Hyper-Accelerating Scientific Discovery via Inverse Design on Hybrid non-von-Neumann HPC AI Architectures

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The ability to rationally design materials, chemicals and medical drugs with desired properties is the holy grail of computational materials science, chemistry and pharmaceutical research with an impact that can hardly be overestimated. In a more general setting, the ability to generate optimal samples from a given constructive scientific model is the key to scientific productivity and a broad impact. While the state-of-the-art discriminatory and generative AI techniques have produced impressive results on modern accelerated classical computers, the true revolution may happen when the emerging disruptive computing technologies, like quantum computing, mature enough to deliver much more efficient exploration of exponentially large combinatorial parameter spaces. Yet, such non-von-Neumann computer architectures will not be self-sufficient, mandating tight coupling to classical supercomputers. In particular, the classical supercomputers excel in generating large amounts of data by running high-throughput numerical simulations. They can also efficiently analyze the generated data using advanced AI techniques on accelerated HPC architectures, thus constructing reduced-dimensional, yet very large latent space representations relevant to the optimization problem in hand. However, exploring these large combinatorial spaces by a classical supercomputer is not an easy task. In contrast, a sufficiently efficient quantum computer could potentially excel in exploring and analyzing such inherently exponential in size combinatorial spaces, thus delivering quantum AI acceleration on top of the classical computing capabilities. Therefore, a tight integration of the future quantum computers (and other specialized accelerators) with the classical supercomputers shows a great promise for future scientific discovery delivered by the leadership computing technologies capable of solving some problems much more efficiently than a classical supercomputer by itself. While a great deal of methodological research is ongoing in this direction, we are still quite far from realizing this scenario at the current leadership computing facilities, requiring new hardware solutions, major hybrid quantum/classical algorithmic advances, and scalable and interoperable software components targeting such hugely heterogeneous computer architectures of future [1]. Furthermore, the entire scientific methodology used in this approach will need to be co-designed with evolving hardware and software components that will require a tight cooperation between domain experts, computational and data scientists, hardware vendors, and leadership computing facilities.

References

1. Extreme Heterogeneity 2018 report: DOI: 10.2172/1473756