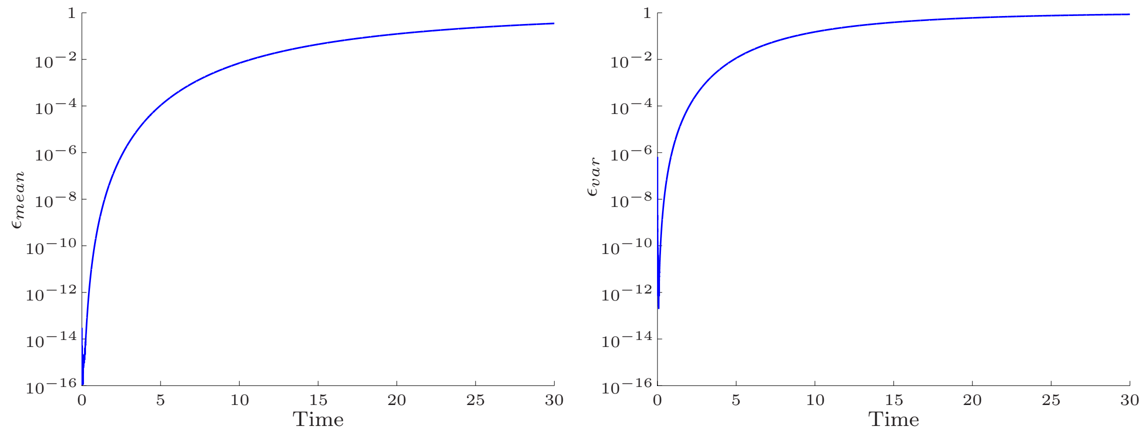
(a) Evolution of the mean (b) Evolution of the variance

Figure 1: Evolution of the mean and variance for 3^{th} order Legendre-Chaos

Figure (1) shows the solution of the mean and variance by employing a 3^{th} 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 really diverges after a while. The same behavior can be observed in the plot showing the evolution of the error, displayed in figure (2). Here, it can be seen that the error ϵ for the mean and variance, respectively defined as

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

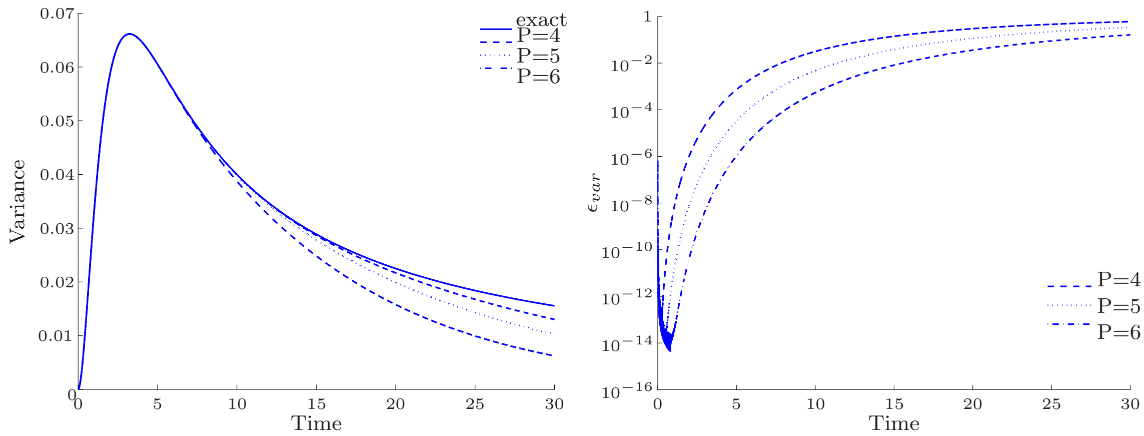
is only acceptable for early times. After this, the error quickly grows to the undesired order of $O(1)$, which is fairly unacceptable.



(a) Evolution of the mean-error (b) Evolution of the variance-error

Figure 2: Evolution of the error for 3^{th} order Legendre-Chaos

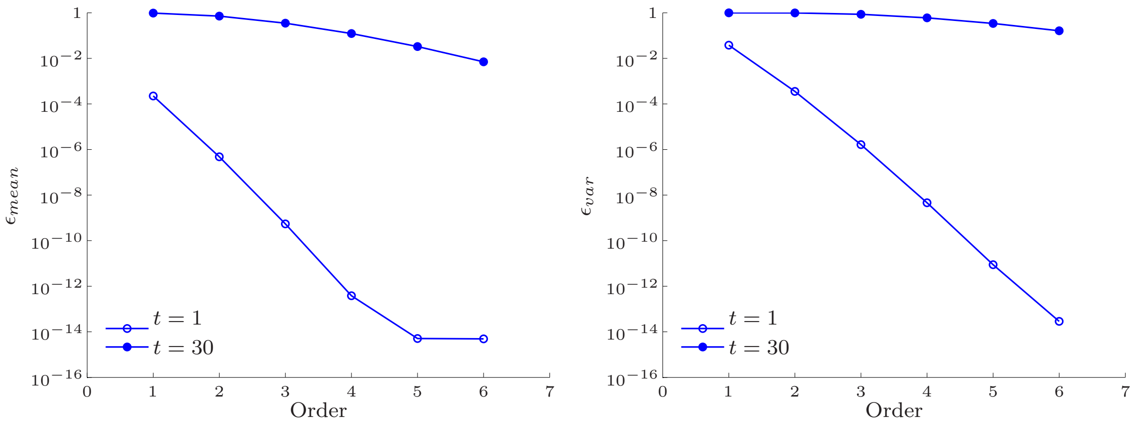
This rather poor behavior can be somewhat alleviated by increasing the expansion order. This is shown in figure (3), where it can be seen that for increasing order, the gPC solution follows the exact solution for a longer period. Here, only the results for the second-order statistics, characterized by the variance, are depicted. Because the gPC-method especially fails in approximating higher order statistics, we will mainly focus on issues related to the variance. The error levels shown in this picture, lie somewhat lower for increasing P. However, for $t = 30$, even for a polynomial order of $P = 6$, the level of the error still cannot be considered as acceptable.



(a) Evolution of the variance (b) Evolution of the variance-error

Figure 3: Behavior of the variance for increasing order Legendre-Chaos

Concerning the convergence, displayed in figure(4), we see that at the end-time, there is still some error convergence, although not as steep, nor exponential, compared to the optimal convergence at early times. However, as the level of the error of the variance itself is unacceptable for all values of P at those late time-levels, this convergence, in a way, does not make sense. For the mean, we can see that the error converges towards values of an order $O(10^{-2})$, which can be considered as acceptable.



(a) Error convergence of the mean

(b) Error convergence of the variance

Figure 4: Error convergence of the mean and variance

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

3.3 Why gPC Fails

Reconsider the gPC expansion of the approximated solution $u(t, \xi)$:

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

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

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

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

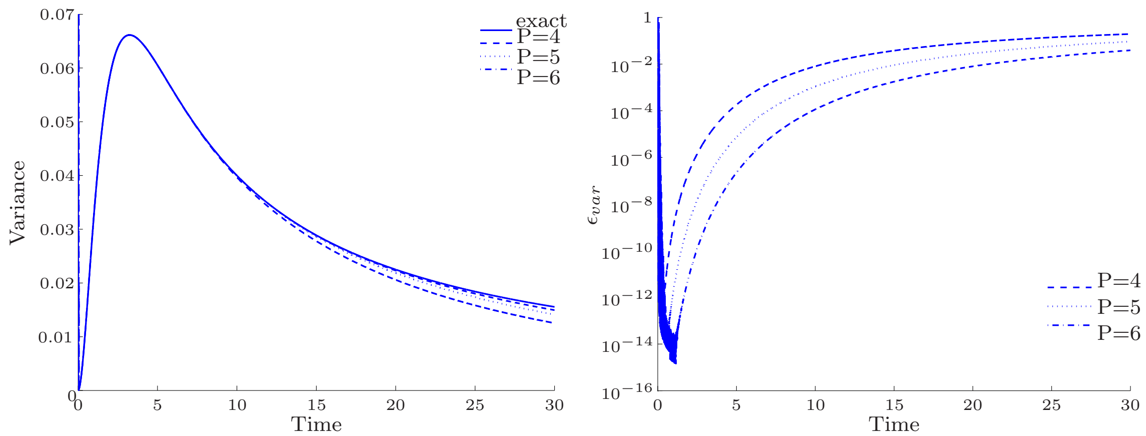
$$\alpha_i(t) = \frac{\langle u_{exact} L_i \rangle}{\langle L_i^2 \rangle} \tag{27}$$

with the ensemble average $\langle \cdot, \cdot \rangle$ defined as in (5). More explicitly, it can be calculated that the Legendre coefficients for the stochastic ODE problem in question, are given by:

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

The only error occurring in the finite Fourier-Legendre series approximation is due to the truncation. In fact, it is the optimal P^{th} order approximation.

Using expression (28) for the coefficients, both the mean and variance of the truncated Fourier-Legendre expansion can be calculated using the relations (22) and (23). Because the expression to calculate the mean exactly, see equation (15), corresponds to the first Legendre coefficient α_0, the mean due to 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 equation (23), where it can be observed that only increasing the polynomial order 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 figure (5) that even the optimal gPC expansion (optimal in the sense of minimal error) is not capable of approximating the second-order statistics in a decent way. Although the



(a) Evolution of the variance (b) Evolution of the variance-error

Figure 5: Behavior of the variance using the Fourier-Legendre chaos expansion

approximation is better than in case of the gPC procedure using a Galerkin projection, which induces an additional error to calculate the coefficients, 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 approximation all the statistics of 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 opts for. This does explain why other approaches such as a least-square projection in random space [12], instead of a Galerkin projection, are not suitable alternatives to attack the long-term integration issues. Also opting for higher order time integration methods will not overcome the problems.

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

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

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 occurs in the second term. This non-linearity in random dimension is essential for the behavior of the solution. For example, it causes the deterministic solution

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

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

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

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

$$\bar{k} = E[k] = \int_0^1 k f_k dk = \frac{1}{2} \tag{32}$$

does not correspond to the mean of the stochastic solution, incorporating the range and distribution of the random parameter k. In figure (6), it can be clearly seen that only for early times, those values do correspond, while for increasing time, their difference does grow. This behavior is known as stochastic drift. This implies that only for early times, the solution can approximated as a linear continuation of the random input. For growing 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 the solution to remember and resemble

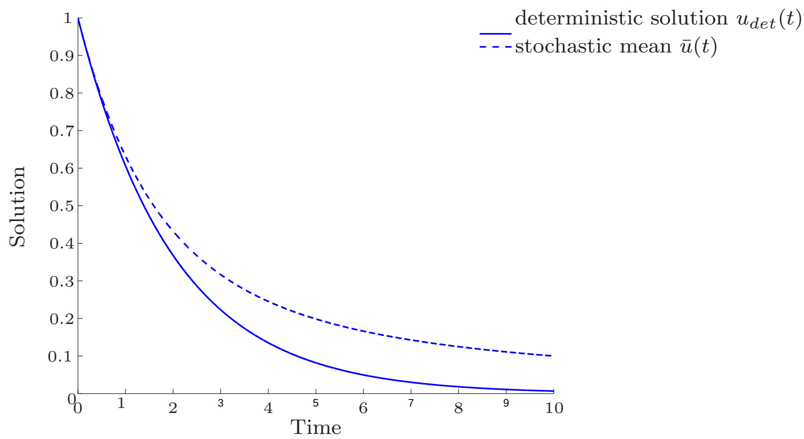


Figure 6: Evolution of deterministic solution and the mean of the stochastic solution

the stochastic input only for early times, while for growing time, the solution starts to forget the input due to the occurring quadratic non-linearity and start to develop its own stochastic characteristics. As a result for high time-levels, expressing the solution in terms of the input parameter requires more and more non-linear expansion terms. In this way, the concept of optimal polynomial chaos as explained in [5], does not really make sense for time-dependent problems involving long-term integration.

4 TIME-DEPENDENT POLYNOMIAL CHAOS

Based on this observation of loss of optimality for long-time integration we here present a time-dependent alternative of polynomial chaos. We first take a look at some basic thoughts that have been postulated on this subject in the late sixties. We then introduce our time-dependent polynomial chaos algorithm before presenting the numerical results showing a proper long-term behavior.

4.1 Background

In 1965, Orszag [13] studied the three mode problem, which can be seen as an inviscid turbulence model, given by the set of ODE's

$$\begin{aligned} \frac{dx_1(t)}{dt} &= x_2(t)x_3(t) \\ \frac{dx_2(t)}{dt} &= x_1(t)x_3(t) \\ \frac{dx_3(t)}{dt} &= -2x_1(t)x_2(t) \end{aligned} \tag{33}$$

This problem was later referred to as the Kraichnan-Orszag problem. Dependent on the initial values of the three modes, the deterministic solution (x_1, x_2, x_3) will in most cases develop as a limit cycle in time. Contrary to those highly dynamic solutions, for some particular initial conditions, the solution converges towards a fixed point.

When considering random initial conditions, it can be shown that for independently distributed Gaussian initial values with zero mean, the solution of each mode x_i converges towards a Gaussianly distributed zero-mean random variable. Inspired by this asymptotic behavior, Orszag expanded the stochastic solution of each mode in a Wiener-Hermite Chaos expansion:

$$x_i(t,\boldsymbol{\xi}) = \sum_{j=0}^{Q} x_j^i(t) H_i(\xi_1, \xi_2, \xi_3) \tag{34}$$

in which he set the first coefficient x_0^i equal to zero because of the zero-mean behavior of the modes. Furthermore, he formulated the expansion in a split form

$$x_i(t,\boldsymbol{\xi}) = x_1^i(t) H_i(\xi_1) + \sum_{j=2}^{Q} x_j^i(t) H_i(\xi_1, \xi_2, \xi_3) \tag{35}$$

in which the first term can be interpreted as the Gaussian part of the solution, while the higher order terms model the deviation of the Gaussian part. Due to the asymptotic behavior of the modes, this expansion seems a suitable solution. The second term should be capable of modeling the non-Gaussian deviation for early times and it should vanish for later times when the solution has converged to a Gaussian process. Orszag solved the three mode problem using this approach and employing a Galerkin projection in random space. The results however, were quite disturbing. Although each mode $x_i(t,\boldsymbol{\xi})$ is a random process being close to Gaussian at all times, the expansion (36) fails to describe the solution properly, even for the converged Gaussian solution.
The problem with this Wiener-Hermite expansion (36) is that while it is perfectly capable of describing a nearly Gaussian process at a fixed time level t_p, it cannot describe a general time-dependent process that is nearly Gaussian at each instant. This can best be understood be considering two solutions of a specific mode at two different time levels t_p and t_q after the solution has converged to a Gaussian process. Those solutions at these fixed time-levels can perfectly be represented using expansion (36), respectively by:

$$x_i(t_p,\boldsymbol{\xi}) = x_1^i(t_\infty)\xi, \qquad x_i(t_q,\boldsymbol{\xi}) = x_1^i(t_\infty)\xi \tag{36}$$

with ξ a zero-mean Gaussian random variable. Although apparently, both expansions seem to be identical, one should bear in mind that, due to the dynamical nature of the solution, the different values of the random variable ξ do not correspond to each other in the expansions. This means that focusing on one sample, resulting from a specific initial condition, the values of ξ in the two expansions above will not correspond to each other. This is because although the statistics of the process do converge to some stationary values, the process itself remains dynamic. For almost every different sample, the solution keeps traveling its resulting limit-cycle for ever. Taking this into account, indeed, it can be seen that the expected converged solution due to the Wiener-Hermite expansion yields a stationary process, while in reality, it continues to be dynamic.

In order to overcome these issues, Imamura et al. [14, 15] presented a method that incorporates the dynamics of the process. They made the Gaussian zero-mean random variables ξ_i to be time-dependent $\xi_i(t)$, allowing to change value when progressing in time, resulting in the following expansion:

$$x_i(t, \boldsymbol{\xi}(t)) = x_1^i(t) H_i(\xi_1(t)) + \sum_{j=2}^{Q} x_j^i(t) H_i(\xi_1(t), \xi_2(t), \xi_3(t)) \tag{37}$$

Although this new expansion does not affect the ability to model the statistics of the process, it does, in addition, make the Wiener-Hermite expansion capable of capturing the dynamic properties of the process. Imamura implemented this approach in a proper way, imposing extra relations modeling the evolution of the random variables ξ_i, which lead to satisfactory results.

4.2 Time-dependent polynomial chaos

Based on Imamura's suggestion, we tried to incorporate the idea of time-dependency with respect to polynomial chaos in order to overcome the long-term integration issues. In order to do so, one should note that what actually happens in Imamura's approach, is that the random variables ξ_i evolve in such a way in time that their values adapt their self to the solution at each time-level. For a more general process than the Kraichnan-Orszag problem with a Gaussian asymptotic behavior, not only the values of random variable should vary in time, also the type of random variable should be able to evolve in time. This means that also the PDF of the random variable should be time-dependent. In the context of gPC, where there is a strict relation between the PDF of the random variable and the employed polynomials, this implies that also the polynomials in the gPC expansion should be time-dependent. In our approach that we will present here, we will implement this time-dependency in a discrete way. We explain this implementation by means of the stochastic ODE from the previous sections.

4.2.1 The procedure

The procedure of the time-dependent polynomial chaos approach works as follows. Consider the same ODE-problem as in section (3.1):

$$\frac{du(t, \xi)}{dt} + k(\xi) u(t, \xi) = 0 \tag{38}$$

Start with the gPC procedure using a Legendre chaos expansion as explained in section (3.2.1)

$$u(t,\xi) = \sum_{i=0}^{P} u_i(t) L_i(\xi) \tag{39}$$

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 important. 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

$$max\left(|u_2(t)|, ..., |u_P(t)|\right) \leq \frac{|u_1(t)|}{\theta} \tag{40}$$

can be used as a suitable stopping criterion. Increasing the threshold value θ does improve the accuracy.

Suppose we halt the gPC procedure at $t = t_1$. For previous mentioned reasons, advancing in time employing the same gPC expansion would be disadvantageous for the accuracy of the approximation. That is why it makes sense to change the expansion. And because for early times, the solution can be approximated well using a linear approximation, it is reasonable to create a new gPC expansion based on the solution at the new time-level t_1. In order to do so, first introduce a new random variable equal to the solution u at $t = t_1$, given by

$$\psi = u(t_1,\xi) = \sum_{i=0}^{P} u_i(t_1) L_i(\xi) = T(\xi) \tag{41}$$

If the PDF of ξ is given by $f_\xi(\xi)$, then the PDF of ψ is given by [16]:

$$f_\psi(\psi) = \sum_n \frac{f_\xi(\xi_n)}{\left|\frac{dT(\xi)}{d\xi}\big|_{\xi=\xi_n}\right|} \tag{42}$$

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

$$\psi = T(\xi) \tag{43}$$

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, on forehand unknown, solution and is in this sense arbitrary, 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

$$\begin{aligned} \phi_0(\psi) &= 1 \\ \int \phi_i(\psi)\phi_j(\psi)f_\psi(\psi)d\psi &= c_i\delta_{ij} \qquad i,j=1,\ldots,P \end{aligned} \tag{44}$$

As mentioned before, various alternatives have been presented by Wan [10] and Witteveen [11] in order to create this set of polynomials numerically. In this work, we choose to create the orthogonal polynomial basis using a Gram-Schmidt orthogonalization, as proposed by Witteveen. In this way, a new proper gPC expansion of the solution has been created. With respect to this new orthogonal system the solution u can be represented as:

$$u(t,\psi) = \sum_{i=0}^{P} u_i(t)\Phi_i(\psi) \tag{45}$$

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 following expansion

$$u(t_1,\psi) = u_0(t_1)\Phi_0(\psi) + \Phi_1(\psi) \tag{46}$$

in which $u_0(t_1)$ is equal to the value of $u_0(t_1)$ due to the old expansion. Note that this is a linear expansion.
Finally, also the stochastic input k, known in terms of the original random variable ξ, should be translated in of the new random variable ψ. Because both $k(\xi)$ and $\psi(\xi)$ are known in terms of the random variable ξ, it is possible, using numerical interpolation, to establish a relation $k(\psi)$ for specific values of ψ. In this work we used a piecewise cubic interpolation for this purpose.

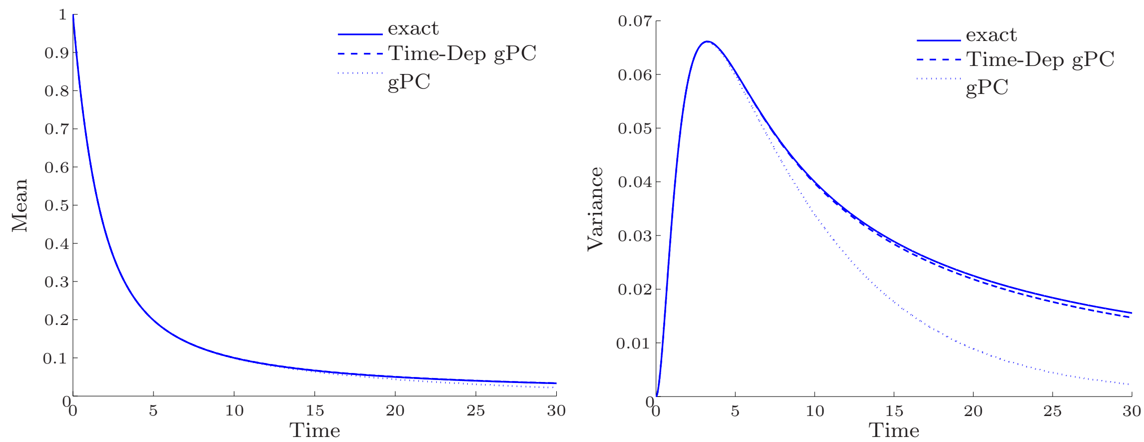
This new expansion should then be employed until a next time level t_2, at which criterion (40) is fulfilled again. Then, the algorithm should be repeated. In this way, one can march throughout the time domain, reinitializing the gPC expansion at certain discrete time-levels. The whole idea of transforming 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 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* $max\big(|u_2(t_i)|, ..., |u_P(t_i)|\big) \leq \frac{|u_1(t_i)|}{\theta}$
- *define a random variable* $\psi_{new} = u(t_i)$
- *calculate the PDF of* ψ_{new}
- *Gram-Schmidt orthogonalization: create a random trial basis* $\{\Phi_i(\psi_{new})\}$
- *generate new initial conditions:* $u(t_i, \psi_{prev}) \rightarrow u(t_i, \psi_{new})$
- *update k:* $k(\psi_{prev}) \rightarrow k(\psi_{new})$
- *construct a new ODE system employing gPC*
- *calculate mean and variance*
- *postprocessing*

4.2.2 Numerical results

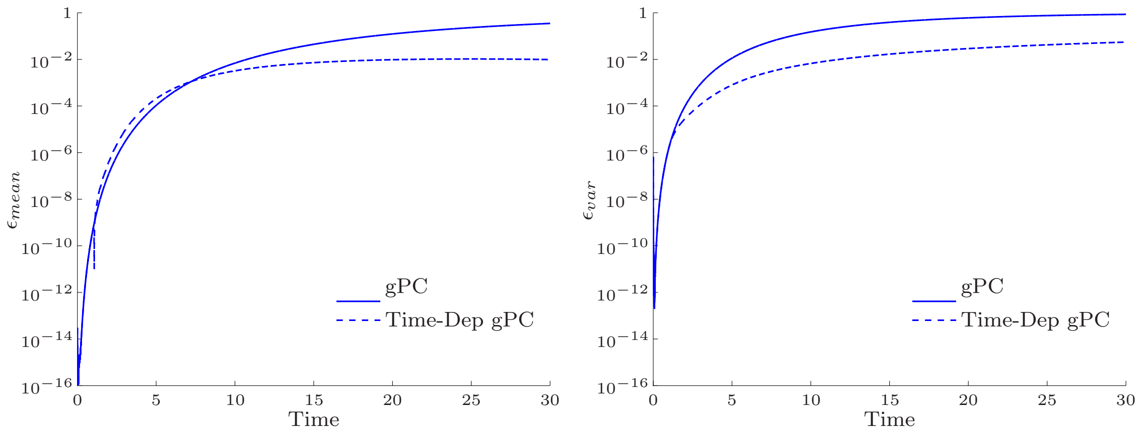
If we analyze the results of this discrete time-dependent approach applied on the ODE in question, it can be observed in figure (7), that for a polynomial order of $P = 3$, the results really outperform the standard gPC approach. In order to generate the results, the threshold parameter is set equal to $\theta = 6$ in the remainder of this work. Especially



(a) Evolution of the mean (b) Evolution of the variance

Figure 7: Evolution of the mean and variance for 3^{th} order time-dependent gPC

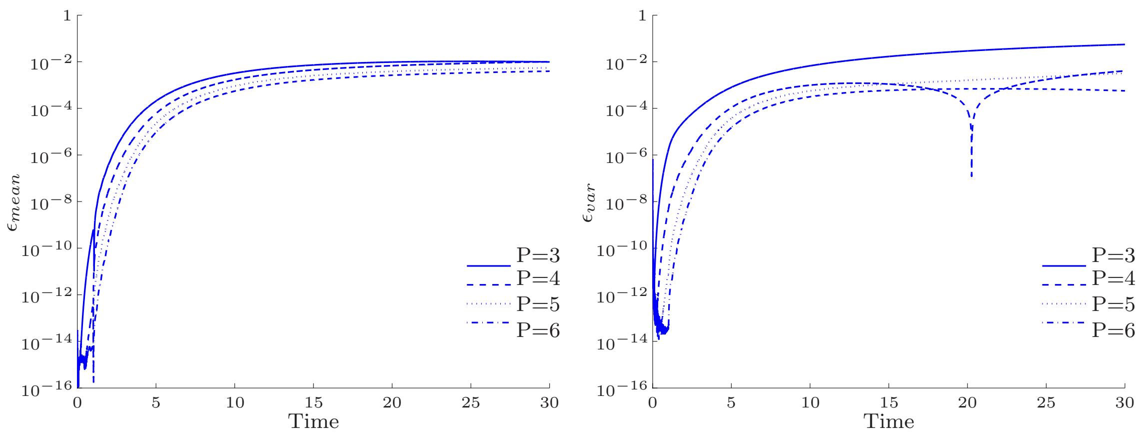
for the second order statistics, which in particular was a bottleneck for the standard gPC, the improvement is truly significant. It so happens that the time-dependent gPC approximation is now capable of following the evolution of the variance. The same behavior can be seen from figure (8), displaying 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



(a) Evolution of the mean-error (b) Evolution of the variance-error

Figure 8: Evolution of the error for 3^{th} order time-dependent gPC

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 order P. As from a polynomial order of $P = 4$, in a plot depicting the evolution the mean and variance analogue to figure (7), the time-dependent gPC approximation would be undistinguishable from the exact solution. In figure (9), the error-evolution of mean and variance are depicted for different expansion orders. It can be seen that mainly the accu-



(a) Evolution of the mean-error (b) Evolution of the variance-error

Figure 9: Evolution of the error for 3^{th} order time-dependent gPC

racy of the variance benefits from increasing the polynomial order. Taking a look at the error-convergence, depicted in figure (10) for $t = 30$, we see differences when compared with the standard gPC solution. First of all, although, for the considered values of P, the

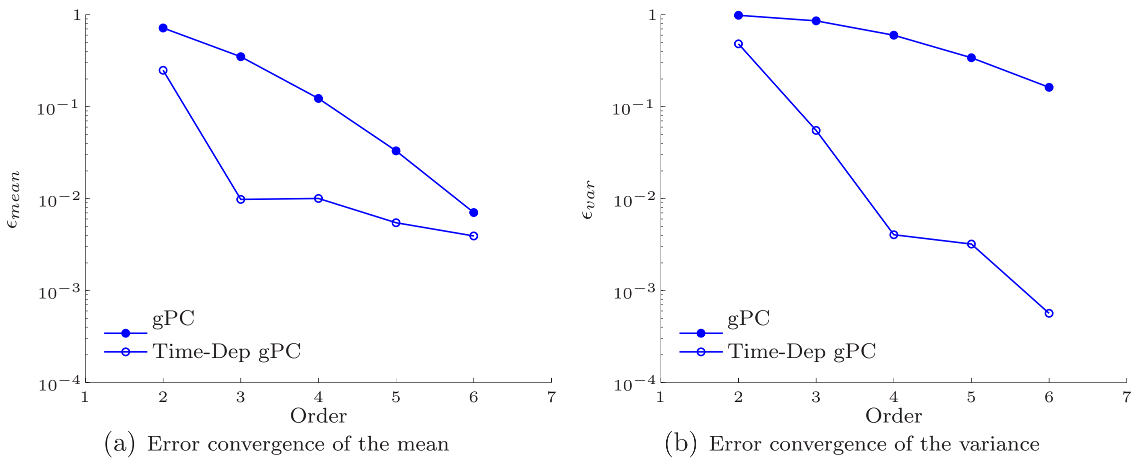


Figure 10: Error convergence of the mean and variance at $t = 30$

convergence of the mean-error for the time-dependent approach is not as steep as for the gPC approach, the level of the error itself is still lower. For the variance, the difference is more pronounced. Where in case of the gPC approximation, the accuracy was only of order $O(1)$ and showing not really significant convergence, for the time-dependent gPC solution, the error converges exponentially towards values of $O(10^{-3})$ for an order $P = 6$, which are acceptable and workable accuracies.

5 CONCLUSIONS AND RECOMMENDATIONS

After the conclusions, which will be presented first, we will discuss some considerations on which role the time-dependent gPC can play in the future.

5.1 Conclusions

Based on the observation that a standard gPC approach fails to describe the solution of a stochastic ODE for growing time due to the governing non-linearity in random space, we presented a time-dependent gPC alternative capable of dealing with the long term integration issues. We reinitialize the polynomial chaos expansion of the solution discretely in time based on the statistics of the evolved solution at this discrete time level. This allows a low order polynomial expansion at each instant in order to attain acceptable accuracies. This is possible because every newly created gPC expansion is only employed in the time-interval in which the linear development of the solution dominates. This time-dependent gPC approach mainly improves the ability of approximating the process's second order statistics for later time-levels, which was disastrous when employing the standard gPC approach. It has been shown that for the stochastic ODE in question, the accuracy levels of the approximated variance at a late time-level can be raised from the unacceptable order $O(1)$ to the order of magnitude $O(10^{-3})$ (for a polynomial order of $P = 6$) when using the time-dependent alternative. This means that the approximated variance evolves from a value which differs as much of the exact variance as this exact value, to a value which approximates the exact variance within 0.1%.

5.2 Recommendations

Although we showed that the time-dependent polynomial chaos is able to solve a one-dimensional stochastic ODE, it should be extended to cases involving a multi-dimensional random space. It is expected that in these cases, the calculation of the PDF of the solution will not be so straightforward. Also an extension to PDE's, involving random fields, can bring along some difficulties and needs further investigations.

A possible way of implementing this time-dependent approach, is in combination with Wan's [9] multi-element generalized polynomial chaos. In this approach, which has been shown to perform adequate in case of long-term integration and discontinuities, a new polynomial basis is created on-the-fly for each new element. However, this new chaos basis is still based on the initial random input. A creation of this basis based on the solution, as in the time-dependent approach, can maybe lead to better results.

And finally, in the ideal case, the time-dependency of the random variable should be continuous instead of discrete. A continuous formulation of time-dependent polynomial chaos can probably purify this approach, resulting in better approximations.

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