On the importance of scalability and resource estimation of quantum algorithms for domain sciences

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Abstract—The quantum information science community has seen a surge in new algorithmic developments across scientific domains. These developments have demonstrated polynomial or better improvements in computational and space complexity, incentivizing further research in the field. However, despite recent progress, many works fail to provide quantitative estimates on algorithmic scalability or quantum resources required —e.g., number of logical qubits, error thresholds, etc.—to realize the highly sought “quantum advantage.” In this paper, we discuss several quantum algorithms and motivate the importance of such estimates. By example and under simple scaling assumptions, we approximate the capabilities needed of a future quantum device for a high energy physics simulation algorithm to achieve superiority over its classical analog. We assert that a standard candle is necessary for claims of quantum advantage.

Index Terms—quantum computing, algorithms, simulation, scalability

I. INTRODUCTION

Quantum computation and information are interdisciplinary marvels born out of the convergence of arguably the two most transformational sciences in human history: Physics and Computer Science. By Dennard scaling, and the laws of Moore and Amdahl, we are nearing the physical limitations of classical computing. Quantum information processing promises exponential gains in terms of computational and space complexity for special classes of problems across scientific domains and industrial applications. Exploiting quantum mechanical phenomena—such as superposition, interference, and entanglement—holds great promise for constructing next-generation devices which will complement traditional von Neumann architectures, enabling researchers to solve currently intractable problems. The development of quantum algorithms, however, requires tremendous ingenuity to leverage the advantages quantum physics offers. Although many such algorithms exist which show a quantum advantage [1–3], the lack of error-correction or fault-tolerance supersedes algorithms’ quantum hallmarks, rendering them either impractical on present day systems or requiring simplification to the point that a classical computer could also perform the task with tractable resource consumption. As such, there exists a serious need for researchers of quantum algorithms to heed practical benefits and considerations when claiming quantum superiority, particularly those primarily motivated by domain science application.

A central area with which the author is familiar is the area of quantum simulation. Here, the task is to use a quantum computing device to simulate the dynamics of a quantum mechanical or field theoretic system of physical interest. While this is a problem that is of clear physical interest to many different subfields of physics and chemistry, it is also clear that the reach of direct quantum simulation of these areas is severely limited in the current area of weak and relatively unreliable quantum computers, often only able to access small lattice sizes which are classically simulable, or requiring dramatic simplification to the point of straining physical applicability. While doing some simulations of this type is useful for proof-of-principle, doing large numbers of such simulations is perhaps not, without a clear and attainable scientific goal.

Something that would be useful in this regard, however, is far more detailed benchmarking of quantum simulation algorithms for domain science in terms of resource requirements in, e.g., gate depth or qubit number. Such estimates would much better enable scientists to determine when quantum computing technology has sufficiently advanced in order to study scientifically relevant questions using quantum simulation. Such benchmarking should be done with current qubit and gate quality in mind, and should be updated with the progression of quantum computing technology. In this way, it will by construction provide an upper bound on the number of years/advances required in order to run a scientifically useful quantum algorithm that grows ever closer with both the passing of time and the development of the technology.

II. QUANTUM ALGORITHMS

A. Quantum Fourier Transform

The Quantum Fourier Transform (QFT) [3] (and its inverse) applies (inverse) Fourier transformation to the wave function amplitudes. It is a linear transformation over the states of
qubits, which is the quantum analogue of the discrete (inverse) Fourier transform. QFT is a basic component of many well-known quantum algorithms, including Shor’s algorithm [1], quantum phase estimation [4], hidden subgroup problem [5], etc. Fig. 1 shows the scaling of the number of gates and particularly CNOT gates with respect to the number of qubits for QFT from 5 to 25. As can be seen, the number of gates and CNOT gates scale exponentially with increased qubits.

B. Grover’s Algorithm

Grover’s algorithm [2] is a quantum algorithm for searching in a database, offering quadratic speedup over classical searching methods. It takes a black-box oracle realizing the function: \( f(x) = 1 \) if \( x = y \), \( f(x) = 0 \) if \( x \neq y \), and find \( y \) within a randomly ordered sequence of \( N \) items using \( O(\sqrt{N}) \) operations and \( O(N \log N) \) gates with a probability of \( p \geq 2/3 \). Grover’s algorithm is appealing in that it determines with high probability the unique input given the output is pre-known. Grover’s algorithm is one of the fundamental quantum algorithms given the importance of searching in data-driven sciences.

C. Harrow-Hassidim-Lloyd

Harrow-Hassidim-Lloyd algorithm (HHL) is one of the fundamental algorithms expected to offer substantial speedup over the classical one and of great interest in many domains. HHL algorithm is a quantum algorithm for linear systems of equations. Given a sparse system with a low condition number \( \kappa \), for a scalar measurement of the solution vector, the HHL algorithm can demonstrate a runtime of \( O(\log(N)\kappa^2) \) where \( N \) is the number of variables, comparing to the best known classical approach of \( O(N\kappa) \).

D. Hybrid Quantum-Classical Algorithms

The variational quantum algorithm is to optimize a parameterized quantum circuit ansatz applied to some initial state for minimizing a cost function defined according to the output state [6, 7]. When applied in quantum simulation, the goal of the algorithm is often to prepare ground states. The cost function is often the expectation value of a Hamiltonian. If the

initial state is \( |\psi\rangle \), the Hamiltonian is \( H \), the ansatz is \( U(\vec{\theta}) \) where \( \vec{\theta} \) is the variational parameter, then the cost function is \( E(\vec{\theta}) = \langle \psi | U(\vec{\theta})^\dagger H U(\vec{\theta}) | \psi \rangle \).

The quantum approximate optimization algorithm (QAOA) [8] is another variational quantum algorithm that is particularly interesting, given its ability to tolerant certain degree of noise through the unique quantum-classic hybrid algorithm design. QAOA is designed to solve combinatorial optimization problems, such as in graph analytics. In QAOA, a quantum subroutine is embedded in a classical search loop. The quantum state is prepared according to a number of variational parameters. These parameters are adjusted based on the measurement result per iteration.

III. Considerations for claims of “Quantum Advantage”

Quantum computing is inherently more ‘difficult’ than that of classical; not solely due to the different way of thinking about computation but also due to the complexity of quantum systems and the precise control necessary for manipulating states. As quantum computing systems become larger (qubit count) and increase connectivity (highly entangled), many of today’s algorithms which presently simplify problems can be employed in more real-life scenarios. However, the big questions here are ‘if’ and ‘when’ such systems will be realized. The full potential of practical quantum computing has yet to be realized, and for the sake of this fascinating science and moving beyond the hype, the community must stress the importance of applications on near-future devices. Therefore, we assert that scalability and resource estimation should be just as important in the design of quantum algorithms as the algorithms themselves if we wish to build upon the momentum in this field.

A. Scalability

Scalability studies are needed to determine whether or not a quantum algorithm maintains its advantage over its classical analog (if one exists). Determining scalability of a quantum algorithm, however, is somewhat more involved than in classical computing; one must consider scaling not only as additional computational resources (qubits) are added to solve a problem, but also requirements such as connectivity for highly entangled systems, and noise and error thresholds—both SPAM and those which accrue during execution—which dictate how deep a circuit can reliably execute. For practical reasons, scaling may not be interesting when going from a weakly connected system of 100 qubits to another weakly connected system of 100,000 qubits; rather, from a weakly connected 100 qubit system to a strongly connected system of 1,000 qubits.

As such, there is no single figure of merit for describing a scalable quantum algorithm; algorithm developers need to either consider a collective set of criteria or design algorithms with significant reliance on one over the others. These and other considerations may soon be necessary to demonstrate
further that quantum algorithms are more than merely pen-and-paper demonstrations of solutions to real problems, but can and will be used to advance science.

B. Resource Estimation

Beyond scalability is the need for estimating the computational resources required to execute a quantum algorithm. The estimates can pertain to near-term requirements or longer-term; regardless, while estimates are by definition approximations or judgements based (hopefully) on experience or trends, they give some level of assurance an algorithm will be implemented and executed to solve a full problem—as opposed to an overly simplified one—by some device eventually. Whether ‘eventually’ may be within the next year, five years, decade or later will determine the usefulness of a given quantum algorithm, as one needs to also take into account the rapid technological advances in classical computing. For example, the GNFS and Shor’s algorithms described earlier: despite Shor’s exponential speed-up, the largest number factorizable on today’s quantum systems is four bits (cf. any $10^{100}$ bit numbers, apart from prime powers, that GNFS can factor).

Obviously exponential speed-ups of quantum algorithms over their classical counterparts have been devised, and have also been shown to be scalable. However, will they actually ever be able to run and empirically show the quantum advantage? Part of the answer to this question can be at least partially answered through naïve application of a quantum version of Moore’s Law: the number of qubits in a system doubles every two years. The remaining considerations include: the evolution of qubit coherence times (T1 and T2); noise, fidelity and duration of physical gate sets and thresholds thereof; as well as other device-level capabilities, e.g., mid-circuit measurements. A concrete example is the well-known algorithm for simulating general quantum field theories from Jordan, Lee and Preskill [9]. This marvelous algorithm considers the fundamental stages in quantum simulation: (1) state preparation (vacuum state, $|0\ldots0\rangle$); (2) adiabatic evolution (from non-interacting theory to interacting); (3) Trotterization (time-evolution of interacting theory); and (4) performing a measurement. A back-of-the-envelope estimate of the number of error-corrected (logical) qubits to needed to simulate a single process (e.g., $pp\to\pi\pi\pi\pi$) is $O(10^5)$. Given the current trends, we can expect perhaps $10^5$ to $10^6$ physical qubits within the next decade; this does not consider connectivity or noise. So the question is: what real advantage will there be over classical methods in $\leq 10$ years from now?

The take-home message here is straightforward: it is essential for researchers to give some level of promise that their algorithm will not only one day be demonstrated on real hardware, as well as what advantage can be expected given some rough idea as to the classical computational resources available to solve the same problem (either via classical means or classically simulating quantum computations).

C. Applicability and Relevance of the Algorithm

This is an area where for example the HHL algorithm struggles. While it is true that the solution to the linear system is encoded in the coefficients of the quantum state, an exponential number of queries are needed to extract the full solution, thus negating the computational advantage. Only when a small number of queries of the quantum state are necessary in order to answer a problem of scientific relevance does this algorithm convey a genuine computational advantage over classical solvers.

Because many existent quantum algorithms are targeted at problems in mathematics and computer science that are interesting in large part (or solely) due to their difficulty, this question of physical relevance is unfortunately one that is ubiquitous in the assessment of quantum algorithms: even given an algorithm of known speed-up, worthy scalability characteristics, and reachable resource requirements both now and in the future, there is still a question to be asked of whether such an algorithm is useful for a reason beyond simply its difficulty.

IV. CASE STUDY: A QUANTUM ALGORITHM FOR HIGH ENERGY PHYSICS SIMULATIONS

As described in Sec. III-C, physically-motivated problems tend to be of greater interest than those aiming to solve problems due primarily to their inherent difficulty. Keeping with this theme, we consider a recent quantum algorithm with exponential speed-up in the context of high energy physics (HEP) [10]; specifically, a quantum final state algorithm. The reason for choosing this particular algorithm is four-fold: (1) quantum simulation is a major driver in the community; (2) its physical relevance; (3) it provides a meaningful scaling analysis; and (4) scientific bias [the author(s) of this paper come from a HEP background].

Simulations of physical phenomena are crucial in many aspects of HEP—from conceptualizing to designing a new experiment, to validation and operation. Beyond this, simulations play a major role in many precision measurement and searches for new physics. High energy collisions, such those between protons at the Large Hadron Collider, have to date been simulated classically using perturbative (hard-scatter, shortest distances), nonperturbative (hadronization, longest distances) and Markov Chain Monte Carlo (MCMC; parton showers, intermediate distances) techniques. While these methods describe different length and energy scales sufficiently well, physics analyses are becoming increasingly more sensitive to quantum effects which are not captured classically; in particular, the efficiency of parton shower algorithms stems from the fact that certain quantum effects are neglected. As more precise studies of final state radiation in high energy collisions are performed, quantum effects—such as interference—must be taken into account.

A. Algorithm Overview

The work from Nachman et al. considered here introduces a quantum algorithm targeting final state radiation that gives,
under certain conditions, exponential improvements in both space and time. The algorithm considers a simple quantum field theory with two fermion fields interacting (non-zero couplings) with one scalar boson. It requires a total of six registers to hold information about the particle state (|p⟩) and number of each particle type (|n_α⟩, |n_f_α⟩, |n_f⟩), whether emission took place in a given step (|c⟩) of the algorithm and emission history (|h⟩). Evolution is performed via a sequence of four operations: (1) U_{count} is controlled on the particle state register and applies the counts of each particle type to the corresponding count register; (2) U_e applies Sudakov factors to determine if an emission took place in the step; (3) U_h generates a superposition of all possible emissions to select the particle that emitted; and (4) U_p which updates appropriately the particle register if an emission occurred. These operations are sandwiched between rotations to first change into a diagonal basis and next to create interferences between equivalent final states containing the same intermediate fermions. For N steps of the algorithm, up to N particles can be emitted; a collection of steps comprises an event, and given a large set of events one can then calculate physical observables of the theory.

B. Scaling

For brevity, we discuss here only the dominant space and time complexities of the quantum parton shower algorithm. For full details, we refer the interested reader to the paper’s supplemental material.

The two dominant registers in terms of the number of required qubits are |p⟩, requiring 3(N + n_f) qubits, and |h⟩, requiring N[log(N + n_f)], where N is the number of steps and n_f is the number of initial particles. Note that states with different particle histories (i.e., different emitting particles and different intermediate fermions) do not interfere with each other. Therefore, |h⟩ can be measured after U_h is applied and can then be reset to the state |0⟩. However, at the time the algorithm was developed, mid-circuit measurements were not supported by IBM Quantum (IBM Q) devices and so the particle history register could not be measured and reset in each step. With this capability now available, one needs only [log(2n_f + 1)] number of qubits to store |h⟩.

The depth (time) complexity with mid-circuit measurement is Nn_f^2 log n_f, coming from the the history operator, U_h, where n_f is the number of fermions. Comparing to the classical counterpart, with scaling N_2^n_f/2 that is exponential in the number of fermions, the quantum parton shower algorithm provides advantage when the number of emitted particles becomes larger than 21. This is a promising result, considering charged particle multiplicities alone expected at the High Luminosity LHC will exceed O(100). Moreover, the quantum algorithm is able to efficiently incorporate important interference effects that are ignored in the classical algorithm.

Space Complexity: 3(N + n_f) qubits
Time Complexity: Nn_f^2 log n_f native gates

| Gate         | Error       | Duration [ns] |
|--------------|-------------|---------------|
| U_{3_7,9}, C_{X,3_{10,12}} | 0.0019, 0.0264 | 71.111, 490.6667 |
| U_{3_{10,12}, C_{X,3_{11,12}}} | 0.0022, 0.0184 | 71.111, 298.6667 |
| U_{3_{11}, C_{X,3_{11,12}}} | 0.0015, 0.0265 | 71.111, 481.5556 |
| U_{3_{12}, C_{X,3_{12,13}}} | 0.0015, 0.0167 | 71.111, 348.4444 |
| U_{3_{13}} | 0.0014 | 71.111 |
| Avg. | 0.0017, 0.0209 | 71.111, 393.9556 |

TABLE I: IBM Q Johannesburg qubit properties. Data retrieved August 2020.

| Gate         | Error       | Duration [ns] |
|--------------|-------------|---------------|
| U_{3_{7,9}, C_{X,3_{10,12}}} | 0.0019, 0.0264 | 71.111, 490.6667 |
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| U_{3_{12}, C_{X,3_{12,13}}} | 0.0015, 0.0167 | 71.111, 348.4444 |
| U_{3_{13}} | 0.0014 | 71.111 |
| Avg. | 0.0017, 0.0209 | 71.111, 393.9556 |

TABLE II: IBM Q Johannesburg gate properties. C_X gates are assumed symmetric (C_{X_{ij}} = C_{X_{ji}}) so redundant entries are omitted. Data retrieved August 2020.

C. Resource Estimates

The quantum field theory considered is given by,

$$L = \bar{f}_1(i\phi + m_1)f_1 + \bar{f}_2(i\phi + m_2)f_2 + (\partial \phi)^2$$

$$+ g_1\bar{f}_1\bar{f}_1\phi + g_2\bar{f}_2\bar{f}_2\phi + g_3(\bar{f}_1f_2 + \bar{f}_2f_1)\phi$$

where f_1 and f_2 are fermions and \phi a scalar boson. Despite its simplicity, the resources necessary to simulate fully this theory with non-zero couplings g_1, g_2 are out of reach on current NISQ devices. To realize the quantum parton shower algorithm on a real quantum system, the problem was further simplified by excluding \phi \to \bar{f}f \, splitting, ignoring the running coupling and having a single fermion in the initial state. The noisy quantum systems set further constraints, limiting the algorithm to four steps. The weak connectivity of current quantum devices further complicates matters, as expensive SWAP gates are necessary to operate on qubits without physical connections. Whereas the full theory in Eqn. 1 would require O(10^4) gates for four steps, the (very) simplified version requires 53. However, despite its simplicity, the quantum parton shower algorithm manages to capture important interference effects that are ignored in classical MCMC.

The quantum parton shower algorithm was demonstrated on the now-retired IBM Q Johannesburg system using five (Q7, Q10–Q13) of its 20 qubits. The qubit and gate properties of this device are given in Tables I and II were retrieved from the backend in August 2020. Note the U_3 = U_3(\pi, 0, 0) represent Pauli X gates, and we take C_X gates to be symmetric with respect to error and duration (i.e., C_{X_{ij}} = C_{X_{ji}}). The state-of-the-art IBM Q Montreal device comprises 27 qubits an average T1 of roughly 130 µs, T2 of 97 µs, and mis-measurement probabilities [Pr(0|1), Pr(1|0)] are cut by more than half compared to Johannesburg. Based on report gate properties, C_X errors have also improved by 50% or more. A naïve scaling of resources thus yields roughly double overall performance every two years, perhaps making possible
circuit depths (additional steps) permitting $O(10)$ particle multiplicities within the next five years but otherwise the same limitations mentioned earlier. It is therefore inconceivable a quantum advantage will be realized within the next decade. Notwithstanding, the quantum parton shower algorithm is an examplar demonstration of innovation that has potential to be leveraged as quantum computing devices become more advanced.

V. CONCLUSIONS

In this paper, we discussed and emphasized the need for scalability and resource estimation studies in the context of quantum algorithm design. There is without doubt great excitement in the field, and high hopes the second quantum revolution will be able to provide greater insight into complex phenomena. The tremendous interest among domain scientists in quantum information and computing is well-deserved, but the community best heed caution as the mutual interest from funding agencies may very well subside without practical near-term applications and results, leaving a small number of experts to continue their research in a field become stagnant.

The development of quantum algorithms holds prodigious potential for impact in domain science and beyond. In order to precisely quantify the impact in the near, intermediate, and future terms, we advocate for better benchmarks are needed for novel quantum algorithms, particularly those developed with domain science in mind by scientists without traditional theoretical computer science training. Such benchmarking will allow for clearer understanding for which algorithms can provide lasting impact for domain science.

This paper was not meant to be pessimistic, rather, to fuel further innovations from the community so the science can continue to flourish.

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