BASIC MACHINE LEARNING APPROACHES FOR THE ACCELERATION OF PDE SIMULATIONS

Hannes Ruelmann[1*], Stefan Turek[1]

[1]TU Dortmund University, 44227 Dortmund, Germany
* hannes.ruelmann@math.tu-dortmund.de

Machine Learning empowers several scientific fields and industries, and it fires the hardware markets to adjust their portfolio to it. Meanwhile the wide range from personal devices like smartphones and personal computers up to modern supercomputers contain hardware that is tailored for AI and chip vendors must satisfy an even larger demand since it is still a growing market. For this reason, a fundamental understanding of the design and theory of Machine Learning is needed to exploit the full arsenal of modern soft- and hardware components when it comes to using Machine Learning Methods in Scientific (High Performance-) Computing. It is not only necessary to adjust existing methods in the field of artificial neural networks to existing simulation pipelines but also a careful performance modelling and -engineering is required.

When it comes to real-world simulations the discretisation of Partial Differential Equations (PDEs) leads to a large but sparse global system matrix since we have to deal with a high number of degrees of freedom. The sheer amount of computational effort direct methods need for such problems makes them obsolete, hence iterative solvers are the only choice.

Usually the linear solver is the largest chunk in the simulation pipeline and by adapting them to the system to be solved and specially tailoring them to target modern hardware, such as General Purpose GPUs and Tensor Processing Units (TPUs), as well, we can accelerate the whole simulation by orders of magnitude. Based on the observations that smoothers in multigrid methods as well as strong preconditioners like Sparse Approximate Inverses (SPAI) have a deficit in the course of the assembly phase, we demonstrate in a simple and yet comprehensive way, how Machine Learning methods can fill this gap [1,2]. We discuss the design, implementation and potential of the Neural Networks that we trained for this task.

In addition we provide insight into other practical situations where Machine Learning can be applied in simulation pipelines, especially in the parts of the linear solver, and discuss the limits and opportunities concerning implementation, functionality and performance.

References

[1] Ruelmann, H., Geveler, M., and Turek, S. 2018. On the prospects of using machine learning for the numerical simulation of PDEs: Training Neural Networks to assemble Approximate Inverses. ECCOMAS newsletter issue 2018, 27-32.

[2] Ruelmann, H. 2017. Approximation von Matrixinversen mit Hilfe von Machine Learning. Master’s thesis, TU Dortmund, Dortmund, Germany.