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Polynomial Chaos Expansions For Damped Oscillators

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ABSTRACT: Uncertainty quantification is the state-of-the-art framework dealing with uncertainties arising in all kind of real-life problems. One of the framework's functions is to propagate uncertainties from the stochastic input factors to the output quantities of interest, hence the name *uncertainty propagation*. To this end, *polynomial chaos expansions* (PCE) have been effectively used in a wide variety of practical problems. However, great challenges are hindering the use of PCE for time-dependent problems. More precisely, the accuracy of PCE tends to decrease in time. In this paper, we develop an approach based on a *stochastic time-transform*, which allows one to apply low-order PCE to complex time-dependent problems.

1. INTRODUCTION

Uncertainty quantification has become a key topic in modern engineering in the last decade due to the increasing complexity of physical systems and associated computational models. One of the objectives of the framework is to propagate uncertainties from the stochastic input factors of the model to the output quantities of interest, hence the name *uncertainty propagation*. For this purpose, polynomial chaos expansions (PCE) have been widely used as approximate models (or metamodels) that substitute computationally expensive ones.

PCE, however, face challenges when applied to time-dependent problems, *e.g.* involving structural or fluid dynamics or chemical systems. The greatest challenge hindering the use of PCE is the decrease of the accuracy in time (Ghosh and Iaccarino, 2007; Le Maître et al., 2010).

The causes of the decaying accuracy of PCE in time-dependent problems can be classified into an *approach-related* cause and an *inherent* cause. The approach-related cause refers uniquely to the intrusive approach, which requires manipulation of the mathematical equations describing the considered problem. In particular, the intrusive approach solves a system of reformulated differential equations, which are derived from the original system by substituting PCE for the quantity of interest (Le Maître et al., 2010). The error due to the approximate solution is accumulated over time and will certainly be excessive at some point. In contrast, the non-intrusive approach considers the computational model as a black-box model in which responses at different instants can be examined independently, which prevents the accumulation of error at late instants. The inherent cause refers to the increasing complexity in the system's response with time. Often, as time elapses, the relationship between the output quantity and the input factors becomes increasingly complicated, *i.e.* non-linear, non-smooth or discontinuous. This makes the representation of the system's response with PCE increasingly hard.

Existing approaches in literature for dealing with time-dependent problems may be classified in different categories. The high-order PCE approach includes the decomposition of the complex problem into simpler sub-problems (non-intrusive low-

rank separated approximations (Doostan et al., 2013), intrusive reduced PCE (Pascual and Adhikari, 2012), factorized (resp. logarithmic) polynomial dimensional decomposition F-PDD (resp. L-PDD) (Yadav and Rahman, 2013)). It also includes methods for reducing the size of the high-order PCE basis (sparse PCE (Blatman and Sudret, 2011), two-step PCE (Peng et al., 2010)) and advanced computational techniques for computing the high-order PCE (*e.g.* decoupled PCE (Pham et al., 2014)).

The local PCE approach consists in dividing the input space into subspaces according to the detected discontinuities or dissimilarities. One then builds a local PCE in each subspace and combines those local PCE models to obtain a global metamodel. This approach includes multi-element PCE (Wan and Karniadakis, 2006b), simplex stochastic collocation method (Witteveen and Iaccarino, 2013) and mixture of PCE (Nouy, 2010).

There exist additional approaches involving the modification or update of the polynomial chaos basis: enriched PCE (Ghosh and Ghanem, 2008), time-dependent PCE (Gerritsma et al., 2010), flow map composition (Luchtenburg et al., 2014), hybrid PCE (Heuveline and Schick, 2014), dynamically bi-orthogonal decomposition (Choi et al., 2014) and wavelet-based Wiener-Haar expansion (Sahai and Pasini, 2013).

An attractive approach that was proposed recently is to transform the response trajectories in order to make the relationship between the output and the input factors less complex. Witteveen and Bijl (2008) and Desai et al. (2013) represented the dynamic response trajectories as functions of the phase ϕ instead of time t in order to obtain in-phase vibrations. The phases are extracted from the observations based on the local extrema of the time series. The response trajectories are then transformed from time-histories to phase-histories. Finally PCE are applied in the phase space. This approach relies on the assumption that the phase is well defined as a function of time t. In case this assumption does not hold, the general solution will not be straightforward.

Le Maître et al. (2010) represented the responses in a rescaled time τ such that the dynamic responses vary in a small neighborhood of a reference trajectory. The reference trajectory is chosen so that the variability of the uncertain parameters does not induce significant changes in the trajectory. In general, the scaled time τ is not a linear function of t, *i.e.* the "clock speed" $\dot{\tau} = \frac{\mathrm{d}\tau}{\mathrm{d}t}$ is not constant. This relation depends on the difference between the dynamic response and the reference trajectory. In the mentioned paper, $\dot{\tau}$ is adjusted in an *intrusive way* at each step so that the difference is minimized.

As a summary, PCE fail to represent long-term time-dependent system responses because of their inherent increasing complexity. So far, there has not been a versatile tool that helps overcome the problem. The objective of this paper is to introduce a non-intrusive approach that allows the use of PCE for time-dependent problems. The proposed approach relies on a *non-intrusive stochastic time-transform* of the response trajectories which aims at *maximizing the similarities in frequency and phase content* of sampled time-histories.

The paper is organised as follows: in Section 2, the fundamentals of PCE are recalled. In Section 3, we propose a non-intrusive PCE approach for time-dependent problems and use a benchmark example of stochastic dynamics to illustrate it.

2. POLYNOMIAL CHAOS EXPANSIONS

Let us consider a computational model $Y = \mathscr{M}(\boldsymbol{X})$ where $\boldsymbol{X} = (X_1, \ldots, X_M)^\mathsf{T}$ is a M-dimensional random input vector with the probability density function $f_{\boldsymbol{X}}$ defined in the probability space $(\Omega, \mathscr{F}, \mathbb{P})$. Without loss of generality, we investigate the case when the input random variables are independent. Assume that the scalar output Y is a second order random variable, *i.e.* $\mathbb{E}\left[Y^2\right] < +\infty$. Then, Y belongs to a Hilbert space $\mathscr{H}$ of square-integrable functions of random vector $\boldsymbol{X}$. Denote by $\mathscr{H}_i$ the Hilbert space associated with the marginal probability measure $\mathbb{P}_{X_i}(\mathrm{d}x_i) = f_{X_i}(x_i)\mathrm{d}x_i$, in which one selects a basis of associated orthonormal univariate polynomial functions $\{\psi_k^i, k \in \mathbb{N}\}$. For instance, when X_i is a uniform (resp. standard normal) random variable, those are orthonormal Legendre (resp. Hermite) polynomials. The generalized polynomial chaos representation of Y can be

written as follows (Xiu and Karniadakis, 2002):

$$Y = \sum_{\boldsymbol{\alpha} \in \mathbb{N}^M} y_{\boldsymbol{\alpha}} \psi_{\boldsymbol{\alpha}}(\boldsymbol{X}) \tag{1}$$

in which $\psi_{\boldsymbol{\alpha}}(\boldsymbol{X}) = \psi^1_{\alpha_1}(X_1) \dots \psi^M_{\alpha_M}(X_M)$ are multivariate orthonornal polynomials with respect to $f_{\boldsymbol{X}}(\boldsymbol{x})$, $\boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_M)$ are multi-indices with $\{\alpha_i, i = 1, \dots, M\}$ denoting the degree of the univariate polynomial of X_i and $y_{\boldsymbol{\alpha}}$'s are the corresponding polynomial chaos coefficients or "coordinates" of Y in the space spanned by the polynomial chaos basis.

In practice, the use of infinite series as in Eq. (1) is not tractable and thus, an approximate truncated representation is utilized:

$$Y \approx \sum_{\boldsymbol{\alpha} \in \mathscr{A}} y_{\boldsymbol{\alpha}} \psi_{\boldsymbol{\alpha}}(\boldsymbol{X}) \tag{2}$$

in which $\mathscr{A}$ is the set of truncated multi-indices $\boldsymbol{\alpha}$. Different choices can be made for the truncation scheme. For instance, the total degree of the expansion is set to be not larger than a prescribed value, *i.e.* :

$$\mathscr{A} = \{\boldsymbol{\alpha} \in \mathbb{N}^M : \quad \| \boldsymbol{\alpha} \|_1 = \alpha_1 + \dots + \alpha_M \leqslant p\} \tag{3}$$

The computation of the coefficients $y_{\boldsymbol{\alpha}}$ can be performed by means of the intrusive approach (*i.e.* spectral stochastic finite element method (Ghanem and Spanos, 2003)) or non-intrusive approaches (*e.g.* projection, regression methods). The reader is refered to Sudret (2007) for further details. In the following, we will use the adaptive sparse polynomial chaos expansions (Blatman and Sudret, 2011), which is a non-intrusive approach based on least-square minimization. The accuracy of PCE is estimated by means of the leave-one-out error (Blatman, 2009).

3. POLYNOMIAL CHAOS EXPANSIONS FOR TIME-DEPENDENT PROBLEMS

An intrusive time-transform of the trajectories was proposed by Le Maître et al. (2010) aiming at representing the time-histories in a small neighborhood of a reference trajectory so as to reduce their variability. This is done by minimizing the Euclidean distance between the distinct trajectories and a reference counterpart. Herein, we propose a non-intrusive transform, which consists in finding a suitable *stochastic mapping* of the time line that increases the *similarity* between different trajectories, thus allowing low-order PCE to be applied. "A neighborhood of a reference trajectory" (Le Maître et al., 2010) is characterized by similarity in terms of distance, whereas "in-phase vibrations" (Witteveen and Bijl, 2008) are characterized by similarity in terms of frequency and phase content. In the current paper, the proposed approach focuses on increasing the similarity both in frequency and phase.

3.1. Proposed approach

Consider a time-dependent system (*e.g.* a structural dynamic or chemical system) whose response is modelled by a system of first-order ordinary differential equations:

$$\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} = \boldsymbol{f}(\boldsymbol{x}, \boldsymbol{\xi}, t) \tag{4}$$

where $t \in [0, T]$, the initial conditions $\boldsymbol{x}(t = 0) = \boldsymbol{x}_0$ are deterministic and the random vector $\boldsymbol{\xi}$ denotes the uncertain parameters governing the system behavior, *e.g.* masses, stiffness, reaction parameters. $\boldsymbol{\xi}$ comprises independent second-order random variables defined in the probability space $(\Omega, \mathscr{F}, \mathbb{P})$. Note that when a non-intrusive approach is used, it is not required to know explicitly the equations, *i.e.* only runs of the available solver for realizations of $\boldsymbol{\xi}$ will be used. The initial conditions can also be uncertain, in which case they become random variables belonging to $\boldsymbol{\xi}$. The time-dependent response of the system is denoted $\boldsymbol{x}(t, \boldsymbol{\xi})$. Without loss of generality, one can consider one component of the response, *e.g.* $x(t, \boldsymbol{\xi})$ with the initial condition $x(t = 0) = x_0$. At each time instant, $x(t, \boldsymbol{\xi})$ is a second-order random variable. As in Witteveen and Bijl (2008), we assume that $x(t, \boldsymbol{\xi})$ is an oscillatory response.

We conduct the time transform operation that makes the trajectories similar in frequency and phase content as follows:

- One first chooses a reference trajectory $x_r(t)$ which is for instance obtained by considering the mean values of the input vector $\boldsymbol{\xi}$, *i.e.*

$x_r(t) = x(t, \boldsymbol{\xi}_r = \mathbb{E}[\boldsymbol{\xi}])$. In general, $x_r(t)$ may be any realization of the response quantity $x(t)$ obtained for a specific sample of $\boldsymbol{\xi}$. For the example considered in this paper, the choice of $x_r(t)$ shall not affect the final results.

- One determines the fundamental frequency f_r and period T_r of the reference trajectory $x_r(t)$. We emphasize that herein $x_r(t)$ is assumed to be a monochromatic signal, *i.e.* f_r is the only frequency contained in $x_r(t)$. The case when $x(t, \boldsymbol{\xi})$ is multichromatic will be considered in a future work. To estimate f_r and T_r, one can use two techniques. The first technique is based on the Fourier transform of $x_r(t)$, *i.e.* it is applied in the frequency domain. The frequency corresponding to the peak of the frequency spectrum of $x_r(t)$ is the expected value of f_r and $T_r = 1/f_r$. The second technique is based on directly examining the trajectory of $x_r(t)$ in the time-domain. One measures the average time interval between consecutive maxima (or minima) of $x_r(t)$ which is the approximate value of T_r. This quick and simple estimation is found sufficiently effective in the example in this paper.

- The following pre-processing consists in transforming the time line with the purpose of increasing the similarity between different realizations of the output $x(t, \boldsymbol{\xi})$. Assume that one is given a set of trajectories $x_i(t) \equiv x(t, \boldsymbol{\xi}_i)$, $i = 1, \ldots, n$ for n realizations $\boldsymbol{\xi}_i$ of the input random vector. For each i the following steps are performed:

  - Determine the fundamental frequency f_i and period T_i of the considered trajectory $x_i(t)$.
  - Define a linear time transform operator $\tau = k_i t + \phi_i$. This operator consists of two actions, namely scaling and shifting, respectively driven by parameters k_i and ϕ_i. The time line is stretched (resp. compressed) when $k_i > 1$ (resp. $0 < k_i < 1$) and is shifted to the left (resp. to the right) when $\phi_i < 0$ (resp. $\phi_i > 0$). In general, the time transform is defined based on the considered problem and a nonlinear transform shall be possible. When $x(t, \boldsymbol{\xi})$ is monochromatic, a linear transform is however sufficient.
  - Determine (k_i, ϕ_i) as the global maximizer of the similarity measure between the considered trajectory and the reference counterpart. We propose the following similarity measure as a function of k and ϕ:

$$g(k, \phi) = \frac{\left| \int_0^T x_i(kt + \phi) x_r(t) \mathrm{d}t \right|}{\|x_i(kt + \phi)\| \|x_r(t)\|}, \quad (5)$$

in which $\int_0^T x_i(kt + \phi) x_r(t) \mathrm{d}t$ is the inner product of the two considered time-histories and $\|\cdot\|$ is the associated l^2-norm, *e.g.* $\|x_r(t)\| = \sqrt{\int_0^T x_r^2(t) \mathrm{d}t}$. In practice, trajectories are discretized over a grid and the inner product (resp. the l^2-norm) is reduced to the classical dot product of the two considered vectors (resp. the Euclidean length). By Cauchy-Schwarz inequality, this similarity measure always takes values in the interval $[0, 1]$. In fact, if (k, ϕ) is a solution then so is $(k, \phi \pm T_r/2)$, *i.e.* when the transformed-function is shifted by a distance equal to $T_r/2$ (whether to the left or to the right), the similarity measure reaches another global maximum (see Figure 1 for example).

To ensure the uniqueness of the solution, constraints on the support of the parameters need to be imposed. If $T_r/4 \leq \phi \leq T_r/2$ (resp. $-T_r/2 \leq \phi \leq -T_r/4$) comprises a solution, then $\phi - T_r/2$ (resp. $\phi + T_r/2$) in the interval $[-T_r/4, T_r/4]$ is also a maximizer. Thus, it is sufficient to consider ϕ in the interval $[-T_r/4, T_r/4]$. In addition, the scaling factor k is as-

sumed to be positive. Finally, one has:

$$(k_i, \phi_i) = \arg \max_{\substack{k \in \mathscr{R}^+ \\ |\phi| \leqslant T_r/4}} g(k, \phi) \qquad (6)$$

  - Represent $x_i(t)$ on the transformed time line τ. For this purpose, one chooses a grid line of τ with the desired time interval. In fact, the finer the grid is, the smaller is the error introduced by the interpolation. Herein, the time step in the time line τ is chosen equal to the discretization step in the original time t. The trajectory $x_i(t)$ is projected onto $\tau_i = k_i t + \phi_i$ to obtain $x_i(\tau_i)$. Finally, the latter is linearly interpolated on τ yielding $x_i(\tau)$.

- One builds PCE of $k(\boldsymbol{\xi})$, $\phi(\boldsymbol{\xi})$ and $x(\tau, \boldsymbol{\xi})$ using the realizations $\{k_i, \phi_i, x_i(\tau, \boldsymbol{\xi}), i = 1, \ldots, n\}$ as experimental design (or training set). Because $k(\boldsymbol{\xi})$ and $\phi(\boldsymbol{\xi})$ are scalar quantities, the computation of their PCE models is straightforward. Note that the computation of PCE of the vector-valued response $x(\tau, \boldsymbol{\xi})$ might be computationally expensive when the time horizon T is large. This computational cost can be reduced significantly by means of principal component analysis (Blatman and Sudret, 2013). Although we are aware of this useful tool, we will not use it in this paper because the considered duration T is relatively short (30 s); in addition, the response in the transformed time line becomes a smooth function of the input variables $\boldsymbol{\xi}$ and requires only low-order PCE which are not expensive to compute.

Given a new realization of input parameters $\boldsymbol{\xi}_0$, one can predict the corresponding responses of the system using PCE as follows:

- One predicts $x(\tau, \boldsymbol{\xi}_0)$, $k(\boldsymbol{\xi}_0)$ and $\phi(\boldsymbol{\xi}_0)$ using the computed PCE models.

- One maps $x(\tau, \boldsymbol{\xi}_0)$ into $x(t, \boldsymbol{\xi}_0)$ using $t = \dfrac{\tau - \phi(\boldsymbol{\xi}_0)}{k(\boldsymbol{\xi}_0)}$

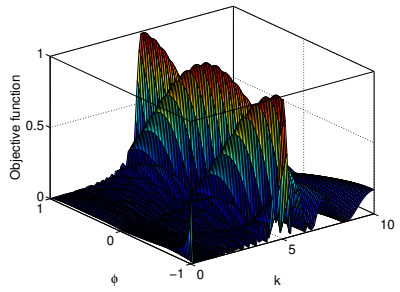

Figure 1: Similarity measure $g(k, \phi)$ (see Eq. (5))

3.2. Example

Let us consider a non-linear single-degree-of-freedom Duffing oscillator under free vibration. The equation of motion reads:

$$\ddot{x}(t) + 2\,\omega\,\zeta\,\dot{x}(t) + \omega^2\,(x(t) + \varepsilon\,x^3(t)) = 0 \qquad (7)$$

with the initial conditions $x(t=0) = 1$ and $\dot{x}(t = 0) = 0$. The motion of the oscillator is driven by three uncertain parameters described as follows:

$$\begin{cases} \zeta = 0.05(1 + 0.05\xi_1), & \xi_1 \sim \mathscr{U}(-1, 1) \\ \omega = 2\pi(1 + 0.2\xi_2), & \xi_2 \sim \mathscr{U}(-1, 1) \\ \varepsilon = -0.5(1 + 0.5\xi_3), & \xi_3 \sim \mathscr{U}(-1, 1) \end{cases} \qquad (8)$$

We aim at building PCE of $x(t)$ as a function of the random variables $\boldsymbol{\xi} = (\xi_1, \xi_2, \xi_3)^\mathsf{T}$.

Figure 2 shows 20 trajectories of $x(t)$ from an experimental design comprising 200 realizations. The trajectories are oscillatory signals, however, they are not periodic. Tenth-order PCE applied directly to this experimental design (*i.e.* without preprocessing the trajectories) result in the leave-one-out (LOO) error depicted in Figure 3. Although it is acceptable in the early time instants, this error starts to be excessive at $t = 5$ s. For illustration, we compare the prediction of this direct PCE model for a particular realization $\boldsymbol{\xi}_0 = (-0.95, -0.64, -0.89)^T$ with the corresponding actual response (Figure 4). It is clear that the prediction fails after 5 seconds.

We now apply the time-transform approach to the above problem. Using tenth-order PCE, we can model the parameters k and ϕ accurately. For a validation set $\mathscr{X} = \left\{\boldsymbol{\xi}^{(1)}, \ldots, \boldsymbol{\xi}^{(n)}\right\}$ of size $n = 200$, Figure 5 depicts the values of k and ϕ predicted by the PCE versus the actual values. The LOO errors of the PCE models of k and ϕ are 9.3×10^{-6}

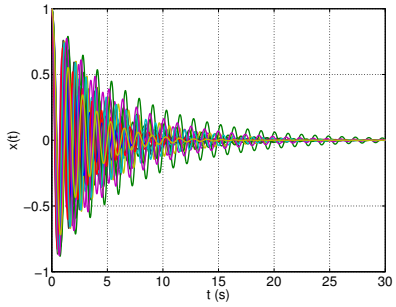

Figure 2: Twenty different trajectories $x(t)$ in the original time line t

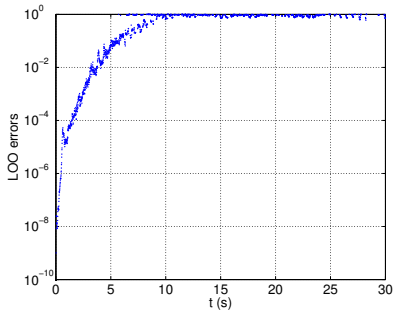

Figure 3: Evolution of the leave-one-out error of PCE in the original time line t

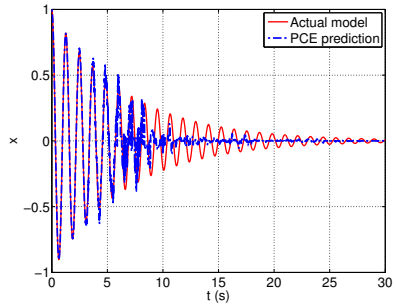

Figure 4: Prediction of $x(t)$ by PCE vs. *actual response trajectory*

and 5.2×10^{-3}, respectively. The transformed trajectories become in-phase vibrations, as shown in Figure 6. For the sake of comparison, PCE of order up to ten are used to model $x(\tau)$. However, the analyses show that the optimal order of the PCE to obtain the largest accuracy is around six. The resulting LOO error normalized by the amplitude envelope $|x_e(\tau)|$ is depicted in Figure 7. One notices that the LOO error has a similar oscillatory feature as observed in Wan and Karniadakis (2006a). The error oscillates around 10^{-4} and attains its minima (resp. maxima) at the instants when $x(\tau)$ reaches its maximal or minimal amplitude (resp. zero amplitude) during an oscillation cycle. For the same validation set $\mathscr{X}$, Figure 8 (resp. Figure 9) compares the response trajectories in the transformed time line τ (resp. in the original time line t) predicted by PCE with the actual response trajectories for two realizations of the input vector, namely $\boldsymbol{\xi}_1 = (-0.02, 0.47, -0.38)^\mathsf{T}$ and $\boldsymbol{\xi}_1 = (-0.95, -0.64, -0.89)^\mathsf{T}$. The results illustrate the accuracy of the proposed time-transform approach.

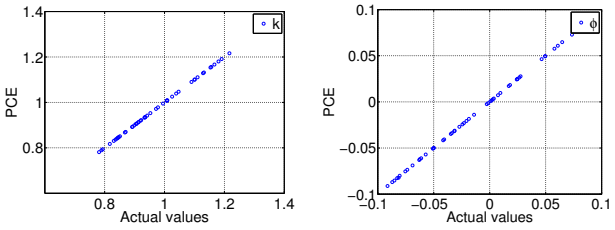

Figure 5: Prediction of k and ϕ by PCE vs. *actual values*

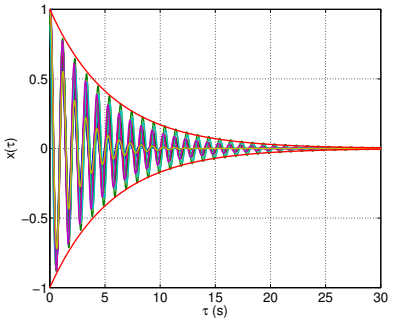

Figure 6: Twenty different trajectories $x(\tau)$ in the transformed time line τ. The red curves are the amplitude envelopes of the trajectories which are defined by $|x_e(\tau)| = \exp(-0.18\tau)$.

4. Conclusions and Perspectives

Polynomial chaos expansions (PCE) constitute an effective metamodelling technique which has been used in several practical problems in a wide variety of domains. However, PCE are known to fail when time-dependent complex systems are considered. The failure is associated with the large dissimilarities between the time-dependent system responses corresponding to different realizations of the uncertain parameters.

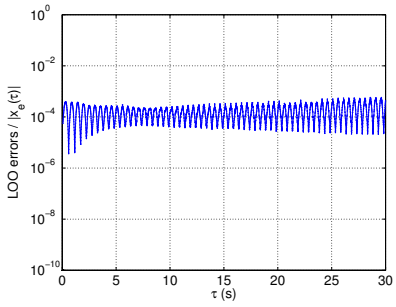

Figure 7: Evolution of the leave-one-out error of PCE in the transformed-time τ

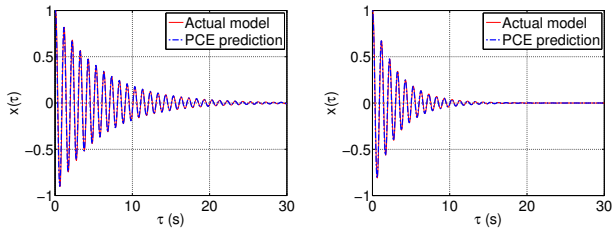

Figure 8: Prediction of $x(\tau)$ by PCE vs. *actual models in the transformed time line τ*

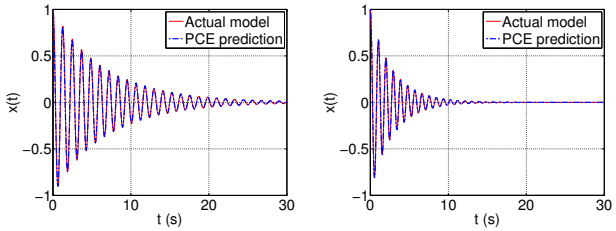

Figure 9: Prediction of $x(t)$ by PCE vs. *actual models in the original time line t*

We proposed an approach which consists in representing the responses into a transformed time line where the similarities between different response trajectories are maximized. The parameters governing the stochastic time transform are determined by means of a global optimization problem with a newly introduced objective function that quantifies the similarity between two trajectories. The proposed approach allows one to solve time-dependent problems using only low-order PCE. In the considered mechanical example, the approach proves effective in terms of accuracy and computational cost.

Further developments are required in order to apply the proposed approach to more complex problems. The formulation in this paper is based on the assumption that the stochastic responses are monochromatic. In the case of multi-chromatic signals (*i.e.* signals which are richer in frequency content), one may decompose the signals into monochromatic components and then apply a similar time-transform to each component. One may also employs a non-linear time-transform in the same context. Other objective functions based on different criteria, *e.g.* a displacement-based measure, may also be developped according to the considered problem.

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