Towards trustworthy use of scientific machine-learning in large scale numerical simulations

Alena Kopaničáková

Abstract

Recently, scientific machine learning (SciML) has expanded the capabilities of traditional numerical approaches by simplifying computational modeling and providing cost-effective surrogates. However, SciML models suffer from the absence of explicit error control, a computationally intensive training phase, and a lack of reliability in practice. In this talk, we will take the first steps toward addressing these challenges by exploring two different research directions. Firstly, we will demonstrate how the use of advanced numerical methods, such as multilevel and domain-decomposition solution strategies, can contribute to efficient training and produce more accurate SciML models. Secondly, we propose to hybridize SciML models with state-of-the-art numerical solution strategies. This approach will allow us to take advantage of the accuracy and reliability of standard numerical methods while harnessing the efficiency of SciML. The effectiveness of the proposed training and hybridization strategies will be demonstrated by means of several numerical experiments, encompassing the training of DeepONets and the solving of linear systems of equations that arise from the high-fidelity discretization of linear parametric PDEs using DeepONet-enhanced multilevel and domain-decomposition methods.

References

[1] Kopaničáková, and G. Karniadakis. DeepOnet Based Preconditioning Strategies For Solving Parametric Linear Systems of Equations. Under review, 2024.

[2] A. Kopaničáková, and G. Karniadakis. Operator Learning Recycling and Augmentation Strategies for Enhancing Convergence of Linear Krylov Methods. Under review, 2024.

[3] A. Kopaničáková, H. Kothari, G. Karniadakis and R. Krause. Enhancing training of physics-informed neural networks using domain-decomposition based preconditioning strategies. SIAM Journal on Scientific Computing , 2024.

[4] Y. Lee, A. Kopaničáková, and G. Karniadakis. Two level overlapping additive Schwarz preconditioner for training scientific machine learning applications. Under review, 2024.

[5] A. Kopaničáková. On the use of hybrid coarse-level models in multilevel minimization methods. Domain Decomposition Methods in Science and Engineering XXVII, 2023.