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MUQ-hIPPYlib: A Bayesian Inference Software Framework Integrating Data with Complex Predictive Models under Uncertainty

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Recent years have seen a massive explosion of datasets across all areas of science, engineering, technology, medicine, and the social sciences. The central questions are: How do we optimally learn from data through the lens of models? And how do we do so taking into account uncertainty in both data and models? These questions can be mathematically framed as Bayesian inverse problems. While powerful and sophisticated approaches have been developed to tackle these problems, such methods are often challenging to implement and typically require first and second order derivatives that are not always available in existing computational models. In this paper, we present an extensible software framework MUQ-hIPPYlib that overcomes this hurdle by providing unprecedented access to state-of-the-art algorithms for deterministic and Bayesian inverse problems. MUQ provides a spectrum of powerful Bayesian inversion models and algorithms, but expects forward models to come equipped with gradients/Hessians to permit large-scale solution. hIPPYlib implements powerful large-scale gradient/Hessian-based solvers in an environment that can automatically generate needed derivatives, but it lacks full Bayesian capabilities. By integrating these two libraries, we created a robust, scalable, and efficient software framework that realizes the benefits of each to tackle complex large-scale Bayesian inverse problems across a broad spectrum of scientific and engineering areas.

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