

UKACM & GACM AUTUMN SCHOOL 2025

Open-Source Codes for High-Performance Computing

Hands-on Session 4C & QUEENS

30.09.2025 and 01.10.2025



QUEENS

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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.



https://survey.unibw.de/ukacm_gacm_2025/

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 Brandstätter¹, Maximilian Dinkel², Lea Häusel², Jonas Nitzler², Gil Robalo Rei²

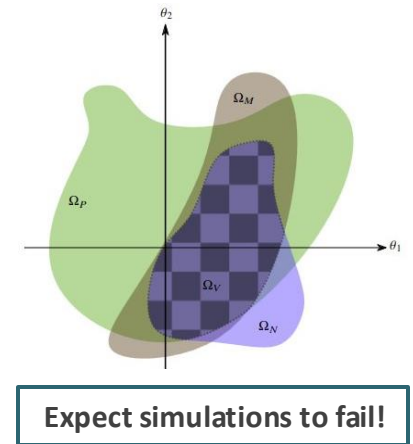
¹ Institute for Mathematics and Computer-Based Simulation | University of the Bundeswehr Munich

² Institute for Computational Mechanics | Technical University of Munich



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)



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!**



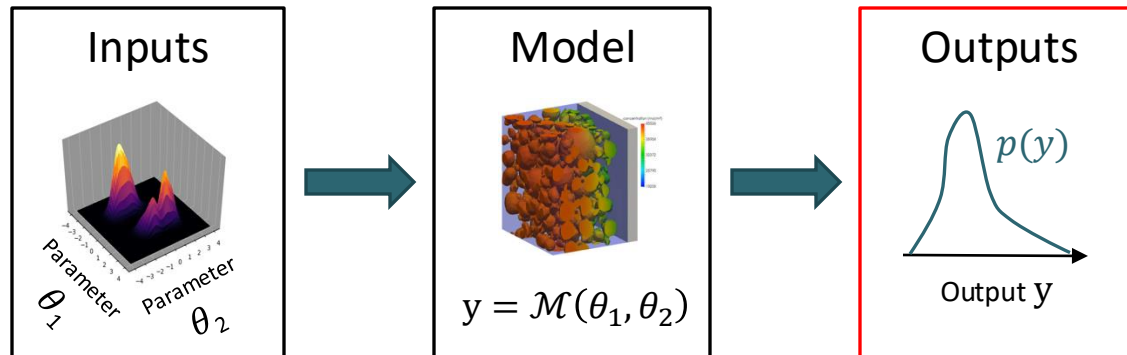
How to quantify uncertainties?

Uncertainty Propagation

Forward Uncertainty Quantification (UQ)

Quantification of uncertainties in the output

Forward UQ

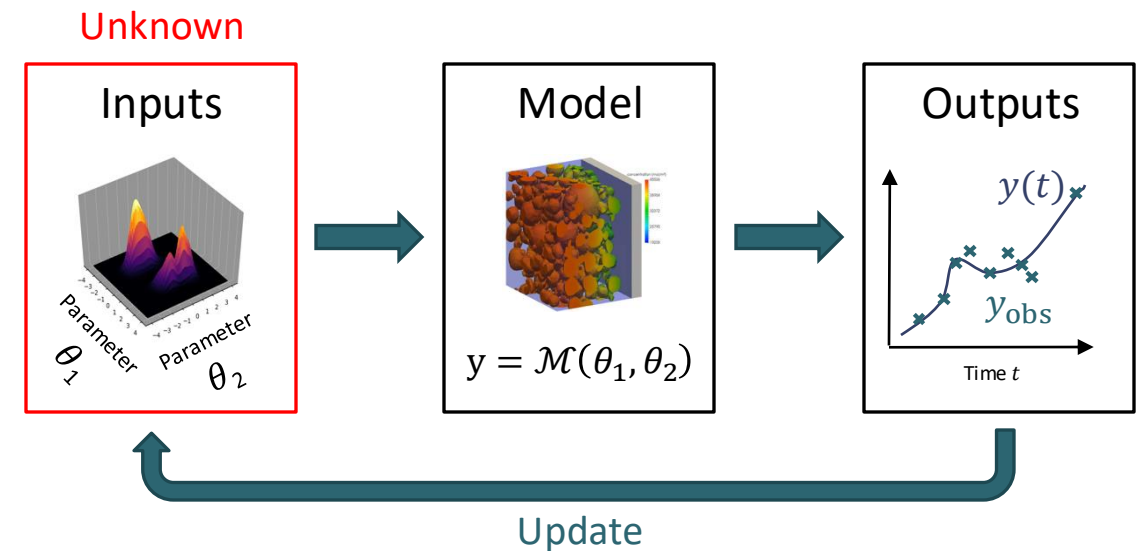


Inverse Analysis (IA)

Backward Uncertainty Quantification (UQ)

Quantification of uncertainties in the input

Backward UQ





Forward UQ – Our research

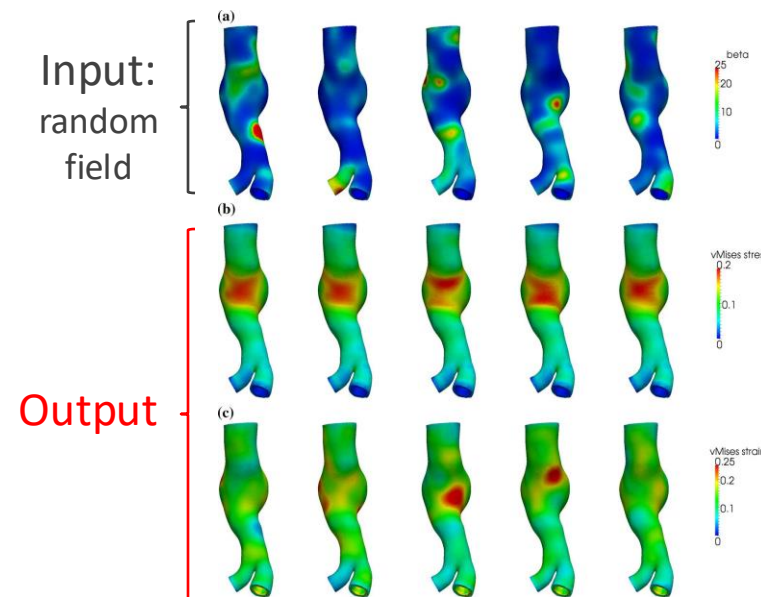
Uncertainty Quantification based on a Bayesian **multi-fidelity scheme**:

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

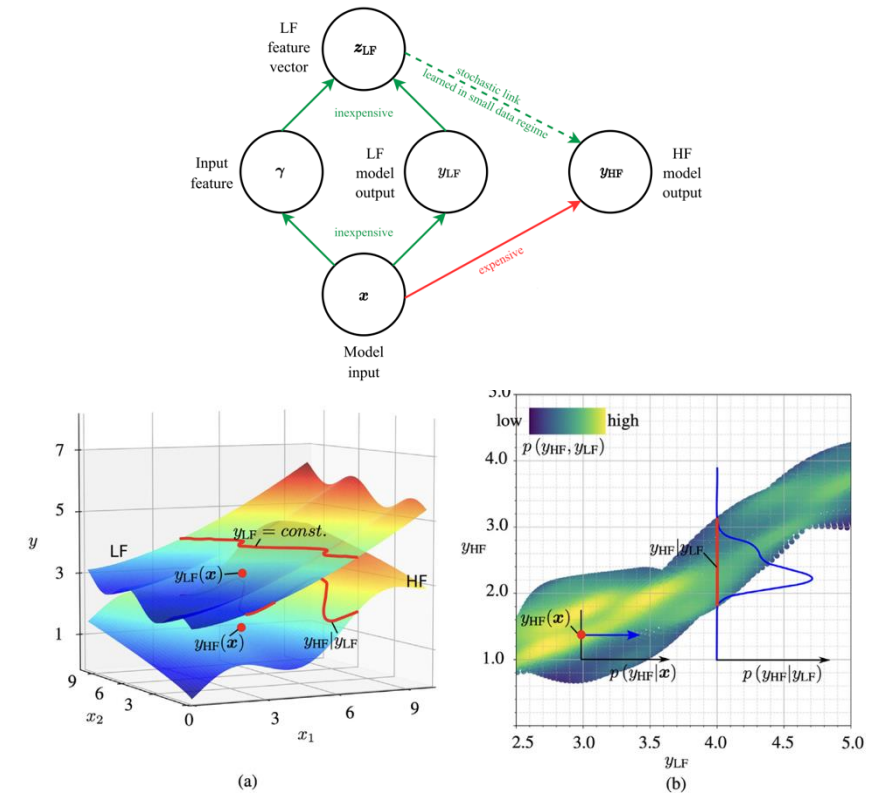


Available in
QUEENS

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



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.



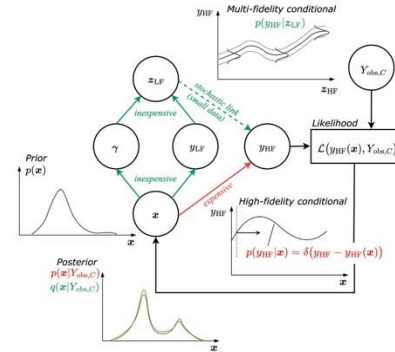
Nitzler, J., Biehler, J., Fehn, N., Koutsourelakis, P., & Wall, W. A. (2022). A generalized probabilistic learning approach for multi-fidelity uncertainty quantification in complex physical simulations. *Computer Methods in Applied Mechanics and Engineering*, 400, 115600.



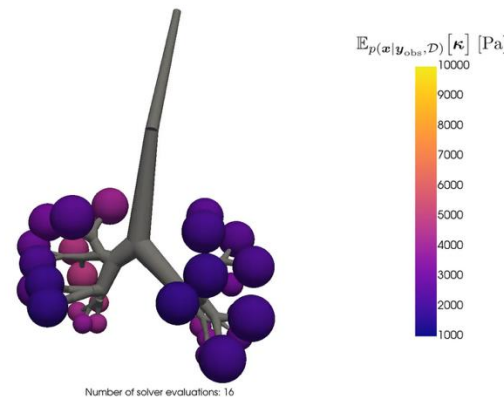
Bayesian inverse analysis – Our research



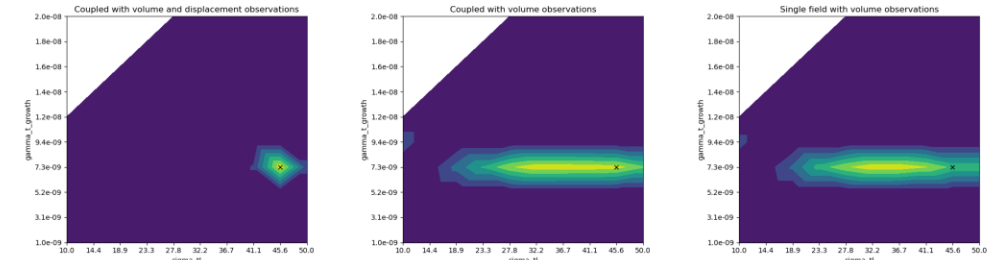
- Markov Chain Monte Carlo (in-house & pymc-based)
- Sequential Monte Carlo (in-house & particles-based)
- Variational inference
- Bayesian multi-fidelity inverse analysis



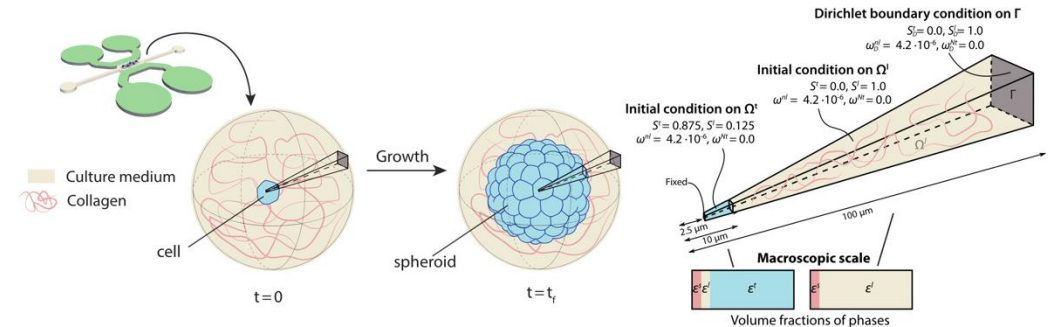
Nitzler, J., Wall, W. A., & Koutsourelakis, P.-S. (2023). *Bayesian multi-fidelity inverse analysis (BMFIA) for expensive, non-differentiable, physics-based simulations in high stochastic dimensions*. 5th International Conference on Uncertainty Quantification in Computational Science and Engineering.



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.



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.



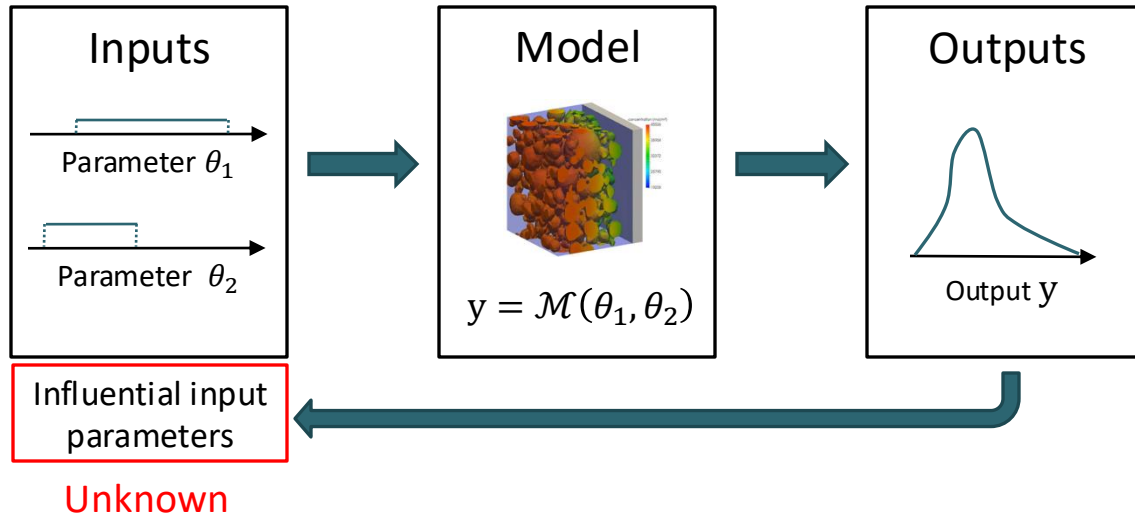
Hervas-Raluy, S., Wirthl, B., Guerrero, P. E., Robalo Rei, G., Nitzler, J., Coronado, E., De Mora Sainz, J. F., Schrefler, B. A., Gomez-Benito, M. J., Garcia-Aznar, J. M., & Wall, W. A. (2023). Tumour growth: An approach to calibrate parameters of a multiphase porous media model based on in vitro observations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



Exploiting uncertainties

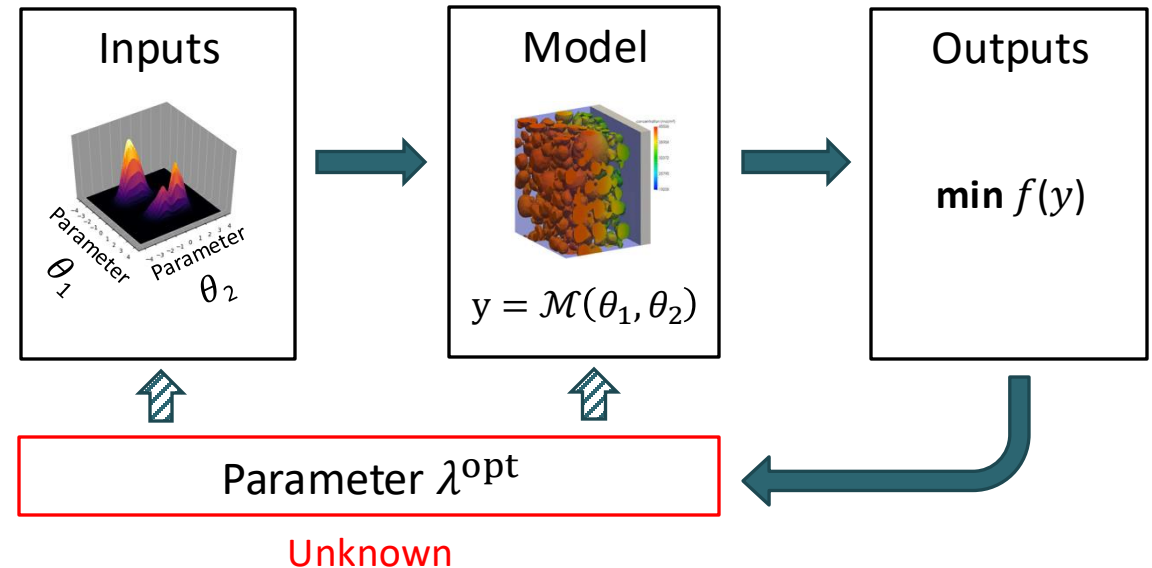
Global Sensitivity Analysis (GSA)

Identification of the most promising input parameters



Optimization Under Uncertainty (OUU)

Find the optimal solutions under uncertain conditions

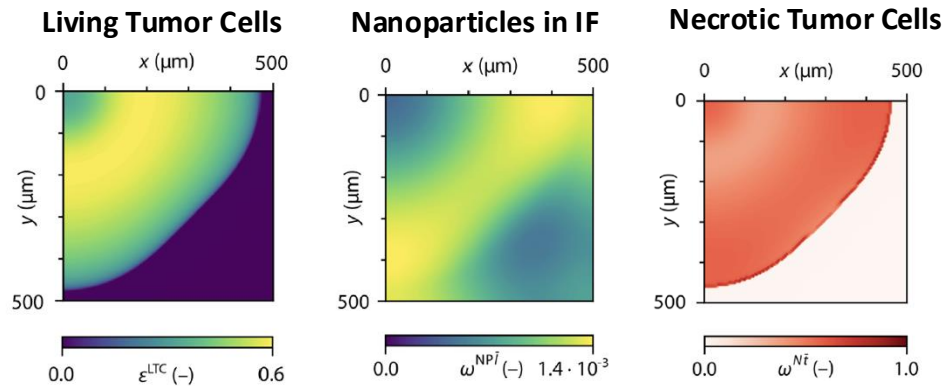
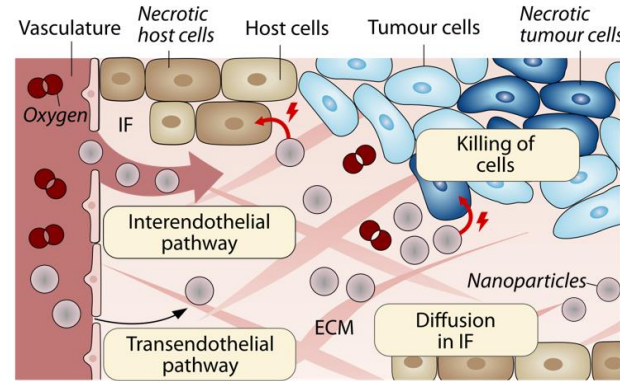




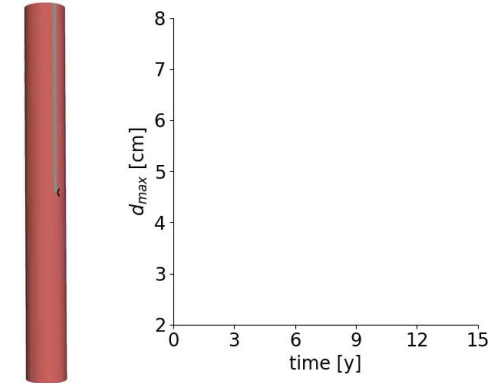
Global sensitivity analysis – Our research



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

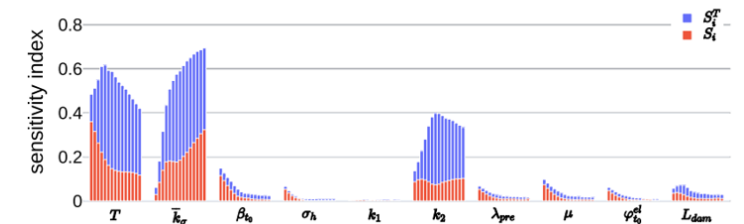


Wirthl, B., Brandstaeter, S., Nitzler, J., Schrefler, B. A., & Wall, W. A. (2023). Global sensitivity analysis based on Gaussian-process metamodeling for complex biomechanical problems. *International Journal for Numerical Methods in Biomedical Engineering*, 39(3), e3675.



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

Sobol indices of ten independent parameters:



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.

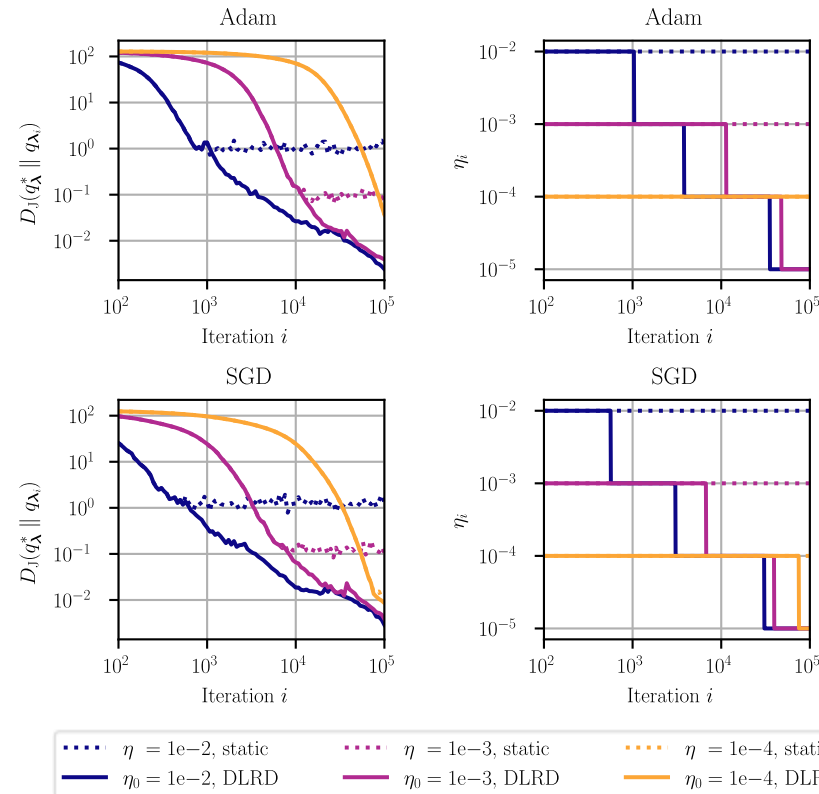


Optimization - Our research

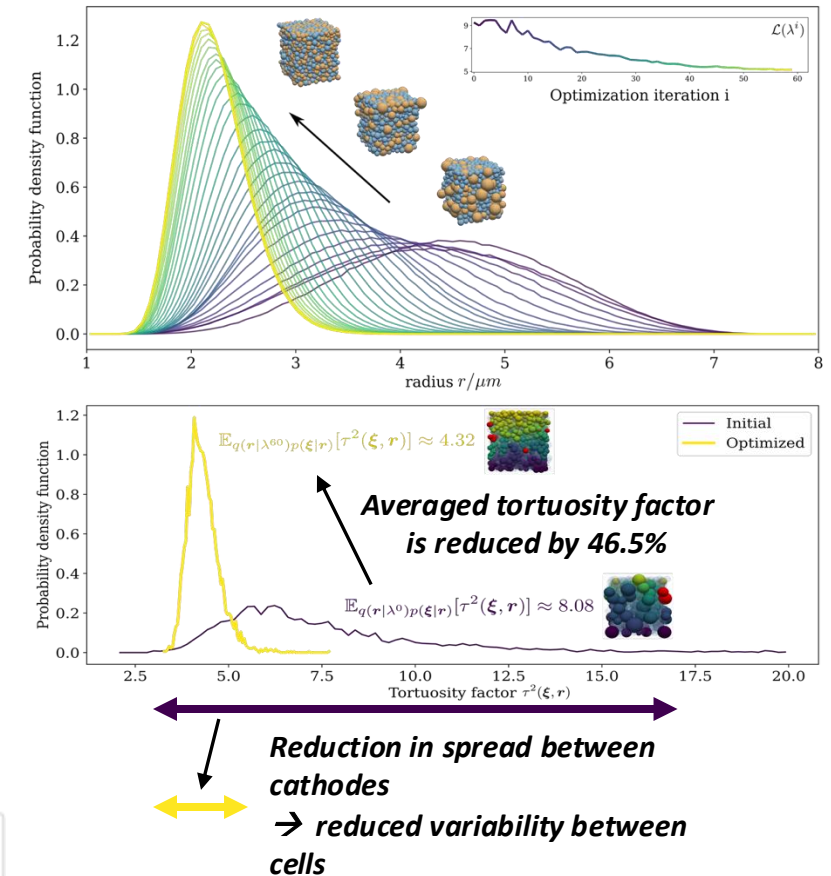


Available in
QUEENS

- 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



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 $\tilde{\mathcal{M}}(\theta)$ to the computational model $\mathcal{M}(\theta)$

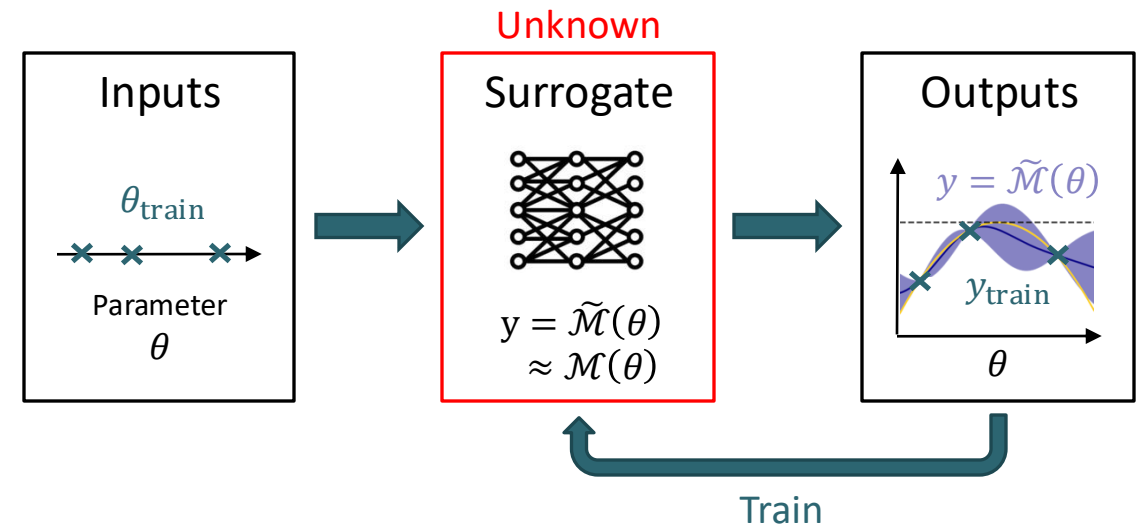
Approximation: $\tilde{\mathcal{M}}(\theta) \approx \mathcal{M}(\theta)$

Known:

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

Unknown:

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



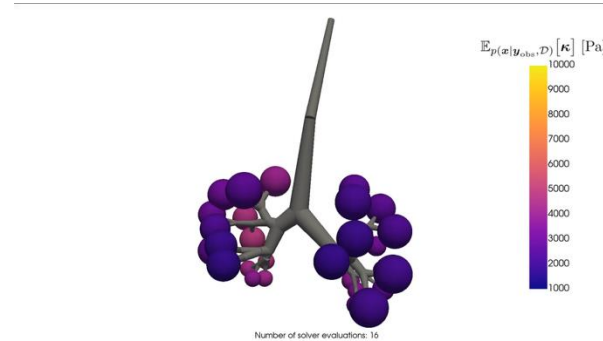


Surrogate modeling - Our research

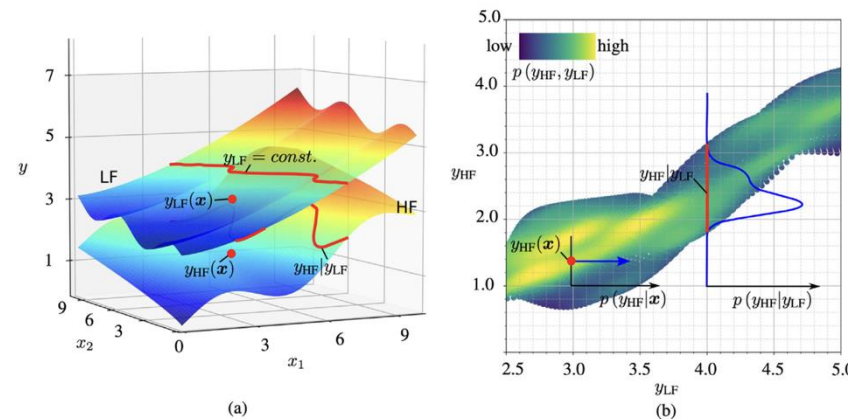


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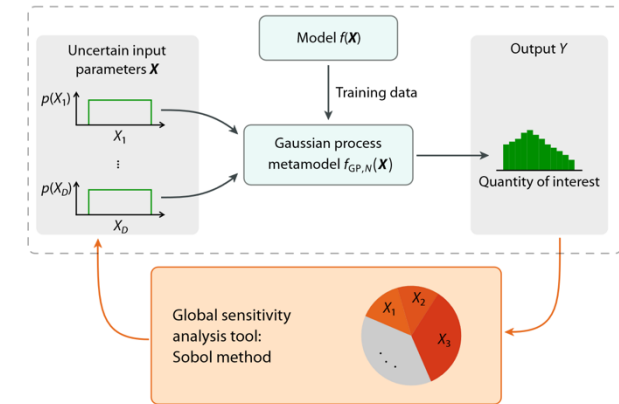
- Gaussian processes (heteroskedastic & variational)
- Gaussian neural networks
- Bayesian neural networks
- Multi-fidelity surrogates



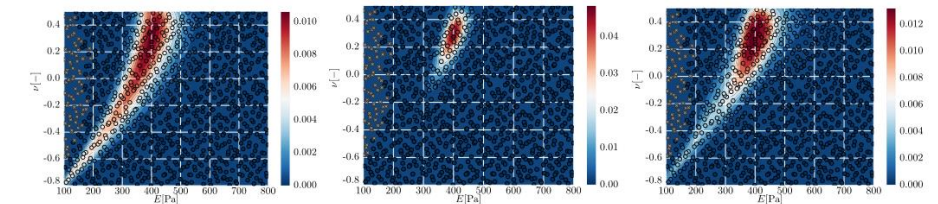
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Nitzler, J., Biehler, J., Fehn, N., Koutsourelakis, P., & Wall, W. A. (2022). A generalized probabilistic learning approach for multi-fidelity uncertainty quantification in complex physical simulations. *Computer Methods in Applied Mechanics and Engineering*,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



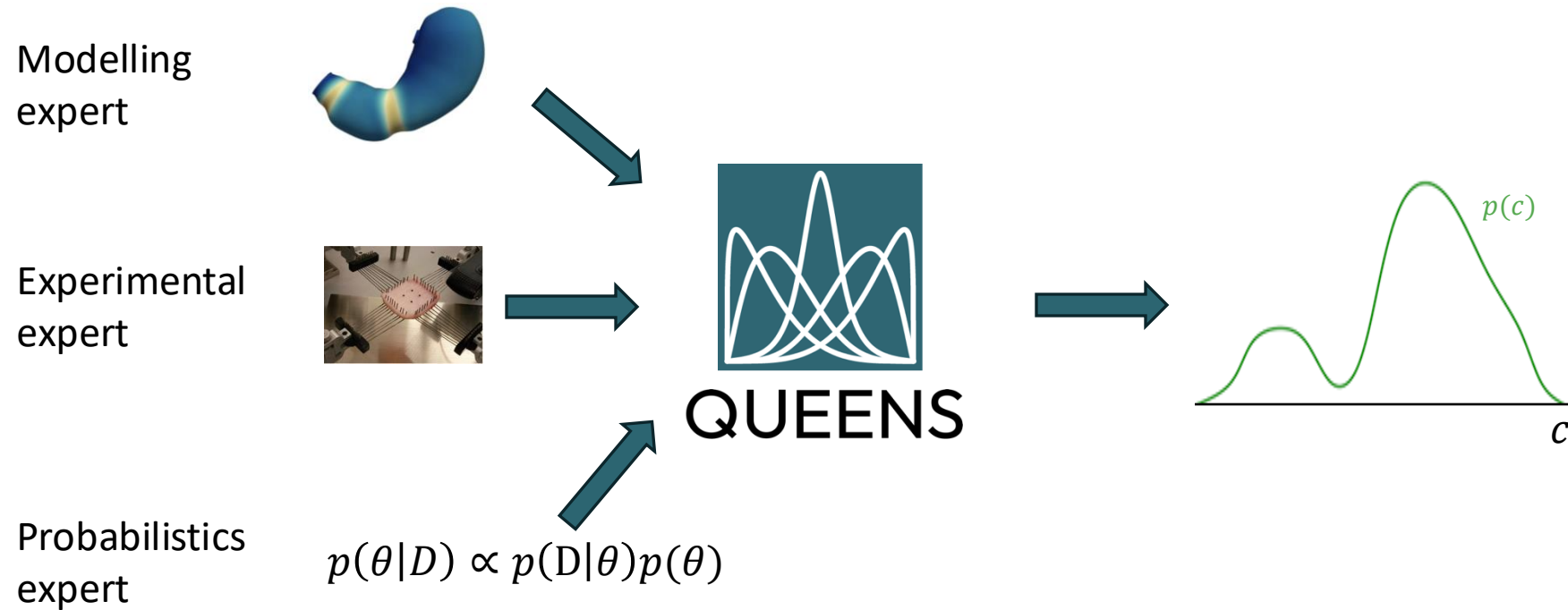
Wirthl, B., Brandstaeter, S., Nitzler, J., Schrefler, B. A., & Wall, W. A. (2023). Global sensitivity analysis based on Gaussian-process metamodeling for complex biomechanical problems. *International Journal for Numerical Methods in Biomedical Engineering*, 39(3), e3675.



Willmann, H., Nitzler, J., Brandstätter, 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:



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



AutoM(Q)Ate your research

For coding:

- Automate your parameter sweeps
- Automate your verification and validation

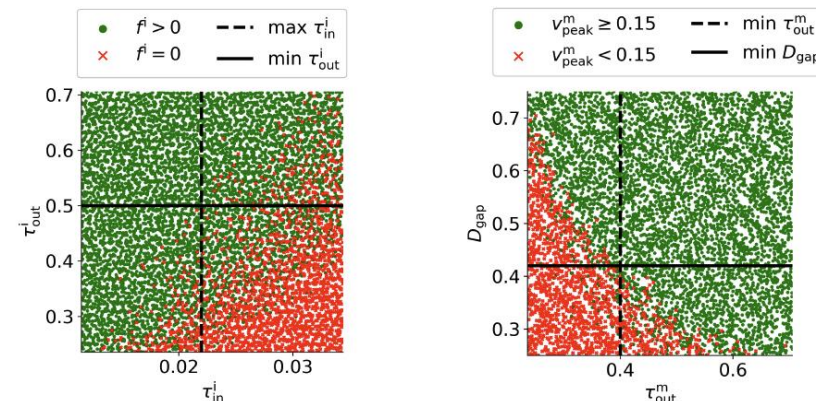
For publications:

- 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



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Maximilian
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Lea
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Contributors

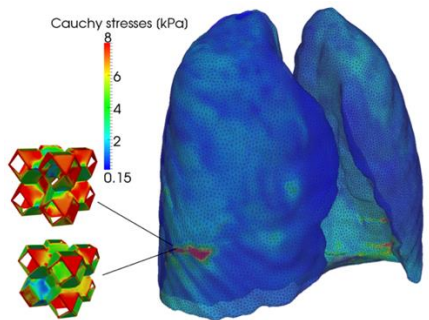
You are welcome to join!
Connect with us on GitHub.



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



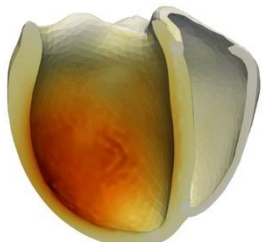
An open-source parallel multiphysics research code
based on FEM, HDG, SPH & DEM



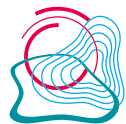
[Lena Yoshihara, LNM, TUM]



github.com/4C-multiphysics/4C



[Amadeus M. Gebauer, LNM, TUM]



hereon

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BOCHUM

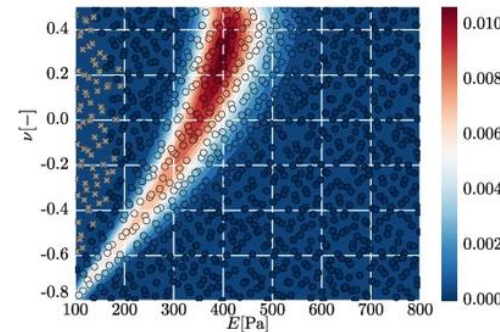
RUB

TUHH



QUEENS

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



github.com/queens-py/queens

Applications:

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



der Bundeswehr
Universität 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](https://arxiv.org/abs/2508.16316).

Thank you for your participation!



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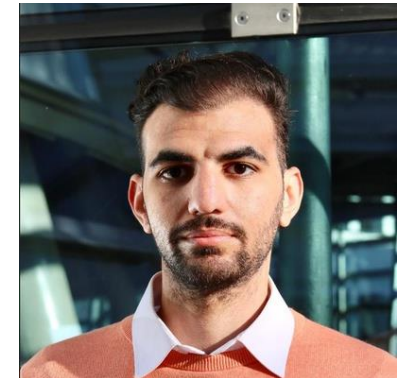
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