Bayesian multi-fidelity inverse analysis for computationally demanding models in high stochastic dimensions

J. Nitzler^{1,2} , W. A. Wall^{1,3} , and P.-S. Koutsourelakis^{2,3}

¹Institute for Computational Mechanics ²Professorship of Data-driven Materials Modeling ³Munich Data Science Institute (MDSI - Core Member), www.mdsi.tum.de Technical University of Munich

The biggest challenges in (Bayesian) inverse analysis of large-scale numerical models are posed by the high computational demands in combination with a high stochastic dimension. The latter is often caused by inverse problems that involve random fields, i.e., in the case of unknown boundary conditions, elastography problems, unknown microstructure distributions or geometric quantities, to name a few examples. The solution process is further impeded when model derivatives are inaccessible as it is often the case in legacy codes and coupled problems.

We propose Bayesian multi-fidelity inverse analysis (BMFIA) which overcomes the aforementioned difficulties by employing computationally inexpensive, lower-fidelity models and constructing a multi-fidelity likelihood function. The approach builds upon previous developments of the authors in the field of uncertainty quantification [1, 2, 3, 4]. The multi-fidelity likelihood is learned robustly from a small number of high-fidelity simulations and reflects the uncertainty, not only in the original inverse problem, but also due to the (small) training data employed. We specifically address challenges imposed by the small data regime and demonstrate how the the multi-fidelity dependency can be learned with higher accuracy in an extended space that is equipped with low-dimensional, informative features of the input. BMFIA is independent of the problem's stochastic dimension as it primarily relies on the dependence between the outputs of models of varying fidelities and not on the input.

Furthermore, improved efficiency is attained since the inference process, which can be performed using state-of-the-art sampling-based or variational methods, requires solely evaluations of the low-fidelity model(s). The latter can be chosen or constructed such that they provide model derivatives (e.g., from adjoint formulations) which further expedite inference. The performance can be even further increased when the low-fidelity model is given by a physics-informed surrogate model or physical knowledge is incorporated directly in the multi-fidelity likelihood function.

We demonstrate our approach on large-scale biomechanical and coupled multi-physics problems and compare them with state-of-the-art single- and multi-fidelity methods.

References

- J. Biehler, M. W. Gee, and W. A. Wall. 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, 2015.
- [2] J. Biehler, M. Mäck, J. Nitzler, M. Hanss, P.-S. Koutsourelakis, and W. A. Wall. Multifidelity approaches for uncertainty quantification. *GAMM-Mitteilungen*, 42(2):e201900008, 2019.
- [3] P.-S. Koutsourelakis. Accurate uncertainty quantification using inaccurate computational models. SIAM Journal on Scientific Computing, 31(5):3274–3300, 2009.
- [4] J. Nitzler, J. Biehler, N. Fehn, P.-S. Koutsourelakis, and W. A. Wall. A generalized probabilistic learning approach for multi-fidelity uncertainty propagation in complex physical simulations. arXiv:2001.02892, 2020.