Quantum Sustainability Working Group (25w7008)

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Consequences of mathematical theories have real-world implications. When we write out a model, its solution so closely mirrors physical processes that we can use mathematics to forecast real life. For the cases considered in this workshop report, the mathematics are vast and wide. The Quantum Sustainability Working Group focuses on key challenges facing the modern world and draws on many different mathematical formulations to make a positive good for society. Such audacious directions require a broader discussion at the interface between mathematics, technology, and policy. The following report focuses on highlighting the multiple areas of applications that are under study within the working group. We discuss these areas broadly due to the technical challenges of going into each area, largely focusing on what formulation and algorithm will yield the best result on the quantum computer of pre-existing theory.

1 Overview of the Field

Quantum computing currently sits at an inflection point. Hardware has advanced at a rapid pace and this now makes possible many applications that were proposed for a quantum computer. However, the large-scale use of the quantum computer has not yet been demonstrated definitively. We may be on the cusp of such an advancement in the near-term, but we expect that the discussion of a quantum advantage will start taking place earnestly over the next year. Our question is: what do we do if we have a quantum computer that can run new tasks at scale?

The responsible use of a quantum computer will require the mobilization of the entire community to ensure that the eventual use of a quantum computer is aligned with the goals of forwarding society and ensuring that fair practices are implemented. Without planning for sustainable outcomes, we risk repeating some of the technological limitations that classical computations led to. With the power of the quantum computer potentially at hand, it would be prudent to understand how to truly derive the best outcomes from the quantum computer in a sustainable way.

Sustainability has many possible meanings, but each has a common understanding of using resources efficiently. This ultimately ensures that either:

- Possibility 1: the quantum computation will be more energy efficient, or
- Possibility 2: that the quantum computer will lead to results that transform modern society in a way to be more resource efficient.

Either of which would be valuable from the perspective of making computations more beneficial in a sustainability sense.

The Quantum Sustainability Working Group is committed to exploring applications for both possibilities. Sustainable computation, in the sense of using fewer resources in any form, is an opportunity that the new paradigm of quantum computing brings to the solution of existing problems.

Part of the goal of this working group will be to obtain useful applications of quantum algorithms–and potentially new quantum algorithms–to bring quantum computing from speculative to useful with a quantum advantage over classical computation in the area of sustainability.

2 Recent Developments and Open Problems

The Sustainability Quantum Working Group is divided into several focus groups. These focus groups range between two predominant topics:

- Energy - in alignment with the United Nations' Sustainable Development Goals we explore the potential for quantum computing to address challenges such as renewable energy, grid optimization, and energy storage technologies. Power grid organizations worldwide share similar challenges, including modernizing grids to accommodate renewables and electric vehicles. Many energy applications are linked to optimization problems. The mathematical formulation of these problems is very diverse and problem dependent. Some are more amenable–such as quadratically unconstrained binary optimization (QUBO) [**?**]–to implementation on the quantum computer than others.
- Materials - Finding new materials is a challenging problem in quantum chemistry. Suggesting properties of a material and then trying to determine what chemical formulae will give these properties is very difficult, as this is an inverse problem. But it is crucial to have compelling methods to advance current materials research for future technology. Solving for new materials in quantum chemistry requires a solution of the many-body problem,
$$H = \hat{T} + \hat{V}_{\text{ee}} + \hat{V} \tag{1}$$
where $\hat{T}$ is the kinetic energy for electrons, $\hat{V}_{\text{ee}}$ is the Coulomb interaction between electrons, and $\hat{V}$ is the external potential energy. It is hoped that this problem can be well treated on the quantum computer because the solution is framed naturally in quantum mechanics.

Both of these areas present their own difficulties in finding efficient solutions and have large spaces to search through for correct answers. Optimization in particular represents a good test of quantum computation since many strategies for optimization scale with computer size, allowing for a direct scaling against the number of qubits used on the quantum computer. Quantum materials have been studied rigorously for decades and use knowledge of the properties of quantum solutions in local quantum chemistry models to find solutions more efficiently. As with all quantum computation solutions at this stage, however, the path to practical implementation at an impactful scale is actively being paved. Understanding how to identify and define problems in both the energy and materials sectors such that they map appropriately to near-term quantum computers is one part of the process, while the other is exploring and establishing the mathematical solutions themselves through current and new algorithms. Participants discussed state of the art research focused on both problem definition and revolutionary quantum solutions. These discussions inspired new directions for ongoing research, as well as several entirely new directions.

3 Presentation Highlights

3.1 Quantum chemistry on quantum computers

Recent advances with IBM quantum computers using new varieties of algorithms including sample-based quantum diagonalization (SQD) [**?**] may lead a pathway to full quantum utility if not outright quantum advantage, as presented by Antonio Mezzocampo from IBM. The present goal for IBM is to demonstrate quantum advantage by the end of 2026 and create algorithms that quantum computers can run that are reliable alternatives to existing classical state of the art techniques.

3.2 Scalable quantum dynamics with quantum machine learning

Advances in the compilation of quantum circuits have allowed for a reduced number of gates for certain quantum circuits. In this presentation, by Lukasz Cincio from Los Alamos National Lab, recent work on more efficient compilations of quantum circuits were applied to quantum machine learning applications [?]. Future advances in these methods may yield an improvement in future algorithms, bringing far-term quantum algorithms down to existing devices.

3.3 Towards performing useful and reliable computations with noisy quantum computers

The supply chain for semiconductors requires careful optimization in order to function in the most efficient way. LG Electronics–represented by Thi Ha Kyaw–has investigated the use of quantum hardware for optimization in this area for a more sustainable supply chain [?]. More precisely, they investigate how near-term quantum algorithms, error mitigation and mapping techniques can lead to improvements solving practical problems.

3.4 Hybrid quantum hyperparameter optimization

This talk by Barry Sanders and Mahkame Salimi from the UCalgary summarized his group at the Unversity of Calgary's work on flood susceptibility prevention. Hybrid quantum genetic algorithm were applied for this use case and work will be done with local authorities to determine if quantum computers can be an advantage here [?].

3.5 Distributed quantum software

This talk presented the work done at G2Q Computing, represented by Utkash Singh, a quantum software startup, using quantum computers to address the challenges of imagine classification, distributed optimization, fraud detection and other financial applications.

4 Group projects

There is a search ongoing for useful application of the quantum computer in several domain areas ranging from quantum chemistry to optimization problems. Several focus groups presented their current progress and one-year roadmaps in a variety of areas.

4.1 Focus on batteries and concrete

Batteries and concrete represent two possible application areas for quantum computing. Making improvements in our ability to simulate quantum matter would allow for new technologies that cost less carbon to make or store energy for a lower material cost. The major challenge will be to construct methods that can solve many Hamiltonians on the quantum computer to fully compete with classical methods such as *ab initio* molecular dynamics (MD). This will be a focus of the working group going forward as well as characterizations of when outcomes from the quantum computer are sustainable.

This working group (represented by Thomas E. Baker from the University of Victoria) added new members and generated a new roadmap for an upcoming formalization of the previous activities. These will include a series of meetings to ensure that domain experts are fully comfortable with the recent algorithmic advances in quantum computing. A planning structure was created during the meeting and several meetings will be held to generate the first draft.

All participants will be given knowledge to make quantum algorithm studies of their own, and some new algorithms are being discussed [?].

4.2 Quantum Gaussian Regression for AC Powerflow

Powerflow calculations in transmission lines represent a challenging task computationally for several reasons. First, the diversification of energy sources, often with fluctuating renewables like wind and solar, adds uncertainties and fluctuation on the electrical grid which impacts the powerflow of power lines. Second, temperature, wind and precipitations can have drastic effects on the powerline and the vegetation integrity.

The question this team is aiming to answer is: Is there a useful way to use quantum computation for time series forecasting of AC powerflow in the grid, by accounting for uncertainty in renewable energy generation? And the chosen approach is a real-life data-driven model based on quantum kernels. The collaboration was represented by Marc-André Dubois, Hydro-Québec.

Early results show that the quantum approach is at least as accurate as state-of-the-art classical models. The team will now run their algorithm on real quantum hardware and investigate the scaling of the method.

4.3 Quantum Reservoir Computing

This team (represented by Francesco Tacchino from IBM) is investigating the use of the Quantum Reservoir Computing to treat time series data with applications to climate modeling, energy or stock market data, rare events among many others. They have already tested their methods to up to 30 qubits on IBM quantum computers and are actively investigating how circuits could scale to the utility scale, at around 80 qubits.

4.4 Optimization for power grid problems

Dr. Adam Bene Watts presented the ongoing project on utility scale unit commitment to better manage power outputs of generators in a network. This project has many similarities to work Professor Steven Rayan at the University of Saskatchewan is pursuing with SaskPower on energy grid storage modelling [?]. Because of their similarities, the working groups chose to merge focuses and mutually benefit from shared knowledge.

It is hoped that improved methods of finding optimized solutions for quantum problems will be available from these efforts.

4.5 New Projects

Five existing projects were expanded to include new collaborators and have updated their project roadmaps accordingly. Additionally, seven new cross-disciplinary projects were defined. While the previously existing projects focus largely on the energy sector, new projects have broadened the group's focus to include other areas of sustainability. Supporting a diversity of topics creates a stronger possibility of obtaining a near term quantum-focused solution in the field of sustainability.

Professor Viki Kumar Prasad from the University of Calgary who proposed projects centered around identifying new materials for carbon capture and catalysts. Other topics include wildfire prevention, semiconductor supply chain optimization, forest management, and carbon capture, utilization, and storage. Soon after the workshop, one of the project on forestry was awarded a grant by the IBM Sustainability Accelerator program.

4.6 Sustainability vision

The broader message of sustainabiliy was a focal point during our discussion regarding a sustainability and quantum manifesto to be presented at COP30 this year. The discussion was facilitated by Institut Quantique (Université de Sherbrooke) who is drafting the report with the Open Quantum Institute as led by Dr. Karl Thibault. The key takeaways are that there is a fundamental need from institutions and governments alike to fund researchers and the programs that support them [?]. This means grants for groups to both hire and train new talent, as well as ensure continued access to state-of-the-art classical and quantum computing resources. Workforce readiness inherently requires funding, but these efforts will only go so far unless the trainees and their advisors have access to the latest technologies. This is particularly crucial for groups pursuing real-world use cases with quantum computers. Additionally, to further encourage sustainable solutions, the group agreed that it would be greatly helpful if each funding source allocated a percentage of financial support for quantum to efforts in solving sustainability challenges. Without this, the necessary advocacy is unlikely to materialize on its own, exacerbating an already urgent need for sustainable methods and technologies and furthering the delay between quantum technical progress and impactful solutions.

This conversation inspired a collaboration with other present researchers from Natural Resources Canada (led by Dr. Ahmed Ragab) to kick start a project on using quantum computation for wildfire prevention.

5 Outcome of the Meeting

Each project is establishing regular meetings with all collaborators to make progress following the 1-year roadmaps they drafted while at BIRS. Several group-wide virtual meetings will also take place to check-in as a wider team. While the next group- wide in-person meeting is on the schedule for 2026, there are several other in-person events later this year featuring the Sustainability Quantum Working Group. The Sustainability Working Group will be at the IEEE Quantum Week conference in September 2025 in Albuquerque, New Mexico. There they are co-hosting a workshop with the 4 other Quantum Technical Working Groups for the first time. Additionally, the group's work will inform a quantum for climate initiative at the Quantum World Congress in September. The group is also working with several other organizations (Institut Quantique, Open Quantum Institute, IBM Chief Sustainability Office) and governments (Québec) to coordinate a quantum presence at COP30 in November. It is also likely that as the projects progress, there may be further talks and publications from the Sustainability Quantum Working Group at various forums within the next year.

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