An adaptive hierarchy of certified machine learning and reduced basis surrogates for parametrized PDEs*

B. Haasdonk[1], H. Kleikamp[2], M. Ohlberger[2], F. Schindler[2], and T. Wenzel[1]

[1] *Institute of Applied Analysis and Numerical Simulation, Pfaffenwaldring 57, 70569 Stuttgart, Germany (*`haasdonk@mathematik.uni-stuttgart.de`*,* `tizian.wenzel@ians.uni-stuttgart.de`*).*

[2] *Mathematics Münster, Westfälische Wilhelms-Universität Münster, Einsteinstr. 62, 48145 Münster, Germany (*`hendrik.kleikamp@wwu.de`*,* `mario.ohlberger@wwu.de`*,* `felix.schindler@wwu.de`*)*

In the context of parametrized partial differential equations (PDE)s, we are interested in efficiently and accurately approximating time-dependent quantities of interest $f_h\colon \mathcal{P} \to L^2([0,T])$ (for an end time $T > 0$), which are given by applying an output operator to state-trajectories obtained from solving an underlying PDE. We assume we are given a full order model (FOM) to evaluate f_h (e.g., stemming from a spatio-temporal discretization of the PDE), that is however costly to evaluate in the sense that while we may compute $f_h(\mu)$ for few parameters $\mu \in \mathcal{P} \subset \mathbb{R}^p$, for $p > 0$, it is computationally infeasible to evaluate f_h in the context of uncertainty quantification or PDE-constrained optimization. We are in particular interested in the case where this cost does not only stem from a high spatial resolution, but where in addition a high temporal resolution or long-time integration $T \gg 1$ is required.

In our earlier work [1], we used model order reduction by reduced basis (RB) methods to generate an RB-reduced order model (ROM) approximation f_{rb} of f_h by means of the method of snapshots, to generate enough certified data to train a machine learning (ML) based model f_{ml} as an efficient surrogate for f_h. The need for an additional ML surrogate stems from the fact that, while the RB-ROM evaluations might be orders of magnitudes faster than the FOM evaluations, they are still inherently iterative in time, limiting their use in aforementioned scenarios. While demonstrated to perform well, the approach in [1] has two main systematic drawbacks: (i) the a-priori choice of training sets and accuracies for the RB-ROM as well as the ML model (yielding models of fixed size and accuracy) and (ii) more critically, as with most ML surrogates, there is no bound on the prediction error $\|f_h(\mu) - f_{\text{ml}}(\mu)\| \leq ?$ available.

This contribution addresses both shortcomings: (ii) by learning the RB coefficients of the intermediate state, instead of learning the output directly, we propose a certified ML-ROM which combines approximation quality and certification of RB-ROMs with the online efficiency of ML predictions. This allows to certify ML-ROM predictions a posteriori and helps to address (i): we propose an adaptive model hierarchy of FOM, RB-ROM and ML-ROM, where (starting from trivial RB-ROM and ML-ROM) each model is used to generate training data for the next, but only if the online certification indicates a need for enrichment, which we demonstrate in the context of PDE-constrained minimization.

References

[1] P. Gavrilenko, B. Haasdonk, O. Iliev, M. Ohlberger, F. Schindler, P. Toktaliev, T. Wenzel, and M. Youssef. A full order, reduced order and machine learning model pipeline for efficient prediction of reactive flows. In *Large-Scale Scientific Computing*, pages 378–386. Springer International Publishing, 2022.

*Funded by BMBF under contracts 05M20PMA and 05M20VSA. Funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) under contracts OH 98/11-1 and SCHI 1493/1-1, as well as under Germany's Excellence Strategy EXC 2044 390685587, Mathematics Münster: Dynamics – Geometry – Structure, and EXC 2075 390740016, Stuttgart Center for Simulation Science (SimTech).