

Quantum Computing Simulation Platform for High-Energy Physics

Snowmass 2021 Frontiers of Interest: Computational Frontier, Quantum Computing (CF6) Theory Frontier, Quantum Information Science (TF10)

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1 Executive Summary

Quantum technologies have the potential to revolutionize science and society in the next five to ten years, but require resources that are not mainstream today. The High-Energy Physics community can be at the forefront of this revolution, setting up collaborations across HEP institutes and organizations, as well as dedicated national and international initiatives. Through such endeavors, we can work to develop new computing, detectors and communications systems, in addition to advancing knowledge of quantum systems and quantum information processing. CERN has recently established a Quantum Technology Initiative based on almost two years of pilot collaborations and investigations to explore possible applications to HEP in close collaboration with the community. An initial three-year roadmap and a research programme are being defined in collaboration with the HEP and quantum-technology research communities. In addition to joint research, one of the main goals of the initiative is to build skills and capacity and help preparing the researchers to understand how to apply quantum technologies to HEP activities, through the establishment of collaborative platforms and educational and training activities.

At the core of this capacity-growth objective is the definition and set up of a shared quantum computing simulation facility to enable the development of algorithms and tools, to experiment with different simulators and resources, and to share knowledge.

2 Quantum Computing Simulation Platform

Over recent years, quantum algorithms, characterized by lower computational complexity than their classical counterparts, have been developed and evolved. These algorithms, however, require large scale fault-tolerant quantum computers, whereas today we have access to *Noisy Intermediate-Scale Quantum* (NISQ) hardware dominated by short coherence time (noise), small number of qubits (from a few tens up to few thousands, in the case of quantum annealers) and limited lattice connectivity (in most cases, only the nearest neighboring qubits interact).

These limitations have sparked intense R&D towards the design and optimization of NISQ algorithms that demonstrate quantum advantage over current hardware. Early experiments have revealed high potential, however, with varying projected roadmaps for practical quantum computers being moved from not less than 20 years to as close as the next 5 years.

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Many classes of workloads typical of high-energy physics rely on optimization algorithms, from Monte-Carlo many-body simulations, to event reconstruction and classification. A special class of algorithms is represented by machine-learning (ML) and deep-learning (DL) algorithms; today, quantum machine learning (QML) is a lively research field. Quantum linear-algebra routines are faster than their classical counterparts and make up most of the computational workload in ML/DL algorithms, meaning QML models could profit from this kind of acceleration. Encoding a ML model as a quantum system opens the possibility of entirely new learning patterns that could be implemented first on NISQ and then on ideal devices.

The work necessary to advance the state of the art in quantum algorithms and software does not, however, require a full commitment to physical quantum devices. Efficient quantum computing simulation programs running on classical hardware of sufficient capabilities are today an excellent way to build skills, design realistic algorithms prototypes and assess trends. They are essential for understanding hardware behavior, gate operations fidelity, correctness and scaling performance, and robustness against errors, as well as for designing error-correction strategies on NISQ devices. Classical simulation of quantum hardware is a difficult task: its complexity scales exponentially with the number of qubits. With n qubits 2^n amplitudes are needed to describe a quantum system and the memory scales exponentially. The processing is tightly coupled and requires low-latency tools, like MPI over thousands of cores. High-performance simulators, relying on CPU or GPU architectures exist; their performance has been studied on HPC clusters or cloud services.

An effort within the HEP community to build a reliable quantum-computing simulation infrastructure, capitalizing on the existing unique expertise of the community in distributed computing would allow us to assess the potential of quantum computers in HEP research, accelerating innovation and enabling the development of expertise for future applications.

Traditional high-throughput computing systems, which represent the bulk of HEP computing are not well suited for large-scale coupled computations. Purpose-designed quantum simulators and HPC systems with adequate memory and network fabric are needed to perform medium to large-scale quantum simulations. CERN can rely on its developing relationship with HPC providers and its existing expertise in data management and large-scale distributed computing to support quantum-simulation development activities.

We propose and support any collaboration to:

- Formalize and extend the existing catalogue of use cases and examples of possible applications of quantum computing to HEP workflows and algorithms.
- Collect and share information about existing resources, tools, libraries, and collaborations across the community, with a special focus on simulators (e.g. IBM Qiskit, Google Cirq, Intel IQS, Amazon Braket, Strawberry Fields, $\text{t|ket}>$ and more cf. <https://quantiki.org/wiki/list-qc-simulators>).
- Capitalize on years of experience of HEP collaborative initiatives like WLCG or HSF to design and deploy a distributed infrastructure for quantum computing and simulation, based on existing distributed computing expertise, to make resources and tools easily accessible to researchers, thus enabling investigations to be performed as part of community projects.
- Identify and coordinate access to computing resources, both for simulators and actual quantum hardware, in collaboration with other Institutes or companies. Resources can come from on-premise, cloud and HPC providers.
- Use the infrastructure to set up R&D projects to adapt or design algorithms for quantum platforms and benchmark their current and potential performance.

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