Interleaved AI for Next-Generation Science Campaigns

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Emerging new patterns of scientific research - interleaved AI with simulation and experimental facilities, which requires a rethinking of computational facilities and science campaigns.

Domain Science Avatars: The rapid growth and wide applicability of AI frameworks poses challenges to computing facilities which need to deploy and support the software, and also to domain scientists who have to keep up with the system environment and scale up scientific exploration through AI. To shield scientific discovery from ever-increasing complexities stemming from complexity in computer architecture and AI methods, computing facilities aspire to provide turnkey interfaces to science users. We propose having a domain science 'Avatar' - an assistant that can advise users of approaches and recent developments, support their search queries, take domain specific language as input and generate initial block diagrams of interleaved simulation-and-AI composable workloads on cross-facility resources, and steer outcomes that can facilitate the decision making. A rudimentary form of the solution is a scientific gateway, providing AI as a service to scientific users, especially those from experimental facilities generating streaming data such as SNS, APS, etc. This gateway will provide automated processing of AI workflows. Developments would be required to customize the workflow components for individual scientific domains, and the 'Avatar' should be smart enough (an AI tool by itself) to compose optimized computing workflow based on domain specific languages.

General AI for informed science campaigns: With the rise of smart facilities and the expected breakthroughs in deep learning, AI informed science campaigns will be a reality in the future, driven by a rapid convergence of AI and scientific simulation. Algorithms will be redesigned to have deep learning components, and even the most common deep learning workflows (i.e., launch deep learning application to analyze the data after the HPC simulation or the completion of the observation or experiment) will change profoundly. Almost all in the AI community agree that the next breakthrough in AI will not be in supervised learning. The interaction between data and AI will be much more dynamic than it is today. This will result in a much more sophisticated learning from the algorithm, and we think that the combination of simulation and experimental observations would be a key part for this to succeed.

This more-general AI will take full advantage of the computing at the edge and naturally bridge experimental facilities, such as SNS, and leadership HPC facilities. The AI will intercept and steer observational data, and directly interact with the simulation, producing learned surrogate models and/or parts of simulation, learning the fundamental theories at microscopic level from simulation, and adjust on the fly macroscopic quantities directly from the experimental observational facilities. This will revolutionize the way science is performed across domains, since the knowledge would be transferable by model rather than data. It is important to study this new general AI informed science campaigns early on since it will also have a large impact on the optimal specialized AI hardware that would be used in the leadership HPC facilities.