UKACM & GACM AUTUMN SCHOOL 2025

Open-Source Codes for High-Performance Computing

Hands-on Session 4C & QUEENS

30.09.2025 and 01.10.2025

Sebastian Brandstäter[1], Georg Hammerl[2], Matthias Mayr[1,3],
Gil Robalo Rei[4], Ingo Scheider[2], Christoph P. Schmidt[4]

[1] Institute for Mathematics and Computer-Based Simulation | University of the Bundeswehr Munich
[2] Institute for Material Systems Modeling | Helmholtz-Zentrum Hereon
[3] Data Science & Computing Lab | University of the Bundeswehr Munich
[4] Institute for Computational Mechanics | Technical University of Munich

Feedback Time

Please take the next **5 minutes** to fill out the feedback form.

Your input is highly valued and will help us improve future sessions.

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Thank you for sharing your thoughts!

UKACM & GACM AUTUMN SCHOOL 2025
Open-Source Codes for High-Performance Computing

QUEENS

STATE-OF-THE-ART RESEARCH WITH QUEENS

Sebastian Brandstäter[1], Maximilian Dinkel[2], Lea Häusel[2], Jonas Nitzler[2], Gil Robalo Rei[2]

[1] Institute for Mathematics and Computer-Based Simulation | University of the Bundeswehr Munich
[2] Institute for Computational Mechanics | Technical University of Munich

Forward Uncertainty Quantification

Goal:
Propagate uncertainties from input quantities θ to output quantities y using a computational model $\mathcal{M}$

$$p(y) = \mathbb{E}_{p(\theta)}[\delta(\mathcal{M}(\boldsymbol{\theta}) - y)]$$

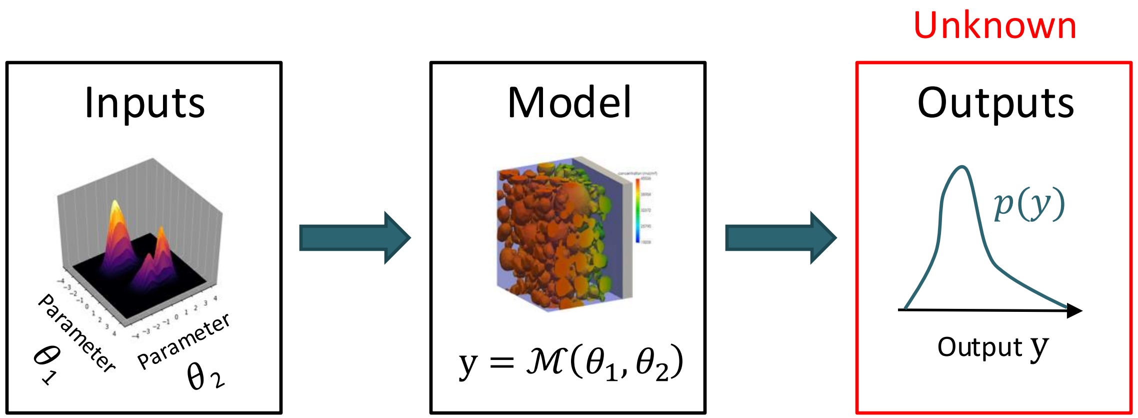
$\delta(.)$ is the Dirac mass delta

Known:

- Probability density function $p(\boldsymbol{\theta})$ of uncertain model inputs $\boldsymbol{\theta}$
- Model $\mathrm{y} = \mathcal{M}(\boldsymbol{\theta})$

Unknown:

- Probability density function $p(y)$ of uncertain output y



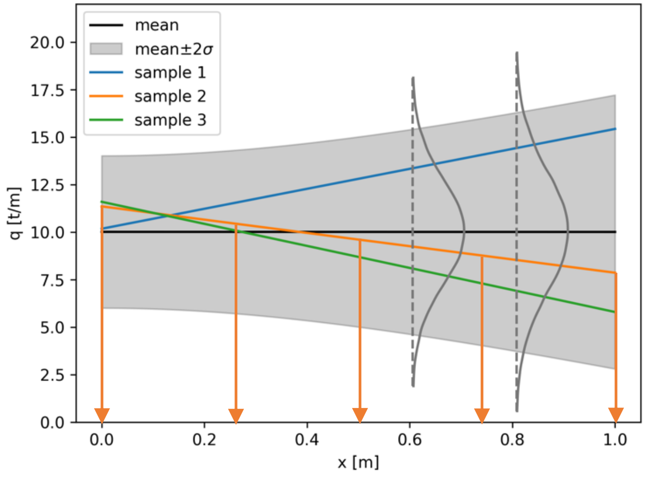
Forward UQ – Beam example

Inputs

$$\boldsymbol{\theta} = [\theta_1, \theta_2]^{\mathrm{T}}$$

$$\theta_1 \sim \mathcal{N}(\mu = 10.0,\ \sigma^2 = 4.0)$$
$$\theta_2 \sim \mathcal{N}(\mu = 0.0,\ \sigma^2 = 9.0)$$

load $q(x, \boldsymbol{\theta}) = \theta_1 + \theta_2 x$

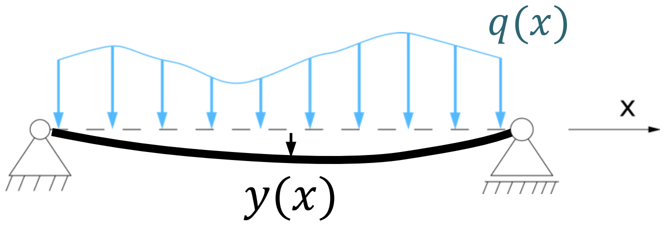


Model

$$y(x) = \mathcal{M}(x, \boldsymbol{\theta})$$

Where $\mathcal{M}(x, \boldsymbol{\theta})$ models a static Euler-Bernoulli beam:

$$EI \frac{\partial^4 y}{\partial x^4}(x) = q(x, \boldsymbol{\theta})$$

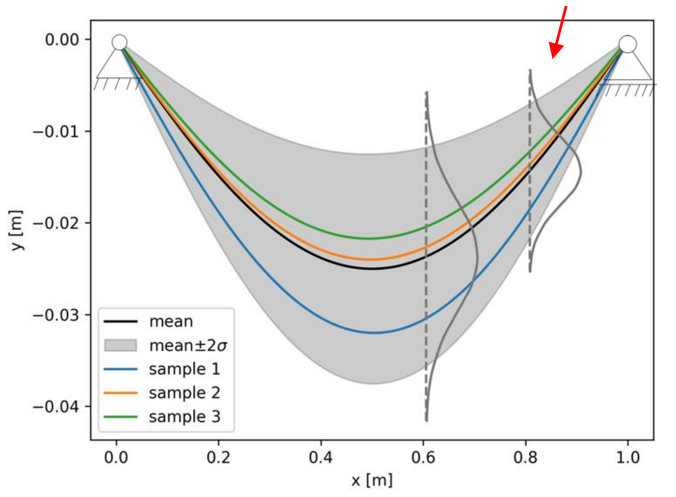


Unknown

Outputs

bending line $y(x)$

Variance smaller towards support



Forward UQ – Our research

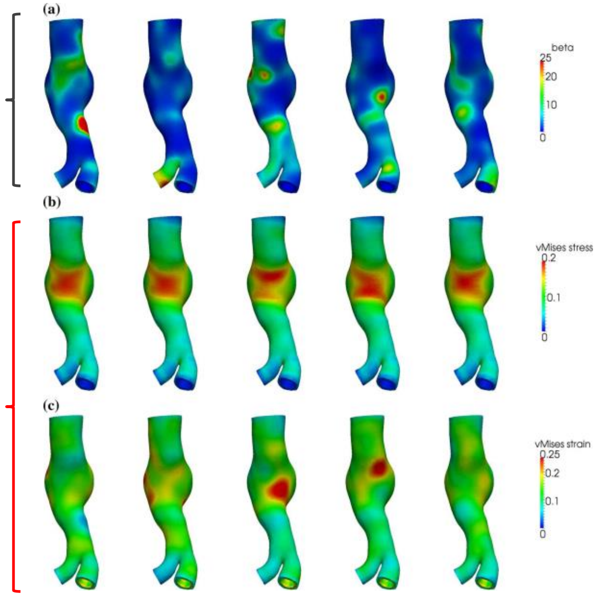
Available in QUEENS

- Monte Carlo sampling
- Collocation-based polynomial chaos expansion (chaospy-based)
- Bayesian multi-fidelity Monte Carlo

Uncertainty Quantification based on a Bayesian **multi-fidelity scheme**:

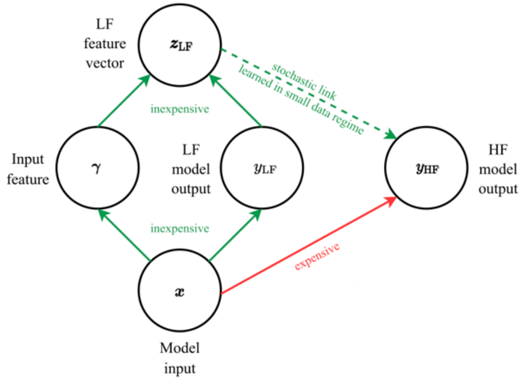
Input: random field

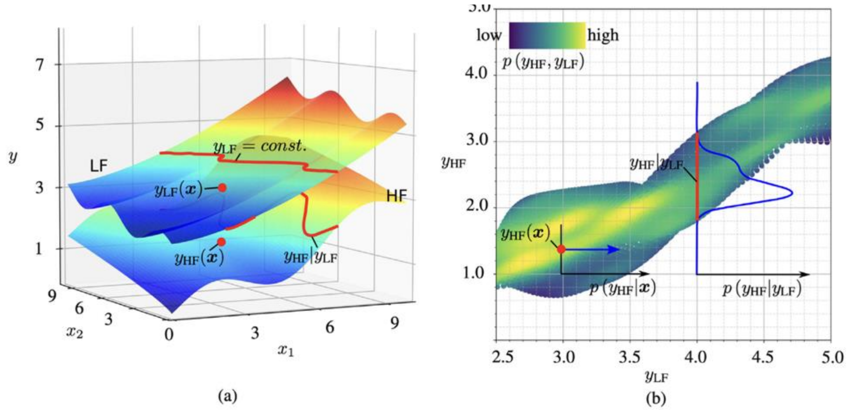
Output



Biehler, J., Gee, M. W., & Wall, W. A. (2014). Towards efficient uncertainty quantification in complex and large-scale biomechanical problems based on a Bayesian multi-fidelity scheme. *Biomechanics and Modeling in Mechanobiology*, *14*(3), 489–513.

Generalized formulation of multi-fidelity scheme using **informative features γ**:





Nitzler, J., Biehler, J., Fehn, N., Koutsourelakis, P., & Wall, W. A. (2022). A generalized probabilistic learning approach for multi-fidelity uncertainty quantification in complex physical simulations. *Computer Methods in Applied Mechanics and Engineering*, *400*, 115600.

Bayesian inverse analysis / Backward UQ

Goal:
Given experimental data y_{obs} and a model $\mathcal{M}$, estimate the unknown input quantities θ and the uncertainty in this estimate

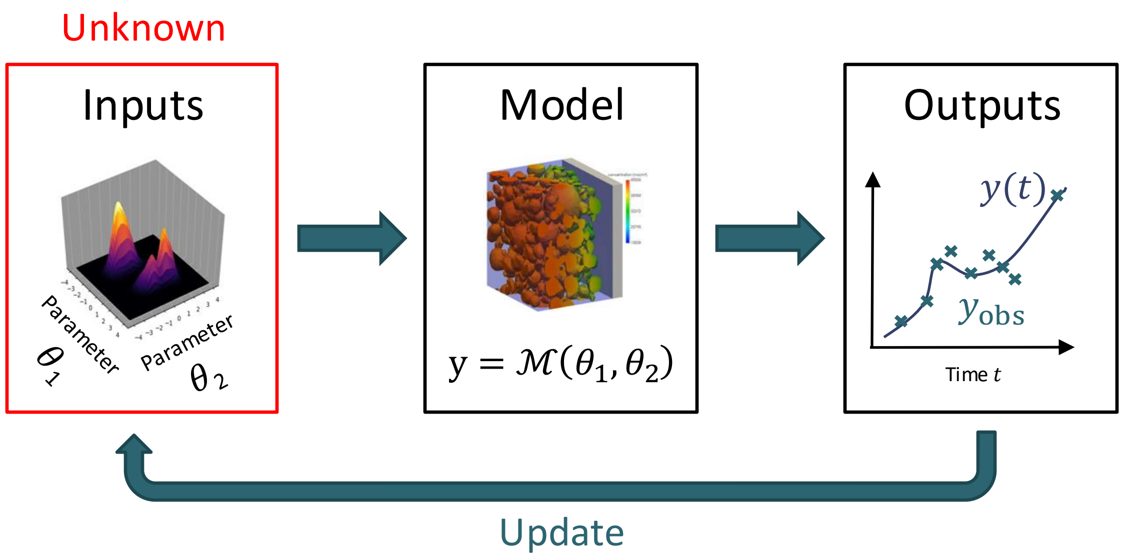
Bayes‘ rule: $p(\theta|y_{obs}) = \frac{p(y_{obs}|\theta)p(\theta)}{p(y_{obs})}$

Known:

- Observations $\boldsymbol{y}_{\text{obs}}$
  e.g. from experiments
- Prior $p(\boldsymbol{\theta})$
  over uncertain model inputs $\boldsymbol{\theta}$
- Model $\mathrm{y} = \mathcal{M}(\boldsymbol{\theta})$
- *Optional but desirable:*
  Model derivative $\frac{\partial \mathcal{M}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}}$

Unknown:

- Posterior $p(\boldsymbol{\theta}|\boldsymbol{y}_{\text{obs}})$
  over uncertain model inputs $\boldsymbol{\theta}$



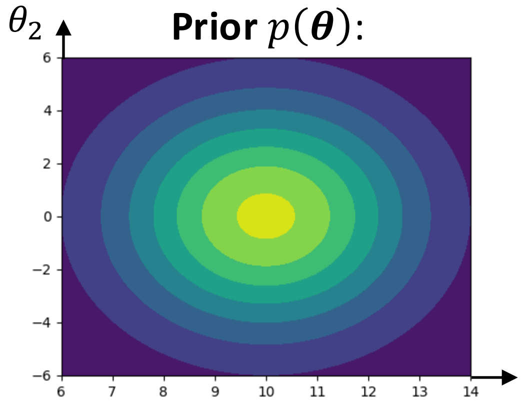
Bayesian inverse analysis – Beam example

Inputs

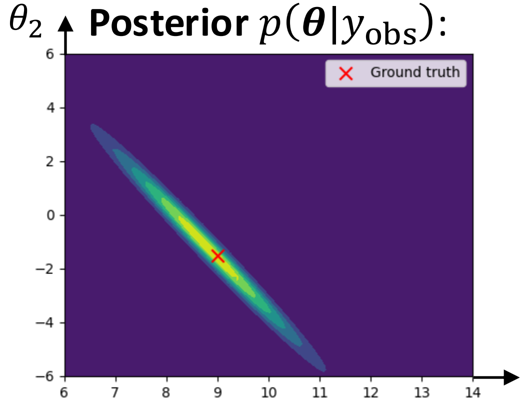
$\boldsymbol{\theta} = [\theta_1, \theta_2]^{\mathrm{T}}$

load $q(x, \boldsymbol{\theta}) = \theta_1 + \theta_2 x$

Prior $p(\boldsymbol{\theta})$:



Posterior $p(\boldsymbol{\theta}|y_{\mathrm{obs}})$:

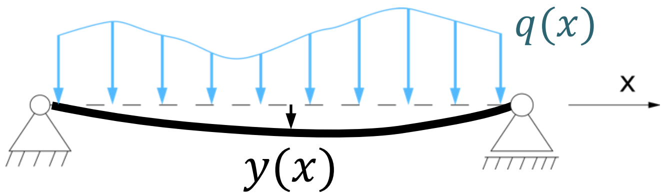


Model

$$y(x) = \mathcal{M}(x, \boldsymbol{\theta})$$

Where $\mathcal{M}(x, \boldsymbol{\theta})$ solves:

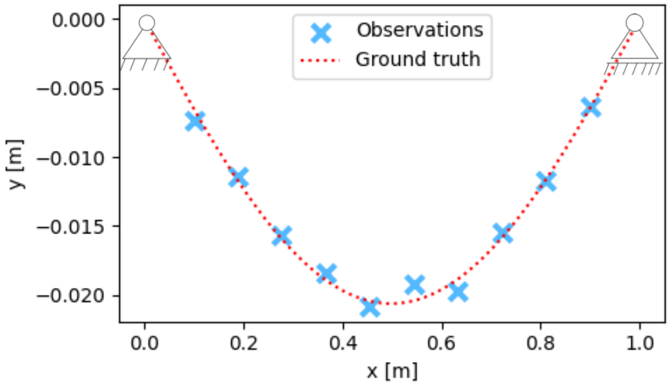
$$EI \cdot \frac{\partial^4 y}{\partial x^4}(x) = q(x, \boldsymbol{\theta})$$



Outputs

bending line $y(x)$

Observations y_{obs}:

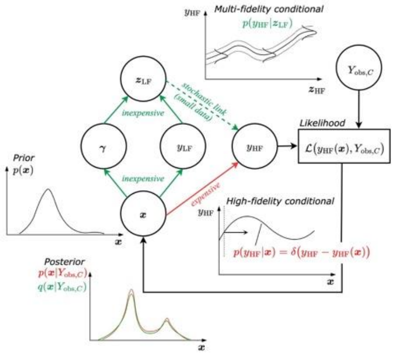


Unknown

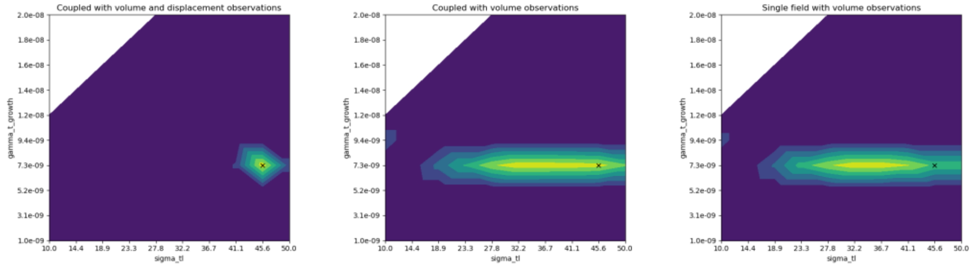
Bayesian inverse analysis – Our research

Available in QUEENS

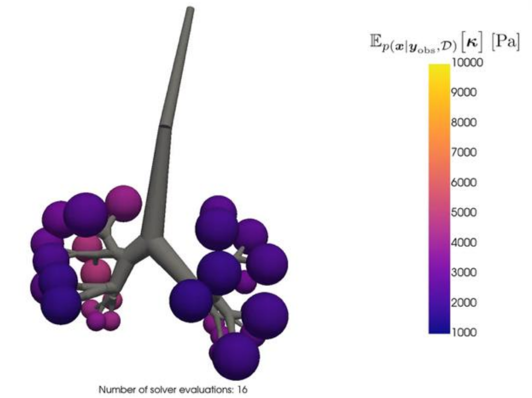
- Markov Chain Monte Carlo (in-house & pymc-based)
- Sequential Monte Carlo (in-house & particles-based)
- Variational inference
- Bayesian multi-fidelity inverse analysis



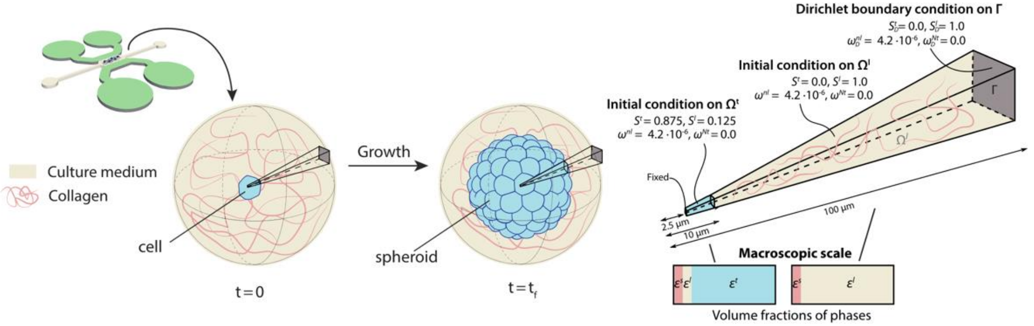
Nitzler, J., Wall, W. A., & Koutsourelakis, P.-S. (2023). *Bayesian multi-fidelity inverse analysis (BMFIA) for expensive, non-differentiable, physics-based simulations in high stochastic dimensions*. 5th International Conference on Uncertainty Quantification in Computational Science and Engineering.



Wall, W. A., Dinkel, M., Nitzler, J., Robalo Rei, G., & Wirthl, B. (2023). *Enhancing Bayesian inverse analysis via multi-physics modeling*. 5th International Conference on Uncertainty Quantification in Computational Science and Engineering, Athens, Greece.



Dinkel, M., Geitner, C. M., Robalo Rei, G., Nitzler, J., & Wall, W. A. (2024). Solving Bayesian inverse problems with expensive likelihoods using constrained Gaussian processes and active learning. *Inverse Problems*, *40*(9), 095008.

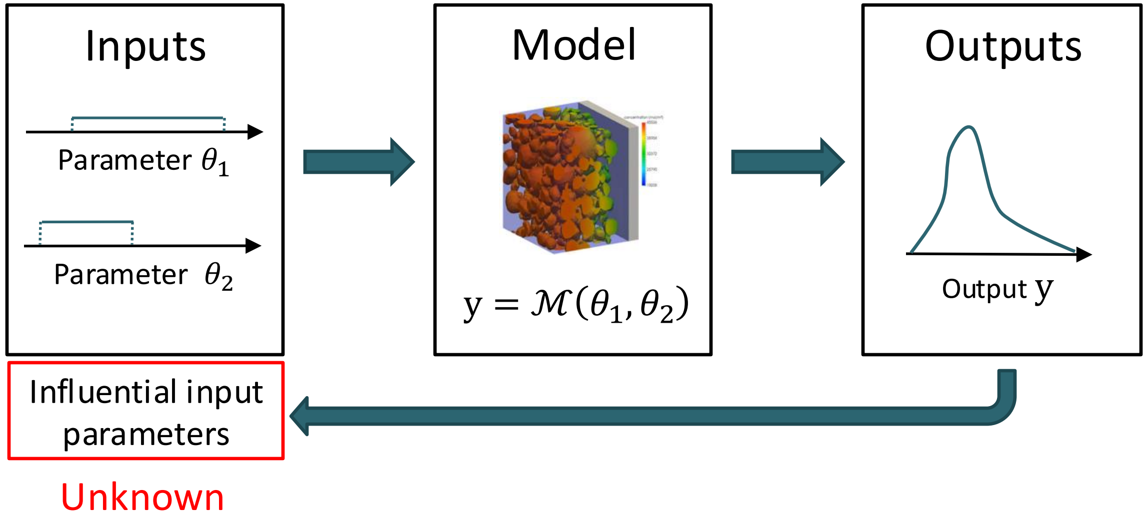


Hervas-Raluy, S., Wirthl, B., Guerrero, P. E., Robalo Rei, G. , Nitzler, J., Coronado, E., De Mora Sainz, J. F., Schrefler, B. A., Gomez-Benito, M. J., Garcia-Aznar, J. M., & Wall, W. A. (2023). Tumour growth: An approach to calibrate parameters of a multiphase porous media model based on in vitro observations of Neuroblastoma spheroid growth in a hydrogel microenvironment. *Computers in Biology and Medicine*, *159*, 106895.

Exploiting uncertainties

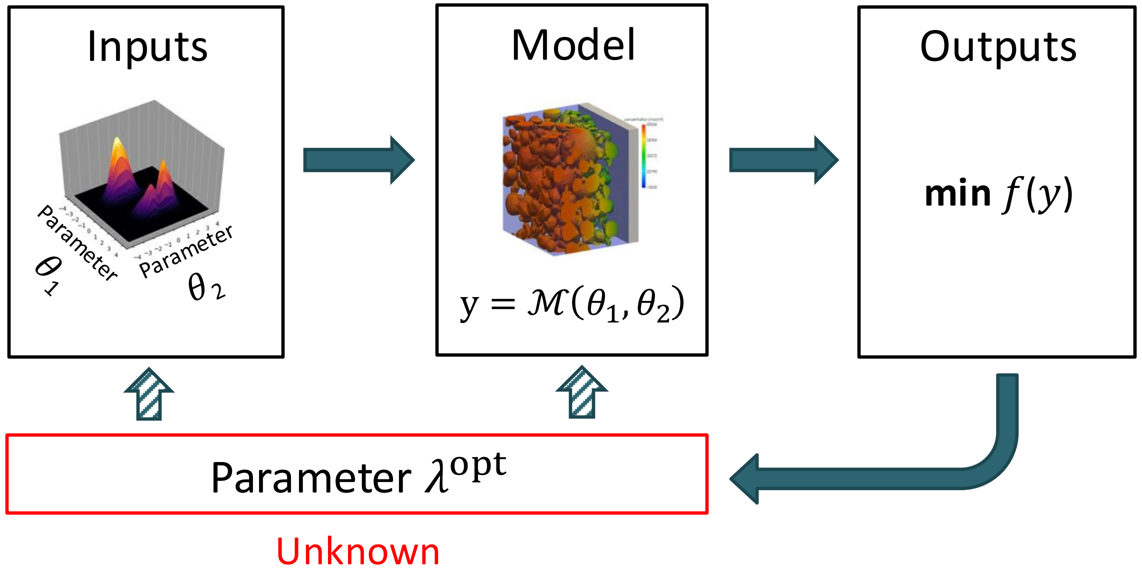
Global Sensitivity Analysis (GSA)

Identification of the most promising input parameters



Optimization Under Uncertainty (OUU)

Find the optimal solutions under uncertain conditions



Global sensitivity analysis

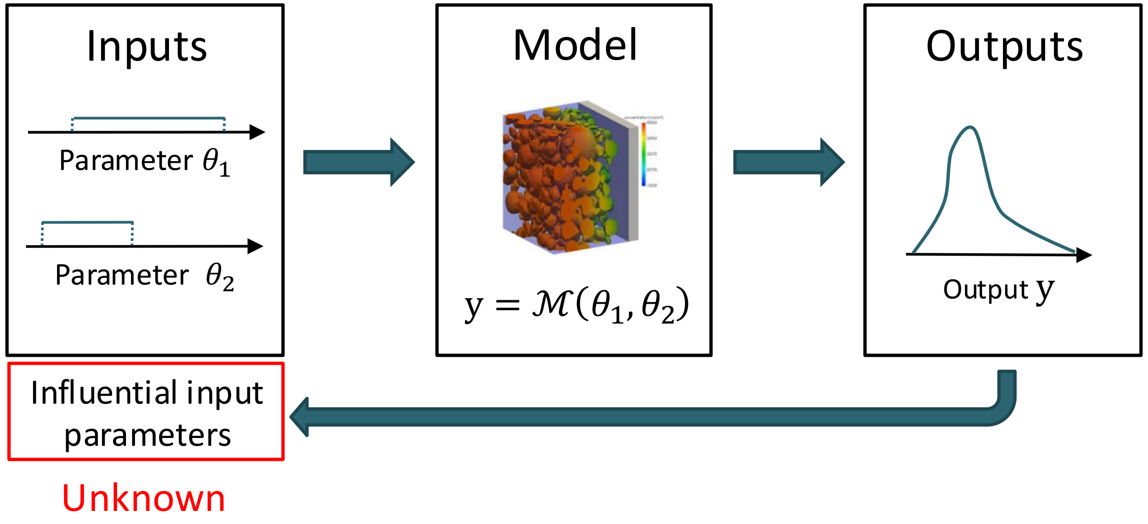
Goal:
Quantify which uncertain input quantity θ influences the uncertainty in the output quantity y the most

Sobol indices: $S_i = \frac{\mathbb{V}_{\theta_i}\left[\mathbb{E}_{\boldsymbol{\theta}_{\sim i}}[\mathcal{M}(\boldsymbol{\theta})|\theta_i]\right]}{\mathbb{V}_{\boldsymbol{\theta}}[\mathcal{M}(\boldsymbol{\theta})]}$

Known:
- Probability density function $p(\boldsymbol{\theta})$ of uncertain model inputs $\boldsymbol{\theta}$
- Model $\mathrm{y} = \mathcal{M}(\boldsymbol{\theta})$

Unknown:
- Influence of variance in inputs $\boldsymbol{\theta}$ on variance in outputs y

  → measured with sensitivity indices



Global sensitivity analysis – Beam example

Inputs

$$\boldsymbol{\theta} = [\theta_1, \theta_2]^{\mathrm{T}}$$

$$\theta_1 \sim \mathcal{N}(\mu = 10.0,\ \sigma^2 = 4.0)$$
$$\theta_2 \sim \mathcal{N}(\mu = 0.0,\ \sigma^2 = 9.0)$$

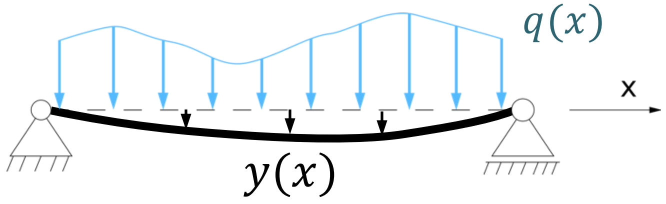
load $q(x, \boldsymbol{\theta}) = \theta_1 + \theta_2 x$

Model

$$y(x) = \mathcal{M}(x, \boldsymbol{\theta})$$

Where $\mathcal{M}(x, \boldsymbol{\theta})$ solves:

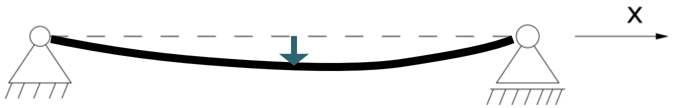
$$EI \cdot \frac{\partial^4 y}{\partial x^4}(x) = q(x, \boldsymbol{\theta})$$



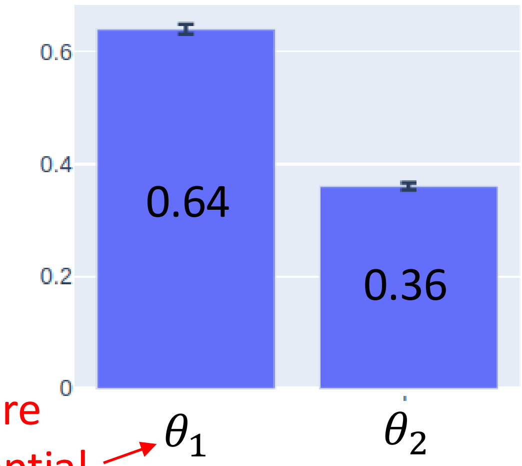
Outputs

bending at mid-length of the beam

$$y(x = 0.5)$$



First-Order Sobol Indices



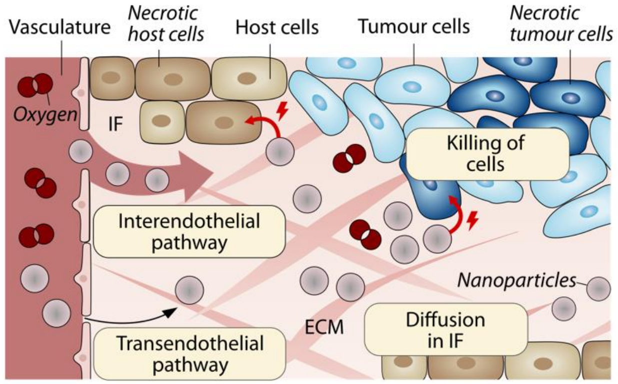
more influential

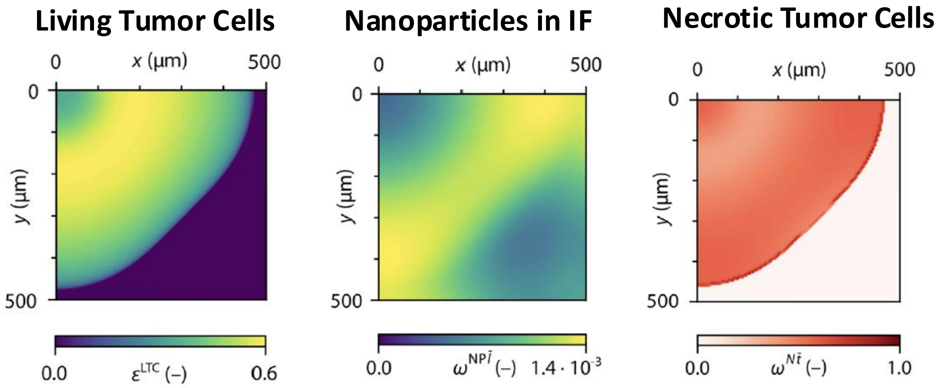
Unknown

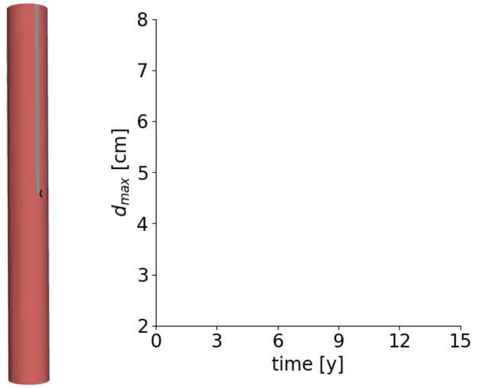
Global sensitivity analysis – Our research

Available in QUEENS

- Sobol indices (1st, 2nd, and total order) (SALib-based)
- Sobol indices with model uncertainty
- Elementary effects / Morris method

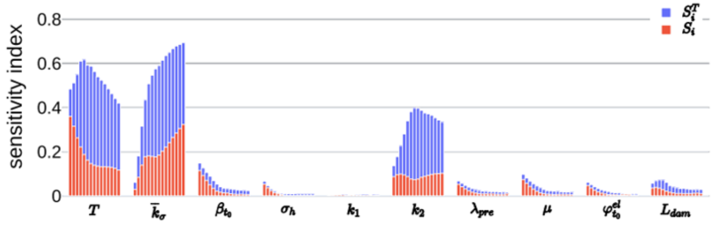






$$d_{max}(t) = \begin{cases} d(t), & \text{if } d(t) < 8\,\mathrm{cm} \\ 8\,\mathrm{cm}, & \text{else} \end{cases}$$

Sobol indices of ten independent parameters:



Wirthl, B., Brandstaeter, S., Nitzler, J., Schrefler, B. A., & Wall, W. A. (2023). Global sensitivity analysis based on Gaussian-process metamodelling for complex biomechanical problems. International Journal for Numerical Methods in Biomedical Engineering, 39(3), e3675.

Brandstaeter, S., Fuchs, S.L., Biehler, J., Aydin, R.C., Wall, W.A., Cyron, C.J. (2021) 'Global Sensitivity Analysis of a Homogenized Constrained Mixture Model of Arterial Growth and Remodeling', Journal of Elasticity, 145(1–2), pp. 191–221.

Optimization (under Uncertainty)

Goal:
Find an optimal parameter λ^{opt} while accounting for uncertainties in the input quantities θ

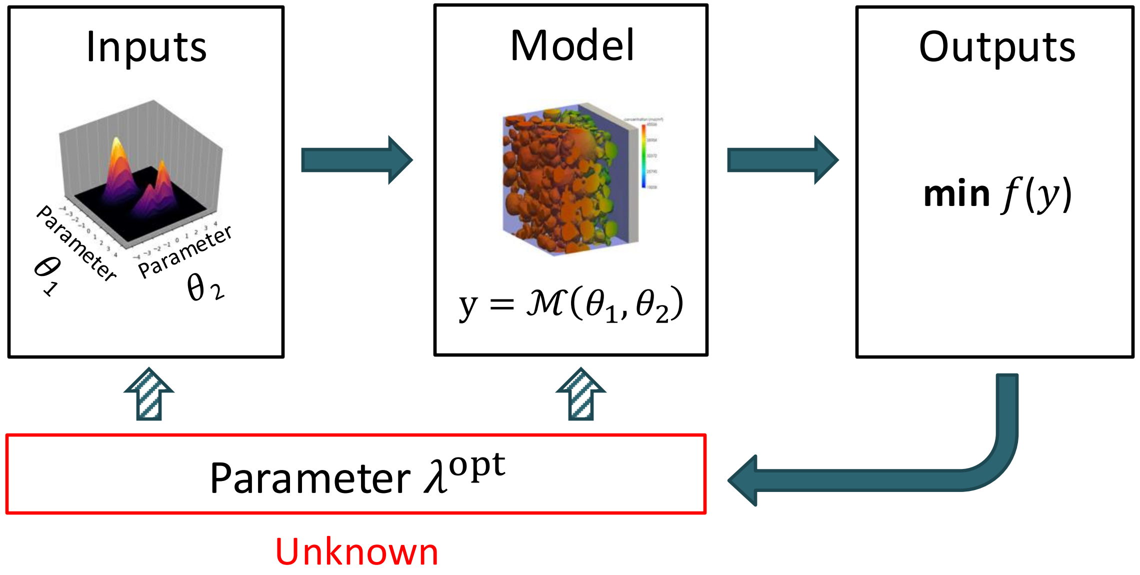
Objective: $\lambda^{\text{opt}} \in \arg\min_{\lambda} \mathbb{E}_{p(\theta)}\left[f\left(y = \mathcal{M}(\theta)\right)\right]$

Known:

- Probability density function $p(\boldsymbol{\theta})$ of uncertain model inputs $\boldsymbol{\theta}$
- Model $\mathrm{y} = \mathcal{M}(\boldsymbol{\theta})$
- Objective function $f(y)$

Unknown:

- Optimal parameter λ^{opt} that minimizes the expected value of the objective function $f(y)$
  - λ can be a parameter of either $p(\boldsymbol{\theta})$ or $\mathcal{M}(\boldsymbol{\theta})$

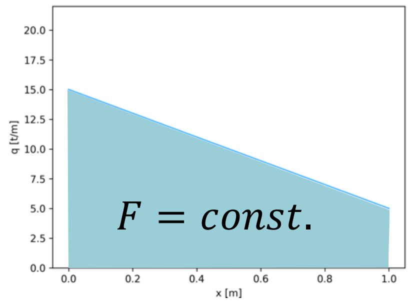


Optimization - Beam example

Inputs

$\theta \sim \mathcal{N}(\mu = \lambda, \sigma^2 = 9.0)$

load $q(x, \theta) = \frac{F}{l} + \left(x - \frac{1}{2} l\right) \theta$

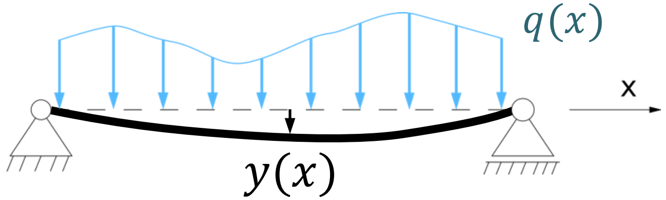


Model

$y(x) = \mathcal{M}(x, \boldsymbol{\theta})$

Where $\mathcal{M}(x, \boldsymbol{\theta})$ solves:

$$EI \cdot \frac{\partial^4 y}{\partial x^4}(x) = q(x, \boldsymbol{\theta})$$

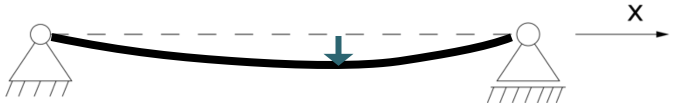


Outputs

bending line $y(x)$

<u>Objective:</u>
minimize the maximum bending:

$$f(y) = \max_x |y(x)|$$



Parameter

$$\lambda^{\text{opt}} \in \arg\min_{\lambda} \mathbb{E}_{p(\theta|\lambda)} \left[\max_x |y(x)|\right]$$

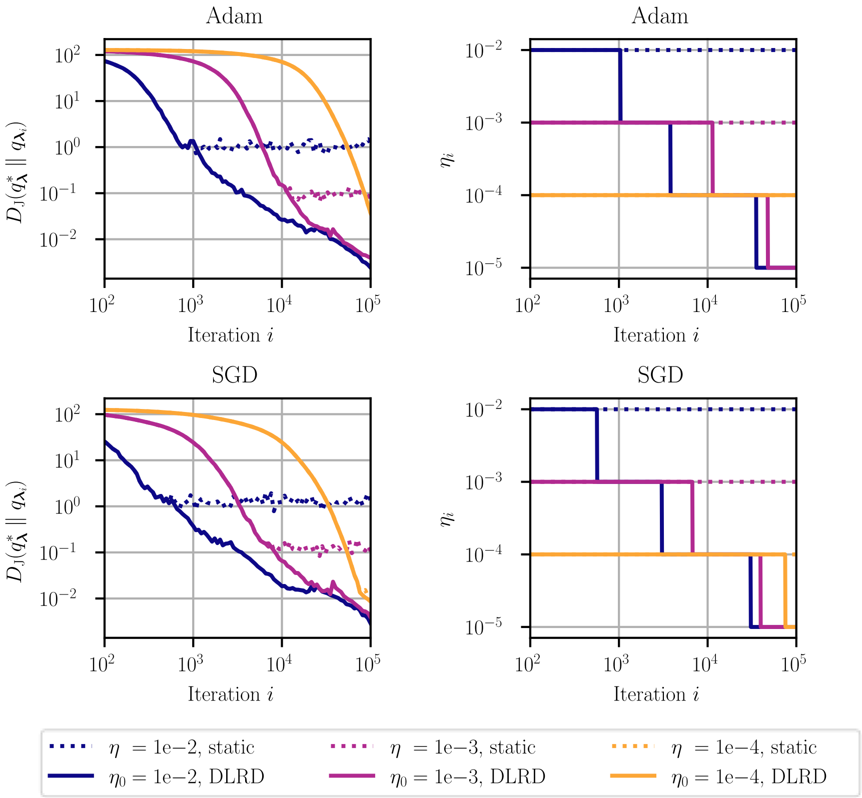
$$\rightarrow \quad \lambda^{\text{opt}} = 0.0$$

Unknown

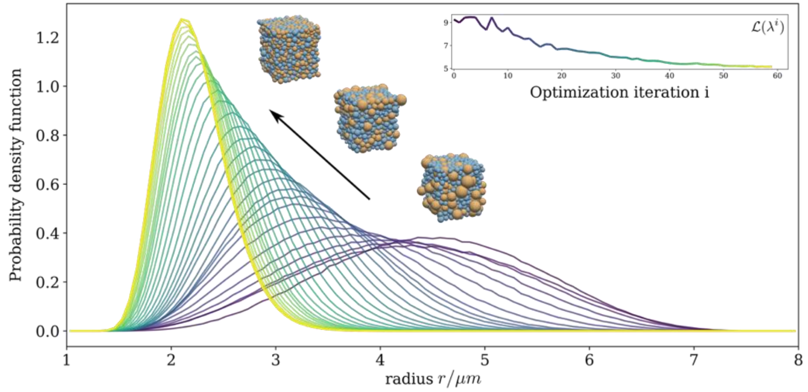
Optimization - Our research

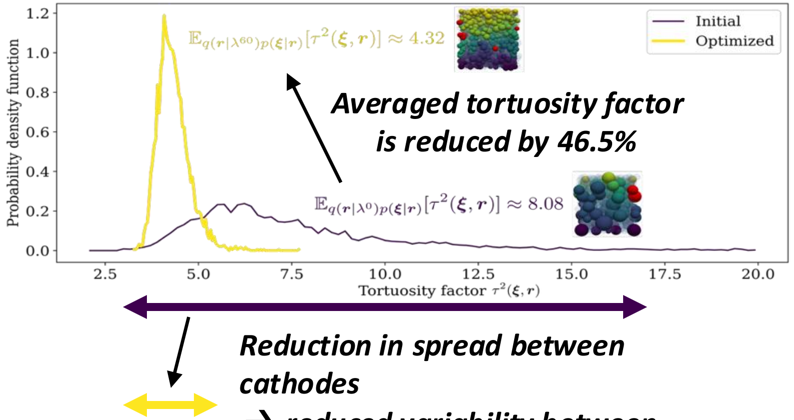
Available in QUEENS

- Deterministic optimizers (based on scipy)
- Stochastic optimizers
- Levenberg-Marquardt algorithm



Dinkel M., Robalo Rei G., Wall W. A., Dynamic Learning Rate Decay for Stochastic Variational Inference





Reduction in spread between cathodes
→ reduced variability between cells

Robalo Rei G., Schimdt C.P., P.M. Praegla, W.A. Wall, Enhancing Physical Powder System Properties through Particle Size Distribution Optimization and Non-Differentiable Stochastic Models

Surrogate modeling

Goal:
Find an inexpensive approximation $\widetilde{\mathcal{M}}(\theta)$ to the computational model $\mathcal{M}(\theta)$

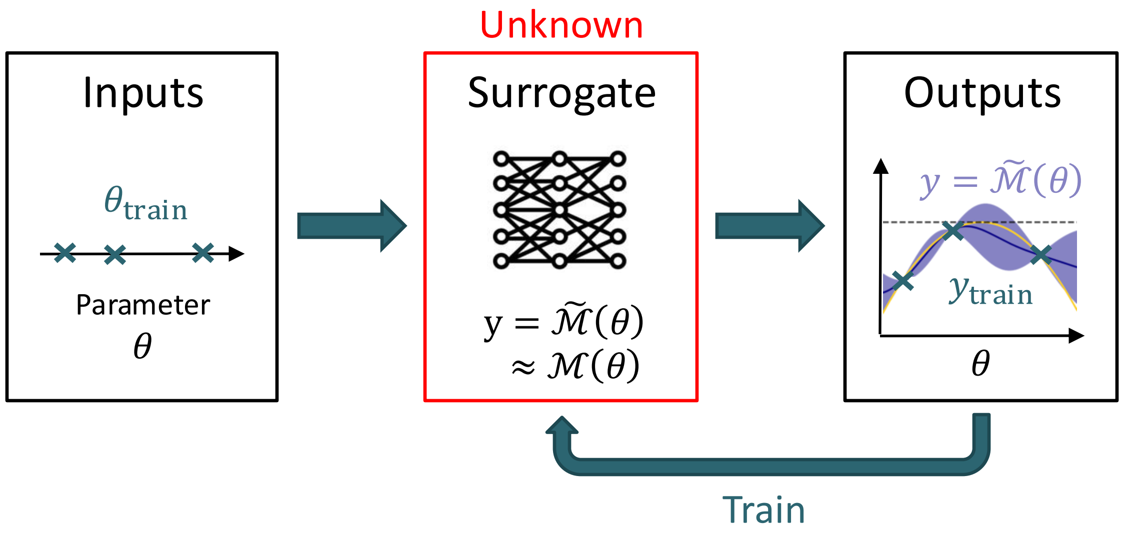
Approximation: $\widetilde{\mathcal{M}}(\theta) \approx \mathcal{M}(\theta)$

Known:

- Training inputs θ_{train}
- Training outputs $y_{\text{train}} = \mathcal{M}(\theta_{\text{train}})$

Unknown:

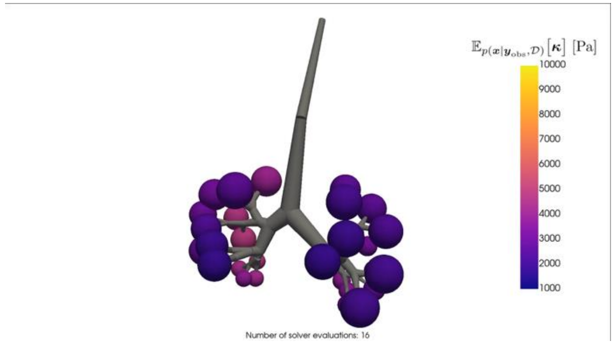
- inexpensive approximation $\widetilde{\mathcal{M}}(\theta)$ to the computational model $\mathcal{M}(\theta)$



Surrogate modeling - Our research

Available in QUEENS

- Gaussian processes (heteroskedastic & variational)
- Gaussian neural networks
- Bayesian neural networks
- Multi-fidelity surrogates



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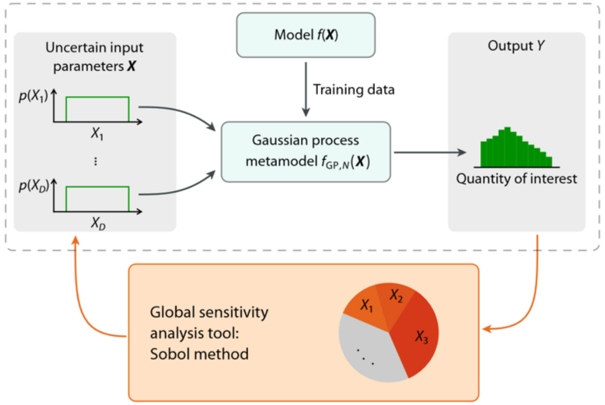
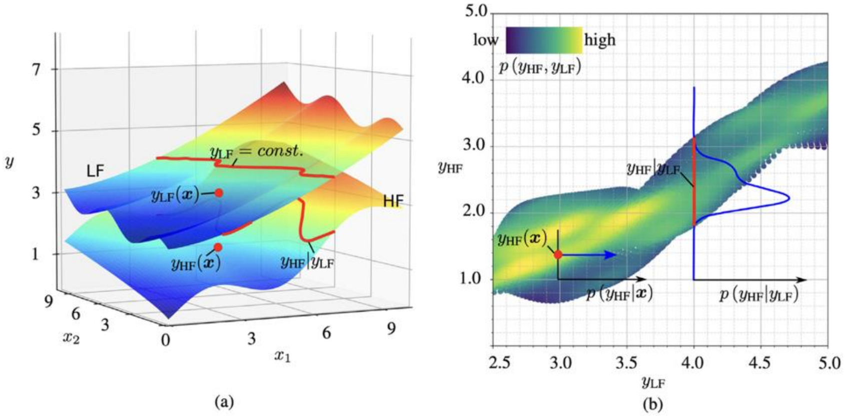
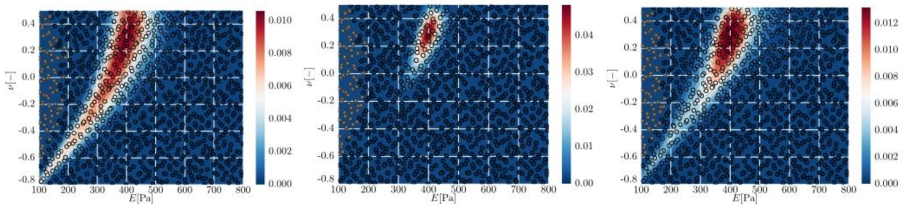


Wirthl, B., Brandstaeter, S., Nitzler, J., Schrefler, B. A., & Wall, W. A. (2023). Global sensitivity analysis based on Gaussian-process metamodelling for complex biomechanical problems. International Journal for Numerical Methods in Biomedical Engineering, 39(3), e3675.



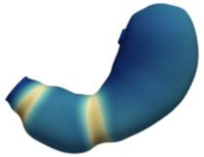
Nitzler, J., Biehler, J., Fehn, N., Koutsourelakis, P., & Wall, W. A. (2022). A generalized probabilistic learning approach for multi-fidelity uncertainty quantification in complex physical simulations. *Computer Methods in Applied Mechanics and Engineering*, *400*, 115600.



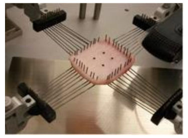
Willmann, H., Nitzler, J., Brandstäter, S. *et al.* Bayesian calibration of coupled computational mechanics models under uncertainty based on interface deformation. *Adv. Model. and Simul. in Eng. Sci.* 9, 24 (2022). https://doi.org/10.1186/s40323-022-00237-5

Collaboration is essential:

Modelling expert



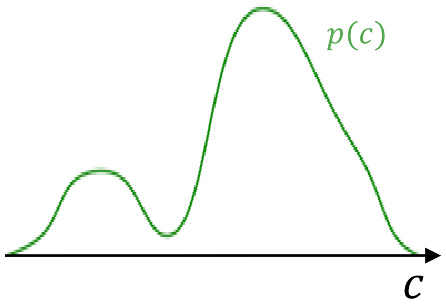
Experimental expert



Probabilistics expert

$$p(\theta|D) \propto p(\mathrm{D}|\theta)p(\theta)$$

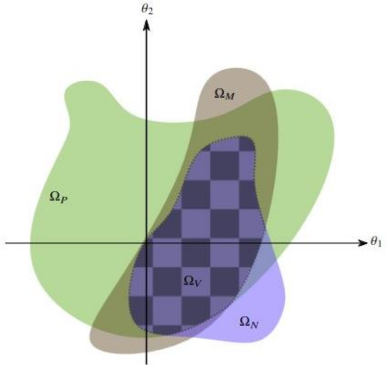
QUEENS



Probabilistic methods help bridge the gap between numerical simulations and experimental work!

Challenges for Multi-Query Analyses

- **Extreme Computational Cost**
- **High-Dimensional Parameter Spaces**
- **Limited or Noisy Data**
- **Model Error as Epistemic Uncertainty**
- **Scalability and Parallelisation (on HPC cluster)**



Expect simulations to fail!

Methodological Solution Strategies

- Dimension Reduction
- Adaptive Sampling
- Surrogate Models
- Multi-Fidelity Methods

Building the infrastructure for MQA takes significant time and effort.
We tackle the challenges, so you don’t have to!

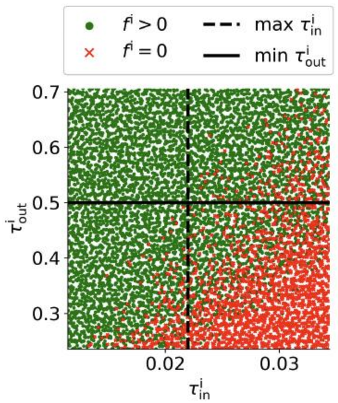
AutoM(Q)Ate your research

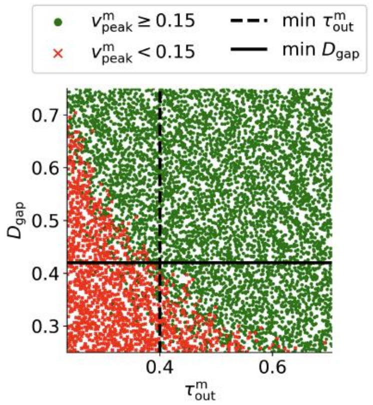
For coding:
- Automate your parameter sweeps
- Automate your verification and validation

For publications:
- Automate your parameter studies
- Automate model comparisons

If your model will be evaluated many times, you can use QUEENS to do so.

Some recent examples
- Identification of physiological parameter ranges
- Temporal and or spatial convergence studies
- Automated comparison of time integration schemes
- Testing various parameter combinations
- Testing different unit systems and check convergence rates
- Verify effect of penalty parameters on solution quality
- Quantify nonlinear solver iterations w.r.t. varying input





Community

Maintainer team


Sebastian Brandstäter


Maximilian Dinkel


Lea Häusel


Jonas Nitzler


Gil Robalo Rei

Contributors


Daniel Wolff


Silvia Hervás Raluy


Regina Bühler


Bishr Maradni

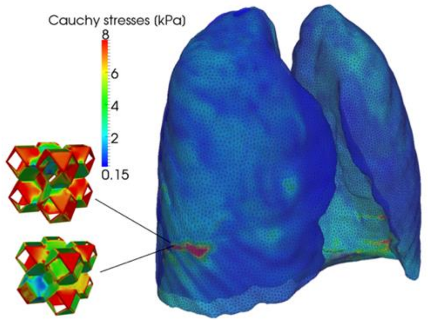
Universität der Bundeswehr München

You are welcome to join!
Connect with us on GitHub.

https://github.com/queens-py/queens

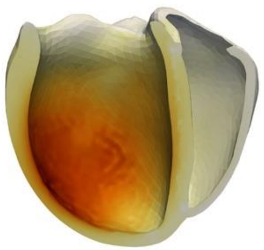
4C — Comprehensive Computational Community Code

An open-source parallel multiphysics research code based on FEM, HDG, SPH & DEM



[Lena Yoshihara, LNM, TUM]

github.com/4C-multiphysics/4C

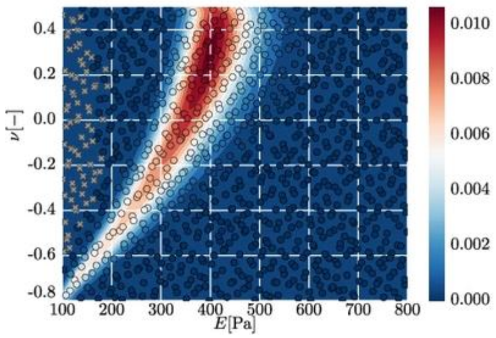


[Amadeus M. Gebauer, LNM, TUM]

TUM — Universität der Bundeswehr München — Helmholtz-Zentrum hereon — Ruhr Universität Bochum RUB — TUHH

QUEENS

An open-source Python framework for solver-independent multi-query analyses of large-scale computational models.



queens-py.org

Applications:

- Parameter identification
- Sensitivity analysis
- Uncertainty quantification
- Bayesian inverse analysis

TUM — Universität der Bundeswehr München

Biehler, J., Nitzler, J., Brandstaeter, S., Dinkel, M., Gravemeier, V., Haeusel, L. J., Rei, G. R., Willmann, H., Wirthl, B., & Wall, W. A. (2025). *QUEENS: An Open-Source Python Framework for Solver-Independent Analyses of Large-Scale Computational Models*. arXiv.2508.16316.

Thank you for your participation!

Dr.-Ing. Sebastian Brandstäter
University of the Bundeswehr Munich

Dr.-Ing. Georg Hammerl
Helmholtz-Zentrum Hereon

Dr.-Ing. Matthias Mayr
University of the Bundeswehr Munich

Regina Bühler, MSc
University of the Bundeswehr Munich

Gil Robalo Rei, MSc
Technical University of Munich

Dr.-Ing. Ingo Scheider
Helmholtz-Zentrum Hereon

Christoph Schmidt, MSc
Technical University of Munich

Bishr Maradni, MSc
University of the Bundeswehr Munich