Quantum Computing: Advancing Fundamental Physics

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The field of Quantum Information Science (QIS) is a rapidly growing field, with an expanding number of potential applications that explore the capabilities of currently available noisy quantum devices and promise to eventually solve problems beyond anything that classical systems can accomplish. In the past few years, this expectation for transformational applications has translated to a lot of attention, both from the media (reaching the scientific community and the general public) and the government funding agencies and technology industry. Examples of this attention include the National Quantum Initiative in the USA [1] that has already generated significant funding (e.g., \$625 million investment from the Department of Energy for Quantum Centers over the next 5 years [2]), and major efforts to design and deploy quantum computers by major companies such as Google, IBM, and Microsoft, as well as a plethora of dynamic start-ups with similar goals, such as Rigetti and IonQ. More importantly, however, is that significant advances have been made in developing new techniques and algorithms and advancing quantum technologies, resulting in applications that are addressing real problems (albeit simplified, in most cases, or very specialized). I am expecting that most of the readers are familiar with the paper by Google [3] claiming ‘quantum supremacy’ [4], and the many discussions and publications it generated. Independently of what one concludes from this debate, this event and the discussions it generated are proving that quantum computers, despite being at their infancy, can be very powerful. Therefore, it is very important to understand what the implications for high energy physics (HEP) are.

The field of QIS, in general, exploits quantum properties, such as coherence, superposition, and entanglement, for acquiring, communicating, and processing information. Of course, in order to take advantage of quantum systems for practical applications, it is imperative that we understand

and control their behavior in the imperfect, classical world, in which they have to operate in order to mitigate and protect from the noise and information loss induced by interactions with the classical environment. Quantum computing (including quantum simulation, which sometimes is considered independently) is one of the major QIS application areas that also includes quantum sensing and quantum communications. Although in this discussion we will focus on the potential impact of quantum computing to HEP, we cannot ignore the other two areas, since, as we will see that due to some potentially very impactful applications for HEP, the whole ecosystem is relevant.

The discussion on the concept of quantum computers and their potential transformational impact on fundamental science began in 1981 with Richard Feynman, providing a HEP connection from the very beginning of this field. Feynman asked the question: Can we simulate physics on a (classical) computer? The answer, of course, is not all of physics, since quantum mechanical systems require far too many variables for classical computers to handle (the dimension of the Hilbert space of a quantum system of many particles grows exponentially with the number of particles). This was true then and it is still true now, although today quantum simulators running on classical computing resources can simulate up to about 50 qubits. Feynman then postulated that if we cannot simulate quantum physics on a classical computer, maybe we can build a quantum mechanical computer, which would perform better than the classical systems. His exact quote, referenced in many talks (at least in the HEP community) “Nature isn’t classical, dammit, and if you want to make a simulation of nature, you’d better make it quantum mechanical, and by golly it’s a wonderful problem, because it doesn’t look so easy,” also admits the fact that simulating a quantum system using another, presumably more controllable, is indeed difficult. A quantum computer is nothing more than an artificial quantum system that encodes information into quantum states and computes by performing quantum operations on it. Quantum computers were formally defined by David Deutsch in 1985 [5], where the notion of a ‘quantum Turing machine’ was introduced. Today there are two

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main approaches for implementing a quantum computer, the universal digital quantum computer, based on qubits and quantum circuits, and analog quantum computing, with quantum annealing being the most widely used variation.

The gain in computing power arises from storing and manipulating information using quantum states and operations. Let us use qubits (two-level quantum systems) to summarize how that works, although there are other representations that are possible. Similar to a classical bit, a qubit has two states, but unlike the classical bit, a qubit may be in a weighted superposition of the two states, allowing functions to be evaluated for both values simultaneously. A quantum register of n qubits can hold a superposition of all the 2^n possible values and can be used to compute on all of them at the same time. This is the principle of quantum parallelism. Of course, the state of the quantum register collapses when the system is measured, settling to one of the states that was part of the superposition, based on their relative weights. The most important element of a successful quantum algorithm is to apply operations on the system that minimize the probabilities of unwanted states and maximize the probabilities of desirable states, in order to get a solution in the fewest possible steps. Another important and necessary element of a quantum algorithm is to map the problem space of the desired computation to the Hilbert space of the qubits. This is the principle of interference for quantum computation. Because of these two principles (quantum parallelism and quantum interference), we know that fully functioning quantum computers will be better than classical computers not only in simulating quantum systems but also in factoring integers [6] or searching for a rare pattern in a large amount of data [7].

In order to realize the quantum advantage we have been discussing so far, we need fault-tolerant quantum computers with a large number of qubits. The devices that are currently available are limited by noise (due to the interactions of the qubits with the environment) that affects both the lifetime of the stored information (the ‘coherence’ time) and the fidelity of the operations (the ‘gate fidelity’). In addition, current engineering and technology limitations allow for devices that only scale up to $O(100)$ qubits (this is for universal digital quantum computers) and architectures that support low qubit connectivity (in some pattern of nearest neighbors), which, in general, increases the number of gates required for a given application. Because of these limitations, current quantum computing applications have to contend with small problem size, shallow circuit depth (thus few operations), and fidelity issues. This is the case in general, although different technologies and implementations perform better in some of these metrics than others, i.e., some might achieve better coherence but have intrinsically slower gate operations, while others are the other way around. There is a broad and multi-faceted Research and Development (R&D)

program pursued by both academia and industry to improve on and, as the ultimate goal, eliminate these limitations. This program includes efforts to improve on the engineering and scaling up of existing technologies, to increase the number of qubits as well as the speed with which gates operate, basic research for better understanding of the physics of decoherence, to improve materials and increase coherence time, and investigations on new approaches with better overall characteristics. One of these potential new approaches involves the native HEP technology of superconducting RF cavities, with their long coherence time, adapted to the quantum regime [8]. Ultimately, the goal is to develop systems of a very large number of qubits (or other, more complex, representations) that will allow the application of error correction codes to protect against qubit noise and faulty gates and measurements. Quantum error correction is another very important area of research for the success of quantum computing. Because quantum information cannot be copied, these error correction protocols rely on storing information on a larger number of entangled qubits in ways that allow the extraction of the original data in the presence of (currently limited types of) errors. This larger number of physical qubits that are combined in the error correction protocol constitute a ‘logical qubit’. In general, to encode a given number of logical qubits we need orders of magnitude more physical qubits. Furthermore, error correction codes do not account for coherent errors across a number of qubits (for example from cosmic ray showers), imposing additional constraints and requirements in the development of large quantum computer facilities.

Despite the large number of challenges and required R&D for developing fully functioning quantum computers, the QIS field is advancing constantly with both device, system engineering, and algorithmic improvements. Very recently, Google put forward a 10-year roadmap to develop a 1-million physical qubit quantum computer to enable operating computations on a few logical qubits [9]. Even if 10 years might be considered aggressive, this roadmap points to a time scale for potentially impactful applications to the currently planned HEP program. What is then an essential strategy for HEP (as well as any other domain science or industry with significant computational challenges) is to identify the potential applications where a clear benefit is expected compared to classical computing, develop the algorithmic approaches, and build the know-how and capacity through implementations for scaled-down problems on available quantum devices. Here ‘benefit’ or ‘advantage’ should be understood either as a computation that cannot be performed classically (e.g., quantum simulation applications) or a runtime speed-up over the classical implementation for the same task. This approach ensures that the community will be ready to take advantage of these devices when they

are capable of large-scale computations, with the right applications to deploy. It also provides an opportunity to carry out some interesting science and even improve on the classical computational approaches, a positive side-effect that has already been realized both in HEP [10] and in other areas that have started to investigate quantum computing applications.

Simulation of quantum systems remains one of the flagship scientific applications of quantum computing, with simulation of quantum field theories (QFTs) of great relevance to HEP, since a capable quantum computer can be transformational. Although the concept of ‘simulation’ could be used to describe a broad class of problems, in this case, we focus on calculating the dynamical properties of the system. Other scientific domains (especially quantum chemistry) have made good progress in developing approaches and applications for systems of fermions and HEP is also benefiting from their advances. One specific focus of our field has been to develop efficient boson representations, as well as fermion–boson interaction approaches [11–13]. This has also led to calculations of reduced problems that have been deployed on current devices and are providing insight both on the algorithmic performance and the physics [14]. Another focus area is on developing algorithms and approaches for describing the quantum properties of parton showers [15], as well as taking advantage of quantum optimization to improve on the numerical performance of color reconnection models. In the near term, there is a coordinated effort (at least in the USA) for an incremental approach (tracking the evolution of hardware capabilities) for developing QFT applications. Although it is not envisioned (in the near term) to reach the problem size necessary for impactful science results, this is a positive first step, since, after all, “the purpose of computing is insight, not numbers” [16].

Beyond HEP theory, it is important to survey and understand the potential benefits and impact of quantum computing on data processing and analysis for HEP experiments. This is very well motivated—in the next decade and beyond, accelerator experiments such as HL-LHC and DUNE and observatory surveys such as LSST will produce very large and complex datasets that will require computing resources of an unprecedented scale. In addition, experiments performing searches for dark matter require unprecedented precision. Because of these requirements, machine learning has been attracting a lot of attention as a potential solution to many different problems in particle physics and cosmology, leading to a substantial number of successful applications. Investigating the potential of quantum machine learning (QML) to provide additional benefits (either in speed-up or capabilities) has been a natural extension of these research activities. Initial investigations involved the utilization of a quantum annealer as a sampling engine for Higgs event classification at the

LHC [17], as well as sampling engines for a set of classes of machine-learning approaches for image classification in astrophysics [18]. Most recently, interest has shifted to the development of QML applications using digital quantum computers, e.g., for event classification using variational quantum circuits for different LHC physics searches [19] and even tracking applications, extending the approach of Farrell et al. [20] who introduced a representation based on space-points in connected graphs to take advantage of the high dimensionality and sparsity of the tracking data to utilize quantum graph neural networks. These research projects provide insight and facilitate the development of the know-how necessary for the HEP community to take advantage of quantum computing technology advancements. Nevertheless, it is not clear that QML approaches could have a significant advantage (in terms of a speed-up) when applied on classical data, and this is a topic for discussion independently of HEP [21, 22]. One very interesting class of QML applications that could provide a definitive advantage over classical methods is when dealing with data from a set of quantum sensors. Dark matter search experiments are already utilizing quantum technologies, and the next generation of these experiments could be collecting data from arrays of distributed, networked, quantum sensors [23]. Designing optimal quantum configurations and measurements to maximize fidelity and suppress noise is therefore an essential task of quantum metrology and algorithm design. In this context, the utilization of QML both in the analysis (possibly real time) and the on-chip (quantum) modeling of the system to optimize the design parameters could be transformational [24, 25].

Will quantum computers and QIS technologies in general deliver fully in their promise? We do not know for sure, but there are many possibilities with the potential for a big impact for HEP, so we need to maintain our engagement so we can fully explore these technologies as they evolve. Quantum computers provide a clear path for transformational applications in theory, for QFT simulation and foundational physics, as they continue to improve in scale and performance. Investigations on the applicability and advantage of other applications such as optimization or QML will continue to build the capacity and know-how necessary to make the best use of these devices for HEP applications. Given the recent aggressive timelines for deploying large systems (such as the Google plan), emphasis should also be put on exploring the potential for impactful applications utilizing a handful of fully error-corrected qubits. In a few years, as major activities (such as the NQI centers in the USA) are concluding their first phase of R&D, we will be able to evaluate overall progress and re-assess our plans and understanding for applications with advantage compared to classical approaches.

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