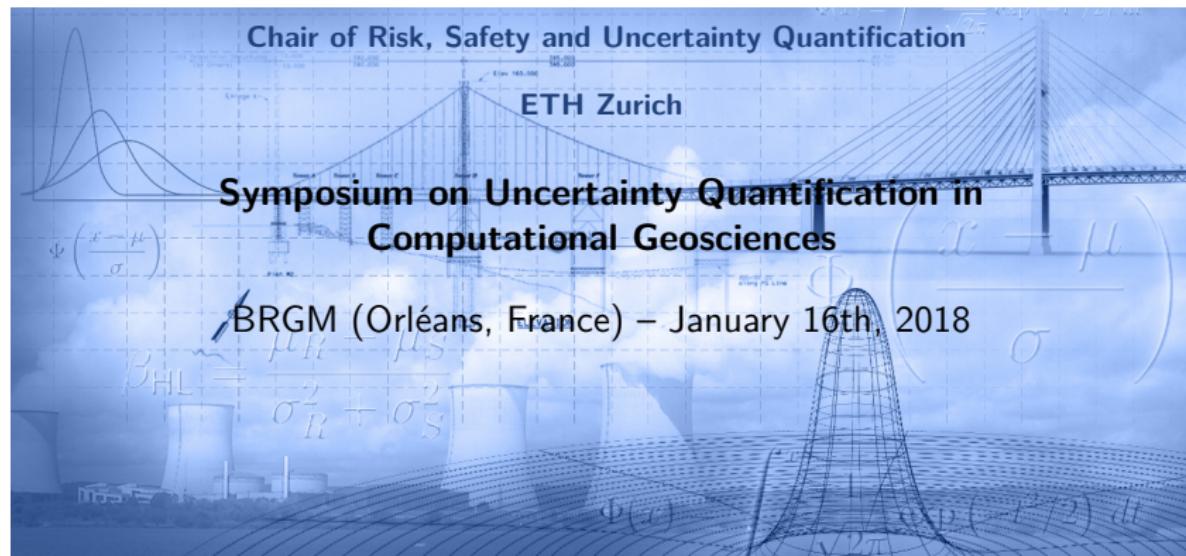


Surrogate models for uncertain dynamical systems: applications to earthquake engineering

Bruno Sudret



Chair of Risk, Safety and Uncertainty quantification

The Chair carries out research projects in the field of uncertainty quantification for engineering problems with applications in structural reliability, sensitivity analysis, model calibration and reliability-based design optimization

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- Structural reliability analysis
- Surrogate models (polynomial chaos expansions, Kriging, support vector machines)
- Bayesian model calibration and stochastic inverse problems
- Global sensitivity analysis
- Reliability-based design optimization



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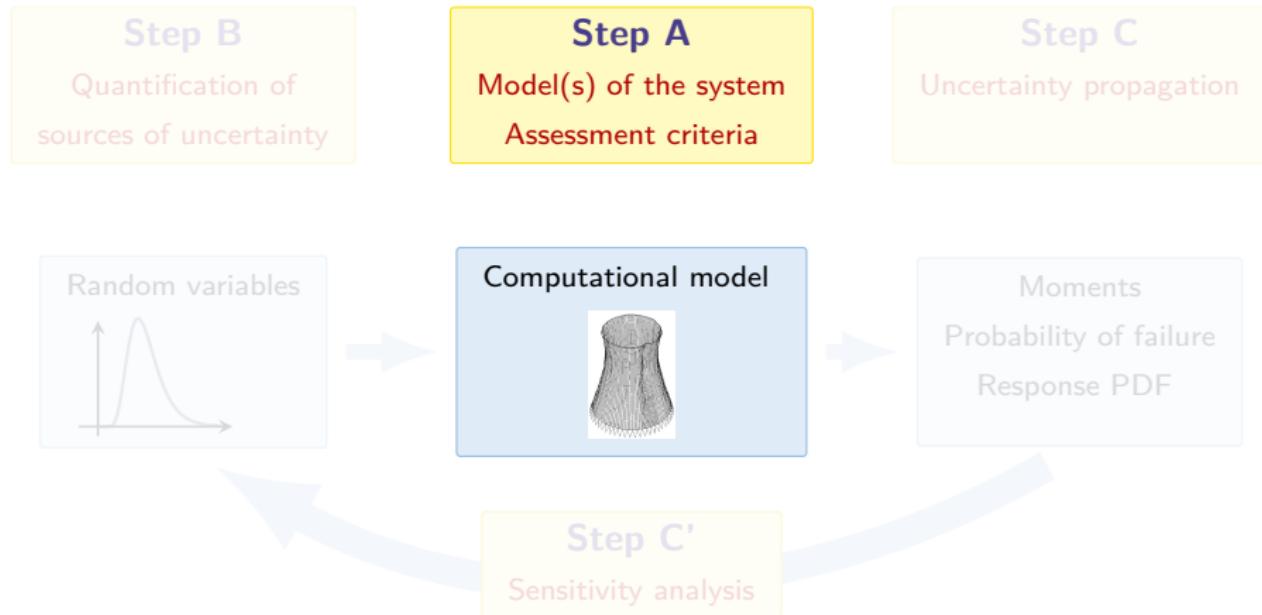
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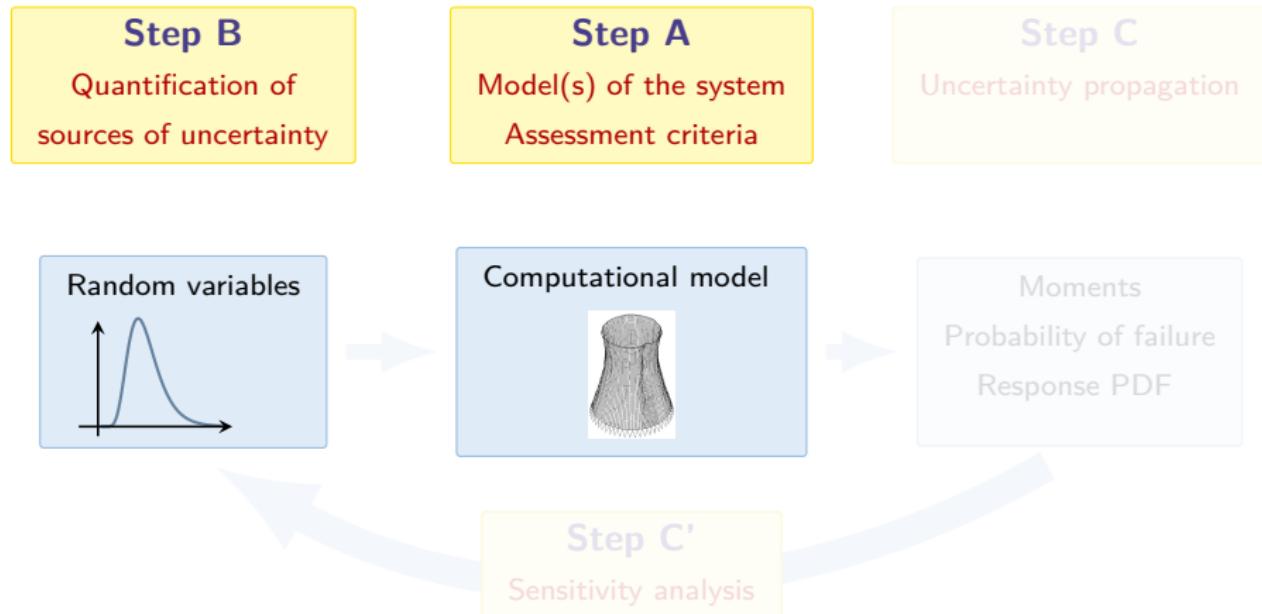
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Global framework for uncertainty quantification



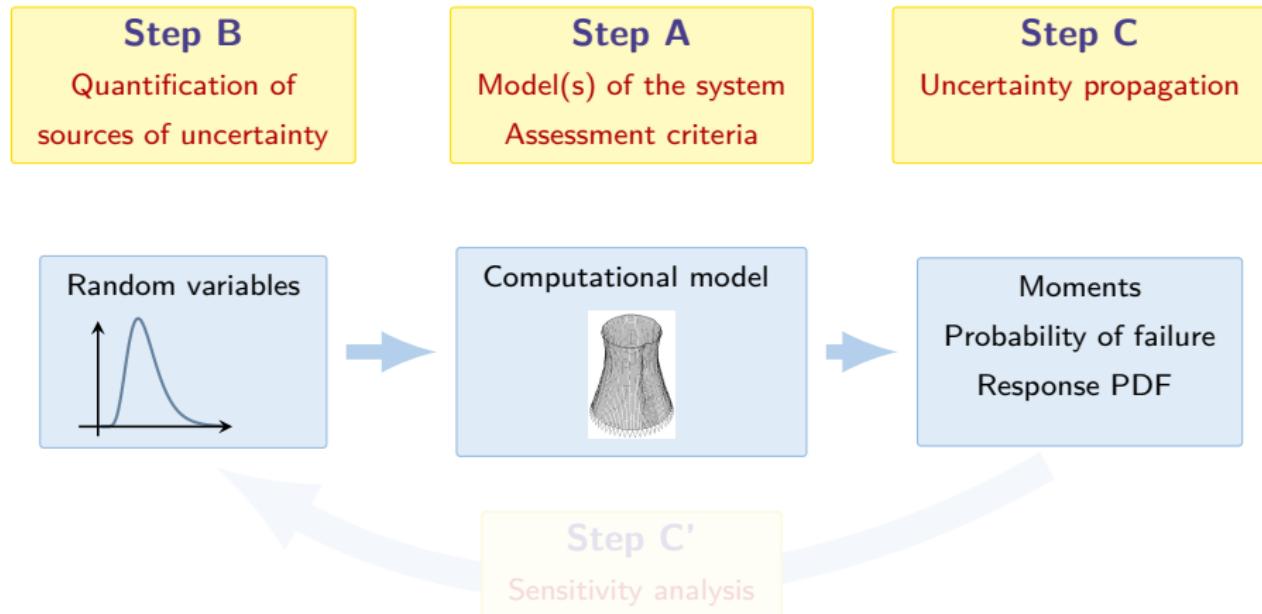
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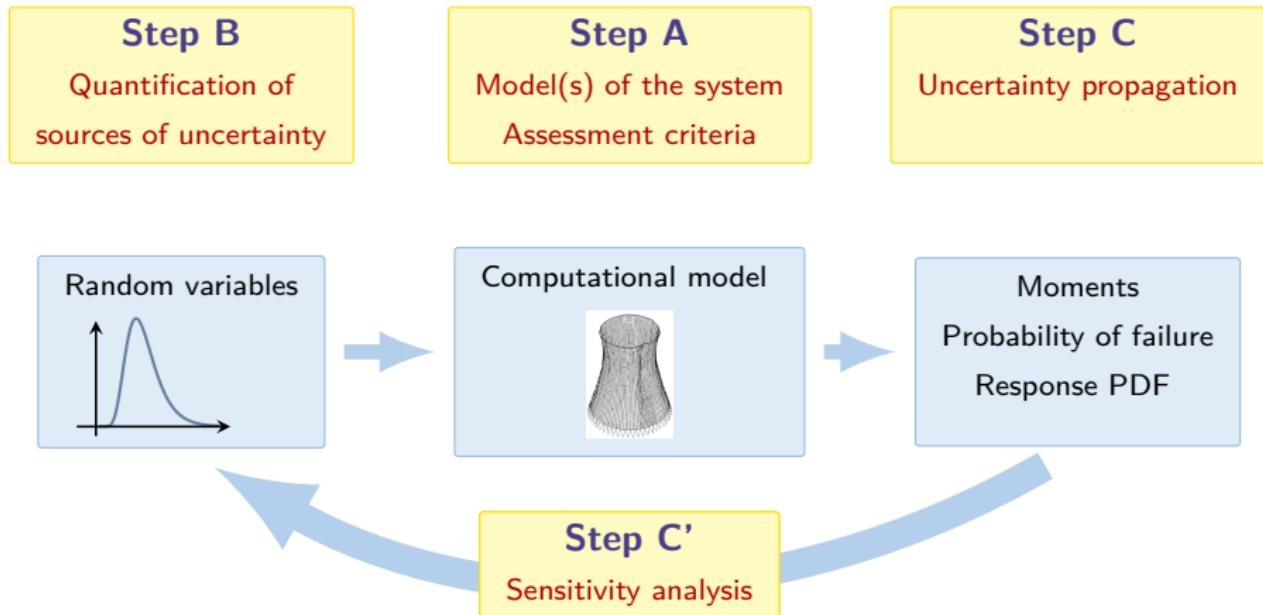
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Surrogate models for uncertainty quantification

A surrogate model $\tilde{\mathcal{M}}$ is an approximation of the original computational model \mathcal{M} with the following features:

- It is built from a limited set of runs of the original model \mathcal{M} called the experimental design $\mathcal{X} = \{x^{(i)}, i = 1, \dots, n\}$
- It assumes some regularity of the model \mathcal{M} and some general functional shape

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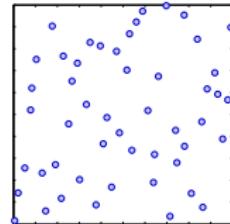
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Name	Shape	Parameters
Polynomial chaos expansions	$\tilde{\mathcal{M}}(\boldsymbol{x}) = \sum_{\alpha \in \mathcal{A}} a_\alpha \Psi_\alpha(\boldsymbol{x})$	a_α
Low-rank tensor approximations	$\tilde{\mathcal{M}}(\boldsymbol{x}) = \sum_{l=1}^R b_l \left(\prod_{i=1}^M v_l^{(i)}(x_i) \right)$	$b_l, z_{k,l}^{(i)}$
Kriging (a.k.a Gaussian processes)	$\tilde{\mathcal{M}}(\boldsymbol{x}) = \beta^\top \cdot \mathbf{f}(\boldsymbol{x}) + Z(\boldsymbol{x}, \omega)$	$\beta, \sigma_Z^2, \theta$
Support vector machines	$\tilde{\mathcal{M}}(\boldsymbol{x}) = \sum_{i=1}^n a_i K(\boldsymbol{x}_i, \boldsymbol{x}) + b$	a, b

Ingredients for building a surrogate model

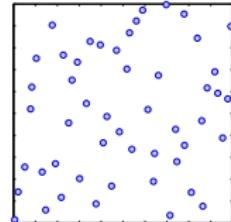
- Select an **experimental design** \mathcal{X} that covers at best the domain of input parameters: **Latin hypercube sampling (LHS)**, **low-discrepancy sequences**
- Run the **computational model** \mathcal{M} onto \mathcal{X} exactly as in **Monte Carlo simulation**
- Smartly post-process the data $\{\mathcal{X}, \mathcal{M}(\mathcal{X})\}$ through a **learning algorithm**



Name	Learning method
Polynomial chaos expansions	sparse grid integration, least-squares, compressive sensing
Low-rank tensor approximations	alternate least squares
Kriging	maximum likelihood, Bayesian inference
Support vector machines	quadratic programming

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Advantages of surrogate models

Usage

$$\mathcal{M}(\boldsymbol{x}) \approx \tilde{\mathcal{M}}(\boldsymbol{x})$$

hours per run seconds for 10^6 runs

Advantages

- Non-intrusive methods: based on runs of the computational model, exactly as in Monte Carlo simulation
- Construction suited to high performance computing: “embarrassingly parallel”

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Challenges

- Need for rigorous validation
- Communication: advanced mathematical background

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Efficiency: 2-3 orders of magnitude less runs compared to Monte Carlo

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① Introduction

② Polynomial chaos expansions

PCE in a nutshell

Why brute-force PCE fails in dynamics?

③ PC-NARX expansions

NARX model

Calibration of a PC-NARX model

Application to Bouc Wen model

④ Fragility curves

Theory

Application: steel frame

Polynomial chaos expansions in a nutshell

Ghanem & Spanos (1991); Xiu & Karniadakis (2002); Soize & Ghanem (2004); Lemaître & Knio (2010)

- Consider the input random vector \mathbf{X} ($\dim \mathbf{X} = M$) with given probability density function (PDF) $f_{\mathbf{X}}(\mathbf{x}) = \prod_{i=1}^M f_{X_i}(x_i)$
- Assuming that the random output $Y = \mathcal{M}(\mathbf{X})$ has finite variance, it can be cast as the following polynomial chaos expansion:

$$Y = \sum_{\alpha \in \mathbb{N}^M} y_{\alpha} \Psi_{\alpha}(\mathbf{X})$$

where :

- $\Psi_{\alpha}(\mathbf{X})$: basis functions
- y_{α} : coefficients to be computed (coordinates)
- The PCE basis $\{\Psi_{\alpha}(\mathbf{X}), \alpha \in \mathbb{N}^M\}$ is made of multivariate orthonormal polynomials

Computing the coefficients by least-square minimization

Isukapalli (1999); Berveiller, Sudret & Lemaire (2006)

Principle

The exact (infinite) series expansion is considered as the sum of a truncated series and a residual:

$$Y = \mathcal{M}(\mathbf{X}) = \sum_{\alpha \in \mathcal{A}} y_\alpha \Psi_\alpha(\mathbf{X}) + \varepsilon_P \equiv \mathbf{Y}^\top \boldsymbol{\Psi}(\mathbf{X}) + \varepsilon_P(\mathbf{X})$$

where : $\mathbf{Y} = \{y_\alpha, \alpha \in \mathcal{A}\} \equiv \{y_0, \dots, y_{P-1}\}$ (P unknown coef.)

$$\boldsymbol{\Psi}(\mathbf{x}) = \{\Psi_0(\mathbf{x}), \dots, \Psi_{P-1}(\mathbf{x})\}$$

Least-square minimization

The unknown coefficients are estimated by minimizing the mean square residual error:

$$\hat{\mathbf{Y}} = \arg \min \mathbb{E} \left[(\mathbf{Y}^\top \boldsymbol{\Psi}(\mathbf{X}) - \mathcal{M}(\mathbf{X}))^2 \right]$$

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Discrete (ordinary) least-square minimization

An estimate of the mean square error (sample average) is minimized:

$$\hat{\mathbf{Y}} = \arg \min_{\mathbf{Y} \in \mathbb{R}^P} \frac{1}{n} \sum_{i=1}^n (\mathbf{Y}^\top \Psi(\mathbf{x}^{(i)}) - \mathcal{M}(\mathbf{x}^{(i)}))^2$$

Procedure

- Select a truncation scheme, e.g. $\mathcal{A}^{M,p} = \{\boldsymbol{\alpha} \in \mathbb{N}^M : |\boldsymbol{\alpha}|_1 \leq p\}$
- Select an experimental design and evaluate the model response

$$\mathbf{M} = \{\mathcal{M}(\mathbf{x}^{(1)}), \dots, \mathcal{M}(\mathbf{x}^{(n)})\}^\top$$

- Compute the experimental matrix

$$\mathbf{A}_{ij} = \Psi_j(\mathbf{x}^{(i)}) \quad i = 1, \dots, n ; j = 0, \dots, P-1$$

- Solve the resulting linear system

$$\hat{\mathbf{Y}} = (\mathbf{A}^\top \mathbf{A})^{-1} \mathbf{A}^\top \mathbf{M}$$

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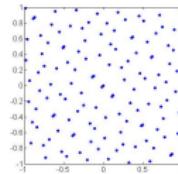
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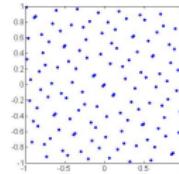
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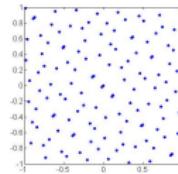
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Simple is beautiful !

Error estimators

- In least-squares analysis, the generalization error is defined as:

$$E_{gen} = \mathbb{E} \left[(\mathcal{M}(\mathbf{X}) - \mathcal{M}^{PC}(\mathbf{X}))^2 \right] \quad \mathcal{M}^{PC}(\mathbf{X}) = \sum_{\alpha \in \mathcal{A}} y_{\alpha} \Psi_{\alpha}(\mathbf{X})$$

- The empirical error based on the experimental design \mathcal{X} is a poor estimator in case of overfitting

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Leave-one-out cross validation

- From statistical learning theory, model validation shall be carried out using independent data

$$E_{LOO} = \frac{1}{n} \sum_{i=1}^n \left(\frac{\mathcal{M}(\mathbf{x}^{(i)}) - \mathcal{M}^{PC}(\mathbf{x}^{(i)})}{1 - h_i} \right)^2$$

where h_i is the i -th diagonal term of matrix $\mathbf{A}(\mathbf{A}^\top \mathbf{A})^{-1} \mathbf{A}^\top$

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- ③ PC-NARX expansions
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Why brute-force PCE fails in dynamics?

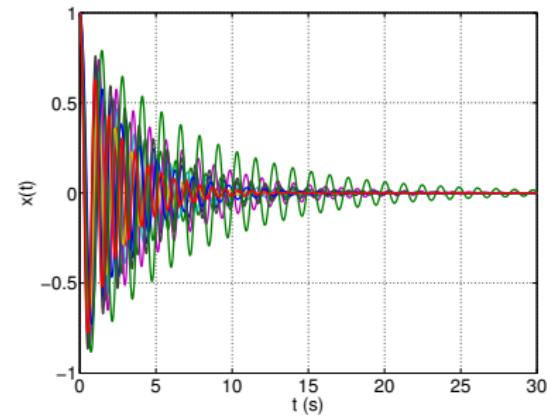
Non-linear SDOF Duffing oscillator

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

Initial conditions: $x(0) = 1, \quad \dot{x}(0) = 0$

Input: 3 uniform random variables

RV	Distribution	Values
ζ	Uniform	$\mathcal{U}[0.015, 0.045]$
ω	Uniform	$\mathcal{U}[\pi, 3\pi]$
ε	Uniform	$\mathcal{U}[-0.25, -0.75]$



Samples of trajectories

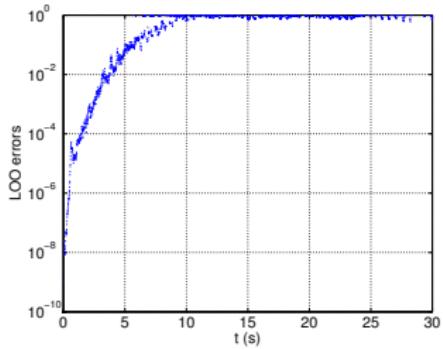
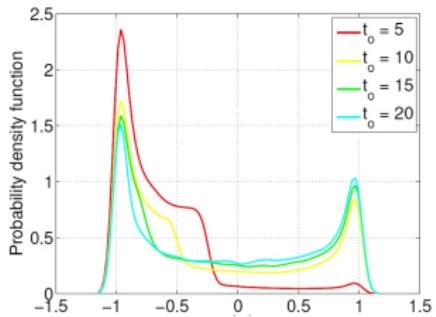
Time-frozen PCE

$$(\zeta, \omega, \varepsilon) = (0.03, 8.92, -0.34)$$

$$(\zeta, \omega, \varepsilon) = (0.04, 3.18, -0.33))$$

Why time-frozen PCE does not work?

- The map $\xi \mapsto \mathcal{M}(\xi, t)$ becomes increasingly non linear with time
- The time-frozen distribution of the output at time t_0 becomes more complex (e.g. multimodal)
- Expansions of higher degree would be required to keep sufficient accuracy with time
- For a fixed experimental design, the LOO error blows up



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Some literature

- Multi-elements PCEs: decomposition of the random space into non-overlapping sub-elements Wan & Karniadakis, 2005
- Constant phase interpolation: responses interpolated in the phase space Witteveen & Bijl, 2008
- Asynchronous time integration: intrusive transformed time variable introduced to reduce variability Le Maître et al., 2010
- Time-dependent PCEs: new random variables added on-the-fly Gerritsma et al., 2010
- PC flow map composition: long-term response obtained by composing intermediate PCE-based flow maps Luchtenburg et al., 2014
- PC-NARX: future state determined by current and past states Spiridonakos & Chatzi, 2015

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Nonlinear AutoRegressive with eXogenous input model

NARX model

Billings, 2013

Based on a time-dependent input excitation $x(t)$ and corresponding system response $y(t)$, the dynamics is captured through:

$$y(t) = \mathcal{F}(x(t), \dots, x(t - n_x), y(t - 1), \dots, y(t - n_y)) + \varepsilon_t$$

where:

- $\mathbf{z}(t) = (x(\textcolor{red}{t}), \dots, x(t - n_x), y(\textcolor{red}{t - 1}), \dots, y(t - n_y))^T$ is the vector of current and past values
- n_x and n_y denote the maximum input and output time lags
- $\varepsilon_t \sim \mathcal{N}(0, \sigma_\varepsilon^2(t))$ is the residual error
- $\mathcal{F}(\cdot)$ is a functional of NARX terms, usually linear-in-parameters:

$$y(t) = \sum_{i=1}^{n_g} \vartheta_i g_i(\mathbf{z}(t)) + \varepsilon_t$$

PC-NARX model

Spiridonakos *et al.*, 2015a, 2015b

Computational model with uncertainties

$$y(t, \xi_x, \xi_s) \stackrel{\text{def}}{=} \mathcal{M}(x(t, \xi_x), \xi_s)$$

- ξ_x : uncertainty in the input excitation
- ξ_s : uncertainty in the system

PC-NARX expansion

$$y(t, \xi) = \sum_{i=1}^{n_g} \vartheta_i(\xi) g_i(z(t)) + \varepsilon_g(t, \xi) \quad \xi = (\xi_x, \xi_s)$$

The NARX stochastic coefficients $\vartheta_i(\xi)$ are represented by PCEs:

$$\vartheta_i(\xi) = \sum_{\alpha \in \mathcal{A}_i} \vartheta_{i,\alpha} \psi_\alpha(\xi)$$

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Interpretation

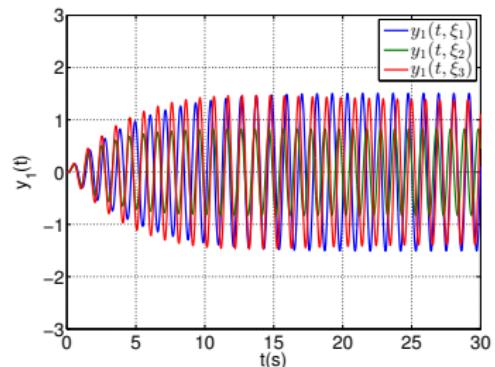
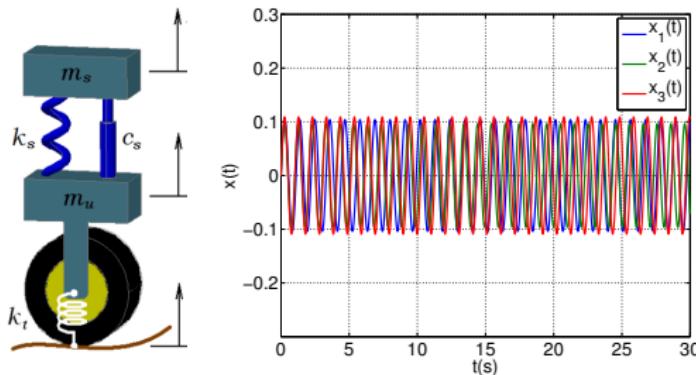
- PC-NARX is a NARX model in which each (random) coefficient is expanded as a PCE
- Compared to time-frozen PCE, a specific dynamics of the random coefficients is imposed
- Similar to flow map composition since the response at current instant is used to predict the response at future instants

Experimental design

Data

- N realizations of the input excitation, cast as $(x_k[1], \dots, x_k[T])^T$, $k = 1, \dots, N$ (T time instants)
- The corresponding system response computed by a simulator, cast as $(y_k[1], \dots, y_k[T])^T$

Example: quarter car model



Deterministic NARX calibration

For a particular realization ξ_k

- Select NARX model (candidate terms):

$$\begin{aligned} z(t) &= (x(t), \dots, x(t - n_x), y(t-1), \dots, y(t - n_y))^T \\ \phi(t) &= \{g_i(z(t)), i = 1, \dots, n_g\}^T \end{aligned}$$

- Use least angle regression ([LARS](#)) to select the best explanatory subset of terms
- Compute the coefficients ϑ_k by ordinary least-squares

Efron et al. , 2004

Prediction error (of model $\#k$ on trajectory l)

$$\varepsilon_l^{\#k} = \frac{\sum_{t=1}^T (y(t, \xi_l) - \hat{y}^{\#k}(t, \xi_l))^2}{\sum_{t=1}^T (y(t, \xi_l) - \bar{y}(t, \xi_l))^2}$$

Common NARX basis

Premise

To expand the NARX coefficients onto a PC basis, it is necessary to have a common NARX model for all trajectories

Procedure

- Select $K \leq N$ trajectories ("NARX learning set"), e.g. with the strongest non linear behaviour (peak displacement, velocities, etc.)
- Determine the sparse deterministic NARX models for realizations $k = 1, \dots, K$, which leads to $P \leq K$ different possible models called $\#1, \dots, \#P$
- Compute the NARX coefficients of the N trajectories, for each model $\#p$, and evaluate an average error:

$$\varepsilon_p = \frac{1}{N} \sum_{k=1}^N \varepsilon_k^{\#p}$$

- Select the final best NARX model that minimizes ε_p

PCE of the NARX coefficients

PCE calibration

- Once a common NARX basis has been found, N realizations of the NARX coefficients are available:

$$\mathcal{ED} = \{\vartheta_{i,k}, i = 1, \dots, n_g; k = 1, \dots, N\}$$

- n_g different sparse PC expansions are built from this experimental design, using least-angle regression (LAR)

Blatman & Sudret, 2011

$$\vartheta_i(\boldsymbol{\xi}) = \sum_{\alpha \in \mathcal{A}_i} \vartheta_{i,\alpha} \psi_\alpha(\boldsymbol{\xi})$$

PC-NARX prediction

- For a new realization of the input parameters $\boldsymbol{\xi}_0$, the NARX coefficients are first evaluated from PCEs
- Then they are plugged into the NARX model

Bouc-Wen model

Governing equations

Kafali & Grigoriu (2007), Spiridonakos & Chatzi (2015)

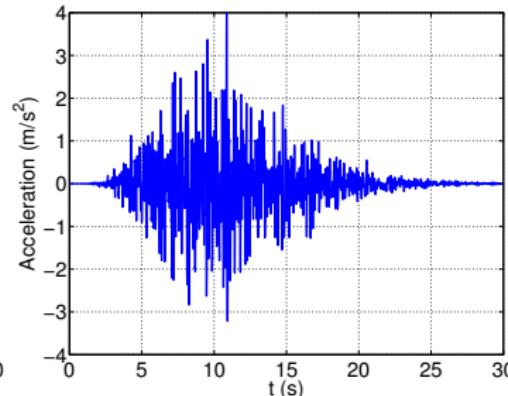
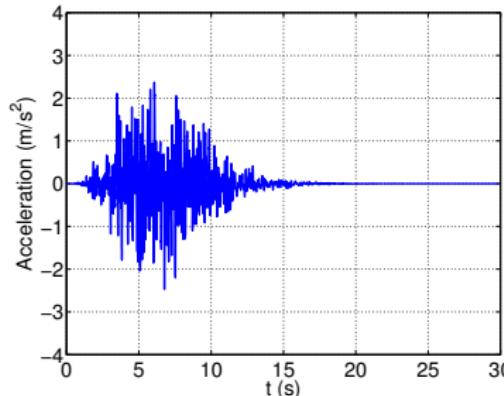
$$\begin{aligned}\ddot{y}(t) + 2\zeta\omega\dot{y}(t) + \omega^2(\rho y(t) + (1 - \rho)z(t)) &= -x(t), \\ \dot{z}(t) &= \gamma\dot{y}(t) - \alpha |\dot{y}(t)| |z(t)|^{n-1} z(t) - \beta \dot{y}(t) |z(t)|^n,\end{aligned}$$

Excitation

$x(t)$ is generated by a probabilistic ground motion model

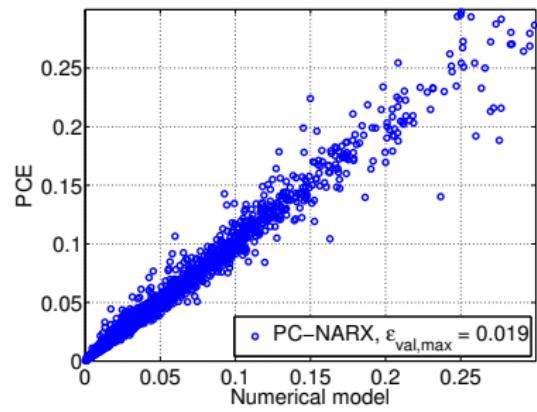
Rezaeian & Der Kiureghian (2010)

$$x(t) = q(t, \boldsymbol{\alpha}) \sum_{i=1} s_i(t, \boldsymbol{\lambda}(t_i)) U_i$$

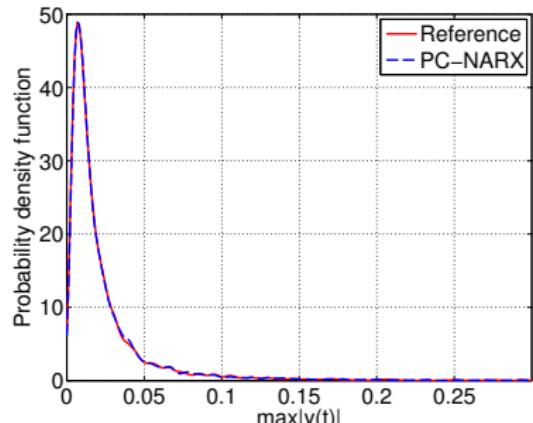


Bouc-Wen model: prediction

Bouc-Wen model: prediction



Maximal displacements



PDF of maximal displacements

Outline

- ① Introduction
- ② Polynomial chaos expansions
- ③ PC-NARX expansions
- ④ Fragility curves
 - Theory
 - Application: steel frame

Introduction to fragility curves



- Earthquake engineering aims at assessing the performance of structures and infrastructures w.r.t recorded or potential quakes
- Due to uncertainties in the localization, magnitude, structural behaviour and resistance, etc. **probabilistic approaches** are commonly used

Fragility curves

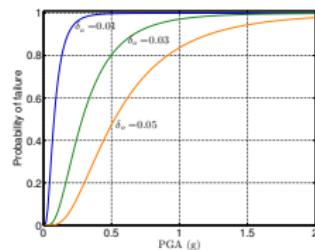
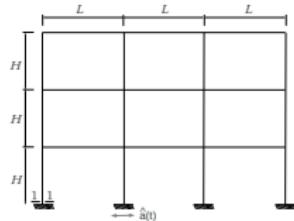
For a given performance criterion $g \leq g_{adm}$, the fragility curve represents the **conditional probability of failure given an intensity measure IM** :

$$\text{Frag}(IM; g_{adm}) = \mathbb{P}(g \geq g_{adm} | IM)$$

Example

- $g = \max_k \max_{t_i \in [0, T]} |\delta_{t_i}^k|$ (k -th interstorey drift)
- IM : peak ground acceleration (PGA), pseudo-spectral acceleration (PSa), cumulative absolute velocity (CAV), etc.

Fragility curves



Classical approach

- Select a set of ground motions (recorded / synthetic)
- Compute the transient structural response (finite element analysis)
- Assume a **parametric** shape for the fragility curve, e.g. a **lognormal shape**:

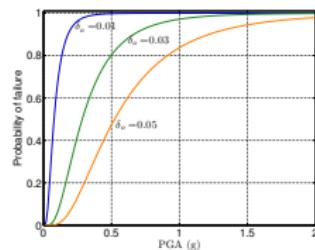
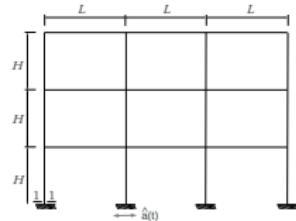
$$\text{Frag}(IM; \delta_o) = \mathbb{P}(\Delta \geq \delta_o | IM) = \Phi\left(\frac{\log IM - \alpha}{\beta}\right)$$

- Fit the parameters (α, β) form data

Limitations

- Predefined shape of the curve
- Subject to epistemic uncertainties when the number of ground motions is small

Fragility curves



Classical approach

- Select a set of ground motions (recorded / synthetic)
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New proposal

- Use **non parametric statistics** for the fragility curves
- Use **surrogate models** of the transient analysis based on polynomial chaos expansions

Parametric methods

Linear regression (LR)

Ellingwood (2001)

- Probabilistic demand model:

$$\log \Delta = A \log IM + B + \zeta Z \quad Z \sim \mathcal{N}(0, 1)$$

- A and B determined by ordinary least squares estimation in a log-log scale
- Results in a lognormal-like fragility curve:

$$\begin{aligned} \widehat{\text{Frag}}(IM; \delta_o) &= \mathbb{P} [\log \Delta \geq \log \delta_o] = 1 - \mathbb{P} [\log \Delta \leq \log \delta_o] \\ &= \Phi \left(\frac{\log IM - (\log \delta_o - B) / A}{\zeta / A} \right). \end{aligned}$$

Maximum likelihood estimation (ML)

Shinozuka et al. (2000)

- Lognormal shape:

$$\widehat{\text{Frag}}(IM; \delta_o) = \Phi \left(\frac{\log IM - \log \alpha}{\beta} \right)$$

- Estimation of α and β by maximum likelihood for each δ_o :

$$\mathcal{L}(\alpha, \beta, \{IM_i\}_{i=1}^N) = \prod_{IM_i: \Delta_i \geq \delta_o} \left[\widehat{\text{Frag}}(IM_i; \delta_o) \right] \prod_{IM_i: \Delta_i < \delta_o} \left[1 - \widehat{\text{Frag}}(IM_i; \delta_o) \right]$$

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Non parametric methods

Binned Monte Carlo estimate

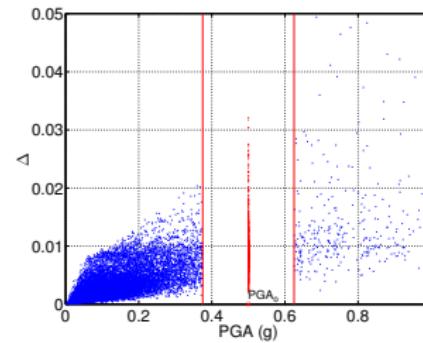
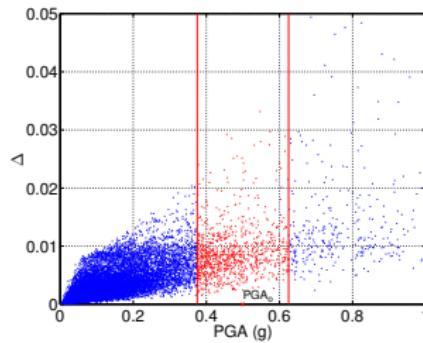
Mai, Konakli & Sudret, Frontiers Struct. Civ. Eng., (2017)

- Suppose N_s analyses are available for $IM = IM_o$, with N_f such that $\Delta \geq \delta_o$. The fragility curve in this point could be estimated by Monte Carlo simulation:

$$\widehat{\text{Frag}}(IM_o) = \frac{N_f (IM_o)}{N_s (IM_o)}$$

- From the data cloud, a bin centered on IM_o is considered, and points within the beam are “projected” onto the vertical line $IM = IM_o$ by linearization

$$\widetilde{\Delta}_j(IM_o) = \Delta_j \frac{IM_o}{IM_j}.$$



Kernel density estimation

Fragility curves as a conditional CCDF

Mai et al., Frontiers Struct. Civ. Eng., (2017)

$$\text{Frag}(a; \delta_o) = \mathbb{P}(\Delta \geq \delta_o | IM = a) = \int_{\delta_o}^{+\infty} f_\Delta(\delta | IM = a) d\delta$$

where:

$$f_\Delta(\delta | IM = a) = \frac{f_{\Delta, IM}(\delta, a)}{f_{IM}(a)}$$

Kernel density estimation

- The joint- and the marginal PDFs are estimated by:

$$\hat{f}_X(x) = \frac{1}{Nh} \sum_{i=1}^N K\left(\frac{x - x_i}{h}\right) \quad \hat{f}_{\mathbf{X}}(x) = \frac{1}{N|\mathbf{H}|^{1/2}} \sum_{i=1}^N K\left(\mathbf{H}^{-1/2}(x - x_i)\right)$$

NB: Use of a constant bandwidth in the logarithmic scale

Mai, C., Polynomial chaos expansions for uncertain dynamical systems – Applications in earthquake engineering, PhD Thesis, ETH Zurich, 2016

Kernel density estimation

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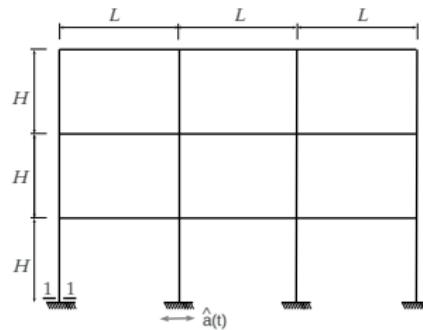
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Zurich, 2016

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Application : steel frame



- 2D steel frame submitted to synthetic ground motions
- Synthetic earthquakes generated in time domain

Parameter	Distribution	Mean	Standard deviation	C.o.V
f_y (MPa)	Lognormal	264.2878	18.5	0.07
E_0 (MPa)	Lognormal	210000	630	0.03

Stochastic ground motion

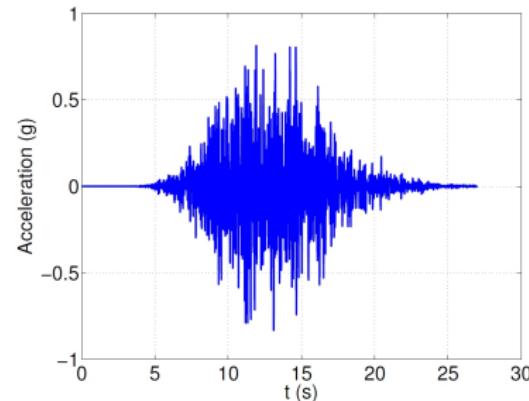
Stochastic excitation

- Obtained by a modulated filtered white noise process

Rezaeian & Der Kiureghian (2010)

$$x(t) = q(t, \boldsymbol{\alpha}) \sum_{i=1}^n s_i(t, \boldsymbol{\lambda}(t_i)) \cdot \xi_i \quad \xi_i \sim \mathcal{N}(0, 1)$$

- Parameters of the filter $\boldsymbol{\lambda} = (\omega_{mid}, \omega', \zeta_f)^T$ are calibrated on recorded signals
- Global parameters (Arias intensity I_a , duration D_{5-95} , strong phase peak t_{mid}) are transformed into the parameters $\boldsymbol{\alpha}$ of the modulation function $q(t, \boldsymbol{\alpha})$ (e.g. gamma distribution)



Stochastic ground motion

Parameters of the excitation

Parameter	Distribution	Support	Mean	Standard deviation
I_a (s.g)	Lognormal	(0, $+\infty$)	0.0468	0.164
D_{5-95} (s)	Beta	[5, 45]	17.3	9.31
t_{mid} (s)	Beta	[0.5, 40]	12.4	7.44
$\omega_{mid}/2\pi$ (Hz)	Gamma	(0, $+\infty$)	5.87	3.11
$\omega'/2\pi$ (Hz)	Two-sided exponential	[-2, 0.5]	-0.089	0.185
ζ_f (.)	Beta	[0.02, 1]	0.213	0.143