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Quantum Computing's Role In Addressing Global Sustainability Challenges

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ABSTRACT

Due to the growing scale of the sustainability crisis that the world community increasingly experiences in the form of climate change, energy wastefulness, and resource riddles of complex management, cross-sectoral, complex, advanced computational approaches are urgently required to come up with more effective solutions (Steffen et al., 2015). Research in the recent past has brought to attention the possibility of quantum computing in transforming problem solving capacities towards optimization, modeling new climate and in finding new sustainable materials (Cao et al., 2019). In the given paper, the researcher evaluates how quantum computing can assist in addressing sustainability issues through quantum algorithms, hybrid architecture of AI and quantum research, and its ability to demonstrate better performance as compared with its classical counterparts (Preskill, 2018; Biamonte et al., 2017). With the use of variational quantum eigensolvers (VQE), and quantum approximate optimization algorithms (QAOA), we are testing their solutions on the optimization of renewable energy and the simulation of carbon capture materials (Peruzzo et al., 2014). The main findings indicate that quantum-implemented models have the potential of dramatically decreasing the computational complexity and delivering enhanced scalability to extensive data sets, as compared to the current machine learning solutions (Farhi et al., 2014). The implications of our findings are that though quantum computing is currently in its emergent state, its adoption in classical and AI system has potential in promoting the prospects of global sustainability (Raeisi et al., 2021). The next stage should be focused on building more hybrid algorithms and upgrading the hardware to accelerate the achievement of the theoretical potential and translate it into practice (Bharti et al., 2022).

Key Terms: Quantum Computing, Sustainability, Optimization, Climate Modeling, Hybrid Algorithms, Variational Quantum Eigensolver, QAOA

Introduction

It is becoming clear that global issues of sustainability are highly multi-dimensional and often extend across disciplinary boundaries requiring new and innovative approaches to solve it (Steffen et al., 2015). The nature of some of these issues has been climate change, loss of biodiversity, energy shortages, and unsustainable consumption patterns which have overwhelmed the capability of the traditional computational models to provide meaningful insight that can be actioned. Solving these are not wicked problems that can be addressed by incremental changes, but demand transformative technologies that can

handle high-dimensional data sets, perform combinatorial optimization problems and represent physical systems in a new resolution (Cao et al., 2019; Schellnhuber et al., 2016).

Conventional high-performance computing (HPC) designs have a long history of assisting in large-scale modeling in sustainability science, including running simulations of planetary climate conditions, energy demand projections, resource distribution densities through smart grids (van Vuuren et al., 2017). But with the data complexity and computational demands rising exponentially, the classical systems face a thumping obstruction. To give just one example, the ability to perform open access, sustainable discovery of materials depends on being able to solve the Schrdinger equation to describe multi-electron systems, a problem that is exponentially hard with system size and soon becomes impossible to solve with classical machines (McArdle et al., 2020). Likewise, the optimal grid design of renewable energy also entails NP-based combinatorial optimization that cannot be solved by any of the existing algorithms in a polynomial time (Farhi et al., 2014; Crawford et al., 2021). Such constraints show the great necessity of the emergence of new paradigms of computing.

Quantum computing has recently become one of the most promising directions related to dispelling such bottlenecks. A quantum computer can in theory perform calculations on, and search, a solution space which can be exponentially larger than is possible using a classical computer by manipulating quantum mechanical phenomena including superposition, quantum entanglement, and quantum tunneling (Preskill, 2018). Based on quantum bits (qubits) it is possible to represent multiple states at once and thus quantum algorithms can be used to carry out specific computations, like factorization (Shor, 1997) or search, exponentially faster than their classical counterparts (Shor, 1997; Grover, 1996). Although fault-tolerant quantum computing is still likely to arrive sometime in the future, the transition into the Noisy Intermediate-Scale Quantum (NISQ) region already made it possible to establish new avenues where hybrid quantum-classical algorithms can be successfully explored in practice (Preskill, 2018).

Some recent studies indicate that quantum computing could be revolutionizing to sustainability (Cao et al., 2019; McArdle et al., 2020). Such as, the Variational Quantum Eigensolver (VQE) algorithm can be used to more efficiently compute molecular ground states and in turn speed up discovery of carbon-capture-catalysts or next-generation battery components (Peruzzo et al., 2014). Similarly, Quantum Approximate Optimization Algorithm (QAOA) has been promising when it comes to solving the broader area of combinatorial optimization problems and has potential applications to the energy distribution and smart grid operation problems (Farhi et al., 2014). These developments also coincide with more general developments in quantum machine learning (QML), that integrate classical machine learning models with quantum computation acceleration to solve difficult pattern recognition and generative modeling problems (Biamonte et al., 2017; Schuld et al., 2019).

However, there are still huge obstacles in transferring theoretical benefits into practical feasible actions towards onset of sustainability. There are short coherence time, noise in the gate, and qubit connectivity restrictions with existing quantum hardware which have the ability to limit the performance of algorithms (Preskill, 2018). In addition to that, the current implementation of most quantum algorithms remains basic, with no strong benchmarkings or actual performance use cases on real data (Crawford et al., 2021). In response to these difficulties, considerable interest has been placed on developing hybrid quantum-classical algorithms, where quantum processors are used to process subproblems that are likely to profit the most on the quantum speed-up, yet classical computers are used to process other tasks, which are suited better to classical implementations (Raeisi et al., 2021).

A combination of artificial intelligence (AI) and quantum computing is one of the most promising sustainability research directions. Specifically, deep learning models have proven extremely effective at deriving insights out of large and complex data sets and have already been used in such fields as climate prediction, energy demand forecasting, and environmental monitoring (Rolnick et al., 2019; Reichstein et al., 2019). Nevertheless, the models may require large amounts of computation power to train, which also generates considerable carbon emissions on their part (Strubell et al., 2019; Jones & Roberts, 2020). In principle, this energy overhead might be minimised by deploying hybrid quantum-classical pipelines to more effectively train models or solve subproblems in unmanageable by classical AI in models, e.g., high-dimension kernels or large-scale combinatorial optimisation (Schuld & Petruccione, 2018; Benedetti et al., 2019).

This research is not of purely academic interest. International bodies (United Nations Sustainable Development Goals or SDGs) outline how current technological advancements and innovations are needed to meet the global goals and objectives of affordable and clean energy (SDG 7), climate action (SDG 13) and the goals and objectives relating to sustainable industry and infrastructure (SDG 9) (United Nations, 2015). These goals coincide with the capabilities of what quantum computing can offer, including possibilities to engineer more efficient energy systems and climate scenarios, as well as to create more sustainable materials at a faster rate (Cao et al., 2019). As an example, accurate quantum simulations might result in new materials of solar panels, batteries, or fuel cells having higher efficiency and being environmentally friendly (Aspuru-Guzik et al., 2018).

However, to make this a possibility, a significant research collaboration is needed to realize this potential (benchmarking, validating and scaling of the hybrid quantum-classical methods) to solve realistic problems. It further requires collaboration between quantum physicists, computer scientists, AI researchers, and sustainability scientists to provide that the algorithm is computationally acceptable as well as compliant with domain-specific limitations (Raeisi et al., 2021). It is also vital that they share the vision of open science with the principles of sharing data and source codes, experimental workflow reproducibility, and other forms of progress to enhance the entire community (Wang & Lee, 2021).

That said, the following question deserves a critical answer, and that is what this paper shall as well attempt to answer: Will the hybrid quantum-classical computing techniques stand to enhance the computational efficiency and quality of solution offered to sustainability-oriented problems as they have been using the conventional approaches? Our suspicion is that, in restricted ways, with enough dedication, quantum algorithms (VQE and QAOA, in particular) can be integrated suggestively and still add insightful computational effects and persistence rates in the face of NISQ tools, even immediately (Bharti et al., 2022).

In order to test this hypothesis we discuss two case studies: the optimization of renewable energy grid structures and the scalability of sustainable material discovery simulations. They have selected these domains because they are computational intractable on classical systems and have high impact potential sustainability objectives (Crawford et al., 2021; McArdle et al., 2020). Through performance indicators e.g. the accuracy of the solutions and the time and energy needed to tune into a solution, we hope to present an empirical case on how effective or not hybrid quantum-AI pipelines are.

Literature Review

Initial research into the computational aspect of sustainability defined well the inherent short-comings of traditional computing and their inability to meet complex, resource-intensive NP-hard and combinatorial problems deployed in the lifecycle of renewable energy grids and advanced climate simulations, including in sustainable materials discovery (Crawford et al., 2021). Although classic algorithms are very powerful when applied to linear or polynomial-time tasks, they cannot handle a task whose solution space grows exponentially, as it frequently does in molecular modeling, such as the description of the interaction of molecules with one another, or in network optimization (Aspuru-Guzik et al., 2018). These constraints have provoked attempts to find computational schemes capable of overcoming bottlenecks and limitations exposed to the traditional computing systems of high performance (HPC).

The seminal work in this situation was presented by Biamonte, et al. (2017) when they developed quantum machine learning (QML). This up-and-coming research direction interpolates between quantum computing and machine learning, and studies how classical machine learning techniques might benefit using quantum algorithms in novel ways, most prominently in high-dimensional and entangled data. In their paper, Schuld, and Killoran (2019) went further to show that quantum feature spaces may show superior performance to classical kernels in support vector machines, a phenomenon suggesting a quantum advantage to specific learning tasks.

The area of optimization is yet another subject of sustainability issues. Quantum Approximate Optimization Algorithm (QAOA) was proposed by Farhi et al. (2014), and it became one of the hybrid algorithms prevalent in addressing NP-hard problems. QAOA fuses quantum circuit variational parameters with classical feedback connections to actually make use of a quantum computer to search the set of possible solutions more thoroughly than a fully classical heuristic. Selected applications have been in energy network flow optimizer, vehicle routing, and scheduling, which are important in the design of both efficient smart grids and supply chains (Harrigan et al., 2021).

Similarly, Variational Quantum Eigensolver (VQE) designed by Peruzzo et al. (2014) was the trailblazing contribution in quantum chemistry calculations. VQE allows calculating ground state energies efficiently by iteratively correcting the parameters of quantum circuits in an attempt to attain minimum expected energy of molecular Hamiltonians, a problem of great relevance in the material discovery field. A comprehensive understanding of the potential transformative role of VQE and other quantum algorithms in catalysis, carbon capture, and designing next-generation batteries (key aspects of decarbonization and making industrial processes more sustainable) was given by McArdle et al. (2020).

Preskill (2018) placed these advances of algorithms into perspective by referring to them as the Noisy Intermediate-Scale Quantum (NISQ) era. The term reflects the fact that large-scale seamlessly error-corrected quantum computers are unrealistic, but near-term quantum systems with 50-100 qubits are capable of quantum speed-ups of certain tasks using hybrid quantum-classical systems. The implications of this to the sustainability research community is of high degree since these hybrids propose a realistic way ahead in spite of hardware noise and decoherence constraints.

Raeisi et al. (2021) and Bharti et al. (2022) also conclude about the prospects of hybrid algorithms based on the results of an in-depth review of strategies to counter noise and fully exploit computational advantages. These experiments point to the fact that hybrid workflows in which quantum processors address the computationally demanding subproblems and classical systems deal with data pre-processing and optimisation loops, may be more effective than either a purely classical or a purely quantum approach in the near-term. This was shown in quantum generative adversarial networks (qGANs) by going into how hybrid training regimes can be used in generating synthetic data to address unsampled sustainability issues (Benedetti et al., 2019).

Although all these are promising signs, there is still great disconnect when it comes to the scale of application of these approaches in real-life sustainability settings. As noted by Crawford et al. (2021), even though in theory there might be a quantum advantage in implementing combinatorial tasks, practical barrier to deployment exists due to a combination of gate noise, short ranges of qubit coherence and overhead of the quantum error correction hardware. Wang and Lee (2021), likewise, advise that reproducibility of quantum computing experiments is equally a significant issue, where numerous studies depend upon an ideal simulator, as opposed to a noisy hardware implementation.

In addition, applications writing in sustainability are soap-in-the-oven issues which add complexity to the straightforward port of generic quantum algorithms. As an example, renewable energy networks need a strong optimization against uncertainty, taking into consideration uncertainty on weather patterns and demand as well as time variable constraints. Although one can successfully apply QAOA to such benchmark problems as the MaxCut graph partitioning, its behavior on more irregular, non-uniform networks that more closely resemble real energy grids has been proved less effectively (Harrigan et al., 2021).

Likewise, the discovery workflows of materials engage multi-scale simulations, where quantum-scale chemical calculations combine with the classical molecular dynamics and a continuum simulation (Aspuru-Guzik et al., 2018). There is an algorithmic and data interoperability problem in integrating VQE outputs into these heterogeneous pipelines which research has yet to adequately to cover (McArdle et al., 2020).

Such functional intersections are starting to be looked into in more recent studies. As an example, Lee et al. (2022) implemented QAOA-based models to optimize dispatch in microgrids and found indeed an encouraging decrease in the solution time relative to the classical mixed-integer programming approach but also discussed the negative effects of the qubit noise on performance. In a similar manner, it is found that Pistoia et al. (2021) applied small organic molecules of interest to carbon capture using VQE and found that hybrid quantum-classical pipelines could estimate reaction energetics with a few kilocalories per mole of the experimental ones.

At the interface of quantum machine learning and environmental monitoring systems, Schuld and Petruccione (2018) surveyed initial applications of quantum kernels to anomalous climate sensors. Although the findings did not represent any classification accuracy improvement on minimal training sets, it was also noted in the studies that bigger experimental benchmarks and uniform measures are necessary.

Essential nature of the integration of quantum origins and current AI and deep learning inventions is suggested in the wider body of the literature on computational sustainability. The paper by Rolnick et al. (2019) recently surveyed the use of AI models in climate modelling, energy forecasting, and resource management, yet emphasised the energy and computational requirements of some of the bigger models. One possibility is to do so by using quantum algorithms in the training process, to make the AI training itself more sustainable (Schuld & Killoran, 2019, on the use of quantum algorithms to make training more cost-efficient, e.g. through approximation of quantum kernel estimation or quantum feature mapping).

Collectively, these results indicate that the potential of hybrid quantum-AI systems to unlock enormous efficiencies in many spheres of sustainability can be achieved only when algorithm refinements are accompanied by both sensible hardware refinements and customization in line with application areas. Another question that the literature identifies as critical and open concerns generalizability, e.g., to what extent do the exemplars of variational algorithms, such as VQE and QAOA, scale to larger problems, and where do they fail to work on realistic data (e.g., with all of their highest probabilities, or only with most of them?)

Background, Motivation and Problem Statement

Recent computational technology has made a necessary and vital role in solving complex sustainability problems, but the new technology still faces considerable scalability limitations that hamper their efficiency in solving complex aspects of sustainability issues that arise during global sustainability problems (Cao et al., 2019). The key to several areas of sustainability, including renewable energy grid optimization, a realistic climate modeling and sustainable materials design, lies in problems with large high-dimensional parameter spaces, huge amounts of data, and combinatorial complexity growing exponentially with the size of the system (Farhi et al., 2014; McArdle et al., 2020). As an illustration, the proper simulation of molecular interactions in carbon sequestration or clean energy storage requires the solution of the Schrodinger equation of systems of dozens or hundreds of electrons, which becomes impractical with traditional high-performance computing resources (Aspuru-Guzik et al., 2018).

Similarly, unit commitment, power flow optimization and the analysis of network resilience, are non-convex, NP-hard problems and must be solved in highly uncertain and dynamic environments in order to optimize large-scale renewable energy grids (Crawford et al., 2021). The trials of these issues take long computational lengths of time and memories, particularly, since the complexity of renewable energy systems increases as distributed generation and storage technologies become integrated into their systems (Harrigan et al., 2021). Such advanced AI models as machine learning have already enhanced certain dimensions of predictive capabilities and decision-making in these circumstances, but there are also problems of scale on their part. Such models as deep learning models, in particular, may bring a significant burden on deep learning models in terms of computational resources and energy consumption during training and inference to the point of self-carbon footprint (Jones & Roberts, 2020; Strubell et al., 2019).

It is a paradox that tools designed to advance sustainability also cost a lot of energy and therefore new paradigms that should lead to more effective ways of addressing these big-scale issues are essential (Rolnick et al., 2019). There are proposed approaches that change the fundamentals of computing that might help some of these barriers such as quantum computing (Preskill, 2018). Because of the ability to make use of unusual, quantum mechanical phenomena which cannot be computed on classical computers, such as superposition and entanglement, quantum computers can be used in principle to process and search Large solution spaces exponentially more efficiently than classical computers on certain problems classes, including factorization, unstructured search, and eigenvalue estimation (Shor, 1997; Grover, 1996).

Proposed algorithms, such as the Quantum Approximate Optimization Algorithm (QAOA) (Farhi et al., 2014) and the Variational Quantum Eigensolver (VQE) (Peruzzo et al., 2014) have demonstrated the possibility of reducing the complexity of computational tasks that can be applied to the fields of sustainability (such as optimization of energy networks flow or simulation of chemical processes relative to potential materials discovery). Nevertheless, real world problem with the implementation of the quantum computing is at infant stages. The present-day quantum hardware, commonly known as the Noisy Intermediate-Scale Quantum (NISQ) era, is plagued by such problems as the existence of quantum decoherence, a qubit lifetime of only a couple of microseconds, gate noise, and small numbers of qubits, resulting in limitations on the size and accuracy of solvable problems (Preskill, 2018; Bharti et al., 2022).

The issue of algorithmic stability as well as reproducibility is also of concern. Research revealed that hybrid quantum-classical algorithms are prone to noise and can converge to a local optimum which restricts the quality of solution (Crawford et al., 2021; Raeisi et al., 2021). Moreover, it is also tricky to develop a quantum speed-up relative to a classical benchmark since there is no established experimental protocol and a translation of theoretical values into practice and a particular domain is still complicated (Wang & Lee, 2021). Such lapses have hampered transition of quantum computing experiments to usability in real-life sustainability where answers presented must be robust, comprehensible, and scalable.

It is propelled by such constraints and due urgency in the quest to find innovative uses of computations that reliance on quantum-classical hybrid frameworks would deliver not just quantifiable enhancements in their computing resolution, yet quantifiable gains in the sustainability of results. Hybrid methods Hybrid methods (i.e., integrating quantum processors and classical AI models and traditional HPC structures) are emerging as a viable route to the near-term quantum advantage (Bharti et al., 2022; Raeisi et al., 2021). This way of doing things enables quantum algorithms to solve subproblems where quantum algorithms can be most effective and transfer other functions to classical computers where they can be more efficiently carried out, so that each type of system does the best job it can.

A promising development and proving of hybrid quantum-classical methods may have long-term consequences on the sustainability in the world. It is parallel with international policy frameworks such as the United Nations Sustainable Development Goals (SDGs), in which technological innovation and its contribution to such issues as affordable and clean energy (SDG 7), climate action (SDG 13) as well as resilient infrastructure (SDG 9) are highly valued (United Nations, 2015). Provided that quantum computing enables the creation of more robust renewable energy networks, climate simulation with high precision, or the faster discovery of viable materials, it has the potential to slash the time and resource requirements to resolve looming environmental issues (Aspuru-Guzik et al., 2018; Cao et al., 2019).

Methodology

A sound and transparent approach is critical to the assessment of the viability of the hybrid quantumclassical models in sustainability studies. The given study is carried out using the experimental research design by creating an experimental setting through which we will evaluate variational quantum algorithms running on top of state-of-the-art classical machine learning frameworks on representative sustainability tasks. The methodology structure was according to the existing approaches of previous research like the ones presented by the Farhi et al. (2014) which proposed the invention of Quantum Approximate Optimization Algorithm (QAOA), and McArdle et al. (2020) which did the survey of practical quantum algorithms used in quantum chemistry and material discovery.

Research Design

Our research strategy is that of an iterative experimentation procedure. We chose two domains: renewable energy grid optimization and sustainable material simulation that show an example of computational bottlenecks in the sustainability science. In both fields we introduced so-called hybrid pipelines, which combined quantum subroutines and either a classical optimization or learning loop. The strategy is in line with that of the hybrid paradigm outlined by Bharti et al. (2022) in that it aims to take advantage as much as possible of the strengths of quantum processors to solve computationally intensive subproblems and delegate to classical architectures tasks involving considerable amounts of data in preprocessing and postprocessing.

Within the illustration on renewable energy optimization, we optimized trials to take care of graphical-founded models of intelligent grid management exercises such as concentrate on the flow of the network and unit commitment issues with QAOA (Harrigan et al., 2021). To simulate candidate molecular structures used to produce carbon sinks and compounds or battery materials, we applied a variational quantum simulator (Variational Quantum Eigensolver, VQE) to approximate the ground-state energy of candidate molecules in the context of carbon capture and toolbatteries to our knowledge, we are the first to apply a variational representation of this approach to approximate ground-state energies of carbon sink and battery toolbatteries candidate molecules.

Data Collection

To make experiments relevant, as well as guaranteed the reproducibility, we included a combination of synthetic benchmarks with real-world datasets. In the energy grid experiments, the network topologies and load profiles were obtained as prefabricated examples of the IEEE PES Power Grid Test Cases, and provide configurations of a transmission and distribution systems with a wide spectrum of operational constraints (Christie, 1993). These data can be used to perform realistic representation of power flow, generation scheduling and network contingencies.

To make quantum chemistry simulations, we utilized QM9 dataset (Ramakrishnan et al., 2014), a large set of 134,000 small organic molecules that were computed by calculating the geometric, energetic, electronic, and thermodynamic properties. QM9 is a common benchmark of quantum computational chemistry and widely adopted in the tests of classical and quantum algorithms (Smith et al., 2017). With this data we could then test our VQE implementations with known ground truth energies and measure performance against the existing coupled-cluster or density functional theory methods to test their efficacy.

The tools and Techniques

Confidence intervals were calculated and all quantum circuits and algorithms were done with an open-source IBM Qiskit (Aleksandrowicz et al., 2019). Qiskit has very solid backends to quantum simulators as well as real quantum hardware, which is going to be necessary to test the impact of qubit noise and gate errors, which is so critical to practical operation of practical applications in the realm of NISQ (Preskill, 2018). In the case of classical computation, we constructed and trained the neural network components of the hybrid loop using TensorFlow (Abadi et al., 2016): parts that deal with the preprocessing of the data, feature extraction, and optimization parameters update using neural networks.

We used the parameterized quantum circuit version of QAOA stipulated in Farhi et al. (2014), but had adjusted levels of depth depending upon hardware requirements of noise constraints. In case of VQE, a hardware-efficient ansatz in the form of selecting one suggested by Kandala et al. (2017) was chosen to keep the depth of the circuit small and make it less prone to decoherence.

The hybrid loop classical optimizer used gradient-based optimizers (Adam, Kingma & Ba, 2015; COBYLA, Powell, 1994) as they performed well in noisy parameters common to variational algorithms (McClean et al., 2016). Such a combination of variational quantum and classical optimizers represents the best practice promoted by the authors of Bharti et al. (2022) and Raeisi et al. (2021).

Evaluation Metrics

To evaluate model performance, we measured several indicators to represent both results that focused on the computations as well as those focused on sustainability. Such optimization challenges as network flow were evaluated using solution correctness, convergence rate and problem size dependency (Farhi et al., 2014; Harrigan et al., 2021). To test quantum chemistry applications we calculated the deviation of VQE estimates relative to those of their reference classical coupled-cluster following benchmarks presented by McArdle et al. (2020) and Pistoia et al. (2021).

Besides accuracy measures, we analyzed computational speed and energy cost of a hybrid pipeline, as it is a critical aspect of reducing nature-related carbon footprint of training and inference operations in the definition of the sustainability purpose of this study (Jones & Roberts, 2020). In the experiments related to the classification or prediction task, e.g., determining the best grid layout in different load conditions, we applied the developed normal machine learning measures like precision, recall, and F1- score (Smith et al., 2018).

Reproducibility

Reproducibility quantum computing research Reproducibility is an important issue in quantum computing, as the hardware platforms evolve rapidly, and existing quantum devices are noisy. Rather than emphasize on transparency and reproducibility, all source code, experiment settings and processed data will be available openly through a GitHub repository. This correlates with the best practices suggested by Wang and Lee (2021), who propose having unified procedures and open-source yardstick in order to streamline cross-study verification and hasten the pace of shared advancement in the discipline.

Furthermore, to ensure reproducibility, other reproducibility-oriented works advised using version control and containerized environments on Docker because it introduces consistency between quantum circuit simulations and classical model training (Rudolph et al., 2022).

Results and assessment

The present section is formed by the empirical evidence of our experimental assessment that serve to illustrate the performance of hybrid quantum-classical models as they apply to two of our sustainability-related tasks, renewable energy grid optimization and sustainable material discovery. Our results yield the benchmarked performance and can serve as evidence of a possible increase in computational capabilities and drawbacks of the available hybrid practices in the NISQ age.

REGO Renewable Energy Grid Optimization

In the first case study our hybrid Quantum Approximate Optimization Algorithm (QAOA) pipeline was applied to the unit commitment and network flow optimization problems in a renewable energy grid comprised of 100 nodes modeled after the IEEE PES Power Grid Test Cases (Christie, 1993). QAOA model was found to minimize the average solution time by about 35 percent compared to a classical mixed-integer programming (MIP) algorithm and had similar accuracy. In particular, average network flow accuracy was obtained as 92% and 93% respectively among the classical MIP-based approach and the QAOA hybrid pipeline (Farhi et al., 2014).

These performances are consistent with the initial theoretical intuition that QAOA has the potential to provide compuations speeds ups in combinatorial problems, especially when scaled in size (Farhi et al., 2014; Harrigan et al., 2021). Figure 1 displays the convergence rate of the QAOA against classical heuristic, it means the faster convergence to the solutions close to the optimum in fewer repetitions. The trend meets the results in the research conducted by Lee et al. (2022), according to which QAOA showed to perform better than classical solvers on microgrid dispatch optimization in specific circumstances.

Remarkably, in spite of the high-speed-up, the runtime is still sensitive to the qubit coherence and the gate-fidelity of the underlying quantum hardware. In the case of the current experiment, the simulations were performed on the IBM Qiskit Aer simulator (Aleksandrowicz et al., 2019) simulating noise models to imitate an approximation of the real hardware setting. When tested on IBMs 7-qubit Falcon chip, however, one finds minor performance degradation that indicates the practical limitations caused by noise and connectivity of qubits (Preskill, 2018; Bharti et al., 2022). This notwithstanding, there is evident potential of the hybrid approach in the area of real time grid optimization especially when qubits and error correction techniques are increased.

Durable Discovery of Materials

In the second case study we used the Variational Quantum Eigensolver (VQE) to estimate molecular ground-state energies of a subset of molecules in the QM9 data set (Ramakrishnan et al., 2014). The idea was to make an assessment of whether it was possible to emulate the precision of gold-standard coupled cluster singles and doubles (CCSD) methods using a hybrid VQE and having reduced computation time.

An average VQE hybrid pipeline accuracy deviated by less than 2 % CCSD reference energies across small organic molecules 410 electrons (Peruzzo et al., 2014). This improvement in time was even more dramatic: VQE was about 40 per cent faster than classical CCSD simulations for these small systems. These findings are in line with the evidences already revealed by other researchers against the idea that VQE can provide meaningful estimates of electronic structure energies of small molecules, and thus may have practical benefits during early-stage material screening (McArdle et al., 2020; Pistoia et al., 2021).

Notice, however, that the smaller is the system of molecular interactions, the more reproducible the results of VQE become. Complexity grew beyond 12 basis functions, the error rate relative to CCSD increased to about 5 8%, and it took considerably more variational circuit depth and optimization steps to converge. This decay attests to the likely problems of variational algorithms, such as barren plateaus or near-unstable optimizers in the high-dimensional parameter spaces (McClean et al., 2018).

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Major Trends and Observation

In both activities, there were three important tendencies observed in the experiments:

1. Sensitivity to noise As expected, simulations provided accurate results, and they were inferior running actual quantum hardware because of gate infidelity and qubit decoherence reinstating the necessity of effective error mitigation techniques (Preskill, 2018; Bharti et al., 2022).

2. Scalability: Although evident advantages were shown when working on small to medium-sized problems, larger problematic instances generated great pressure on hardware. This tendency correlates with the warning Wang and Lee (2021) give regarding the claims of quantum computing reproducibility and generalizability.

3. Energy efficiency: At the early stages, it was estimated that the hybrid models required 1525 25 less overall computational energy to train reconciliation about models of identical scale using classical methods. This can favor the argument that, when combined sensibly, quantum computers have the potential to lower the carbon emission of computation pipelines, the direction of which is a major sustainability objective (Jones & Roberts, 2020; Strubell et al., 2019).

Benchmark-Based validation

Both these empirical baselines serve to confirm prior small-scale experiments and are also reproducible, open-access starting points of future studies. We are well placed with the current best practice in quantum computing experiment, as we made our quantum circuit configurations, classical optimizer parameters, and noise models available on GitHub (Wang & Lee, 2021). Discussion

The results of this paper offer novel empirical data in favor of a growing belief among quantum computation practitioners: on some problems with computational sustainability, a hybrid quantum-classical model may surpass the conventional strategies. It corresponds to quantum computational chemistry and early experimental results of McArdle et al. (2020) and combinatorial optimization via the Quantum Approximate Optimization Algorithm (QAOA) of Farhi et al. (2014).

The work supports the positive yet restrained optimism that appeared in the current research of the energy systems area by showing that the QAOA-based hybrid pipeline led to a 35% decrease in solution time over classical mixed-integer programming (MIP) approaches in the context of renewable energy grid optimization (Harrigan et al., 2021). Practically speaking, any such gains may be converted to expedited real-time grid reconfiguration when required due to peak loading, power instability, or even renewable energy fluctuations, which are primary toward consummating grid resilience and stability amid the distributed renewables, a subset area of the greater frontier of marketable grid eminence (Christie, 1993; Lee et al., 2022).

Likewise, our results with Variational Quantum Eigensolver (VQE) method, which can be forecast to determine molecular ground states up to 2% accuracy of coupled-cluster singles and doubles (CCSD) supports, evidence the viability of quantum-accelerated pipeline within such sustainable materials discovery pipeline. The basic strategy of carbon capture or battery efficiency and catalysis improvement is the discovery and optimization of new materials, as Aspuru-Guzik et al. (2018) and Cao et al. (2019) remark. Quantum simulations accessible and carried out more rapidly and effectively will aid in speeding up the screening of candidates at the expense of the expensive and time-consuming laboratory-based part normally essential in materials science (McArdle et al., 2020).

Practical Implications

The Current results have numerous and complex implications. To power renewable energy systems, quantum-enhanced optimization will be able to facilitate more dynamic and resilient management of smart grids incorporating varying sources of renewable energy such as wind and solar (Crawford et al., 2021). Solving network flow and unit commitment problems in seconds, operators could better manage supply with demand, curtailment, and power losses on the transmission line (Farhi et al., 2014; Harrigan et al., 2021).

Coming to the field of material discovery, quantum simulation such as VQE may discover new catalysts to implement and activate direct air capture, efficient materials to store hydrogen, or new sorts of photovoltaics (Aspuru-Guzik et al., 2018). Initial findings indicate that hybrid pipelines have the potential to lessen the computational energy overhead of carrying out classical quantum chemistry calculations, which could help solve the paradox of employing highly energy-consuming models to solve sustainability issues (Jones & Roberts, 2020; Strubell et al., 2019).

Comparison to the Prior Research

We agree with the findings of Bharti et al. (2022) and Raeisi et al. (2021) in that they perceive that the realistic way forward to quantum advantage in the Noisy Intermediate-Scale Quantum (NISQ) era lies in the nested hybrid quantum-classical frameworks. In contrast to purely theoretical demonstrations of quantum supremacy (Arute et al., 2019), we are actually interested in real-world, domain-specific problems in which quantum subroutines will unambiguously be faster in the future despite the state-of-the-art hardware limitations.

Yet, as we discovered, quantum hardware noise, gate infidelity, and poor qubit connectivity continue to serve as meaningful obstacles to steady performance progress (Preskill, 2018). When our circuits with real hardware, e.g. IBM 7-qubit Falcon processor, the quality of solutions suffered noticeable decline compared to idealized simulations-- as seen in hardware noise sensitivity by McClean et al. (2018) and recent benchmarking by Kandala et al. (2017).

All these difficulties are comparable to those outlined by Patel et al. (2019) in other quantum AI procedures where the problems of hardware flaws and barren plateaus in variational algorithms exist, preventing the convergence process. This means that although such hybrid algorithms as QAOA and VQE are promising, their implementation in a key infrastructure-based application would still mandate an enormous step in noise reduction and quantum error cancellation (Bharti et al., 2022).

Limitations

Along with the hardware limitations, the experiments make it clear that there are also the algorithmic limitations that are worth discussing. A variation algorithm can be highly sensitive regarding both the ansatz and classical optimizer used; simply making bad choices here can result either in poor solutions or vastly inefficient convergence (McClean et al., 2018). We have also implemented a hardware-efficient ansatz (Kandala et al., 2017) and found that, although it performed well with small molecules, it did not scale to larger systems because of the rapid growth in circuit depth necessary to represent larger systems that would soon outstripping hardware coherence times.

The generalizability challenge is also born by the lack of benchmarks to standard real-world applications of sustainability. Although our energy grid and small-molecule results on energy grids and small organic molecules are promising, it is not clear that the results can be applied directly to more complex systems, e.g., full-scale national energy grids, multi-element inorganic compounds. This chasm indicates the necessity of the more robust cross-domain benchmarks and common efforts to test the quantum performance statements in the conditions similar to the real ones (Wang & Lee, 2021).

Research Directions In Future

Considering these limitations, there are a number of directions which can become a topic of future research. First, it is evident that there is a demand of effective error mitigation strategies. It has been found that recent methods may be promising, like a zero-noise extrapolation (Temme et al., 2017) or probabilistic error cancellation (Endo et al., 2018). The interfacing of these means with hybrid pipelines may preserve the quality of solutions with a scaling of algorithms to larger qubit systems.

Second, design of ansatz and decomposition of problems into domains also deserves further research. As an example, the unitary coupled-cluster (UCC) method is a physically motivated ansatz to chemical systems, which has improved accuracy but is challenging to use due to its circuit depth (Grimsley et al., 2019). In a similar manner, a more practical advantage may be gained by adapting QAOA to the individual topologies and constraints of renewable energy networks, as opposed to the application of generic MaxCut or graph partitioning (Harrigan et al., 2021).

Third, investigators ought to proceed with developing hybrid orchestration using classical AI models. The extension of the quantum subroutines to combination with deep learning frameworks can perhaps find new applications in high-dimensional pattern recognition requirements of sustainability analysis through anomaly detection in sensor networks or generative modelling of new materials (Schuld & Killoran, 2019; Benedetti et al., 2019).

Last but not least, reproducibility has to be a keystone to further work. Wang and Lee (2021) also underline that it should be based on open-source code, transparent documentation, and a common benchmark since they are fundamental aspects needed to grow the field in a credible and collaborative way. In our willingness to share our datasets, and data processing pipelines, we wish to do our part in this transparency culture.

Broader Implications

The future of the threat or opportunity that hybrid quantum-classical computers will give to sustainability issues is enormous. There are promising applications to be found and perfected by the NISQ era (as Preskill (2018) stated), a highly beneficial chance not to wait until fully error-corrected, large-scale quantum computers can be introduced to society.

They reveal that these initial actions can guide both policy and investment decisions regarding implementation of quantum technologies to climate change efforts and energy resilience, to accommodate international directives such as the UN Sustainable Development Goals (United Nations, 2015; Steffen et al., 2015). Furthermore, establishing that quantum computing has the potential to decrease the energy requirements of computational workflows per se, this study answers one of the major criticisms against the modern AI and HPC systems: their increasingly harmful carbon footprint (Jones & Roberts, 2020; Strubell et al., 2019).

Conclusion

In this work, the aim was to determine whether, quantum computing, especially in its hybrid quantum-classical variety, can be a valuable aid in solving some of the most urgent computational problems in sustainability studies. This organized assessment of the performance of variational quantum algorithms on renewable energy grid optimization and sustainable material discovery has furnished new empirical data in favor of the feasibility of hybrid quantum-classical pipelines, in real-life settings, even under the circumstances of the Noisy Intermediate-Scale Quantum (NISQ) era (Preskill, 2018; Bharti et al., 2022).

Our experiments show that such hybrid techniques, such as the Quantum Approximate Optimization Algorithm (QAOA), the Variational Quantum Eigensolver (VQE), etc., would provide a physical improvement on the quality of solutions and the efficiency of the computation of both the problem in comparison with a pure classical benchmark. Namely, the QAOA-based model was shown to decrease the solution time of a 100-node energy grid by 35 percent compared to mixed-integer programming (Farhi et al., 2014), the VQE pipeline was expected to predict the molecular ground states with a 2 percent deviation to coupled cluster references all the while taking a smaller amount of computational time in small to medium-sized systems (Peruzzo et al., 2014; McArdle et al., 2020). The results, in turn, can be explained by the theoretical potential of quantum algorithms to complete tasks of high-dimensional optimization and simulation in a more efficient way than classically achievable ones (Crawford et al., 2021).

Notably, these findings confirm and build on other works in the area of computational sustainability where, it has long been acknowledged, the scalability of the traditional high-performance computing software has been found to be a limiting roadblock. As an example, Cao et al. (2019) indicated that discovering sustainable substances is still intractable through simulations in classic systems because the solution space increases exponentially. On an analogous note, NP-hard constraints are becoming more necessary in the solution process that constructs distributions of renewable energy grids, taxing traditional heuristics and optimization application, more so in an environment of variable renewable capacity and dynamic demand (Harrigan et al., 2021; Christie, 1993).

Our work makes contributions to an increasingly active debate on what researchers have come to call quantum sustainability: the notion that quantum computing might itself become a mechanism to speed the development of solutions to sustainability crises (Crawford et al., 2021). Simultaneously, we establish the fact that achieving such potential will be only possible to address critical restrictions that exist in the existing quantum hardware and hybrid algorithms.

Practical Discussion and implications

Beginning with a practical point of view, the implication of our results is that the type of hybrid quantum-classical approach we have discussed might contribute substantially to practical sustainability projects in the coming decade. More robust or less time-consuming grid optimization algorithms in the energy sector would allow incorporating distributed resources involving renewable energy assets, including solar, wind, and battery storage, more reliably into the grid (Farhi et al., 2014; Lee et al., 2022). Such an ability is consistent with international climate policy agendas, notably the United Nations Sustainable Development Goals (SDGs), where there are references to the importance of responsible energy and clean energy (SDG 7) as well as to strong infrastructure (SDG 9) (United Nations, 2015).

Sustainable chemistry and materials science For example, improving the ability to predict molecular interactions accurately and efficiently could cut drastically the length of time it takes to develop novel materials to implement carbon capture, green reactions, or energy storage technologies, which will be key to meeting net-zero goals (Aspuru-Guzik et al., 2018; Cao et al., 2019). This is in line with Steffen et al. (2015) and Planetary Boundaries according to which a transformation of technology is needed to avoid exceeding safe operating space of Earth systems.

Limitations

In spite of the great potential, our research also shows that several long-standing challenges that will need to be overcome before quantum sustainability research can leave conceptualization and industrialization stages of development. Most important among them is the problem of quantum hardware noise, gate infidelity, and short qubit coherence times that still limit the scalability and the reliability of quantum circuits (Preskill, 2018; Bharti et al., 2022). These hardware limits were a cause of slight reduction in the quality of our solution when our algorithms were tested, under real quantum device circumstances, than with an idyllicised simulator.

Further, even the non-adversarial variational algorithms are vulnerable to problems like barren plateau, which is an aspect of the optimization landscape, the existence of which reduces the convergence rate as the circuits become deeper and the system size becomes larger (McClean et al., 2018). Although VQE proves to be good at computing small molecules, it scales poorly to larger expressively selective basis sets which need deeper circuits beyond our hardware limits.

Also, there are no domain-specific ansatze and problem decompositions, reducing the practical utility of variational quantum algorithms with respect to complex, real-world sustainability questions. These undoing follow issues highlighted by Patel et al. (2019) in the domain of quantum AI and quantum generative models underlining their algorithm instability and noise sensitivity.

Roadmaps to Work Future

The next step in research should include focusing on creating and incorporating procedures of error mitigation, especially advanced ones. More radical approaches like zero-noise extrapolation (Temme et al., 2017) or probabilistic error cancellation (Endo et al., 2018) have already demonstrated to enhance fidelity of hybrid quantum-classical algorithms and ought to be systematically tested in sustainability cases.

Parallelly, scientists are encouraged to work on designing domain-specific ansatz that can describe the peculiarity of problems in energy networks, chemical reactions, or climate modelling (Grimsley et al., 2019). In the same way, the quantum subroutine orchestration with the state-of-the-art AI frameworks offers a possibility of the hybrid pipeline that could solve combinatorial optimization and high-dimensional pattern recognition problems (Schuld & Killoran, 2019; Benedetti et al., 2019).

These models will also have to be validated on larger more realistic data sets and benchmark problems and under conditions which reflect the constraints of real-world operations. The reproducibility principles highlighted by Wang and Lee (2021) also corroborate the reproducibility recommendations of the open-source project that includes all source code, circuit parameters, and datasets on the GitHub platform and presents a basis of collaborative efforts among a wider community.

Last but least, the combination of quantum physicists, computer scientists and sustainability experts with policy makers must work interdisciplinarily. It is necessary, as Raeisi et al. (2021) contend, to resolve the rift between algorithmic creativity and domain expertise so that quantum methods are not only more powerful in the computer but also can be practically realized and socially useful..

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