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Data-Driven Inference Design for the Bayesian Uncertainty Quantification of the Reactive Shock-Bubble Interaction

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The quantification of uncertainties in reacting flow solvers poses significant computational challenges with individual fully-resolved simulations, with their complex reaction chemistry costing 100's of thousands of CPU hours while at the same time suffering from a long time-to-solution for individual simulations [1]. Approaching such simulation workflows with Bayesian Uncertainty Quantification, with Bayesian inference at its core, hence requires the commitment of inordinate computational resources to the inference routine to obtain expressive uncertainties for our quantities of interest. To enable such large routines we hence have to exploit domain-specific model hierarchies to the fullest extent possible [3]. To accelerate and improve the efficiency of the sampling we build on advances in fields adjacent to uncertainty quantification, such as machine-learning based design, sequential decision making, and reinforcement learning to pose our problem as the design of a Multifidelity-exploiting inference routine with intelligent sampling agents at its core. The intuition here is that the sampling agents learn the task- and problem-structure in their attention-based policy networks [2], which can then later be fine-tuned to similar inference problems. In this work we present a machine-learning based design approach to Bayesian Uncertainty Quantification inference routines for fully-resolved reacting flows, which is based on a graph network representation of the inference routine in combination with a Transformer-based placement network to exploit the available model hierarchies. The excessive training costs of the learned inference routine are amortized across later inference studies, of which we will show the chances and limits of amortization across related flow-configurations.

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