Other - Colloquium on Artificial Intelligence Research and Optimization

Machine Learning Techniques for Simulation-Driven Design Optimization

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Abstract:

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An important component of the design process of new reactive flow devices lies in optimizing them for efficiency under constraints relating to undesirable emissions, thermo-mechanical limits, and stability. Computational modeling can play a vital role in this process, whereby design optimization can be performed using computational fluid dynamics (CFD) simulations to identify promising designs for experimental prototyping. However, CFD simulations of such systems are compute-intensive because they involve capturing multi-physical processes that include turbulent gas dynamics, liquid spray injection and breakup, chemical kinetics, heat transfer, and their complex interactions. In this talk, I will present a mixture of deep experts approach that automatically divides modeling tasks amongst specialized learners, leading to simulations that capture experimental trends with reduced computational costs. Efficient simulation-driven design optimization depends, not solely on tractable and predictive computational models, but also on optimizers that can drive design decisions by utilizing these simulations to quickly identify promising designs. Accordingly, I will also talk about a novel approach that employs reinforcement learning to rapidly discover domain-specific and simulation-efficient optimizers. I will conclude my talk by outlining lingering challenges and future directions.

Speaker's Bio:

Opeoluwa (Ope) Owoyele has been an Assistant Professor of Mechanical Engineering at Louisiana State University since August 2021. Before joining LSU, he was a Postdoctoral Appointee in the Computational Multi-Physics Research Section at Argonne National Laboratory (ANL). Prior to this, he was a recipient of the ORISE postgraduate fellowship to perform research at the National Energy Technology Laboratory (NETL). He obtained his Master's and Ph.D. degrees in Mechanical Engineering from North Carolina State University. At ANL, he received an Impact Argonne Award in the category of Innovation and a Postdoctoral Performance Award in the Engineering Research category. He is also the recipient of the R&D 100 Award for developing a machine learning-genetic algorithm for rapid product design optimization. His research interests lie at the intersection of numerical methods, data science, machine learning, and high-performance computing for design optimization and data-derived reduced-order modeling.

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