DAC WorkGroup on Scientific AI Agents
University of Notre Dame

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Building a Science Assistant

I will discuss our recent efforts to build a science assistant, with the goal of using LLM technology to accelerate the practice of science. In particular we focus on the manual creation of software to support computational experiments, using an AI system that creates expert-level scientific software whose goal is to maximize a quality metric. The system uses a Large Language Model and a variant of Monte Carlo Tree Search to systematically improve the quality metric and intelligently navigate the large space of possible solutions. I will demonstrate the system on various types of computational problems, showing how it achieves expert-level results when it explores and integrates complex research ideas from external sources. Examples range from analysis of single cell RNA sequencing data, where the method discovers 40 novel methods for single-cell data analysis to epidemiology (where it generated 14 models that outperformed the CDC ensemble and all other individual models for forecasting COVID-19 hospitalizations) to applied math problems of various types that might be of interest to this audience, ranging from very difficult problems in applied math 201, to solving nonlinear PDEs, and beyond. Paper https://arxiv.org/pdf/2509.06503

Tue, Feb. 3, 2026
3:30 – 4:30 PM
On Zoom

Seminar Zoom Link