Towards the second year milestone: the UQLab development roadmap

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S. Marelli and B. Sudret

Chair of Risk, Safety and Uncertainty Quantification

UNCECOMP 2017, Rhodes Island, Greece, 15 June 2017

Introduction

Computer simulations and uncertainty quantification

- Computer simulations increasingly substitute expensive experimental investigations
- Massive increase in availability of computational resources and computational algorithms
- Logarithmic decrease of cost/flop in High Performance Computing infrastructures
- Computer models only provide a **simplified** representation of reality and are prone to intrinsic model errors and uncertainty

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> **Uncertainty quantification** aims at making the best use of computer models by dealing rigorously with variability, lack of knowledge, measurement- and model errors

Outline

Global framework for managing uncertainties

Probabilistic Input Model

Quantification of sources of uncertainty

Physical Model

Model(s) of the system

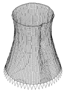
Assessment criteria

Uncertainty Analysis

Uncertainty propagation

Random variables

Computational model



Moments

Probability of failure

Response PDF

Iteration

Sensitivity analysis

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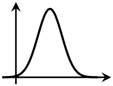

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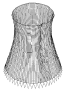

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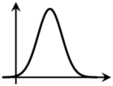

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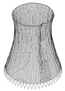

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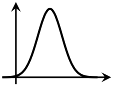

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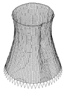

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The physical model

Computational models of physical and engineering systems

- Solution of differential equations (*e.g.* FEM, FD, PS, *etc.*)
- Multi-physics simulations (*e.g.* Comsol, *etc.*)

Surrogate models

- Gaussian process regression (Kriging)
- Polynomial chaos expansions
- Support vector machines/Neural networks

Measurements/databases

- Experimental data from literature
- New in-situ measurements

A physical model $\boldsymbol{Y} = \mathcal{M}(\boldsymbol{X})$ is the (possibly abstract) map that connects a set of entities $\boldsymbol{X}$ (the inputs) to a set of quantities of interest $\boldsymbol{Y}$ (the responses)

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Surrogate models

Definition

- A surrogate model is an **inexpensive to evaluate analytical function** that accurately approximates a computational model
- It is built from a relatively small sample of full model evaluations, known as the *experimental design*:

$$\mathcal{X} = \left\{ \boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(N)} \right\}, \quad \mathcal{Y} = \left\{ \mathcal{M}(\boldsymbol{x}^{(1)}), \ldots, \mathcal{M}(\boldsymbol{x}^{(N)}) \right\}$$

Selected surrogate modelling techniques

Polynomial chaos expansions (PCE):

$$\mathcal{M}^{PC}(\boldsymbol{X}) = \sum_{j=0}^{P} a_j \boldsymbol{\Psi}_j(\boldsymbol{X})$$

Gaussian process modelling (Kriging):

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The probabilistic input model

Experimental data available

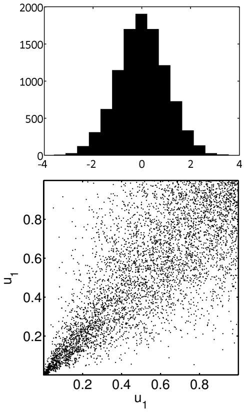
- Descriptive Statistics: moments, histograms, kernel smoothing
- Statistical inference: fitting marginals, copula

Only prior/expert knowledge

- Maximum entropy principle: maximize information under constraints
- Prior knowledge: *e.g.* physical constraints on system variables, literature

Scarce data + expert information

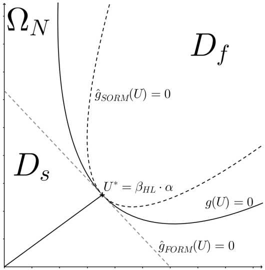
- Bayesian inference methods to combine expert judgment and experimental information



The statistical analysis

Many possibilities

- Analysis of the moments
- Full response characterization (distribution analysis)
- Reliability analysis (rare events simulation)
- Sensitivity analysis/model reduction
- Stochastic/parametric inversion
- Model calibration
- Design optimization



Examples

- Monte Carlo Simulation
- Approximation methods (FORM/SORM)
- Sensitivity analysis: Morris' and Sobol' indices
- Surrogate-model-based analyses: AK-MCS, PCE-based Sobol'

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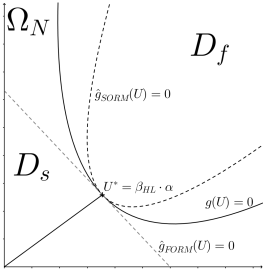

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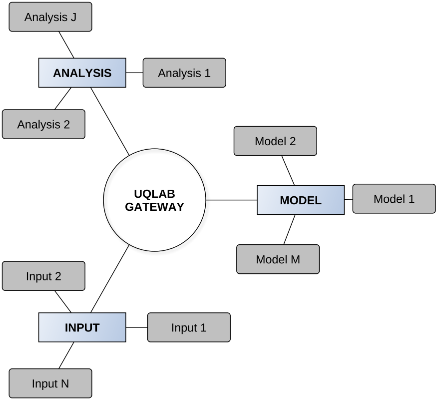
The UQLab Software Framework



UQLab: Uncertainty Quantification Lab

Focus on:

- Generality
- Ease of use
- Documentation
- Non-intrusiveness
- Extendibility
- Collaboration

Current Features of UQLab

Representation of

- **The physical model**
  - Matlab*-based functions (m-files, strings, function handles)*
  - *Support for model parameters*
  - *Simple API to connect to external solvers*
  - *Pre-computed surrogate models*
- **The probabilistic input model (copula formalism)**
  - *Standard marginals (support for user-defined)*
  - *Truncation of marginals (including user-defined)*
  - *Gaussian copula*
  - *Generalized isoprobabilistic transforms*
  - *Sampling strategies (MC, LHS, quasi-random sequences)*
- **[Upcoming] UQLink: easily connect external solvers to UQLab**

Current Features of UQLab (cont'd)

Surrogate modelling (1)

- **Polynomial Chaos Expansions**
  - *Full and sparse (Smolyak) quadrature*
  - *Least-square analysis*
  - *Sparse expansions (LARS,OMP)*
  - *Polynomials orthogonal to arbitrary distributions*
- **Gaussian process modelling (Kriging)**
  - *Simple, ordinary and universal Kriging*
  - *Arbitrary trends (function handles)*
  - *Maximum Likelihood- and Cross-Validation- based hyperparameters estimation*
  - *Local, global and mixed hyperparameter optimization*
  - *Support for user-defined correlation families/functions*

Current Features of UQLab (cont'd)

Surrogate modelling (2)

- **Polynomial Chaos-Kriging**
  - *Fully configurable PCE and Kriging components*
  - *Sequential and optimal construction*
  - *Built from the existing PCE and the Kriging modules*
- **Low Rank Tensor approximations**
  - *Low-rank basis elements built from orthogonal polynomials*
  - *Alternating least-squares construction strategy*
  - *Cross-validation-based error estimation*
  - *Polynomial degree- and maximum rank-adaptive construction*
- **[Upcoming] Support Vector Machines (Regression/Classification)**

Current Features of UQLab (cont'd)

Uncertainty quantification methods

- **Reliability analysis**
  - Monte-Carlo reliability analysis with advanced sampling (LHS/Quasi-Monte-Carlo)
  - Approximation methods: FORM and SORM with revisited algorithms
  - Importance Sampling (FORM-based, or user specified)
  - Subset Simulation
  - Surrogate-modelling-based adaptive-sampling (AK- and APCK-MCS)
- **Global sensitivity analysis**
  - Screening: Correlation analysis, Standard regression coefficients (SRA/SRRA), Cotter measure, Morris method
  - Variance decomposition: Sobol' indices
  - PCE- and LRA-based Sobol' indices
- **[Upcoming] Bayesian model calibration**
- **[Upcoming] Reliability-based design optimization**

Outline

Timeline

End of 2012 official start of the UQLab project at ETH Zürich at the Chair of Risk, Safety and Uncertainty Quantification (Prof. Sudret)

End of 2013 initial development and first collaborations between ETH groups using UQLab PCE tool

2013-2015 development of the scientific modules, including Probabilistic modelling, Kriging, Sensitivity Analysis, Structural reliability

July 1st 2015 public release of the UQLab Beta (closed source)

March 1st, 2016 release of the Structural reliability module

April 28, 2017 UQLab Version 1.0.0: open source release of the scientific code (modules). Release of the low-rank approximations and PC-Kriging metamodelling tools

UQLab in Numbers

Since release of the public beta (July 1st, 2015):

- 870+ users from 55 countries worldwide...
- ...and counting!

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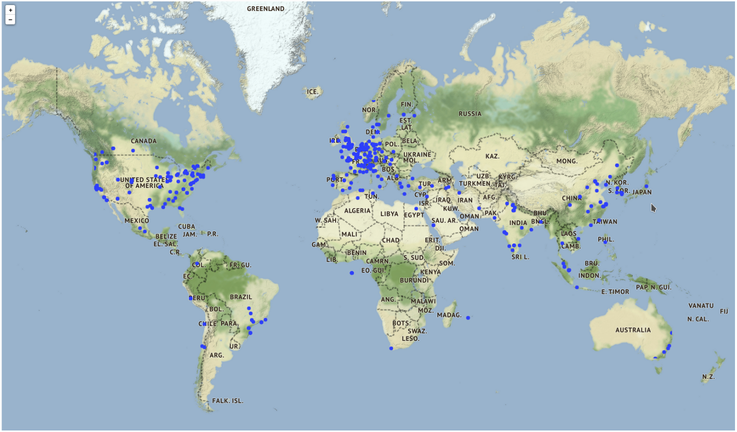

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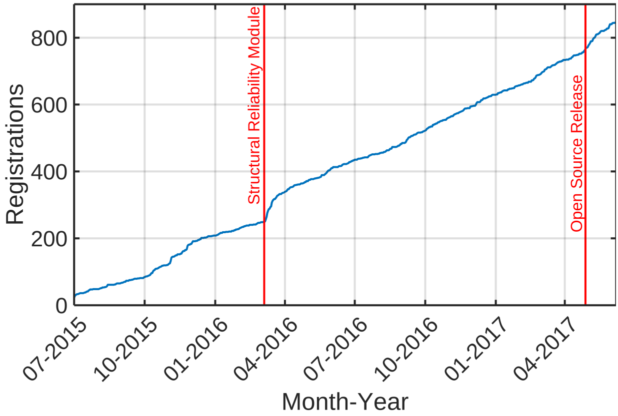

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Upcoming milestones

Tools under active development

- Random fields toolbox
- Support vector machines (classification and regression)
- Bayesian model calibration
- Reliability-based design optimization (RBDO)
- Advanced dependence inference and modelling (vine copulas)

Collaborative development/community

- **End of 2017** Community kickstart (forums, file exchange)
- **2018** Contributors infrastructure: documentation, distribution of contributed modules/codes (first contributions already received!!)
- **2018+** Establish a network/community of UQLab developers

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Thank you very much for your attention!

UQLab

The Framework for Uncertainty Quantification

www.uqlab.com

Chair of Risk, Safety & Uncertainty Quantification

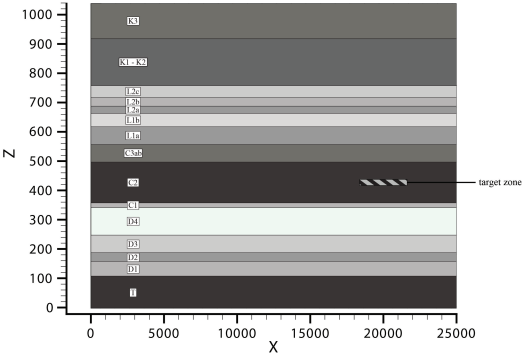
http://www.rsuq.ethz.ch

Outline

4 Case studies
- Subsurface contaminant diffusion
- Foundation settlement
- Example gallery

Case Study I: Sensitivity analysis in long-term nuclear waste storage

Joint work with University of Neuchâtel



- Idealized model of the Paris Basin
- Two-dimensional cross section

  (25 km long / 1,040 m depth) with 5×5 m mesh (10^6 elements)
- 15 homogeneous layers
- Steady-state flow with Dirichlet boundary conditions:

$$\nabla \cdot (\mathbf{K} \cdot \nabla H) = 0$$

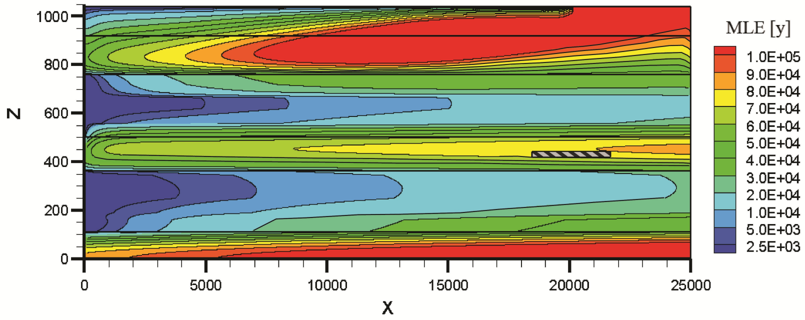
Question: which parameters affect most the time needed for contaminants to escape the region?

Deman, Konakli, BS, Kerrou, Perrochet & Benabderrahmane, Using sparse polynomial chaos expansions for the global sensitivity analysis

The physical model: mean life-time expectancy

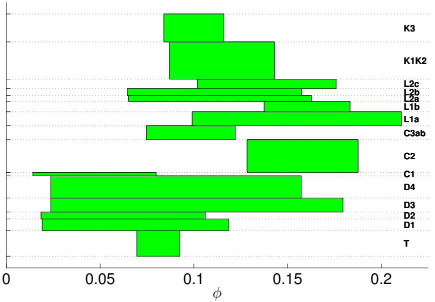
Definition

The Mean Lifetime Expectancy $MLE(\boldsymbol{x})$ is the time required for a molecule of water at point $\boldsymbol{x}$ to get out of the boundaries of the model



Map of mean lifetime expectancy (nominal case)

Probabilistic input model: porosity and conductivity

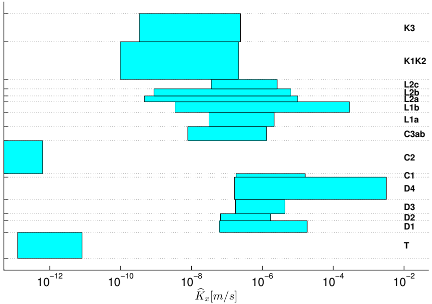


- In each layer, bounds on porosity:

$$\phi^i \sim \mathcal{U}[\phi^i_{min}\,,\,\phi^i_{max}]$$

- Deterministic mapping to the conductivity

Probabilistic input model: porosity and conductivity



Nominal conductivity (K_x) vs. porosity

Layer	K_x [m/s]	ϕ [-]
K3	9.01E−09	0.0100
K1-K2	4.53E−09	0.1150
L2c	1.10E−06	0.1389
L2b	3.46E−07	0.1110
L2a	1.62E−07	0.1139
L1b	1.49E−05	0.1604
L1a	1.17E−06	0.1549
C3ab	4.59E−08	0.0984
C2	1.99E−13	0.1580
C1	1.89E−06	0.0470
D4	1.65E−05	0.0905
D3	1.76E−06	0.1016
D2	2.62E−07	0.0623
D1	3.23E−06	0.0688
T	1.95E−12	0.0810

- In each layer, bounds on porosity:

$$\phi^i \sim \mathcal{U}[\phi^i_{min}\,,\,\phi^i_{max}]$$

- Deterministic mapping to the conductivity

$$\log_{10}(K^i_x) = f_i(\phi^i) \qquad \text{(layer-dependent)}$$

Additional parameters

Parameter	Notation	Range
Porosity	$\phi^i,\ i = 1, \ldots, 15$	$[\phi^i_{min}\ ,\ \phi^i_{max}]$
Anisotropy of hydraulic conductivity tensor	$A^i_K,\ i = 1, \ldots, 15$	$[0.01\ ,\ 1]$
Euler angle of hydraulic conductivity tensor	$\theta^i,\ i = 1, \ldots, 15$	$[-30\ ,\ 30](\mathrm{deg})$
Longitudinal component of dispersivity tensor	$\alpha^i_L,\ i = 1, \ldots, 15$	$[5\ ,\ 25]$
Anisotropy of dispersivity tensor	$A^i_\alpha,\ i = 1, \ldots, 15$	$[5\ ,\ 25]$

Hydraulic gradient $(10^{-3} m/m)$		
Dogger sequence	∇H_D	[0.64 , 0.96]
Oxfordian sequence	∇H_O	[2.40 , 3.60]
Top of the model	∇H_{top}	[2.72 , 4.08]

78 independent variables with uniform distributions

Statistical analysis: PCE-based Sobol' sensitivity indices

Sensitivity analysis

- **Method:** Sobol' indices postprocessed from PCE coefficients Sudret, 2008
- **Surrogate model:** Sparse degree-adaptive PCE Blatman and Sudret, 2011
- **Training:** 200 maximin latin hypercube samples (LHS)

Results:

Total cost: $N_{PCE} = 200$ model runs.
MCS-based calculation $N_{MCS} \approx 10^4 \cdot 78 = 780000$:

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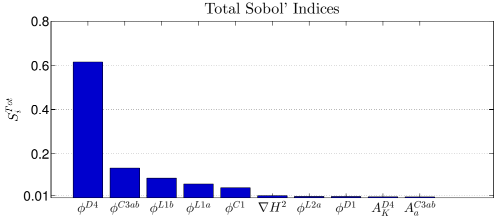

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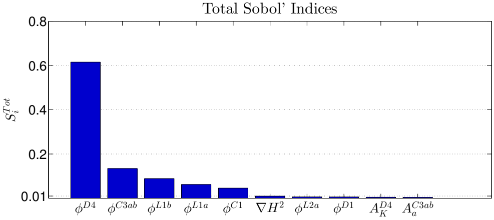

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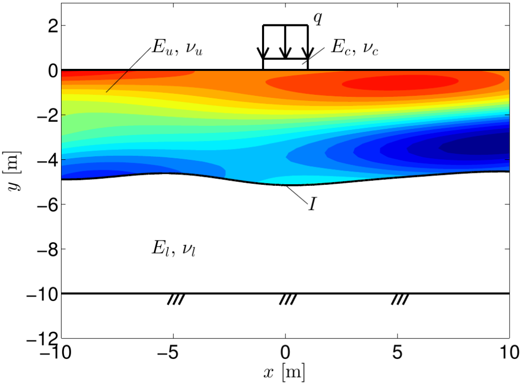
Case study II: Foundation settlement

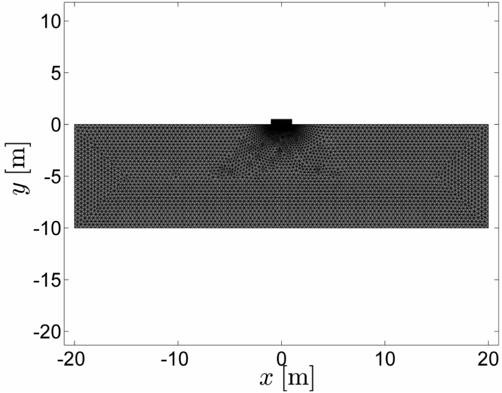
Reliability analysis of a high dimensional foundation settlement problem



Question: What is the probability that the settlement of the foundation exceeds some safety threshold u_{adm}?

The physical model: FEM structure

- FEM model
- ~ 8500 elements
- Output: mid-foundation deflection
- Computed with COMSOL multiphysics FEM module



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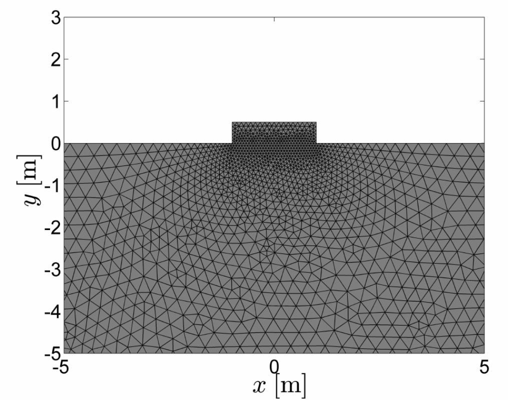

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Stochastic input model

Structural Parameters:

Name	Distribution	Mean	CoV
Load	Gumbel	200lkPa	15%
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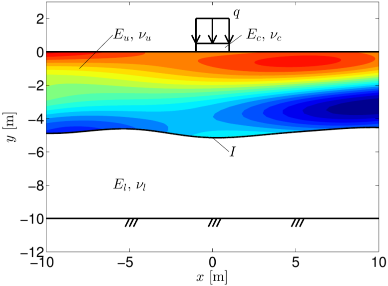

First Layer:

- Lognormal random field
- Mean: 10MPa
- CoV: 15%
- Correlation: squared exp.
- Corr length: 10m (x), 2m (y)

Interface:

- Gaussian random field
- Mean: -5m
- CoV: 30%
- Correlation: squared exp.
- Corr. length: 5m

After KL-based random field discretization: 45 standard normal random variables for the first layer, 11 for the interface
Total of $45 + 11 + 2$ random inputs

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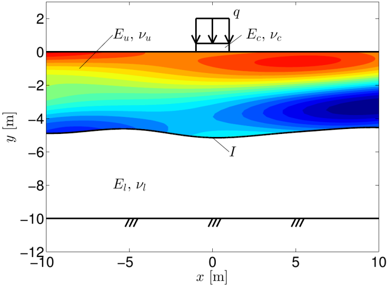

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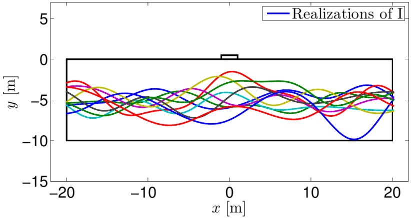

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- Corr length: 10m (x), 2m (y)

Interface:

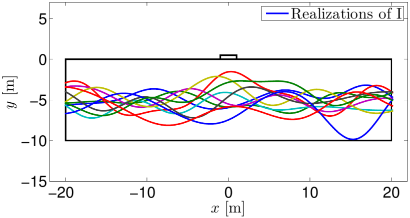
- Gaussian random field
- Mean: -5m
- CoV: 30%
- Correlation: squared exp.
- Corr. length: 5m

After KL-based random field discretization: 45 standard normal random variables for the first layer, 11 for the interface
Total of $45 + 11 + 2$ random inputs

Stochastic input model

Structural Parameters:

Name	Distribution	Mean	CoV
Load	Gumbel	200lkPa	15%
E-Low	Lognormal	MPa	15%



First Layer:

- Lognormal random field
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Reliability analysis with PCE

Reliability analysis

- **Method:** direct Monte Carlo Simulation ($N = 10^7$) on a surrogate model

$$P_f = N_{exceed}/N$$

- **Surrogate model:** sparse degree-adaptive non-intrusive PCE
- **Training:** 1000 maximin latin hypercube samples (LHS)

Results

u_{adm}	P_f	β_{HL}
5 cm	$2.71 \cdot 10^{-2}$	1.93
6 cm	$2.85 \cdot 10^{-3}$	2.76
7 cm	$2.80 \cdot 10^{-4}$	3.45
8 cm	$2.49 \cdot 10^{-5}$	4.06

Total cost: 1000 model runs

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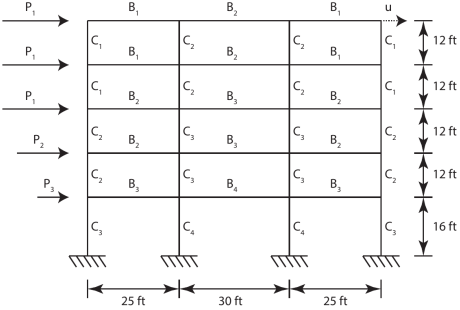
Example Gallery

Multi-level Meta-modelling in Imprecise Structural Reliability Analysis

Schöbi and Sudret, APSSRA 2016

- Multi-storey building subject to random loads
- Random material properties with imprecise distributions
- Complex correlation structure between inputs
- Parametric and non-parametric p-boxes



Problem: probability range of maximum inter-storey drift being higher than a safe threshold

Solution: multi-level adaptive-Kriging Monte-Carlo Simulation (AK-MCS).

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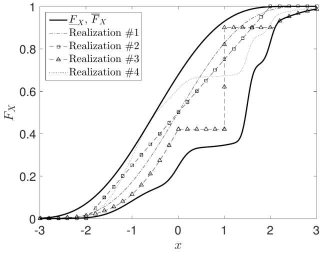

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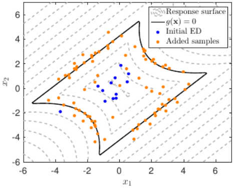
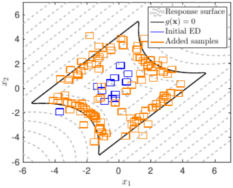


$\boldsymbol{\mathcal{X}}$ for $\mathcal{G}^{(K)}$



Optim. for $\underline{\mathcal{G}}^{(K)}$

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Sparse polynomial chaos expansions of frequency response functions

Yaghoubi et al. 2016, submitted to PEM

- System with 6 degrees of freedom
- 16 random inputs
- $\sim 10^5$ outputs
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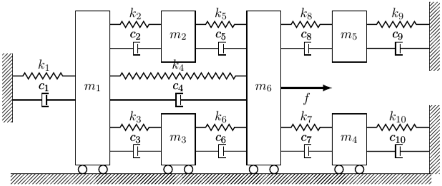
- Eigenmodes depend on the inputs



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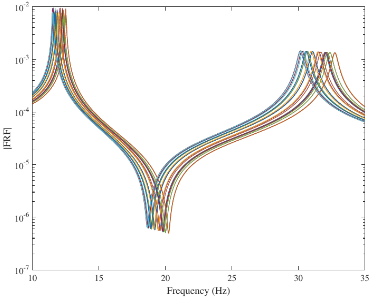

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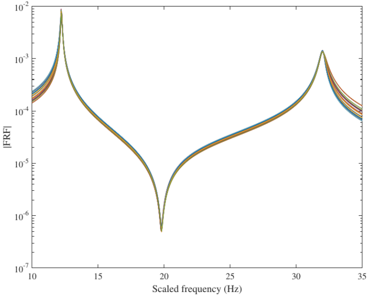

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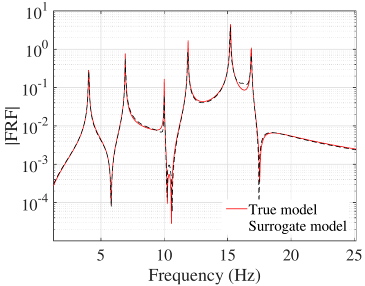

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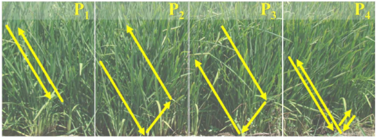

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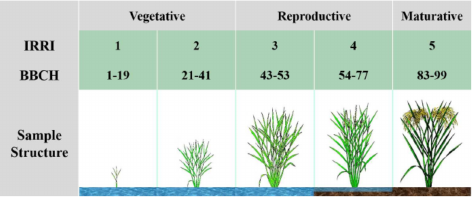

	Vegetative		Reproductive		Maturative
IRRI	1	2	3	4	5
BBCH	1-19	21-41	43-53	54-77	83-99
Sample Structure					

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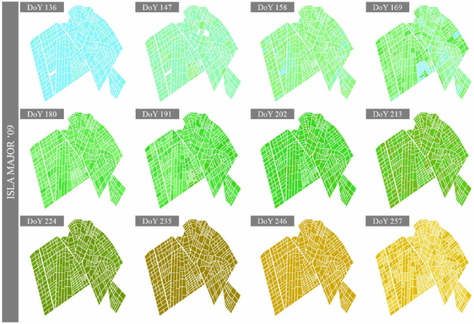

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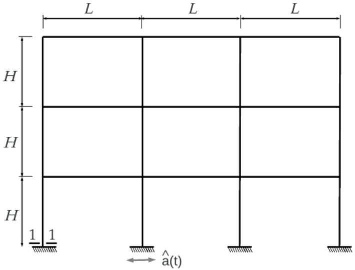

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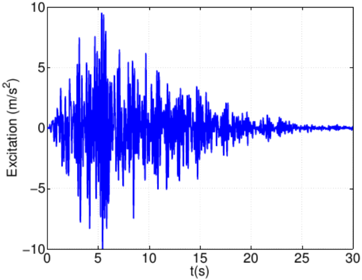

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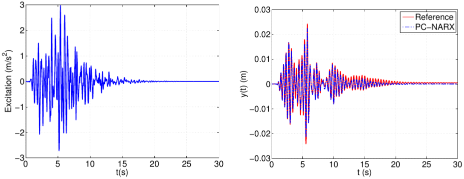

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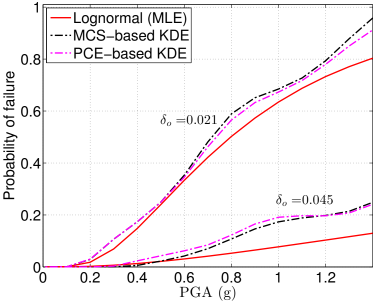

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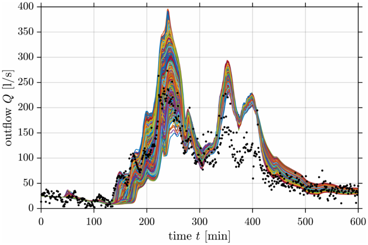
- 8-random input variables
- Calibration with 600 outflow recordings



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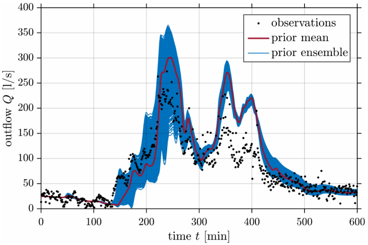

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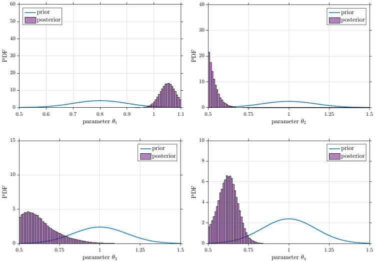

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