A new certified hierarchical and adaptive RB-ML-ROM surrogate model for parametrized PDEs

Bernard Haasdonk[†], **Hendrik Kleikamp**[*], **Mario Ohlberger**[‡], **Felix Schindler**[‡], **Tizian Wenzel**[†]

[†] Institute for Applied Analysis and Numerical Simulation
University of Stuttgart
Pfaffenwaldring 57, 70569 Stuttgart, Germany

[*],[‡] Institute for Analysis and Numerics, Mathematics Münster
University of Münster
Orléans-Ring 10, 48149 Münster, Germany

ABSTRACT

In this talk, we present a new surrogate modeling technique for efficient approximation of solutions and output quantities of parametrized partial differential equations [1]. The model is hierarchical as it is built on a full order model (FOM), reduced order model (ROM) and machine-learning (ML) model chain. The model is adaptive in the sense that the ROM and ML model are adapted on-the-fly during a sequence of parametric requests to the model. To allow for a certification of the model hierarchy, as well as to control the adaptation process, we employ rigorous a posteriori error estimates for the ROM and ML models, see [3]. The model is therefore able to fulfill fixed or adaptively chosen error tolerances for every requested parameter. In particular, we provide an example of an ML-based model that allows for rigorous analytical quality statements. Numerical experiments showcase the efficiency of our approach in different scenarios, for instance a parameter optimization problem and uncertainty quantification. Here, the ROM is instantiated by Reduced Basis Methods [2] and the ML model is given by a neural network, similar to [4], or a VKOGA kernel model, see [5]. However, a wide range of ML algorithms is applicable within the modeling chain while maintaining the certification of the results.

REFERENCES

[1] B. Haasdonk and H. Kleikamp and M. Ohlberger and F. Schindler and T. Wenzel, “A new certified hierarchical and adaptive RB-ML-ROM surrogate model for parametrized PDEs”, *arXiv preprint*, https://arxiv.org/abs/2204.13454, (2022).

[2] M. Ohlberger and S. Rave, “Reduced Basis Methods: Success, Limitations and Future Challenges”, *Proceedings of the Conference Algoritmy*, pp. 1–12, (2016).

[3] M. A. Grepl and A. T. Patera, “A posteriori error bounds for reduced-basis approximations of parametrized parabolic partial differential equations”, *ESAIM: Mathematical Modelling and Numerical Analysis*, Vol. **39**, pp. 157–181, (2005).

[4] J. S. Hesthaven and S. Ubbiali, “Non-intrusive reduced order modeling of nonlinear problems using neural networks”, *J. Comput. Phys.*, Vol. **363**, pp. 55–78, (2018).

[5] G. Santin and B. Haasdonk, “Kernel Methods for Surrogate Modeling”, in *Model Order Reduction*, Eds. P. Benner and S. Grivet-Talocia and A. Quarteroni and G. Rozza and W. Schilders and L. M. Silveira, Vol. **2**, pp. 311–353, (2021).