Seminar

SciML Lab · CDS

Wednesday, April 17, 2024
12:00–13:30
Seminar Room 1
Mathematical Institute
University of Cologne
Weyertal 86–90

Center for Data and Simulation Science

Speaker:

Prof. Dr. Uwe Naumann

RWTH Aachen University

Derivatives and Applications for Learning Derivatives

Surrogates for numerical simulations can be learned (by "machines") through sampling inputs to the simulation to obtain desired outputs. Adequate matching of the latter is likely to not be sufficient for the numerical methods (e.g. calibration or optimal control) to be applied to the simulations and hence to their surrogates. Consistency of simulation and surrogate up to a certain order of differentiation may be required. The "machine" needs to learn values as well as first and possibly higher derivatives. Algorithmic differentiation [1] helps to generate this data.

We discuss two rather different recent applications of differential machine learning (also known as Sobolev training). [2] addresses pruning of oversized artificial neural networks based on interval adjoint significance analysis. A new exact matrix-free Newton method is presented in [3]. Its extension to surrogates of appropriate structure is the subject of ongoing research.

[1] Naumann: The Art of Differentiating Computer Programs. SIAM 2012. [2] Kichler, Afghan, Naumann: Towards Sobolev Pruning. Under review for PASC'24. See also arXiv:2312.03510. [3] Naumann: A Matrix-Free Exact Newton Method. To appear in SISC, SIAM. See also arXiv:2305.01669.

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