CompBioMed Conference 2019

AI for Science

Rick Stevens

Argonne National Laboratory

University of Chicago

In this talk, I will describe an emerging initiative at Argonne National Laboratory to advance the concept of Artificial Intelligence (AI) aimed at addressing challenge problems in science. We call this initiative "AI for Science". The basic concept is threefold: (1) to identify those scientific problems where existing AI and machine learning methods can have an immediate impact (and organize teams and efforts to realize that impact); (2) identify areas of where new AI methods are needed to meet the unique needs of science research (frame the problems, develop test cases, and outline work needed to make progress); and (3) to develop the means to automate scientific experiments, observations, and data generation to accelerate the overall scientific enterprise. Science offers plenty of hard problems to motivate and drive AI research, from complex multimodal data analysis, to integration of symbolic and data intensive methods, to coupling large-scale simulation and machine learning to drive improved training to control and accelerate simulations. A major sub-theme is the idea of working toward the automation of scientific discovery through integration of machine learning (active learning and reinforcement learning) with simulation and automated high-throughput experimental laboratories. I will provide some examples of projects underway and lay out a set of long-term driver problems.