International Research Training Group IRTG 2657
Computational Mechanics Techniques in High Dimensions

Augmenting Transport Maps with Metamodel Tools for an Accurate and Efficient Bayesian Framework for Dynamical Systems

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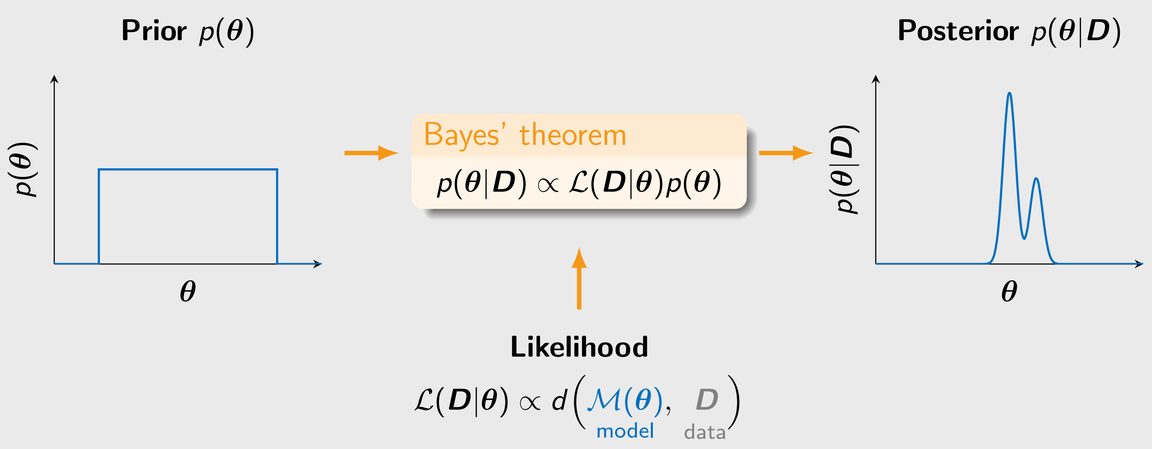
Second Cohort – Starting Date: 01.09.2024

Bayesian Inference under Hybrid Uncertainties

Bayesian Model Updating (BMU)

Let $\boldsymbol{\theta}$ be the parameters of a computational model $\boldsymbol{y} = \mathcal{M}(\boldsymbol{\theta})$.
Infer parameters $\boldsymbol{\theta}$ based on a set of measurements of the output:

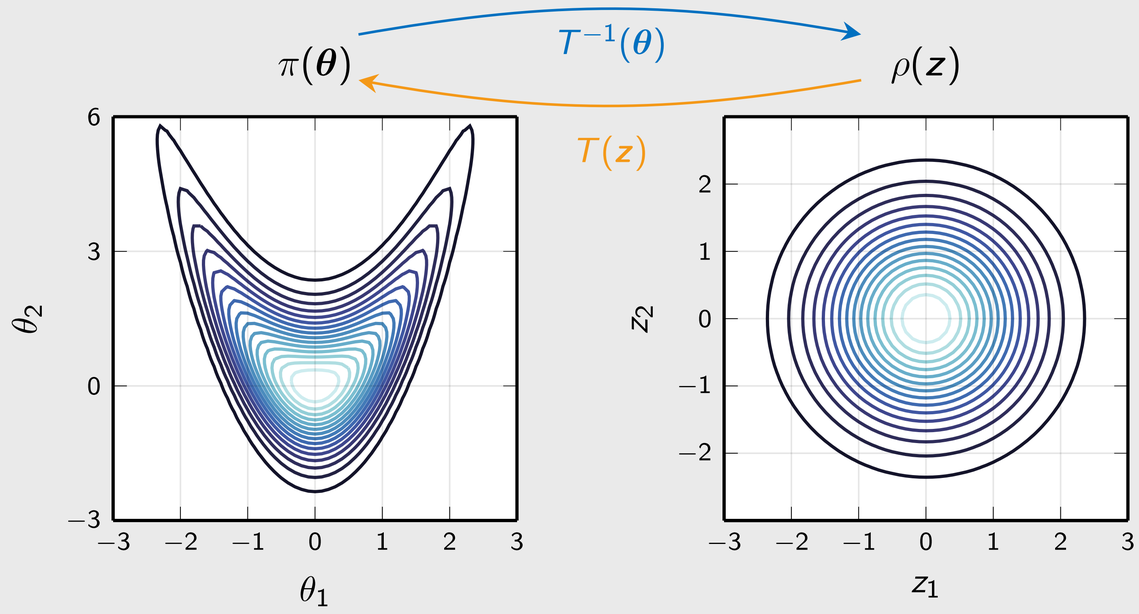


Challenges

- **Implicit posterior:** unnormalized, requires costly model evaluations
- **Hybrid uncertainties:** increases computational cost
  - Handling of parameters that are both epistemic (unknown) and aleatory (random)
- **Dynamical systems:**
  - Need compact feature extraction from multivariate time series

Bayesian Inference with Transport Maps

Approximate the posterior by mapping a reference measure $\rho(z)$ to the target measure (= posterior) $\pi(\boldsymbol{\theta})$ through an invertible transformation:



Transport Map (TM) Construction

1. Choose a **parameterized basis for the map**, e.g., orthogonal polynomials, neural networks, sum-of-square functions, etc.
2. Approximate target distribution by mapping from the reference:

$$\pi(\boldsymbol{\theta}) \approx \hat{\pi}(\boldsymbol{\theta}; \boldsymbol{a}) = \rho\left(T^{-1}(\boldsymbol{a}, \boldsymbol{\theta})\right) \; |\det \nabla T^{-1}(\boldsymbol{a}, \boldsymbol{\theta})|$$

3. Find parameters $\boldsymbol{a}$ that **minimize** the Kullback-Leibler divergence $\mathcal{D}_{\mathrm{KL}}$:

$$\min_{\boldsymbol{a}} \; \mathcal{D}_{\mathrm{KL}}\left(\hat{\pi}(\boldsymbol{\theta}; \boldsymbol{a}) || \pi(\boldsymbol{\theta})\right)$$
$$\text{s.t. } \nabla T \succ 0 \quad \text{(invertibility)}$$

Current Work

- Building an open-source Julia framework for transport maps

Future Work

- TMs for problems with hybrid uncertainties
- **Data-driven state estimation of dynamical systems**
  - Use TMs to improve state estimation
  - Enhance state estimation with system identification (i.e., SINDy) to learn model purely from data

Applications

NASA and DNV UQ Challenge 2025 [2]

- Parameter inference, uncertainty propagation, and reliability-based optimization of a black-box model
  - Efficient handling of hybrid uncertainties by use of Kriging surrogate
  - Feature extracting by observing manifold of multivariate outputs
- **Successful participation:** 3rd overall, 2nd in model calibration

Time-Dependent Biofilm Growth Model [3]

Time evolution of biofilm growth of interacting species due to nutrients c^* and antibiotics α^*

$$\Psi = -\frac{1}{2}c^*\overline{\boldsymbol{\phi}} \cdot \boldsymbol{A} \cdot \overline{\boldsymbol{\phi}} + \frac{1}{2}\alpha^*\boldsymbol{\psi} \cdot \boldsymbol{B} \cdot \boldsymbol{\psi}$$

- Hybrid uncertainty model (random growth dynamics & unknown parameters)
- Application of BMU to infer material parameters in $\boldsymbol{A}$ and $\boldsymbol{B}$
- Novel approach to reduce computational cost of BMU:
  - Reduced order model (ROM) constructed using time-separated-stochastic mechanics (TSM)

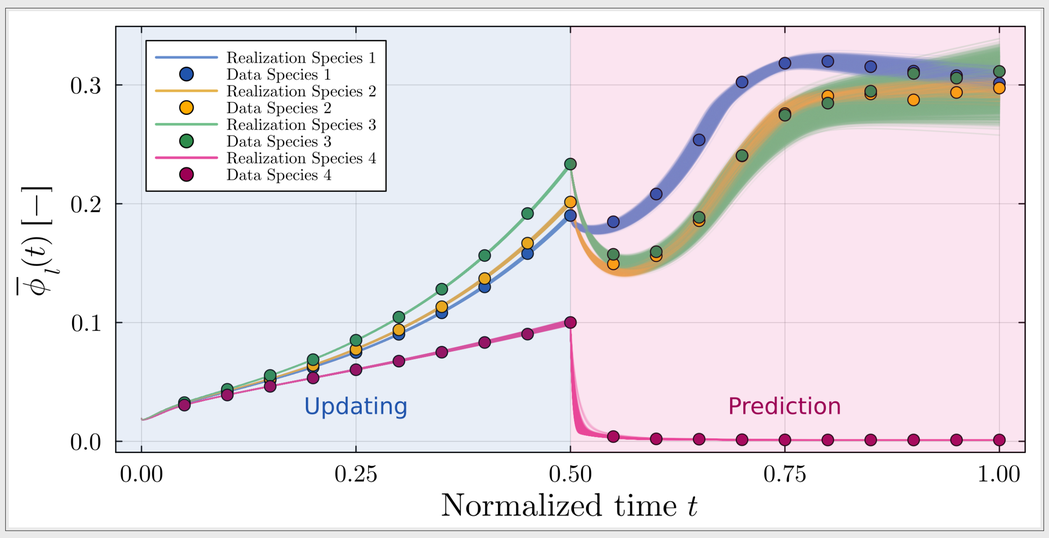


Figure: Biofilm concentrations (model output $\overline{\phi}$) over time for four different species without antibiotics ($t < 0.5$) and with antibiotics ($t \geq 0.5$) applied.

Transport map implementation in Julia together with Jan Grashorn:
https://github.com/lukasfritsch/TransportMaps.jl

Publications

Published

[1] **Lukas Fritsch**, Matteo Broggi, and Michael Beer. "Bayesian Updating for Reliability with Imprecise Probabilities: Julia Implementation and Application to the NASA Langley UQ Challenge 2019". In: *Proceedings of the 35th European Safety and Reliability & the 33rd Society for Risk Analysis Europe Conference*. Singapore: Research Publishing, 2025.

[2] Nataly Manque, **Lukas Fritsch**, Chao Dang, Jan Grashorn, Zhouzhou Song, Marius Bittner, Thomas Potthast, Pei-Pei Li, Marcos Valdebenito, Matteo Broggi, and Matthias Faes. "Taking on the NASA and DNV Challenge 2025: Bayesian Calibration and Optimization under Hybrid Uncertainty". In: *Proceedings of the 35th European Safety and Reliability & the 33rd Society for Risk Analysis Europe Conference*. Singapore: Research Publishing, 2025.

In Preparation

[3] **Lukas Fritsch**, Hendrik Geisler, Jan Grashorn, Felix Klempt, Maisam Soleimani, Matteo Broggi, Philipp Junker, and Michael Beer. "Bayesian Updating of Bacterial Microfilms under Hybrid Uncertainties with a Novel Surrogate Model". (submitted to Computational Mechanics).

IRTG Environment

- Spokesperson of the doctoral candidates of IRTG (German side)
- **Collaboration**: The spirit of the IRTG enabled for interdisciplinary collaboration to combine TSM-ROM with Bayesian inference and apply it to the biofilm model
- **Stay at ENS Paris-Saclay**: Nov. 2026 - Apr. 2027

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