Polynomial chaos expansions for time-dependent problems

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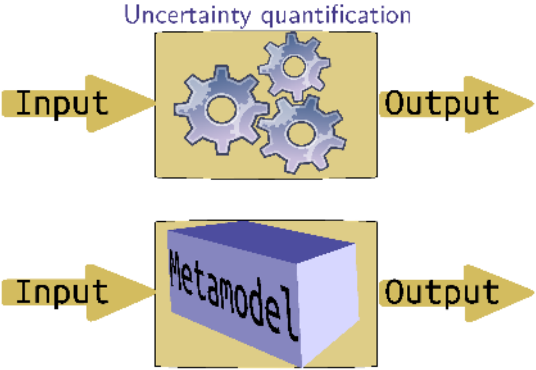
Chair of Risk, Safety & Uncertainty Quantification

MascotNum, April 8th, 2015

Uncertainty quantification

Uncertainty quantification



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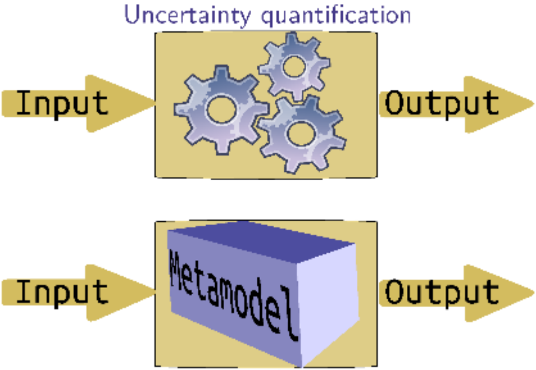


Polynomial Chaos Expansions

Outline

Outline

Polynomial chaos expansions

Ghanem and Spanos, 2003; Soize and Ghanem, 2004

PCE

$$Y(\boldsymbol{\xi}) = \sum_{\boldsymbol{\alpha} \in \mathbb{N}^M} y_{\boldsymbol{\alpha}} \boldsymbol{\psi}_{\boldsymbol{\alpha}}(\boldsymbol{\xi})$$

where:

- $\boldsymbol{\xi} = \{\xi_1, \ldots, \xi_M\}$ is the vector of uncertain input parameters,
- $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_M)$ is a multi-index,
- $\boldsymbol{\psi}_{\boldsymbol{\alpha}}(\boldsymbol{\xi})$ is a multivariate polynomial function

$$\boldsymbol{\psi}_{\boldsymbol{\alpha}}(\boldsymbol{\xi}) = \prod_{i=1}^{M} \psi^{(i)}_{\alpha_i}(\xi_i)$$

- $y_{\boldsymbol{\alpha}}$'s are expansion coefficients.

Polynomial chaos expansions

PCE for time-dependent problems

$$Y(t, \boldsymbol{\xi}) = \sum_{\boldsymbol{\alpha} \in \mathbb{N}^M} y_{\boldsymbol{\alpha}}(t) \psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi})$$

Frozen-in-time PCE

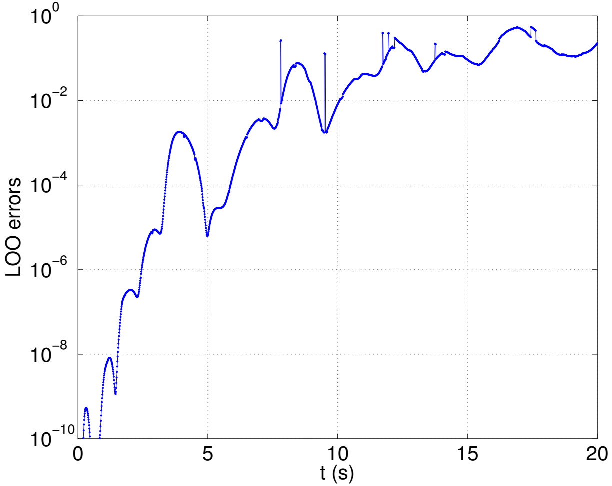
Computing PCE

- Intrusive approach — Le Maître and Knio, 2010
- Non-intrusive approach
  - Projection method
  - Least squares method

Leave-one-out (LOO) cross-validation

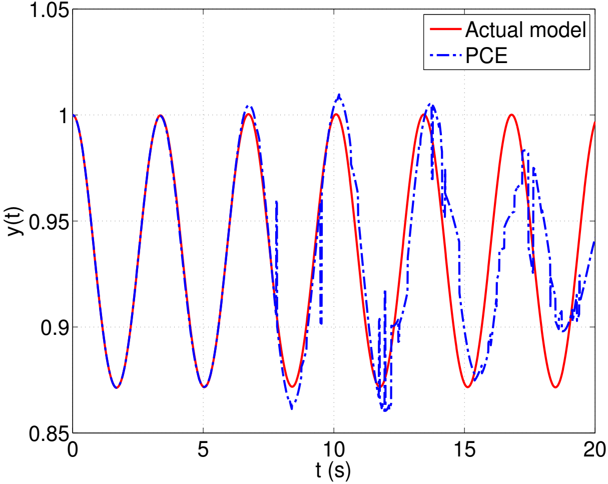
Adaptive sparse PCE based on least-angle-regression — Blatman and Sudret, 2011

PCE for time-dependent systems



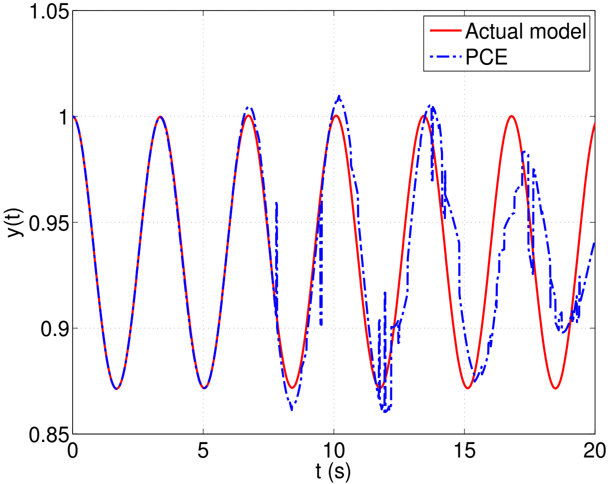
LOO errors *vs.* time (Rigid body dynamics)

PCE for time-dependent systems



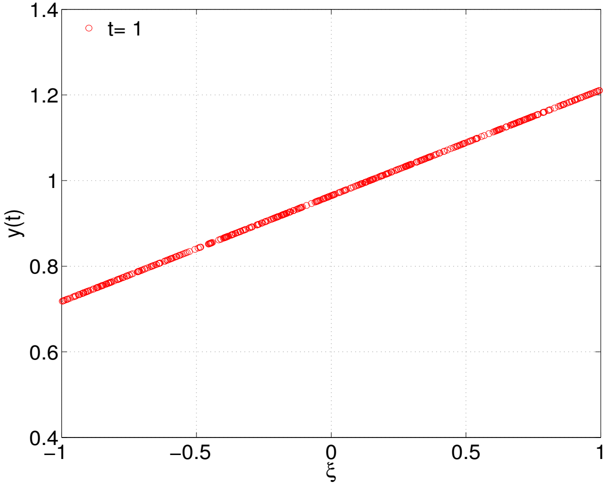
Prediction by PCE *vs.* actual response

PCE for time-dependent systems



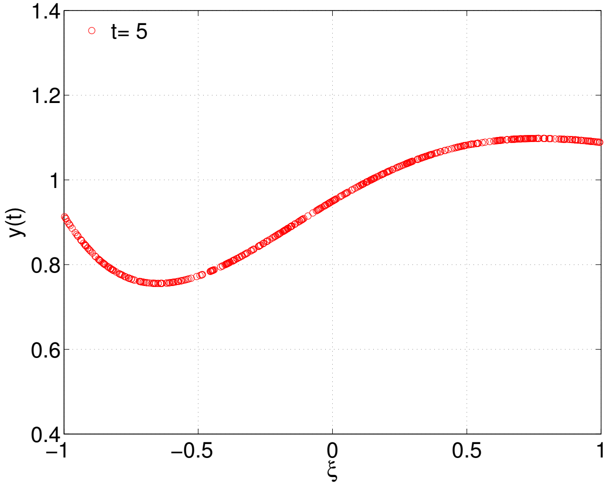
Problem: accuracy decreases over time

PCE for time-dependent systems



Time-dependent input-output relationship (Rigid body dynamics)

PCE for time-dependent systems



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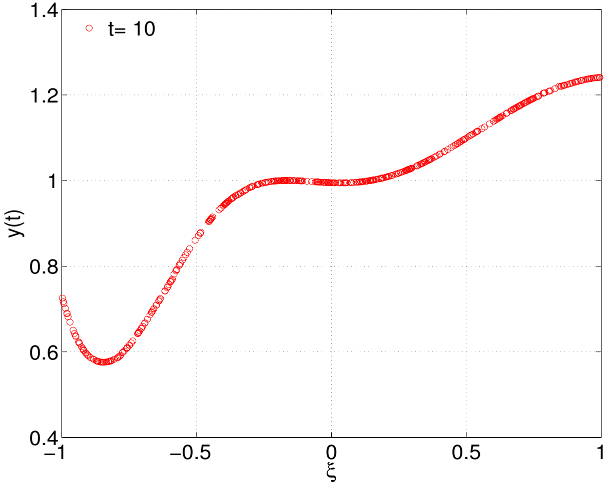

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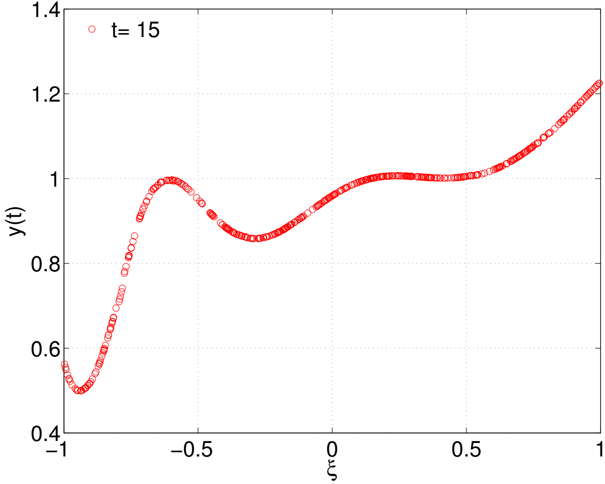

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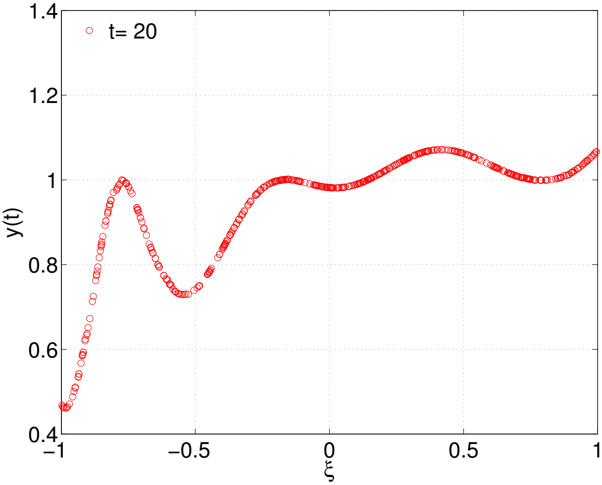

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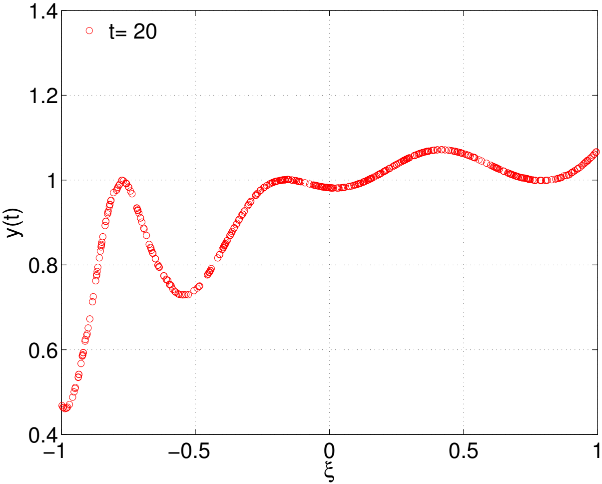
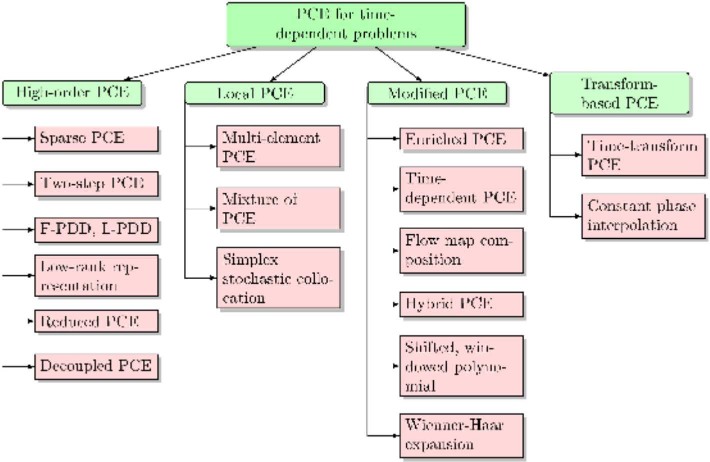


Complexity increases over time (nonlinearity, discontinuity, *etc.*)

PCE for time-dependent systems



Existing PCE approaches that can be used for time-dependent problems

Intrusive time-transform

Intrusive time-transform

Le Maître, Mathelin, et al., 2010

$$\begin{aligned}
\frac{d\boldsymbol{x}^r}{dt}(t) &= \boldsymbol{f}^r(\boldsymbol{x}^r(t)), \\
\frac{d\boldsymbol{y}}{dt}(t;\boldsymbol{\xi}) &= \dot{\tau}(t;\boldsymbol{\xi})\boldsymbol{f}(\boldsymbol{y}(t;\boldsymbol{\xi});q(\boldsymbol{\xi})), \\
\frac{d\dot{\tau}}{dt}(t;\boldsymbol{\xi}) &= -\alpha_0\dot{\tau}(t;\boldsymbol{\xi})\Delta(t;\boldsymbol{\xi}) + \alpha_1\left[1-\dot{\tau}(t;\boldsymbol{\xi})\right], \\
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Application: limit-cycle oscillations

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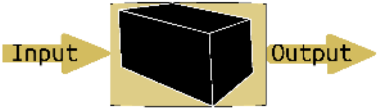


Outline

Stochastic time transform

Focus on

- Oscillatory systems: limit-cycle oscillators, harmonic oscillators, *etc.*

System of type "black box"

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

in which

- $\boldsymbol{x}(t=0) = \boldsymbol{x}_0$: initial condition
- $\boldsymbol{\xi}$: parameter vector of independent second-order random variables defined in the probability space $(\Omega, \mathcal{F}, \mathbb{P})$

What to to

- Represent the system's output in a transformed time scale in which the similarity in the frequency and phase content of distinct trajectories is maximized.

Similarity measure

Similarity measure between two trajectories $x_1(t)$ and $x_2(t)$:

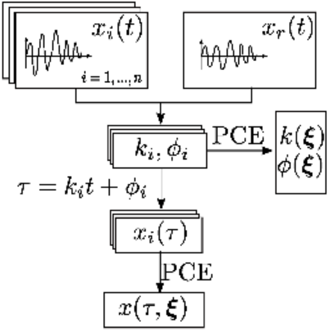
$$f(x_1(t), x_2(t)) = \frac{\left| \int_0^T x_1(t) x_2(t) \mathrm{d}t \right|}{\|x_1(t)\| \|x_2(t)\|}$$

- $\int_0^T x_1(t) x_2(t) \mathrm{d}t$ is the inner product of the two considered time histories
- $\| \cdot \|$ is the associated l^2-norm

Stochastic time transform

Time-transform PCE

- Choose a reference trajectory $x_r(t)$
- Define a linear stochastic time transform $\tau = k\,t + \phi$
- For $i = 1, \ldots, n$,
  - Determine $\{k_i, \phi_i\}$ as solution of an optimization problem.
  - Represent $x_i(t)$ on the transformed time line τ, yielding $x_i(\tau)$.
- Compute PCE $x(\tau, \xi) = \sum x_\alpha(\tau)\psi_\alpha(\xi)$ using $\{x_i(\tau, \xi), i = 1, \ldots, n\}$
- Compute PCE $k(\xi) = \sum k_\beta \psi_\beta(\xi)$ and $\phi(\xi) = \sum \varphi_\gamma \psi_\gamma(\xi)$ using $\{k_i, \phi_i, i = 1, \ldots, n\}$



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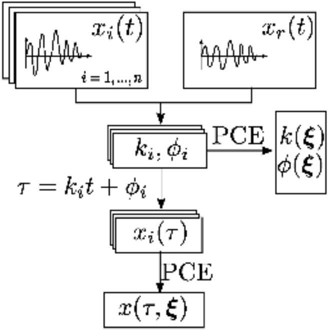

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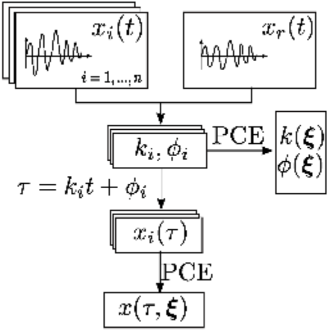

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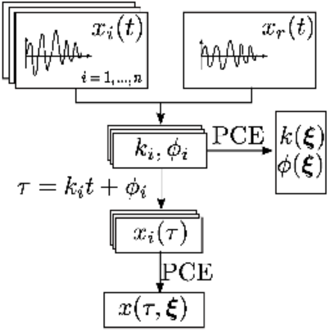

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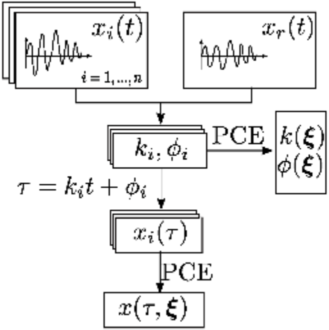

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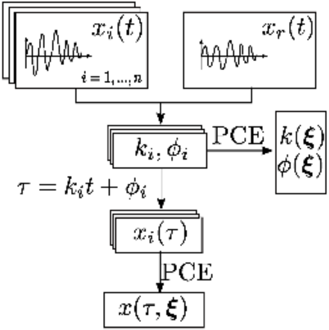

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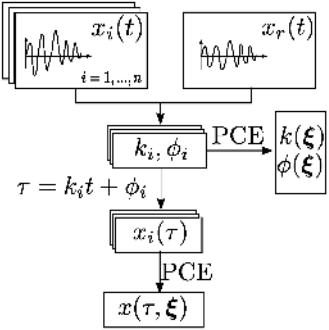

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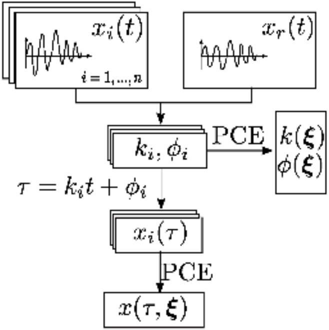

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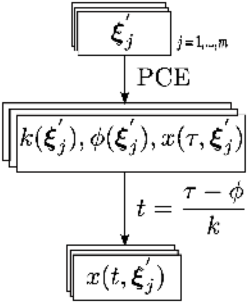

Prediction by time-transform PCE

- Predict $x(\tau, \xi')$, $k(\xi')$ and $\phi(\xi')$ using the computed PCE.
- Map $x(\tau, \xi')$ into $x(t, \xi')$ using $t = \frac{\tau - \phi(\xi')}{k(\xi')}$

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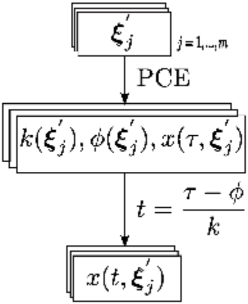

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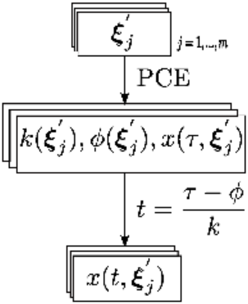

Optimization-based time transform

Maximize the similarity measure between the considered trajectory and the reference one

$$(k, \phi) = \arg \max_{\substack{k \in \mathcal{R}^+ \\ |\phi| \leqslant T_r/4}} g(k, \phi)$$

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where

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

Outline

Rigid body dynamics

http://www.esa.int/spaceinimages/Missions/Rosetta

Rigid body dynamics

http://www.esa.int/spaceinimages/Missions/Rosetta

Rotation of a rigid body described by Euler's equations

$$\begin{cases} M_x = I_{xx}\,\dot{\omega}_x - (I_{yy} - I_{zz})\,\omega_y\,\omega_z \\ M_y = I_{yy}\,\dot{\omega}_y - (I_{zz} - I_{xx})\,\omega_z\,\omega_x \\ M_z = I_{zz}\,\dot{\omega}_z - (I_{xx} - I_{yy})\,\omega_x\,\omega_y \end{cases}$$

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- $M_x = M_y = M_z = 0$
- $x(0) = 0,\ y(0) = 1,\ z(0) = 1$
- $I_{xx} = \dfrac{1-c}{2} I_{yy},\ I_{zz} = \dfrac{1+c}{2} I_{yy}$

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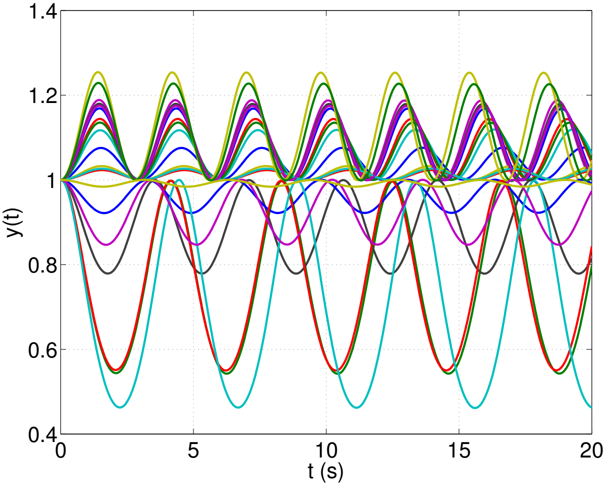
$$\begin{cases} \dot{x} = yz \\ \dot{y} = c \times xz \\ \dot{z} = -xy \end{cases}$$

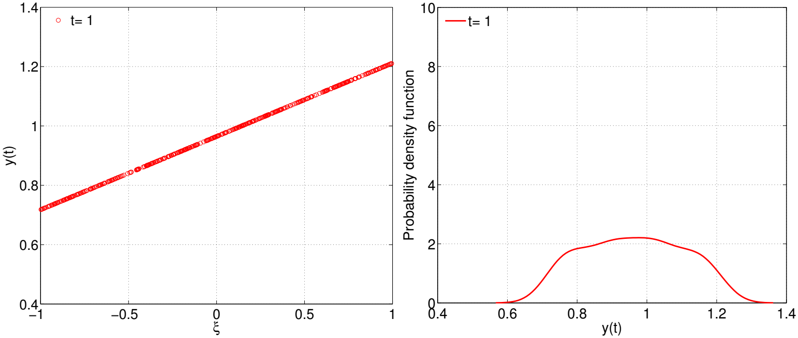
$$c = 0.1(7 \times \xi - 1);$$
$$\xi \sim \mathcal{U}(-1,1)$$

PCE for rigid body dynamics



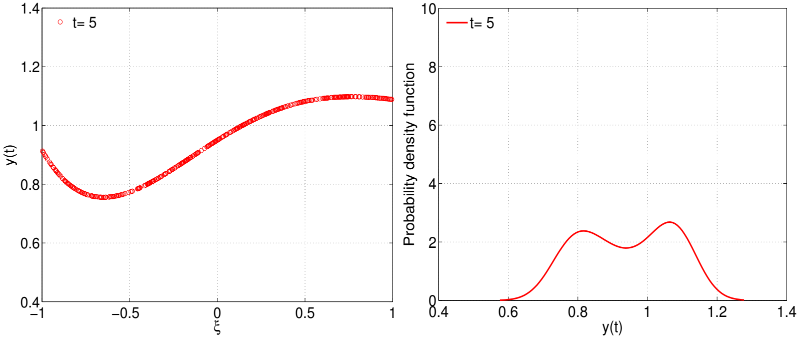
Distinct response trajectories in the original time t

PCE for rigid body dynamics



Input-output relationship in t and output's PDF

PCE for rigid body dynamics



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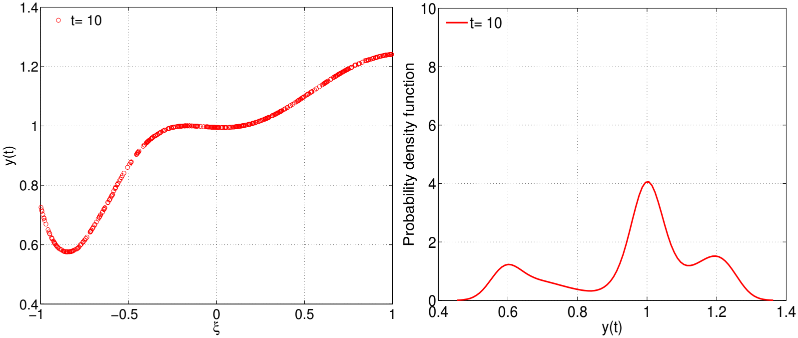

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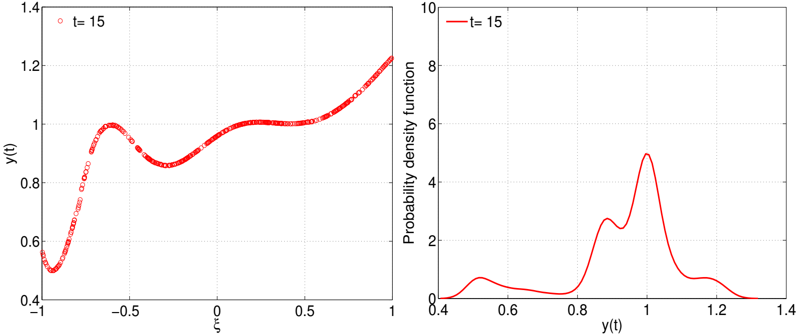

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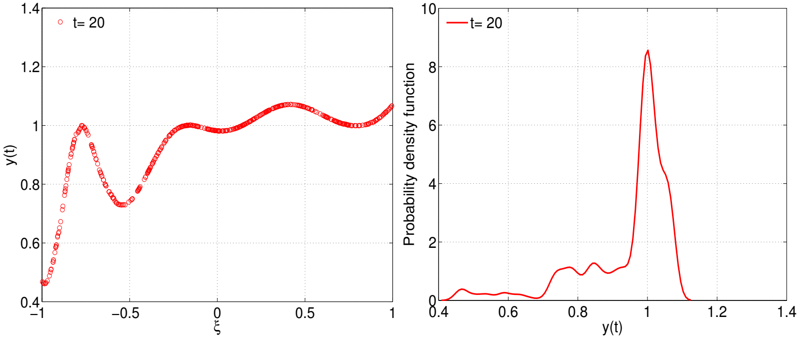

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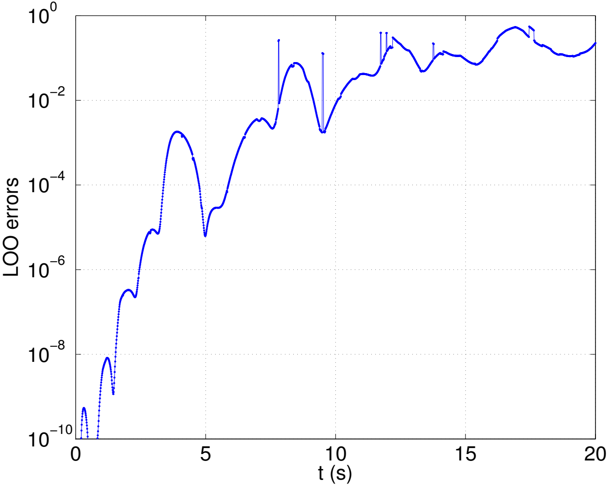
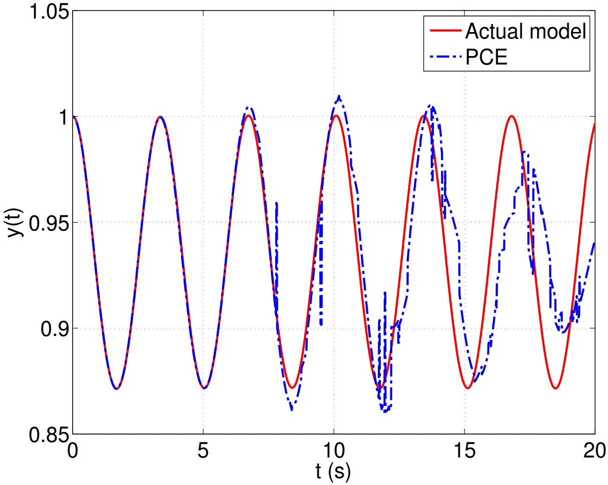
PCE prediction *vs.* actual response trajectory



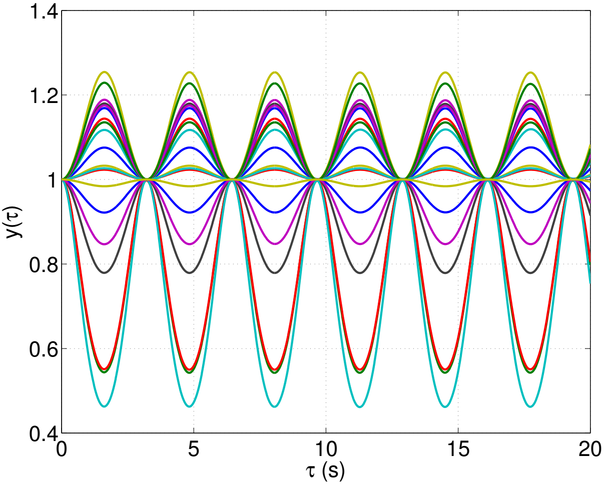
LOO errors *vs.* time t

PCE prediction *vs.* actual response trajectory



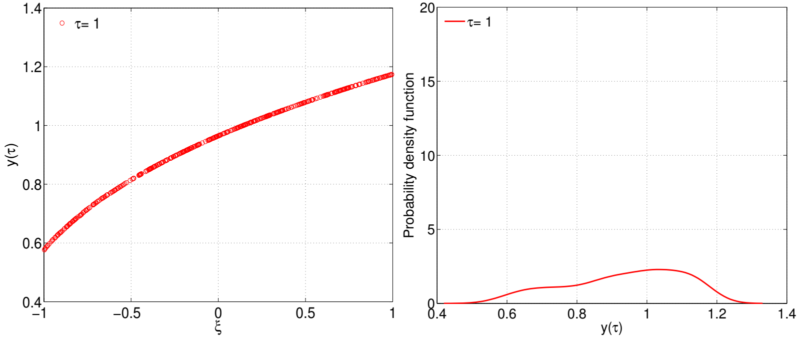
Frozen-in-time PCE *vs.* numerical model

PCE for rigid body dynamics



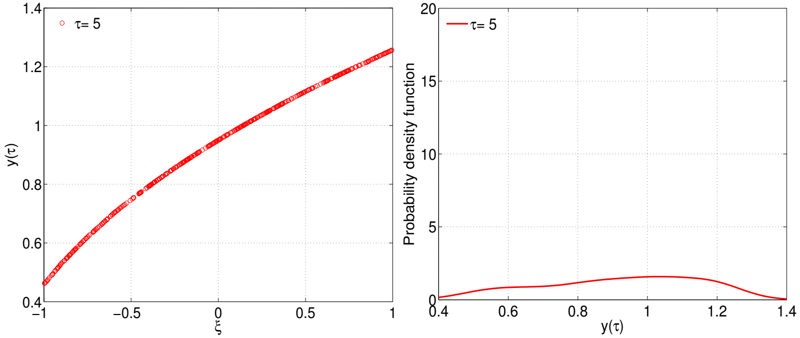
Distinct response trajectories in the time τ

PCE for rigid body dynamics



Input-output relationship in τ and output's PDF

PCE for rigid body dynamics



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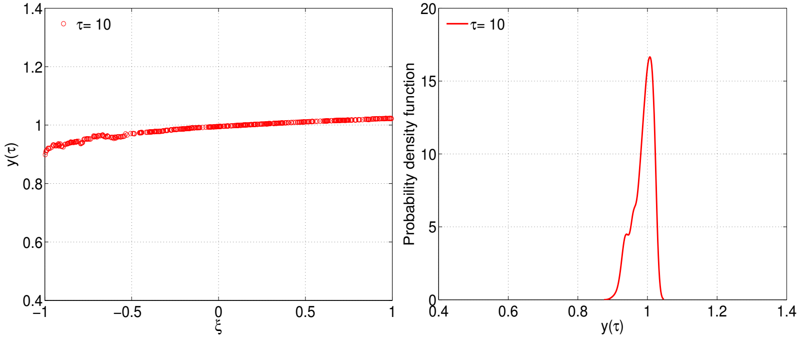

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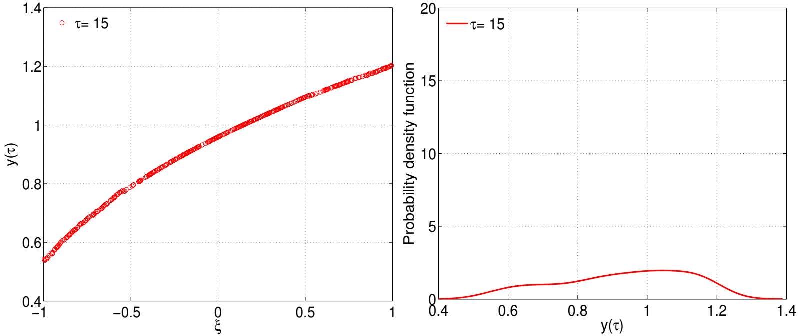

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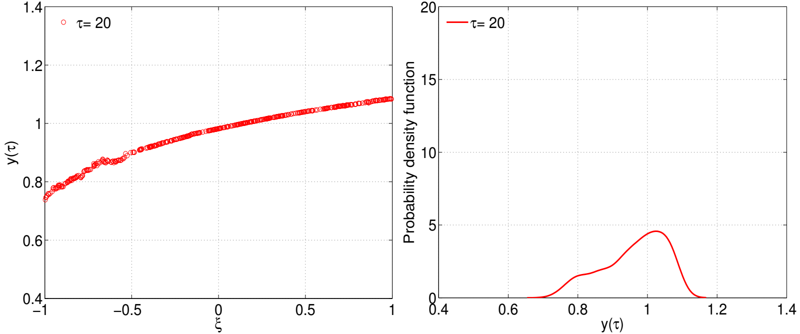
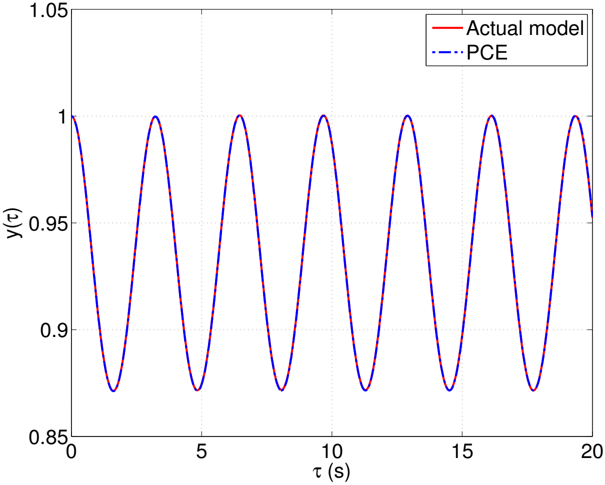


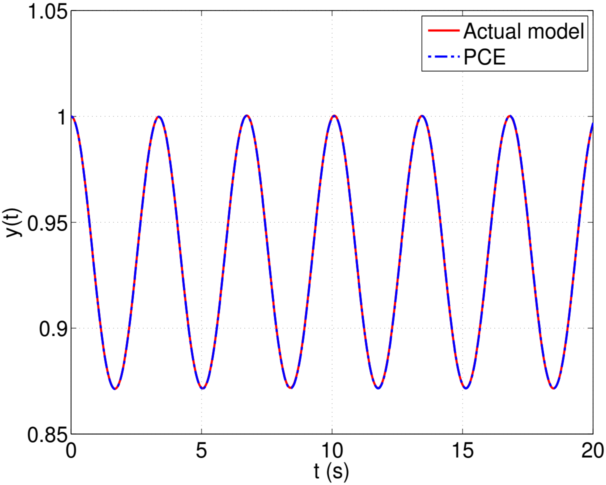
Input-output relationship in τ and output's PDF

PCE prediction *vs.* actual response trajectory



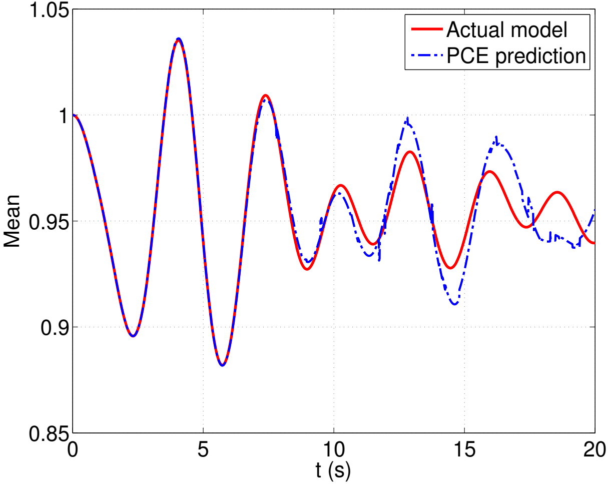
in the transformed time τ

PCE prediction *vs.* actual response trajectory



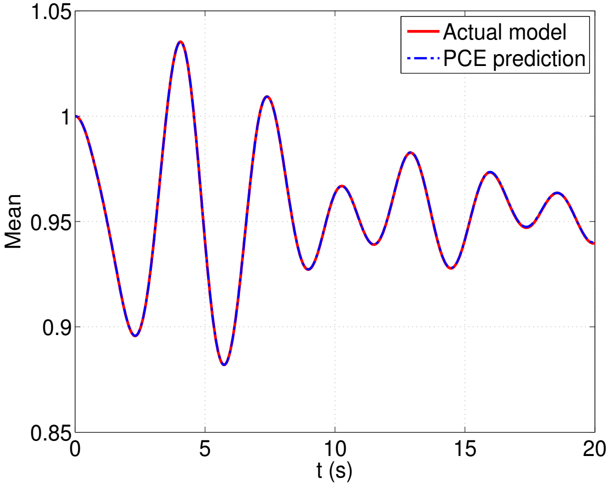
in the original time t

PCE *vs.* MCS



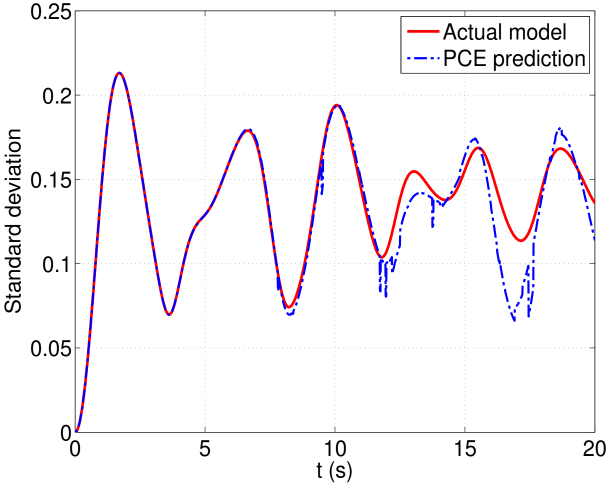
Frozen-in-time PCE *vs.* MCS (10000 runs)

PCE *vs.* MCS



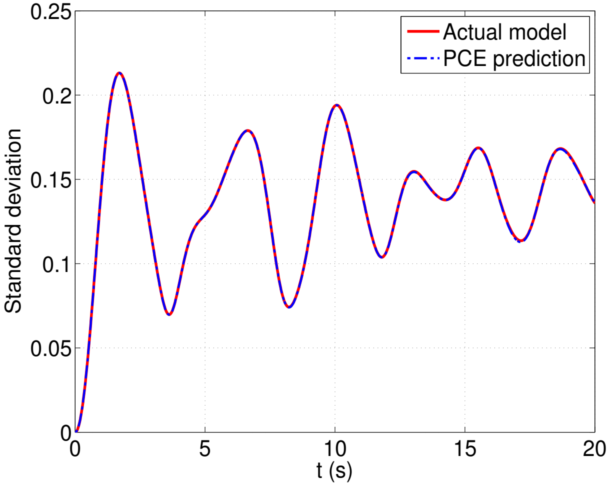
Time-transform PCE *vs.* MCS (10000 runs)

PCE *vs.* MCS



Frozen-in-time PCE *vs.* MCS (10000 runs)

PCE *vs.* MCS



Time-transform PCE *vs.* MCS (10000 runs)

Duffing oscillator

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Duffing oscillator

3d-pictures.picphotos.net

Non-linear SDOF Duffing oscillator:

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

where

- $\zeta = 0.05(1 + 0.05\xi_1), \quad \xi_1 \sim \mathcal{U}(-1, 1)$
- $\omega = 2\pi(1 + 0.2\xi_2), \quad \xi_2 \sim \mathcal{U}(-1, 1)$
- $\epsilon = -0.5(1 + 0.5\xi_3), \quad \xi_3 \sim \mathcal{U}(-1, 1)$
- $x(t = 0) = 1$ and $\dot{x}(t = 0) = 0$.

Duffing oscillator

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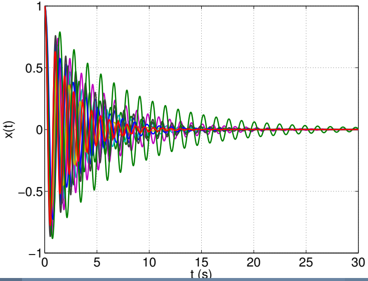
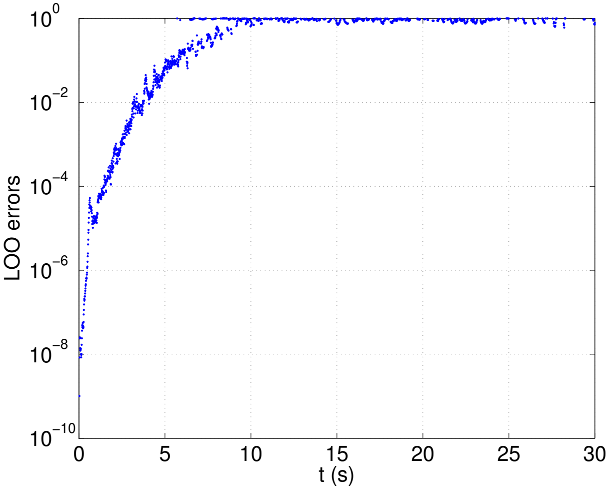
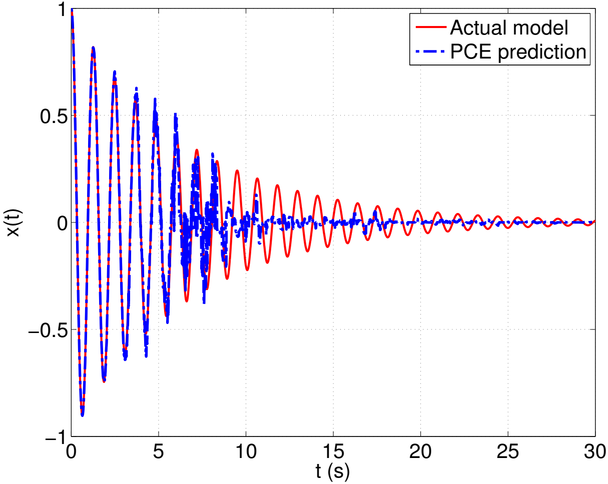


PCE for Duffing oscillator



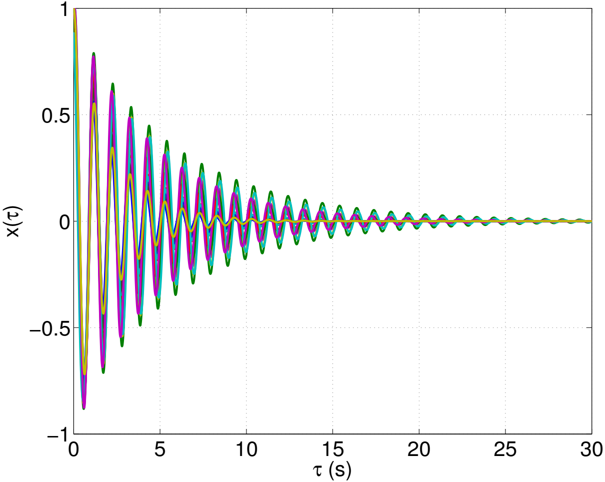
LOO errors *vs.* time

PCE for Duffing oscillator



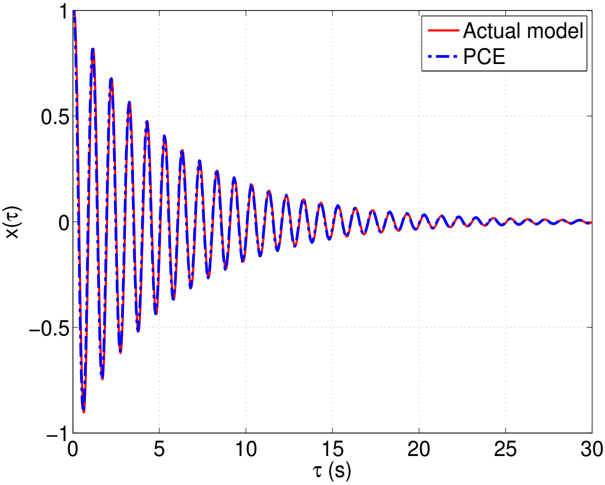
Frozen-in-time PCE *vs.* numerical model in time t

PCE for Duffing oscillator



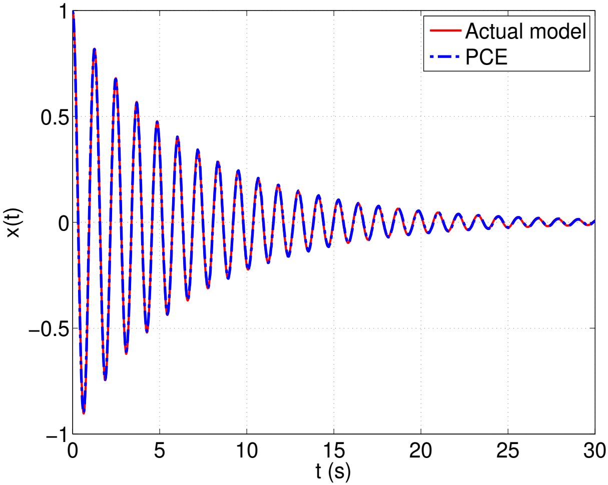
Distinct responses in the transformed time τ

PCE for Duffing oscillator



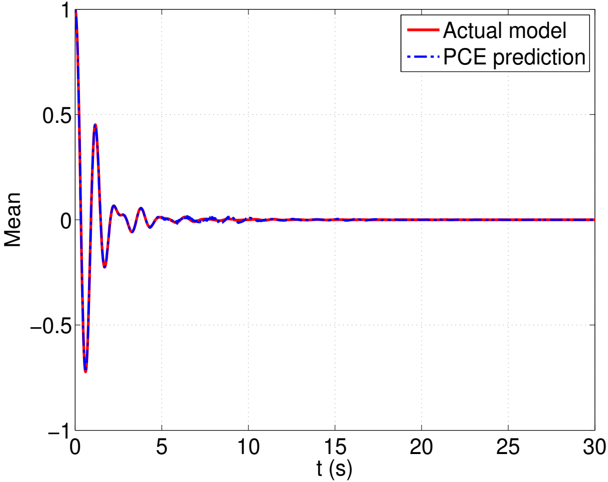
in time τ

PCE for Duffing oscillator



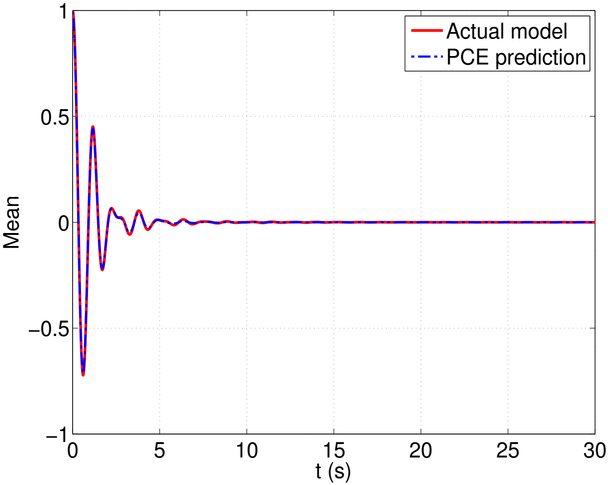
in time t

PCE *vs.* MCS



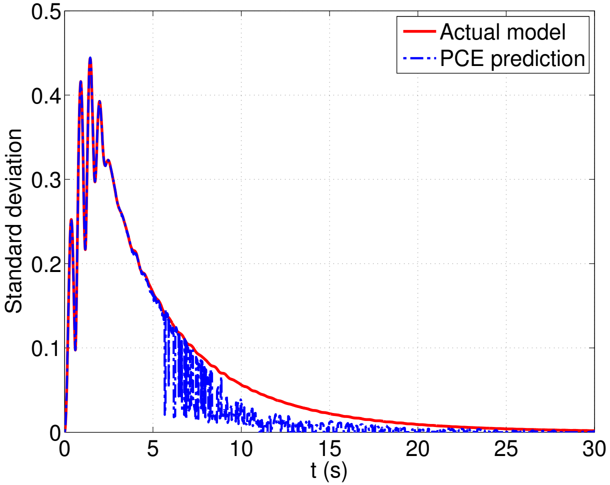
Frozen-in-time PCE *vs.* MCS (10000 runs)

PCE *vs.* MCS



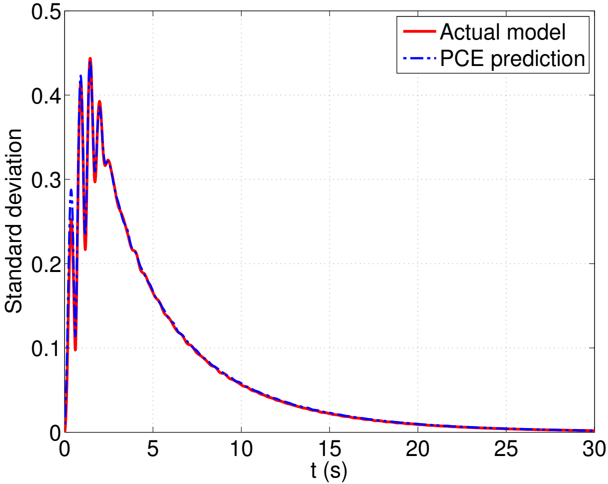
Time-transform PCE *vs.* MCS (10000 runs)

PCE *vs.* MCS



Frozen-in-time PCE *vs.* MCS (10000 runs)

PCE *vs.* MCS



Time-transform PCE *vs.* MCS (10000 runs)

Oregonator model

Le Maître, Mathelin, et al., 2010

The Oregonator model describes the dynamics of a well-stirred, homogeneous chemical system governed by a three species coupled mechanism:

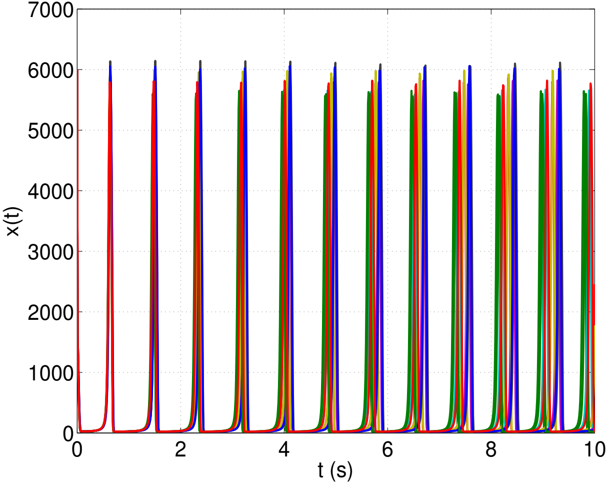
$$\begin{cases} \dot{x} = k_1\, y(t) - k_2\, x(t)\, y(t) + k_3\, x(t) - k_4\, x(t)^2 \\ \dot{y} = -k_1\, y(t) - k_2\, x(t)\, y(t) + k_5\, z(t) \\ \dot{z} = k_3\, x(t) - k_5\, z(t) \end{cases}$$

dreamstime.com

in which

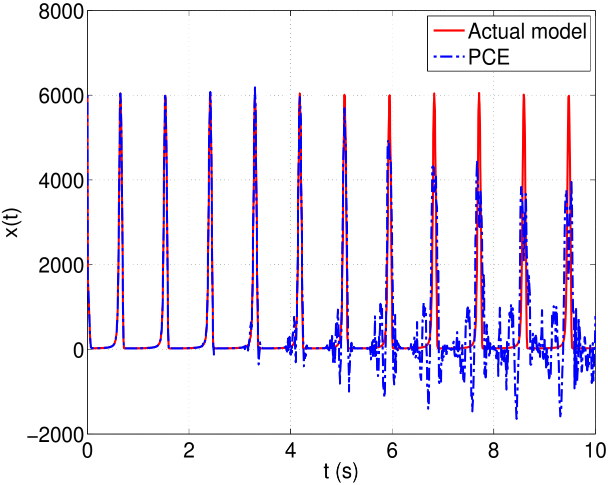
- (x, y, z) indicates the three species concentration
- the initial condition $(x_0, y_0, z_0) = (6000, 6000, 6000)$ corresponds to a deterministic mixture.
- $k_i,\ i = 1, \ldots, 5$ are the reaction parameters.
  - $k_1 = 2,\ k_2 = 0.1,\ k_3 = 104$
  - $k_4 = 0.008(1 + 0.05\xi_1), \qquad \xi_1 \sim \mathcal{U}(-1, 1)$
  - $k_5 = 26(1 + 0.1\xi_2), \qquad \xi_2 \sim \mathcal{U}(-1, 1)$

PCE for Oregonator model



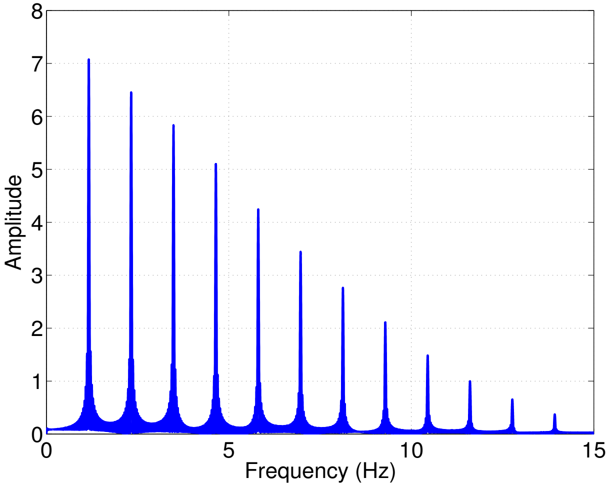
Responses in t

PCE for Oregonator model



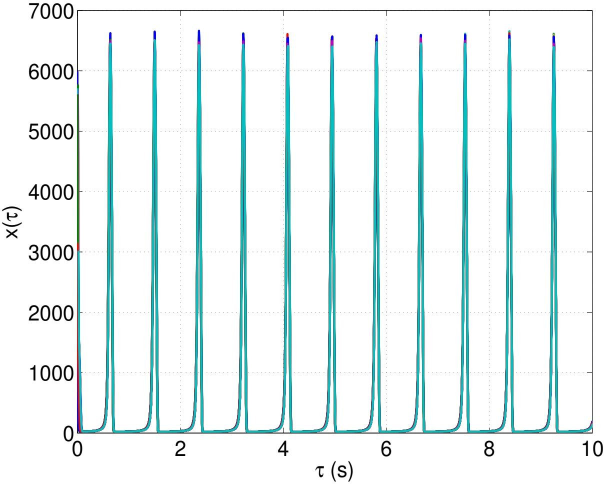
PCE prediction *vs.* actual response in t

PCE for Oregonator model



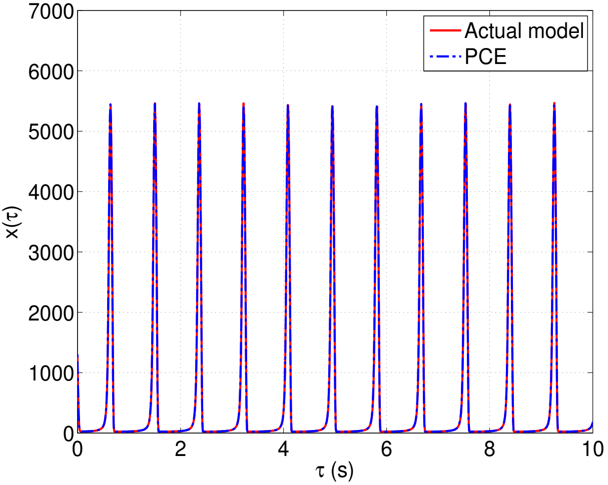
Amplitude spectrum of an output trajectory

PCE for Oregonator model



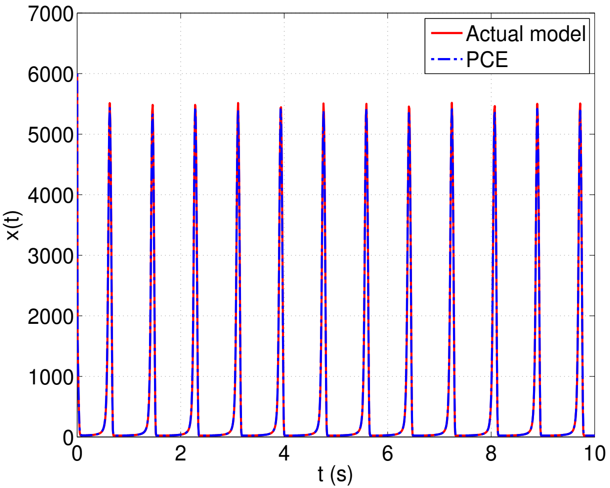
Responses in τ

PCE prediction *vs.* actual response trajectory



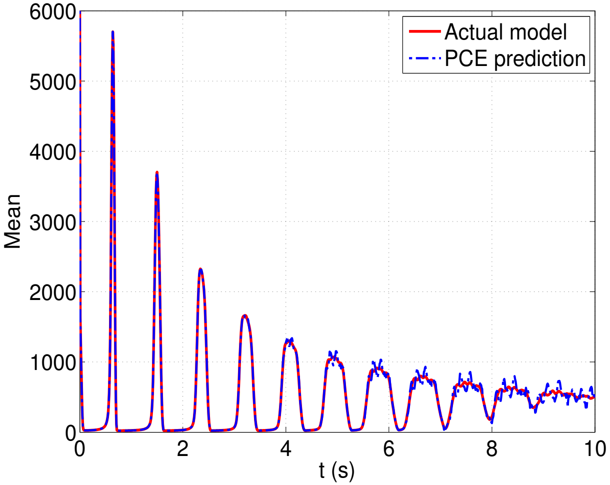
in the transformed time τ

PCE prediction *vs.* actual response trajectory



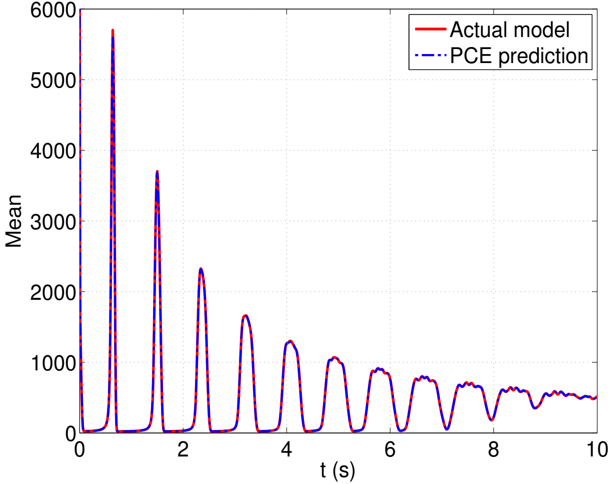
in the original time t

PCE *vs.* MCS



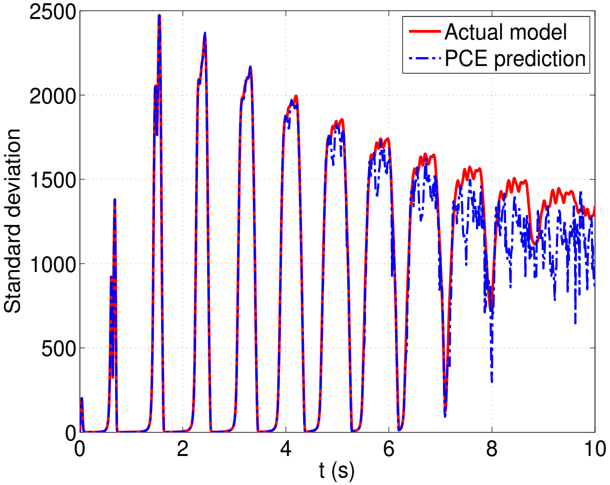
Frozen-in-time PCE *vs.* MCS (10000 runs)

PCE *vs.* MCS



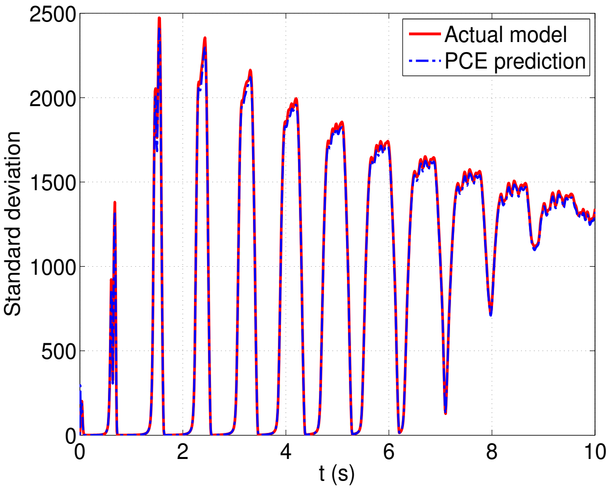
Time-transform PCE *vs.* MCS (10000 runs)

PCE *vs.* MCS



Frozen-in-time PCE *vs.* MCS (10000 runs)

PCE *vs.* MCS



Time-transform PCE *vs.* MCS (10000 runs)

Outline

Conclusions and perspective

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- Polynomial chaos expansions are facing challenging issues when modelling time-dependent systems.
- A non-intrusive stochastic time transform approach is proposed to solve the problems of non-linear oscillators.
- The approach is proved effective in some examples.

Perspective

- Further investigation is required to extend the approach to more complex problems involving output signals which are rich in the frequency content.

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Questions ?

Thank you very much for your attention !

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`http://www.rsuq.ethz.ch`

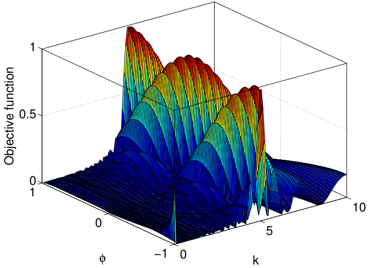
UQLAB ...

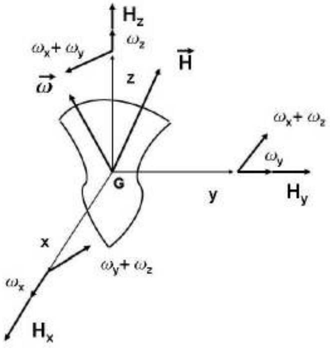
... The Uncertainty Quantification Laboratory

Backup slides

Optimization-based time transform

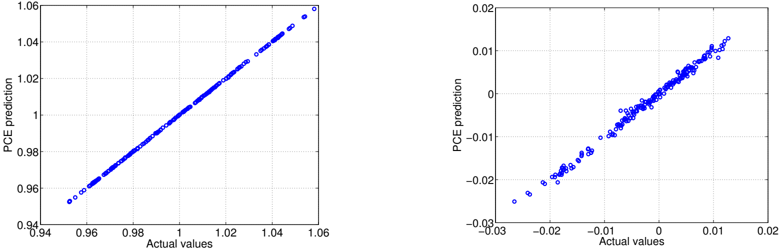
The constraint on the support of the parameters is adopted to ensure the uniqueness of the solution.





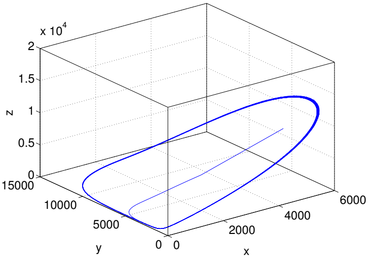
Rigid body dynamics

PCE for Oregonator model



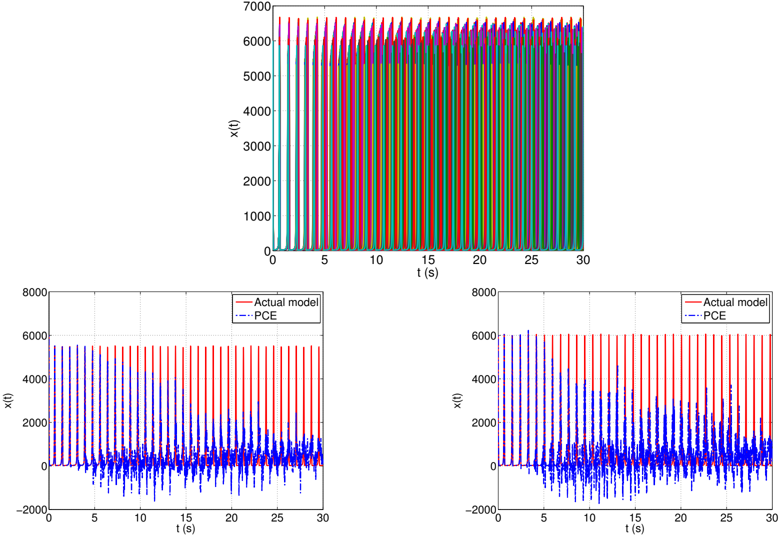
Prediction of k (left) and ϕ (right) by PCE *vs.* actual values

Oregonator model

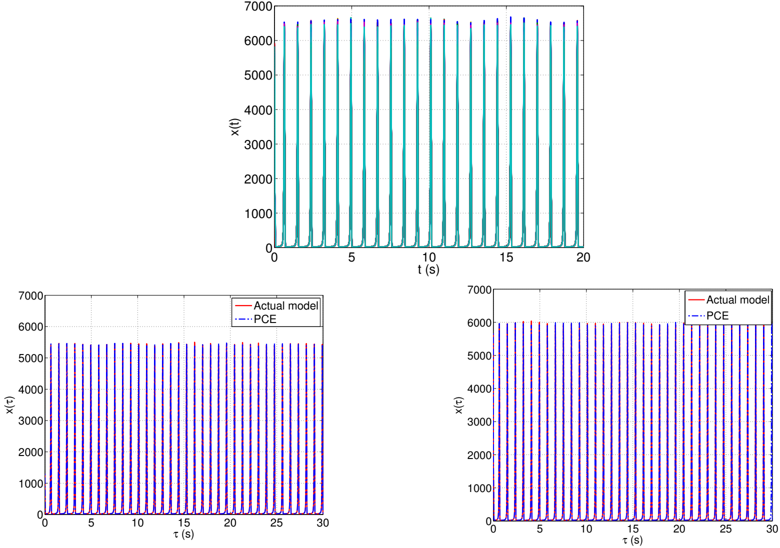


Limit cycle oscillation

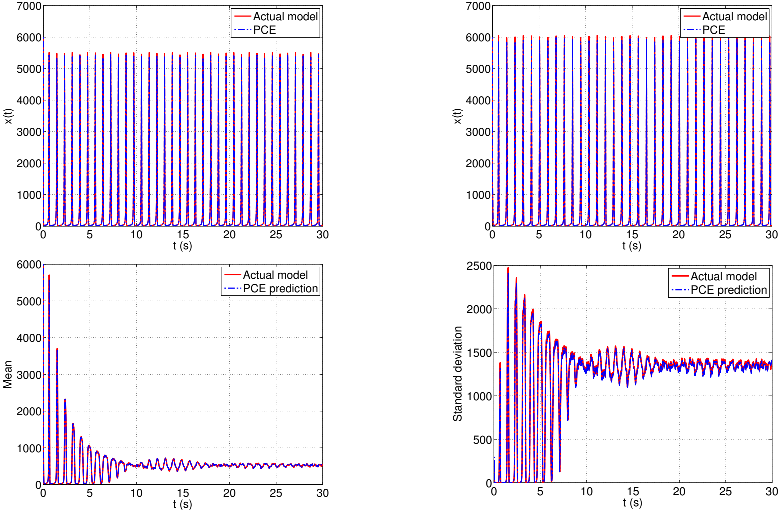
PCE for Oregonator model



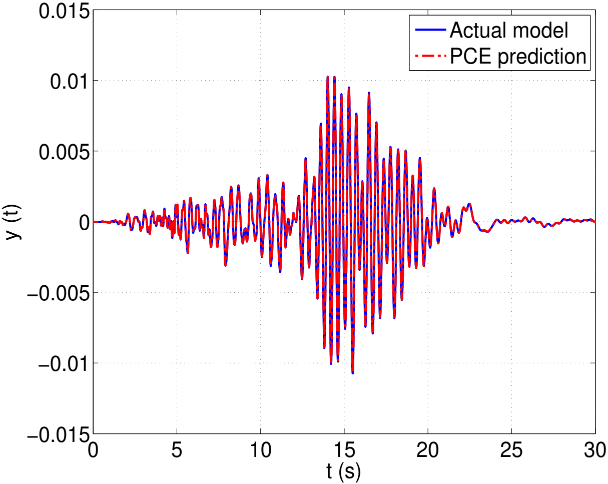
PCE for Oregonator model



PCE for Oregonator model



PCE for seismic analysis



First story displacement of a non-linear steel frame subject to random seismic excitation