APS Scientific Computation Seminar Series

Speaker:
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Title:
Navigating the Data Deluge: AI, Infrastructure, and Decision-Making in the Era of Big Data

Date:
January 29, 2024

Time:
1:00 p.m. (Central Time) – Seminar **[In-person or Zoom]**
9:30-10:30 a.m. and 2:00-4:00 p.m. (Central Time)
Half-hour Individual Discussions (In-person or Teams)
Sign-up here:
https://docs.google.com/spreadsheets/d/1UMQ2ujZ3PpkNjQcYxyNlBqijju4wOpasnYQ8e0_hWtI/edit?usp=sharing

Seminar Location (hybrid):
In-person: Bldg. 401/A5000
Join ZoomGov Meeting
https://argonne.zoomgov.com/j/1601444470?pwd=N1phbHZVdCtmcVR5cGh0c1Zhc0orZz09

Hosts:
Mathew Cherukara and Nicholas Schwarz

Abstract:
Science has traditionally leveraged data to guide decision-making processes. In the past, data dimensions were sufficiently manageable for human analysis. However, with the advent of advanced sensing technologies across various fields, we now face an influx of vast, high-velocity data streams emanating from diverse, sometimes unreliable sources. This deluge has rendered traditional human-centric methods inadequate. Despite significant progress in AI and the advent of large language models like ChatGPT, their capabilities are not without limitations. Predominantly, current AI algorithms excel in interpolation rather than extrapolation, resulting in outputs that can be unrealistic or nonsensical when pushed beyond the scope of their training data. This presentation delves into the convergence of massive data growth and artificial intelligence, underscoring their combined strengths and weaknesses in augmenting decision-making processes, especially in the realm of data-driven infrastructure. We explore the co-design of experimental systems, encompassing algorithms, comprehensive software solutions, and hardware, all aimed at actualizing scientific machine learning. We then tackle the challenges inherent in applying machine learning within the context of materials science, where concepts like order, symmetry, and periodicity form essential semantic relationships. Our discussion extends to the development of high-availability computational frameworks designed for deploying resilient, self-repairing services in science, thus facilitating materials science at the exascale. Additionally, we spotlight innovations in parsimonious neural networks, adept at learning geometric transformations in reciprocal space. We emphasize the role of stochastic averaging in enhancing noise robustness, surpassing traditional algorithmic approaches. Finally, we examine the progress in AI co-design, wherein algorithms are optimized for programmable logic. This optimization enables rapid, intelligent analysis, decision-making, and control on ultra-low-cost, low-power devices at unparalleled speeds. We illustrate how this approach is instrumental in real-time data analysis, data reduction, and dose-controlled imaging across various scientific platforms, including electron microscopy.