

Polynomial Chaos for the Computation of Failure Probabilities in Periodic Problems

Roland Pulch

Abstract Numerical simulation of electric circuits uses systems of differential algebraic equations (DAEs) in general. We examine forced oscillators, where the DAE models involve periodic solutions. Uncertainties in physical parameters can be described by random variables. We apply the strategy of the generalised polynomial chaos (gPC) to resolve the stochastic model. In particular, failure probabilities are determined using the approximation from gPC. We present results of numerical simulations for a system of DAEs modelling a Schmitt trigger.

1 Introduction

Mathematical modelling of electric circuits yields time-dependent systems of ordinary differential equations (ODEs) or differential algebraic equations (DAEs), see [1]. The solutions consist of unknown node voltages and branch currents. Typically, the systems include many physical parameters like capacitances, inductances, resistances, etc. Assuming some uncertainties, we replace several parameters by random variables. Accordingly, the solution of the DAEs becomes a random process. The generalised polynomial chaos (gPC) provides techniques for solving the stochastic model approximately, see [2, 3].

We consider forced oscillators, where a periodic boundary value problem of the DAEs results for each realisation of the parameters. A Galerkin approach yields a larger coupled system of DAEs for the finite representation in the polynomial chaos. Thus a periodic boundary value problem of the larger system has to be solved, which can be done by well-known techniques like shooting methods, finite difference schemes or harmonic balance, cf. [4]. Previous work on periodic problems of ODEs or DAEs using the strategy of gPC is given in [5–7]. Moreover, a numerical

Lehrstuhl für Angewandte Mathematik und Numerische Mathematik, Bergische Universität Wuppertal, Gaußstr. 20, D-42119 Wuppertal, Germany. e-mail: pulch@math.uni-wuppertal.de

solution of the coupled system from gPC can be used to determine failure probabilities of the problem, see [2, 8].

In this article, we consider the circuit of a Schmitt trigger, which converts an analogue input signal into a digital output signal. The mathematical model that is used represents the circuit as a system of DAEs. Assuming a random capacitance, we solve numerically the periodic problem of the corresponding gPC system from the Galerkin method, i.e., one random parameter appears. An according strategy and simulations with several random parameters are presented for ODEs in [5, 6]. We compute failure probabilities with respect to the behaviour of the output signal based on the gPC approximation using a common approach. Thereby, failure means that some result exceeds a reference value, which can be determined in a post-processing of a time integration. The numerical results illustrate the performance of the gPC expansions.

2 Problem Definition

We consider a system of DAEs in the form

$$A(\mathbf{p})\dot{\mathbf{x}}(t, \mathbf{p}) = \mathbf{f}(t, \mathbf{x}(t, \mathbf{p}), \mathbf{p}). \quad (1)$$

The matrix $A \in \mathbb{R}^{n \times n}$ and the right-hand side $\mathbf{f} : [t_0, t_1] \times \mathbb{R}^n \times \mathbb{R}^q \rightarrow \mathbb{R}^n$ depend on parameters $\mathbf{p} = (p_1, \dots, p_q)^\top$. Hence the solution $\mathbf{x} : [t_0, t_1] \times \mathbb{R}^q \rightarrow \mathbb{R}^n$ becomes also parameter-dependent. Let $\mathbf{p} \in Q$ for some relevant set $Q \subseteq \mathbb{R}^q$ of parameters. Typically, a parameter p_j is included either in the matrix A or in the right-hand side \mathbf{f} .

We assume that independent input signals in the right-hand side force a periodic solution for each parameter. Thus it holds $\mathbf{x}(t, \mathbf{p}) = \mathbf{x}(t+T, \mathbf{p})$ for all $t \in \mathbb{R}$ and each $\mathbf{p} \in Q$, where the period $T > 0$ is known from the input signals. We set $[t_0, t_1] = [0, T]$ in the following.

Let the chosen parameters exhibit some uncertainty. Consequently, we arrange random variables $\mathbf{p} : \Omega \rightarrow Q$ with respect to a probability space (Ω, \mathcal{A}, P) . We assume that each random variable p_j exhibits a classical distribution like uniform, beta, Gaussian, etc. Consequently, the solution of the DAEs (1) becomes a random process $\mathbf{X} : [0, T] \times \Omega \rightarrow \mathbb{R}^n$. We are interested in the properties of the random process like expected values and variances or more sophisticated quantities. In particular, we will investigate failure probabilities in Section 4.

For a function $f : \mathbb{R}^q \rightarrow \mathbb{R}$ depending on the parameters, we denote the corresponding expected value (if exists) by

$$\langle f(\mathbf{p}) \rangle = \int_{\Omega} f(\mathbf{p}(\omega)) dP(\omega) = \int_{\mathbb{R}^q} f(\mathbf{p}) \rho(\mathbf{p}) d\mathbf{p}$$

using the probability density function $\rho : \mathbb{R}^q \rightarrow \mathbb{R}$. We apply this operation component-wise also to vector-valued or matrix-valued functions. The expected value implies the inner product $\langle f(\mathbf{p})g(\mathbf{p}) \rangle$ for functions $f, g : \mathbb{R}^q \rightarrow \mathbb{R}$ with $f, g \in L^2$.

3 Generalised Polynomial Chaos

Now we examine the stochastic process solving the DAEs (1) with random parameters. Assuming finite second moments, the stochastic process exhibits the representation

$$\mathbf{X}(t, \mathbf{p}(\omega)) = \sum_{i=0}^{\infty} \mathbf{v}_i(t) \Phi_i(\mathbf{p}(\omega)), \quad (2)$$

see [2]. The functions $(\Phi_i)_{i \in \mathbb{N}}$ with $\Phi_i : \mathbb{R}^q \rightarrow \mathbb{R}$ represent a complete basis of multivariate polynomials. We apply an orthonormal basis, i.e., it holds $\langle \Phi_i \Phi_j \rangle = \delta_{ij}$ with the Kronecker-delta. The coefficient functions $\mathbf{v}_i : [0, T] \rightarrow \mathbb{R}^n$ are unknown a priori. The periodicity of the stochastic process \mathbf{X} implies periodic coefficient functions with rate T , see [7].

We truncate the series (2) to achieve the finite representation

$$\mathbf{X}^m(t, \mathbf{p}(\omega)) = \sum_{i=0}^m \mathbf{v}_i(t) \Phi_i(\mathbf{p}(\omega)). \quad (3)$$

Approximations for expected values and variances are obtained component-wise by

$$\langle X_j^m(t, \mathbf{p}) \rangle = v_{0,j}(t), \quad \text{Var}(X_j^m(t, \mathbf{p})) = \sum_{i=1}^m v_{i,j}(t)^2 \quad \text{for } j = 1, \dots, n \quad (4)$$

with $\mathbf{X}^m = (X_1^m, \dots, X_n^m)^\top$ and $\mathbf{v}_i = (v_{i,1}, \dots, v_{i,n})^\top$. The coefficient functions can be computed approximately by stochastic collocation, see [3, 9]. Alternatively, we construct a system of DAEs for the coefficient functions. Inserting the finite approximation (3) in the DAEs (1) yields the residual

$$\mathbf{r}(t, \mathbf{p}) \equiv A(\mathbf{p}) \left(\sum_{i=0}^m \dot{\mathbf{v}}_i(t) \Phi_i(\mathbf{p}) \right) - \mathbf{f} \left(t, \sum_{i=0}^m \mathbf{v}_i(t) \Phi_i(\mathbf{p}), \mathbf{p} \right).$$

Due to the Galerkin method, we demand that the residual is orthogonal to the space of the applied basis polynomials with respect to the inner product of L^2 in the probability space. It follows a larger coupled system of DAEs

$$\sum_{i=0}^m \langle \Phi_l(\mathbf{p}) \Phi_i(\mathbf{p}) A(\mathbf{p}) \dot{\mathbf{v}}_i(t) \rangle = \left\langle \Phi_l(\mathbf{p}) \mathbf{f} \left(t, \sum_{i=0}^m \mathbf{v}_i(t) \Phi_i(\mathbf{p}), \mathbf{p} \right) \right\rangle \quad (5)$$

for $l = 0, 1, \dots, m$ with the coefficient functions $\mathbf{v}_i(t)$ of (3) as unknowns. Although the solutions of (5) are not identical to the coefficients in (2), we apply the same

symbol for convenience. A periodic boundary value problem of the system (5) has to be solved, which can be done by according numerical methods, see [4].

In models of electric circuits, the matrix A typically includes parameters like capacitances C and inductances L , for example. We assume the structure of parameter-dependence of the matrix A motivated in [10], namely

$$A(\mathbf{p}) = A_0 + \sum_{j=1}^q \eta_j(p_j) A_j$$

with constant matrices $A_0, A_1, \dots, A_q \in \mathbb{R}^{n \times n}$ and scalar functions $\eta_j : \mathbb{R} \rightarrow \mathbb{R}$. We can write the complete system using Kronecker products as

$$\left[I_{m+1} \otimes A_0 + \left(\sum_{j=1}^q S_j \otimes A_j \right) \right] \dot{\mathbf{v}}(t) = \mathbf{F}(t, \mathbf{v}) \quad (6)$$

with $\mathbf{v} = (\mathbf{v}_0^\top, \mathbf{v}_1^\top, \dots, \mathbf{v}_m^\top)^\top$, the identity matrix $I_{m+1} \in \mathbb{R}^{(m+1) \times (m+1)}$ and an abbreviation \mathbf{F} for the right-hand side. The matrices S_j are defined via

$$S_j = (\sigma_{li}^j) \in \mathbb{R}^{(m+1) \times (m+1)}, \quad \sigma_{li}^j := \langle \eta_j(p_j) \Phi_l(\mathbf{p}) \Phi_l(\mathbf{p}) \rangle.$$

In case of a single parameter and $\eta_1(p_1) \equiv p_1$, the constant matrix in the left-hand side of (6) becomes block-tridiagonal, since the matrix S_1 is tridiagonal due to the orthogonality of the basis polynomials.

4 Determination of Failure Probabilities

If the solution of the DAEs (1) exhibits specific critical values, the corresponding electric circuit may produce a failure. We describe the state of the solution via a function $g : [t_0, t_1] \times \mathbb{R}^n \rightarrow \mathbb{R}$, where $g \leq 0$ represents the undesired cases. For example, we define as failure that a component x_j for a particular $j \in \{1, \dots, n\}$ becomes smaller or larger than some threshold value $\theta \in \mathbb{R}$, i.e.,

$$g(t, \mathbf{x}(t, \mathbf{p})) \equiv x_j(t, \mathbf{p}) - \theta \quad \text{or} \quad g(t, \mathbf{x}(t, \mathbf{p})) \equiv -x_j(t, \mathbf{p}) + \theta. \quad (7)$$

In the general case, the failure probability at each time point reads

$$P_F(t) := \int_{\mathbb{R}^q} \chi(g(t, \mathbf{X}(t, \mathbf{p}))) \rho(\mathbf{p}) \, d\mathbf{p} \quad \text{with} \quad \chi(g) := \begin{cases} 0 & \text{for } g > 0, \\ 1 & \text{for } g \leq 0. \end{cases} \quad (8)$$

In a Monte-Carlo or quasi Monte-Carlo simulation, the integrals (8) are approximated using realisations $\mathbf{p}^k \in Q$ for $k = 1, \dots, K$. For each realisation, a periodic boundary value problem of the DAEs (1) has to be solved. Alternatively, we apply the solution of the system (5) from the gPC. The computation of this solution can be more costly than the (quasi) Monte-Carlo simulation with same accuracy. Nev-

ertheless, the gPC solution includes more information and may be available from a previous simulation for another purpose. We insert the approximation (3) in the integral (8) and thus obtain

$$P_F(t) \doteq \int_{\mathbb{R}^q} \chi(g(t, \mathbf{X}^m(t, \mathbf{p}))) \rho(\mathbf{p}) \, d\mathbf{p}. \quad (9)$$

The formulation (9) can be evaluated by (quasi) Monte-Carlo sampling again. Given a numerical solution for the coefficients $\mathbf{v}_0, \dots, \mathbf{v}_m$, just polynomials have to be evaluated in an approximation of (9), i.e., no further DAE systems have to be resolved, since we apply $\mathbf{X}^m(t, \mathbf{p})$ instead of $\mathbf{x}(t, \mathbf{p})$. Sophisticated techniques have been constructed for this purpose in case of parameters \mathbf{p} with Gaussian distributions and/or small failure probabilities, see [2, 8].

We consider w.l.o.g. the first case in (7). Since we examine periodic boundary value problems, the total probability of failure $\hat{P}_F \in [0, 1]$ corresponds to the time-independent function

$$g(\mathbf{x}(\cdot, \mathbf{p})) = \left(\min_{t \in [0, T]} x_j(t, \mathbf{p}) \right) - \theta. \quad (10)$$

Typically, this probability is computed by a discretisation $0 \leq t_1 < \dots < t_R < T$ and identification of the minimum value in the grid points.

5 Illustrative Example: Schmitt Trigger

We apply the circuit of a Schmitt trigger illustrated in Figure 1. The Schmitt trigger converts an analogue input signal u_{in} into a digital output signal u_{out} . A mathematical modelling yields a system of DAEs (1) for five unknown node voltages with differential index 1, see [1]. More precisely, the system exhibits the form

$$A(C)\dot{\mathbf{u}} = \mathbf{f}(t, \mathbf{u}), \quad \mathbf{u} : [t_0, t_1] \rightarrow \mathbb{R}^5.$$

Figure 1 also shows the singular matrix A , which depends on the linear capacitance C only. We use a sinusoidal input signal with period $T = 2$ ms. Thus all node voltages become periodic functions.

Let the capacitance be a random variable with uniform distribution in a certain interval. We consider two cases in the simulation, namely

$$\text{case (a): } C \in [10^{-9} \text{ F}, 10^{-7} \text{ F}], \quad \text{case (b): } C \in [1 \cdot 10^{-10} \text{ F}, 2 \cdot 10^{-10} \text{ F}].$$

The first case involves large uncertainties for demonstration and corresponds to the results displayed in Figure 2 and 3. The second case is more realistic and serves for the computation of failure probabilities only.

We solved all periodic boundary value problems via a finite difference method, see [4], using the unsymmetric difference formula of second order (BDF2) at

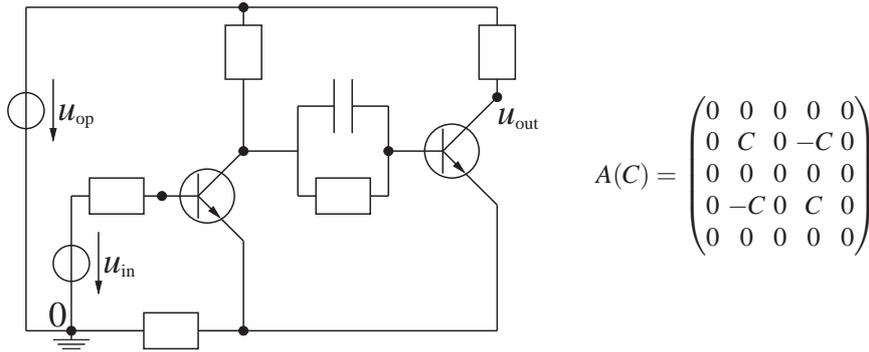


Fig. 1 Schmitt trigger circuit (left) and capacitance matrix of the mathematical model (right).

equidistant distributed time points. Thereby, the same accuracy was demanded in each Newton iteration and we arranged 200 grid points.

We employ the strategy of gPC based on the representation (2), where the orthonormal basis functions are the Legendre polynomials in case of the uniform distribution. We discuss the periodic problems of the coupled systems of DAEs (5) for different orders m .

Figure 2 demonstrates the expected value and the standard deviation of the output voltage in case (a) with $m = 3$ calculated via (4). Moreover, three samples of the output voltage for specific values of the capacitance are given. Figure 3 shows the other coefficient functions of (3). Although the solutions are computed in $[0, T]$ only, the figures show the domain $[0, 2T]$ for a better impression of the signals.

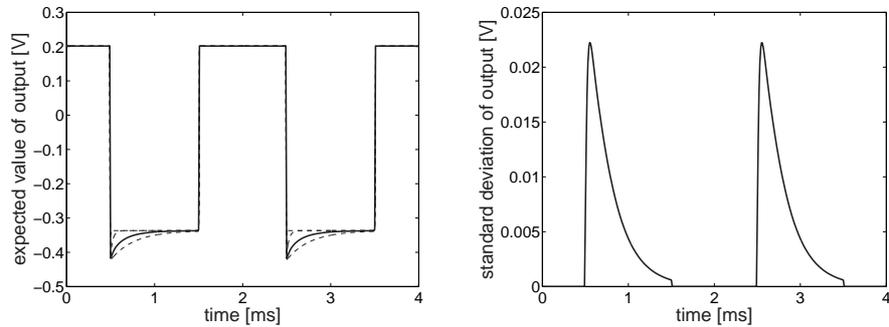


Fig. 2 Expected value (left, solid line) together with three samples for $C = 10^{-j}$ F with $j = 7, 8, 9$ (left, dashed lines) and standard deviation (right) of output u_{out} computed by gPC with $m = 3$.

In the case (a), we recognise that variations in the capacitance do not influence the upper value of the digital output signal. In particular, the standard deviation evidences the critical time intervals. Using $C = 10^{-10}$ F of case (b), the behaviour at the lower value becomes the same as at the upper value, which represents the desired

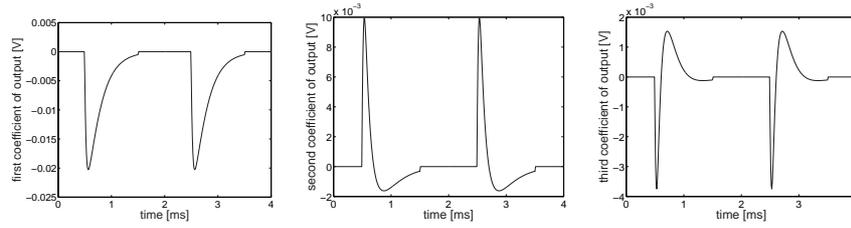


Fig. 3 Coefficient functions v_1, v_2, v_3 for output voltage u_{out} obtained by gPC with $m = 3$.

behaviour. An overshoot appears for larger parameters $C > 10^{-10}$ F. However, this effect decreases again for even larger capacitances $C > 10^{-7}$ F.

To illustrate the convergence of the periodic coefficient functions in (2), we compute the corresponding maximal values within $[0, T]$ for a simulation using $m = 8$. Table 1 presents these maxima with respect to the output signal in case (a) as well as case (b). The other components exhibit a similar behaviour. We recognise the convergence of the gPC representation (2) in both situations. However, case (a) implies a much slower convergence due to the large range of the random parameter.

Next, failure probabilities are determined in this example. We demand that the periodic output voltage must not decrease below some threshold value, which corresponds to the definition (10). We arrange the threshold values $\theta = -0.415$ for case (a) and $\theta = -0.34$ for case (b). The corresponding total failure probability \hat{P}_F is determined by the values in the grid points.

For large numbers of random parameters, (quasi) Monte-Carlo methods have to be used in solving (8). Since one random parameter is considered here (only C), we apply equidistant realisations C_k for $k = 1, \dots, K$, which represents the special case of a quasi Monte-Carlo technique. On the one hand, a reference solution of (8) is computed by solving $K = 10^4$ systems (1). On the other hand, we sample approximations (9) with $K = 10^3$ using solutions of (5) with different numbers m . Remark that the probability in (8) and (9) does not depend on time here, since (10) is observed. The results are shown in Table 2. We note that the approximation becomes more accurate for increasing orders m . In case (b), the usage of $m = 2$ already yields a sufficient result. However, a linear approximation ($m = 1$) is too rough, which indicates that the application of the gPC as a nonlinear approach is necessary.

Table 1 Maximum values of coefficients v_i for output u_{out} in gPC simulation using $m = 8$.

i	1	2	3	4	5	6	7	8
case (a)	$2 \cdot 10^{-2}$	$1 \cdot 10^{-2}$	$5 \cdot 10^{-3}$	$3 \cdot 10^{-3}$	$2 \cdot 10^{-3}$	$1 \cdot 10^{-3}$	$6 \cdot 10^{-4}$	$3 \cdot 10^{-4}$
case (b)	$9 \cdot 10^{-4}$	$1 \cdot 10^{-5}$	$2 \cdot 10^{-7}$	$5 \cdot 10^{-9}$	$1 \cdot 10^{-10}$	$2 \cdot 10^{-12}$	$5 \cdot 10^{-14}$	$1 \cdot 10^{-14}$

Table 2 Computed total failure probabilities from gPC system with $m = 1, \dots, 8$ and reference solution from solving the original systems.

m	1	2	3	4	5	6	7	8	ref.
case (a)	0.940	0.759	0.775	0.802	0.821	0.830	0.830	0.820	0.8177
case (b)	0.082	0.079	0.079	0.079	0.079	0.079	0.079	0.079	0.0786

6 Conclusions

We have applied the technique of the generalised polynomial chaos to periodic boundary value problems of DAEs with time-dependent input signals. The resulting larger coupled systems of DAEs are solved successfully for the electric circuit of a Schmitt trigger. Moreover, the computed numerical solution provides a cheap method to determine failure probabilities a posteriori. In the used examples, it follows that the accuracy of the achieved failure probabilities is adequate if the order of the polynomial chaos is chosen sufficiently high. The construction of techniques based on generalised polynomial chaos is feasible also for autonomous oscillators with a priori unknown periods, which will be part of further research.

Acknowledgements This work has been supported by the PostDoc programme of 'Fachgruppe Mathematik und Informatik' from Bergische Universität Wuppertal (Germany). The author is indebted to Prof. Robert D. Skeel (Purdue University, Indiana, U.S.A.) for helpful discussions.

References

1. Kampowsky, W., Rentrop, P., Schmitt, W.: Classification and numerical simulation of electric circuits. *Surv. Math. Ind.* 2, 23–65 (1992).
2. Augustin, F., Gilg, A., Paffrath, M., Rentrop, P., Wever, U.: Polynomial chaos for the approximation of uncertainties: chances and limits. *Euro. Jnl. of Applied Mathematics* 19, 149–190 (2008).
3. Xiu, D.: Fast numerical methods for stochastic computations: a review. *Comm. Comput. Phys.* 5 (2-4), 242–272 (2009).
4. Günther, M., Feldmann, U., ter Maten, E.J.W.: Modelling and discretization of circuit problems. In: Schilders, W.H.A., ter Maten, E.J.W. (eds.), *Handbook of Numerical Analysis, Vol. XIII: Numerical Methods in Electromagnetics*, pp. 523–659, Elsevier, N. Holland (2005).
5. Lucor, D., Karniadakis, G.E.: Adaptive generalized polynomial chaos for nonlinear random oscillators. *SIAM J. Sci. Comput.* 26 (2), 720–735 (2004).
6. Lucor, D., Su, C.H., Karniadakis, G.E.: Generalized polynomial chaos and random oscillators. *Int. J. Numer. Meth. Engng.* 60, 571–596 (2004).
7. Pulch, R.: Polynomial chaos for analysing periodic processes of differential algebraic equations with random parameters. To appear in: *Proc. Appl. Math. Mech.*
8. Paffrath, M., Wever, U.: Adapted polynomial chaos expansion for failure detection. *J. Comput. Phys.* 226, 263–281 (2007).
9. Xiu, D., Hesthaven, J.S.: High order collocation methods for differential equations with random inputs. *SIAM J. Sci. Comput.* 27 (3), 1118–1139 (2005).
10. Pulch, R.: Polynomial chaos for linear DAEs with random parameters. Preprint, Bergische Universität Wuppertal (2008).