Technische Universität Braunschweig

Institut für Dynamik und Schwingungen

Global Sensitivity Analysis for Vector-Valued Responses of Mechanical Models

Master's Thesis Presentation

Prateek Bhustali, September 27, 2021
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Index

Goal

To study global sensitivities of models with vector-valued responses and demonstrate their efficient computation using surrogate models.

Outline

1. Uncertainty Quantification Primer
2. Surrogate modeling
3. Sensitivity Analysis
4. Chaboche Model
5. Results

What is Uncertainty Quantification?

Uncertainty Quantification (UQ) deals with the quantitative characterization and reduction of uncertainties in mathematical models [Sul15, LMK10, Xiu10].

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Types of uncertainties:

- **Aleatory Uncertainty**: inherent, irreducible uncertainties
- **Epistemic Uncertainty**: lack of knowledge, reducible uncertainties

Example: Mechanical oscillator

Example from [AGS20]:

$$\ddot{y} + 2\alpha\dot{y} + (\alpha^2 + \beta^2)y = 0,$$
$$y(0) = \ell, \dot{y}(0) = 0.$$

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$$\alpha \sim \mathcal{U}(3/8, 5/8),$$
$$\beta \sim \mathcal{U}(10/4, 15/4),$$
$$\ell \sim \mathcal{U}(-5/4, -3/4).$$

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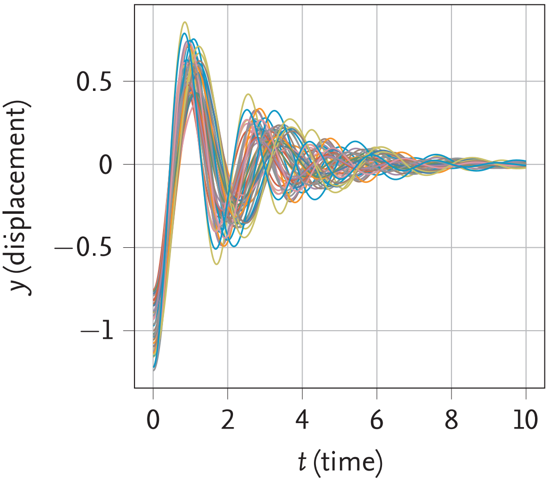

Monte Carlo methods

Let's estimate the mean position of the block at $t = 2$s using N Monte Carlo (MC) samples,

$$\tilde{\mathbb{E}}[y_{t=2}] = \frac{1}{N}\sum_{k=1}^{N} y(t = 2; \xi^{(k)})$$

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Due to the sampling error ϵ_N, the estimate above differs from the true mean $\mathbb{E}[y_{t=2}]$ given as:

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- MC convergence rate: $\mathcal{O}(1/\sqrt{N})$

$\implies$ MC methods are slow and expensive

Surrogate modeling

Idea: *Approximate the solution manifold Υ using models that are computationally inexpensive to evaluate.*

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Input(s)

$$\boldsymbol{\xi} = [\xi_1, \xi_2, \ldots\ldots, \xi_{N_p}]$$
$$t_s \in \mathcal{T}$$
$$s \in \{1, \ldots, m\}$$

Model

$$\mathcal{M}(t_s, \boldsymbol{\xi})$$

$$\wr\wr$$

Surrogate

$$\tilde{\mathcal{M}}(t_s, \boldsymbol{\xi})$$

Output(s)

$$\boldsymbol{\Upsilon} = (\Upsilon_{t_1}, \ldots, \Upsilon_{t_m})$$
$$\tilde{\boldsymbol{\Upsilon}} = (\tilde{\Upsilon}_{t_1}, \ldots, \tilde{\Upsilon}_{t_m})$$

Surrogate modeling

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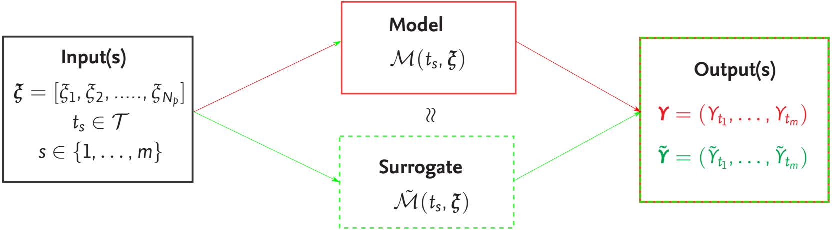

For example: **Polynomial Chaos Expansions, Karhunen-Loève Expansion with PCE approximated modes**, Neural Networks, Gaussian Processes etc.

Polynomial Chaos Expansion (PCE)

A *spectral method* that approximates the solution manifold Υ using a polynomial basis [LMK10].

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$$\mathcal{M}(t, \xi) \approx \tilde{\mathcal{M}}^{PC}(t, \xi) = \sum_{k=1}^{N_{PC}} c_k(t) \Psi_k(\xi),$$

$\{\Psi_k(\xi)\}_{k=1}^{N_{PC}}$: multivariate orthonormal polynomial basis and $\{c_k\}_{k=1}^{N_{PC}}$: basis coefficients.

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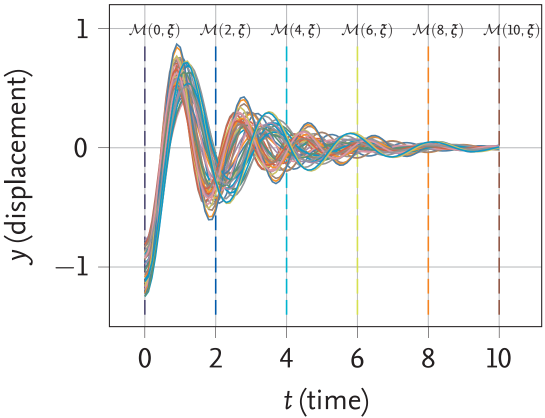
- Local surrogate must be built at each point in time (time-frozen surrogates).



Karhunen-Loève Expansion

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Karhunen-Loève Expansion (KLE):

$$\mathcal{M}(t, \xi) \approx \tilde{\mathcal{M}}^{KL}(t, \xi) = \sum_{i=1}^{N_{kl}} \Phi_i(\xi) \boldsymbol{e}_i(t),$$

$\{\boldsymbol{e}_i(t)\}_{i=1}^{N_{kl}}$: eigenfunctions of the covariance operator of $\mathcal{M}(t, \xi)$ and $\{\Phi_i(\xi)\}_{i=1}^{N_{kl}}$: expansion coefficients.

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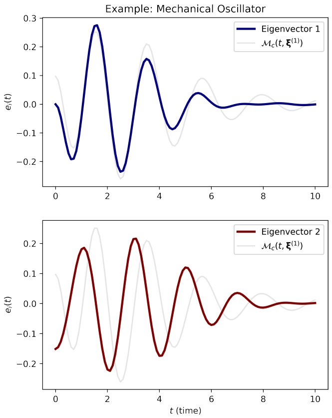

Karhunen-Loève Expansion with PCE approximated modes

However, $\Phi_i(\xi)$ are approximated using PCE, which leads to

$$\Phi_i(\xi) \approx \sum_{k=1}^{N_{PC}} f_{\Phi_i}^{(k)} \mathcal{F}_{\Phi_i}^{(k)}(\xi).$$

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The new surrogate model

$$\tilde{\mathcal{M}}^{KL+PC}(t, \xi) = \sum_{i=1}^{N_{kl}} \sum_{k=1}^{N_{PC}} f_{\Phi_i}^{(k)} \mathcal{F}_{\Phi_i}^{(k)}(\xi) e_i(t),$$

is called **Karhunen-Loève Expansion with PCE approximated modes** (KLE + PCE) [BS14].

Sensitivity Analysis

How can the uncertainties in the model output be *apportioned* or *allocated* to the uncertainties in the model inputs? [Sal08]

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Motivation:

- Which input variables make large contributions towards the output uncertainty?
  Factor Prioritisation $\implies$ Reduce parameter uncertainty
- Which input variables have the least contribution towards the output uncertainty?
  Factor Fixing $\implies$ Model simplification
- Identify experimental settings under which a variable is most responsive
  Experiment Design $\implies$ Model calibration

Local v/s Global Sensitivity Analysis

Local Sensitivity Analysis

- Example: $\Delta_i y = f(\xi_i + \Delta\xi_i, \boldsymbol{\xi}^0_{\sim i}) - f(\boldsymbol{\xi}^0), \;\; \boldsymbol{\xi} \in [0,1]^n$
- Provides local information about the model sensitivities
- Not meaningful if model inputs are uncertain

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Global Sensitivity Analysis

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Global Sensitivity Analysis

- Assign PDF(s) to input random variable(s) using domain knowledge
- **Variance-based methods (Sobol indices)**, density-based methods (Borgonovo indices), Monte Carlo filtering, regression-based methods etc.

Sobol indices

- For non-additive, time-independent models $\mathcal{M}(\xi)$, we use the following generalisation: *How much will the output variance decrease, if we know the value of an input with certainty?*

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- First-order Sobol index

$$\mathcal{S}_i := 1 - \frac{\mathbb{E}_{\xi_i}[\mathbb{V}_{\xi|\xi_i}[\mathcal{M}(\xi) \mid \xi_i]]}{\mathbb{V}[\mathcal{M}(\xi)]} = \frac{\mathbb{V}_{\xi_i}[\mathbb{E}_{\xi|\xi_i}[\mathcal{M}(\xi) \mid \xi_i]]}{\mathbb{V}[\mathcal{M}(\xi)]}.$$

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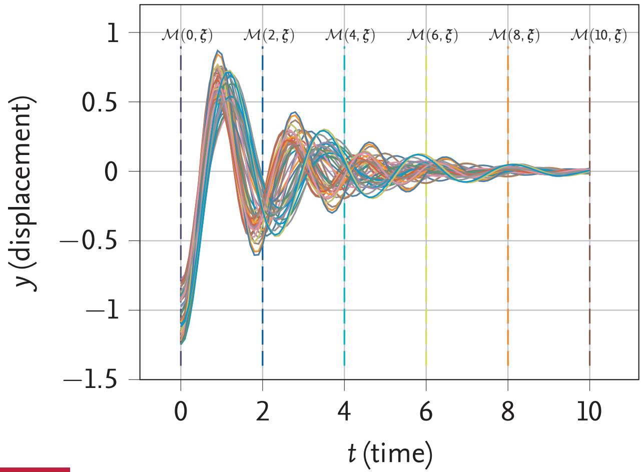
- $0 \leq \mathcal{S}_i \leq 1.$
- Computing using PCE surrogate: $\mathcal{S}_i = \sum_{k \in \mathcal{K}_i} c_k^2.$

Example: Mechanical oscillator



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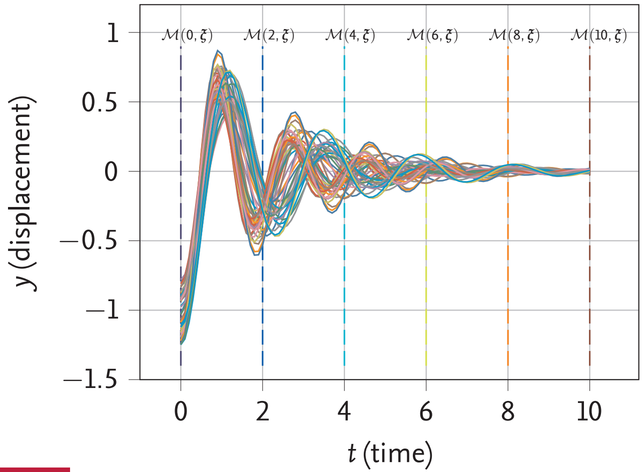
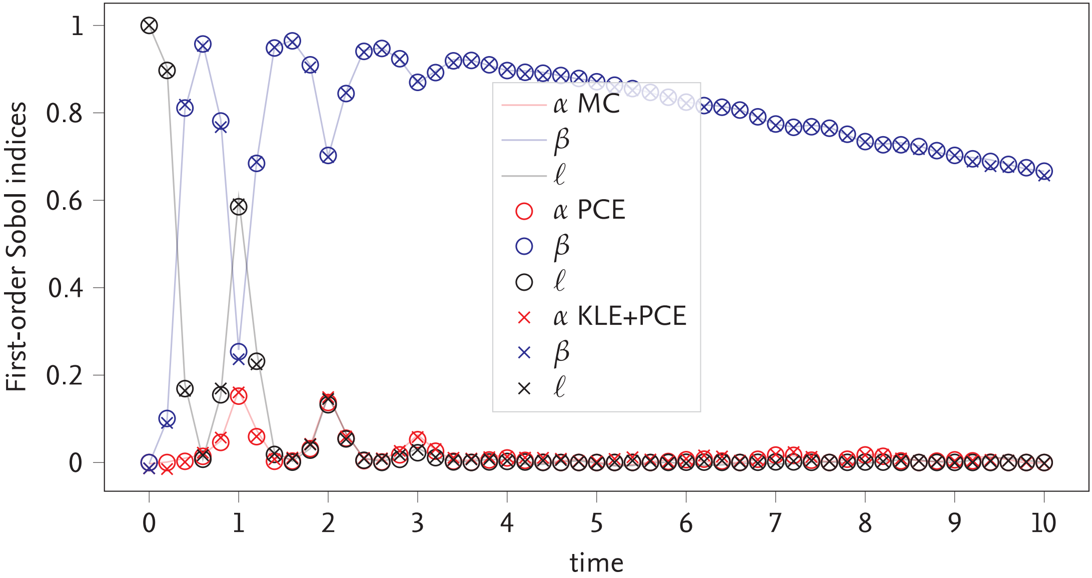


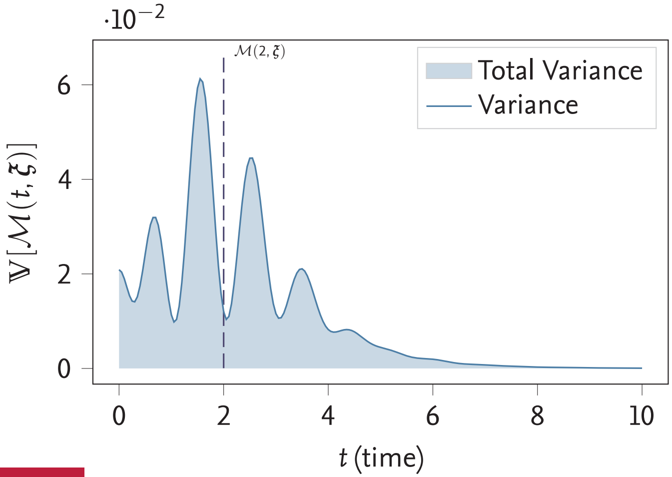
$$\mathcal{M}(t_s,\xi) = \ell e^{-\alpha t_s}\left(\cos\beta t_s + \frac{\alpha}{\beta}\sin\beta t_s\right)$$

$$\mathcal{S}_i(t_s) = \frac{\mathbb{V}_{\xi_i}[\mathbb{E}_{\xi|\xi_i}[\mathcal{M}(t_s,\xi)|\xi_i]]}{\mathbb{V}[\mathcal{M}(t_s,\xi)]}$$

Pointwise-in-time Sobol indices



Shortcomings



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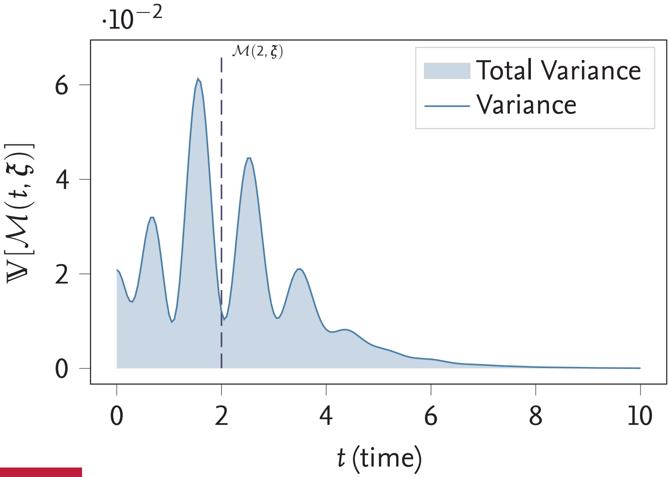

- Sensitivity metric - variance, changes over time
- Cannot provide holistic overview of sensitivities
- Solution: Use total integrated variance as a metric [AGS20, GJKL13].

Generalised Sobol Indices

For time-dependent processes, the generalised Sobol indices are the ratio of the time integrals of the numerator and denominator of the Sobol indices [AGS20].

$$\mathcal{G}_i(\mathcal{T}) := \frac{\int_{\mathcal{T}} \mathcal{S}_i^{num}(\mathcal{M};t)\,\mathrm{d}t}{\int_{\mathcal{T}} V(\mathcal{M};t)\,\mathrm{d}t} = \frac{\int_{\mathcal{T}} \mathbb{V}_{\xi_i}[\mathbb{E}_{\boldsymbol{\xi}|\xi_i}[\mathcal{M}(t,\boldsymbol{\xi}) \mid \xi_i]]\,\mathrm{d}t}{\int_{\mathcal{T}} \mathbb{V}[\mathcal{M}(t,\boldsymbol{\xi})]\,\mathrm{d}t},$$

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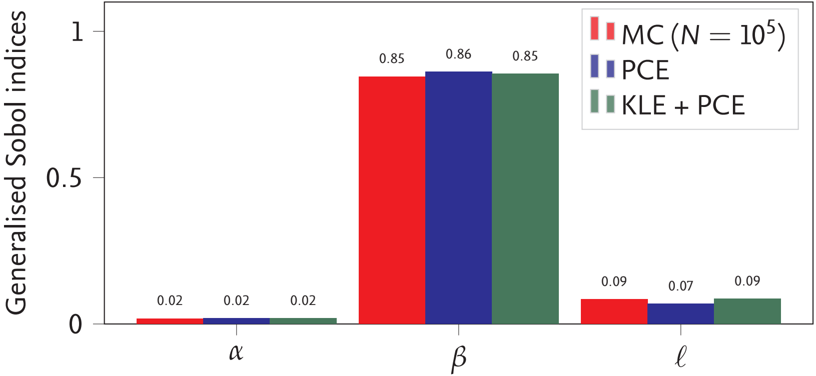
where $\mathcal{T}$ is the time interval.

- Computing using PCE surrogates:

$$\mathcal{G}_i^{PC}(\mathcal{T}) \approx \left(\sum_{j=1}^{N_{\mathrm{quad}}} \sum_{k\in\mathcal{K}_i} w_j\, c_k^2(t_j)\right) \Big/ \left(\sum_{j=1}^{N_{\mathrm{quad}}} \sum_{k=2}^{N_{PC}} w_j\, c_k^2(t_j)\right).$$

Example: Mechanical oscillator

- Generalised Sobol indices for $\mathcal{T} = [0, 10]$s.
- Computed using MC simulation, PCE and KLE+PCE surrogate.



Chaboche Model

- A constitutive material model that describes the behaviour of viscoplastic materials (such as steel) when subjected to time-dependent loading.

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- System of ODEs for a $1D$ bar:

$$\begin{bmatrix} \dot{\varepsilon}_{xx} \\ \dot{K} \\ \dot{X}_{xx} \end{bmatrix} = \begin{bmatrix} E^{-1} \cdot \dot{\sigma}_{xx} + \frac{1}{\sigma_\nu}(\sigma_{xx} - X_{xx}) \cdot \left\langle \frac{\sigma_{ex}}{D} \right\rangle^n \cdot \dot{\varepsilon}_0 \\ b_{iso} \cdot (Q_{iso} - K) \cdot \left\langle \frac{\sigma_{ex}}{D} \right\rangle^n \\ b_{kin} \left(\frac{2}{3} Q_{kin} \cdot \frac{1}{\sigma_\nu}(\sigma_{xx} - X_{xx}) - X_{xx} \right) \cdot \left\langle \frac{\sigma_{ex}}{D} \right\rangle^n \end{bmatrix}$$

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- Stress response: $\mathcal{M}(t, \xi) = \sigma_{xx}(t; E, \sigma_{y_0}, Q_{iso}, b_{iso}, n, D, Q_{kin}, b_{kin})$, when subjected to strain $\varepsilon_{xx}(t)$.

Physical Model setup [Hei21]

- Monotonic loading: $\mathcal{M}(t, \xi) = \sigma_{xx}(t; E, \sigma_{y_0}, Q_{iso}, b_{iso}, n, D)$

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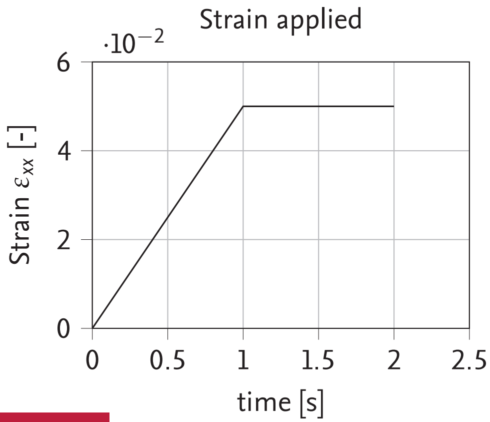

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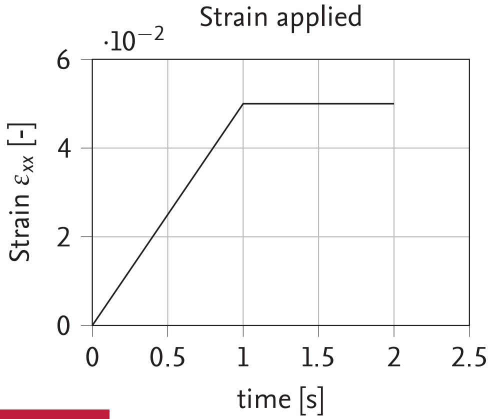
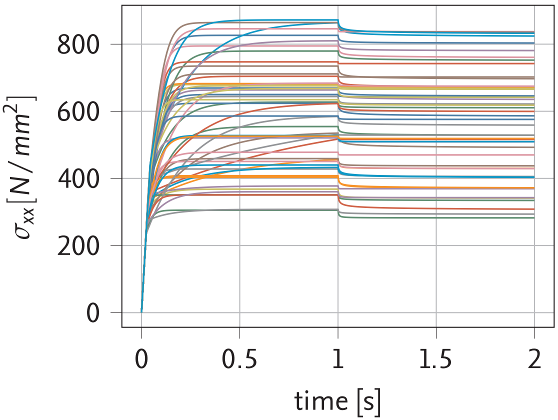
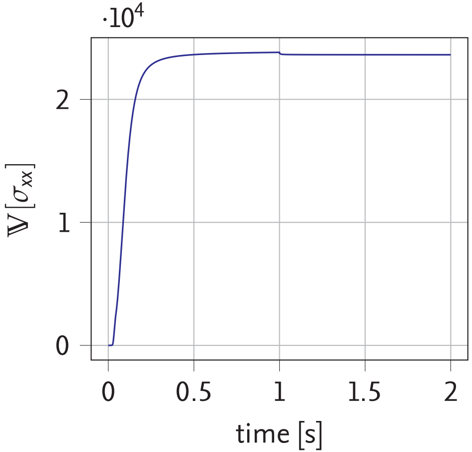


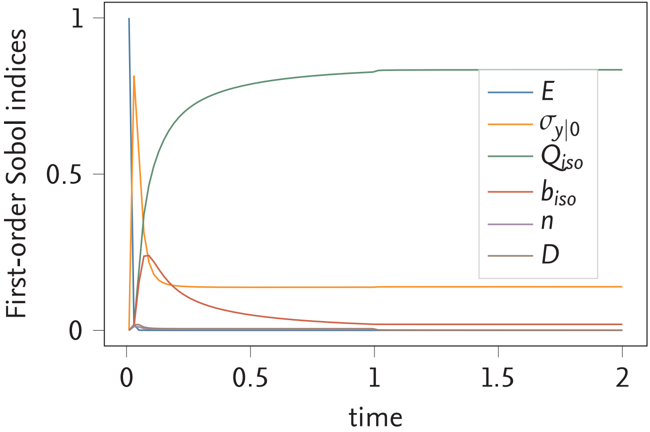
#	ξ	Distribution	a	b	Mean	Variance	Unit
1	E	Uniform	200, 000	210, 000	205, 000	8, 333, 333.33	N/mm^2
2	σ_{y0}	Uniform	200	400	300	3, 333.33	N/mm^2
3	Q_{iso}	Uniform	0	500	250	20, 833.33	N/mm^2
4	b_{iso}	Uniform	0	1000	500	83, 333.33	-
5	n	Uniform	1	6	3.5	2.08	-
6	D	Uniform	1	100	50.5	816.75	N/mm^2

Chaboche Model Response





Pointwise-in-time Sobol indices



- Estimated using time-frozen PCE surrogates.

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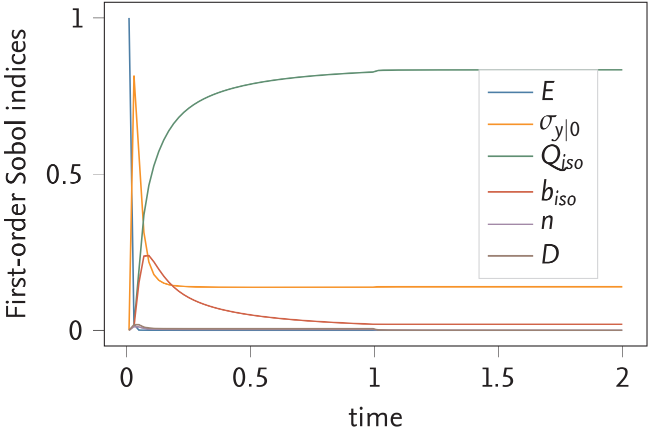
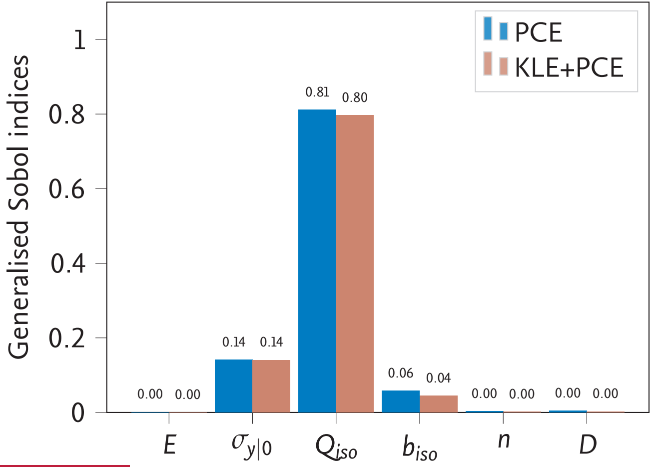


- Estimated using time-frozen PCE surrogates.
- In literature [GR18, WSK19], it has been observed that sensitivity can be a good indicator for parameter identifiability $\Longrightarrow$ calibration time-points are now available.

Generalised Sobol indices



- Estimation using MC simulations not feasible.

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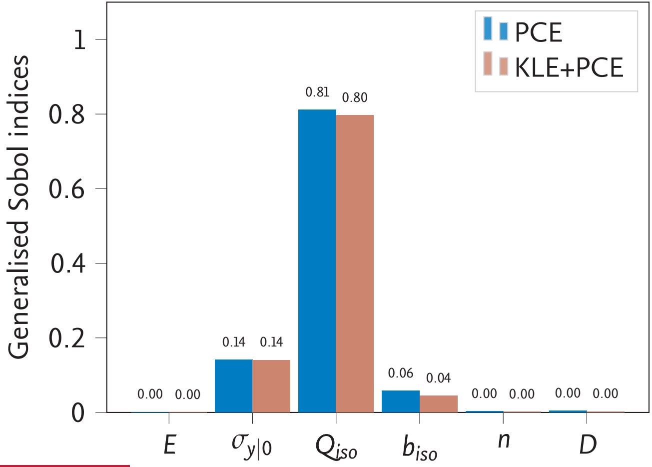

- Estimation using MC simulations not feasible.
- The uncertainty in parameter Q_{iso} must be reduced to reduce overall output uncertainty.

Bayesian Calibration

Bayes' rule:

$$\underbrace{\pi(\xi \mid \mathcal{Y})}_{\text{Posterior}} = \frac{\overbrace{\mathcal{L}(\xi, \mathcal{Y})}^{\text{Likelihood}} \overbrace{\pi(\xi)}^{\text{Prior}}}{\underbrace{\mathbb{E}_{\pi}(\boldsymbol{y})}_{\text{Evidence}}}$$

- Young's Modulus E has sensitivity highest in the initial elastic region $[0, 0.019]$s, therefore calibrated at $t = 0.01$s.

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- Young's Modulus E has sensitivity highest in the initial elastic region $[0, 0.019]$s, therefore calibrated at $t = 0.01$s.
- True parameter value assumed $E = 200,000$ N/mm^2 and thus model response $\hat{\sigma}_{xx} = E \cdot \dot{\varepsilon} \cdot t_1 = 200,000 \cdot 5 \times 10^{-2} \cdot 0.01 = 100$ N/mm^2.

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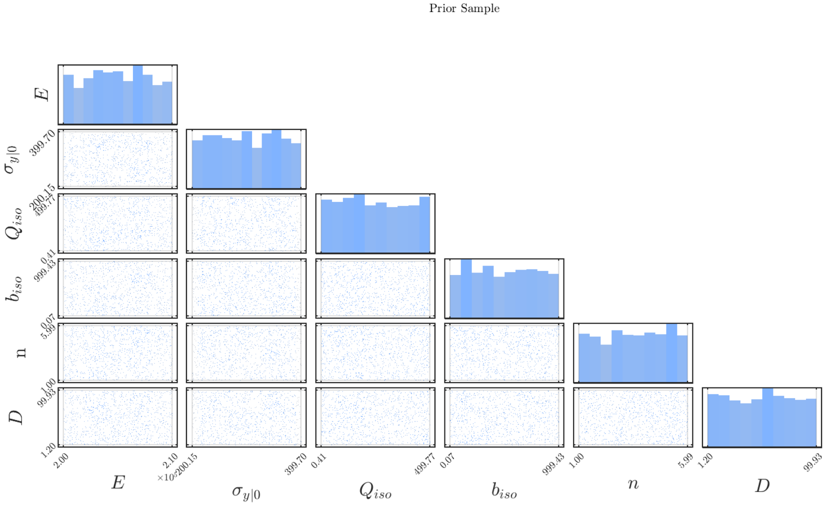
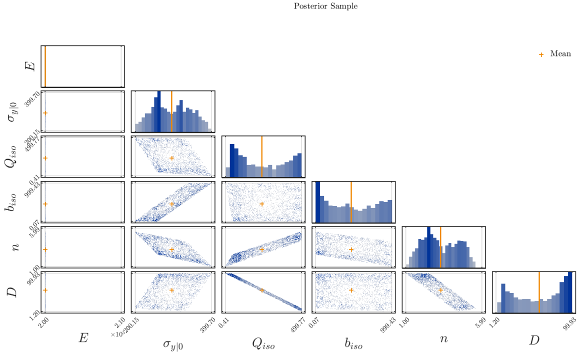
- Calibrated E using 10 samples from mock data: $y_i \sim \mathcal{N}(100, 10^{-4})$ (coefficient of variation = 0.01%).

Model Priors

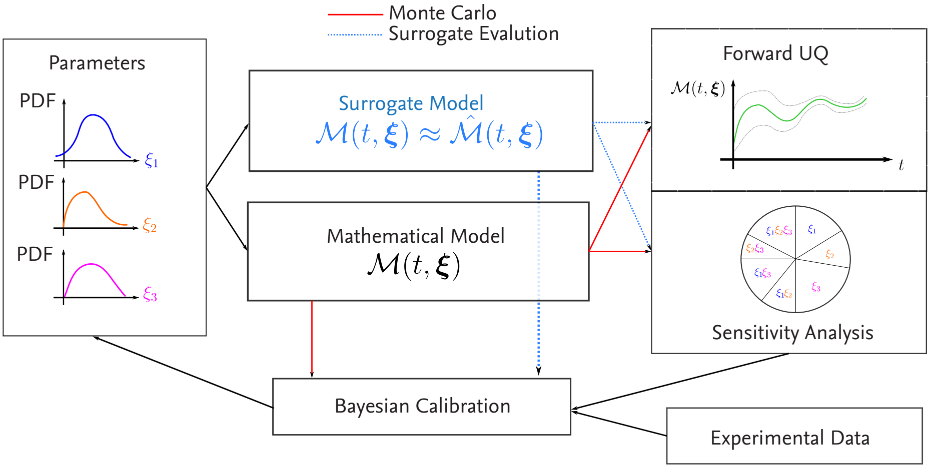


Posterior Marginals



- Successfully calibrated E using PCE surrogate to replace model evaluations in MCMC.

Summary


Monte Carlo
Surrogate Evalution
Parameters
PDF
ξ_1
PDF
ξ_2
PDF
ξ_3
Surrogate Model
$\mathcal{M}(t,\boldsymbol{\xi}) \approx \hat{\mathcal{M}}(t,\boldsymbol{\xi})$
Mathematical Model
$\mathcal{M}(t,\boldsymbol{\xi})$
Forward UQ
$\mathcal{M}(t,\boldsymbol{\xi})$
t
$\xi_1\xi_2\xi_3$
ξ_1
$\xi_2\xi_3$
ξ_2
$\xi_1\xi_3$
ξ_3
$\xi_1\xi_2$
Sensitivity Analysis
Bayesian Calibration
Experimental Data

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