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Machine Learning-enhanced Polytopal Finite Element Methods

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The new paradigm of Polytopal Finite Element methods has emerged in recent years. Polytopal methods are Galerkin-type projection methods that construct the discretisation space using a computational grid made of arbitrarily polygonal/polyhedral (polytopal, for short) elements. This talk discusses how to integrate Machine Learning techniques to boost the accuracy and performance of Polytopal methods as well as their efficiency for large-scale applications. We demonstrate the capabilities of the proposed approach by considering two families of Polytopal methods, namely the Virtual Element method and the Polytopal Discontinuous Galerkin method. We show that these strategies can be effectively employed to enhance accuracy and reducing overall computational cost, and they can be efficiently employed for multiphysics problems modelled by heterogeneous partial differential equations, which are relevant to many engineering and applied science fields.

Physics-Informed Neural Networks for Power Systems Applications

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A power system consists of several critical components necessary for providing electricity to the consumers from the producers. Monitoring the lifetime of power system components becomes vital since they are subjected to electrical currents and high temperatures, which affect their aging. As the data is limited and complex in the field of components' aging, Physics-Informed Neural Networks (PINNs) can help overcome the problem. PINNs exploit the prior knowledge stored in partial differential equations (PDEs) or ordinary differential equations (ODEs), modeling the involved systems. This prior knowledge becomes a regularization agent, constraining the space of available solutions and consequently reducing the training data needed. This talk presents how we design and implement PINNs for monitoring the aging of power system components by highlighting the method's advantages and limitations in the field.

Computational Paradigms in Scientific Machine Learning

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Scientific Machine Learning (SciML) has emerged as a powerful tool for solving partial differential equations (PDEs) and addressing a wide spectrum of real-world challenges. This surge in interest has led to a reassessment and rethinking of traditional numerical methods, highlighting the need for more efficient and reliable approaches that integrate both model-driven and data-driven methodologies. In this context, Physics-Informed Neural Networks (PINNs) are novel deep learning frameworks for solving forward and inverse problems associated with nonlinear PDEs. Although PINNs have showcased remarkable effectiveness, several emerging Artificial Intelligence (AI) methodologies warrant consideration in addressing even more intricate and demanding applications. In this presentation, we will explore some novel theoretical and applied challenges related to the fascinating world of AI as it intersects with SciML.

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Graph-informed neural network and discontinuity learning

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In several applications related to rather complex problems, the availability of reliable surrogate models is of paramount importance. This is the case, for example, of multi-query tasks, such as uncertainty quantification analyses or optimization problems. In order to reduce the computational complexity of such processes, recent literature shows that it is worth considering the application of neural networks (NN) to perform regression tasks.

In several applications (such as transportation systems, epidemic spread, and social interactions), network analyses come into play, and graphs have a key role in such frameworks. Recently, new key contributions have been proposed by the neural network (NN) community, extending deep learning (DL) approaches to graphs via the so-called graph neural networks (GNNs) and the more recent graph convolutional networks (GCNs). Despite the good results of GCNs in many applications, some challenges still exist: (i) building deep GCNs with good performances; (ii) building GCNs scalable for large graphs.

In this talk, we present a new type of layer designed for regression tasks on graphs, a framework for which GCNs are not well suited and the use of multi-layer perceptrons (MLPs) is usually preferred. The new graph layer exploits the graph structure to improve the NN training (compared to an MLP). Moreover, it allows the building of deep NNs and it is scalable for large graphs. This new layer is called graph-informed (GI) layer [1]. Numerical experiments show the potentiality of the graph-informed NNs (GINNs), highlighting in particular improved regression abilities of the GINNs on maximum-flow regression problems, with respect to MLPs' performances on the same problem.

GI-layers have been recently exploited also to develop a new algorithm based on sparse grids for detecting discontinuity interfaces of n-dimensional piece-wise continuous functions; this task is of interest for example in UQ analyses, as in some applications the Quantity of Interest may be a discontinuous function in the space of stochastic parameters, thus preventing from the effective application of stochastic collocation strategies.

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Accelerating Numerical Simulations by Model Reduction with Scientific and Physics-Informed Machine Learning

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Partial differential equations (PDEs) are invaluable tools for modeling complex physical phenomena. However, only a limited number of PDEs can be solved analytically, leaving the majority of them requiring computationally expensive numerical approximations. To address this challenge, reduced order models (ROMs) have emerged as a promising field in computational sciences, offering efficient computational tools for real-time simulations. In recent years, deep learning techniques have played a pivotal role in advancing efficient ROM methods with exceptional generalization capabilities and reduced computational costs. In this talk we explore how classical ROM techniques can be elevated through the integration of deep learning models.

Our discussion encompasses a review of existing approaches to enhancing ROM, from graph neural network to multifidelity models by means of neural operators. We will introduce Physics-Informed Neural Networks (PINNs), highlighting their recent advancements in inverse modeling, discretive PINNs, and multiphase modeling and application to fluid dynamics.

Recent advances and failures in the machine-learning enhanced solution of PDEs

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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 talk 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 [2] and shock capturing [1, 3]. 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.

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