Towards Data-Driven Computational Fluid Dynamics

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Machine learning in scientific applications including computational fluid dynamics (CFD) is a growing field of research. The broad range of machine learning techniques available and their ability to learn unknown, complex and possibly nonlinear correlations enable a large spectrum of applications, from game theory, image/speech recognition to applied mathematics. State-of-the-art data-driven methods generally originate from computer science, rendering a straight forward application to applied mathematics difficult. There are various reasons for this, depending on the problem under consideration. First, physical constraints given by the underlying equation system can be invaluable to obtain reasonable predictions, but are generally not considered by construction. Another problem is that numerical simulations, especially high-order methods, are susceptible to instabilities due to inaccurate predictions, which the learning algorithm has to account for and is particularly critical if discontinuities in the solution are present. Moreover, the definition of a suitable input space and loss function is a crucial and difficult task due to the highly nonlinear and mostly unknown mapping which has to be learned. Thus, the utilized machine learning algorithm has to be consistent to the considered numerical discretization. With these considerations in mind, the focus of recent research has concentrated on reinforcement learning or physics-informed methods applied to CFD, where the former enables to consider time-evolutions, while the latter inherently considers the physical constraints given by the given equation system.

This talks seeks to provide an overview about recent advances and failures in the application of deep learning techniques to enhance the solution of nonlinear, hyperbolic PDEs, from supervised to reinforcement learning. This will be demonstrated using two examples from CFD, turbulence modeling and shock capturing. First, depending on the equation system utilized, turbulent structures can appear in the solution, which either have to be resolved or adequately modeled, depending on the resolution requirements and computational resources available. The detailed physical behavior of turbulence is still unknown, rendering turbulence modeling difficult. Second, since nonlinear, hyperbolic PDEs admit discontinuities in the solution, adequate numerical methods are necessary to detect and handle such discontinuities, especially if high-order polynomial approximations are considered, denoted as shock capturing.