technische universität dortmund

Chair for Reliability Engineering

Quantification and propagation of uncertainties in expensive simulation models

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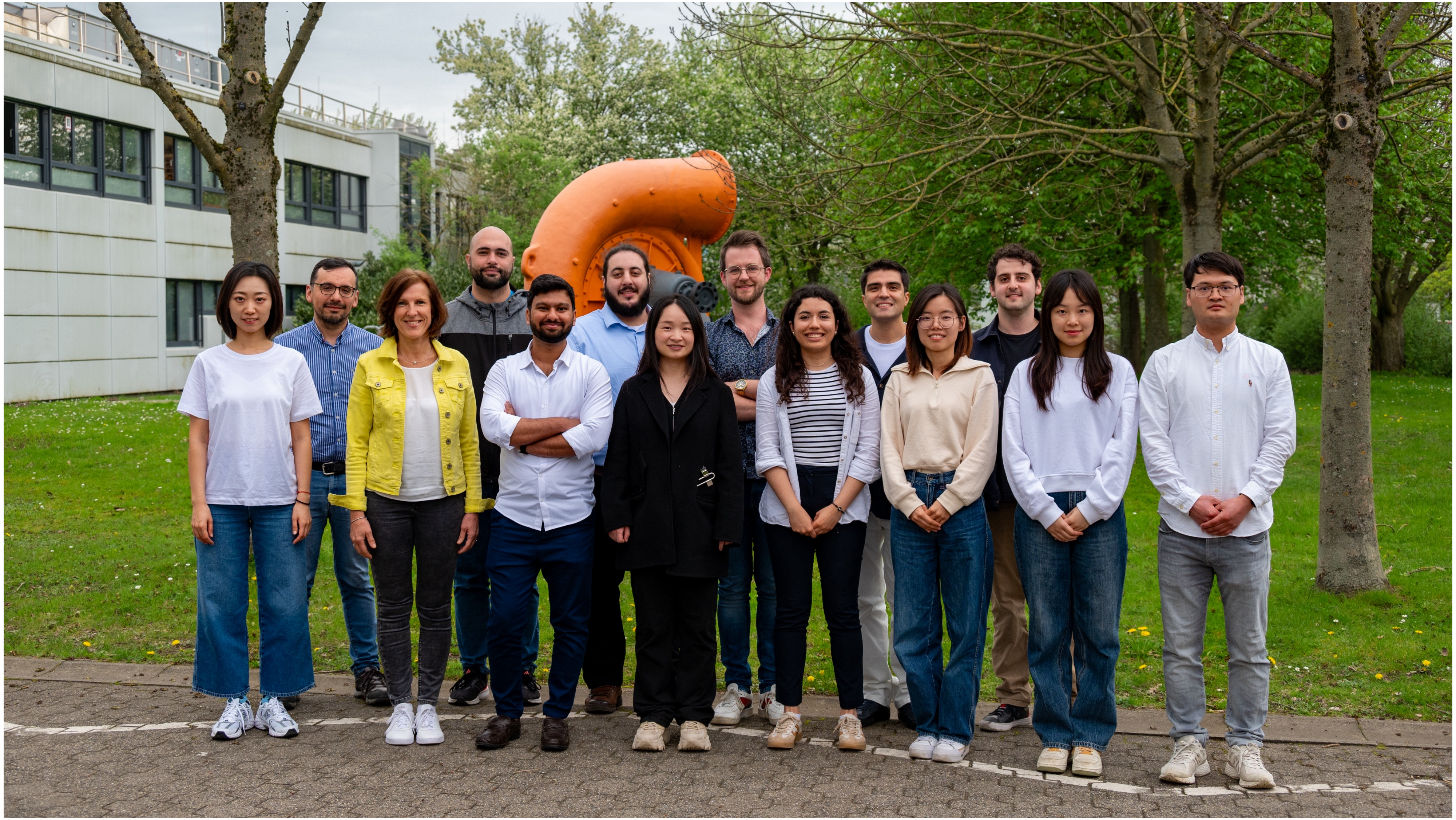
Professor in Reliability Engineering
TU Dortmund University

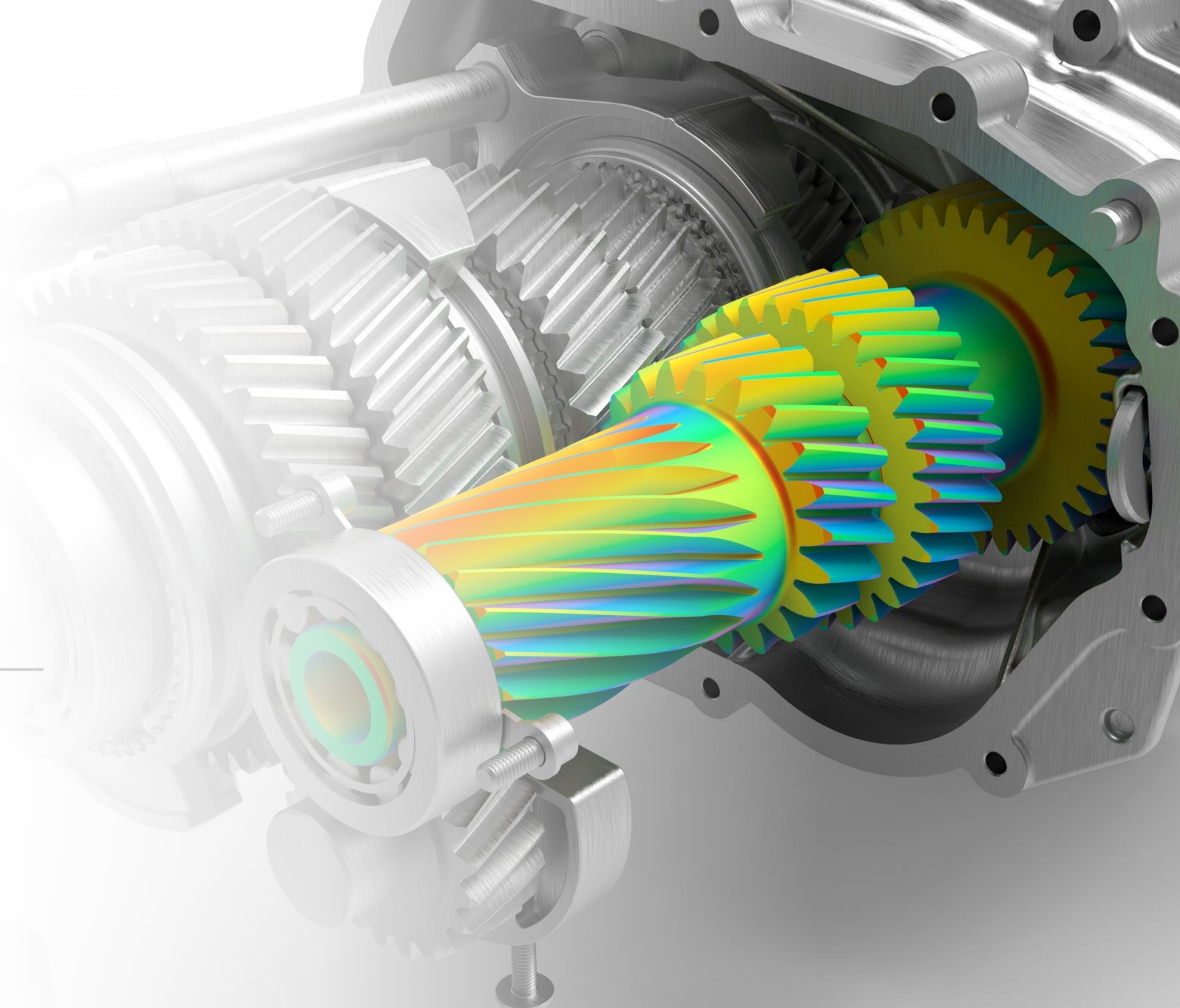
A big thanks to the team @ CRE – TU Dortmund



Not in the picture:




Numerical simulation tools allow for designing complex components



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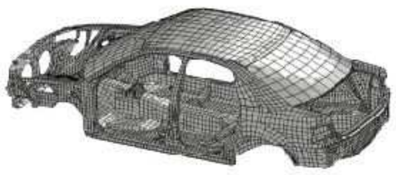
Computational models in engineering

- Complex engineering systems are designed and assessed using computational models
- A computational model consists of:
  - A mathematical description of the physical phenomena (i.e., the governing equations)
  - Discretisation techniques that transform continuous equations into linear algebraic formulations
  - Algorithms to solve the discretized equations

$$\mathrm{div}\ \boldsymbol{\sigma} + \mathbf{f} = 0$$

$$\boldsymbol{\sigma} = \mathbf{D} \cdot \boldsymbol{\epsilon}$$

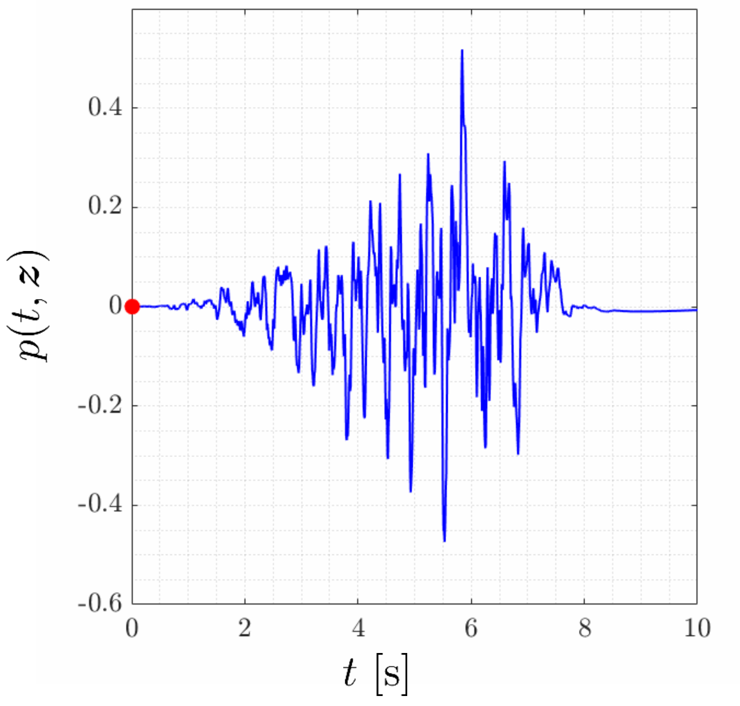
$$\boldsymbol{\epsilon} = \frac{1}{2}\left(\Delta \boldsymbol{u} + {}^{\mathrm{T}}\Delta \boldsymbol{u}\right)$$



Computational models : another viewpoint

Finite Element Model

Ground Acceleration



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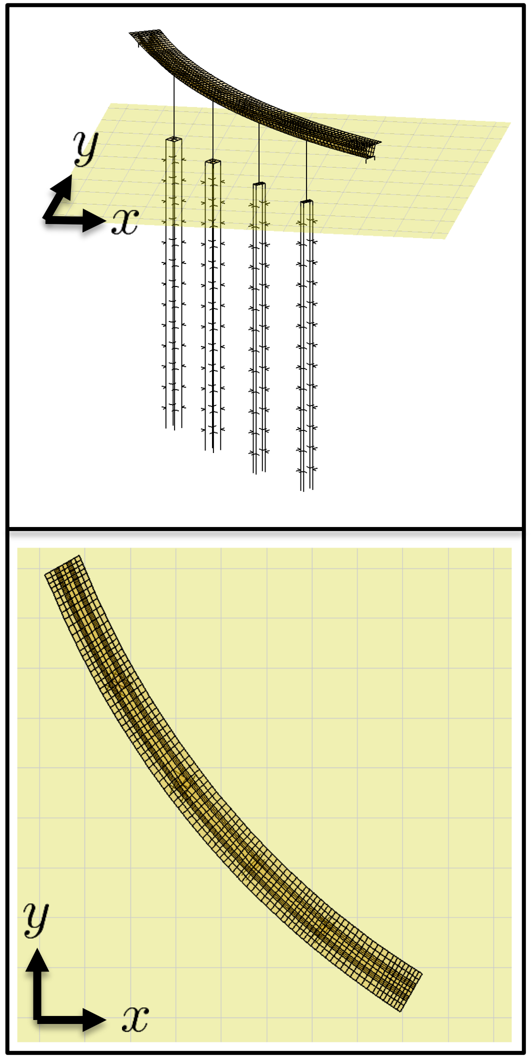
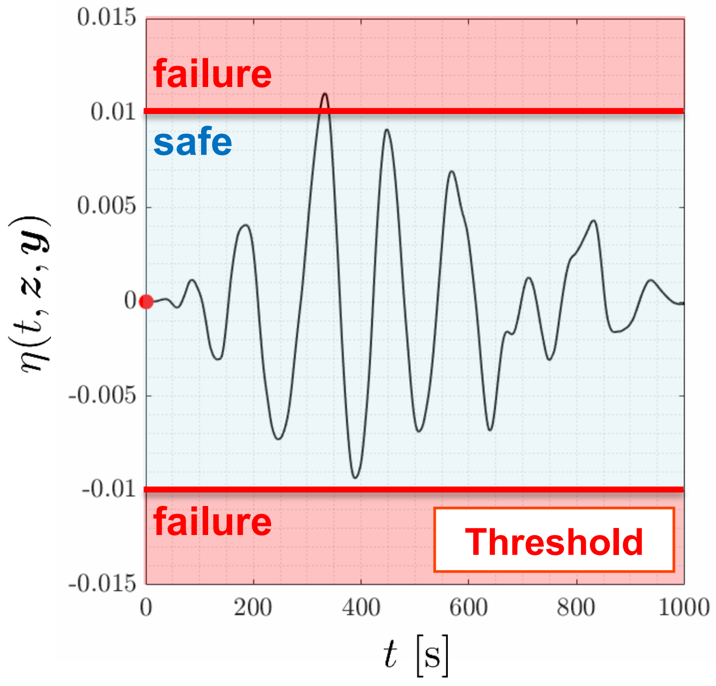


Response of interest



Response

Computational models : another viewpoint

Finite Element Model

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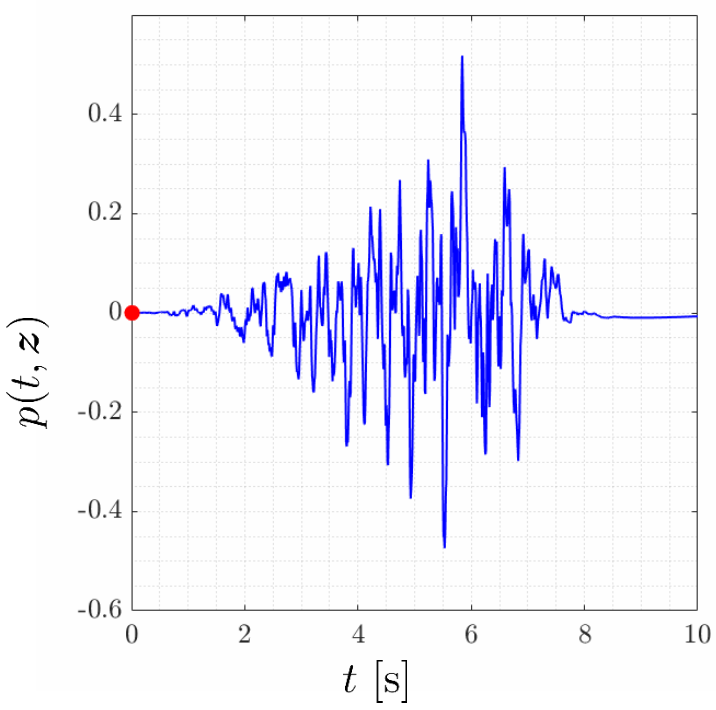

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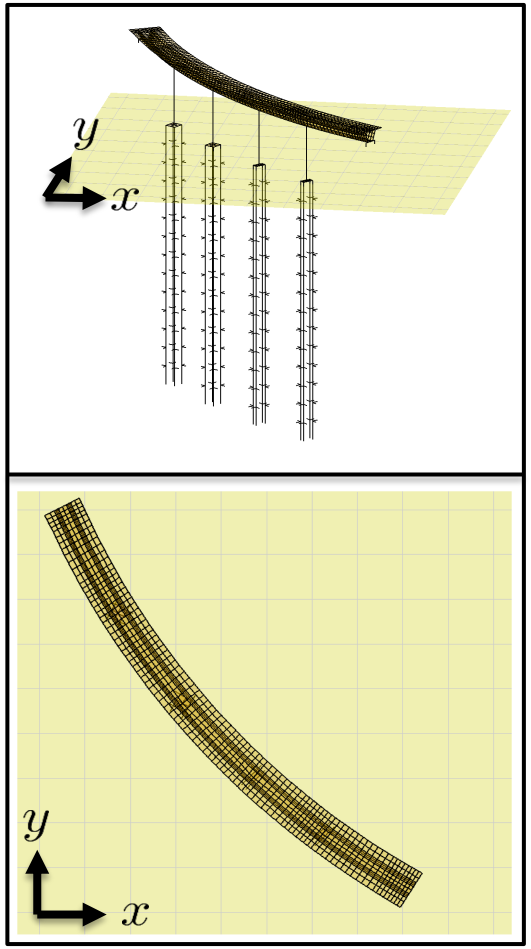
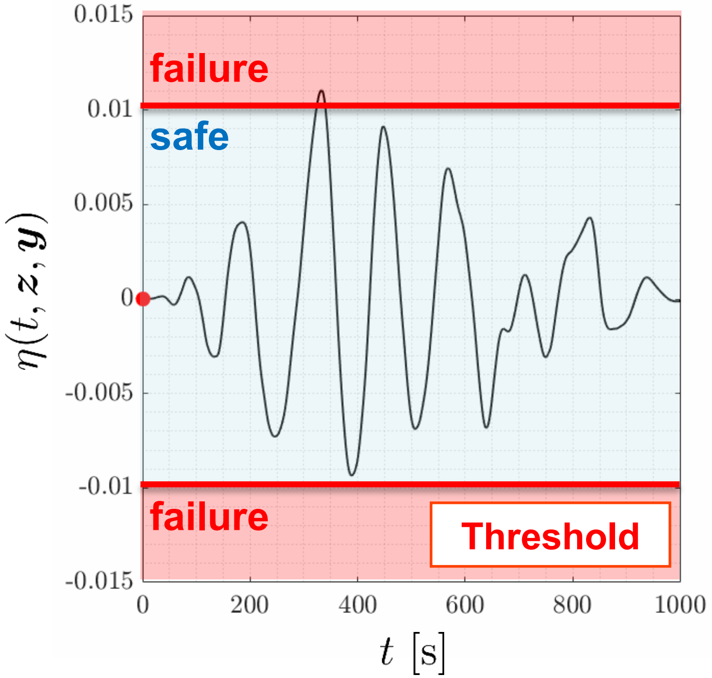


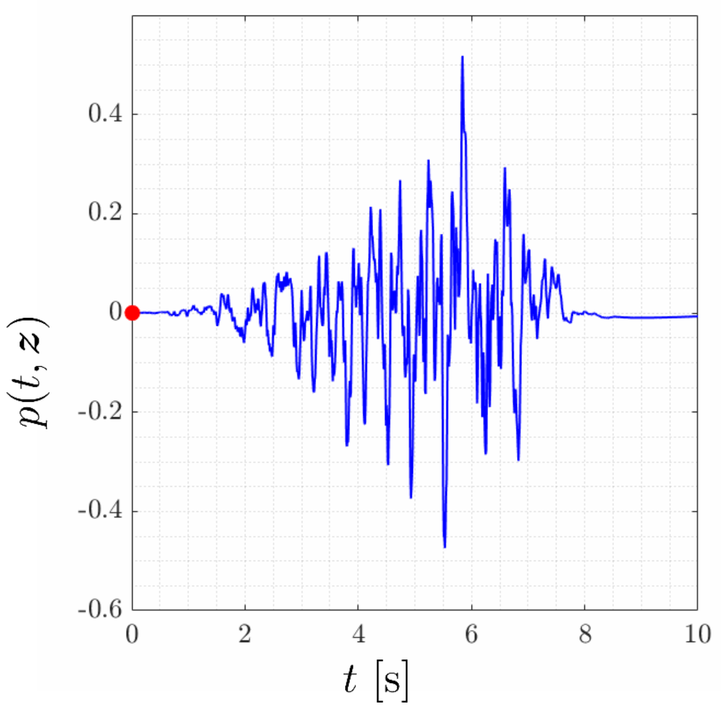
Response of interest



Response

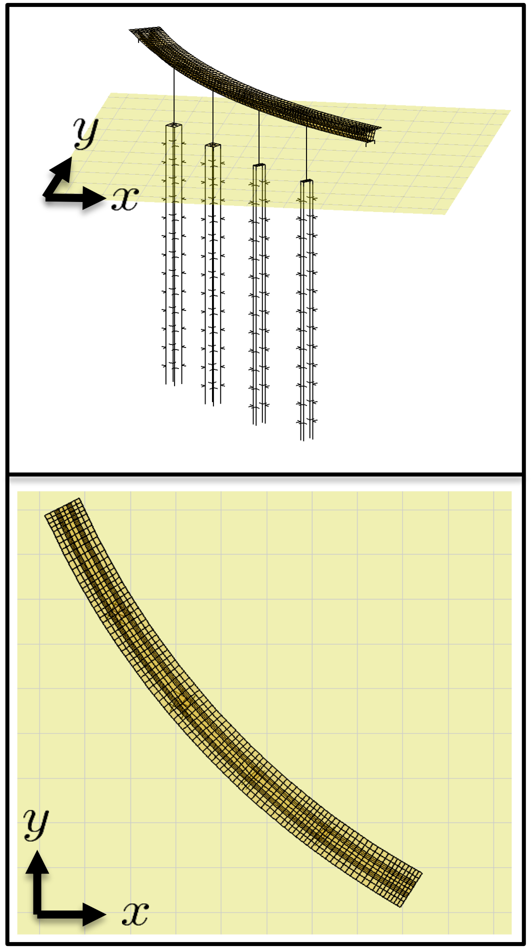
Computational models : another viewpoint

Ground Acceleration



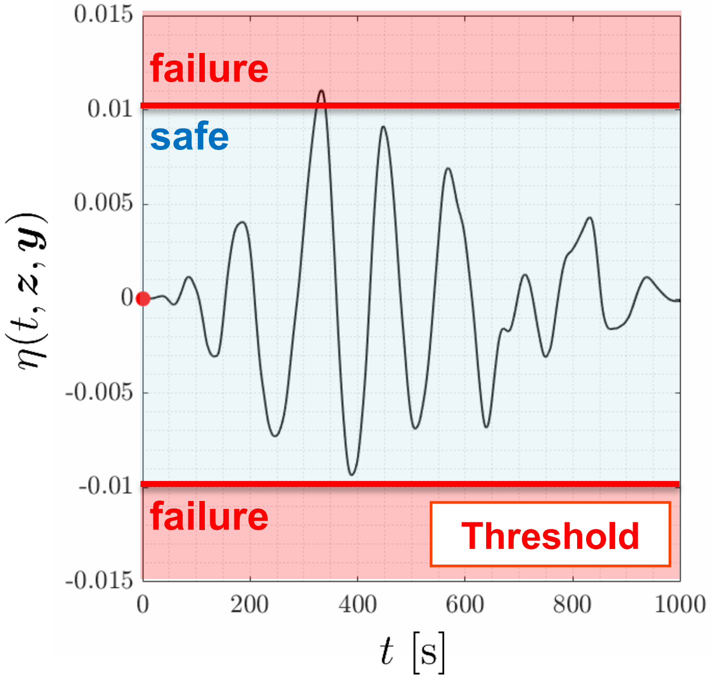
Stochastic process

Finite Element Model



Uncertain model properties

Response of interest



Stochastic response

General uncertainty quantification overview

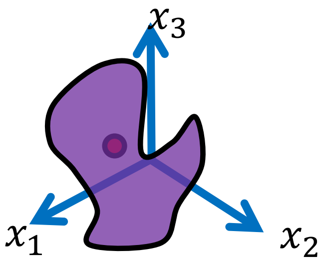
Step 2:
Quantification of sources of uncertainty

Step 1:
Model the system and assessment criteria

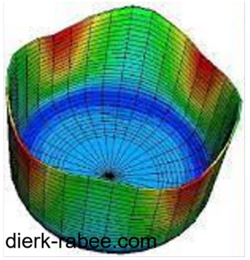
Step 3:
Uncertainty propagation

Step 2':
Stochastic model updating

Random variables



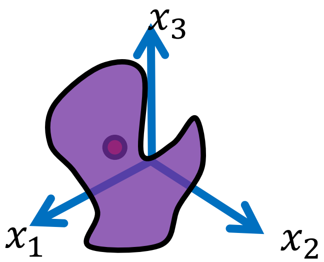
Computational model



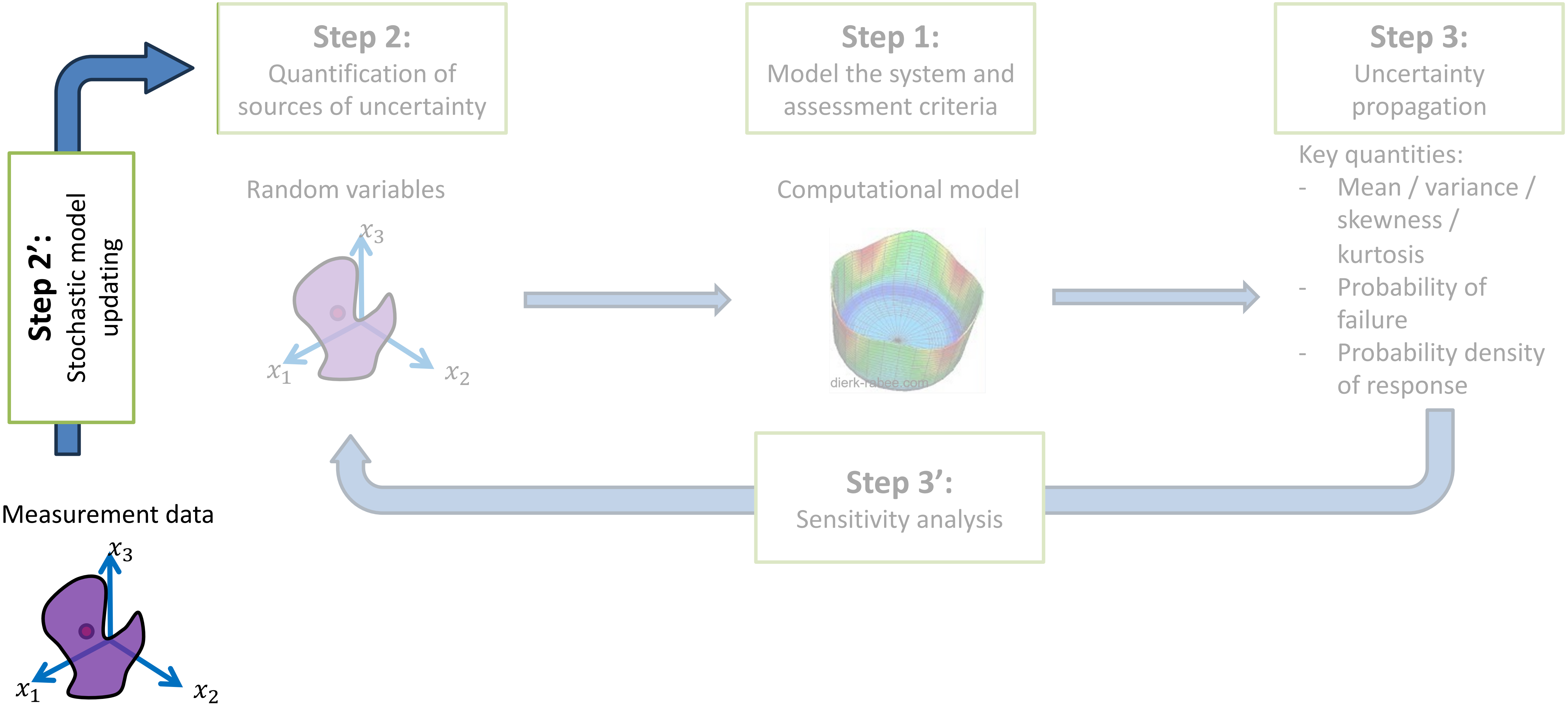
Key quantities:
- Mean / variance / skewness / kurtosis
- Probability of failure
- Probability density of response

Step 3':
Sensitivity analysis

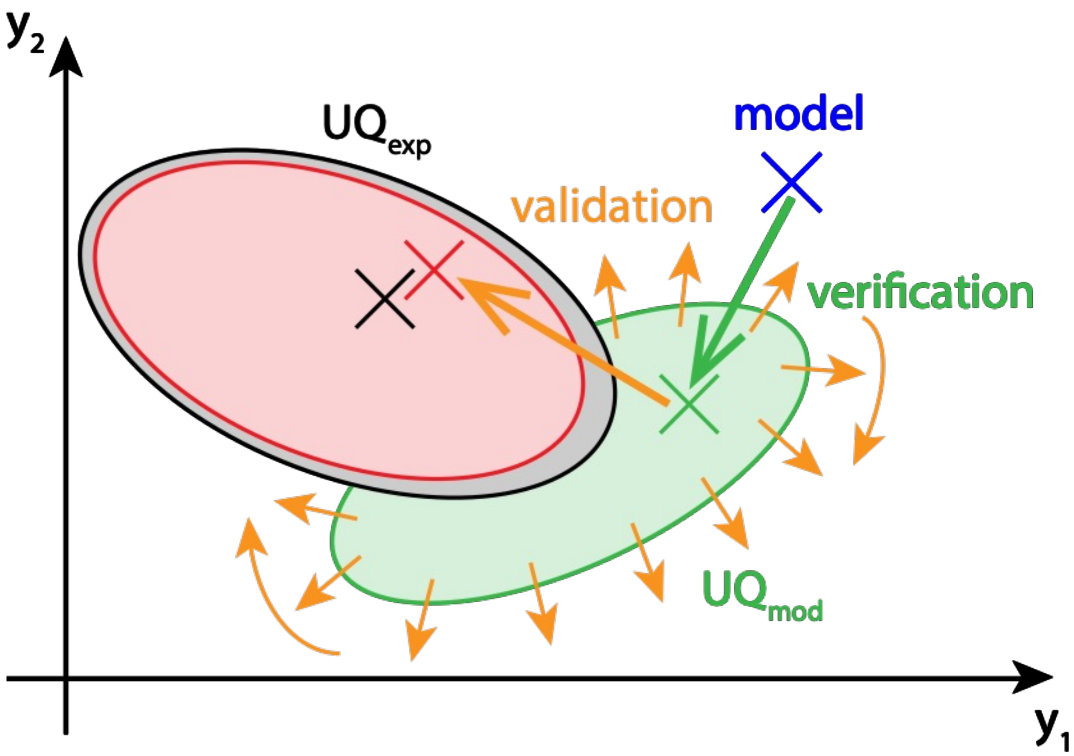
Measurement data



General uncertainty quantification overview



Step 2’: Stochastic model updating



Step 1: modelling

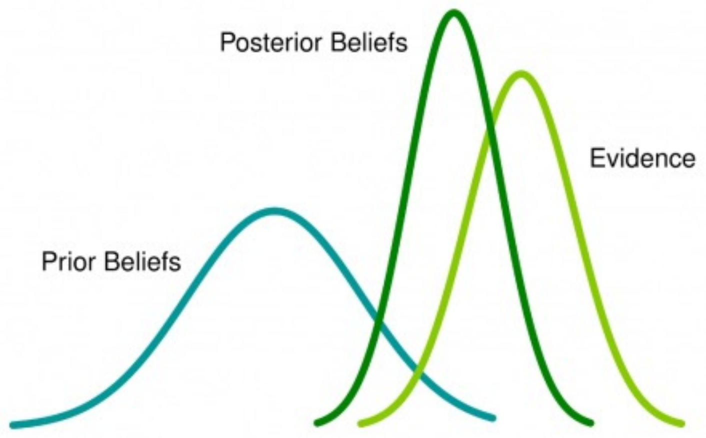
Step 2: uncertainty modelling

Step 2’: stochastic model updating

Experimental quantification of probabilistic variability

- Bayesian updating

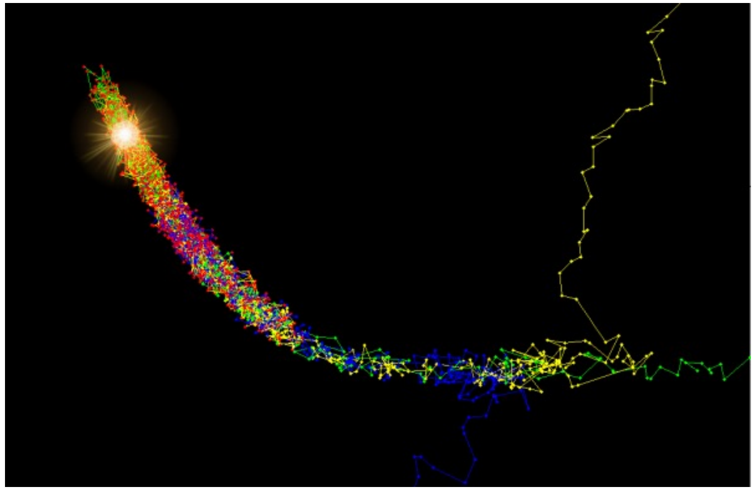
$$f(\theta|D,M) = \frac{f(D|M,\theta)\cdot f(\theta|M)}{f(D|M)}$$



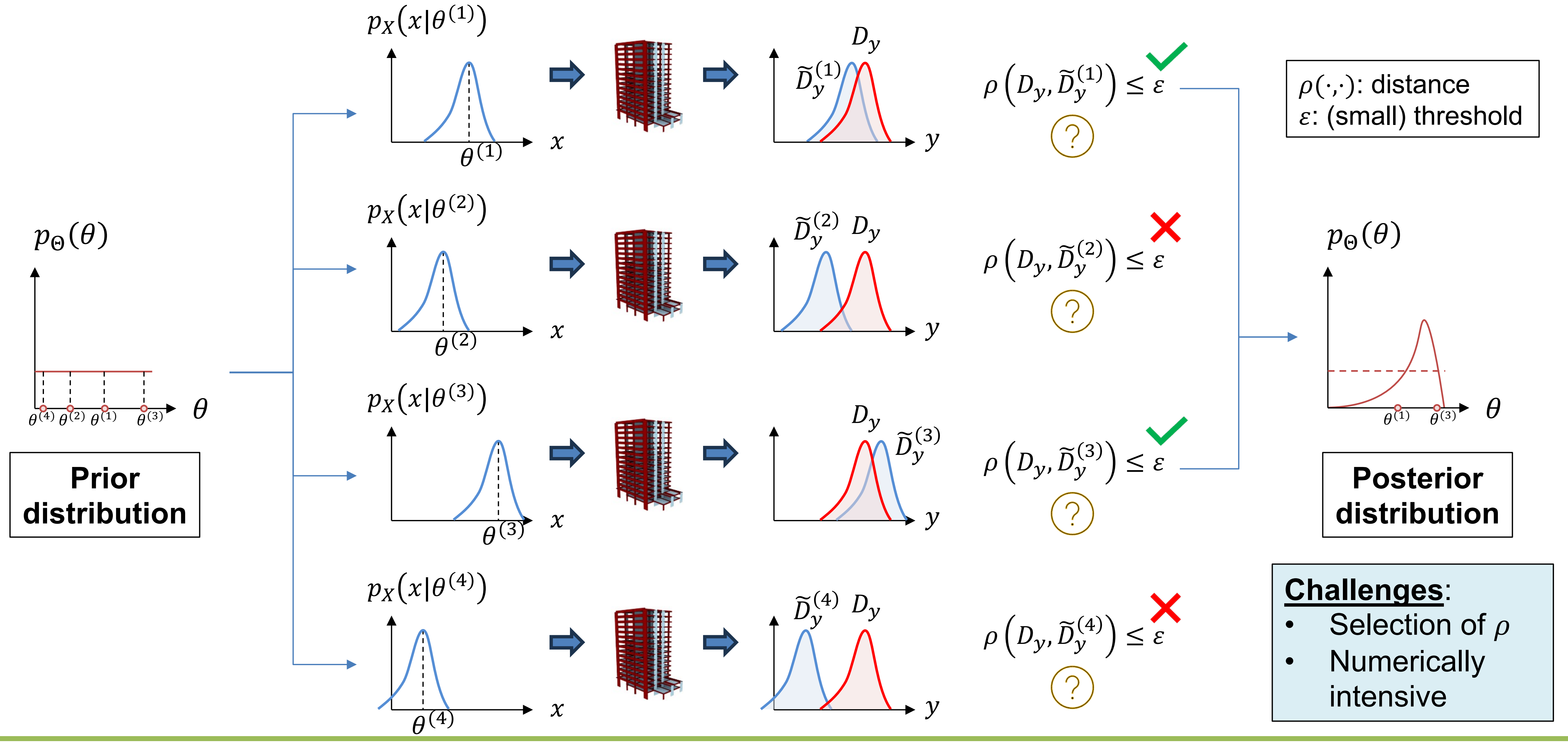
- $f(D|M,\theta)$ often based on a zero-mean Gaussian white noise with covariance Σ

$$f(D|M,\theta) \propto \prod_{i=1}^{N} \exp\left(-\frac{1}{2}\epsilon_i^T(\theta)\Sigma^{-1}\epsilon_i(\theta)\right)$$

- Model evidence $f(D|M)$ is a tool for model selection
- However:
  - Need for expensive Markov Chain Monte Carlo based simulators (MCMC, TMCMC, HMCMC)
  - Gaussian assumption of error usually not realistic



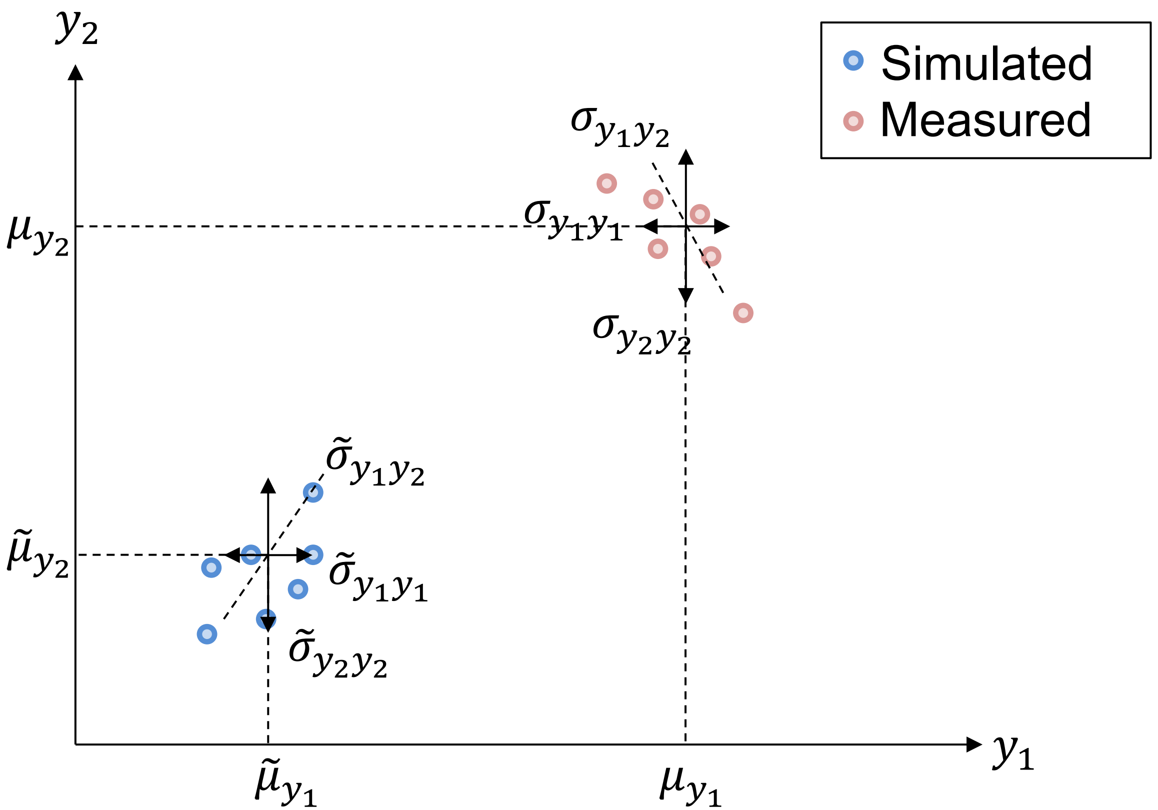
Approximate Bayesian Computation (ABC)



Challenges:
- Selection of ρ
- Numerically intensive

Distance ρ: Selection

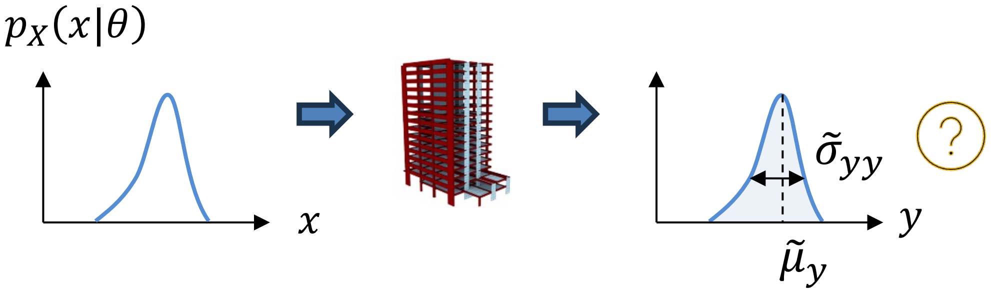
- Different distance metrics available, e.g. Euclidian distance, Mahalanobis distance, Bhattacharyya distance, etc.
- This contribution: **summary statistics**



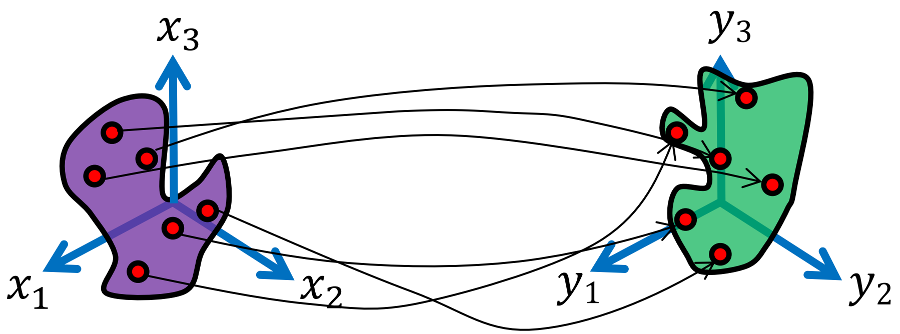
$\rho\left(D_y, \tilde{D}_y\right)$: maximum relative difference between **second order statistics** of simulated and measured data

Distance ρ: Calculation

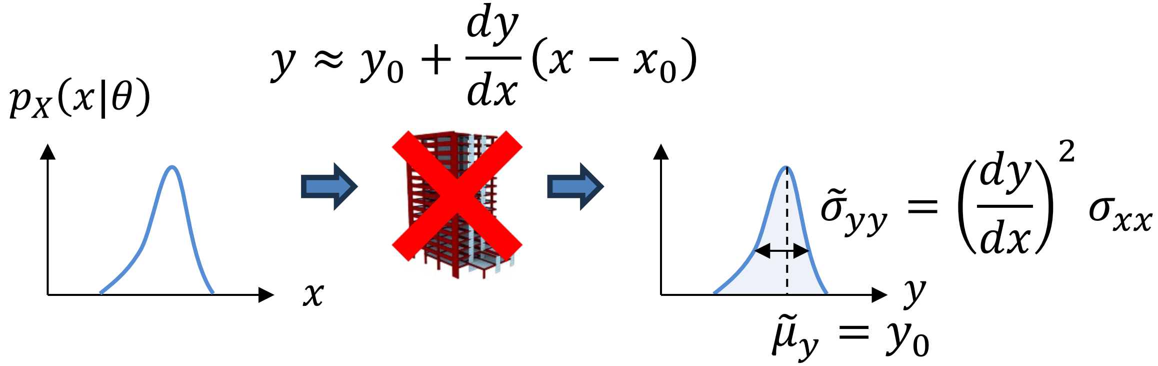
- Distance ρ demands knowledge on **mean** and **covariance** of simulated data



  - Monte Carlo simulation+ divergence: accurate but numerically demanding, noisy estimators

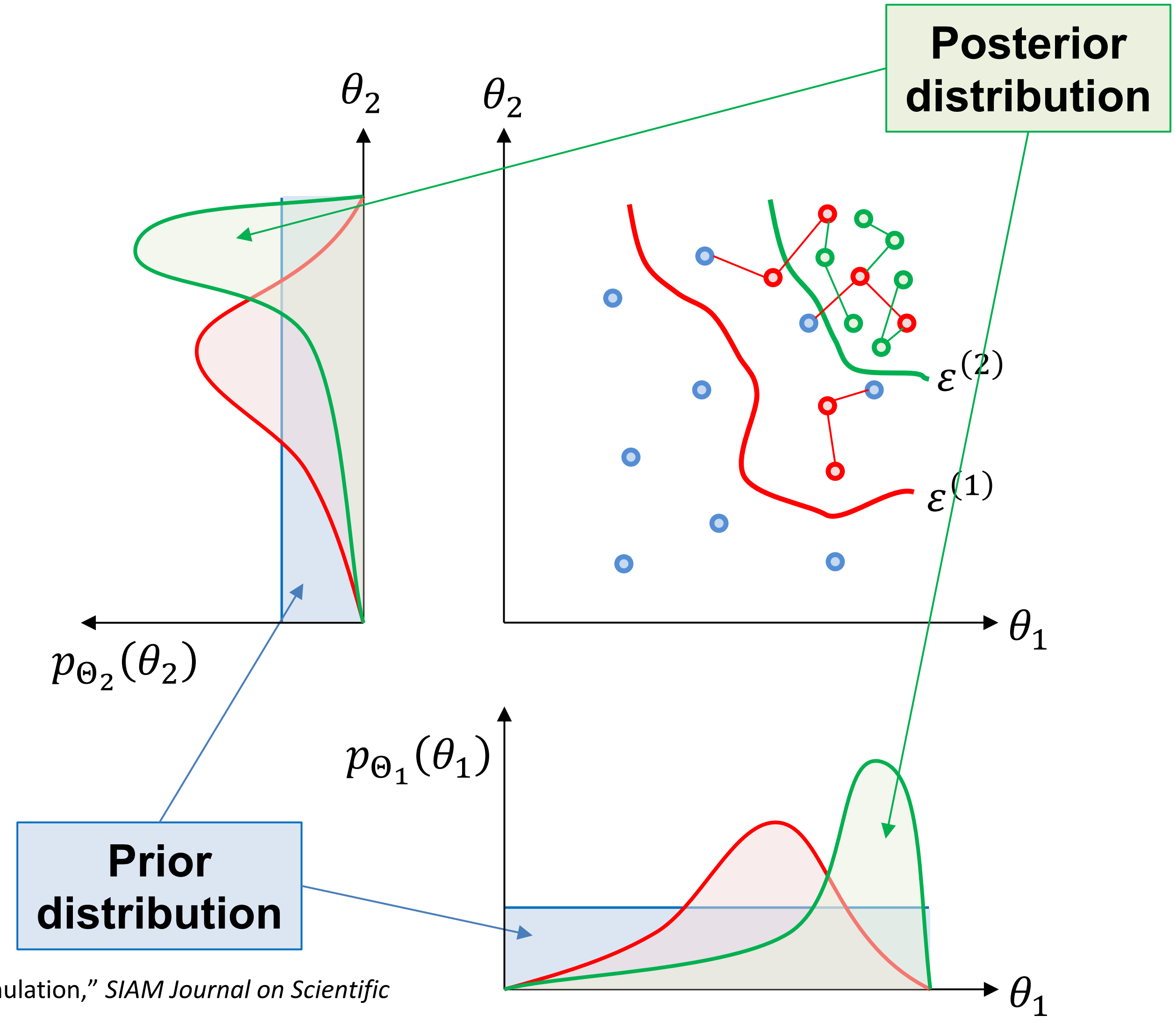


  - **Perturbation**: accuracy depends on nonlinearity, highly efficient, precise estimators



Practical Implementation: Subset Simulation

- Subset simulation*
  - Small batches of simulated data at each stage
  - Threshold levels $\varepsilon^{(1)} \geq \varepsilon^{(2)} \geq \cdots$ selected adaptively
  - **Gradual approach** from prior to sought posterior distribution
  - Samples of $\boldsymbol{\theta}$ conditioned on $\rho \geq \varepsilon^{(i)}$ are generated with **preconditioned Crank – Nicolson** algorithm**

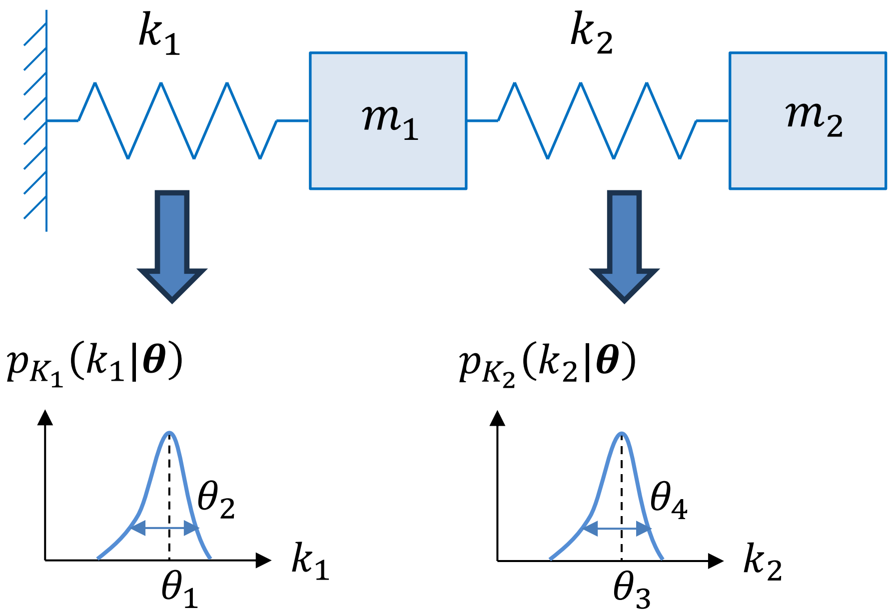


*M. Chiachio, J. L. Beck, J. Chiachio, and G. Rus, "Approximate Bayesian computation by subset simulation," *SIAM Journal on Scientific Computing*, vol. 36, Art. no. 3, 2014.

**A. Beskos, G. Roberts, A. Stuart, and J. Voss, "MCMC methods for diffusion bridges," *Stochastics and Dynamics*, vol. 8, Art. no. 03, 2008.

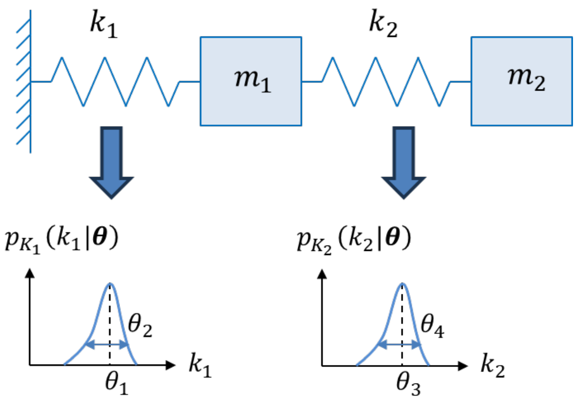
Example

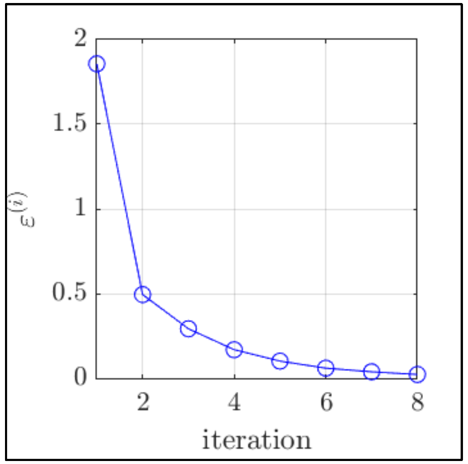
- Two-degree-of-freedom oscillator
  - Uncertain stiffnesses k_1 and k_2 (lognormal distribution)
  - Epistemic uncertainty regarding mean value (θ_1, θ_3) and standard deviation (θ_2, θ_4) of each stiffness
  - 30 measurements of natural frequencies (synthetically generated)

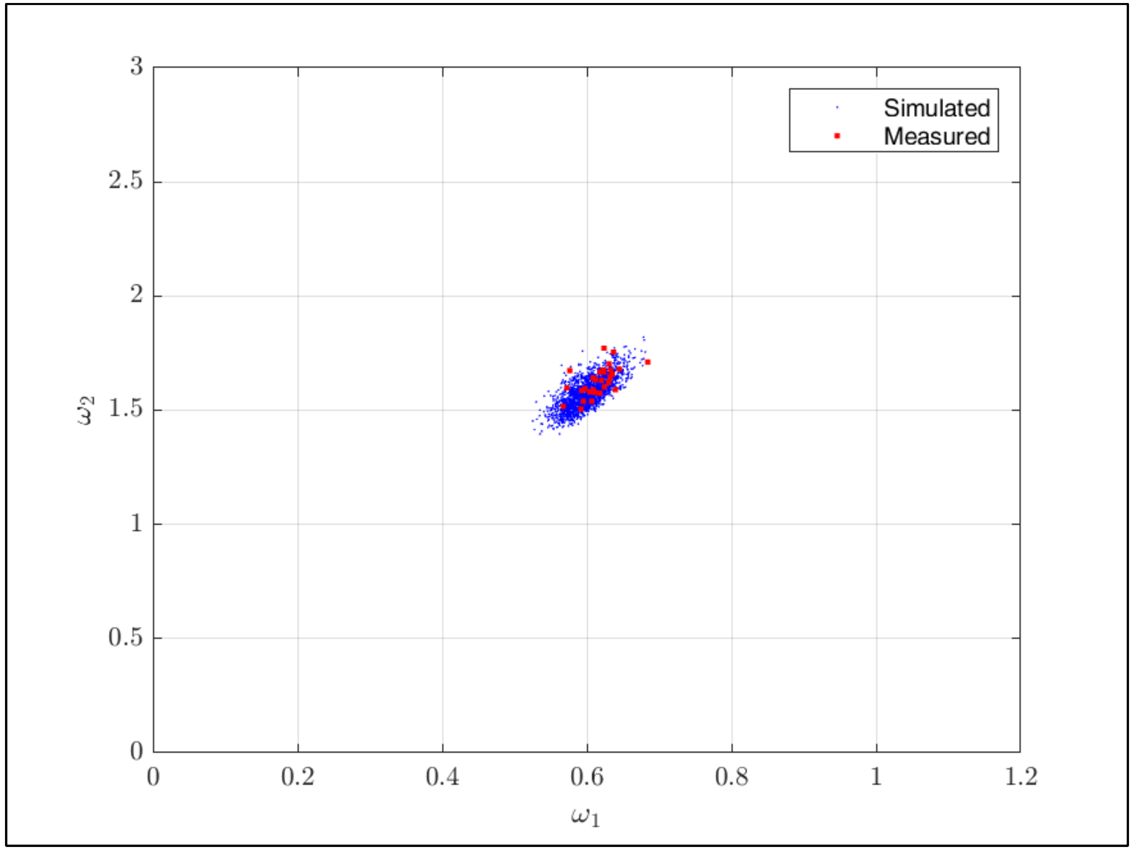


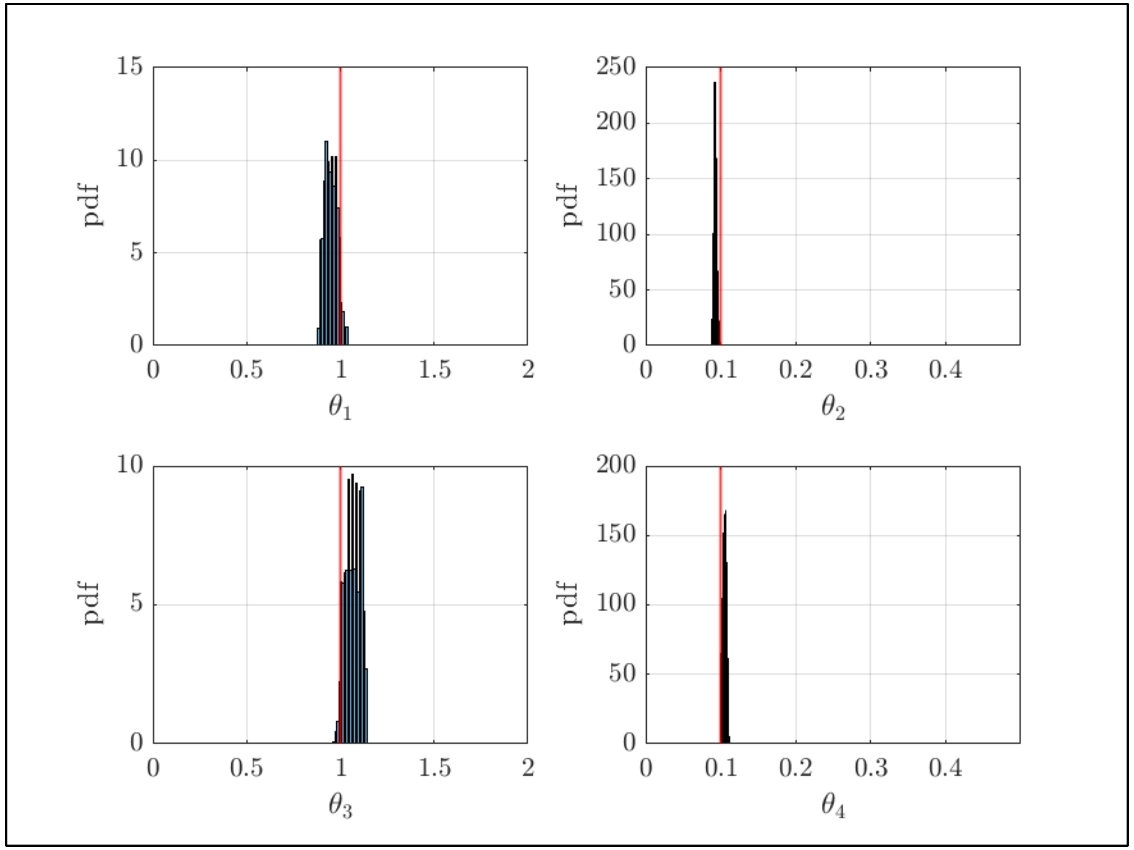
Example

- Two-degree-of-freedom oscillator









Faes, Matthias GR, Nadja Klein, Markus Pauly, Marcos A. Valdebenito, and Mauricio A. Misraji. "Approximate Bayesian Computation for Parameter Identification in Computational Mechanics."

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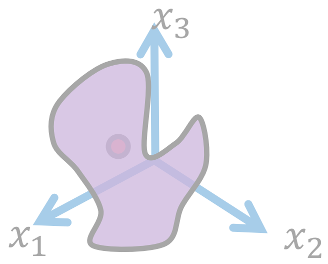
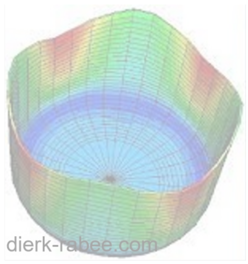
Random variables



Computational model



Key quantities:
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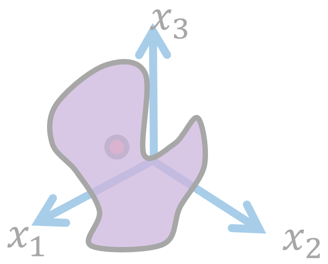
Step 3':
Sensitivity analysis

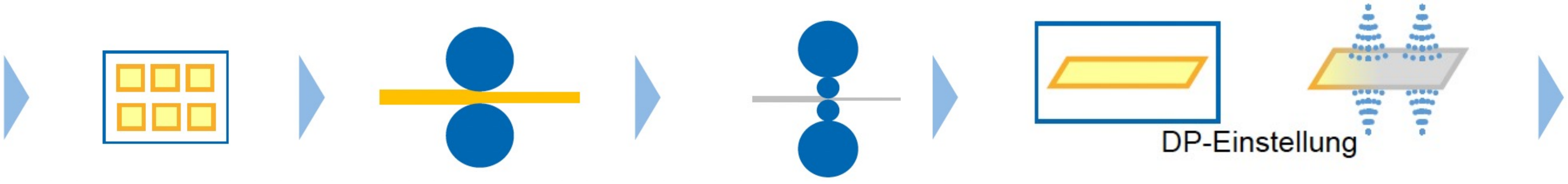
Measurement data



Step 3’: sensitivity analysis

Casting | Hot rolling | Cold rolling | Heat treatment

Base material



Resulting properties

Grain sizes
Grain boundaries
Initial damage
Stress-strain curves as-cast
Residual stresses
Plate material dimensions before rolling
…

Grain size and shape after rolling
Damage after cold rolling
Mechanical performance of as-rolled material
Residual stresses
Damage in the material
…

Final dimensions
Functional properties
…

Chemical composition
Alloy
Impurities

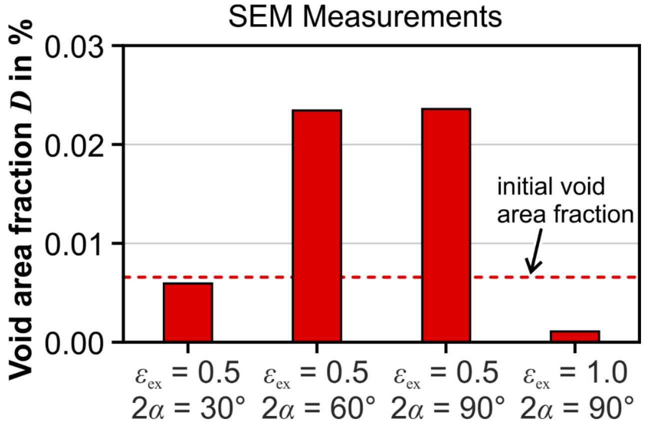
Plate dimensions after rolling
Residuals stresses
Strain-stress curves as-rolled
Damage after rolling
…

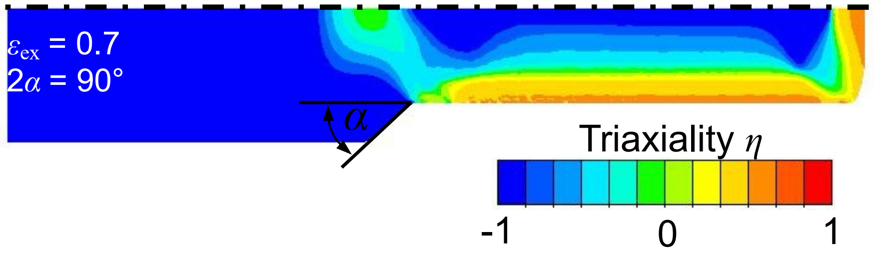
Grain size, type and shape after heat treatment
Mechanical performance
Damage state
…

Application of probabilistic methods in metal forming

- Damage is introduced during forward rod extrusion process
- Goal: predict damage numerically to optimize process a priori and *in silico*
- Challenge: many sources of uncertainty
  - Material parameters
    - Elastic
    - Damage model
  - Manufacturing parameters
    - Friction in the die
    - Flow characteristics

- Need for sensitivity analysis!





Böddecker, M., Faes, M. , Menzel, A., Valdebenito, M. (2023). Effect of uncertainty of material parameters on stress triaxiality and Lode angle in finite elasto-plasticity - a variance-based global sensitivity analysis. Advances in Industrial and Manufacturing Engineering. Volume 7 , November 2023, 100128

Application of probabilistic methods in metal forming

- First order sensitivity index (S_i)
  - Fraction of the variance of y that can be attributed to θ_i alone

$$S_i = \frac{\mathbb{V}_{\Theta_i}\left[\mathbb{E}_{\boldsymbol{\Theta}_{-i}}\left[y|\theta_i\right]\right]}{\mathbb{V}_{\boldsymbol{\Theta}}\left[y\right]}$$

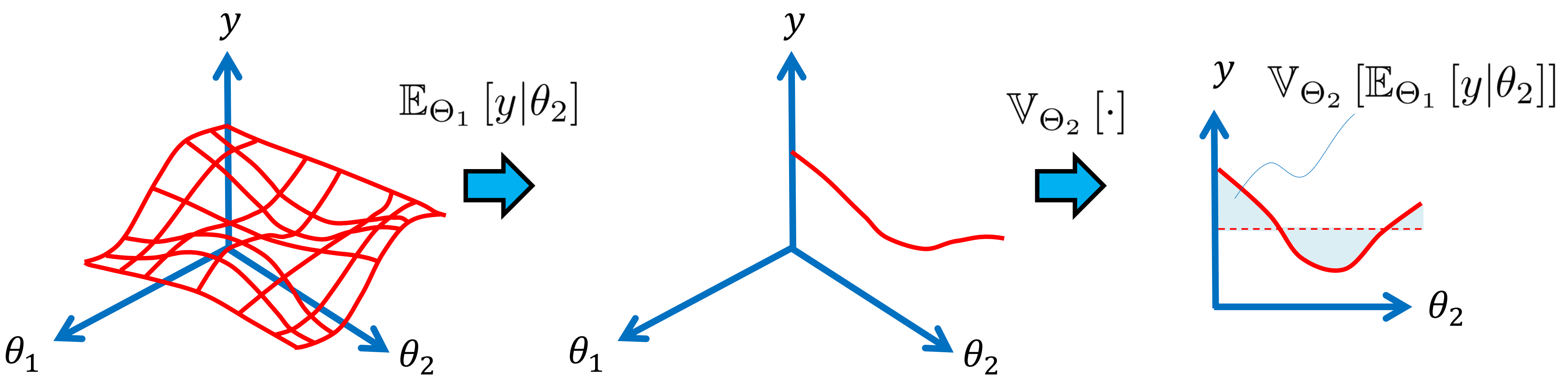
$\mathbb{E}_{\boldsymbol{\Theta}}[\cdot]$: Expected value w.r.t. $\boldsymbol{\Theta}$

$\mathbb{V}_{\boldsymbol{\Theta}}[\cdot]$: Variance w.r.t. $\boldsymbol{\Theta}$

$\boldsymbol{\Theta} = \{\Theta_1, \ldots, \Theta_{n_\theta}\}$

$\boldsymbol{\Theta}_{-i} = \{\Theta_1, \ldots, \Theta_{i-1}, \Theta_{i+1}, \Theta_{n_\theta}\}$

  - Example: calculation of S_2 for model $y(\theta_1, \theta_2)$

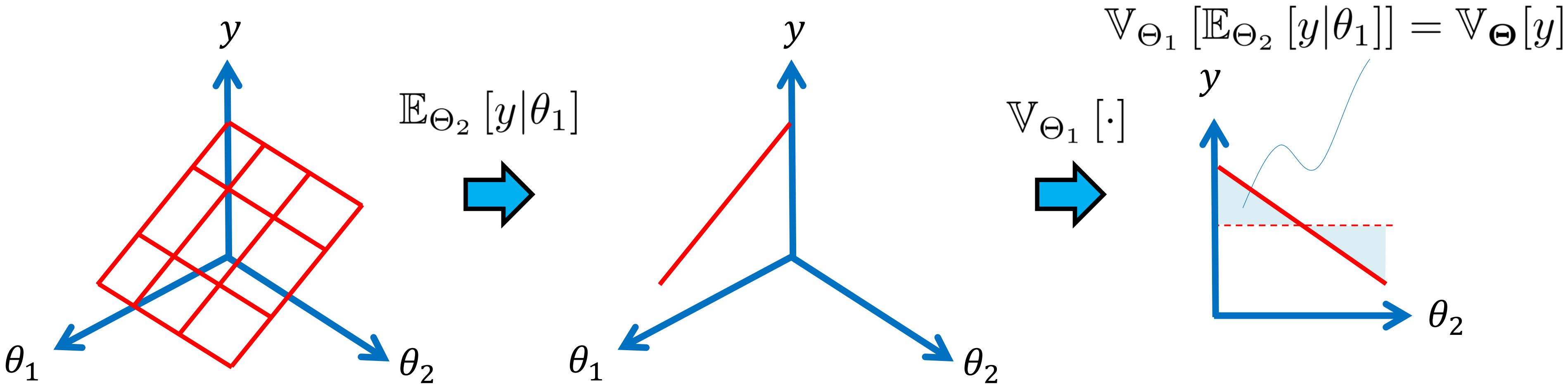


Application of probabilistic methods in metal forming

- Total sensitivity index (S_{T_i})
  - Fraction of the variance of y that can be attributed to θ_i and all its interactions with other variables

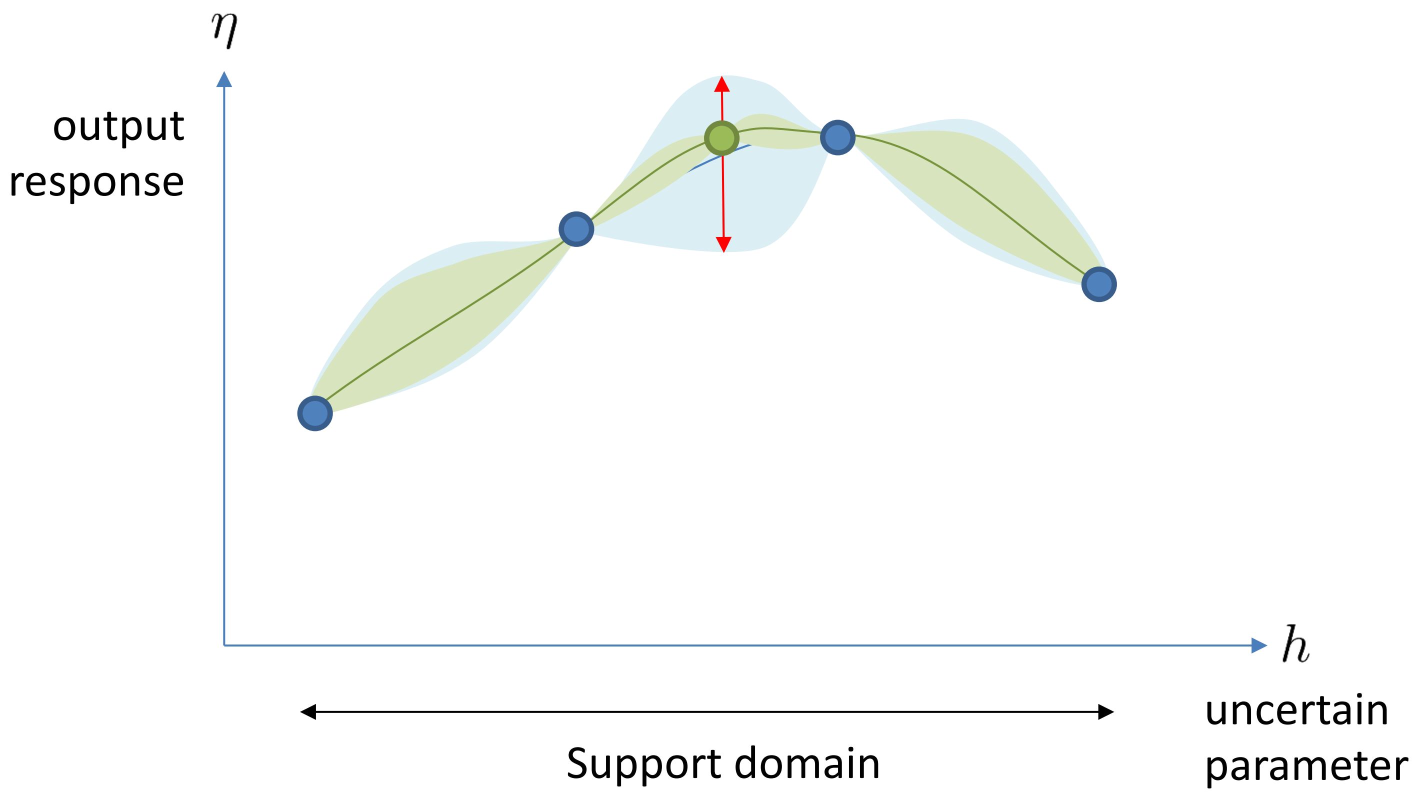
$$S_{T_i} = 1 - \frac{\mathbb{V}_{\boldsymbol{\Theta}_{-i}}\left[\mathbb{E}_{\Theta_i}\left[y|\boldsymbol{\theta}_{-i}\right]\right]}{\mathbb{V}_{\boldsymbol{\Theta}}\left[y\right]}$$

  - Example: calculation of S_{T_2} for model $y(\theta_1, \theta_2)$, $S_{T_2} = 0$



Application of probabilistic methods in metal forming

- Surrogate model is used to replace finite element simulations
- Bayesian active learning for Sobol indices



(1) Design of experiments / full system analyses

(2) Interpolation & confidence bounds

(3) Active learning / locate critical point

(4) Additional system analysis

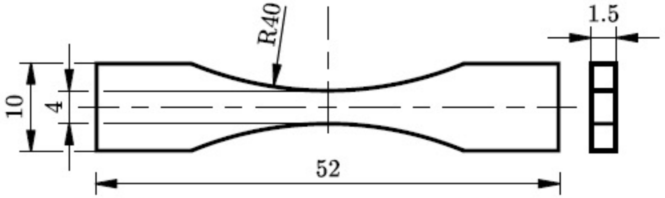
(5) Improve surrogate

J. Song, P. Wei, M. A. Valdebenito, M. Faes, and M. Beer, 'Data-driven and active learning of variance-based sensitivity indices with Bayesian probabilistic integration', *Mechanical Systems and Signal Processing*, vol. 163, p. 108106, Jan. 2022,

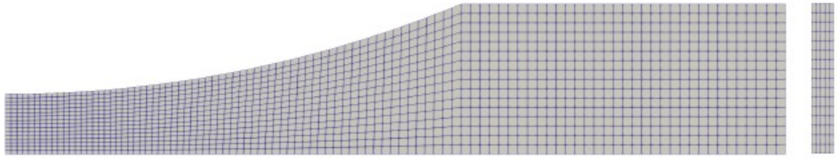
Application of probabilistic methods in metal forming

- Summary of results (1/2)

Model

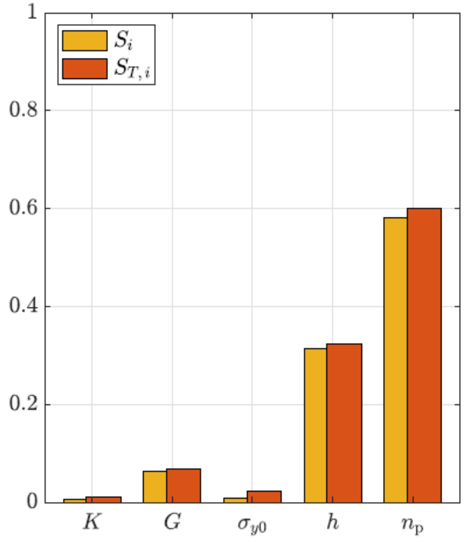


(a) Tensile test specimen geometry and dimensions.



(b) Spatial discretization of the tensile test specimen.

Results



(a) First-order and total order Sobol' sensitivity indices S_i and $S_{T,i}$ associated with maximum stress triaxiality η.

Table 3
First-order and total Sobol' sensitivity indices of stress triaxiality before active learning for different n_d and after convergence.

n_d	S_K [-]	S_G [-]	$S_{\sigma_{y0}}$ [-]	S_h [-]	S_{n_p} [-]
10	0.0000	0.1394	0.0000	0.3586	0.4857
30	0.0133	0.0812	0.0255	0.2778	0.5640
60	0.0185	0.0530	0.0075	0.3125	0.5682
60 + 145	0.0065	0.0622	0.0087	0.3134	0.5825
	$S_{T,K}$ [-]	$S_{T,G}$ [-]	$S_{T,\sigma_{y0}}$ [-]	$S_{T,h}$ [-]	S_{T,n_p} [-]
10	0.0000	0.1550	0.0000	0.3721	0.5027
30	0.0236	0.0915	0.0443	0.2938	0.6006
60	0.0322	0.0662	0.0134	0.3403	0.5980
60 + 145	0.0107	0.0690	0.0221	0.3234	0.6015

Böddecker, M., Faes, M. , Menzel, A., Valdebenito, M. (2023). Effect of uncertainty of material parameters on stress triaxiality and Lode angle in finite elasto-plasticity - a variance-based global sensitivity analysis. Advances in Industrial and Manufacturing Engineering. Volume 7 , November 2023, 100128

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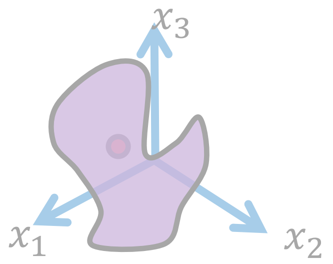
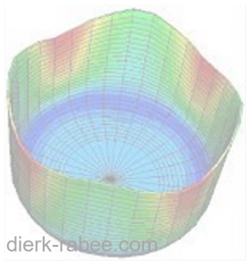


Computational model



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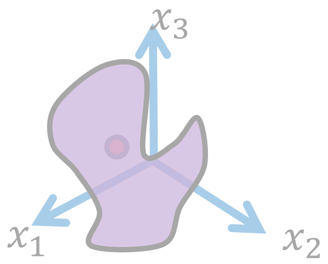
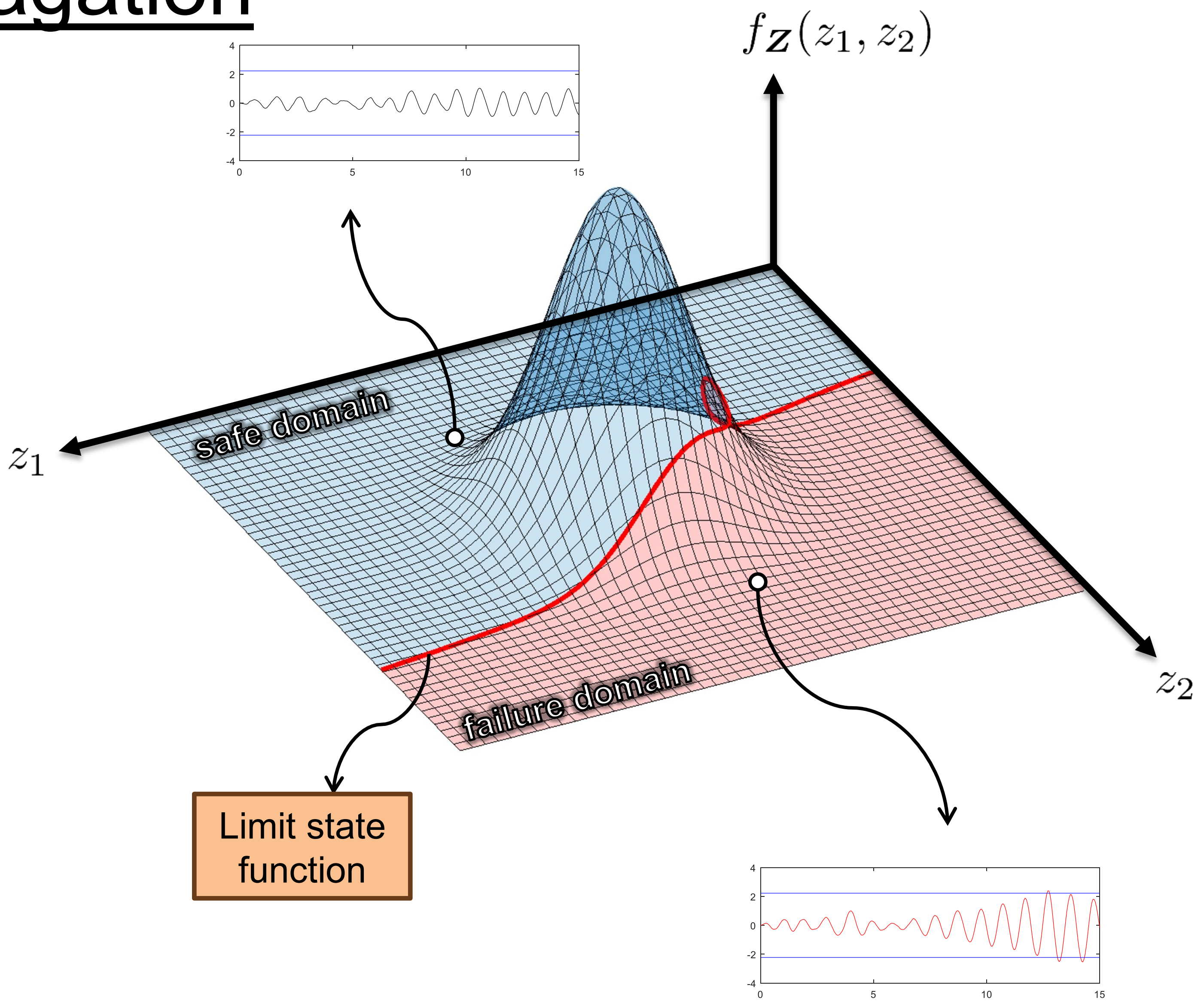


Step 3: uncertainty propagation

Gaussian Loading $\Rightarrow$ $p(t, \boldsymbol{z})$

Structural Properties $\Rightarrow$ $\boldsymbol{y} = \begin{Bmatrix} y_1 \\ y_2 \\ y_3 \\ \dots \end{Bmatrix}$

Design variables vector



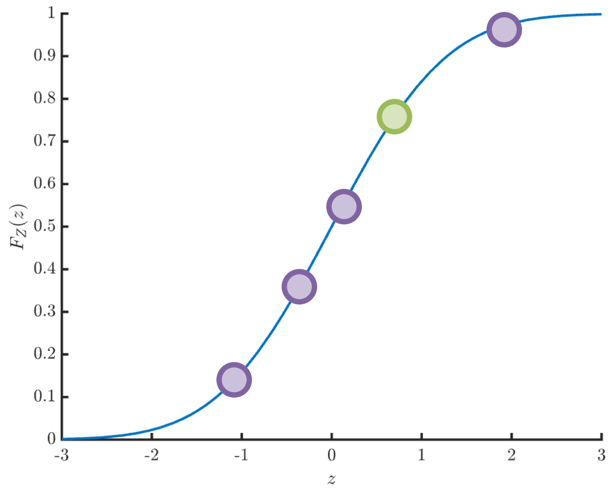
Of interest: first excursion probability:

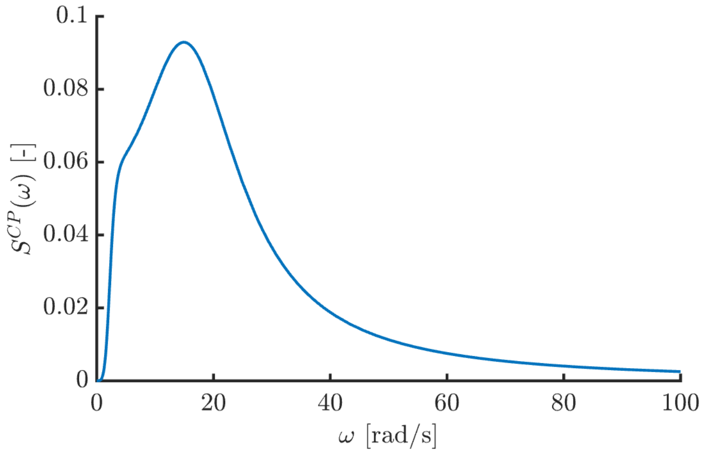
$$p_F = \int_{\boldsymbol{z} \in \mathbb{R}^{n_D}} I_F(\boldsymbol{y}, \boldsymbol{z}) \, f_Z(\boldsymbol{z}) d\boldsymbol{z}$$

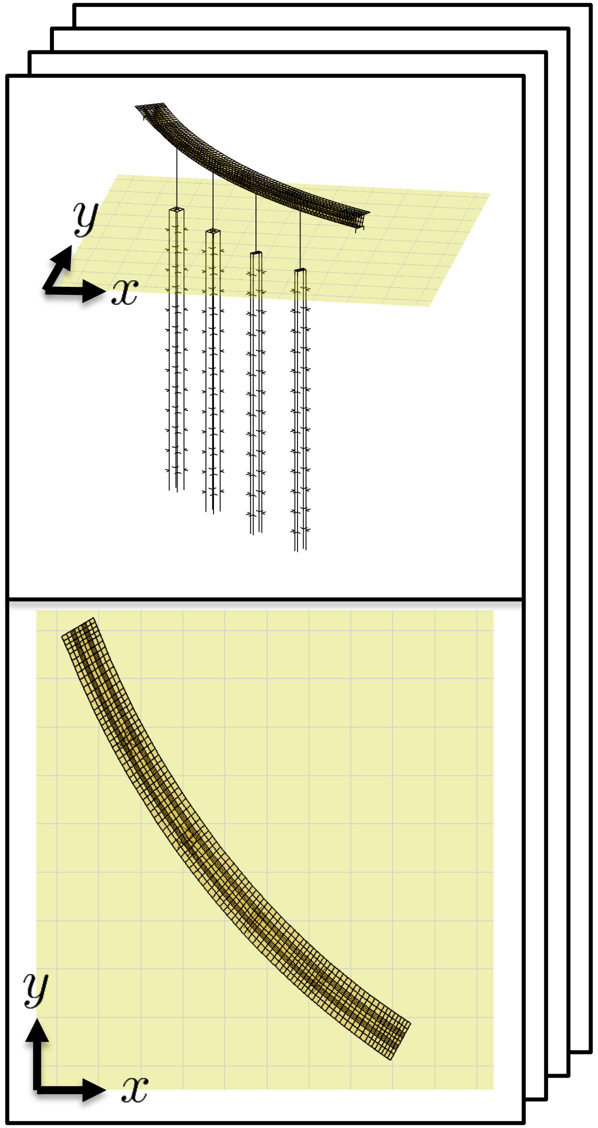
Indicator function

PDF, excitation

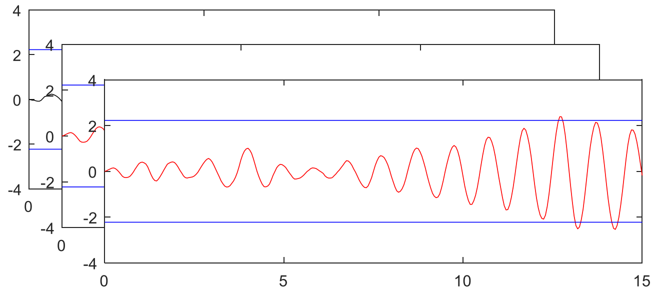
Reliability analysis





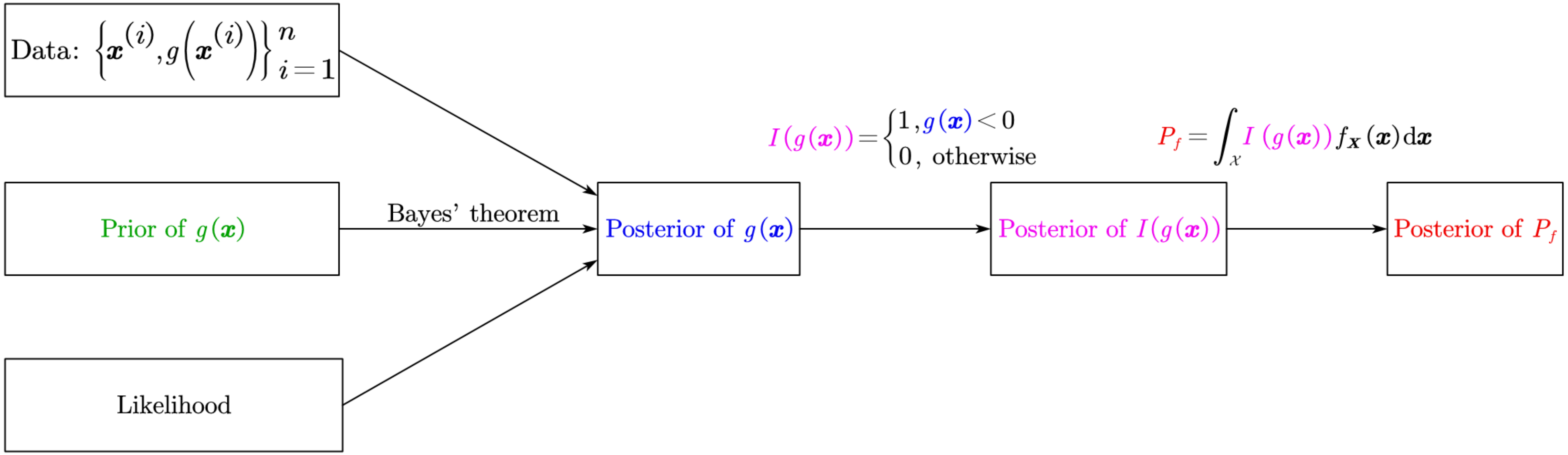


Aleatory	Deterministic model
p_F	$\eta(t)$



$$p_F = \int_{\boldsymbol{z}\in\mathbb{R}^{n_D}} I_F(\boldsymbol{y},\boldsymbol{z}) f_Z(\boldsymbol{z}) d\boldsymbol{z}$$

Bayesian active learning



Dang, Chao, Marcos A. Valdebenito, Matthias G.R. Faes, Pengfei Wei, and Michael Beer. "Structural Reliability Analysis: A Bayesian Perspective." *Structural Safety* 99 (November 2022): 102259.

Step 3: Bayesian active learning of the failure probability

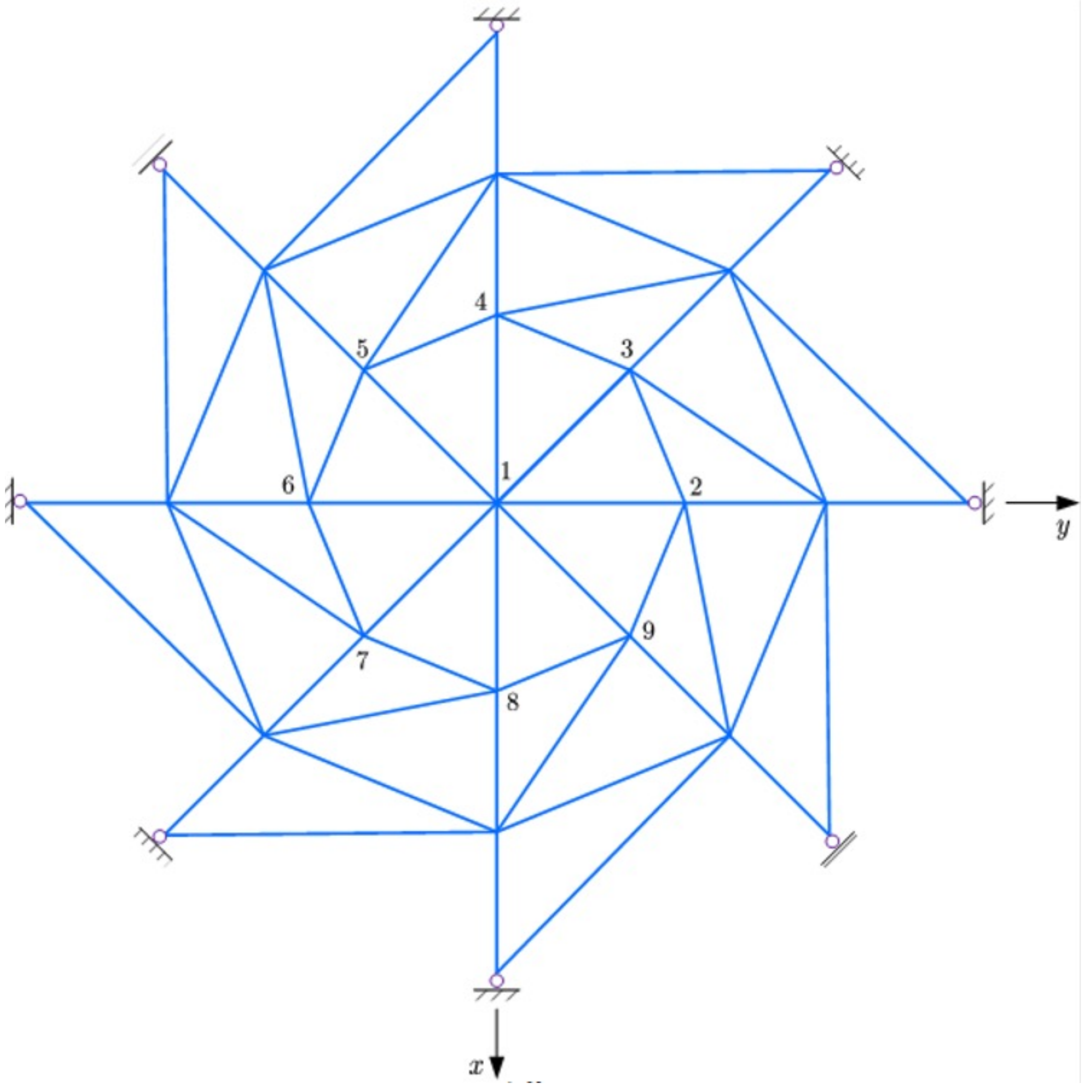
Idea	Method	Stopping Criterion	Learning function
Using the posterior mean	PBALQ [1]	$\frac{\int_{\mathcal{X}}\left[\Phi\left(-\frac{m_{g_n}(\boldsymbol{x})}{\sigma_{g_n}(\boldsymbol{x})}\right)-\Phi\left(-\frac{m_{g_n}(\boldsymbol{x})}{\sigma_{g_n}(\boldsymbol{x})}-b\right)\right]f_{\boldsymbol{X}}(\boldsymbol{x})\mathrm{d}\boldsymbol{x}}{\int_{\mathcal{X}}\Phi\left(-\frac{m_{g_n}(\boldsymbol{x})}{\sigma_{g_n}(\boldsymbol{x})}\right)f_{\boldsymbol{X}}(\boldsymbol{x})\mathrm{d}\boldsymbol{x}}<\epsilon$	$\mathrm{LF}(\boldsymbol{x})=\left[\Phi\left(-\frac{m_{g_n}(\boldsymbol{x})}{\sigma_{g_n}(\boldsymbol{x})}\right)-\Phi\left(-\frac{m_{g_n}(\boldsymbol{x})}{\sigma_{g_n}(\boldsymbol{x})}-b\right)\right]f_{\boldsymbol{X}}(\boldsymbol{x})$
Using the posterior variance also, but with simplification	QBALC [2]	$\frac{\sqrt{\tilde{\rho}}\int_{\mathcal{X}}\sqrt{\Phi\left(-\frac{m_{g_n}(\boldsymbol{x})}{\sigma_{g_n}(\boldsymbol{x})}\right)\Phi\left(\frac{m_{g_n}(\boldsymbol{x})}{\sigma_{g_n}(\boldsymbol{x})}\right)}f_{\boldsymbol{X}}(\boldsymbol{x})\mathrm{d}\boldsymbol{x}}{\int_{\mathcal{X}}\Phi\left(-\frac{m_{g_n}(\boldsymbol{x})}{\sigma_{g_n}(\boldsymbol{x})}\right)f_{\boldsymbol{X}}(\boldsymbol{x})\mathrm{d}\boldsymbol{x}}<\epsilon$	$\mathrm{LF}(\boldsymbol{x};p)=\sqrt{\Phi\left(-\frac{m_{g_n}(\boldsymbol{x})}{p\sigma_{g_n}(\boldsymbol{x})}\right)\Phi\left(\frac{m_{g_n}(\boldsymbol{x})}{p\sigma_{g_n}(\boldsymbol{x})}\right)}f_{\boldsymbol{X}}(\boldsymbol{x})$
	WBALC [3]	$\frac{\hat{\lambda}_{\hat{I}_n}}{\hat{m}_{\hat{P}_{f,n}}}<\epsilon$	$LF(\boldsymbol{u})=\sigma_{\tilde{\mathcal{G}}_n}(\boldsymbol{u})\boldsymbol{\Phi}\left(-\frac{m_{\tilde{\mathcal{G}}_n}(\boldsymbol{u})}{\sigma_{\tilde{\mathcal{G}}_n}(\boldsymbol{u})}\right)\boldsymbol{\Phi}\left(\frac{m_{\tilde{\mathcal{G}}_n}(\boldsymbol{u})}{\sigma_{\tilde{\mathcal{G}}_n}(\boldsymbol{u})}\right)\phi(\mathbf{u})$

[1] Dang, Chao, Matthias G.R. Faes, Marcos A. Valdebenito, Pengfei Wei, and Michael Beer. “Partially Bayesian Active Learning Cubature for Structural Reliability Analysis with Extremely Small Failure Probabilities.” *Computer Methods in Applied Mechanics and Engineering* 422 (March 2024): 116828.
[2] Dang, Chao, Alice Cicirello, Marcos A. Valdebenito, Matthias G.R. Faes, Pengfei Wei, and Michael Beer. “Structural Reliability Analysis with Extremely Small Failure Probabilities: A Quasi-Bayesian Active Learning Method.” *Probabilistic Engineering Mechanics* 76 (April 2024): 103613.
[3] Dang, Chao, Tong Zhou, Marcos A. Valdebenito, and Matthias G.R. Faes. “Yet Another Bayesian Active Learning Reliability Analysis Method.” *Structural Safety* 112 (January 2025): 102539.

An example: a 56-bar truss structure

$$g(P_1, P_2, \cdots, P_9, E, A) = \Delta - V_1(P_1, P_2, \cdots, P_9, E, A),$$

Method	ε	N_{call}	$\widehat{P}_f$	$\delta\widehat{P}_f$
IS	–	66,107	$4.94 \cdot 10^{-8}$	1.00%
AK-MCMC	–	465.00	$4.97 \cdot 10^{-8}$	2.92%
PBALC	$\varepsilon_2 = 5.00\%$	26.90	$4.85 \cdot 10^{-8}$	4.61%
SBALQ	$\varepsilon = 4.00\%$	31.40	$4.77 \cdot 10^{-8}$	5.32%
QBALC	$\varepsilon = 5.00\%$	29.20	$4.69 \cdot 10^{-8}$	6.42%
WBALQ	$\varepsilon = 4.00\%$	26.30	$4.87 \cdot 10^{-8}$	5.57%



General uncertainty quantification overview

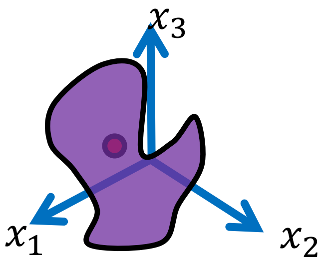
Step 2:
Quantification of sources of uncertainty

Step 1:
Model the system and assessment criteria

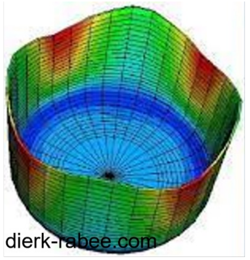
Step 3:
Uncertainty propagation

Step 2':
Stochastic model updating

Random variables



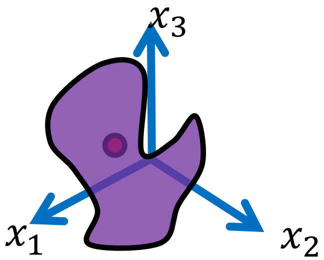
Computational model



Key quantities:
- Mean / variance / skewness / kurtosis
- Probability of failure
- Probability density of response

Step 3':
Sensitivity analysis

Measurement data



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We are always happy to host guests from other groups to set-up and maintain joint collaborations, as well as to support the application of CSC and Humboldt Fellowships.