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Neural Differentiable Physics: Unifying Numerical PDEs and Deep Learning for Data-Augmented Computational Physics

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ABSTRACT:

Predictive modeling and simulation are essential for understanding, predicting, and controlling complex physical processes across many engineering disciplines. However, traditional numerical models, which are based on first principles, face significant challenges, especially for complex systems involving multiple interacting physics across a wide range of spatial and temporal scales. (1) A primary obstacle stems from our often-incomplete understanding of the underlying physics, which results in inadequate mathematical models that fail to accurately capture system behavior. (2) Additionally, the high computational demands of traditional solvers represent another substantial barrier, especially when real-time control or many repeated model queries are required, as in design optimization, inference, and uncertainty quantification. Fortunately, the continual evolution of sensing technology and the exponential increase in data availability have opened new avenues for the development of data-driven computational modeling frameworks. Bolstered by advanced machine learning and GPU computing techniques, these models hold the promise of greatly enhancing our predictive capabilities, effectively tackling the challenges posed by traditional numerical models. While data science and machine learning offer novel methods for computational mechanics models, challenges persist, such as the need for extensive data, limited generalizability, and lack of interpretability. Addressing existing challenges for predictive modeling issues requires innovative computational methods that integrate advanced machine learning techniques with physics principles. This talk will introduce some of our efforts along this direction, spotlighting the Neural Differentiable Physics, a novel SciML framework unifying classic numerical PDE solvers and advanced deep learning models for computational modeling of complex physical systems. Our approach centers on the integration of numerical PDE operators into neural architectures, enabling the fusion of prior knowledge of known physics, multi-resolution data, numerical techniques, and deep neural networks through differentiable programming. The way for integrating physics into the deep learning model represents a novel departure from existing SciML frameworks, such as Physics-Informed Neural Networks (PINNs). By combining the strengths of known physical principles and established numerical techniques with cutting-edge deep learning and AI technology, this innovative framework promises to inaugurate a new era in the understanding and modeling of complex physical systems, with far-reaching implications for science and engineering applications.

BIOGRAPHY:

Dr. Jian-Xun Wang is the Robert W. Huether Collegiate Associate Professor of Aerospace Engineering in the Department of Aerospace and Mechanical Engineering at the University of Notre Dame. He earned his Ph.D. in Aerospace Engineering from Virginia Tech in 2017 and worked as a Postdoctoral Scholar at UC Berkeley before joining Notre Dame in 2018. Dr. Wang has a multidisciplinary research background that spans Scientific Machine Learning, Data Assimilation, Bayesian Computing, Uncertainty Quantification, and Computational Fluid Dynamics. His research focuses particularly on the in-depth integration of advanced AI/ML techniques with physics-based mathematical models and classic numerical methods, aiming to revolutionize the field of computational modeling in the era of "big data" and significantly enhance the predictive simulation capabilities. He has led research projects sponsored by multiple agencies, including NSF, ONR, AFSOR, DARPA, Google, and others. Dr. Wang is a recipient of the 2021 NSF CAREER Award and the 2023 ONR YIP Award. He is also an elected vice chair of the US Association for Computational Mechanics (USACM) Technical Thrust Area on Data-Driven Modeling.