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From Ansätze to Z-gates: a NASA View of Quantum Computing

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Abstract. For the last few years, the NASA Quantum Artificial Intelligence Laboratory (QuAIL) has been performing research to assess the potential impact of quantum computers on challenging computational problems relevant to future NASA missions. A key aspect of this research is devising methods to most effectively utilize emerging quantum computing hardware. Research questions include what experiments on early quantum hardware would give the most insight into the potential impact of quantum computing, the design of algorithms to explore on such hardware, and the development of tools to minimize the quantum resource requirements. We survey work relevant to these questions, with a particular emphasis on our recent work in quantum algorithms and applications, in elucidating mechanisms of quantum mechanics and their uses for quantum computational purposes, and in simulation, compilation, and physics-inspired classical algorithms. To our early application thrusts in planning and scheduling, fault diagnosis, and machine learning, we add thrusts related to robustness of communication networks and the simulation of many-body systems for material science and chemistry. We provide a brief update on quantum annealing work, but concentrate on gate-model quantum computing research advances within the last couple of years.

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1. Introduction

The power of quantum computation comes from encoding information in a non-classical way, enabling quantum algorithms to harness effects at the heart of quantum mechanics – interference, tunneling, entanglement, measurement, many-body delocalization – for

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computational purposes. Several quantum algorithms are known that provably outperform the best classical algorithms [1][3]. The field has matured rapidly from its birth in the early 1980s, blossoming with Shor’s 1994 breakthrough discovery of polynomial-time quantum algorithms for the cryptographically important integer factoring and discrete logarithm problems [4].

While large-scale universal quantum computers are likely decades away, the next few years will see the emergence of prototype quantum processors that can run a wide variety of quantum algorithms whose simulation is beyond the reach of even the most powerful supercomputers. The advent of such hardware opens up empirical exploration of quantum algorithms far beyond what has been possible to date, including the potential to establish novel quantum heuristic algorithms. Heuristic algorithms commonly serve as the leading approaches to solving many of the world’s most challenging computational problems. With the advent of more sophisticated early quantum hardware, and the empirical exploration it enables, we expect a substantial broadening of established applications of quantum computing. Target applications include optimization, machine learning, simulation of quantum chemistry and material science, and beyond.

The earliest available quantum computing hardware were D-Wave quantum annealers, special-purpose processors that could run one type of quantum algorithm, quantum annealing, an optimization metaheuristic. The world is now entering the Noisy Intermediate-Scale Quantum (NISQ) [5] era, with prototype universal gate-model quantum processors, including superconducting processors at Google [6], IBM [7], and Rigetti [8], as well as more sophisticated quantum annealers. Universal quantum processors are on the verge of “quantum supremacy” [9], the ability to perform computations beyond the reach of even the largest supercomputers. However, useful quantum supremacy - the ability of a quantum processor to provide a solution to a practical problem that cannot be found by supercomputers - is still some years away. In the meantime, emerging quantum processors provide an unprecedented opportunity to explore quantum algorithms, providing the means to test quantum algorithms at sizes beyond classical simulation. A critical question for the NISQ era is what should be run on these early devices to give the most insight into quantum algorithms, the quantum mechanisms that can be harnessed for computation, the breadth of applications of quantum computing, and the design of quantum processors. Here, we describe efforts to provide partial answers to that question, focusing on those efforts which, through our involvement, we know best.

We discuss novel gate-model approaches to exact and approximate optimization and sampling, particularly the quantum alternating operator ansatz. This extension of the quantum approximate optimization algorithm supports NISQ exploration of a broader array of problems, particularly those with hard constraints, by allowing more general mixing operators. This extension makes possible more efficient mixing that keeps the evolution within the feasible subspace, and supports mixing operators that are more easily implemented on NISQ hardware. We briefly touch on quantum annealing for network problems, for sampling with a quantum-assisted associative adversarial network, and for quantum variational autoencoders. Prior work on quantum annealing, including for planning and scheduling, fault diagnosis, and machine learning, was described in [10]. We also describe novel classical and quantum methods for simulating many-body quantum systems, with potential applications to material science and chemistry, particularly strongly-correlated quantum systems. Quantum computing has inspired novel classical algorithms, from optimization to the simulation of quantum systems. We focus
on advanced quantum Monte Carlo (a quantum-mechanics-inspired classical algorithm) and other physics-based classical algorithms for optimization. These classical algorithms give insights into their quantum counterparts and also provide benchmarks against which any speedup claimed for a quantum algorithm can be assessed.

Research into the roots of quantum computation in quantum physics and quantum information theory grounds the algorithmic work. We discuss recent studies providing a deeper understanding of thermalization in quantum annealers, making use of new features on the 2000Q D-Wave annealers that support more flexible annealing schedules. We review recent work suggesting the potential to harness many-body delocalization effects for quantum optimization. Critical to this effort is the development of tools, including high-performance computing (HPC) simulation of quantum circuits, methods for compiling quantum circuits to realistic hardware, and state-of-the-art classical algorithms (including physics-inspired algorithms) against which to compare quantum algorithms.

This paper discusses contributions to:

- Advancing gate-model quantum algorithms for optimization, both exact and approximate, and for sampling
- Advancing quantum annealing approaches to optimization and sampling
- Physics-inspired classical algorithms for optimization and sampling
- Quantum algorithms for simulating quantum many-body systems arising in material science and chemistry
- Empirical testing of quantum approaches, both gate-model and annealing, applied to problems of interest
- Novel methods, including temporal-planning-based methods, for compiling algorithms to near-term quantum processors
- Optimized HPC for simulation of near-term quantum circuits
- Fundamental insights into the mechanisms of quantum computation.

The rest of this paper is organized as follows. Sec. 2 surveys recent work on quantum algorithms for optimization, both exact and approximate, and for sampling with applications to optimization and machine learning. Sec. 3 turns to applications of quantum computing to simulating quantum systems, with applications in material science and chemistry. Sec. 4 covers tools to support quantum computing investigations going forward, including a novel HPC method for simulating quantum circuits, methods for compiling quantum circuits to near-term hardware, and quantum subroutines for scientific computing. Sec. 5 looks at recent work illuminating mechanisms of quantum computation, focusing on two topics, thermalization and many-body delocalization. In Sec. 6, we conclude with some thoughts on the future outlook for quantum computing.

2. Quantum Algorithms for Optimization and Sampling

At present, relatively few applications are known for which quantum computing provably outperforms classical (i.e. non-quantum) computation [1,2]. Yet this scarcity of proven applications is unsurprising at this stage of the technology. Challenging computational problems arising in the practical world are frequently tackled by heuristic algorithms. Heuristic algorithms often work well in practice, but by definition have not been analytically proven to be the best approach, or even proven to outperform the best previous ap-
proach on all instances. Instead, heuristic algorithms are empirically tested on benchmark problems in, for example, satisfiability (SAT), planning, and machine learning competitions, and on real-world problems. Due to the typically exponential slowdown for simulating quantum algorithms on classical hardware, prior to the emergence of quantum hardware, quantum heuristics could only be tested on tiny problems, usually capable of giving only inconclusive results. Further, hardware constraints greatly limit the scope of problems embeddable on existing quantum annealers, and it remains unclear to what degree these devices can provide advantages [11-14]. Emerging universal quantum computers will enable a substantial broadening of the types of quantum heuristics that can be investigated. Empirical testing of quantum algorithms on quantum hardware in the coming decades will substantially broaden the applications for which quantum computing is known to outperform classical approaches. The immediate question is: what experiments should we prioritize that will give us insight into quantum heuristics?

2.1. The Quantum Alternating Operator Ansatz

One leading candidate is the quantum approximate optimization algorithm (QAOA) metaheuristic. QAOA circuits were first proposed by Farhi et al. [15], subsequently leading to a number of tantalizing results [16-24]. At the high-level, QAOA circuits have a particularly simple form. Given a cost function \( f(x) \) to optimize, a QAOA circuit alternates between “phase separation operators” \( U_P = e^{-i\beta H_P} \), which apply phases to computational basis states \( |x\rangle \) depending on the cost \( f(x) \), and “mixing operators” \( U_M = e^{-i\beta H_M} \), which generate transitions between the eigenstates of the cost-function Hamiltonian \( H_P \).

QAOA circuits are parameterized by a set of real numbers \( \{\gamma, \beta\} \equiv \{\gamma_j, \beta_j\}_{j=1}^p \), indicating the length of time the cost function Hamiltonian \( H_P \) and the mixing Hamiltonian \( H_M \) at each level are applied, where parameter \( p \) is the number of iterations. A QAOA circuit creates the quantum state \( |\gamma\beta\rangle = U_M(\beta_p)U_P(\gamma_p)\cdots U_M(\beta_1)U_P(\gamma_1)|s\rangle \), where \( |s\rangle \) is a suitable initial state such as the uniform superposition state. By choosing a good parameter set, quantum interference results in a concentration of amplitude in computational basis states with low cost.

Recent work [22, 25] extends this framework to the Quantum Alternating Operator Ansatz (retaining the acronym QAOA), enabling alternation between more general families of operators. The essence of this extension is the use of alternating mixing and phase-separation operators drawn from more general one-parameter families of unitaries rather than only those corresponding to time-evolution under a fixed Hamiltonian for a time specified by the parameter. For example, \( U_M(\beta) \) may take the form \( U_M(\beta) = U_m(\beta)U_{m-1}(\beta)\cdots U_1(\beta) \), where \( U_i(\beta) = e^{-i\beta H_i} \), where \( \{H_i\}, 1 \leq i \leq m \), is a fixed set of Hamiltonians. This ansatz supports the representation of a larger, and potentially more useful, set of states than the original formulation, with potential for broad long-term impact on exact optimization, approximate optimization, and sampling. For many optimization problems, this extension allows simpler constructions, significantly expanding the implementability of QAOA on NISQ hardware.

Prior work on QAOA focused almost exclusively on cases in which all bit strings are feasible solutions, and hence the mixing operator takes an exceptionally simple forms: independent flips of single qubits. When there are constraints that must be satisfied (hard constraints), it is desirable to design the algorithm so that the state evolution stays within the feasible subspace, a subspace in which all constraints are satisfied, usually an ex-
ponentially smaller subspace of the Hilbert space (while still exponentially large itself). Our recent results on graph coloring problems confirm the advantages of mixers that constrain the evolution to the feasible subspace \[26\]. In \[22\], we lay out design criteria for mixing operators. We detail mappings for a diverse array of problems with different types of constraints and solution space structure, including many prototypical NP-hard optimization problems such as Maximum Independent Set, Graph Coloring, Traveling Salesperson, and Single Machine Scheduling.

Gate-model quantum computing is implemented through a sequence of local quantum unitaries, each involving a few qubits. In QAOA, expanding the set of possible mixers enables more efficiently implementable mixers, particularly for optimization problems with hard constraints. If a mixing Hamiltonian takes the form of a sum \( H_M = \sum_k H_k \), where each \( H_k \) involves a small number of qubits, the Hamiltonian-based unitary \( U_M = e^{-i\beta H_M} \) can still be quite complicated to implement because the \( H_k \) typically do not mutually commute. A unitary of the form \( U_M = \prod_k e^{-i\beta H_k} \) with any given ordering of \( k \) also keeps the states in the feasible subspace so can serve as a mixing operator, but one that is often much easier to implement.

Current QAOA research includes mapping a wider variety of problems and applications, including problems related to resource allocation and robust communication networks, and exploring tradeoffs between alternative QAOA mappings. Evaluating the performance of QAOA on small problems using near-term hardware and classical simulation of quantum circuits, enables us to explore tradeoffs between QAOA mappings with a variety of alternative mixers and initial states. Additionally, we continue to advance techniques for compiling QAOA circuits to NISQ hardware (see Sec. 4.3).

A critical research thrust is finding effective sets of parameters \( \{\beta, \gamma\} \). Generally, finding a global optimum \( \{\beta, \gamma\} \) in parameter space is NP-hard (to see this, consider the circuit that rotates each qubit individually into a bit string that minimizes the cost function). However, a set of QAOA parameters does not have to be global-optimal in order for the resulting algorithm to demonstrate quantum advantage \[17, 20\]. Analysis of the algorithm and its parameter landscape benefits from identifying symmetries in the system \[20, 24\]. Understanding the landscape of parameter values of QAOA is a complicated quantum control problem, and numerical search can be hindered by not only local minima, but also by large flat areas in the energy landscape where the gradient is very close to zero. We illustrate these aspects in the following two examples.

### 2.1.1. QAOA algorithm for Grover’s search problem

For a Boolean function \( f \) that takes value 0 on all \( n \) bit strings except for a single unknown bit string \( x \), Grover’s unstructured search problem \[27\] is to find the \( x \) such that \( f(x) = 1 \), given only a black-box oracle for computing \( f(x) \). Classical deterministic or randomized algorithms must access the oracle at least \( \Theta(2^n) \) times to solve this problem in the worst-case, whereas Grover’s algorithm \[27, 28\] showed a quantum computer requires only \( \Theta(2^{n/2}) \) oracle calls. Thus, quantum computers achieve a quadratic improvement in query complexity for this problem. The QAOA approach \[20\] reproduces this quadratic improvement with an entirely new algorithm. It is also the first QAOA result for large \( p < \infty \). A unitary operator built from the standard mixing Hamiltonian \( H_M \) and the cost (oracle) Hamiltonian \( H_P \) are applied to the system periodically

\[
W(\gamma) = e^{-i\pi H_M/n} e^{i\gamma H_P} e^{-i\pi H_M/n} e^{-i\gamma H_P},
\] (1)
where there is only one free parameter $\gamma \in (0, \pi]$. Analysis shows that such a quantum circuit yields a nearly optimal query complexity of $T \approx \sqrt{N}\left(\frac{\pi}{2}\sqrt{2}\right)$. Future work includes evaluating the effectiveness of periodic parameters for QAOA in other settings.

### 2.1.2. Analysis of QAOA parameter landscape for the problem of ring-of-disagrees

Another problem in which algorithm parameter setting and performance can be informed by analytical treatment is maximum cut (MaxCut) on the 1-d cycle (ring) graph, known as the “ring of disagrees” [17]. On general graphs, MaxCut is NP-hard. For MaxCut on a ring, the optimal solutions are known: a bitstring of alternating values. From numerical results for QAOA$_p$ on a ring with an even number of vertices $n$, the approximation ratio achieved is $1$ for $p > n/2$, and is $(2p + 1)/(2p + 2)$ for $p \leq n/2$ when the algorithm parameters are optimized [17]. We apply a fermionic transformation to this problem in [24], transforming it into a problem involving $n/2$ rotating non-interacting individual spins. All spins are initialized evenly on the unit circle in the x-z plane. Applying the cost and mixing unitaries correspond to rotating each spin along the z-axis and a direction specific to each spin in the x-z plane, respectively. The goal is to line up all spins along the $-z$-axis by the end of the algorithm. From the symmetry observation that certain transformations bring the two axes on equal-footing, we infer that optimal parameters must live in a submanifold defined by symmetry $\beta_i + \gamma_{p+1-i} = 0$. This reduces the number of parameters to search by half, and provides significant speedup in the search.

![Figure 1](image.png)  
**Figure 1.** (Color online). Trap-free landscape of the space of parameter values for QAOA$_2$ on the problem of ring-of-disagrees, formulated as a minimization problem, in the sub-manifold xx. The four darkest spots indicate the global minima. The origin (0, 0) is a saddle point. No local minima are observed.

### 2.1.3. Some general comments on parameter setting

For parameterized quantum circuits, the landscape of the parameter space affects the ease with which good parameters can be found. We discuss two barriers that affect numerical search. One is controllability and the existence of local minima, and the other is barren plateau. In quantum control theory, assuming controllability (i.e., evolution between any
two states is achievable via the set of controls given), the landscape of parameter values generically has only global minima [29-31]. Without controllability, the quantum control landscape in general is rugged and admits local minima ("traps") [32]. In the case of QAOA, the controls are constrained in a specific way: if an infinite number of controls are allowed, i.e., $p \rightarrow \infty$, then the system is controllable. The finite number of control steps dictated by finite $p$ limits the controllability. For QAOA on the problem of ring of disagrees, our results suggest that although the system is not controllable, within the symmetry-defined sub-manifold the landscape is trap-free, see Figure 1. This simple problem demonstrates that the landscape of QAOA parameters can be complicated and calls for further studies into the relation with quantum control theory.

Besides local minima, barren plateau may form another severe challenge. In some circumstances, such as random quantum circuits, the gradient will be effectively zero over vast reaches of parameter space [33], known as barren plateaus. Barren plateaus foil gradient-based numerical optimization procedures. Although the framework of QAOA does not fall exactly into the conditions of this argument, finding good parameters for QAOA may face a similar challenge. Detailed study of quantum control is required to further understand both case-specific and general feature of the landscape of parameter space for applications of QAOA, and as suggested in McClean et al. [33], good ansätze, such as those found in quantum chemistry, may be needed here.

We are interested in analytical results and numerical experimentation that can lead to a better understanding of how best to find good parameters for QAOA algorithms, design trade-offs for the mixers, robustness under errors, and error mitigation approaches tailored to these circuits. The ring of disagrees analysis provides a promising start, as did the work of Yang et al. [34]. We intend to explore further ideas for leveraging control theory, machine learning, and spectral properties and quantum transport techniques to provide deeper insights and better parameter-setting methods.

2.2. Update on Quantum Annealing Work

Quantum annealing is a quantum metaheuristic for optimization [35,36]. Quantum annealers are quantum hardware that are designed to run this metaheuristic. Given a classical cost function $C(x)$ with binary input $x \in \{0,1\}^n$, a quantum annealer works by encoding the binary variables $x$ as qubits, and slowly varying the Hamiltonian that governs the quantum evolution of the qubits from a Hamiltonian $H_0$ whose ground state is the uniform superposition of all bit strings, to a Hamiltonian $H_1$ that is constructed based on the cost function such that the global minimum of $C(x)$ is the ground state of $H_1$.

Quantum annealing has been a major research focus of the QuAIL team [10]. Our previous studies range from obtaining physical insights into and intuitions for quantum annealing, studying programming and parameter setting for quantum annealers, and application-specific as well as general classical solvers. Older investigations of quantum annealing and quantum-classical hybrids to potential application areas, included planning and scheduling [37,42], fault diagnosis [43], and machine learning [44,48]. In [49], we pioneered the use of subsystem codes in the context of error suppression in quantum annealing, showing that subsystem codes circumvent a no-go theorem for stabilizer codes, enabling effective error suppression with just two-local terms. Marvian [50] has taken this approach further, deriving performance bounds and new two-local constructions. We refer the reader to [10] and references therein, for a survey of the older work.
Here, we look first at work on quantum annealing applied to robust network design, and then turn, in Sec. 2.2.2, to a hybrid quantum-classical machine learning algorithm of the generative adversarial network (GAN) class. Later, Sec. 5 discusses lower-level advances related to quantum annealing that may be generally applicable.

2.2.1. Quantum Annealing for Network Problems

Driven by application-related network problems, we examined the spanning tree with bounded degree problem with quantum annealing. As motivation, we start with a testing model in an aeronautic communication network problem. Consider a given number, say four, of unmanned vehicles with known trajectories and a pre-determined network disruption area $S$, where vehicles outside $S$ can talk directly to the ground control station but vehicles inside $S$ must route communication through vehicles not in $S$ to reach the ground station. If each vehicle can connect to at most $\Delta$ other vehicles (including the ground station), how should communications be routed so that the overall communication distance is minimized?

This problem simplifies to minimizing the total edge weight of bounded-degree spanning trees of a graph specified by the problem instance. The spanning tree problem forms the basis of many network related applications. In the above case, the graph is a complete graph of five vertices (four vehicles and a ground station) with some edges removed (between the ground station and the vehicles inside $S$). For an arbitrary graph, deciding whether or not a degree-constrained spanning tree exists is a NP-complete problem, and finding a degree-constrained spanning tree that optimizes certain cost functions on the graph is NP-hard. We developed three mappings of this problem to the quadratic unconstrained binary optimization (QUBO) form for input to quantum annealer hardware. These mappings can be readily embedded on the D-Wave annealer. We performed sample runs for the different mappings on complete graphs of small size, and confirmed the ability of the quantum annealer to solve these problems.

We describe one of these mappings, the “level-based mapping,” for a simple spanning-tree problem to illustrate the mapping process. Given a graph $G = (V,E)$, $|V| = n$, $|E| = m$, we aim to find a spanning-tree of $G$ through mapping it as a global minimum of QUBO. Since a tree can be equivalently rooted at any node, we fix vertex $v = 1$ to be the root. We assign two types of binary variables. For each vertex $v$, a binary variable $x_{u,v}$ for $\{u,v\} \in E$ indicates whether vertex $u$ is the parent of $v$, and another binary variable $y_{v,l}$ indicates whether $v$ is at level $l$. We allow $l$ to run from 1 to $n$. The root $v = 1$ is at level 1 and has no parent. Constraints that guarantee the graph to be a tree includes: that each vertex $v \in (1,n]$ has exactly one parent; that each vertex $v$ is assigned exactly one level; and that the parent vertex of $v$ must be of lower level than $v$. The constraints are mapped to polynomial binary optimization terms as $(\sum_{v \neq v'} x_{v,v'} - 1)^2$, $(\sum_{l=2}^{n} y_{v,l} - 1)^2$, and $y_{v,l} \sum_{l=2}^{n} y_{v',l} x_{v,v'}$, where the first two are in QUBO form and the last term can be further transformed into quadratic terms through ancilla qubits [41].

2.2.2. Quantum-Assisted Associative Adversarial Network Learning

Near-term utilization of quantum annealers in service of machine learning requires that the number of variables used be small and the algorithms resistant to noise. The aim of these algorithms is to turn over classically computationally expensive subroutines, such as sampling, to quantum hardware in hybrid architectures. Interest in integrating quan-
tum Boltzmann machines and their restricted variants into deep learning architectures is driven by a potential increase in speed of sampling for some graph structures and the ability to learn quantum models. We developed and evaluated a learning algorithm: Quantum Assisted Associative Adversarial Network (QAAAN) learning [51]. This algorithm learns a latent variable generative model using a generative adversarial network (GAN) with an informed prior probability distribution. In our approach, the canonical noise input to a generative adversarial network is replaced by samples from an informed prior. The prior is a model of a feature space taken from a low-dimension representation in the discriminative network and is learned by a Boltzmann machine. The output of the algorithm is a latent variable generative model, where sampling from the prior can be performed by sampling from the distribution with a quantum annealer or Markov chain Monte Carlo methods. We evaluated the algorithm on the MNIST, a standard machine learning dataset of images of handwritten digits. We found close performance between classical and quantum implementations when evaluated using the Frechet inception distance (29 and 23, respectively) and the inception score (5.6 and 5.7, respectively), drawing the conclusion that the quantum device can be successfully integrated into the classical framework. We also demonstrated the classical architecture on the more complex dataset LSUN bedrooms, concluding the algorithm can be scaled. This work expands the set of deep learning algorithms that exploit near-term quantum annealers [45, 52, 53].

2.2.3. Quantum Variational Autoencoders

An Alternative Approach [52] to integrate quantum Boltzmann machines into deep generative models uses Variational Autoencoders (VAE) [54] with discrete latent variables [55, 56]. VAE are directed generative models that can be efficiently trained by maximizing a variational lower bound (ELBO) of the model log-likelihood. The use of variational inference and low-variance estimators of the training gradients [54] makes this possible. In addition to achieving state-of-the-art performance in generative modeling (unsupervised learning), VAE are an important tool in semi-supervised learning [57].

When applied to natural image processing, VAE are very good at extracting coarse-grained features but struggle to reproduce the fine-details. This problem can be cured using a fully autoregressive decoder such as PixelCNN [58, 59] at the cost of having a less informative latent space [60, 61]. We recently demonstrated that RBM priors enable an informative discrete latent space, state-of-the-art performance on common datasets such as MNIST and CIFAR10, and sharp image generation [62]. This work demonstrates that quantum priors (which define distributions on discrete variables) can be used to train state-of-the-art quantum/classical hybrid generative models.

On important advantage of VAE is the potential to quantitatively evaluate trained models (by computing the ELBO or estimating the log-likelihood on the test set), enabling iterative improvement of the generative model. We demonstrated [63] using this approach that convolutional VAE can be successfully trained with D-Wave DW200Q quantum annealers to achieve close to state-of-the-art performance on MNIST. The same paper demonstrates improved performance of VAE when using D-Wave if the structure of the convolutional encoder and decoder is crafted to the D-Wave Chimera architecture.
3. Quantum Computing for Simulation

The accurate simulation and characterization of systems of interacting fermions was one of the original motivations for the development of quantum computers \[64\, 66\]. There is optimism that for relatively near-term quantum computers that we will be able to perform some type of characterization of ground and excited state properties of quantum chemical systems \[67\, 71\]. The field of interacting fermions (and other quantum particles) has applications in physics, chemistry and material science. Due to broad applicability of fermionic simulations, efficient quantum simulation techniques would significant impact all of these fields. Recent estimates of the quantum resources \[72\] needed to perform phase estimation on FeMoco, a transition metal center that splits the nitrogen dimer in a nitrogenase enzyme, are high compared to current quantum hardware, but represents a concrete goal for future quantum computers.

It is a challenge for quantum computers to achieve an advantage over classical computers in this domain, given the decades of work on, and myriad classical tools for, treating quantum systems. However, the quantum information processing viewpoint has proven fruitful for the discovery of advanced purely classical algorithms and analysis techniques (e.g. \[73\, 79\]). In this regard, our research focuses developing new techniques for both classical and quantum hardware from different perspectives. This covers a range of systems including \textit{ab initio} simulations, Hubbard models, spin Hamiltonians, interacting Fermi liquids, solid state systems, and molecular systems \[80\, 86\]. While the long-term impact of quantum computing for simulations of quantum chemistry and materials is promising, we are in the early days; none of the experiments realized so far perform even close to state-of-the-art classical simulations. For these reasons, near-term research will focus on advancing classical, and quantum-classical hybrid, as well as quantum algorithms, and on estimating the quantum resources, and designing quantum hardware architectures, for simulations of practical interest, so as to determine when and how such simulations can be realized.

An understanding of classical algorithms, and their strengths and weaknesses, can suggest where a quantum advantage may be most likely, as well as suggesting issues that may arise for quantum simulation approaches both in the near term and the long term. In order to understand the feasibility of different quantum simulations broadly, we work at the interface between classical and quantum simulations. For example, in \[86\] we used leading classical simulations to start providing resource estimates for aspects of quantum simulations that are crucially important but often neglected: initiating the starting wave function used in quantum methods such as phase estimation. Efficient \textit{state preparation}, finding and creating an effective initial state, must be part of any efficient quantum simulation algorithm. We designed a new approach to creating correlated wave functions on a quantum device, and demonstrated this new approach to generating effective initial states with classical algorithms. We investigated state preparation for a series of difficult physics- and chemistry-relevant Hamiltonians, demonstrating the plausibility of generating good initial states for problems that may not be solved to high accuracy with current classical algorithms.

Other recent work \[87\] showed that faster quantum simulation algorithms may be obtained by considering Hamiltonian structure. For simulating the sum of many Hamiltonians, we split the Hamiltonians into groups, simulate each group separately, and then combine the partial results, with each simulation tailored to the properties of each group.
We illustrated our results using the electronic structure problem of quantum chemistry, in which the second-quantized Hamiltonian is typically given by a sum in which relatively few terms are substantial in norm. Separately grouping the large norm and small norm terms significantly improved simulation cost estimates under mild assumptions.

Another promising research direction is improving existing quantum methods. Two of the most discussed methods, phase estimation and variational quantum eigensolvers (VQE) require significant quantum computing resources, prompting work to find less resource-intensive alternatives. For example, while the variational quantum eigensolver \[67, 69, 88\] approach has early experimental demonstrations \[69, 89, 92\], it is far from settled whether or not it will be possible to overcome difficulties involved in choosing a useful ansatz, optimizing many thousands of parameters \[33\], and scaling of noise and measurement challenges \[93, 95\]. Some of these challenges were addressed for spinless Hubbard models, where a suitable circuit’s structure was proposed based on the entanglement properties of the examined Hamiltonians and achievable speed of convergence \[96, 97\]. Much research remains to be done in this direction, with many wave function ansätze to explore \[98\] to advance variational quantum eigensolvers.

Phase estimation, a method for determining eigenstate energies, is useful for the accurate simulation of long-time dynamics and the determination \[99, 100\], but requires a large number physical qubits and quantum gates \[72, 101, 103\]. While quantum phase estimation has been experimentally implemented for small molecules on a variety of quantum computing architectures, including with quantum optics \[104\], nitrogen-vacancy centers \[105\] and superconducting qubits \[89\], its application to larger molecules of practical interest, such as FeMoco, is estimated to need a gate depth several orders of magnitude beyond what is currently feasible \[72\]. We are therefore interested in trying to improve techniques for these types of simulations.

In addition to finding new algorithms for quantum simulation, tools for maximally utilizing NISQ hardware, such as methods for compiling quantum circuits to near-term architectures, can reduce the quantum resources required compared to more straightforward implementations. Sec. 4.3.2 describes one novel approach to compilation of circuits for simulation (and also for other near-term algorithms such as QAOA).

### 4. Tools for Quantum Computing Investigations

Quantum computing research requires an array of tools, and the creation of new or improved tools. Here, we discuss advances in methods for simulating quantum circuits on classical computers, in physics-inspired optimization algorithms for benchmarking quantum algorithms, in compiling quantum circuits to near-term hardware, and in efficient implementation of subroutines commonly used in scientific computing.

#### 4.1. Classical Methods for Simulating Quantum Circuits

Classical simulation of quantum circuits not only provides insight into quantum heuristics: it is key to validating early quantum hardware \[6, 106\]. The direct comparison of results from NISQ devices and from classical simulations will enable prioritization of hardware improvements to best support these algorithms. The computational effort involved in simulating quantum circuits grows exponentially with the number of qubits,
| Circuit size         | Target fidelity (%) | Runtime (hours) | Energy cost (MWh) |  |
|----------------------|---------------------|-----------------|-------------------|---|
|                      |                     | Pleiades | Electra | Pleiades | Electra |
| $7 \times 7 \times (1 + 40 + 1)$ | 0.51 | 62.4 | 59.0 | 2.73 x 10^2 | 96.8 |
| $8 \times 8 \times (1 + 32 + 1)$ | 0.78 | 1.38 | 1.59 | 6.91 | 2.61 |
| $8 \times 8 \times (1 + 40 + 1)$ | 0.58 | 1.18 x 10^4 | 1.23 x 10^4 | 5.15 x 10^4 | 2.02 x 10^4 |
| $8 \times 9 \times (1 + 32 + 1)$ | 0.51 | 14.8 | 15.2 | 73.9 | 24.9 |
| Bris.-70 $\times (1 + 32 + 1)$ | 0.50 | 145 | 178 | 723 | 293 |

Table 1. Estimated runtimes and energy costs for the computation of $10^6$ amplitudes with fidelity close to 0.5% on NASA HPC Pleiades and Electra systems. The $7 \times 7 \times (1 + 40 + 1)$ and $8 \times 8 \times (1 + 40 + 1)$ grid jobs do not fit in Sandy Bridge nodes, due to their memory requirements; for that reason, the portion of Pleiades with Sandy Bridge nodes is not considered, in the energy cost estimations for these two cases.

| Circuit size         | Fidelity (%) | Runtime (hours) | Energy cost (MWh) |  |
|----------------------|--------------|-----------------|-------------------|---|
|                      |              | Pleiades | Electra | Pleiades | Electra |
| $7 \times 7 \times (1 + 40 + 1)$ | 100.0 | 1.22 x 10^-2 | 1.16 x 10^-2 | 5.35 x 10^-2 | 1.89 x 10^-2 |
| $8 \times 8 \times (1 + 32 + 1)$ | 100.0 | 1.77 x 10^-4 | 2.04 x 10^-4 | 8.66 x 10^-4 | 3.34 x 10^-4 |
| $8 \times 8 \times (1 + 40 + 1)$ | 100.0 | 2.03 | 2.12 | 8.88 | 3.48 |
| $8 \times 9 \times (1 + 32 + 1)$ | 100.0 | 2.90 x 10^-3 | 2.98 x 10^-3 | 1.45 x 10^-2 | 4.89 x 10^-3 |
| Bris.-70 $\times (1 + 32 + 1)$ | 100.0 | 2.89 x 10^-2 | 3.57 x 10^-2 | 1.45 x 10^-1 | 5.85 x 10^-2 |

Table 2. Estimated effective runtimes and energy cost for the computation of a single amplitude with perfect fidelity on NASA HPC Pleiades and Electra systems. The $7 \times 7 \times (1 + 40 + 1)$ and $8 \times 8 \times (1 + 40 + 1)$ grid jobs do not fit in Sandy Bridge nodes, due to their memory requirements; for that reason, the portion of Pleiades with Sandy Bridge nodes is not considered in the energy cost estimations for these two cases.

making even low-depth circuits challenging to simulate [6, 107, 108]. In recent years, new classical techniques have been devised to take advantage of regular structures of near-term implementable quantum algorithms such as QAOA, instantaneous quantum computation (IQP), random circuits, and Variational Quantum Eigensolvers (VQE). Among the classical techniques to simulate quantum circuits, the most promising ones to simulate near-term devices are the tensor network contraction [109] and the Bravyi-Gosset stabilizer approach [110]. While the former technique is more suitable for shallow quantum circuits, the latter works the best for deep quantum circuits with non-Clifford gates.

Utilizing NASA Ames’s supercomputer resources and expertise to optimize code based on the aforementioned techniques, in collaboration with the Quantum AI team at Google, and ORNL [111][112], we devised a simulator that pushes the boundary on the size and complexity of near-term quantum circuits that can be simulated. The resulting simulator can simulate random circuits on Google Bristlecone QPU [6][113]. The simulator can compute both exact amplitudes, a task essential for the verification of the quantum hardware, as well as low-fidelity amplitudes to mimic NISQ devices. For instance, our simulator is able to output single amplitudes with depth 1+32+1 for the full 72-qubit Google Bristlecone QPU in less than $(f \cdot 4200)$ hours on a single core, where $0 < f < 1$ is the target fidelity, on 2 x 20-core Intel Xeon Gold 6148 processors (Skylake). We also estimate that computing $10^6$ amplitudes (with fidelity 0.50%) needed to sample from the full Google Bristlecone QPU with depth (1+32+1) would require about 3.5 days using the NASA Pleiades and Electra supercomputers combined. Table 1 and Table 2 report our latest numerical estimations [111] to classically simulate quantum random circuits.
for 2-D grids, including the Google Bristlecone QPU. Tables I and II report estimated runtimes and energy costs for the computation of $10^6$ noisy amplitudes, with target fidelity of 0.5% (Table I) or single perfect amplitudes (Table II). As comparison, the power needed by 1 million inhabitants city is \(\sim 1500\) MW. Our analysis is supported by extensive simulations on NASA HPC clusters Pleiades and Electra (further details in [111]).

For the most computationally demanding simulation we had, the two HPC clusters combined reached a peak of 20 Piflop/s (single precision), that is 64% of their maximum achievable performance. To date, this numerical computation is the largest in terms of sustained Piflop/s and number of nodes utilized ever run on NASA HPC clusters. We also performed numerical benchmarks on Summit, currently the fastest supercomputer in the world [112]. After porting qflex for GPU architectures, we were able to reach an average performance of 281 Piflop/s (true single precision, corresponding to the 68% of the maximum achievable), with peaks of 381 Piflop/s (true single precision, corresponding to the 92% of the maximum achievable). All numerical simulations can be found at the QuAIL@NASA repository [114].

State of the art algorithms for simulating quantum algorithms are parameterized; their resource requirements scale exponentially only in some property of an instance rather than its size, e.g. the number of T-gates for the stabilizer approach. Tensor network contraction was shown to be parameterizable by the treewidth of the line graph of the tensor network’s graph; we found an alternative characterization of this result in terms of tree embeddings and vertex congestion [115]. The characterization in terms of vertex congestion is conceptually clearer and exactly quantifies the running time when the contraction is done as a series of matrix multiplications. It also yields a characterization, in terms of edge congestion, of the memory used, which is often the bottleneck in practice.

4.2. Physics-inspired Classical Algorithms and Benchmarking of Quantum Algorithms and Applications

We continue to push the state-of-the-art in classical optimization techniques, particularly physics-inspired techniques. Quantum Monte Carlo [116–118] and iso-energetic cluster moves [119] provide a fair comparison of quantum heuristics to classical techniques [13][120][121] and a reference for claims of quantum advantage. Key to evaluation of quantum advantage is characterizing different kinds of quantum speed-ups [11][13].

In addition to both classical and quantum heuristics for hard-optimization problems, we developed novel quantum and hybrid quantum-classical approaches for real-world applications in the areas of planning and scheduling [37][42], fault diagnosis [43], and machine learning applications [45–47]. In contexts in which diverse solutions are valued, aspects of the cost function are not available ahead of time, or the problems change quickly with time, having multiple optimal and quasi-optimal solutions is of utmost importance. To this end, we are also advancing classical optimization approaches through physics-based advances in classical algorithms for sampling [122][123].

As part of the effort to detect and identify quantum speed-ups, the QuAIL team’s work developing benchmark problems sets including the theory, identification, and generation of parameterized families of hard problems [121], containing small problems suitable for near-term, prototype quantum processors [124][125], generation of problems with planted solutions and fine-tuned complexity [126]. Figure 2 shows an example in
Figure 2. Time-to-solution (TTS) for the parallel tempering iso-energetic cluster method (PT+ICM), the Hamze-de Freitas-Selby (HFS) heuristic, as well for the D-Wave 2000Q (DW2000Q) quantum chip (see [121] for more details).

which the D-Wave quantum device shows a better pre-factor (but a similar scaling and comparable energy consumption) if compared to the state-of-the-art classical heuristics once the problem parameters are properly tuned. We will use these benchmark problem sets for evaluating early quantum hardware, both to evaluate the utility of annealing capabilities newly available on the D-Wave quantum annealers such as the anneal offset, pause and quench, and reverse annealing [127], and to evaluate the effectiveness of gate-model approaches such as QAOA (see Sec. 2.1). We will extend this approach to the evaluation of quantum-classical hybrid methods as well.

4.3. Compiling Quantum Circuits to Realistic Hardware

Compilation is required to take descriptions of quantum algorithms and generate implementations on near-term hardware. There are multiple aspects of compiling, including addressing the limited connectivity of many NISQ devices. One way to overcome limited connectivity is to insert swaps in the circuit so that states can be moved to adjacent qubits where logical operations can be performed. The problem of doing so optimally is referred to as the “Å‘qubit routing” problem. Here, we consider two types of routing approaches, one based on temporal planning, the other on Jordan-Wigner reordering.

4.3.1. Temporal Planning for Quantum Circuit Compilation

Temporal planning is an effective approach for qubit routing of quantum circuits to near-term hardware [128]. Temporal planning [129], a subdomain of Automated Planning and Scheduling, is concerned with choosing actions, among a large finite set of possibilities, to achieve a specific goal, incorporating temporal constraints or time optimization objectives. Our mapping of compilation to planning allows us to exploit highly optimized, off-the-shelf planners. Temporal planners minimize the makespan, a refinement of circuit depth that takes into account gate times, namely the time it takes to run a circuit. NISQ hardware does not have the resources to implement error correction, and thus suffers from decoherence, making the makespan a quantity of critical relevance.

The temporal-planning approach is particularly effective for circuits, such as QAOA circuits, with many commuting gates, in which the space of possible compilations is larger than for circuits with more restricted ordering. More recently, we integrated the
temporal planning approach with constraint programming \cite{130}, and have started working on more sophisticated hybrids of temporal planning and constraint programming (CP), including adaptive switching approaches. Results are encouraging, as temporal planning if properly tuned and hybridized with CP, can deliver provably optimal results for the instances tested in \cite{128}.

We developed software components for a fully-fledged module that supports temporal-planning and CP-based compilation to NISQ processors, currently instantiated for Google’s Bristlecone architecture and MaxCut problems. The software supports visualization (Fig. 3) and interactive tuning of the compiled circuits. See \cite{131} for details. We are extending our evaluation from QAOA MAXCUT circuits to QAOA circuits for a variety of problems \cite{22,25}, starting from Graph Coloring. The automated reasoning framework is broad enough to incorporate more hardware constraints and capabilities such cross-talk, measurement, and feedback. Another important research direction is to extend this approach beyond superconducting architectures.

4.3.2. Jordan-Wigner-Based Compilation for Quantum Simulation and Beyond

The near-term algorithms in Sec. 2 and Sec. 3 are typically based on one of two primitive steps: Trotterized time evolution or Hamiltonian-based variational ansätze. From a compilation perspective, these have essentially the same structure, namely a gate for each term in the Hamiltonian. While these gates do not necessarily commute, there is significant freedom in how they are ordered, and compilation efficiency may be the dominant criterion therefor. Using the standard Jordan-Wigner transformation from fermionic operators to qubit operators, each term in the Hamiltonian corresponds to a gate whose locality depends on the differences of the indices in the relevant fermionic modes. However, fermionic swap gates can be used to reorder the indexing of the modes so that each gate has minimum locality (i.e. it acts on the same number of qubits as the corresponding number of fermionic modes). Previous work \cite{68} showed how to compile circuits corresponding to quadratic fermionic Hamiltonians on $n$ modes in $O(n)$ depth. However, these
quadratic Hamiltonians derive from particular bases that are likely unsuitable for molecular systems. We generalized the approach to arbitrary bases, showing how to get the optimal depth of $O(n^3)$ for a general chemical Hamiltonian $[132]$. Using similar methods, we also show how to achieve $O(n^2\eta)$ depth for Unitary Coupled Cluster with $n$ modes and $\eta$ electrons, as well as $O(n)$ depth for Unitary Paired Coupled Cluster $[98]$. Importantly, the optimality of this scaling is independent of the connectivity of the hardware and shows that the parallelization can address the locality problem of the Jordan-Wigner transformation for free. For “low-rank” instances, other approaches $[133]$ may provide more efficient compilations, but our techniques are unconditional.

This approach to compiling fermionic gates by reordering the Jordan-Wigner string to get certain modes adjacent $[70]$ is equivalent to compiling local qubit operators to a physical line of qubits. Therefore the techniques are equally applicable, e.g., to QAOA circuits for constraint satisfaction problems. In this context, the approach can be considered an instance-independent compilation; for any particular instance, the compilation may be suboptimal, but with the advantage that there is no instance-specific compilation time, which is important for practically benchmarking against classical methods.

4.4. Quantum Subroutines for Scientific Computing

Algorithms for scientific computing applications often require modules, i.e., building blocks, implementing elementary numerical functions that have well-controlled numerical error, are uniformly scalable and reversible, and that can be implemented efficiently. We showed explicit quantum circuits, at the level of basic addition and multiplication operators, for a variety of numerical functions important in scientific computing in $[134]$. The decomposition into basic addition and multiplication operations, and hence the corresponding error and cost bounds, are largely agnostic to the underlying hardware. This allows for easy portability between different quantum architectures, and straightforward derivation of the cost in terms of primitive quantum gates.

In particular, in $[134]$ we derive quantum algorithms and circuits for computing square roots, logarithms, and arbitrary fractional powers of numbers, and derive worst-case error and cost bounds. We describe a modular approach to quantum algorithm design as a first step towards numerical standards and mathematical libraries for quantum scientific computing. Ongoing work seeks to explore the tradeoffs between different low-level realization of these circuits, such as between circuit depth and the number of qubits required for scratchpad space, and between the resources required for different implementations of the underlying quantum circuits for addition and multiplication.

In $[135]$, we showed a methodical approach to mapping classical Boolean and real functions to quantum Hamiltonians in terms of Pauli operators. Quantum circuits for simulating these Hamiltonians and their costs then follow immediately from these mappings. In particular, this allows for efficient construction and of a wide variety of QAOA phase operators. Nevertheless, it remains an ongoing research direction to explore when these constructions are optimal with respect to a fixed gate-set, i.e., when the cost of the construction obtained from the Hamiltonian mapping cannot be improved upon significantly. Furthermore, the results of $[135]$ are also applicable to quantum annealing, where they give a methodical approach to mapping general objective functions to Hamiltonians acting on quantum spins, and to constructing Hamiltonians implementing penalty functions in the case of constrained optimization.
5. Mechanisms of Quantum Computation

Here, we discuss recent work that deepen understanding and quantum mechanisms. The first is research into thermalization in quantum annealers and the effect of annealing schedules on performance. The second is many-body delocalization with potential implications for quantum computing. An overview of our past work, including [12, 116, 117, 122, 136–141] can be found in [10].

5.1. Thermalization and Sampling

In [127], we investigated alternative annealing schedules on current generation 2000 qubit quantum annealing hardware (the D-Wave 2000Q), including the use of forward and reverse annealing with an intermediate pause. This work provides new insights into the inner workings of these devices, and quantum devices in general, particularly into how thermal effects govern the system dynamics. On benchmark problems native to the D-Wave architecture, we showed that a pause mid-way through the anneal dramatically changes the output distribution. Upon pausing the system in a narrow region shortly after the minimum gap, the probability of finding the ground state of the problem Hamiltonian can be increased by several orders of magnitude, compared to not pausing or when pausing outside of this region. By identifying three relevant time-scales, we provide evidence suggesting thermalization is indeed occurring during such a pause. We related this effect to relaxation (i.e. thermalization) after diabatic and thermal excitations that occur in the region near the minimum gap. For a set of small native problems, for which the minimum gap can be computed, we confirmed this relation. For a set of large-scale native problems of up to 500 qubits, we demonstrate that the distribution returned from the annealer closely matches a (classical) Boltzmann distribution of the problem Hamiltonian, albeit one with a temperature higher than the (effective) temperature of the annealer. An encouraging result is that larger problems appear more likely than smaller problems to thermalize to a classical Boltzmann distribution, suggesting the potential use of quantum annealers as Boltzmann sampling subprocessors in quantum-classical hybrid machine learning algorithms. Our model is general, suggesting that similar thermal effects could apply to different types of quantum devices, and within quantum annealing, the results should hold for other classes of problem. This work suggests that not only pausing, but alternative annealing schedules more generally, are a promising way to improve time-to-solution for a wide range of optimization problems.

5.2. Many-body Delocalization

A deeper understanding of many body dynamics will aid quantum computing, from hardware design to novel algorithms. Of particular interest are quantum effects that could be harnessed for quantum computational purposes. Many-body delocalization is potentially one of those effects. Many-body localization (MBL) is the robust breakdown of ergodicity in quantum disordered systems, when an isolated quantum system does not properly function as a bath for its own local subsystems, which therefore fail to thermalize [142]. Localization/delocalization transitions are typically driven by a parameter controlling the relative strength of kinetic and disorder terms affecting a quantum system. In the strong disorder phase (also called the localized phase), these systems develop quasi-local
integrals of motion that constrain its dynamics in a “frozen” regime where transport is suppressed. This is detected by localized spatial configuration of the eigenfunctions of the system’s Hamiltonian: delocalized systems have wavefunctions whose amplitudes are roughly equal ($|\psi_i|^2 \approx 1/\text{Vol}$) over all spatial sites, while the amplitudes of localized wavefunctions concentrate in a finite region and decay exponentially away from it. Although originally defined for tight-binding models of electrons hopping on a lattice, MBL was generalized to quantum spin models and spin glasses.

The connection between localization and quantum computing was first drawn in . Writing the standard quantum annealing Hamiltonian $H(t) = H_{cl} + B(t) \sum \sigma_i^x$ in the (classical) computational basis, one recovers the Hamiltonian

$$H = \sum_i \epsilon_i |i\rangle\langle i| + B(t) \sum_{\langle i,j \rangle} \left( |i\rangle\langle j| + |j\rangle\langle i| \right),$$

where the sum is over all pairs $\langle i,j \rangle$ of classical states connected by exactly one spin flip (a Boolean hypercube graph structure). The Hamiltonian of Eq. (2) is analogous to the Anderson model Hamiltonian

$$H_{AM} = \sum_i \epsilon_i a_i^\dagger a_i + t \sum_{\langle i,j \rangle} \left( a_i^\dagger a_j + a_j^\dagger a_i \right)$$

restricted to the one-particle sector of its Fock space. The Anderson model describes the theory of free electrons hopping in a $d$-dimensional cubic lattice, scattered by a disordered local potential with uncorrelated energies $\epsilon_i$. It undergoes a localization/delocalization transition in dimensions $d \geq 3$. An open question is whether the same is true for the when the energies $\epsilon_i$, the costs that appear in the (local) combinatorial optimization problem $H_{cl}$, show correlations. The emergence of localized dynamics for such systems would suppress quantum tunnelling and thus negatively impact the performance of quantum annealers in the part of the anneal when $B(t)$ is small.

In light of the similarity between the spectra of various spin glasses models and combinatorial optimization problems, the current effort by the scientific community to detect the appearance and the exact extent of the MBL phase in various quantum spin glass models is of clear interest to quantum computing as it provides a theoretical tool for the analysis of how effectively quantum annealing (and other optimization methods that exploit the quantum dynamics of local Hamiltonians) explores the complicated energy landscapes of combinatorial problems.

MBL was proposed in as a physical mechanism behind the appearance of superexponentially closing gaps in the spectra of Hamiltonians in this later part of a quantum annealing run, with avoided crossing happening at a point that approaches the final time of the anneal, $N^{-1/8}$. A more precise analysis refining the results of , and showed that these avoided crossings happen more realistically at a time that is $O(1)$ away from the end of the anneal.

A further attempt to understand the dynamics of quantum spin glasses considers a simplified “impurity band” model with a low-energy subspace composed of $M$ classical states whose energies are contained within a narrow interval, separated from the rest of the spectrum by an extensive energy gap (for simplicity it was assumed that the energies of states inside of the band are negative while all the others are zero). The dynamics of the system is defined by adding a transverse field term to the band Hamiltonian
in order to induce transitions between different states. At $t = 0$ the wavefunction of system is taken to be localized at one of the classical states $|i\rangle$ inside of the band. The dynamics generates multi-channel tunnelling from the initially populated site $i$ to other sites in the system. These tunnelling processes are mediated by the excited states that lie outside of the impurity band. This quantum process is expected to be hard to simulate classically; it is not captured by path-integral quantum Monte Carlo, which can be used to study tunnelling dynamics in potentials where tunnelling is dominated by a single path, such as the standard double-well potential [116, 155].

After some time $t_{\text{PT}}$ the wavefunction will have spread to a superposition of some number $\Omega$ of states in the impurity band. This number of states turns out to be dependent on the fractal properties (controlled by the choice for $B_\perp$) of the eigenstates of the down-folded Hamiltonian that effectively describes the band. The best choice for $B_\perp$ is a compromise between two opposing considerations: ideally, one desires to tunnel to as many states inside of the impurity band as possible (and make $\Omega$ as large as possible), but one does not want to lose significant amplitude to excited states above the band. The optimal choice is achieved when the system is in a “bad metal” phase between the “insulating” (localized) phase and the “conducting” (ergodic, extended) phase. In this phase, the eigenstates of the system are delocalized over a number of sites proportional to $N^\alpha$, for some value $0 < \alpha < 1$. Thus, the support of these states for all finite system sizes is not compact (that is, $O(1)$ in $N$, as in the case of localized states), but the fraction of sites in the support goes to zero in the thermodynamic limit (unlike ergodic extended states, where instead it approaches a finite value). States with these intermediate properties are called non-ergodic, extended (NEE) states.

The typical time required to achieve this delocalization effect over a number $\Omega$ of states is given by the population transfer time $t_{\text{PT}}$, which was found to be

$$t_{\text{PT}} \propto \left( \frac{2N}{\Omega \log \Omega} \right)^{1/2} e^{\Omega/(2B_\perp^2)},$$

which gives a scaling with $N$ and $\Omega$ that is comparable (up to a factor of $e^{\Omega/(2B_\perp^2)}$) to the scaling multiple-target Grover search, but is obtained through a different mechanism. The hope is that investigating the dynamics of population transfer on more realistic examples of quantum spin glasses, and better understanding the role that non-ergodic, extended states play, will lead to a new class of quantum algorithms for optimization and sampling.

6. Future Outlook

Since its birth as musings of Richard Feynman [156] and Yuri Manin [157], quantum computing has blossomed from speculative idea into one with solid theoretical foundations, inspiring feats of engineering that are taking quantum computing into a new era. Many mysteries remain, from the fundamental to the practical. Key questions include:

- From which quantum effects does the power of quantum computing arise, and how best to harness these effects for computational purposes?
How and when will quantum computers sufficiently large and robust to support the solution of application-scale problems be built?

How broad will the applications of quantum computing ultimately be?

The emergence of quantum information processors large and coherent enough to be beyond the power of the world’s largest supercomputers to simulate opens up new ways of working that will provide insight into the key questions in the field. How soon such processors arrive depend not only on hardware efforts, but also on the developing software ecosystem of algorithms and tools that make efficient use of quantum resources. Quantum computing work in the coming decades will require a different skill set and mindset that adds tool building and exploration of quantum algorithms through numerical experimentation to theoretical analysis that has been the predominant means of progress prior to the advent of quantum hardware of non-trivial size and coherence.

With respect to the breadth of applications, it is instructive to look at the classical case. For the vast majority of computations run on a supercomputer, there is no mathematical proof that the algorithm being run is the best possible, or even a mathematical proof that it is better than last year’s algorithm; the analysis of these algorithms on problem classes of interest is just too complex to carry out. Instead, algorithms are tested empirically, with practitioners comparing notes on their performance and formal competitions held, in SAT [158], machine learning [159], and planning [160], among others. Until recently this empirical approach was not possible for most quantum algorithms given the limited quantum hardware available and the exponential overhead in simulating the algorithms on supercomputers in the general case. The next decades, as the quantum hardware matures to support larger and more varied quantum algorithms, particularly quantum heuristic algorithms for which formal analysis is intractable on problem classes of interest, we strongly conjecture that the areas in which quantum computing is known to have an advantage will substantially broaden. After all, given the status in the classical case, what is the chance that most algorithms for which quantum computing provides a speed up are algorithms for which we can mathematically prove that they provide such a speed up? It seems quantum computers only significantly outperform classical computers on problems for which the analysis is simple enough to provide a mathematical proof, given that this standard of proof is rare even for classical algorithms for most computationally challenging real-world problems.

To understand the current status of the field, a historical perspective can be helpful. In 1972, under the guidance of Hans Mark, director of NASA Ames Research Center at the time, the “massively parallel” Illiac IV [161][162] computer, was brought to Ames. It consisted of sixty-four 64-bit processors and, with a 50 MFLOP peak, was the fastest computer in the world at the time. Finding problems that demonstrated the potential of such parallel computers was challenging. It was not until 1975 that a usable service could be offered, but at a slower rate of operations [163], and proponents had to continue to field questions as to whether such machines could ever compete with state-of-the-art approaches at the time, such as wind tunnels. The overwhelming progress of the succeeding decades makes it hard for us not to smile at these doubts in the early 70s. The NASA QuAIL team looks forward to working with other teams around the world to realize the potential of quantum computing building on our work to date from fundamental theory, through tools, to exploration of applications. If quantum computing has even a fraction of the success of massively parallel computers, its practical impact on the future will be great, with diverse applications including those beyond what we can imagine today.
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About the NASA QuAIL team

The mandate of the NASA’s Quantum Artificial Intelligence Laboratory (QuAIL) is to assess the potential impact of quantum computers on computational problems that will be faced by NASA missions in decades to come. Successful and increasingly ambitious NASA missions require the solution of myriad challenging computational problems. QuAIL’s home, the NASA Ames Research Center, has long had one of the most powerful supercomputers in the world. This work requires highly interdisciplinary teams of theoretical and experimental physicists, computer scientists, and domain experts in the various application domains. The QuAIL team members, physicists, computer scientists, and mathematicians, come from a wide variety of backgrounds, with complementary expertise. The team has strong collaborations with application domain experts in and outside NASA, and with groups implementing quantum hardware, including Google and Rigetti with whom NASA has Space Act Agreements. NASA’s QuAIL team has particular expertise in efficient utilization of near-term quantum computing hardware to evaluate the potential impact of quantum computing.

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