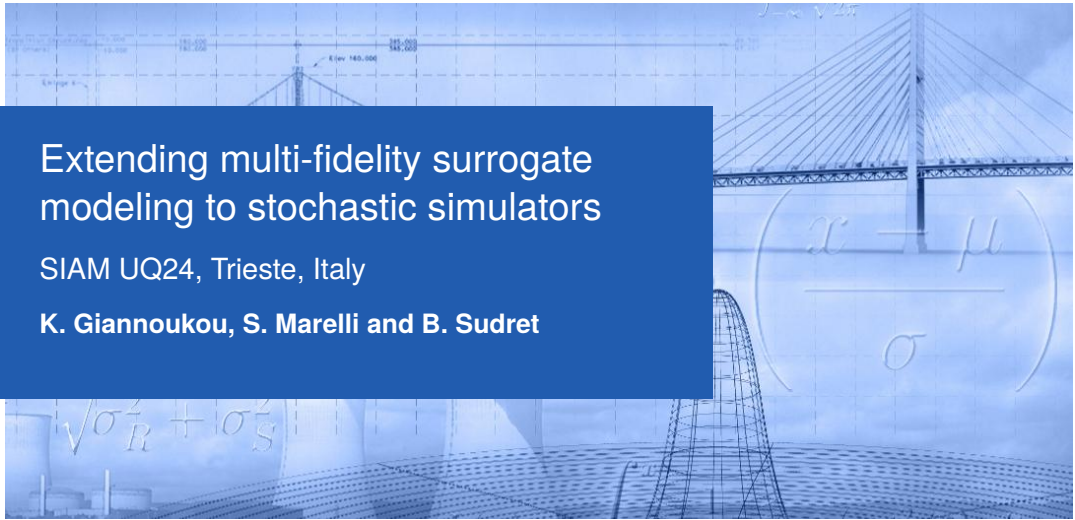
Extending multi-fidelity surrogate modelling to stochastic simulators

ETH zürich

Risk, Safety & Uncertainty Quantification



Extending multi-fidelity surrogate modeling to stochastic simulators

SIAM UQ24, Trieste, Italy

K. Giannoukou, S. Marelli and B. Sudret

Multi-fidelity surrogate modeling

	Accuracy	Cost	Available data	Examples		
				Mathematical/ Physical model	Discretization	Experiments/ Simulations
High fidelity	High	High	Little	Complex	Fine	Physical experiments
Low fidelity	Low	Low	More	Simplified	Coarse	Computer simulations

Image modified from Perez-Moreno *et al.* (2016) *Roadmap to the multidisciplinary design analysis and optimisation of wind energy systems*, J. Phys.: Conf. Ser.

Multi-fidelity surrogate modeling for deterministic simulators

Set-up

- Two levels of fidelity considered
- High-fidelity data $(\boldsymbol{\mathcal{X}}_{\mathsf{H}}, \mathcal{Y}_{\mathsf{H}})$

$$y_{\mathsf{H}}(\boldsymbol{x}) = \psi_{\mathsf{H}}(\boldsymbol{x}) + \varepsilon_{\mathsf{H}}, \quad \varepsilon_{\mathsf{H}} \sim f_{\varepsilon_{\mathsf{H}}}(\varepsilon_{\mathsf{H}}), \quad \mathbb{E}\left[\varepsilon_{\mathsf{H}}\right] = 0.$$

- Low-fidelity data $(\boldsymbol{\mathcal{X}}_{\mathsf{L}}, \mathcal{Y}_{\mathsf{L}})$

$$y_{\mathsf{L}}(\boldsymbol{x}) = \psi_{\mathsf{L}}(\boldsymbol{x}) + \varepsilon_{\mathsf{L}}, \quad \varepsilon_{\mathsf{L}} \sim f_{\varepsilon_{\mathsf{L}}}(\varepsilon_{\mathsf{L}}), \quad \mathbb{E}\left[\varepsilon_{\mathsf{L}}\right] = 0.$$

- PCE model $\hat{\psi}_{\mathsf{L}}(\boldsymbol{x}) \approx \psi_{\mathsf{L}}(\boldsymbol{x})$ trained on $(\boldsymbol{\mathcal{X}}_{\mathsf{L}}, \mathcal{Y}_{\mathsf{L}})$

Information fusion

$$\hat{\psi}_{\mathsf{H}}^{\mathsf{MF}}(\boldsymbol{x}) = \rho \cdot \hat{\psi}_{\mathsf{L}}(\boldsymbol{x}) + \delta(\boldsymbol{x}).$$

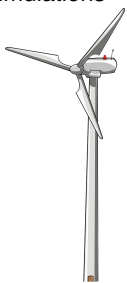
Beyond unbiased homoscedastic noise

Sources of stochasticity

- Unidentified variables
- Unmodeled low-importance variables
- Very high-dimensional problems

Application examples

- Physical experiments
- Epidemiology: disease spread models
- Wind turbine simulations



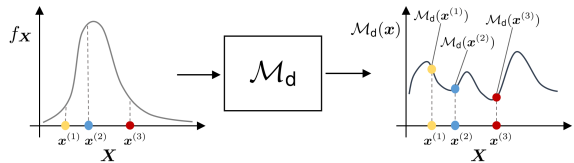
Implications

- Non deterministic input-output relation
- The model response at each point is a random variable

Stochastic simulators - formal definition

Deterministic simulators

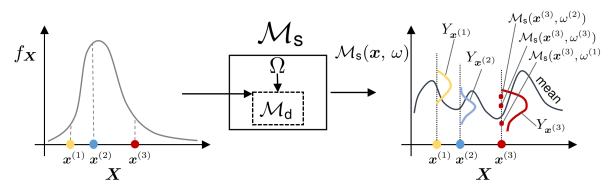
$$\mathcal{M}_{\mathsf{d}} : \mathcal{D}_{\boldsymbol{X}} \to \mathbb{R},$$
$$\boldsymbol{x} \mapsto \mathcal{M}_{\mathsf{d}}(\boldsymbol{x})$$



Stochastic simulators

$$\mathcal{M}_{\mathsf{s}} : \mathcal{D}_{\boldsymbol{X}} \times \Omega \to \mathbb{R},$$
$$(\boldsymbol{x}, \omega) \mapsto \mathcal{M}_{\mathsf{s}}(\boldsymbol{x}, \omega)$$

- For fixed $\boldsymbol{x}_0$, $Y_{\boldsymbol{x}_0} := \mathcal{M}_{\mathsf{s}}(\boldsymbol{x}_0, \omega) : \Omega \to \mathbb{R}$ is a random variable.
- For fixed ω_0, $\mathcal{M}_{\mathsf{s}}(\boldsymbol{x}, \omega_0) : \mathcal{D}_{\boldsymbol{X}} \to \mathbb{R}$ is a deterministic function (trajectory).



Emulating stochastic simulators

Need for stochastic emulators:

- High cost of stochastic simulators
- Tasks like uncertainty quantification, optimization, etc., require lots of runs

Current approaches:

- Replication-based approaches
  - Ankenman, Nelson & Staum (2010), Operations Research
  - Zhu & Sudret (2020), International Journal for Uncertainty Quantification
- Statistical approaches
  - McCullagh & Nelder (1989), Monographs on Statistics and Applied Probability
  - Zhu & Sudret (2021), SIAM/ASA Journal on Uncertainty Quantification
  - Zhu & Sudret (2023), International Journal for Uncertainty Quantification
- Random field-based approaches
  - Azzi, Huang, Sudret & Wiart (2019), International Journal for Uncertainty Quantification
  - Lüthen, Marelli & Sudret (2023), Computer Methods in Applied Mechanics and Engineering

Multi-fidelity stochastic emulators

Set-up

- High-fidelity stochastic simulator $\mathcal{M}_{\mathsf{s,H}}(\boldsymbol{x}, \omega)$ and $(\boldsymbol{\mathcal{X}}_{\mathsf{H}}, \mathcal{Y}_{\mathsf{H}}) = (\boldsymbol{x}_{\mathsf{H}}^{(i)}, y_{\mathsf{s,H}}^{(i)}),\ i = 1, ..., N_{\mathsf{H}}$. $\mathcal{M}_{\mathsf{s,H}}(\boldsymbol{x}, \omega)$ is evaluated once at each $\boldsymbol{x}_{\mathsf{H}}^{(i)}$.
- Low-fidelity deterministic simulator $\mathcal{M}_{\mathsf{L}}(\boldsymbol{x})$ and $(\boldsymbol{\mathcal{X}}_{\mathsf{L}}, \mathcal{Y}_{\mathsf{L}}) = (\boldsymbol{x}_{\mathsf{L}}^{(i)}, y_{\mathsf{L}}^{(i)}),\ i = 1, ..., N_{\mathsf{L}}$

Goal

Emulate the response PDF $Y_{\boldsymbol{x}} = Y|\boldsymbol{X} := \boldsymbol{x}$ of $\mathcal{M}_{\mathsf{s,H}}(\boldsymbol{x}, \omega)$ at each $\boldsymbol{x}$

Assumption

$$\mathcal{M}_{\mathsf{s,H}}(\boldsymbol{x}, \omega) = \underbrace{\rho \cdot \psi_{\mathsf{L}}(\boldsymbol{x})}_{\text{deterministic}} + \underbrace{\delta_{\mathsf{s}}(\boldsymbol{x}, \omega)}_{\text{stochastic}}$$

Multi-fidelity stochastic emulators: our approach

$$\widehat{\mathcal{M}}^{\mathsf{MF}}_{\mathsf{s,H}}(\boldsymbol{x},\omega) = \hat{\rho}\cdot\hat{\psi}_{\mathsf{L}}(\boldsymbol{x}) + \hat{\delta}_{\mathsf{s}}(\boldsymbol{x},\omega)$$

1. Train PCE model $\hat{\psi}_{\mathsf{L}}(\boldsymbol{x}) = \sum_{\alpha\in\mathcal{A}_{\mathsf{L}}} c_{\alpha,\mathsf{L}}\Psi_{\alpha}(\boldsymbol{x})$ on $(\boldsymbol{\mathcal{X}}_{\mathsf{L}}, \mathcal{Y}_{\mathsf{L}})$

2. $\hat{\rho} = \mathbb{E}_{\boldsymbol{x}}\left[\dfrac{\mathcal{M}_{\mathsf{s,H}}(\boldsymbol{x},\omega)}{\hat{\psi}_{\mathsf{L}}(\boldsymbol{x})}\right] \approx \dfrac{1}{N_H}\sum_{i=1}^{N_H}\dfrac{y^{(i)}_{\mathsf{s,H}}}{\hat{\psi}_{\mathsf{L}}(\boldsymbol{x}^{(i)}_{\mathsf{H}})}$

3. Construct stochastic emulator for $\delta_{\mathsf{s}}(\boldsymbol{x},\omega)$

   3.1 Obtain $(\boldsymbol{\mathcal{X}}_{\delta}, \mathcal{Y}_{\delta}) = (\boldsymbol{\mathcal{X}}_{\mathsf{H}}, \{y^{(i)}_{\mathsf{s,H}} - \hat{\rho}\widehat{\psi}_{\mathsf{L}}(\boldsymbol{x}^{(i)}_{\mathsf{H}}), i = 1,...,N_{\mathsf{H}}\})$

   3.2 Train stochastic emulator $\hat{\delta}_{\mathsf{s}}(\boldsymbol{x},\omega)$

Zhu & Sudret (2021) *Emulation of stochastic simulators using generalized lambda models.*, SIAM/ASA J. Unc. Quant.

Generalized lambda models (GLaM)

Zhu & Sudret (2021), SIAM/ASA J. Unc. Quant.

- Assumption: $Y_{\boldsymbol{x}} = Y|\boldsymbol{X} = \boldsymbol{x}$ belongs to the family of generalized lambda distribution (GLD)

$$Y_{\boldsymbol{x}} \sim \mathrm{GLD}\left(\lambda_1(\boldsymbol{x}), \lambda_2(\boldsymbol{x}), \lambda_3(\boldsymbol{x}), \lambda_4(\boldsymbol{x})\right)$$

- The GLD can approximate the most common unimodal distributions, e.g.: Gaussian, Lognormal, Exponential, Weibull, etc.
- The GLD parametrizes the quantile function $Q = F^{-1}(u)$:

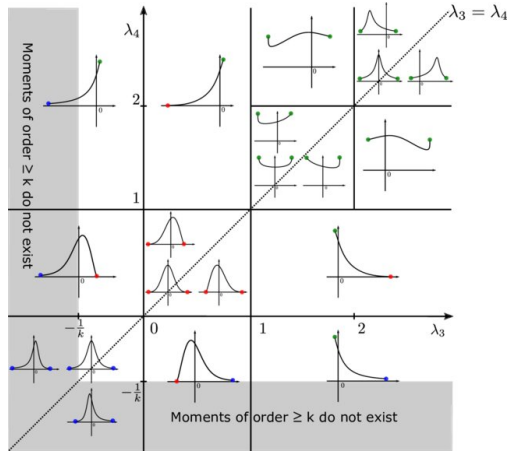
$$Q(u;\boldsymbol{\lambda}) = \lambda_1 + \frac{1}{\lambda_2}\left(\frac{u^{\lambda_3}-1}{\lambda_3} - \frac{(1-u)^{\lambda_4}-1}{\lambda_4}\right)$$

The PDF is given by

$$f_Y(y;\boldsymbol{\lambda}) = \frac{1}{Q'(u;\boldsymbol{\lambda})} = \frac{\lambda_2}{u^{\lambda_3-1}+(1-u)^{\lambda_4-1}}\mathbb{1}_{[0,1]}(u), \qquad u = Q^{-1}(y;\boldsymbol{\lambda})$$

GLD parameters

- λ_1: location parameter
- $\lambda_2 > 0$: scaling parameter
- λ_3, λ_4: shape parameters
  - Shape:
    - $\lambda_3 = \lambda_4$: symmetric PDFs
    - $\lambda_3, \lambda_4 < 1$: bell-shaped PDFs
  - Boundedness:
    - $\lambda_3 > 0$: PDF support left-bounded
    - $\lambda_4 > 0$: PDF support right-bounded



Zhu & Sudret (2020) *Replication-based emulation of the response distribution of stochastic simulators using generalized lambda distributions* , Int. J. Unc. Quant.

Generalized lambda models

$$Y_{\boldsymbol{x}} \sim \mathrm{GLD}\left(\lambda_1(\boldsymbol{x}), \lambda_2(\boldsymbol{x}), \lambda_3(\boldsymbol{x}), \lambda_4(\boldsymbol{x})\right)$$

Polynomial chaos expansions for $\boldsymbol{\lambda}$:

$$\lambda_k(\boldsymbol{x}) \approx \lambda_k^{\mathrm{PC}}(\boldsymbol{x}; \boldsymbol{c}) = \sum_{\boldsymbol{\alpha} \in \mathcal{A}_k} c_{k,\boldsymbol{\alpha}} \psi_{\boldsymbol{\alpha}}(\boldsymbol{x}), \quad k = 1, 3, 4$$

$$\lambda_2(\boldsymbol{x}) \approx \lambda_2^{\mathrm{PC}}(\boldsymbol{x}; \boldsymbol{c}) = \exp\left(\sum_{\boldsymbol{\alpha} \in \mathcal{A}_2} c_{2,\boldsymbol{\alpha}} \psi_{\boldsymbol{\alpha}}(\boldsymbol{x})\right)$$

Fitting procedure:

- Global model for the joint PDF of inputs and outputs: $f_{\boldsymbol{X},Y}(\boldsymbol{x}, y) = f_{Y|\boldsymbol{X}}(y \mid \boldsymbol{x}) \cdot f_{\boldsymbol{X}}(\boldsymbol{x})$
- GLD model for the conditional PDF: $f_{\boldsymbol{X},Y}^{\mathrm{GLD}}(\boldsymbol{x}, y; \boldsymbol{c}) = f_{Y|\boldsymbol{X}}^{\mathrm{GLD}}\left(y; \boldsymbol{\lambda}^{\mathrm{PC}}(\boldsymbol{x}; \boldsymbol{c})\right) \cdot f_{\boldsymbol{X}}(\boldsymbol{x})$
- Estimate the coefficients by minimizing the Kullback-Leibler divergence between $f_{\boldsymbol{X},Y}$ and $f_{\boldsymbol{X},Y}^{\mathrm{GLD}}$:

$$\hat{\boldsymbol{c}} = \arg\max_{\boldsymbol{c}} \frac{1}{N} \sum_{i=1}^{N} \log f_{Y|\boldsymbol{X}}^{\mathrm{GLD}}\left(y^{(i)}; \boldsymbol{\lambda}^{\mathrm{PC}}\left(\boldsymbol{x}^{(i)}; \boldsymbol{c}\right)\right)$$

Putting everything together

Setting

- High fidelity: stochastic simulator $\mathcal{M}_{\mathsf{s,H}}(\boldsymbol{x}, \omega)$
- Low fidelity: deterministic simulator $\mathcal{M}_{\mathsf{L}}(\boldsymbol{x})$

Goal

Emulate the HF response PDF $Y_{\boldsymbol{x}} := Y|\boldsymbol{X} = \boldsymbol{x}$ at each $\boldsymbol{x}$

Multi-fidelity stochastic emulator

$$\widehat{\mathcal{M}}^{\mathsf{MF}}_{\mathsf{s,H}}(\boldsymbol{x}, \omega) = \hat{\rho} \cdot \hat{\psi}_{\mathsf{L}}(\boldsymbol{x}) + \hat{\delta}_{\mathsf{s}}(\boldsymbol{x}, \omega)$$

$\hat{\rho}$: $\mathbb{E}_{\boldsymbol{x}}\left[\frac{\mathcal{M}_{\mathsf{s,H}}(\boldsymbol{x},\omega)}{\hat{\psi}_{\mathsf{L}}(\boldsymbol{x})}\right]$

$\hat{\psi}_{\mathsf{L}}(\boldsymbol{x})$: PCE

$\hat{\delta}_{\mathsf{s}}(\boldsymbol{x}, \omega)$: GLaM

Toy example: Borehole function

$$f(\boldsymbol{x}) = \frac{2\pi t_u (h_u - h_l)}{\ln(r/r_w)\left(1 + \frac{2lt_u}{\ln(r/r_w) r_w^2 k_w} + \frac{t_u}{t_l}\right)}$$

Variable	Distribution
R_w	$\mathcal{N}([0.1, 0.016])$
H_u	$\mathcal{U}([990, 1110])$
K_w	$\mathcal{U}([9855, 12045])$
R	$\mathcal{LN}([7.71, 1.0056])$
T_u	$\mathcal{U}([63070, 115600])$
T_l	$\mathcal{U}([63.1, 116])$
H_l	$\mathcal{U}([700, 820])$
L	$\mathcal{U}([1120, 1680])$

High-fidelity stochastic model [1]:

- Three input random variables $\mathbf{X}_{\mathsf{H}} = (R_w, H_u, K_w)$
- Five latent variables $\boldsymbol{\Xi} = (R, T_u, T_l, H_l, L)$
- $f_{\mathsf{s,H}}(\boldsymbol{x}_{\mathsf{H}}; \omega) = f(r_w, h_u, k_u; \xi)$

Low-fidelity deterministic model:

- Two input random variables $\mathbf{X}_{\mathsf{L}} = (R_w, H_u)$
- The other variables fixed at their means
- $f_{\mathsf{L}} = \frac{5\mu_{T_u}(h_u - \mu_{h_l})}{\ln(\mu_r/r_w)\left(1.5 + \frac{2\mu_l \mu_{t_u}}{\ln(\mu_r/r_w) r_w^2 \mu_{k_w}} + \frac{\mu_{t_u}}{\mu_{t_l}}\right)}$

[1] Lüthen *et al.* (2023) *A spectral surrogate model for stochastic simulators computed from trajectory samples*, Comput. Meth. Appl. Mech. Eng.

Validation set-up

Global convergence of conditional distributions

- Error measure:

$$\epsilon = \mathbb{E}_{\boldsymbol{X}}\left[\frac{d_{\mathrm{WS}}(\mathcal{M}_{\mathsf{s}}(\boldsymbol{X},\omega),\widehat{\mathcal{M}}_{\mathsf{s}}(\boldsymbol{X},\omega))}{\sigma(\mathcal{M}_{\mathsf{s}}(\boldsymbol{X},\omega))}\right],$$

  where d_{WS} is the *Wasserstein distance of order two* between two random variables with inverse CDF Q_1, Q_2:

$$d_{\mathrm{WS}}\left(Y_1, Y_2\right) = \left\|Q_1 - Q_2\right\|_2 = \sqrt{\int_0^1 \left(Q_1(u) - Q_2(u)\right)^2 \,\mathrm{d}u}.$$

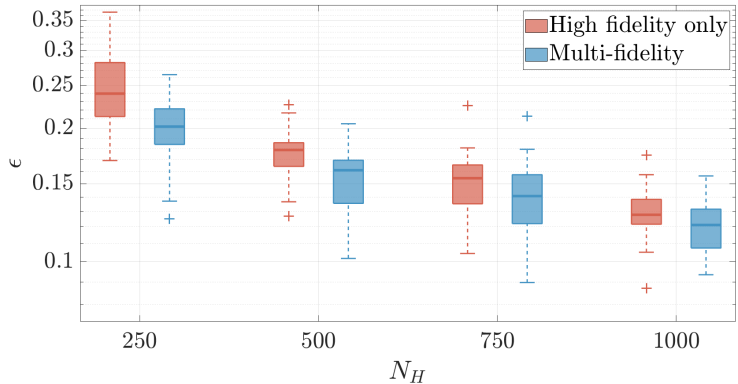
- Test set $\boldsymbol{\mathcal{X}}_{\mathrm{t}}$ of size $N_{\mathrm{t}} = 10^3$; for each $\boldsymbol{x}_{\mathrm{t}} \in \boldsymbol{\mathcal{X}}_{\mathrm{t}},\ N_{\mathsf{v}} = 10^4$ model evaluations for $Y_{\boldsymbol{x}_{\mathrm{t}}}$
- Comparison between $\widehat{\mathcal{M}}_{\mathsf{s},\mathsf{H}}(\boldsymbol{x},\omega)$ and $\widehat{\mathcal{M}}^{\mathsf{MF}}_{\mathsf{s},\mathsf{H}}(\boldsymbol{x},\omega)$

Point-wise approximation of conditional distributions

- Stochastic simulator and emulator responses at selected points

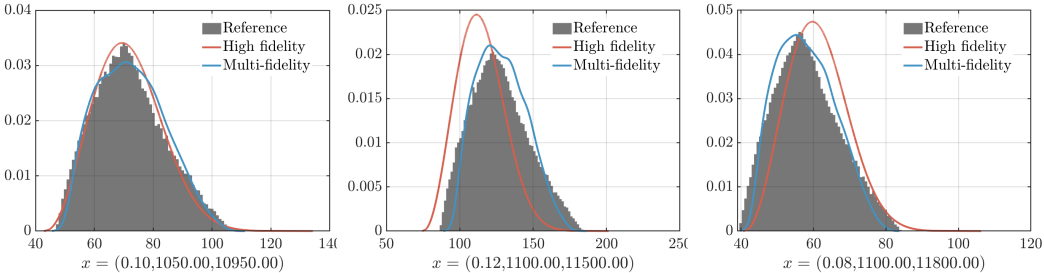
Results: performance vs experimental design size

- HF experimental design of size $N_{\mathrm{H}} \in \{250, 500, 750, 1000\}$
- LF experimental design size fixed: $N_{\mathrm{L}} = 500$
- 25 independent runs for each scenario



Results: point-wise approximation of conditional distributions

- HF experimental design size: $N_{\mathsf{H}} = 250$
- 10^4 replications as a reference



Concluding remarks

Conclusions

- Stochastic simulators necessary due to inherent stochasticity in models and measurements
- Need for stochastic emulators
- Constructed a multi-fidelity stochastic emulator considering a HF stochastic simulator and a LF deterministic simulator
- The MF stochastic emulator can achieve faster global convergence and better point-wise approximation of the conditional distributions
- Stochastic emulator method used: GLaM

Next steps

- Multi-fidelity stochastic emulator for the case where both the HF and LF models are stochastic
- Consider different stochastic emulator methodologies

References

Ankenman, B., B. Nelson, and J. Staum (2010). Stochastic Kriging for simulation metamodeling. *Oper. Res. 58*, 371–382.

Azzi, S., Y. Huang, B. Sudret, and J. Wiart (2019). Surrogate modeling of stochastic functions – application to computational electromagnetic dosimetry. *Int. J. Unc. Quant. 9*(4), 351–363.

Lüthen, N., S. Marelli, and B. Sudret (2023). A spectral surrogate model for stochastic simulators computed from trajectory samples. *Comput. Meth. Appl. Mech. Eng. 406*(115875), 1–29.

McCullagh, P. and J. Nelder (1989). *Generalized Linear Models*, Volume 37 of *Monogr. Stat. Appl. Prob.* Chapman and Hall.

Zhu, X. and B. Sudret (2020). Replication-based emulation of the response distribution of stochastic simulators using generalized lambda distributions. *Int. J. Unc. Quant. 10*(3), 249–275.

Zhu, X. and B. Sudret (2021). Emulation of stochastic simulators using generalized lambda models. *SIAM/ASA J. Unc. Quant. 9*(4), 1345–1380.

Zhu, X. and B. Sudret (2023). Stochastic polynomial chaos expansions to emulate stochastic simulators. *Int. J. Unc. Quant. 13*(2), 31–52.

Thank you for your attention!

Chair of Risk, Safety & Uncertainty Quantification

The GREYDIENT project

The UQ Software:

UQLab

UQ[py]Lab

The project leading to this application has received funding from the European Union's Horizon 2020 research and innovation program under the Marie Skłodowska-Curie grant agreement No 955393