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TOWARDS A HYBRID NUMERICAL METHOD USING GENERALIZED POLYNOMIAL CHAOS FOR STOCHASTIC DIFFERENTIAL EQUATIONS

VINCENT HEUVELINE AND MICHAEL SCHICK

ABSTRACT. Generalized polynomial chaos (gPC) is known to fail for problems involving strong nonlinear dependencies on stochastic inputs, especially arising in the context of long term integration. The reason for this is that gPC is a time-independent projection method, not able to capture a dynamic behavior of probability distributions. Recent developments in addressing this problem are represented by decomposing the random space or employing discrete time-dependent basis functionals, both exhibiting promising results but also introducing increasing computational costs. This work focuses on a numerical analysis of these two approaches as well as their hybrid combination with regard to a simple ODE decay problem subject to a uniformly as well as a Gaussian distributed random input. It is observed that depending on the initial probability distribution strong differences occur with respect to the error developments, which efficiently can be reduced when employing local discrete time-dependent basis functionals.

1. INTRODUCTION

Many practical applications are modeled by differential equations involving parameters. The study of those problems often employs deterministic models, which in practice are not always available and therefore introducing uncertainty into the system. This has influence on the solution, as it can be viewed as a stochastic process, depending on some underlying probability space. Usually one is interested in the statistics (stochastic moments) of the solution to quantify its reaction to the uncertainty. A popular and simple strategy is known as the Monte-Carlo method. Here, a set of samples is generated using some random number generator and a deterministic simulation is performed corresponding to each realization. At a post-processing step, the collected information is evaluated and one obtains the desired statistics by taking weighted averages. The positive feature is that the sampling and determination of the corresponding deterministic solutions can be performed independently, leading to a trivial parallelization technique. A remedy comes along with the cost of Monte-Carlo, since it is usually not known a priori how many samples are required to reach a certain accuracy, since its convergence is based on the “law of large numbers” [2]. However, there exist modifications, such as variance reduction techniques and Quasi-Monte-Carlo techniques, which can reduce the number of samples to improve the convergence rate. A powerful alternative, which got increasing attention within the last two decades is given by the Polynomial Chaos method (PC), initially introduced by Wiener in 1938 [14]. It decomposes a stochastic process by a linear combination of chosen basic functionals in terms of random variables. In its original form, Wiener employed Hermite functionals in terms of Gaussian distributed random variables to represent square-integrable stochastic processes. In 1991, Ghanem and Spanos [5] pioneered the use of PC in combination with the Finite-Element-Method naming it the “Spectral-Stochastic-Finite-Element-Method”. It was successfully applied for problems arising from solid mechanics and turned out to be an

Key words and phrases. Polynomial Chaos, uncertainty quantification, stochastic differential equations, long term integration.

effective way of representing uncertainties. Later, the area of applications was successfully extended to fluid mechanics, e.g. [7, 9]. However, the convergence rate of PC was found out to be poor when trying to represent non-Gaussian processes. In an effort to overcome this restriction Xiu and Karniadakis [15], in 2003, established a correspondence between the chosen basic functionals and the probability distribution of the to be decomposed random variable naming the modification the "generalized Polynomial Chaos" method (gPC), which significantly improved the convergence rate for non-Gaussian stochastic processes.

Ongoing research is focusing on some drawbacks, which come along with gPC, represented mainly by the stationarity, i.e., time independency, of the approach [4, 11, 12, 6, 8]. This leads to difficulties arising when the solutions dependency on the stochastic parameters becomes increasingly nonlinear, which is often the case in highly dynamic systems. First analysis with respect to time-ideal random functions was carried out in 1969 and 1971 by Imamura et al. [3, 10]. Addressing this problem by a local approach, Wan and Karniadakis [11] proposed a variant of gPC, namely an "adaptive multi-element generalized polynomial chaos" method (ME-gPC) in 2005. Its basic idea is to decompose the probability space into a set of probability spaces, in which a gPC is employed subject to a conditional probability distribution function. ME-gPC turned out to be an efficient way of dealing with nonlinearities, yet leading to higher computational costs, since in every element a local problem of the size of the original global problem needs to be solved, assuming that the degree of the gPC expansion remains constant. An alternative was proposed by Gerritsma et al. [4] in 2010, addressing the nonlinearity problem on the global probability space, employing discrete time-dependent chaos polynomials (TD-gPC) based on the ideas of [3, 10]. The basic principle is to transform the system to an optimal basis in terms of new random variables, subject to the same probability distribution as the solution itself at some certain discrete time steps. However, a broad analysis and numerical evaluation is still part of ongoing research. Especially the combination of both ME-gPC and TD-gPC can lead to a powerful method, combining the features of both worlds.

This work is aiming at addressing some modifications to a basic TD-gPC to reduce its complexity and a numerical evaluation of a hybrid approach consisting of TD-gPC and ME-gPC. The numerical analysis is performed on some simple decay model problem. Here, a uniformly and a Gaussian distributed input parameter will be considered. The outline of this paper is as follows: In Section 2 a mathematical background reviewing gPC is given following in Section 3 with the introduction of the model problem. Section 4 briefly reflects the main ideas behind ME-gPC and TD-gPC. In Section 5 both methods as well as their combination are applied to the model problem and are being evaluated. Section 6 closes with drawing conclusions from this work.

2. GENERALIZED POLYNOMIAL CHAOS

2.1. Discrete expansion of a second order random variable. Consider, without loss of generality, a real-valued random variable X defined on some probability space $(\Omega, \mathcal{F}, \mathbb{P})$, whereas Ω denotes the sample space, $\mathcal{F} \subset 2^\Omega$ the filtration, and \mathbb{P} a probability measure. Further, let us assume that X is square-integrable, i.e., $X \in L^2(\Omega) = \{X : \mathbb{E}(X^2) < \infty\}$, whereas

$$(2.1) \quad \mathbb{E}(X) := \int_{\Omega} X \, d\mathbb{P}$$

Case	Probability distribution	Askey–chaos	Support
Continuous	Gaussian	Hermite–chaos	$(-\infty, \infty)$
	Gamma	Laguerre–chaos	$[0, \infty)$
	Beta	Jacobi–chaos	$[a, b]$
	Uniform	Legendre–chaos	$[a, b]$
Discrete	Poisson	Charlier–chaos	$\{0, 1, 2, \dots\}$
	Binomial	Krawtchouk–chaos	$\{0, 1, 2, \dots, N\}$
	Negative binomial	Meixner–chaos	$\{0, 1, 2, \dots\}$
	Hypergeometric	Hahn–chaos	$\{0, 1, 2, \dots, N\}$

TABLE 1. Askey–chaos for selecting polynomials corresponding to certain types of distributions.

denotes the expectation of X . The original polynomial chaos expansion of X can be represented in the form

$$(2.2) \quad X(\omega) = a_0 H_0 + \sum_{i_1=1}^{\infty} a_{i_1} H_1(\xi_{i_1}(\omega)) + \sum_{i_1=1}^{\infty} \sum_{i_2=1}^{i_1} a_{i_1 i_2} H_2(\xi_{i_1}(\omega), \xi_{i_2}(\omega)) \\ + \sum_{i_1=1}^{\infty} \sum_{i_2=1}^{i_1} \sum_{i_3=1}^{i_2} a_{i_1 i_2 i_3} H_3(\xi_{i_1}(\omega), \xi_{i_2}(\omega), \xi_{i_3}(\omega)) + \dots,$$

whereas $H_n(\xi_{i_1}, \dots, \xi_{i_n})$ denote the Hermite polynomials of order n in terms of the multi-dimensional independent standard Gaussian random variables $\boldsymbol{\xi} = (\xi_{i_1}, \dots, \xi_{i_n})$. Note that this expansion is the discrete version of the original decomposition introduced by Wiener [14]. The multi-dimensional Hermite polynomials are constructed by a tensor product of the corresponding one-dimensional Hermite polynomials, resulting in

$$(2.3) \quad H_n(\xi_{i_1}, \dots, \xi_{i_n}) = (-1)^n \exp\left(\frac{1}{2} \boldsymbol{\xi}^T \boldsymbol{\xi}\right) \frac{\partial^n}{\partial \xi_{i_1} \dots \partial \xi_{i_n}} \exp\left(-\frac{1}{2} \boldsymbol{\xi}^T \boldsymbol{\xi}\right).$$

To simplify the notation, equation (2.2) can be rewritten to obtain the form

$$(2.4) \quad X(\omega) = \sum_{i=0}^{\infty} x_i \psi_i(\boldsymbol{\xi}(\omega)),$$

since there exists a one-to-one correspondence between the polynomials $\{\psi_i\}$ and $\{H_n\}$, and between the coefficients $\{a_{i_1}, \dots, a_{i_k}\}$ and $\{x_i\}$. The decomposition is indeed an orthogonal and complete basis in the L^2 -space of Gaussian random variables in terms of

$$(2.5) \quad \langle \psi_i \psi_j \rangle = \langle \psi_i^2 \rangle \delta_{ij},$$

where δ_{ij} denotes the Kronecker–delta and $\langle \cdot \rangle$ denotes the inner product, defined by

$$(2.6) \quad \langle f(\boldsymbol{\xi}) g(\boldsymbol{\xi}) \rangle := \int f(\boldsymbol{\xi}) g(\boldsymbol{\xi}) w(\boldsymbol{\xi}) d\boldsymbol{\xi}$$

with the weight function w given by

$$(2.7) \quad w(\boldsymbol{\xi}) := \frac{1}{\sqrt{(2\pi)^n}} \exp\left(-\frac{1}{2} \boldsymbol{\xi}^T \boldsymbol{\xi}\right)$$

as the joint probability density function of the multi-dimensional independent standard Gaussian random variable $\boldsymbol{\xi}$. Cameron and Martin [1] proved that this expansion converges in mean-square to any second order random variable.

In practical applications, it is desirable that the series in (2.4) converges fast, since for feasible numerical implementations the series needs to be truncated at some finite integer, which should be of small value. Although for the decomposition of Gaussian random variables this is usually the case (exponential convergence is expected, because of the spectral projection nature), other types of non-Gaussian random variable expansions may exhibit poor convergence rates. Therefore, Xiu and Karniadakis [15] introduced the so-called ‘‘Askey-chaos’’ and with it the ‘‘generalized polynomial chaos’’, which essentially replaces the Hermite polynomials $\{\psi_i\}$ by other polynomials, which are orthogonal with respect to the underlying probability density function of the random input. For example, if X is chosen to be represented in terms of uniformly distributed random variables, then $\{\psi_i\}$ are chosen to be Legendre polynomials. It is expected by a generalization of the Cameron and Martin theorem [1], that this kind of expansion will also converge to any second order random variable. The ‘‘Askey-chaos’’ is listed in Table 1 and gives an overview which polynomials correspond to certain types of distributions (continuous and discrete ones). To distinguish between the classical Hermite-chaos in terms of Gaussian random variables ξ and other types of chaos, the notation for the random vector is changed to ζ throughout the rest of this work.

2.2. Application of gPC to stochastic processes and differential equations. Let us consider, without loss of generality, the following scalar problem:

Seek $u = u(\mathbf{x}, t; \omega)$ such that

$$(2.8) \quad \mathcal{L}(u, \mathbf{x}, t; \omega) = f(\mathbf{x}, t; \omega),$$

where \mathcal{L} denotes some differential operator in the space variable $\mathbf{x} \in \mathcal{D} \subset \mathbb{R}^d$, $d \in \mathbb{N}$, and the time variable $t \in [0, T] \subset \mathbb{R}$. Further, $\omega \in \Omega$ denotes a sample from the sample space Ω , representing the stochastic influence within the differential equation. Here, Ω belongs to some underlying probability space $(\Omega, \mathcal{F}, \mathbb{P})$. The stochastic influence is assumed to be parameterized by some vector of independent random variables $\zeta = (\zeta_1, \zeta_2, \dots)$. Hence, problem (2.8) can be reformulated in the way:

Seek $u = u(\mathbf{x}, t; \zeta)$ such that

$$(2.9) \quad \mathcal{L}(u, \mathbf{x}, t; \zeta) = f(\mathbf{x}, t; \zeta).$$

This is the starting point for the discretization technique employing chaos polynomials. Since ζ represents the stochastic input, its probability distribution is known a priori. However, no information about the stochastic distribution of u is available, therefore, gPC constitutes an efficient way of representing u in terms of ζ , leading to

$$(2.10) \quad u(\mathbf{x}, t; \zeta) = \sum_{i=0}^{\infty} u_i(\mathbf{x}, t) \psi_i(\zeta),$$

whereas the notation of ω is dropped for notational convenience. For computational purposes, equation (2.10) is not adequate, since it involves an infinite summation and therefore needs to be discretized by truncation at some finite level N . This is achieved by restricting the size of ζ at some finite level M , resulting in $\zeta \approx \zeta^M = (\zeta_1, \dots, \zeta_M)$ and fixing the maximal polynomial order of the chaos polynomials ψ_i to a finite level P . The expansion now reads

$$(2.11) \quad u(\mathbf{x}, t; \zeta) \approx u^N(\mathbf{x}, t; \zeta^M) = \sum_{i=0}^N u_i(\mathbf{x}, t) \psi_i(\zeta^M),$$

with

$$(2.12) \quad N + 1 = \frac{(M + P)!}{M!P!},$$

$P \setminus M$	1	2	3	4	5	6
1	2	3	4	5	6	7
2	3	6	10	15	21	28
3	4	10	20	35	56	84
4	5	15	35	70	126	210
5	6	21	56	126	252	462
6	7	28	84	210	462	924

TABLE 2. Number of unknowns $N + 1$ in gPC.

which is equal to the number of unknowns u_i within the expansion. Table 2 states some values for $N + 1$ to illustrate the high number of unknowns even for small truncations at low polynomial degrees and low stochastic input sizes. This creates a great numerical task, since each of the unknowns $u_i = u_i(\mathbf{x}, t)$ needs to be discretized further by some deterministic numerical procedure, e.g., the Finite-Element-Method, resulting in a blown up system size in comparison to a single deterministic problem. In literature, this phenomena is often referred to as ‘‘curse of dimensionality’’.

Galerkin Projection. The Galerkin method is one representative of the class of so-called ‘‘weighted residual methods’’. The basic principle lies in formulating a weak equation for the solution u , such that the residual is orthogonal to the space of test respectively ansatz functions. For illustration, consider problem (2.9) and approximate u by u^N , such that

$$(2.13) \quad \mathcal{L}\left(\sum_{i=0}^N u_i \psi_i, \mathbf{x}, t; \zeta^M\right) = f(\mathbf{x}, t; \zeta^M).$$

Here, the space of test and ansatz functions is the same and is equal to $\mathcal{V}_N = \text{span}\{\psi_0, \psi_1, \dots, \psi_N\}$. The next step is to multiply (2.13) by all ψ_j and taking the expectation $\langle \cdot \rangle$ to obtain

$$(2.14) \quad \left\langle \mathcal{L}\left(\sum_{i=0}^N u_i \psi_i, \mathbf{x}, t; \zeta^M\right), \psi_j \right\rangle = \langle f(\mathbf{x}, t; \zeta^M), \psi_j \rangle, \quad \text{for } j = 0, \dots, N.$$

The resulting equation (2.14) is a coupled system of deterministic differential equations, which is larger than one single deterministic problem by a factor of $N + 1$. This can be solved by employing any appropriate deterministic solver, which needs to be modified to take account of the couplings within the system resulting from the stochastic discretization using gPC. Note that the couplings only occur within the left hand side of equation (2.14) and therefore, for linear problems involving only uncertainty in boundary or initial conditions, the system deteriorates to a fully decoupled structure, which is attributed to the orthogonality property of the chaos polynomials $\{\psi_i\}$.

3. A SIMPLE DECAY PROBLEM

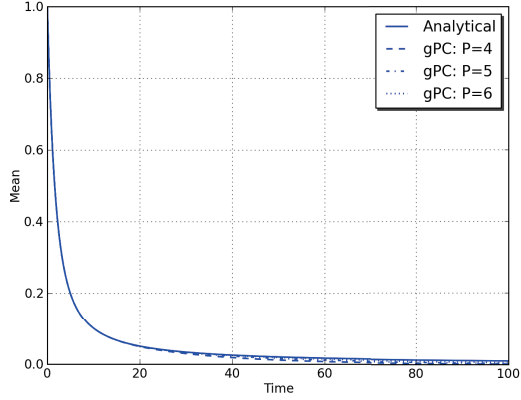
For illustrating the efficiency of gPC for short time simulations and the lack of convergence as time progresses, a simple ODE model problem is studied:

$$(3.1) \quad \frac{\partial}{\partial t} u(t; \zeta) = -k(\zeta)u(t; \zeta),$$

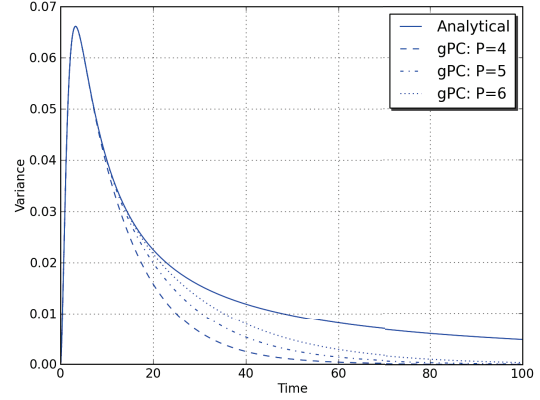
$$(3.2) \quad u(0; \zeta) = 1,$$

whereas $k(\zeta) = \frac{1}{2} + \frac{1}{2}\zeta$. The analytical solution to this ODE is given by

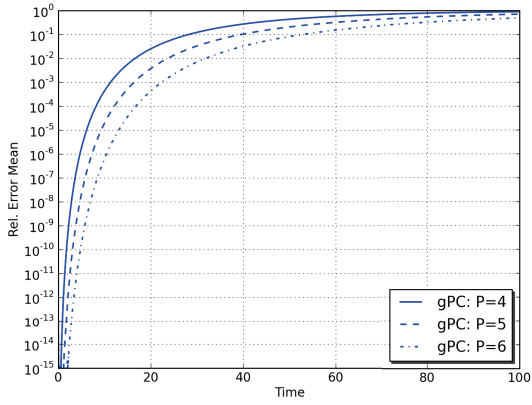
$$(3.3) \quad u(t; \zeta) = \exp(-k(\zeta)t).$$



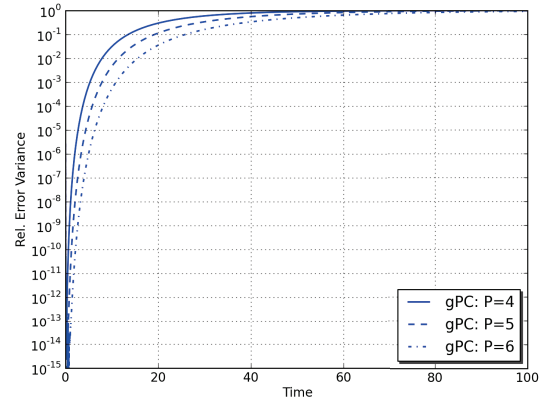
(A) Analytical and computed mean.



(B) Analytical and computed variance.



(C) Relative error mean.



(D) Relative error variance.

FIGURE 3.1. Solutions employing gPC for $P = 4, 5, 6$ and their corresponding relative errors of mean and variance for a uniformly distributed input. An explicit Runge–Kutta Scheme of 4^{th} order with $\Delta t = 0.001$ was used for time discretization.

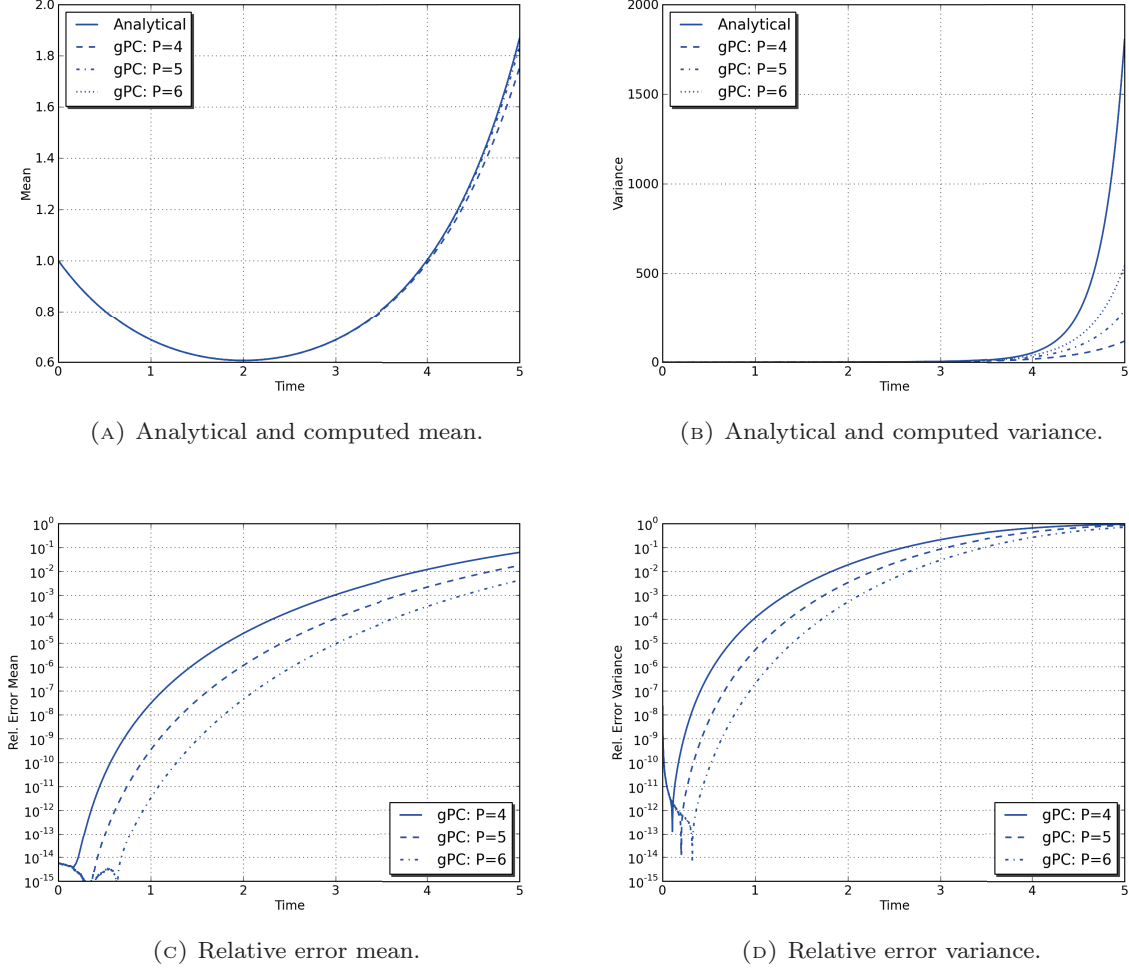
Employing gPC yields the following coupled system of deterministic ODEs:

$$(3.4) \quad \frac{\partial}{\partial t} u_j(t) = - \sum_{i=0}^P u_i(t) \frac{\langle k \psi_i \psi_j \rangle}{\langle \psi_j \psi_j \rangle}, \quad \text{for } j = 0, \dots, P,$$

$$(3.5) \quad u_0(0) = 1,$$

$$(3.6) \quad u_j(0) = 0, \quad \text{for } j = 1, \dots, P.$$

Since we consider a one–dimensional stochastic random variable ζ , the index j of ψ_j denotes its degree and $P = N$.



(A) Analytical and computed mean.

(B) Analytical and computed variance.

(C) Relative error mean.

(D) Relative error variance.

FIGURE 3.2. Solutions employing gPC for $P = 4, 5, 6$ and their corresponding relative errors of mean and variance for a standard Normal distributed input. An explicit Runge–Kutta Scheme of 4th order with $\Delta t = 0.001$ was used for time discretization.

Suppose $\zeta \sim U(-1, 1)$, i.e., ζ is uniformly distributed within $(-1, 1)$. Hence, the analytical solutions for the mean and the variance are given respectively by:

$$(3.7) \quad \mathbb{E}(u)(t) = \frac{1 - \exp(-t)}{t},$$

$$(3.8) \quad \sigma^2(u)(t) = \frac{1}{2t}(1 - \exp(-2t)) - \left(\frac{1 - \exp(-t)}{t}\right)^2.$$

If $\zeta = \mathcal{N}(0, 1)$, i.e., ζ is a standard Normal distributed random variable, then the analytical solutions for the mean and the variance are respectively given by:

$$(3.9) \quad \mathbb{E}(u)(t) = \exp\left(-\frac{1}{2}t + \frac{1}{8}t^2\right),$$

$$(3.10) \quad \sigma^2(u)(t) = \exp\left(-t + \frac{1}{2}t^2\right) - \exp\left(-t + \frac{1}{4}t^2\right).$$

For a uniformly distributed ζ the chaos polynomials ψ_j are selected to be Legendre polynomials L_j , for a standard Normal distributed ζ Hermite polynomials are chosen - both according to the Askey–chaos (see Table 1). The chaos polynomials are orthogonal w.r.t. the probability distribution function of ζ , which is given by

$$(3.11) \quad f(z) = \frac{1}{2}, \quad z \in (-1, 1), \quad \text{for a Uniform distribution,}$$

$$(3.12) \quad f(z) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{z^2}{2}\right), \quad z \in \mathbb{R}, \quad \text{for a standard Normal distribution.}$$

As one can see in Fig. 3.1 and Fig. 3.2, gPC is able to approximate the mean and the variance of the solution for short physical time only. As time progresses gPC is not capable of representing the stochastic moments accurately, leading to relative errors of order $O(1)$ for both mean and variance at later times. This can be explained by taking a closer look on the series representation of the analytical solution itself:

$$(3.13) \quad u(t; \zeta) = \exp(-k(\zeta)t) = \sum_{n=0}^{\infty} (-1)^n \frac{(1 + \zeta)^n t^n}{2^n n!}.$$

It is clear that when t gets large the nonlinear dependency on ζ becomes more dominant. However, only polynomials up to the degree P are used throughout the whole simulation time, therefore restricting the representable nonlinearities in ζ to the order of P , which is only sufficient for early times.

4. MULTI-ELEMENT AND TIME-DEPENDENT APPROACH

4.1. Multi-element generalized Polynomial Chaos (ME-gPC). In their work, Wan and Karniadakis [11, 13] developed an adaptive domain decomposition method of the probability space to split the global problem into independent local ones. The basic principle lies in decomposing the range of ζ into a finite set of intervals of finite or infinite boundaries, i.e., if $\zeta \in (a, b) \subset \mathbb{R}^* = \mathbb{R} \cup \{-\infty, \infty\}$ with $a, b \in \mathbb{R}^*$ then

$$(4.1) \quad (a, b) = \bigcup_{k=1}^N B_k, \quad B_k = (a_k, b_k) \subset \mathbb{R}^*, \quad B_k \cap B_l = \emptyset \text{ if } k \neq l.$$

By defining the indicator function

$$(4.2) \quad I_k = \begin{cases} 1 & \text{if } \zeta \in B_k \\ 0 & \text{otherwise} \end{cases},$$

one obtains a decomposition of the sample space Ω via

$$(4.3) \quad \Omega = \bigcup_{k=1}^N I_k^{-1}(1).$$

In each element B_k a new random variable $\zeta_k : I_k^{-1}(1) \mapsto B_k$ is defined subject to a conditional probability distribution function

$$(4.4) \quad f_{\zeta_k}(z_k | I_k = 1) = \frac{f_{\zeta}(z_k)}{\mathbb{P}(I_k = 1)}.$$

The next step is to employ gPC locally in each element B_k leading to N problems, which can be solved independently from each other. For simplification the focus will lie only on a uniformly

refined probability space, not on an adaptive procedure. Any statistics of the solution u can be obtained by Bayes's rule and the law of total probability by

$$(4.5) \quad \int_B g(u(z))f_\zeta(z) dz \approx \sum_{k=1}^N \mathbb{P}(I_k = 1) \int_{B_k} g(u^{(k)}(z_k))f_{\zeta_k}(z_k|I_k = 1) dz_k,$$

whereas $u^{(k)}$ denotes the solution in element B_k .

Remark 1. Note that since on each element gPC is employed, a set of orthogonal polynomials has to be computed w.r.t. the conditional probability distribution for each element. Also, solving N independent problems leads to higher costs, which increase linearly in N if P is fixed over all elements. Another view on ME-gPC is that the chaos polynomials are replaced by piecewise chaos polynomials, hence allowing for improved accuracy.

4.2. Time-dependent generalized Polynomial Chaos (TD-gPC). Gerritsma et al. [4] introduced a time-dependent approach evaluated for uniformly distributed random variables, which aims at reducing the nonlinear dependency of the solution u on the stochastic input. In contrast to ME-gPC, TD-gPC constitutes a global polynomial chaos discretization of the probability space. Its basic principle lies in the idea of representing the solution u in terms of a new random variable, which is defined as the solution u itself at certain time steps. The procedure can be summarized by the following:

First employ gPC in a standard way. Define a reset criteria for some parameter θ

$$(4.6) \quad \max\{|u_2(t)|, \dots, |u_P(t)|\} \geq \frac{|u_1(t)|}{\theta},$$

which measures the nonlinear dependency, represented by the higher modes, on the random variable ζ . If this criteria is fulfilled, say at time step $t = t_r$, halt the simulation and perform a reset step. First define a new random variable η by

$$(4.7) \quad \eta := u(t_r; \zeta) = \sum_{i=0}^P u_i(t_r)\psi_i(\zeta).$$

Next, employ a gPC representation of u in terms of η , i.e.,

$$(4.8) \quad u(t; \eta) = \sum_{i=0}^P u_i(t)\phi_i(\eta), \quad t \geq t_r,$$

whereas $\{\phi_i\}$ is a set of new chaos polynomials, which are orthogonal to the probability distribution function f_η of η . Computing this polynomials can be done by a Gram-Schmidt orthogonalization procedure starting with $\phi_0 \equiv 1$, using the well known fact that

$$(4.9) \quad \int \phi_i(y)\phi_j(y)f_\eta(y) dy = \int \phi_i(u(t_r; z))\phi_j(u(t_r; z))f_\zeta(z) dz$$

allowing for evaluating all inner products without explicitly computing f_η . The last step is to reformulate the model problem. For (3.1), (3.2) this results in

$$(4.10) \quad \frac{\partial}{\partial t} u(t; \eta) = -k(\eta)u(t; \eta), \quad \text{for } t \geq t_r,$$

$$(4.11) \quad u(t_r; \eta) = u_0(t_r)\phi_0(\eta) + \phi_1(\eta).$$

Since this is a linear expansion in η at $t = t_r$, it is an optimal representation of u in terms of η .

Remark 2. The criteria in (4.6) can be replaced by any other suitable stopping criteria. In the following a decay rate of the variance will be used throughout the numerical simulations, defined by

$$(4.12) \quad \frac{u_P^2(t) \langle \psi_P \psi_P \rangle}{\sum_{i=0}^P u_i^2(t) \langle \psi_i \psi_i \rangle} \geq \theta,$$

since the higher order moments represent the critical quantities.

5. NUMERICAL RESULTS

Throughout this section the model problem (3.1), (3.2) will be analyzed for a uniformly and a standard Normal distributed ζ . Recapitulate that the corresponding analytical solutions for the mean and the variance are given respectively by

$$(5.1) \quad \mathbb{E}(u)(t) = \frac{1 - \exp(-t)}{t},$$

$$(5.2) \quad \sigma^2(u)(t) = \frac{1}{2t}(1 - \exp(-2t)) - \left(\frac{1 - \exp(-t)}{t} \right)^2,$$

for $\zeta \sim U(-1, 1)$ and

$$(5.3) \quad \mathbb{E}(u)(t) = \exp\left(-\frac{1}{2}t + \frac{1}{8}t^2\right),$$

$$(5.4) \quad \sigma^2(u)(t) = \exp\left(-t + \frac{1}{2}t^2\right) - \exp\left(-t + \frac{1}{4}t^2\right),$$

for $\zeta \sim \mathcal{N}(0, 1)$. All calculations were performed using a 4th order explicit Runge–Kutta method with a time step of $\Delta t = 0.001$. Errors are measured in a relative norm, i.e.,

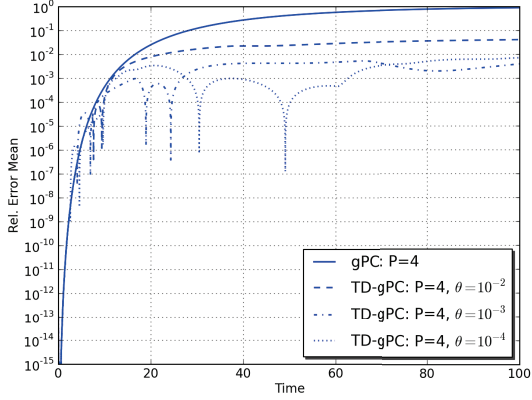
$$(5.5) \quad \epsilon_{mean}(t) := \frac{|\mathbb{E}(u_{analytical})(t) - \mathbb{E}(u_{computed})(t)|}{|\mathbb{E}(u_{analytical})(t)|}$$

$$(5.6) \quad \epsilon_{variance}(t) := \frac{|\sigma^2(u_{analytical})(t) - \sigma^2(u_{computed})(t)|}{\sigma^2(u_{analytical})(t)}.$$

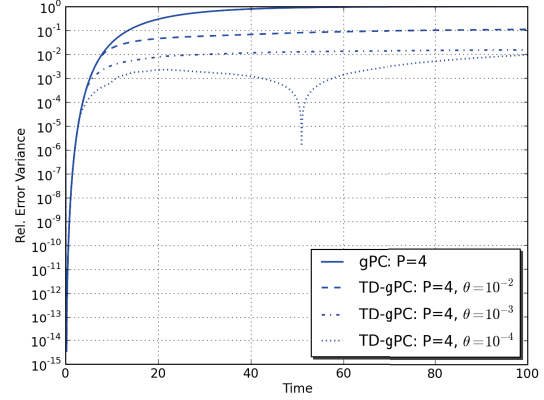
5.1. Numerical results for TD-gPC. First, the time-dependent approach (TD-gPC) for a uniformly distributed ζ is being analyzed. As can be seen in Fig. 5.1 the relative errors both for the mean and the variance are significantly improved in comparison to gPC leading to an error reduction of approximately 3 to 4 orders in the best case. Note that decreasing θ results in a higher number of reset steps throughout the simulation (see Table 3). The optimal θ , however, for which the smallest possible error is obtained, is not necessarily of smallest magnitude. For

θ	$No, P = 4$	$No, P = 6$
10^{-2}	2	1
10^{-3}	3	2
10^{-4}	7	2
10^{-5}	50	2
10^{-6}	184	30
10^{-7}	614	196
10^{-8}	1962	642

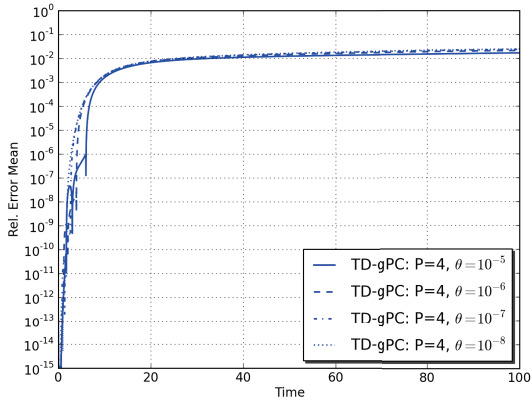
TABLE 3. Number of resets steps No for $P = 4$ and $P = 6$ corresponding to various values of the stopping parameter θ for Uniform distribution.



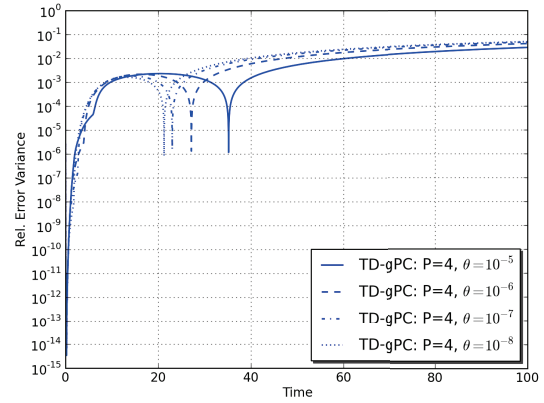
(A) Relative error mean.



(B) Relative error variance.



(C) Relative error mean.

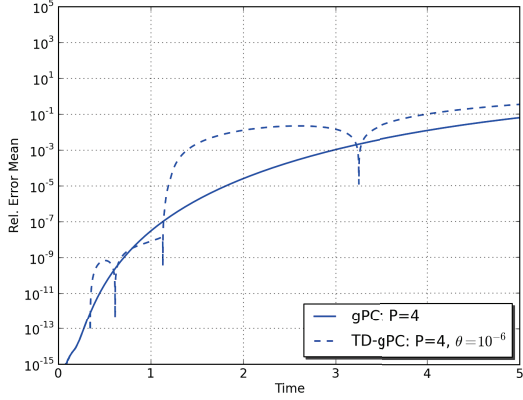


(D) Relative error variance.

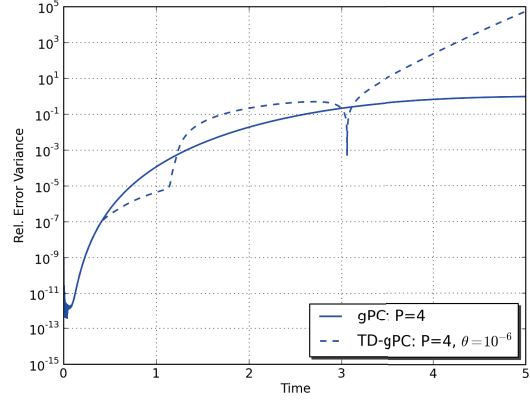
FIGURE 5.1. Relative errors of mean and variance for TD-gPC with $P = 4$ and varying stopping parameter $\theta = 10^{-2}, \dots, 10^{-8}$ for a Uniform distribution.

$P = 6$ optimal results are achieved employing $\theta = 10^{-6}$ leading to an error reduction of 4 orders compared to gPC, whereas only 30 reset steps are sufficient, which makes up for just 0.03% of all time steps (the case $P = 6$ is not shown). Decreasing θ even further, will not improve the relative errors anymore, even making them slightly worse. The case $P = 4$ exhibits a similar behavior, achieving optimal results for $\theta = 10^{-4}$ with an error reduction of 2 to 3 orders requiring only 7 reset steps.

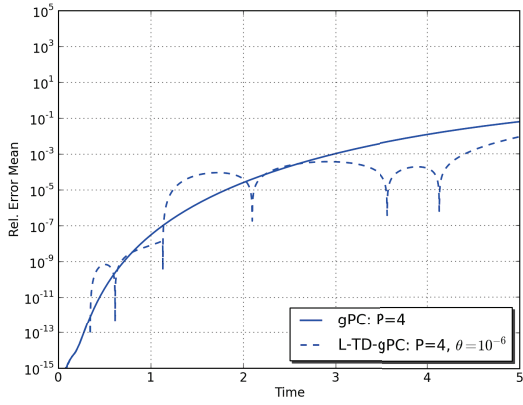
For a standard normal distributed ζ , however, the results exhibit some completely different behaviors (see Fig. 5.2). The plots show a discretization carried out with $P = 4$ and a stopping parameter $\theta = 10^{-6}$ to illustrate the problem. The classical gPC approach is demonstrating an expected development, i.e., error growth in time to the order $O(1)$, in contrast to TD-gPC, which drastically diverges from the exact solution and leads to considerably worse results in comparison to gPC measured in the relative errors. This phenomena can be explained by a numerical loss of orthogonality, i.e., the orthogonality of the time-dependent polynomials cannot be maintained throughout the simulation time. This is due to the solution itself, which at every reset steps defines a new inner product, which evaluation is numerically unstable, if the polynomials differ



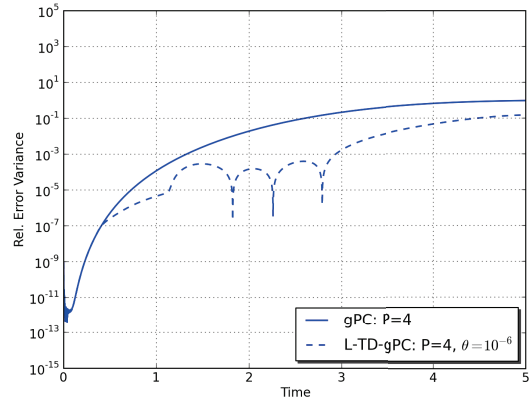
(A) Relative error mean.



(B) Relative error variance.



(C) Relative error mean.



(D) Relative error variance.

FIGURE 5.2. Relative errors of mean and variance for TD-gPC with $P = 4$ and stopping parameter $\theta = 10^{-6}$ for standard Normal distribution. Top TD-gPC, bottom limited TD-gPC.

to much in the magnitudes of their coefficients. Note, that the inner product is approximated by some quadrature rule, in this case a Gauss–Hermite quadrature, which will involve round off errors if terms with highly different magnitudes are summed. To be able to use TD-gPC, one therefore has to restrict the maximum number of reset steps allowed, resulting in an limited time–dependent approach (L-TD-gPC). However, it is not feasible to define a limit a priori, we therefore use the following application dependent criteria to analyze, if the orthogonality is still satisfied:

$$(5.7) \quad \mathbf{if} \max_{i,j,i \neq j} |\langle \psi_i, \psi_j \rangle| > \delta \mathbf{then} \text{ do not reset anymore,}$$

whereas $\delta = 10^{-15}$, which is a quite strong criteria. Fig. 5.2 shows that using this limitation leads to significantly improved results and that L-TD-gPC is also able to reduce the errors compared to gPC even further. Note that for this case, TD-gPC results in 869 steps, whereas L-TD-gPC only allows for 2 reset steps, which are sufficient to decrease the relative errors up to

one order in comparison with gPC. Especially, considering TD-gPC, for the variance a reduction of up to 6 orders is achieved by L-TD-gPC.

A remedy of TD-gPC and L-TD-gPC is that the errors still continue to grow as time progresses, although the growth rate seems to become relatively small for later simulation time. Gerritsma et al. [4] introduced a revised TD-gPC approach, which does consider both the probability distribution of the solution as well as the probability distribution of the initial parameter. Therefore, the modes of the solution are expressed in a gPC in terms of the initial input distribution, i.e.,

$$(5.8) \quad u = u(t; \zeta; \eta) = \sum_{i=0}^{P_1} \sum_{j=0}^{P_2} u_{ij}(t) \phi_i(\zeta) \psi_j(\eta),$$

whereas ζ denotes the random variable of the initial parameter and η the random variable coming from the time-dependent approach as explained previously. Note that $\eta = \eta(\zeta)$, i.e., the expansion now employs two dependent random variables. This modification allows for a better representation of the time derivative of the solution leading to strongly improved results in the reduction of the relative errors throughout the whole time simulation interval for this model ODE problem subject to a uniformly distributed input. However, a drawback of the revised approach is the increasing cost which comes along with introducing two dependent random variables instead of a single one. Especially, the number of unknowns is increased by a factor of $P_1 + 1$ instead of just using $P_2 + 1$ unknowns. This can lead to computational difficulties when considering more complex problems like partial differential equations. Future work will elaborate in detail on this modification.

Remark 3. The observable peaks in the error throughout the simulation time are due to the change of sign in the corresponding absolute error, resulting in jumps of the relative errors at exact these time steps.

5.2. Numerical results for ME-gPC. Next the numerical results concerning the multi-element approach (ME-gPC) as introduced in [11, 13] are being evaluated. For simplicity a global refined probability space is assumed, i.e., no adaptive refinement strategies will be considered. The partitioning in case of a standard Normal distributed input is carried out employing initially three elements $(-\infty, -a)$, $(-a, a)$, (a, ∞) , whereas $a = 9$ such that $\mathbb{P}(\zeta \notin (-a, a)) = 2.25718 \cdot 10^{-19}$, resulting in a small contribution of the tail elements to the global problem. Therefore, it is sufficient to only refine the middle element $(-a, a)$. For a uniformly distributed input, the interval $(-1, 1)$ is being refined.

The results as seen in Fig. 5.3 and Fig. 5.4 display exponential convergence for a 4th order chaos expansion both for a uniformly and a standard Normal distributed ζ similar to an *h-refinement* in the context of a Finite-Element-Method. This is in good agreement with the results shown in [13]. However, ME-gPC also exhibits an error growth over time which can be decreased if more elements are used at later times, yet leading to higher costs since in every element a gPC problem needs to be solved. Further, comparing the local approach of ME-gPC with the global one of TD-gPC shows, that for a Uniform distribution TD-gPC is capable of achieving the same low relative errors as ME-gPC employing a small number of elements, yet with less costs, since the computation of orthogonal polynomials at every reset step is negligible in comparison to solving the ODE. Even for the case subject to a standard Normal distribution, at least the limited TD-gPC can achieve the same error bounds as ME-gPC for $N = 6$ both for the mean and the variance. Since ME-gPC as well as (L-)TD-gPC provide efficient means of reducing the relative errors, a combination of both of these approaches is expected to lead to even better results concerning the accuracy, yet at less cost than using ME-gPC only, which will be evaluated in the following.

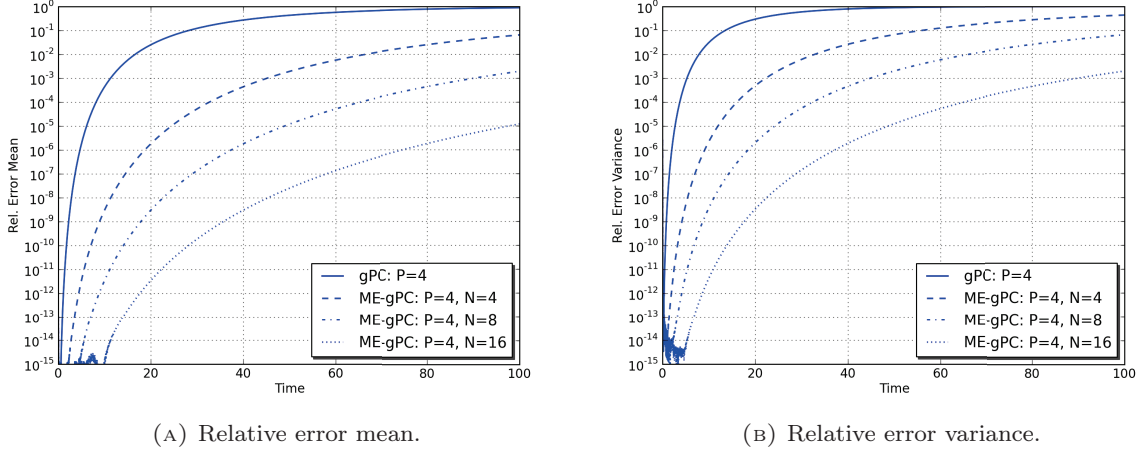


FIGURE 5.3. Relative errors of mean and variance for ME-gPC with $P = 4$ and varying number of elements $N = 1, 4, 8, 16$ for a Uniform distribution.

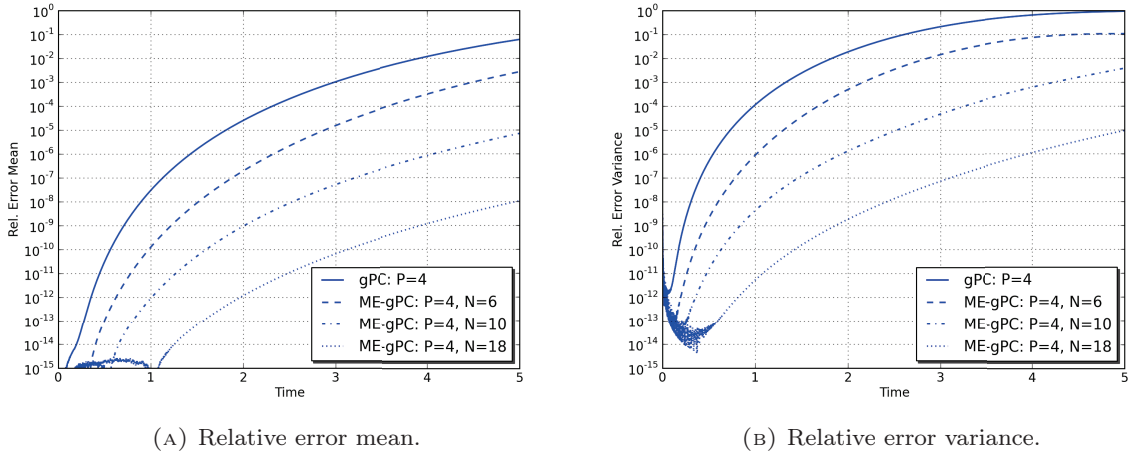
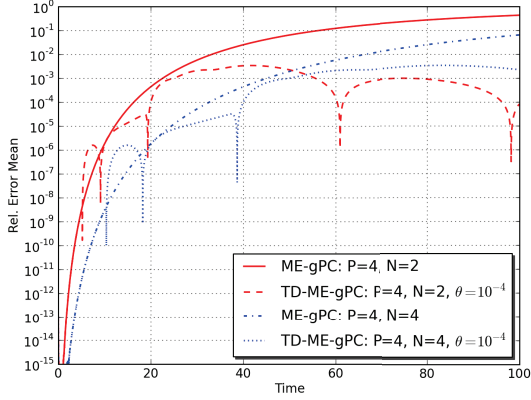


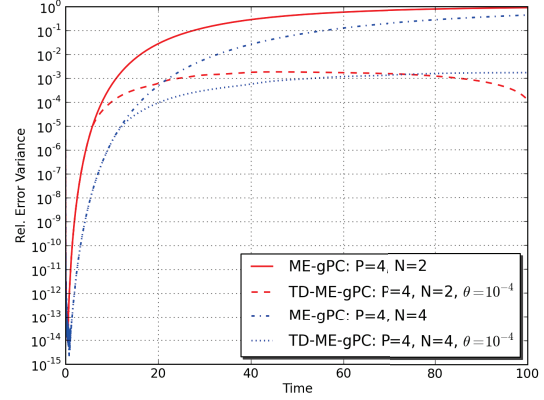
FIGURE 5.4. Relative errors of mean and variance for ME-gPC with $P = 4$ and varying number of elements $N = 1, 6, 10, 18$ for a standard Normal distribution.

Remark 4. The number of elements used in ME-gPC can efficiently be reduced if an adaptive refinement procedure is employed [11, 13]. Also note that the problem in each element can be solved independently from each other, which can be exploited by using appropriate parallelization techniques.

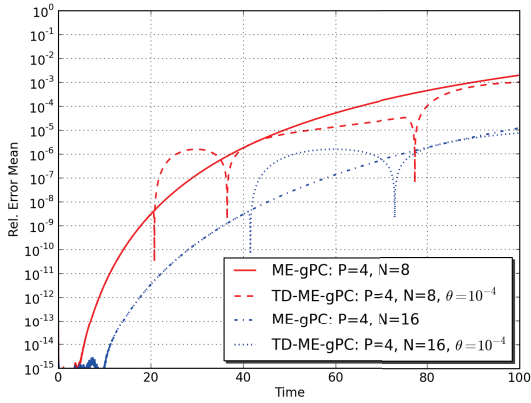
5.3. Time-dependent multi-element gPC. In this section we analyze the effects of the time-dependent approach implemented in every single element resulting from the partitioning of the probability space due to ME-gPC. This approach can play a huge role when dealing with multi-dimensional random input, since then a time-dependent approach on the global probability space becomes quite expensive.



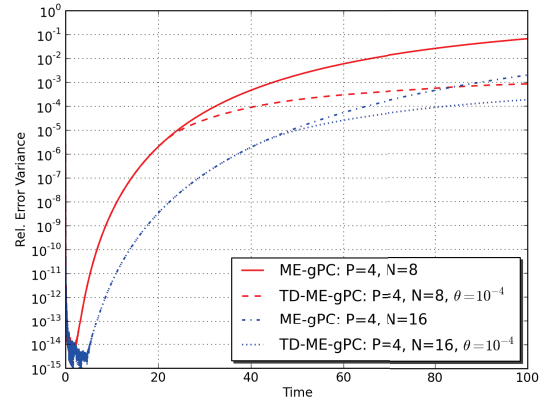
(A) Relative error mean.



(B) Relative error variance.



(C) Relative error mean.

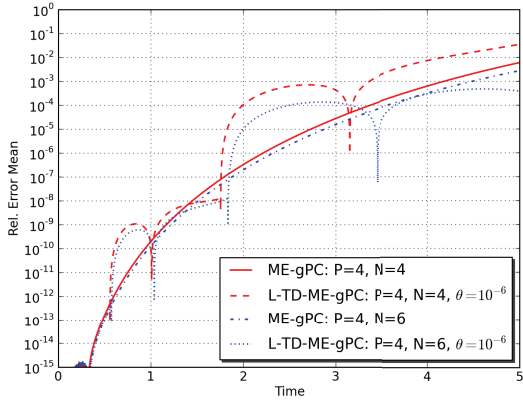


(D) Relative error variance.

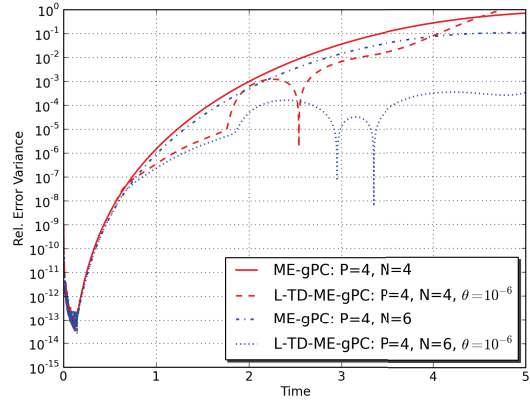
FIGURE 5.5. Relative errors of mean and variance for TD-ME-gPC with $P = 4$, stopping parameter $\theta = 10^{-4}$ and varying number of elements $N = 2, 4, 8, 16$ for a Uniform distribution.

Here, a discretization using 4th order polynomial chaos ($P = 4$) in combination with a stopping parameter $\theta = 10^{-4}$ for the Uniform case and $\theta = 10^{-6}$ for the standard Normal case is carried out employing a varying number of elements. As one can see in Fig. 5.5 and Fig. 5.6, in which the errors resulting from (L-)TD-gPC and ME-gPC are compared to each other, the results exhibit strongly different error developments with respect to the underlying probability distribution and partitioning. For a uniformly distributed ζ (see Fig. 5.5) the improvements, especially for the variance, are significant, whereas the less elements are used, the bigger is the gap between ME-gPC and TD-gPC. For $N = 2$, for example, the error decrease is of the order 3 to 4 for both the mean and the variance for the time-dependent approach. A higher refinement level partitioning, however, has only less benefit from employing TD-gPC elementwise, since in each element, the problem to be solved becomes smoother with respect to stochastic dynamics, hence resulting in less impact of the time-dependent approach.

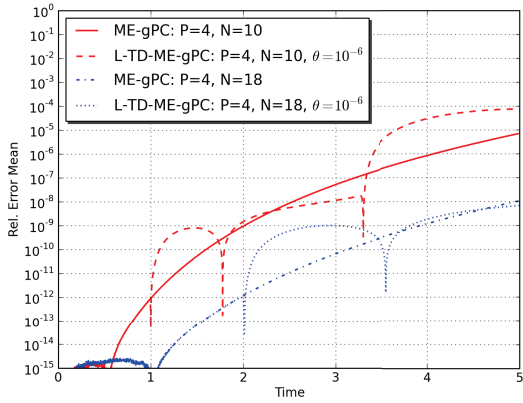
In contrast, looking at the results for the standard Normal distributed ζ (see Fig. 5.6) the relative errors behaviors are different than those for the Uniform case. For $N = 4$, meaning



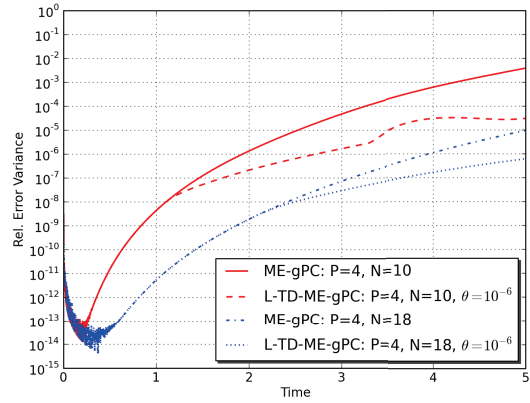
(A) Relative error mean.



(B) Relative error variance.



(C) Relative error mean.



(D) Relative error variance.

FIGURE 5.6. Relative errors of mean and variance for limited TD-ME-gPC with $P = 4$, stopping parameter $\theta = 10^{-6}$ and varying number of elements $N = 4, 6, 10, 18$ for a standard Normal distribution.

that the middle element is refined once, L-TD-ME-gPC is leading to even worse relative errors compared to ME-gPC. However, for the next refinement level, i.e., $N = 6$, this is not the case anymore and L-TD-ME-gPC is achieving significantly improvements up to 3 orders, especially with regard to the variance. For the mean, no such clear error reduction is observable. But it is expected, that choosing different stopping parameters θ and varying the order P of the chaos expansion will lead to different results. This aspects, however, will be addressed in future publications.

6. CONCLUSIONS

Generalized polynomial chaos exhibits poor convergence qualities, when dealing with a highly nonlinear dependency on the random input quantity. Therefore, two recent developments addressing this issues were analyzed, namely a discrete time-dependent generalized polynomial chaos method (TD-gPC, [4]) and a multi-element generalized polynomial chaos method (ME-gPC, [11, 13]). Both approaches were evaluated and analyzed for a simple ODE decay problem

subject to a uniformly and a standard Normal distributed random input. The results were compared and a combination of both methods was proposed and studied, leading to promising improvements in accuracy, which strongly depend on the underlying probability distribution of the input. Especially for the standard Normal case, a restriction of TD-gPC needs to be performed, limiting the maximum number of time resets allowed during one simulation. This is attributed to the loss of orthogonality of the chaos polynomials, which is a problem not occurring for the uniformly distributed input. To overcome this problem, a criteria is suggested checking whether the orthogonality is still satisfied and therefore being dependent only on the application itself. It is expected that the combination of TD-gPC and ME-gPC can play a huge role in the case of multi-dimensional random variables and / or vector-valued differential equations, since a time-dependent “stand alone” approach can lead to very high computational costs very quickly. Future work will give a more detailed analysis on the hybrid formulation. Furthermore, a convergence analysis in terms of the number of chaos polynomials and a study of alternative reset criteria is required. This will also be addressed in future publications, also extending the analysis to the field of partial differential equations, for which it is assumed that due to the dependency on space and time, the challenges and complexity of TD-ME-gPC will increase significantly.

REFERENCES

- [1] R. Cameron, W. Martin, The orthogonal development of nonlinear functionals in series of Fourier-Hermite functionals, *Ann. Math.* 48 (2) (1947) 385–392.
- [2] K. L. Chung, *A Course in Probability Theory*, 3rd ed., Academic Press, Elsevier, 2001.
- [3] M. Doi, T. Imamura, The Wiener-Hermite expansion with time-dependent ideal random function, *Progress of Theoretical Physics* 41 (2) (1969) 358–366.
- [4] M. Gerritsma, J.-B. van der Steen, P. Vos, G. Karniadakis, Time-dependent generalized polynomial chaos, *Journal of Computational Physics* 229 (2010) 8333–8363.
- [5] R. G. Ghanem, P. D. Spanos, *Stochastic Finite Elements: A Spectral Approach*, Springer, New York, 1991.
- [6] O. P. Le Maître, O. M. Knio, *Spectral Methods for Uncertainty Quantification*, Springer, 2010.
- [7] O. P. Le Maître, O. M. Knio, H. N. Najm, R. G. Ghanem, A stochastic projection method for fluid flow I. Basic formulation, *Journal of Computational Physics* 173 (2) (2001) 481–511.
- [8] O. P. Le Maître, L. Mathelin, Asynchronous time integration for polynomial chaos expansion of uncertain periodic dynamics, *Discrete and Continuous Dynamical Systems* 28 (1) (2010) 199–226.
- [9] O. P. Le Maître, M. T. Reagan, H. N. Najm, R. G. Ghanem, O. M. Knio, A stochastic projection method for fluid flow II. random process, *Journal of Computational Physics* 181 (1) (2002) 9–44.
- [10] S. Tanaka, T. Imamura, The Wiener-Hermite expansion with time-dependent ideal random function. II - The three-mode model problem, *Progress of Theoretical Physics* 45 (4) (1971) 1098–1105.
- [11] X. Wan, G. Karniadakis, An adaptive multi-element generalized polynomial chaos method for stochastic differential equations, *Journal of Computational Physics* 209 (2005) 617–642.
- [12] X. Wan, G. Karniadakis, Long-term behavior of polynomial chaos in stochastic flow simulations, *Computer Methods in Applied Mechanics and Engineering* 195 (41-43) (2006) 5582–5596.
- [13] X. Wan, G. Karniadakis, Multi-element generalized polynomial chaos for arbitrary probability measures, *SIAM Journal on Scientific Computing* 28 (3) (2006) 901–928.
- [14] N. Wiener, The homogeneous chaos, *Am. J. Math.* 60 (4) (1938) 897–936.
- [15] D. Xiu, G. Karniadakis, The Wiener-Askey polynomial chaos for stochastic differential equations, *SIAM Journal on Scientific Computing* 24 (2) (2002) 619–644.

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