Title: Towards data-driven high fidelity CFD

Abstract:

In this talk, I will give an overview of recent successes (and some failures) of combining modern, high order discretization schemes of Discontinuous Galerkin (DG) type with machine learning submodels and their applications for large scale computations. This approach can thus for example be employed in cases where current submodels in the discretization schemes currently rely on heuristic data. The primary focus will be on supervised learning strategies, where a multivariate, non-linear function approximation of given data sets is found through a high-dimensional, non-convex optimization problem that is efficiently solved on modern GPUs. I will introduce the basic concepts of machine learning strategies and their mathematical backgrounds and discuss the role the machine learning models can play in conjunction with established PDE solvers.

A prime of example of this is shock detection and shock capturing for high order methods, where essentially all known approaches require some expert user knowledge as guiding input. As an illustrative example, I will show how modern, multiscale neural network architectures originally designed for image segmentation can ameliorate this problem and provide parameter free and grid independent shock front detection on a subelement level. With this information, we can then inform a high order artificial viscosity operator for inner-element shock capturing.

In the second part of my talk, I will present data-driven approaches to LES modeling for implicitly filtered high order discretizations. Whereas supervised learning of the Reynolds force tensor based on non-local data can provide highly accurate results that provide higher a priori correlation than any existing closures, a posteriori stability remains an issue. I will give reasons for this and introduce reinforcement learning (RL) as an alternative optimization approach.

Reinforcement learning (RL) is considered as the third learning paradigm, besides unsupervised and supervised learning. In RL, the learning task is framed as a Markov Decision Process (MDP), which is solved by an optimal policy. This policy is either approximated directly or through the evaluation of a learned value action function. The learned policy represents the current control strategy for solving the MDP. Its parameters are updated through repeated sampling of the policy's proposed action space through interaction with the environment of the MDP, which emits reward signals intermittently and estimating the gradient of the objective w.r.t these parameters. This optimization within the context of a dynamical system makes the RL approach somewhat orthogonal to supervised learning (SL) in that no training samples need to be known a priori, only a definition of a meaningful reward (which could be a single scalar value) is necessary. This more indirect guidance of the learning process makes RL methods relatively sample-inefficient and training stability is less well understood than for SL methods, however, its possible benefits have been demonstrated in a range of applications from autonomous driving, strategic games and flow control.

Our initial experiments with this method suggest that is it much better suited to account for the uncertainties introduced by the numerical scheme and its induced filter form on the modeling task. For this coupled RL-DG framework, I will present discretization-aware model approaches for the LES equations (c.f. Fig. 1) and discuss the future potential of these solver-in-the-loop optimizations.

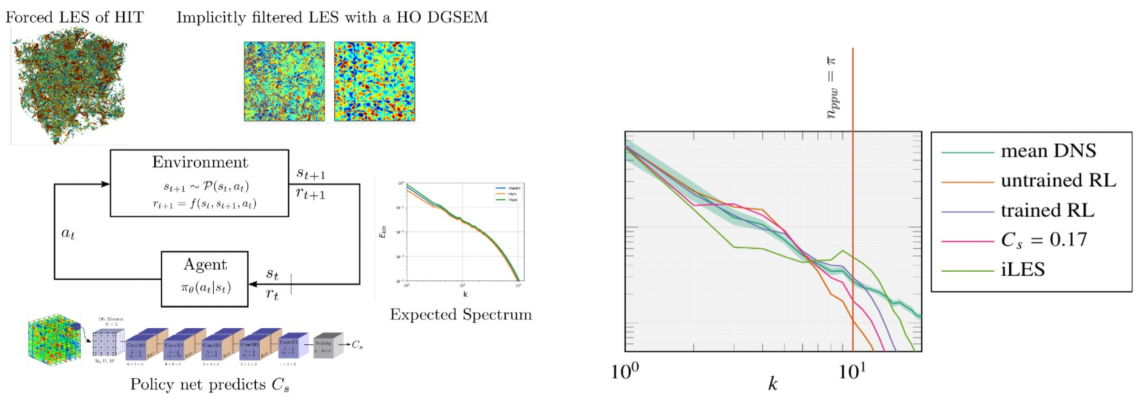

Figure 1: Left: Finding an eddy viscosity closure for LES formulated as an RL-problem. Right: Spectra of turbulent kinetic energy of homogeneous isotropic turbulence: DNS and LES results with different closure models.

In the practical sessions, we will investigate model training for canonical turbulent flows through supervised learning and explore methods to incorporate physical constraints into the ML-based models.

Bio:

Andrea Beck obtained a M.Sc. degree in aerospace engineering with a focus on fluid dynamics from the Georgia Institute of Technology in Atlanta (USA) and a doctoral degree from the University of Stuttgart (Germany) in computational fluid dynamics (CFD). She held the Dorothea-Erxleben professorship at the Institute of Fluid Dynamics and Thermodynamics of the Otto-von-Guericke University in Magdeburg (Germany) from 2020 to 2022 and is currently a professor for numerical methods in fluid dynamics at the faculty of aerospace engineering and geodesy at the University of Stuttgart. Her areas of interest include numerical discretization schemes for multiscale-multiphysics problems, in particular high order methods, high performance computing and visualization, Large Eddy Simulation methods and models, shock capturing schemes, uncertainty quantification methods and machine learning. She is a co-developer of the open-source high order Discontinuous Galerkin CFD framework FLEXI. Recent fields of application include uncertainty quantification of feedback loops in acoustics, particle-laden flow in turbomachines, wake-boundary layer interaction for transport aircraft at realistic flight conditions, shock-droplet interactions and data-driven models for LES closures.