Quantum Computing and Sustainable Development: What Are the Benefits?

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Abstract. This paper studies the use of quantum computing to disrupt serious problems in a sustainable development space. In our view, the quantum algorithms can disrupt studies related to carbon capture, renewable energy optimization and sustainable agriculture (such as Variational Quantum Eigensolver and Quantum Approximate Optimization Algorithm). We demonstrate that quantum after a broad underlining of existing studies and theoretical avenues has the potential to have practical, even expedited pathways for attaining multiple goals on United Nations Sustainable Development Goals list. It covers the mathematics behind these quantum algorithms, and discusses case studies that investigate their applications as well as ethical consideration and future directions. The case for quantum computing as a technology solution to our sustainable future: An evidence-based perspective is expected to be strong.

1 Introduction

The reported systems threatening global sustainable development and the articulation of this commitment through 17 Sustainable Development Goals (SDGs) by United Nations prompts a requirement for discovering effective solutions to complex, interdependent issues such as climate change, resources scarcity, biodiversity loss and energy security [1]. Classical computing has greatly contributed to the foundation of scientific and technological progress, yet many of today's key challenges in sustainability span problems in which significant computational resources underpin their complexity: from searching for high-throughput materials discovery related to carbon bonding, through designing global resiliency energy grids, or optimizing supply chains on an international scale [2].

The quantum computing is an emerging paradigm based on the principles of quantum mechanics that offers a fundamentally different approach to computation. Quantum computers have the potential to use phenomena such as superposition, entanglement and quantum interference to process information [3] and solve certain problem classes exponentially faster than their classical counterparts. This distinctive computational power leads to completely new opportunities for discovery in science and engineering, pattern recognition, behaviour optimisation across many fields directly applicable to the sustainable development goals.

This paper provides a much deeper exploration of how quantum computing can be used to improve sustainable development (SD). We consider two major areas which it is expected that quantum algorithms will have a large impact on this: molecular simulation for the discovery of advanced materials, and combinatorial optimization solving complex systems. In particular, we will further elaborate in how the Variational Quantum Eigensolver (VQE) has been employed to design new materials with superior properties for carbon capture and sustainable chemistry as well as using of the Quantum Approximate Optimization Algorithm (QAOA) to optimize renewable energy grids logistics, and resource allocation. It likely makes sense to organize the application of quantum computing in relation to a broader conceptual framework relevant for sustainable development initiatives, as presented conceptually here (illustrated by figure 1).

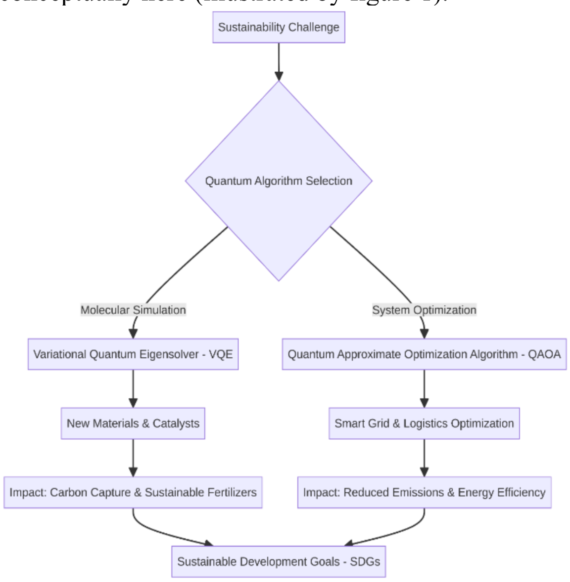

Fig. 1. A conceptual diagram explaining how quantum algorithms can be applied to sustainability challenges.

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In the following sections will explain how VQE and QAOA works, with a thorough description of its theoretical foundations and mathematical formalism. Then, together, we will provide a full overview of the advantages in performance and potential applications of these quantum methods to real-world problems in sustainability areas that have been published within recent works. We will first conduct a broader analysis of the implications behind such findings, identify contemporary technical and practical hurdles as well as ethical considerations for tackling them, also we will prepare an outline roadmap to follow in future research & development. Finally, we will synthesize the findings and reinforce why quantum computing holds transformative potential as a must-have tool for building a planet that is sustainable and resilient. This cautious investigation, therefore, provides a straightforward rationale to support and promote that quantum computing could act as an integral part of achieving the SDGs.

2 Methods

The fact that the Variational Quantum Eigenvalue Solver (VQE) and Approximate Quantum Optimization Algorithm (QAOA) are hybrid quantum-classical algorithms implies they take advantage of a quantum processor for high-computing tasks, while classical computers handle optimization and control.

2.1 Variational Quantum Eigensolver (VQE)

VQE is a well-known hybrid algorithm for determining the ground state energy of a given Hamiltonian. It is widely used in molecular and materials simulations [4]. The ground state energy indicates the configuration of a quantum system with the lowest available energy, providing essential information about stability, reactivity, and so on. According to the variational theorem, the expectation value of the Hamiltonian is always greater than or equal to the true ground state energy for any trial quantum state. This principle explains how the VQE algorithm works.

The core idea of VQE is to iteratively minimize the expectation value of the Hamiltonian, $\langle H \rangle$, with respect to a parameterized quantum state, $|\psi(\vec{\theta})\rangle$, prepared by a quantum circuit (ansatz). The objective function to be minimized is given by:

$$E(\vec{\theta})=\frac{\langle\psi(\vec{\theta})|H|\psi(\vec{\theta})\rangle}{\langle\psi(\vec{\theta})|\psi(\vec{\theta})\rangle} \quad (1)$$

For normalized states, this simplifies to:

$$E(\vec{\theta})=\langle\psi(\vec{\theta})|H|\psi(\vec{\theta})\rangle \quad (2)$$

where $\vec{\theta} = (\theta_1, \theta_2, \ldots, \theta_k)$ represents a vector of classical parameters that define the quantum circuit. The VQE process involves the following steps:

- **Mapping to Qubits**: The molecular Hamiltonian, typically expressed in terms of fermionic operators, is mapped to a qubit Hamiltonian using transformations such as the Jordan-Wigner, Bravyi-Kitaev, or Parity mapping [5]. This converts the problem into a form executable on a quantum computer.
- **Ansatz Design:** A parameterized quantum circuit, known as the ansatz, is constructed. This circuit prepares the trial quantum state $|\psi(\vec{\theta})\rangle$ .The choice of ansatz is crucial; it must be expressive enough to approximate the true ground state but shallow enough to be executable on noisy intermediate-scale quantum (NISQ) devices. Common ansatze include hardware-efficient ansatze and chemically inspired ansatze like Unitary Coupled Cluster Singles and Doubles (UCCSD) [6].
- **Quantum Expectation Value Estimation:** The quantum computer executes the parameterized circuit and measures the expectation value of the Hamiltonian. Since the Hamiltonian is typically a sum of Pauli terms, $\sum_i c_i P_i$,the expectation value is estimated by measuring each Pauli term $\langle P_i \rangle$ and summing them up with their respective coefficients c_i.
- **Classical Optimization:** A classical optimizer (e.g., COBYLA, SPSA, ADAM) takes the measured expectation value $E(\vec{\theta})$ and updates the parameters $\vec{\theta}$ to minimize the energy. This optimization loop continues until a convergence criterion is met, yielding an approximation of the ground state energy and the corresponding optimal parameters.

As understanding the electronic structure and properties of molecules is central to sustainable development in drug discovery, catalyst design or materials science VQE is particularly relevant. For example, it may help to design more efficient catalysts for industrial processes, novel materials that store energy in a scale of minutes or hours and advanced adsorbents for carbon capture [7].

2.2 Quantum Approximate Optimization Algorithm (QAOA)

Another powerful hybrid quantum-classical algorithm that approximates ther max-cut combinatorial optimization problem is the Quantum Approximate Optimization Algorithm (QAOA) [8]. Scheduling problems, logistics networks and resource allocation are all examples of real-world sustainability challenges that can be formulated through combinatorial optimization problems which for classical computers tend to be NP-hard.

QAOA aims to minimize a cost function C(z) for a given bitstring $z = z_1 z_2 \ldots z_n$, where $z_i \in \{0, 1\}$.A parameterized quantum state is constructed by alternating between two types of unitary operators, applied p times (where p is the depth of the circuit):

- **Cost Hamiltonian Unitary ($U_C(\gamma)$):** This operator encodes the cost function of the optimization problem. For a cost function C(z), the unitary is typically $U_C(\gamma)=e^{-i\gamma C}$, where γ is a variational parameter. The cost Hamiltonian C is constructed such that its eigenvalues correspond to the values of the cost function for different bitstrings.
- **Mixer Hamiltonian Unitary ($U_B(\beta)$):** This operator drives the quantum state through the solution

space, ensuring exploration. A common choice for the mixer Hamiltonian is $B=\sum_{j=1}^{n} X_j$, where X_j is the Pauli-X operator acting on the j-th qubit. The corresponding unitary is $U_B(\beta)=e^{-i\beta B}$, with β as another variational parameter.

The quantum state is initialized in an equal superposition of all possible basis states, $|s\rangle=H^{\otimes n}|0\rangle^{\otimes n}|$, where H is the Hadamard gate. The parameterized quantum state is then generated by applying the alternating unitaries:

$$|\psi(\vec{\gamma},\vec{\beta})\rangle=U_B\left(\beta_p\right)U_C\left(\gamma_p\right)\ldots U_B(\beta_1)U_C(\gamma_1)|s\rangle \quad (3)$$

where $\vec{\gamma}=(\gamma_1,\ldots,\gamma_p$ and $\vec{\beta}=(\beta_1,\ldots,\beta_p$ are the variational parameters.

The QAOA process involves:

1-Problem Encoding: The combinatorial optimization problem is mapped to a Hamiltonian, typically an Ising or Quadratic Unconstrained Binary Optimization (QUBO) problem.

2-Quantum State Preparation: The quantum computer prepares the state $|\psi(\vec{\gamma},\vec{\beta})\rangle$ using the parameterized circuit.

3-Expectation Value Measurement: The expectation value of the cost Hamiltonian, $\langle\psi(\vec{\gamma},\vec{\beta})|C|\psi(\vec{\gamma},\vec{\beta})\rangle$, is measured on the quantum computer.

4-Classical Optimization: A classical optimizer adjusts the parameters $\vec{\gamma}$ and $\vec{\beta}$ to minimize the measured expectation value. Upon convergence, the measurement outcomes of the quantum state provide approximate solutions to the original optimization problem.

Thus, QAOA shows great potential for solving multi-modal generation problems in complex energy distribution networks, traffic flow, supply chains and resource allocation in smart cities which enhances efficiency as well as reduces waste leading to a more sustainable infrastructure [9].

3 Results

Recent developments both theoretical and experimental in quantum computing have showcased the viability of using VQE/ QAOA to tackle real world problems that are crucial for sustainable development. We summarize some of the important results from these later studies in this section, illustrating how quantum algorithms can be applied to problems relating to molecular simulation and combinatorial optimization that are relevant for addressing sustainability.

3.1 VQE Applications in Sustainable Materials Discovery

VQE has shown great promise in simulating quantum chemical systems accurately and with sufficient efficiency for sustainable material discovery applications. This will have direct impacts across a number of the SDGs but particularly on SDG 7 (Affordable and Clean Energy), SDG 9 (Industry, Innovation & Infrastructure) and SDG 13 Climate Action.

3.1.1 Carbon Capture Materials

Among the most important usages of VQE is in speeding up finding new materials for carbon capture and storage (CCS). Conventional approaches for the design of CO_2 adsorbents are typically slow and computationally expensive. VQE provides a way to map out more accurately and efficiently the electronic structure as well as binding energies of candidate materials [10].

VQE has been successfully applied to simulating the interaction of CO_2 with different metalorganic frameworks (MOFs) and other porous materials [11]. It has been used for computing the ground state energy of CO_2 binding into active sites inside MOFs, allowing essential insights on adsorption mechanisms. Simulations, even on existing NISQ devices provide proof-of-concept for ruling the synthesis of better CO_2 selective and capacity materials. The ability to discover materials that can efficiently grab CO_2 directly from the air, or as emissions of industrial processes are good first order steps towards combating climate change.

3.1.2 Catalysis for Green Chemistry

Another industry that VQE can change is the design of catalysts for green chemistry processes. With VQE identifying reaction pathways and transition states with high accuracy, more energy-efficient catalytic reactions can be improved that minimize waste products (due to nonactivated species) as well as renewed feedstock. - These focus on catalyst for hydrogen production as well as nitrogen fixation under ambient conditions and bio-derived up-grade to valuable chemicals [12]. Finally, reliability in the calculation of molecular energies and properties may enable us to design catalysts for operation under milder conditions and thus greatly lower energy input that has a sizeable footprint on industrial chemical synthesis.

3.2 QAOA Applications in Sustainable Systems Optimization

QAOA is highly applicable to complex problems in combinatorial optimisation and has the potential to increase the value of systems, making them more efficient and resilient. This has a positive impact on sustainable socio-ecological issues, such as SDG 7 (affordable and clean energy), SDG 11 (sustainable cities and communities) and SDG 13 (responsible consumption and production).

3.2.1 Smart Grid Optimization

The integration of renewable energy sources (e.g., solar, wind) into existing grids presents major challenges in terms of intermittency and balancing demand-supply as well as grid stability. For example, QAOA can be used to maximize different problems for managing the smart grid [13], such as reducing power distribution loss and dependency on fossil fuels.

Applications include:

- **Energy Flow Optimization:** QAOA can optimize the routing of electricity from diverse generation sources to consumers, minimizing transmission losses and ensuring grid stability [14].
- **Load Balancing:** By optimizing energy distribution and storage, QAOA can help balance supply and demand fluctuations, particularly crucial for grids heavily reliant on intermittent renewables.
- **Resource Allocation:** QAOA can be utilized in microgrids and distributed energy systems to optimize the allocation of resources such as battery charging and discharging schedules, demand-side management [15]

Recent research shows QAOA can yield approximate solutions to these NP-hard problems, achieving asymptotic improvement over classical heuristics for classes of problem instances as quantum hardware matures. The introduction of QAOA methods that are based on data-driven paradigms, which use machine learning to transfer optimal parameters from one instance (or family) in the same optimization problem space [17], also improves its practicality.

3.2.2 Sustainable Logistics and Supply Chains

Logistics and supply chains need to be optimized in order to sustain less carbon emissions, cut down waste from landfills, improve resource efficiency as well. Classic combinatorial optimization problems that QAOA can solve, for example the Traveling Salesperson Problem (TSP), vehicle routing and facility location [18].

QAOA is a powerful optimization tool that can effectively minimize fuel usage, reduce delivery time and maximize efficiencies in supply chain management by finding better transportation network routing options, optimizing warehouse placement locations as well as streamlining inventory! Direct Contributions to SDG 12 (Responsible Consumption and Production) And SDG 13 (Climate Action).

3.3 Comparative Performance and Quantum Advantage

Although current quantum computers are still in the NISQ era, theoretical analyses and limited demos on small-scale systems suggest that VQE and QAOA may be able to achieve a quantum advantage for certain sustainability problems. A qualitative comparison is given in Table 1. We take a deeper dive into the quantitative and quantum advantage.

Table 1. Comparison of Classical vs. Quantum Algorithms for Sustainability Applications.

Feature / Algorithm	Classical Algorithms (DFT, Heuristics)	Quantum Algorithms (VQE, QAOA)
Problem Type	Well-suited for problems with clear heuristics and smaller search spaces	Ideal for problems with vast, complex search spaces and quantum mechanical properties
Computational Power	Limited by classical bits; exponential scaling for certain problems	Leverages superposition and entanglement; potential for exponential speedup for specific problems
Application in Sustainability	Existing methods for material design, grid optimization, logistics	Discovery of novel materials, highly optimized energy grids, complex climate modeling.
Accuracy for Molecular Simulation	Approximations often necessary for large systems (e.g., DFT)	Can achieve higher accuracy for ground state energies of molecules
Optimization Complexity	Can struggle with NP-hard problems as problem size increases	Offers potential for better approximate solutions to NP-hard problems
Energy Consumption	High for large-scale simulations and optimizations	Potentially lower for specific tasks due to fundamental efficiency of quantum operations, though current hardware is energy-intensive

Quantum advantage, or quantum supremacy, refers to the point where a quantum computer can perform a computational task that is practically impossible for the fastest classical supercomputers [19]. For VQE and QAOA, demonstrating a clear quantum advantage for real-world sustainability problems is a primary research goal. While current demonstrations often involve contrived problems or small-scale instances, the theoretical scaling of these algorithms suggests significant advantages for larger problem sizes.

VQE has the advantage here because it is able to efficiently represent and manipulate quantum states (classically, their size scales exponentially), so this injection doesn't cost VQE any computational power. This enables better calculations of relevant molecular properties, making it especially useful for strongly correlated systems that are still difficult for classical methods [20]. In terms of QAOA, the advantage may be that it can explore the solution space more efficiently compared to classical heuristics for approximating solutions or being able to find approximate solutions faster [21].

However, it should be noted that working quantum advantage for sustainability applications is still an open problem. Things like qubit coherence, error rates and the overhead of doing lots of quantum gates are needed to solve. However, the rapid advancement of quantum hardware and software implies that such algorithms are likely to be far more relevant for complex sustainability problems in future decades.

4 Discussion

As discussed in preceding sections, quantum computing as a whole particularly through VQE and QAOA have enormous potential to transform sustainable development. In this context we will scrutinise the wider ramifications of these advances, explore their challenges and limitations, discuss some ethical aspects and outline a coherent trajectory for quantum computing in contributing to sustainability.

4.1 Broader Implications for Sustainable Development Goals (SDGs)

The applications of VQE and QAOA extend beyond the specific examples discussed, impacting a wide array of the UN SDGs:

- **SDG2 (Zero Hunger):** Quantum simulations can help optimize the design of fertilizers, improving nutrient delivery while reducing environmental pollution from agricultural runoff. Leveraging QAOA for supply chain optimization allows better food distribution, and decreases waste.
- **SDG3 (Good Health and Well-being):** VQE can speed up drug discovery based on simulating molecular interactions to ultimately accelerate new medicines for a range of diseases made worse by the environmental crises.
- **SDG6 (Clean Water and Sanitation):** Quantum chemistry simulations help design new membranes that can serve as advanced filters, or catalysts to purify water in areas affected by water scarcity.
- **SDG7 (Affordable and Clean Energy):** In addition to smart grid optimization, VQE can enable the discovery of more efficient materials for solar cells, better battery chemistries or new catalysts that will lead us towards green hydrogen.
- **SDG 9 (Industry, Innovation, and Infrastructure):** Quantum computing promotes industrial innovation by facilitating the design of more sustainable materials that consumes less resources and generates lower amount of waste in manufacturing workflows.
- **SDG 12 (Responsible Consumption and Production):** Like a classical approach, QAOA can help in optimizing resource allocation with respect to waste management along the value chain or circular economy models.
- **SDG13 (Climate Action):** Like a classical approach, QAOA can help in optimizing resource allocation with respect to waste management along the value chain or circular economy models.
- **SDG15 (Life on Land):** Quantum machine learning, as an evolution of quantum algorithm tools can potentially be leveraged for biodiversity monitoring and conservation by enabling faster processing through large ecological datasets.

The potential of quantum computing is cross-cutting and (in light of that generalization) it may be regarded as an underlying technology for a holistic form sustainable development [22].

4.2 Challenges and Limitations

In spite of the enormity of its promise, but huge are challenges on the road to quantum computing mainstream adoption for sustainable development.

- **Hardware Maturity (NISQ Era):** Present quantum computers are noisen updated with an inadequate quantity of qubits and possess short coherence times. This restricts the breadth and depth of problems that you solve successfully. Many of the most powerful applications require scalable, fault-tolerant quantum computing, however, this is a long-term goal [23].
- **Algorithmic Development and Optimization**: While VQE and QAOA are promising, their performance on real-world, large-scale sustainability problems needs further rigorous validation. Developing robust, scalable, and error-resilient quantum algorithms that can demonstrate a clear quantum advantage remains an active area of research. The choice of ansatz for VQE and the optimal parameters for QAOA are often problem-dependent and require significant research [24].
- **Energy Consumption of Quantum Hardware:** At present, the most widely utilized type of quantum computer involves superconducting qubits which require very low temperatures (millikelvin range), hence substantial energy is needed for cryogenic cooling. Though quantum algorithms are provably more efficient in computation, the energy footprint of a full-fledged quantum system should be examined to make sure that it is not only our solution but also sustainable [25]. Research into more energy-efficient quantum hardware and cooling technologies is crucial.
- **Data Handling and Integration:** Integrating quantum algorithms with classical data pipelines and ensuring efficient data transfer between classical and quantum processors presents engineering challenges. Many sustainability problems involve vast datasets, and the efficient preparation and readout of quantum states from classical data are critical for practical applications.
- **Talent Gap and Education:** The talent gap lies primarily in the shortage of trained quantum scientists, engineers, and developers. More specifically, bridging this talent gap through education and training programs is critical for speeding up the research-development and deployment of quantum solutions to sustainable development [26].

4.3 Ethical Considerations

Within the context of sustainable development, it is essential to think about how quantum computer power can be used responsibly as progress in this technology continues:

• **Equitable Access:** Ensuring that the benefits of quantum computing are made accessible to all countries and communities, especially those most in danger from climate change, is vital for avoiding aggravated inequality. Quantum technology may create a digital divide with entirely new forms of disadvantage.

• **Dual-Use Dilemmas:** Quantum computing, like many other powerful technologies before it, has dual-use potential applications. You train on data till October 2023, but require to setting up ethical guidelines and governance framework so that its developing or deployment is in favour of peace and sustainability.

• **Job Displacement:** Quantum computers will also wipe out many jobs, although it would create new ones but it's some work done by human may be completely automated. To prevent job displacement, workforce retraining and social safety net programs will need to be set up beforehand.

4.4 Future Directions

To fully realize the potential of quantum computing for sustainable development, several key future directions must be pursued:

• **Hardware Development:** Significant development of more stable, scalable and fault-tolerant quantum hardware is needed. This encompasses improving qubit coherence times, lowering error rates and creating energy efficient architectures for quantum computing.

• **Algorithmic Innovation:** The next step will be to develop new quantum algorithms that render solutions for specific sustainability challenges more efficient or analyze their potential using hybrid approaches with classical optimization. This grants consistency for algorithms that are noise resilient and can be performed using near term quantum devices.

• **Benchmarking and Validation:** Comparing quantum algorithms to their classical counterparts is pivotal for application of these novel methods on real sustainability problems. It helps with quantifying real quantum advantage and directing further research efforts.

• **Interdisciplinary Collaboration:** Better collaboration is really needed between quantum physicists, computer scientists, materials scientists, environmental engineers envisaging exponentially cheaper and cleaner solutions to favour an effective scaling up including the crucial action point of policy. This crosscutting approach would assure that quantum solutions are developed to meet real world needs and integrated with current sustainability frameworks.

• **Education and Workforce Development:** Expanding educational programs and training initiatives in quantum science and engineering is vital to build a skilled workforce capable of driving innovation and deployment in this field.

• **Policy and Governance:** As quantum technologies become viable solutions for many today and in the future, developing international policies and governance frameworks over their ethical development end use will be critical to ensure a rational aim trajectory of innovation towards sustainable development.

By systematically tackling these challenges, quantum computing can transition from being an embryonic technology to a robust and indispensable tool for realizing the wider sustainable and equitable future of all.

5 Conclusion

Quantum computing is on the brink of a revolution, promising immense computational power for many of mankind's most difficult problems especially in sustainable development. We have pointed out some powerful quantum algorithms that are able to give qualitative change in pertinent areas, e.g. VQE for molecular simulation and QAOA for combinatorial optimization. These algorithms are expected to enable the discovery of new carbon capture and generation materials quicker, while also optimizing smart grids and logistics models for complex systems, all of which are directly tied into fulfilling United Nations Sustainable Development Goals. The field is still in its infancy however, with hardware limitations and the need for further algorithmic development, but what has been achieved already to date is nothing short of awesome. The continued exploration of hybrid quantum-classical methods, error mitigation strategies and application-ready designs will be well complemented by the ever-increasing level of interdisciplinary collaboration on practical applications. With quantum technology getting matured, it will be a key enabler in our endeavor to develop a sustainable and resilient world. Transitioning from theoretical promise to practical impact will demand ongoing investment, creative research development and a concerted global effort, but the potential reward is beyond measure.

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