OAK RIDGE National Laboratory

Graph-informed Neural Networks for Multiscale Physics

Presented by

Dr. Eric Hall

Hosted by

Mathematics in Computation

Thursday | May 20 | 3 p.m.–4 p.m.
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Abstract: Modeling complex physical systems plays a vital role in many science and engineering domains, where computational models inform decisions and guide design, particularly when data is sparse. We develop a Graph-Informed Neural Network (GINN), which forms part of a broader strategy for incorporating domain knowledge into deep learning for complex physical systems. This framework utilizes probabilistic graphical models to embed expert knowledge, available data, and design constraints into a physics-based representation. Next, the hidden nodes of a neural network (i.e., learned features) replace computationally intensive nodes in the probabilistic graphical model. The resulting GINN is a learned statistical surrogate that can cheaply generate a large amount of output data for sensitivity analysis and further uncertainty quantification. Incorporating available domain knowledge into machine-learned models has the potential to reduce data requirements while accelerating training and prediction and enhancing the accuracy, interpretability, and defensibility of the surrogate. As a proof of concept, we build two GINNs of interest in energy storage: (1) a multiscale model of electrical double-layer capacitor dynamics and (2) a nonlinear dynamical system describing biomolecular adsorption. We also discuss mutual information-based global sensitivity analysis methods for interrogating surrogate models to accelerate design cycles.

Speaker's Bio: Eric Hall is a Baxter Fellow and Lecturer in Applied Mathematics at the University of Dundee. His research interests focus on uncertainty quantification, stochastic

numerics, and data-driven and predictive modeling. Originally from Philadelphia, Eric graduated with a B.A. in Mathematics from the University of Pennsylvania and earned a Ph.D. in Mathematics (Probability and Stochastic Analysis) at the University of Edinburgh. Subsequently, he was a Göran Gustafsson Postdoctoral Fellow in Numerical Analysis at KTH Stockholm, a Visiting Assistant Professor in Applied Math at the University of Massachusetts Amherst, and a Research Scientist at the Chair of Mathematics for Uncertainty Quantification at RWTH Aachen University.

Host: Pravi Devineni, devinenip@ornl.gov. Please contact host to meet with speaker.

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