College of Engineering
Department of
Mechanical & Industrial Engineering

The Robert W. Courter Seminar Series

9:00-10:00am, Friday, November 21, 2025
1253 Patrick F. Taylor Hall

Generative AI as a Foundation for Computational Discovery

by Dr. Karthik Duraisamy

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Abstract: This talk will highlight some on-going work in building towards a future of AI-augmented science. The first part of the talk will cover MIST, a molecular foundation model that has been scaled to 60B molecules to date, achieving state of the art performance on multiple benchmarks. Notably, our novel lossless tokenizer enables MIST to directly interact with the encoded elemental, electronic, nuclear, and geometric features. MIST is used for a wide range of downstream tasks including battery materials discovery and energetic material property predictions and olfaction characterizations Next, we discuss progress towards developing foundation models in a spatiotemporal physics setting. We show that incorporating physical constraints into diffusion models helps improve performance in forward and inverse problems governed by partial differential equations. We show that score-based diffusion models offer a convenient framework to execute a large number of scientific tasks under one umbrella including forward and inverse problems, data assimilation and sparse reconstruction. Time permitting, the final part of the talk will present ideas towards building a comprehensive framework for AI-augmented scientific discovery combining foundation models that share embedding spaces with dynamic knowledge graphs and AI agents that perform a number of tasks including formal verification and managing interactions with the real world via simulations and experiments.

Biography: Karthik Duraisamy is the Arthur B. Modine Professor of Engineering at the University of Michigan (U-M) where he also directs the Michigan Institute for Computational Discovery and Engineering (MICDE). He holds a PhD in Aerospace Engineering and a Masters in Applied Mathematics from the University of Maryland. His research interests span a broad spectrum of computational science and AI, including data-driven and reduced order modeling, statistical inference, numerical methods, and Generative AI for science. He is the PI of the U-M/Los Alamos Center on Advanced Computational Sciences. He is also the founder and chief scientist of the Silicon Valley-based startup Geminus.AI, which is focused on physics-informed AI to accelerate autonomous industrial operations.