OQI
Open Quantum
Institute

White Paper 2024

SDG Use cases

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Introduction

The Open Quantum Institute (OQI) [1] is a multilateral governance initiative that promotes global and inclusive access to quantum computing and the development of applications for the benefit of humanity. As a novel science diplomacy instrument, it brings together research, diplomacy, private sector and philanthropy stakeholders. OQI is hosted by CERN during its pilot phase (2024-2026).

As part of its mission, one of OQI's four main activities is focusing on accelerating applications for humanity. While quantum computing is still in its early stages of development and computational resources remain limited, there is an opportunity today to join a global effort to explore potential applications of the technology that will positively impact our society and our planet. OQI aims to fully harness the potential of quantum computing by accelerating the development of use cases that contribute to the achievement of the United Nations Sustainable Development Goals (SDGs) and subsequent frameworks.

Through the support of OQI, quantum and subject matter experts from around the world have been collaborating with UN agencies and large NGOs to explore the potential of quantum computing to address global challenges. OQI's use case portfolio contains a growing number of use cases at various phases of their development. A complete overview of this portfolio is illustrated in Figure 1. These use cases primarily address SDG 2 (Zero Hunger), SDG 3 (Good Health and Wellbeing), SDG 6 (Clean Water and Sanitation), SDG 7 (Affordable and Clean Energy), SDG 12 (Responsible Consumption and Production) and SDG 13 (Climate Action). Additionally, they have interconnections with several other SDGs. Quantum approaches in these solutions span from simulation to optimisation and machine learning, utilizing either quantum or quantum-inspired algorithms [3]. None of the suggested approaches would outperform existing state-of-the-art classical approaches on today's quantum computing hardware. Nevertheless, this effort is crucial for building a global community of practice that rigorously explores quantum computing applications for the SDGs and their potential scalability on future quantum devices.

This 2024 OQI Use Case White Paper presents 10 new use cases developed by experts from 22 countries, who have started their work with OQI support since the publication of the 2023 Edition [2]. Some of these use cases are inherited from the OQI incubation phase, while others emerged from OQI's call for ideas in the spring of this year. The development of use case exploration will continue to be pursued, deepening both the scientific methodology as well as the potential societal impact.

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[3] Quantum-inspired algorithms refer to classical algorithms that are inspired by physical nature/ quantum mechanical nature. The categorisation of the approaches and algorithms is done independently of their performance of potential future implementation on quantum processors.

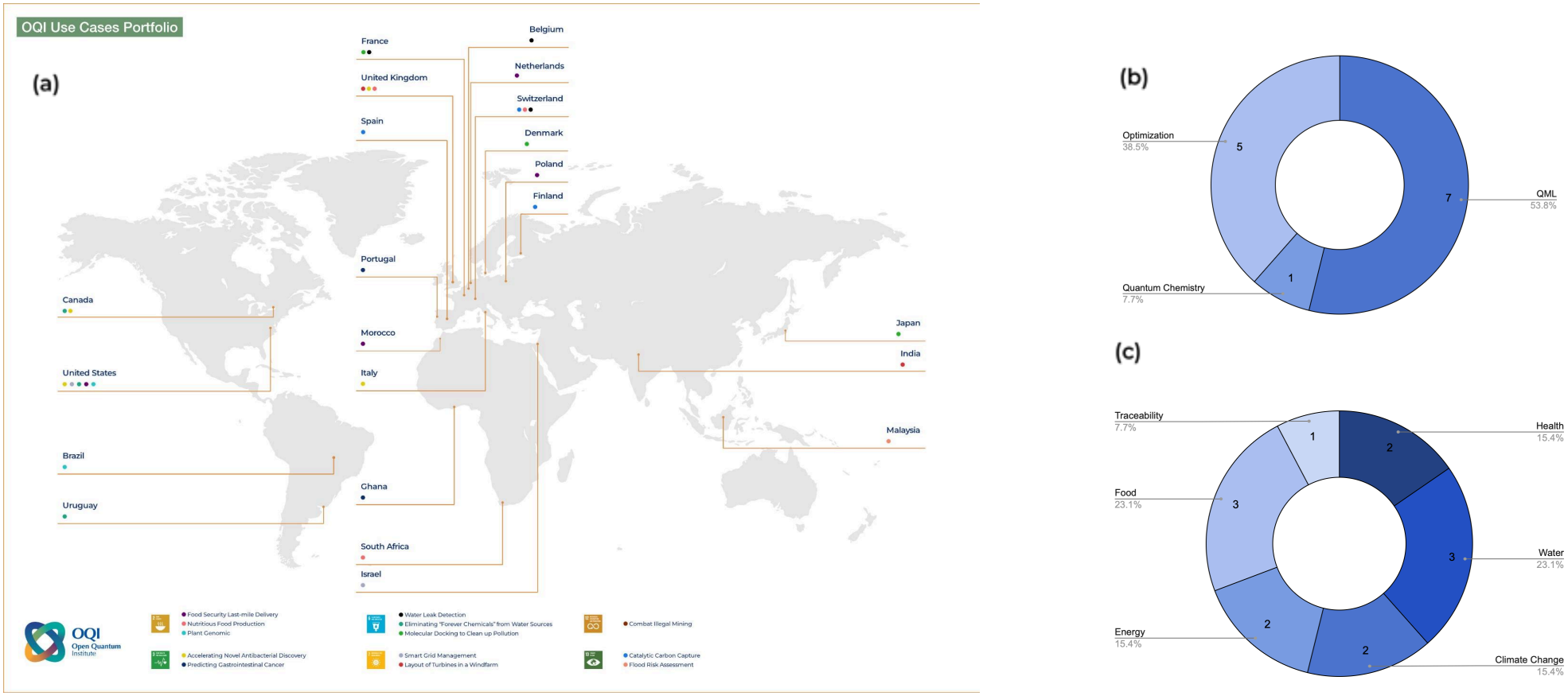

Figure 1. OQI portfolio of active use cases relevant to the UN SDGs
Important to note that OQI has explored additional use case ideas over the past years. This chart shows only the current active use cases, i.e. that have performed substantial development in 2024. (a) Each coloured dot represents a use case team formed by experts from multiple countries to explore the potential of quantum computing for the SDGs. (b) These use cases are leveraging existing quantum approaches that include simulation for chemistry, optimisation and machine learning (QML). (c) The use cases address real-world problems, ranging from food, health, water, energy, traceability and climate.

SDG 2 – Zero Hunger

Plant Genomics

SHORT SUMMARY
Quantum computing solution for sustainable agrifood system by boosting predictive design and gene editing of plants.

QUANTUM APPROACH
Machine Learning

TEAM ORIGINS

Context

The world currently faces one of the greatest challenges to humanity: providing enough nutritious calories for a growing population, while reducing the footprint of agricultural production on the environment. The Food and Agriculture Organisation of the United Nations (FAO) has included as one of its top four priorities to have a better production of food, which includes ensuring resilient and sustainable agrifood systems in a changing climate and environment [1].

Indeed, climate change, along with economic and geopolitical instabilities that directly affect the food supply in the most vulnerable geographies, has increased the urgency of addressing these scientific and societal challenges. Developing countries, such as Brazil, necessitate the optimization of agricultural output in conjunction with conserving natural resources via improved crops and crop management systems. To tackle these challenges, several partnerships have been created among governmental and international agencies and organisations. For instance, the Brazil-FAO International Cooperation Programme focuses on transforming the agri-food system in Brazil and Latin America [2].

Innovative applications of science and technology, including those in biotechnology, may play significant roles in transforming agrifood systems [3]. Representing a recent advancement in genetics, gene editing technology and its application to plant and animal breeding highlights its position for contributing to improvements in various aspects of agricultural production [4]. Gene editing allows modification of a genome with more speed and precision than other forms of breeding. Moreover, it offers an opportunity to address a range of difficult problems, including those associated with increasing yield while reducing the use of natural resources and developing durable resistance to diseases, pests and abiotic stressors. It also offers new options for developing adapted traits in neglected and underutilised crop species.

Gene editing technology advances conventional approaches with greater speed and accuracy for executing gene modification and gene networks leading to desired phenotypes [5]. When the outcome of precision breeding such as gene editing equals that of conventional breeding, the products carry the same risk profile and should be treated equally by regulatory bodies. Regulation and safety issues are being addressed to ensure secure and sustainable use of gene editing in agrifood [6].

In the past two decades, the convergence of technological revolutions in genomics, data analytics and genome editing offers a unique opportunity to contribute to the global challenge of food security [5]. To date, plant biotechnology approaches have been limited by the lack of understanding of the molecular basis of crop performance. With the ability to (i) produce data in target crops at a very competitive cost due to the sequencing technological breakthroughs (ii) the opportunity to efficiently transform the data into knowledge using the ongoing advancements in artificial intelligence technologies and (iii)

using this knowledge to guide the highly precise modification of plant genomes using gene editing technologies, it presents a unique opportunity for a breakthrough in crop improvement.

Computational Challenges

Gene discovery is still a major challenge - particularly for complex traits like yield. New approaches are needed to transform and accelerate the process, with one of the main problems being the need for high levels of computational power to analyse the plant genome. While the existing human reference genome structure is linear, plant genome data is a lot more complex. The wheat genome, for example, is five times the size of the human genome [5]. Even more critically, however, the most impactful characteristics are driven not by one or two native genes, but by intricate networks in which many of these genes work together. One in particular refers to pangenomes, as the complete sequences of multiple individuals of a species or taxonomic units [7].

Pangenomics is a new domain of science. Sequence alignment algorithms involve computing comparisons between high dimensional data – a problem known to be computationally challenging and sometimes ill-formed due to the curse of dimensionality. Current algorithms consume substantial time and space complexity for a single pairwise alignment. Alignment-based searches with millions of potential sequence pairs can therefore produce substantial bottlenecks in sequence processing workflows.

Another important challenge is related to the complexity needed to accurately and efficiently understand the core developmental and biological processes underlying plant complex traits [8]. As the number of genes and interactions increases, the computational resources required to model and predict the behaviour of the genes grow exponentially.

Potential Impact of a Quantum Solution

Quantum computing could help tackle these complex computational challenges. In particular, using sequence graph methods, it could accelerate the key processes of mapping data to graph nodes in the pangenome and finding good routes through the graph [9, 10, 11, 12].

In addition, quantum computers might be used to simulate the behaviour of complex biological networks, potentially uncovering new insights into how genes interact and how these interactions give rise to cellular behaviours [13, 14, 15]. Quantum computing could offer novel approaches to better understand the genetic diversity, adaptation, and evolution of species, and combined with gene editing, positively impact food security, nutrition and environmental sustainability.

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Team

Tommaso Macri (QuEra), Luis Martinez (QuEra), Jonathan Wurtz (QuEra), Pedro Lopes (QuEra), Anderson Fenandes Pereira dos Santos (Venturus), Daniel de Haro Moraes (Venturus), Tiago Santiago do Espírito Santo (Venturus), José Erinaldo da Fonseca (Venturus), Douglas Silva Domingues (University San Paolo), Michael Farruggia (Inari), Sebastien Lefebvre (Inari), Sonali Quantius (Inari), Matthew Robertson (Inari), Dylan Elliott (Inari), Jeremy Pardo (Inari), Wenbin Mei (Inari), Josh Price (Inari), Emily Negrin (Inari), Alex Frieden (Inari), Catherine Feuillet (Inari), Kellye Eversole (Eversoles Associates), Rutendo Mukaratirwa (FAO), Erik VanIngen (FAO).

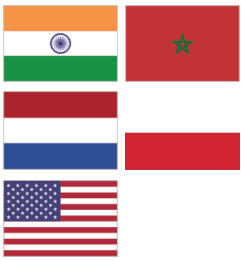
Last-Mile Food Delivery

2 ZERO HUNGER

SHORT SUMMARY
Quantum optimisation solution to optimise last-mile food delivery, minimising waste and costs.

QUANTUM APPROACH
Optimisation

TEAM ORIGINS



Context

Worldwide, 2.33 billion people lack regular access to sufficient nutrition, of whom 864 million are prone to periodically run out of food [1]. Despite widespread food insecurity, one-third of the global food supply post-harvest goes to waste [2]. Nearly 40% of this waste is accounted for by the supply chain connecting producers and retailers [3]. Food logistics, which involves delivering agricultural products from suppliers to end customers via retailers, is the most complex, costly, and inefficient part of the food supply chain [4].

Inefficient delivery of agricultural products has a number of consequences. Transportation is expensive and time consuming, and goods not delivered quickly enough might perish. Consequently, suboptimal routes result in additional fuel consumption and product loss. This results in higher costs for farmers and higher prices for consumers. There is also an environmental cost to this delivery from vehicle emissions: 5.3-5.8% of the global warming potential of the agriculture industry comes from last-mile delivery. Food waste during this stage also contributes to the 6% of greenhouse gas emissions associated with the disposal of food waste, with the resulting pollution negatively impacting the air quality of surrounding communities. Inefficient deliveries increase the number of vehicles on the road and can result in overworked drivers who are more prone to causing accidents [5].

Efficient distribution of agricultural goods is particularly difficult for smallholder farmers who cultivate less than two hectares of land. Although the role of smallholders differs between countries, they account for more than 80% of farms worldwide and produce 35% of the global food supply using only 10% of agricultural land [6]. These farmers typically do not have the same transportation capabilities, market information access, and logistic expertise accessed by larger producers [7]. These conditions limit the ability of smallholdings to secure good prices for their products and effectively distribute them. These producers stand to benefit the most from open-source and generalisable logistics optimisation tools.

Scalable algorithms for determining how to best route goods have the potential to reduce the transportation costs of farmers and manufacturers while reducing food waste and increasing the affordability of food for consumers. This use case focuses on investigating novel approaches to solve this problem using quantum computing.

Computational Challenges

A fundamental challenge in logistics is determining how to optimally make a set of deliveries with a set of vehicles, which is also known as the Vehicle Routing Problem (VRP) [8]. VRP and its variants are NP-complete, meaning it is unlikely that fast (polynomial-time) algorithms will exist to find optimal solutions in all cases. From the mathematical point of view, this particular optimisation problem can be defined as the Multi-Depot Capacitated Vehicle Routing Problem with Time Windows [9]. Some last-mile

food delivery cases can also be defined as the Capacitated Pickup and Delivery Problem with Time Windows [10].

The VRP is a well-studied problem using several exact solution algorithms [11, 12]. For instance, arc-based formulations of the problem use classical methods such as branch-and-bound [13] and branch-and-cut [14] methods, while path-based formulations of the problem use column generation [15] and branch-and-price [16] methods. All of these approaches guarantee optimality upon algorithm convergence but suffer from exponentially increasing computational complexity for larger instances.

As a result, in order to tackle large problems most practical solvers either employ heuristics or are carefully tailored to the given problem. These approaches are significantly faster, but do not have the same optimality guarantee as exact approaches. Examples of these are classical algorithms such as local search and tabu search heuristics [17] or modern algorithms such as Adaptive Large Neighborhood Search (ALNS) heuristics [8]. Designing a good exact solver or heuristic is usually difficult, and these problems can be challenging even for metaheuristics [18].

Some modern approaches to solving VRP use machine learning techniques like reinforcement learning, which can be used to train a policy that solves the VRP to near-optimality [19]–but these methods are limited by the computational cost of dataset generation and training.

The infeasibility of exact solvers, paired with limits in the accuracy of approximate solvers, poses an obstacle to achieving minimal waste in complex food delivery. In addition, solvers used in practice are usually prohibitively expensive for small companies, limiting business efficiency and posing a financial burden; highlighting a need to develop efficient algorithms for optimal food distribution that can minimise waste and reduce prices to make nutritious food more accessible to consumers.

Potential Impact of a Quantum Solution

While classical heuristics for VRP are often insufficiently accurate and difficult to design, quantum algorithms present an alternative. Quantum algorithms have shown promise for efficiently solving complex computational problems, including VRP, in practice. However, there is no theoretical guarantee that quantum algorithms are fast, and more research is needed to determine if they outperform classical algorithms in practice. Present quantum hardware is limited by qubit count, connectivity, and error rates, restricting which quantum circuits can be implemented in practice. This poses a difficulty for testing the scalability of many quantum algorithms, including those for solving VRP. This use case aims at building on previous quantum algorithms for VRP to develop a repository of solvers for last-mile supply chain optimisation as a short-term proof of concept.

Vehicle routing is an example of a constrained combinatorial optimisation problem, as there are many practical limits on routes; such as truck capacity and delivery hours. As a result, VRP can be represented as a Quadratic Constrained Binary Optimisation (QCBO) problem. However, since optimisation with constraints is often difficult on quantum computers, many techniques for solving QCBO problems convert the formulation into a Quantum Unconstrained Optimisation (QUBO) problem. Constraints are added as penalty terms, enforced through projective measurement into the space of valid answers, or through post-selection of valid states.

There are already a number of QUBO formulations available for VRP and some of its variants [9, 11]. However, the number of variables required for these QUBO formulations is quadratic in the number of locations to be visited. This quickly becomes too large for conventional quantum computers for large numbers of locations. As a result, we will also investigate hybrid approaches based on classical road network graph reduction (e.g.,

coarsening, clustering), quantum processing of the smaller instances, and different encoding techniques aiming to reduce the required number of qubits.

There are a number of algorithms for finding the set of variables to minimise the QUBO objective including Quantum Approximate Optimisation Algorithm (QAOA) (and its variants) [20], Variational Quantum Eigensolver (VQE) (and its variants) [21], and Quantum Annealing [9]. QAOA and VQE are both hybrid algorithms which use classic optimisers to determine the parameters of the quantum circuit. Classical algorithms can also be used to find subproblems for the quantum algorithm using graph coarsening techniques [22] or to find good values of relaxation parameters [23].

It is expected that the hybrid approaches may accelerate the process of finding heuristically optimal solutions for VRP, but achieving this state would be long term. In the short term, one could develop a proof of concept of a quantum solver for finding optimal solutions for representative but downscaled vehicle routing problems, with relatively few vehicles (5-15) and deliveries (25-150). It is unlikely that this approach will give an advantage over classical algorithms at this scale, but could offer empirical insight into the scalability of quantum algorithms. This information is valuable for determining if a quantum approach could provide an efficient, scalable, and give way to an accessible solution for reducing waste from food delivery systems across the world.

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Team

Paweł Gora (Quantum AI Foundation), Brennan Lagasse (Yale University), Nouhaila Innan (Hassan II University of Casablanca and New York University Abu Dhabi), Abdullah Kazi (CQI and University of Mumbai), Ronit Dutta (Indian Institute of Technology, Kharagpur), Shreyas Patil (Indian Institute of Technology Bombay), Shaun Pexton (Yale University), Gabriel E. Marous (Yale University) Diya Naik (Yale University), José María Salvador (Yale University), Yuvan Chali (Yale University), Rohan Wassink (Yale University), Patrick Stokkink (Technical University of Delft), Yousef Maknoon (Technical University of Delft), Jose Alcocer (WFP).

SDG 3 – Good Health and Well-Being

Accelerating Novel Antimicrobial Discovery

3 GOOD HEALTH AND WELL-BEING

SHORT SUMMARY
Quantum simulation and quantum machine learning solution to accelerate the antimicrobial discovery and lower resistance.

QUANTUM APPROACH
Machine Learning and Quantum Simulation

TEAM ORIGINS

Context

The United Nations (UN) with the World Health Organization (WHO) have identified antimicrobial resistance (AMR) as one of the top ten threats to global public health [1, 2]. The latest figures estimate that in 2019, nearly five million deaths were associated with, and 1.3 million deaths attributable to, drug-resistant bacterial infections [3]. AMR has the potential to reverse decades of progress in fighting infectious diseases and undermine many aspects of modern medicine. If AMR is left unchecked, its annual death toll is expected to rise considerably, and according to some estimates could cost as much as 3.4 trillion USD to the global economy by 2030 [2].

Despite the pressing need to develop effective treatments for drug-resistant infections, most pharmaceutical companies have left the market to invest in more profitable areas, producing a "market failure" that has hugely exacerbated the AMR crisis. Today, as public and philanthropic investments attempt to overcome this failure, it is becoming increasingly evident that addressing market dynamics alone is insufficient. Promising new treatments often still fail to reach patients due to the lack of additional investment required for research and development; including funding for the discovery stages of fundamental research and preclinical work, to manufacturing and distribution capacity. This funding gap significantly hinders the development of novel antibiotics.

The challenge we face when addressing AMR is both a public health as well as a market failure. The greatest burden of AMR is in low- and middle-income countries with weaker healthcare systems and a greater lack of access to effective antibiotics. If this situation is not addressed, the continuous escalation of AMR will impinge on these health systems even further, with the impact disproportionately felt by people of lower economic standing, irrespective of where they live. It is a reality set to undo critical progress made towards universal health coverage and the sustainable development goals.

GARDP's Discovery and Exploratory programme is actively working in this discovery space in order to tackle these interrelated challenges. By leading discovery and early-stage research and working with relevant stakeholders from the beginning, GARDP accelerates the timely development of new antibiotics on behalf of all populations in need [4].

The current arsenal of clinically used antibiotics has largely resulted from screening efforts designed to identify broad-spectrum molecules that inhibit the growth of bacteria in standard laboratory growth conditions. However, despite an impressive number of compounds – on the order of a hundred used in the clinic – these only represent approximately 20 major structural classes and target a narrow range of cellular processes; namely cell envelope biogenesis, DNA replication, transcription, and protein biosynthesis. The small range of structural and functional classes of these broad-spectrum antibiotics has contributed to the increasing emergence and spread of resistance.

Despite advances in academic and industrial research, there is a limited ability to predict antibacterial activity or cellular accumulation of compounds, especially in gram negative pathogenic bacteria [5], requiring a costly empirical approach of synthesis and testing. A more accurate and higher throughput in-silico prediction of activity and accumulation ahead of experimental steps could create a dramatically more efficient drug discovery process.

Computational Challenges

Our failure to discover new antibiotics stems largely from the inability to thoroughly investigate the vast chemical space, with the largest screens for antibiotics consisting of only a few million molecules. This number is vanishingly small when compared to the theoretical number of drug-like molecules (~10^{60}) and considering that the molecules applied in these screening programs are limited in their structural diversity.

One approach to address this involves the application of machine learning algorithms that can predict antibacterial activity in-silico and lead to the discovery of highly interesting and novel antibacterial compounds [5, 6]. In generative AI, models are trained to build molecules piece by piece, assembling individual atoms and bonds into full molecules that have user-defined properties. The challenge remains in broadening the exploration of chemical spaces [7].

Another major hurdle is the prediction of accumulation of compounds in bacteria. This is a problem that is fundamentally chemical, but compounds must follow the physics-based laws of thermodynamics and classical electrodynamics in order to reach their target, with molecular properties required for different steps in the process. For the penetration of molecules into bacteria, physical properties such as volume, shape, electric charge, and electric dipole play crucial roles [8]. Moreover, the statistical behaviour of these properties is crucial [9]. One approach is to decompose the problem to the physical and chemical parts. This procedure relies on simulating the behaviour of molecules under physiological conditions. Molecular dynamics (MD) simulations are performed classically, while the quantum mechanical nature of molecules and interactions is included implicitly. Going beyond such an approach requires modelling the quantum dynamics of the molecules.

Potential Impact of a Quantum Solution

One alternative is to leverage innovative frameworks like quantum reservoir computing (QRC). Reservoir computing is a computational framework often used for time-series prediction and classification [10]. In its original description, it leverages a recurrent neural network (RNN) with fixed, randomly initialised weights in its hidden layer (the “reservoir"). This is thought to simplify the training by only adjusting the output layer. The reservoir serves as a dynamic system that projects inputs into a high-dimensional latent space, which could assist the capturing of complex relationships and patterns. Despite being mostly explored via the route of RNNs running on classical hardware (CPUs, GPUs), physical systems acting as reservoirs have been explored a great deal.

QRC has the potential to explore a broader range of chemical and biological interactions more efficiently than classical methods, while avoiding the difficulty in loading complex data on quantum computers. Recent studies using neutral-atom quantum computers have demonstrated the scalability, robustness, and general-purpose applicability of QRC for time-series and classification tasks. This suggests it could be particularly effective in predicting not only activity, but also accumulation and permeability properties in antibacterial drug discovery.

Reservoir computing has shown to be highly useful for dynamical property prediction and time series evolution [11, 12]. Both tasks are relevant for another major challenge in drug discovery, namely the prediction of accumulation of compounds in bacteria. Quantum hardware natively implements dynamics in high-dimensional Hilbert space and by encoding a molecule in this Hilbert space, it is natural to investigate the usage of

quantum hardware as a reservoir for molecular systems. Indeed, early studies [13, 14] have demonstrated some promising results.

Overall, there is ample evidence to support the claim that quantum reservoir computing is a potentially useful area of research and short-term application. Since full gate-based operation and logical qubits are not prerequisites, QRC could be explored on modest quantum devices that exist currently. Usage of QRC for higher throughput/accuracy in-silico prediction of activity and accumulation holds the potential to dramatically improve the efficacy and effectiveness of the early antibacterial drug discovery process.

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Team

Alan Hennessy (GARDP), Kenneth Heitritter (qBraid), Tarini Hardika (qBraid), James Brown (qBraid), Jon Stokes (McMaster University), Matteo Ceccerelli (University of Cagliari), Stefan Milenkovic (University of Cagliari), Alain Labrique (WHO).

Predicting Gastrointestinal Cancer

3 GOOD HEALTH AND WELL-BEING

SHORT SUMMARY
Quantum machine learning solution to improve accuracy of gastrointestinal cancer diagnosis and speed up medical treatment and prevention.

QUANTUM APPROACH
Machine Learning

TEAM ORIGINS

Context

More than two million new cases of colorectal cancer are diagnosed every year around the world [1, 2, 3], affecting the entire global population, in particular people above the age of 45-50. The incidence of colorectal cancer in Europe is higher in men (79 cases per 100000 people) than in women (54 per 100000). Colorectal cancer remained the second leading cause of cancer-related deaths, accounting for 12-14% of all cancers recorded in Europe in 2012 [1], and contributes 14 billion USD to annual healthcare costs in the United States alone. In Asia, incidence rates range from 49.3 in Japan, 24.7 in South Korea, and 35.1 in Singapore [4], with rates equally high in many African [5] and South American countries [6]. From the data, it is clear that colorectal cancer is a global challenge, not just a problem in the Western world.

The World Health Organization's (WHO) recommendations for SDG 3 target the reduction of premature mortality from non-communicable diseases by one-third through prevention and treatment and promoting mental health and wellbeing [3], with a specific resolution on colorectal cancer [7].

Current scientific breakthroughs enable the development of non-invasive, high-quality imaging, energy-efficient and miniaturised electronic devices that can travel through the gastrointestinal tract using natural body cavities [2]. The potential of applying non-invasive technology to the screening of large groups in the 45-50 age group, could significantly reduce the number of new cancer cases diagnosed each year at an advanced stage of progression. However, to date, there are only few ingestible devices that have successfully reached clinical practice, partly due to the novelty of the information they provide and due to the challenges of adding this new technology to established clinical paradigms [8].

Computational Challenges

The issue of an advanced medical imaging strategy is that if successfully orchestrated, this paradigm change would produce trillions of gastrointestinal tract images, taking an unprecedented number of hours to process and analyse; presenting an intractable challenge from a human resources (medical teams capable of screening and diagnosing pathologies from manual inspection of images) and computational (high-performance computing data centres) perspective. Despite the challenge of accessing high quality data, medical teams could benefit from novel computational tools and methods to increase prevention and diagnosis on a large scale, with possible support through unconventional and highly efficient novel computational approaches. Such approaches to image analysis could then be explored by both molecular and biologic markers to provide insight into disease risk or onset.

Potential Impact of a Quantum Solution

Quantum computing could offer transformative potential for artificial intelligence in medical imaging, in particular for early colorectal diagnosis, building on current scientific computing technology and algorithms to address future challenges.

Classical machine learning strategies struggle with the computational load of analysing billions of hours of gastrointestinal tract images, and high-performance computing resources are costly and consume significant power. By using quantum computing, we could solve some complex optimisation and pattern recognition tasks more efficiently [9, 10]. This could improve efficiency in image processing and diagnosis, enabling near real-time analysis as well as diagnosis accuracy.

In the classical approach using Convolutional Neural Networks (CNNs), both transfer learning and ensemble learning are used. In a quantum approach, Quantum Neural Networks (QNNs) and Quantum Support Vector Machines (QSVMs) [11] could enhance the efficiency and accuracy of image analysis. Quantum-enhanced features space could provide more nuanced insights from the data– perhaps even improving detection rates. Another possibility could be to exploit Quantum Reservoir Computing (QRC), an extension of the classical Reservoir Computing (RC) paradigm to the quantum domain intersecting quantum computing and neural networks [12, 13].

Developing quantum algorithms specifically tailored for AI tasks and medical imaging is complex. Ensuring reliable and accurate results from quantum computations is also a major hurdle, especially in sensitive applications like medical diagnosis. Efficiently encoding large medical imaging datasets into quantum states and accurately reading out the results are not trivial tasks. Therefore, quantum data encoding methods must be developed to handle the complexity and size of medical imaging data. Given the limited capability of current quantum computers, this medical imaging use case could be explored in the short term with quantum simulators, running artificial intelligence kernels with a higher number of simulated qubits.

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Team

Gabriel Falcão (IT, University of Coimbra), Jorge Lobo (ISR, University of Coimbra), Ana Beatriz Morgado (IT, University of Coimbra), Tomás Costa (University of Coimbra), Laura Scherzberg (University of Coimbra), Iara Bento (University of Coimbra), João Martins (University of Coimbra), Cláudio Gomes (CMU-Portugal), Vitor Silva (IT, University of Coimbra), Sridhar Tayur (Tepper School of Business, CMU), Susana de Noronha (Center for Social Studies), Pedro Narra Figueiredo (Faculty of Medicine, University of Coimbra), Partha Basu (IARC), Alain Labrique (WHO).

SDG 6 – Clean Water and Sanitation

Water Leak Detection

6 CLEAN WATER AND SANITATION

SHORT SUMMARY
Quantum simulation to optimally position sensors and detect water leaks in urban water systems.

QUANTUM APPROACH
Optimisation

TEAM ORIGINS

Context

Our planet is becoming more water-scarce. Not only is the global population, particularly the urban population, expanding at an unprecedented rate, but climate extremes result in droughts and flooding in many parts of the world. The ageing infrastructure to collect and distribute water is unable to cope with such demands. By 2050, close to 70% of the world's population will live in urban space, although 60% of that space has yet to be built [1]. Aside from the usual urbanisation trends, migration due to climate and conflicts further exacerbates the situation.

Along with urban development comes the need for adequate water. As a result of increasing populations, many water supply systems are stretched to supply populations beyond their design capacity. Such systems have often not been properly maintained and lack the necessary investment to ensure service levels, especially amongst marginalised groups. The increasing trend towards privatisation and commercialisation of water services had further impacted investments by diverting funds to shareholders, rather than maintaining the infrastructure [2]. Those most affected by lack of access to water are the underserved communities in urban settings.

Current levels of unaccounted-for-water (UFW) are often in excess of 50% in many urban settings [3]. This means that of the water resources that are collected and treated, at least half is lost through leakage, system losses or illegal connections. Complex water reticulation systems and pipe networks are difficult to monitor. Without this basic level of measurement, interventions to manage the losses are almost impossible.

Many regions of the world are already water-scarce, but the number of countries affected will undoubtedly increase [4], with Arab countries and many African countries severely affected. It can be expected that many developed regions in Europe and North America will be faced with critical “day-zero” type scenarios, which have already been experienced in Cape Town, RSA and Sao Paolo, Brazil [5]. Currently, Mexico City is precariously close to “day-zero” [6].

Leak detection is critical to understanding the management of water distribution networks and is done through the provision of bulk-metering and zoning of the network. By analysing the results on water use, in particular night-flows, it is possible to quantify leakage losses with reasonable accuracy.

Optimising both the position and number of metres required for any given network impacts the ability to provide the information required to quantify losses and examine the various scenarios for repair and rehabilitation. Current methods for metering are based on expert judgement and experience. Having more efficient ways to determine optimum metering would reduce initial investments significantly.

Computational Challenges

A water distribution network can be represented as an undirected graph with nodes (pipe junctions/hydraulic installations) and edges (pipes). The dynamics of the water in the network is typically controlled and monitored with a limited number of sensors located at several places in the network. When a leak occurs at a specific location, there is in general a nonlinear signature in the physical quantities (mostly pressure drop) at different locations in the network.

In most cases, the number of sensors used for localising leaks is determined by the number of devices available [8]. This limitation makes it essential to optimise sensor placement to maximise the monitoring effect of these sensors on the water distribution network. An example is given by the Philadelphia Water Department. With a large and complex water distribution network consisting of over 3,000 miles of pipes, the department has a limited budget for installing sensors to monitor water quality, pressure, and flow rates [9]. The guiding principle is to place sensors with an optimal geolocation spread in order to cover the network as much as possible.

It is, however, conceivable to imagine a more optimal placement of a potentially even smaller number of sensors. This gives rise to considering the sensor placement as an optimisation problem under constraints [10], where one must place an optimal number of sensors at tactical positions. To achieve this, it is necessary to combine multiple features, such as the topology of the water network, sensor data, leak signatures, and give other considerations to factors such as the environmental impact in case of leakage hazards.

Optimising the sensor placement in a given water distribution network can be formulated as a Maximum Weighted Independent Set (MWIS) problem that can be enriched by taking into account a typical budget requirement–such as the maximum number of sensors–and can be formulated as a quadratic unconstrained binary optimisation (QUBO) problem. Like any combinatorial optimisation problem, the MWIS problem can be addressed by either exact or approximate algorithms and heuristic methods.

The main bottleneck to tackle the MWIS is its combinatorial nature (NP-hard), which limits the size of the network that can be efficiently considered. Exactly solving the MWIS problem, especially for large and complex graphs, remains a challenging task, but understanding the structure and properties of specific graphs can lead to solutions more efficiently. For the optimal placement of sensors, it requires searching for approximate high-quality solutions.

Potential Impact of a Quantum Solution

The complexity of this problem makes it a significant focus for research in quantum computing. State-of-the-art quantum approaches to MWIS span hybrid quantum-classical algorithms, quantum annealing (leveraging the QUBO formulation of the problem), gate-model algorithms like Quantum Approximate Optimisation Algorithm (QAOA), integration with classical techniques like branch-and-bound, and quantum-enhanced machine learning.

One quantum approach that looks particularly promising is the use of Neutral Atom Quantum Processors, which have a unique advantage in natively embedding complex graph-structured problems like MWIS at the hardware level, yielding a potential advantage in terms of implementation, scalability and performance. When mapping the water network onto a two-dimensional lattice of individual neutral atoms using optical tweezers, each node of the graph corresponds to one atom in this array.

The first step towards solving the sensor placement problem is to use the analogue quantum computing mode to create a set of potential solutions to the MWIS problem. The next step involves a cost function that maximises the sum of the weights and gives at an output the desired WMIS.

Given the analogue neutral atom quantum computing devices currently available [11, 12], it is possible to consider a small-scale proof of concept of this optimal sensor placement problem, and a larger-scale implementation in the mid-term plan.

While this quantum computing method is particularly suitable for applications such as leak detection in water distribution networks, it is possible to imagine other broader applications involving complex networks that can be modelled in the form of weighted graphs, such as road networks or telecoms networks.

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Team

Laurent Querella (QClavis), Maëlle Toy-Riont-Le Dosseur (Reply), Quentin Ma (Reply), Louis Barcikowsky (Reply), Graham Alabaster (UN Habitat), Mourad Beji (Pasqal), Louis-Paul Henry (Pasqal).

Eliminating "Forever chemicals" From Water Sources

6 CLEAN WATER AND SANITATION

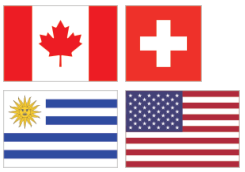
SHORT SUMMARY

Quantum simulation of the decomposition of "forever chemicals" (Poly-fluoroalkyl substances (PFAS)) for more efficient removal in water, limiting physiological and environmental harm.

QUANTUM APPROACH

Quantum Simulation

TEAM ORIGINS



Context

Poly-fluoroalkyl substances (PFAS) are synthetic chemicals ubiquitous in everyday products, such as Teflon pans, food packaging, and water-resistant clothing [1]. Despite their versatility, PFAS negatively impact human health and the environment. PFAS are also known as "forever chemicals" because they persist in the environment and are challenging to eliminate; they are even found in the human bloodstream [2]. The human impacts are so pervasive that when 3M attempted to test the effect of PFAS on human health in 1997, they failed to create a "control" group and could not find anyone without PFAS in their blood, suggesting widespread exposure [3]. PFAS accumulate in the environment and have been detected even in remote areas [4]. Even at low concentrations, PFAS are linked to reproductive problems, immune system dysfunction, and cancer [5]. The overarching goal of this use case is to support Good Health and Wellbeing (Target 3.9: Reduce Illness and Death from Hazardous Chemicals and Pollution) and Clean Water and Sanitation (Target 6.3: Improve Water Quality, Wastewater Treatment, and Safe Reuse) [6, 7] by eliminating PFAS from water sources globally.

Although PFAS are found everywhere, water is a consistent source of exposure, consumed and used by people every day. In a recent study, two of the most widely-used PFAS, Perfluorooctanoic acid (PFOA) and Perfluorooctane sulfonate (PFOS), exceeded limits set by the Environmental Protection Agency (EPA) in both private and public water sources across the United States [8]. According to the EPA, there is technically no safe amount of exposure to PFOA or PFOS. As such, the EPA's maximum contaminant level goal for these PFAS in drinking water is zero exposure [9].

The World Health Organization (WHO), Organization for Co-operation and Development (OECD), and UN-Habitat tackle the harmful effects of substances like PFAS by facilitating global information exchange, finding safer chemical alternatives, and assessing risks [10, 11, 12]. UN-Habitat has recently produced a report on treatment of wastewater [13], indicating we are a long way off reaching the SDG 6.3.1 goal of reducing by half the proportion of wastewater safely treated, and have not yet begun to address many of the micro-pollutants such as PFAS. In 2024, reporting on industrial wastewater treatment remains limited, with data only reported from 22 countries representing 8% of the global population. In these countries, only 38% of industrial wastewater was reported as treated, and only 27% was safely treated. Despite these coordinated efforts, there are no current solutions that completely eliminate PFAS. Rather than putting the burden on the individual user, removal systems installed at the water treatment plant would provide equal access to PFAS-free water. This is especially important in underserved areas, like developing countries, where treatment at the point of use may not be available. Domestic treatment systems usually only address drinking water – excluding water for showers, washing clothes and dishes, or water for lawns, pools, and gardens. Eliminating PFAS at the source would further reduce human exposure from routes other than drinking water.

The impact of widespread PFAS exposure not only decreases overall wellbeing, but also creates an unnecessary economic burden. The Nordic Council of Ministers estimates that

the annual healthcare cost of PFAS exposure in Europe is €52-84 billion [14]. When expanded globally (including remediation costs), the total societal cost of PFAS is staggering, at €16 trillion [15]. Waste streams containing PFAS also contaminate groundwater and negatively impact the environment. PFAS tend to bio-accumulate in animals, acting as an additional source of human exposure [12, 16]. Destroying PFAS instead of filtering them out into concentrated waste would eliminate the need for waste disposal methods and increase the supply of water that can be used for consumption, supporting the Sustainable Cities and Communities SDG. Knowledge gained from this use case could directly inform approaches for regulatory agencies, decrease liability for manufacturers of products with PFAS, and advance technology for mobile and rapidly-deployable solutions to treat PFAS-contaminated water in underserved communities.

Computational Challenges

There are several existing technologies to reduce PFAS contamination, including granular activated carbon, ion exchange, sonochemical degradation, and reverse osmosis. As of yet, none of these solutions completely eliminate PFAS [1, 17]. Breaking PFAS bonds is a particularly difficult chemical challenge; PFAS have a high concentration of fluorine, the most electronegative element. Fluorine's powerful electronegativity causes uneven electron clustering, resulting in a partial ionic charge; the resulting carbon-fluorine interaction is one of the strongest single bonds in chemistry. Modelling PFAS properties and interactions, such as reaction pathways and transition states, can help elucidate mechanisms of enzymatic degradation. Computational modelling can also identify materials such as adsorbents, membranes, or catalysts, which could be used to make better treatment systems or augment existing ones. Historically, modelling PFAS molecules computationally has been challenging due to the high number of carbon-fluorine bonds. Each CF2 bond adds 18 valence electrons, increasing the complexity of calculations needed to model them accurately. Using classical methods, the largest calculations can consider up to 1012 determinants, while PFOA requires 10151 determinants to calculate its exact energy [18].

Computational chemistry modelling is accomplished via classical or quantum mechanical methods. Classical mechanics, also known as the "force field" method, uses existing experimental data and ab initio computation results to determine the forces acting on the molecule. This approximates the molecule's energy, which can be used to predict its dynamics, reaction rates, and mechanisms. Classical methods are generally used when the electronic information is not required to compute a specific property, or when the system size prohibits modelling the system using the Schrödinger equation due to computational requirements. The data and accuracy achieved with classical methods is limited, as only quantum methods can provide structural information at the electronic level. Post-Hartree-Fock methods can be used to include electron-electron interaction, which is essential for bond dissociation modelling or density functional theory (DFT). The latter reduces computation scaling by using the electronic density instead of all the electronic degrees of freedom. Coupled-cluster theory (CCSD(T)) is the gold standard for computational chemistry; it is more accurate than DFT, but is not feasible for large molecules like PFAS [19].

The most accurate PFAS modelling to date was recently accomplished, using the incremental full configuration interaction (iFCI) method [20, 21]. The iFCI method addresses the problem of scalability by separating large molecules into smaller, more manageable pieces. This significantly decreases the number of determinants needed for accurate calculations. These independent molecular problems can be solved simultaneously on distributed computing, shrinking calculation time to less than a day. This novel application of the iFCI method creates a foundation for further research of PFAS chemistry, using quantum methods on quantum computers.

For such quantum solutions, there is a need to access many types of PFAS data, such as the freely available online Data Hub for PFAS, which includes: lists of over 4,000 known PFAS, suspected PFAS that have not been identified yet, PFAS structures and chemical properties, a list of over 40,000 sites in the United States that are suspected sources of PFAS, water quality data, contaminated water sources, compliance information, and PFAS biomonitoring. Additionally, the Forever Pollution Project identifies over 23,000 confirmed and 21,000 suspected contamination sites in Europe [22]. Despite PFAS' presence in all environments, global PFAS data is notably lacking.

Potential Impact of a Quantum Computing Solution

Incremental full configuration interaction molecular type of simulations could be augmented with quantum methods to model increasingly complex PFAS molecules. Accurate representations of PFAS, their interactions, and their respective bond dissociation energies require information at the quantum level. Achieving this would lead to insights on the feasibility of breaking the C-F bonds that make PFAS so challenging to destroy, and would eventually inform paths to materials that can efficiently break the bonds; including materials that could make up treatment systems to best sequester PFAS for destruction. Quantum phase estimation (QPE) and/or quantum imaginary time evolution (QITE) algorithms could be employed on quantum computers to tackle this problem. These algorithms are preferred over variational quantum algorithms (VQAs), such as the variational quantum eigensolver (VQE), because VQAs are prone to barren plateaus and optimisation challenges [23]. QPE and QITE circumvent these issues by not requiring an optimisation algorithm [24], which is necessary to augment iFCI molecular simulations [25, 26, 27].

Alternatively, it would be possible to use a derivative of the QITE algorithm, which uses classical information to construct operations on a quantum computer [28]. Once this is achieved, a proof-of-concept experiment with a simplified approximation of a realistic molecule–such as trifluoroacetic acid (TFA) to represent the family of perfluoroalkyl carboxylic acids, or trifluoromethanesulfonic acid (TFMS) for perfluorosulfonic acids–could be performed on near-term quantum computers. This proof of concept would be possible to perform with today's quantum computing hardware, paving the way in the exploration of more efficient removal of "forever chemicals" in water.

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Team

Valentin Senicourt (SandboxAQ), Alexandre Fleury (SandboxAQ), Erika Lloyd (SandboxAQ), Rafael Sotelo (Quantum South), Pauline Bekkers (UN Habitat), Graham Alabaster (UN Habitat).

Molecular Docking to Clean up Pollution

6 CLEAN WATER AND SANITATION

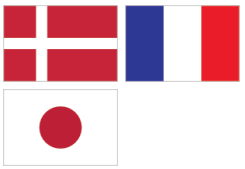
SHORT SUMMARY

Quantum simulation and quantum machine learning solution to accurately model the chemical process of molecular docking involved in removing organic pollutants in water.

QUANTUM APPROACH

Machine Learning and Quantum Simulation

TEAM ORIGINS



Context

Chemical pollutants in soil and wastewater pose a significant and long-lasting environmental and sanitary concern, with their degradation in environmental remediation representing a critical societal challenge. Contaminants, including pesticides, industrial chemicals, and pharmaceuticals, present substantial risks to human health and ecosystems [1]. Addressing this issue is crucial for ensuring environmental sustainability and public health, aligning with several United Nations Sustainable Development Goals (SDGs), particularly SDG 6 - Clean Water and Sanitation [2].

Among various pollutants, phenol stands out as a significant chemical contaminant present in wastewater. There are many variants of phenol molecules with differing levels of toxicity, many of which are classified by the WHO as dangerous in drinking water [3]. Phenol arises from petrochemical and pharmaceutical industries [4] and alongside its vapour contains toxic compounds that can have a serious impact on health. Erosive to the respiratory tract, skin, and eyes, it can cause pulmonary edema, tracheal ulcerations, corneal damage, and blindness [5]. Chronic exposure can also lead to renal, liver, and heart damage, underscoring the urgency of effective remediation strategies [6].

The impact of organic pollutants like phenol is widespread, but certain populations and regions are more vulnerable due to socio-economic factors, geographical location, and industrial activities. Urban populations in cities with significant industrial activities, such as in China, India, and parts of the United States, face high levels of organic pollutants [7]. Rural areas dependent on agriculture often use pesticides and fertilisers containing organic pollutants, leading to soil and water contamination in regions such as Southeast Asia and Latin America, affecting both the environment and human health. Coastal communities, such as those in Southeast Asia, the Gulf of Mexico, and the Mediterranean, are particularly vulnerable to marine pollution from industrial discharges and agricultural runoff, impacting fishing industries and local food supplies. Indigenous populations, often relying on natural resources, are disproportionately affected by pollution. Areas like the Amazon basin and the Arctic face threats from organic pollutants accumulating in the environment, jeopardising traditional ways of life and local ecosystems [8].

The persistence of such pollutants in our environment necessitates innovative approaches leading to more efficient and cost-effective ways for their removal and degradation.

Computational Challenges

Several techniques have been developed to degrade phenol in wastewater, each offering unique benefits but also presenting specific limitations. Advanced Oxidation Processes [9]–particularly photo-Fenton and heterogeneous photocatalysis–are among the most promising methods for phenol degradation. Alternatives are electrochemical oxidation, adsorption, and membrane filtration [10]. The downside of these methods is their high energy costs and the need for specialised equipment. Bioremediation leverages microorganisms to degrade phenol into less harmful products under aerobic or anaerobic conditions [11], although slower and less effective at high phenol concentrations.

Computational tools, such as molecular modelling, enzyme docking, and machine learning, can significantly accelerate the development of optimised treatment strategies. These methods enable researchers to simulate enzyme-substrate interactions and predict how microorganisms or catalysts interact with phenol, leading to more targeted engineering of enzymes or catalysts for enhanced degradation. Additionally, machine learning algorithms can analyse large datasets from treatment processes to identify patterns and optimise operating conditions. Integrating these computational approaches, one can reduce the reliance on trial-and-error experiments, speed up innovation, and develop more effective solutions to the problem of phenol degradation [12].

Currently, the state-of-the-art approach in simulating enzyme docking includes a variety of computational methods that predict how enzymes interact with substrates like phenol. These methods range from molecular docking, which provides fast predictions of binding modes, to more complex techniques, such as molecular dynamics (MD) simulations, quantum mechanics/molecular mechanics (QM/MM) hybrids, and machine learning-based approaches [13]. Molecular Dynamics (MD) [14], Quantum Mechanics/Molecular Mechanics (QM/MM) Hybrid Methods [15] are useful to explore the dynamic behaviour of enzymes and catalytic reactions, while De Novo Design [16] integrates structure-based, dynamics-based, and QM-based approaches to design new enzyme active sites capable of degrading phenol. Alternatively, Machine Learning-Based Methods [12, 17] use algorithms trained on large datasets to predict enzyme-phenol interactions and identify beneficial mutations. Each of these methods offers distinct advantages, from large-scale screening to capturing the nuanced behaviour of enzyme-substrate interactions. However, these methods are limited by the assumptions made during simulations, computational expense, and scalability. Despite their advancements, many existing approaches still fall short in accuracy and efficiency.

However, these methods are constrained by their reliance on approximations and significant computational resources. As a result, classical methods often struggle to accurately model enzyme-substrate interactions, particularly for large, complex systems such as those involved in phenol degradation. These shortcomings slow down the discovery of effective enzymes, increase research costs, and delay the implementation of environmentally beneficial solutions for pollutants like phenol.

Potential Impact of a Quantum Solution

Quantum computing could help to model the complexity of enzyme dynamics, quantum effects in catalysis, and large conformational spaces more efficiently. In particular graph-based methods are promising to model enzyme-substrate interactions. In this reformulation of the molecular docking problem, the binding interaction graph represents potential contacts between the enzyme and the phenol molecule, with each vertex corresponding to a possible interaction point and edges indicating compatible interactions. The complexity of this graph problem is a key factor in why classical methods struggle and why quantum computing offers a potential advantage. Finding the maximum clique or dense subgraph in a large graph is known to be NP-hard, meaning that the required computational resources grow exponentially with the size of the graph for classical algorithms. This exponential scaling makes it infeasible to solve these problems exactly for large molecular systems using classical computers.

Quantum computing, specifically the Boson Sampling approach, offers a way to address this complexity, through single photons identifying dense subgraphs [18]. The quantum nature of the computation could allow for the exploration of the vast solution space more efficiently than classical algorithms. This approach is particularly well suited for implementation on near-term photonic quantum computers.

In addition, fermionic simulations could be leveraged to compute the binding energies of these docking sites. Quantum algorithms such as the Variational Quantum Eigensolver (VQE), are well-suited to modelling the electronic structure of molecular systems in the near-term devices. By accurately evaluating the binding energies of the dense subgraphs generated by Boson Sampling, configurations could be prioritised based on their energetic stability.

A small-scale proof of concept could be run on existing photonic quantum processors, while simulations on GPU-enhanced classical simulators would help to study the scaling of the proposed method for larger systems, providing insights into the potential advantages as we move to more complex enzymes and substrates. With steady advancement of the quantum processors, moderately sized molecules relevant to phenol degradation could be studied to ultimately implement full-scale analyses of complex enzyme-pollutant interactions.

Quantum computing could enable more accurate and faster predictions of enzyme-substrate interactions, leading to better candidate identification for phenol degradation. This, in turn, could accelerate the development of sustainable bioremediation methods, reduce experimental costs, and offer scalable solutions for tackling industrial pollutants, directly aligning with environmental and industrial goals.

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Team

Samuel Horsch (Quandela), Brian Ventura (Quandela), Jiabao Chen (QunaSys), Ronin Wu (QunaSys), Alain Labrique (WHO).

SDG 7 – Affordable and Clean Energy

Layout of Turbines in a Wind Farm

7 AFFORDABLE AND CLEAN ENERGY	**SHORT SUMMARY** Quantum optimisation solution to efficiently layout turbines in a wind farm and maximise the power produced.	**TEAM ORIGINS** 
	QUANTUM APPROACH Optimisation	

Context

Climate change is a global crisis– as the climate becomes increasingly unstable, we can expect more extreme weather events, rising sea levels, and the loss of critical habitats worldwide. A primary driver of climate change is the emissions generated from the burning of fossil or biomass fuels. To combat this, we must look for more renewable ways to produce energy, cutting back our reliance on emission-producing fuels.

According to the United Nations, the world still faces significant challenges in achieving universal energy by 2030; improving the efficiency of wind farms directly supports this goal, by providing a more reliable and cost-effective source of renewable energy. This can help increase energy accessibility, particularly in regions with limited electricity, and contribute to global efforts to meet SDG 7 [1]. Wind energy offers significant potential to reduce our reliance on fossil fuels and mitigate the negative impacts on the environment. By improving the efficiency of wind farms, we can do our part to work towards a sustainable future. This also enables a move towards two urgent targets: energy security and net-zero concerning carbon emissions. Within this, there is a huge increase in wind power required. The latest European Union target for renewable energy requires more than doubling wind power generation from 204 GW (2022) to greater than 500 GW (2030) [2].

Wind farms provide a powerful means for countries to produce independent, clean energy. The efficiency of these farms is crucial, especially for nations with limited financial resources, where optimising energy output is vital. Countries like Argentina, Colombia, Egypt, Indonesia, and Morocco [3], are currently developing wind farms, and will benefit significantly from improved efficiency as a result. Additionally, wind farms contribute to infrastructure development and job creation, driving economic growth (SDG 8). Energy independence also enhances national security and reduces reliance on external sources (SDG 9).

Despite its potential, there are numerous challenges in making wind energy both economically viable and reliable [4]. One of the most significant challenges is optimising the layout of wind farms to maximise energy output. The largest onshore wind farm in the world is the Jiuquan Wind Power Base, also known as the Gansu Wind Farm, containing over 7,000 turbines and with a capacity of 10 GW [5]. Choosing the best placement of all the turbines must account for many factors, including environmental, economic and infrastructural. This involves complex and computationally intensive optimisation problems, especially as windfarms grow to such size and complexity.

Computational Challenges

In wind farm layout optimisation (WFLO), one key factor reducing wind farm efficiency is the wake effect, where upstream turbines disrupt wind flow, and reduce the power generated by downstream turbines. Modelling these wake effects is difficult, as the model should include multiple wind regimes and interactions between more than two turbines.

The Jensen wake model [6] uses the linear superposition expression to accurately capture these effects, calculating the reduced wind speed downstream in a way that can be optimised fairly efficiently. Jensen's wake model is simplistic but easy to compute, which helps during the optimisation process. However, this simplicity ignores some effects, which in individual cases, can lead to misestimation of the velocities in the wake. Other models are available, but can sometimes take much longer to compute.

The WFLO problem is solved classically using advanced (Genetic) Random Search algorithms [7]. These allow for multiple, possibly disconnected, polygons with continuous turbine placements, which have been tested on cases with hundreds of turbines. The WFLO that has so far discussed is specific to onshore or fixed offshore wind turbines. Newer types of turbines, such as floating offshore, have many more degrees of freedom, meaning that further modelling (and more computationally costly evaluations) is needed.

The classical industry standard for finding high-quality solutions to QUBO problems [8] is the Gurobi optimisation software [9]. The precise working of this algorithm is not open source, although it is known to use multiple different algorithms as well as intelligent initial condition selection.

Potential Impact of a Quantum Solution

Quantum computers may offer a way to find high-quality windfarm configurations faster or more accurately than classical approaches. To address WFLO using quantum computing, wind farms can be discretised into a grid and mapped to a quadratic unconstrained binary optimisation (QUBO) problem. Once in this form, the search space grows exponentially with the number of variables, a characteristic that quantum computers can naturally handle by scaling resources linearly, allowing the problem to scale more efficiently on quantum hardware. This QUBO formulation follows previous work for this problem's application to quantum annealers, which allows us to leverage quantum computing through two variational mappings: Hamiltonian and Pauli correlation encoding (PCE).

Using the Hamiltonian mapping, the QUBO problem is transformed into a distinct diagonal Ising Hamiltonian, with its ground state corresponding to our solution as a basis state. When applying the PCE-based method, we map binary variables to the expected values of correlation variables, which can independently range from -1 to 1. Due to their independent variability, we can find a combination that solves the QUBO problem in its spin form. The PCE mapping allows us to have N correlation variables, where N can exceed the number of qubits.

Alongside these variational approaches, quantum annealers are purpose-built machines for QUBO problems, and they might also offer an efficient quantum methodology. We must investigate these to test their relative performance, including issues such as qubit connectivity. Finding high-quality solutions faster will allow better fine-tuning and improved efficiency, leading to a greater share of energy from renewable sources.

There are very few studies that report on the potential use of quantum computers to solve the WFLO problem. The goal is to compare these quantum methods with the industry-standard Gurobi, breaking down their effectiveness on real-world problems, where optimal and near-optimal solutions are crucial. By investigating the scalability of these algorithms, we can evaluate their future usefulness, providing a foundational step in their development. Specifically, comparing approaches with higher qubit counts but smaller parameter spaces versus larger parameter spaces with fewer qubits will help guide the direction of future algorithms.

As part of assessing the usefulness of quantum computing for this optimisation use case with potential impact in transitioning to renewable energy sources, one would also need to explore high-performance computing, including the potential for parallelising the

optimisation process. Tests could be done on circuit-based algorithms on digital quantum processors as well as on quantum annealers. Short term, a standard test case of a 10x10 grid size, requiring 100 qubits for the VQE and ~ 8 qubits for the PCE. Longer term, these high qubit/high gate count circuits would require investigations into error mitigation.

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Team

James Hancock (University of Plymouth), Craig McNeile (University of Plymouth), Matthew Craven (University of Plymouth), Ruthwika Vemulapalli (G.Narayanamma Institute of Technology and Sciences).

Smart Grid Management

7 AFFORDABLE AND CLEAN ENERGY

SHORT SUMMARY
Quantum optimisation solution to improve the management of large energy grids and efficiently distribute energy.

QUANTUM APPROACH
Optimisation

TEAM ORIGINS

Context

Meeting the world's increasing energy demands while incorporating renewable sources for a sustainable future requires efficient and reliable management of electrical grids [4]. By optimising grid management, it is possible to better integrate renewable energy sources, reduce energy losses, and ensure a stable supply of electricity. This is crucial for providing affordable energy and a stable power supply to all, especially in areas with growing energy demands; supporting the transition to sustainable energy systems. According to a report by the US Department of Energy [1], grid modernisation efforts have shown potential for significant improvements in energy efficiency and reliability. This challenge relates to SDG 7 (Affordable and Clean Energy), SDG 9 (Industry, Innovation, and Infrastructure), and SDG 13 (Climate Action). In particular, within SDG 7 it directly aligns with target 7.3 to "Double the improvement in energy efficiency" and target 7.5 to "expand and upgrade energy services for developing countries" [2].

The International Energy Agency (IEA) has also highlighted the importance of electricity grid improvements in their report on 'Electricity Grids and Secure Energy Transitions' [3]. The IEA report emphasises the critical role of grids in clean energy transitions and stresses the need for adding or refurbishing over 80 million kilometres of grids by 2040, equivalent to the entire existing global grid. This expansion is essential to decarbonise electricity supply and effectively integrate renewables. The IEA also notes that modern and digital grids are vital to clean energy transitions, as the need for system flexibility is expected to double between 2022 and 2030, in order to meet national climate goals.

Smart grid management is a cornerstone of modern infrastructure, supporting the development of resilient infrastructure by enhancing the grid's ability to adapt to real-time supply, demand fluctuations and integrate various energy sources.

The challenge of efficient grid management is global in nature, affecting both developed and developing countries. In developing nations, improved grid management can lead to more reliable access to electricity, supporting economic growth and quality of life improvements for millions of people. By optimising the integration and management of renewable energy, this use case would help mitigate the impact of climate change.

Computational Challenges

Currently, smart grid management problems are approached using various classical computational methods [4].

1. Linear and Mixed-Integer Programming: Used for solving resource allocation and scheduling problems.
2. Heuristic Algorithms: Such as genetic algorithms and particle swarm optimization, used for multi-objective optimization problems.
3. Machine Learning: For demand forecasting and anomaly detection in grid operations.

These computational models are useful because they allow for simulation of complex grid scenarios, optimisation of resource allocation, and prediction of demand and supply fluctuation. Available datasets typically include historical and real-time power

consumption data, weather data for renewable energy forecasting, grid topology, and capacity information–alongside energy market pricing data.

Many optimisation problems in grid management, such as resource allocation or power flow optimisation, are NP-hard problems, meaning that as the size of the problem increases, the computational resources required to solve it classically grow exponentially. These methods struggle with the complexity and scale of modern power systems, especially when integrating large-scale renewable energy sources. The main challenges include:

- Real-time optimisation: Classical methods often struggle to provide optimal solutions in real-time for large-scale grid systems.
- Handling uncertainty: Renewable energy sources introduce significant uncertainty, which is difficult to model and optimise using classical methods.
- Multi-objective optimisation: Balancing conflicting objectives like cost minimisation, emission reduction, and stability maximisation is computationally intensive.

The introduction of quantum computing could offer new possibilities to address the challenges mentioned above. Quantum algorithms have the potential to explore larger solution space, providing more efficient solutions for complex grid optimisation problems.

Potential Impact of a Quantum Solution

One quantum approach is to use a Quantum Approximate Optimisation Algorithm (QAOA) [4] for combinatorial optimisation tasks, such as resource allocation and scheduling in grid management. Nested algorithms like HHL [5] within QAOA [6] could be used when linear systems need to be solved as part of the larger optimisation problem, for example in power flow calculations.

While the full potential of QAOA is still being explored, recent research suggests it may offer usefulness for certain optimisation problems. A study of benchmarking quantum algorithms for combinatorial optimisation provides insights into the comparative performance of different approaches [6, 7], anticipating that a first implementation could be anticipated on near-term devices. A nested variational quantum algorithm approach –such as QAOA in QAOA [9] and HHL in QAOA [10]–would allow for both the use of hybrid algorithm approaches and the ability to parallelise compute tasks. This would enable larger quantum algorithms to be subdivided and calculated among multiple quantum hardware simultaneously or single quantum hardware sequentially, allowing for larger quantum algorithms to be developed and executed without the necessity of having larger quantum hardware to run them on.

In the short term, quantum optimisation tools [11, 12] that incorporate these hybrid approaches could be leveraged to explore the potential impact on the efficiency of smart grid management.

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Team

Mohammad Bahrami (Wolfram), John McNally (Wolfram), Yi Yin (Wolfram), Erik Garcell (Classiq), Ron Cohen (Classiq), Tamuz Danzig (Classiq).

SDG 13 – Climate Action

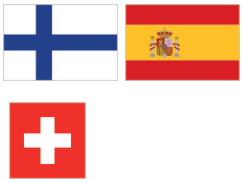
Catalytic Carbon Capture

13 CLIMATE ACTION

SHORT SUMMARY
Quantum machine learning solution to enhance chemical catalysis, reduce the carbon footprint of catalytic processes and refine carbon capture technologies.

QUANTUM APPROACH
Machine Learning

TEAM ORIGINS



Context

Climate change is one of the most pressing global challenges, posing significant threats to ecosystems, human health, and economies worldwide. A primary contributor to climate change is the excessive concentration of carbon dioxide (CO_2) in the atmosphere, mainly from fossil fuel combustion, industrial activities, and deforestation [1]. The rise in CO_2 levels has led to a rapid increase in global temperatures, resulting in extreme weather events, rising sea levels, and disruptions to food and water supplies [2]. Addressing this challenge is crucial for ensuring environmental sustainability, economic stability, and social wellbeing.

The Paris Agreement, adopted under the United Nations Framework Convention on Climate Change (UNFCCC), aims to limit the global temperature increase to well below 2°C, with efforts to keep it to 1.5°C above pre-industrial levels [3]. Achieving these goals requires significantly reducing greenhouse gas emissions, of which carbon capture technologies play a critical role. According to the International Energy Agency (IEA) [4], Carbon Capture, Utilisation and Storage (CCUS) technology is expected to contribute to 15% of the cumulative reduction in CO_2 emissions needed to meet global climate targets by 2070; highlighting the necessity of scaling up these technologies to meet the ambitious goals of the Paris Agreement. The importance of these efforts has been further emphasised in recent discussions, such as those at COP28, where the Global Climate Action agenda highlighted the critical role of innovative technologies in achieving these objectives [5]. Carbon capture technologies are seen as a key component of global strategies to reduce emissions, particularly in sectors where decarbonisation is challenging, such as heavy industry and power generation.

The societal challenge of excessive CO_2 emissions affects populations globally, with particularly severe impacts in regions with high industrial activity and vulnerable ecosystems. Populations in urban areas with dense industrialisation, such as those in developing countries, face increased health risks from air pollution and climate change-related disasters. Additionally, small island and coastal communities are disproportionately affected by rising sea levels and extreme weather events, resulting from increased atmospheric CO_2 concentrations.

This use case seeks to address these challenges by focusing on two critical areas: (i) the development of advanced chemical catalysis techniques to make industrial processes more energy efficient, directly reducing the amount of CO_2 emitted, and (ii) the optimisation of carbon capture methods from sources like power plants and industrial facilities and prevent them from entering the atmosphere.

Computational Challenges

A major challenge in developing sustainable catalytic processes lies in accurately modelling molecular interactions at the atomic level. Classical computational methods are valuable for providing insights into molecular interactions and optimising materials, but they come with significant limitations. Density Functional Theory (DFT) is a widely used computational method for this purpose. In catalysis, DFT is crucial for predicting the adsorption energy of molecules on catalyst surfaces, a key metric for understanding and improving catalyst performance. By simulating different molecular configurations on these surfaces, DFT helps identify optimal catalysts that can enhance reaction efficiency and sustainability. However, the accuracy of Density Functional Theory (DFT) is often constrained by the approximations inherent in classical models, which can lead to potential inaccuracies in predicting molecular behaviours. Additionally, the computational power required to model large and complex systems is immense, which can be prohibitive and slow down the pace of discovery and innovation.

Metal-organic frameworks (MOFs) have emerged as promising materials for Direct Air Capture (DAC) due to their tunable structures [6]. The performance of existing absorbents and adsorbents is often limited by their capacity, selectivity, and regeneration efficiency, presenting further challenges in making DAC a viable and scalable solution for carbon reduction. However, identifying and optimising MOFs involves navigating a vast space of possible configurations, which is a complex and resource-intensive task [7].

One way to tackle this challenge is by using Generative Adversarial Networks (GANs), which consist of two competing neural networks—a generator and a discriminator—working together to produce data that mimics real-world distributions. A main limitation of classical computing, particularly with GANs, is their inability to explore certain regions of the chemical space due to the vast size of the search space. Classical GANs often struggle with training instabilities and require a substantial amount of computational resources to model such large spaces accurately. This limitation hinders the effective discovery and optimisation of novel materials, as these models may converge on suboptimal solutions or fail to capture the underlying chemical complexity fully.

Obviously, for any data-driven approach, high-quality datasets are essential for model performance. Such examples of datasets are from the SwissCAT+ [8], the GDB-17 [9], and The Open Catalyst Project (OCP) [10] initiatives.

Potential Impact of a Quantum Solution

Quantum computing [11], particularly through the Quantum Generative Adversarial Networks (QGANs) method [12], could offer a promising alternative. QGANs could help overcome the classical limitations in the ability to explore certain regions of chemical space or the training instabilities due to the vast search space [13, 14]. Instead of relying solely on classical DFT calculations, QGANs could be employed to generate new chemical catalysts and MOFs more efficiently. The quantum component in QGANs could allow for the creation of quantum layers and leverages the inherent indeterministic properties of quantum mechanics to generate the necessary noise for the generative network, enhancing the ability to explore vast chemical spaces and identify novel materials. One could anticipate that currently available quantum devices could accommodate a first small-scale proof of concept.

As explored for carbon fixation process [14], leveraging quantum computing for carbon capture - in this case leveraging QGANs for chemical catalysts and MOFs - could provide accuracy gains in the modelisation of the chemical processes involved and thus lead to more efficient CO_2 reduction in the fight against climate change.

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Team

Oscar Novo (Universidad Politécnica de Madrid), Carlos Kuchkovsky (QCentroid), Gregory Shutko (QCentroid).

Contributors

Graham Alabaster (UN Habitat), **Jose Alcocer** (WFP), **Dr. Mohammad (Mads) Bahrami** (Wolfram), **Louis Barcikowsky** (Reply), **Ana Beatriz Morgado** (University of Coimbra), **Partha Basu** (IARC), **Pauline Bekkers** (UN Habitat), **Mourad Beji** (Pasqal), **Iara Bento** (University of Coimbra), **James Brown** (qBraid), **Matteo Ceccerelli** (University of Cagliari), **Jiabao Chen** (QunaSys), **Ron Cohen** (Classiq), **Tomás Costa** (University of Coimbra), **Matthew Craven** (University of Plymouth), **Tamuz Danzig** (Classiq), **Dylan Elliott** (Inari), **José Erinaldo da Fonseca** (Venturus), **Kellye Eversole** (Eversoles Associates), **Gabriel Falcão** (University of Coimbra), **Michael Farruggia** (Inari), **Catherine Feuillet** (Inari), **Anderson Fernandes Pereira dos Santos** (Venturus), **Alexandre Fleury** (SandboxAQ), **Alex Frieden** (Inari), **Dr. Erik Garcell** (Classiq), **Cláudio Gomes** (CMU-Portugal), **Paweł Gora** (Quantum AI Foundation), **James Hancock** (University of Plymouth), **Tarini Hardika** (qBraid), **Daniel de Haro Moraes** (Venturus), **Kenneth Heitritter** (qBraid), **Alan Hennessy** (GARDP), **Louis-Paul Henry** (Pasqal), **Samuel Horsch** (Quandela), **Nouhaila Innan** (University of Casablanca and New York University Abu Dhabi), **Abdullah Kazi** (CQI and University of Mumbai), **Carlos Kuchkovsky** (QCentroid), **Alain Labrique** (WHO), **Brennan Lagasse** (Yale University), **Sebastien Lefebvre** (Inari), **Erika Lloyd** (SandboxAQ), **Jorge Lobo** (University of Coimbra), Quentin Ma (Reply), **Tommaso Macri** (QuEra), **Luis Martinez** (QuEra), **João Martins** (University of Coimbra), **Craig McNeile** (University of Plymouth), **Wenbin Mei** (Inari), **Stefan Milenkovic** (University of Cagliari), **Rutendo Mukaratirwa** (FAO), **Nikolay Murzin** (Wolfram), **Emily Negrin** (Inari), **Oscar Novo** (Universidad Politécnica de Madrid), **Shreyas Patil**, **Josh Price** (Inari), **Sonali Quantius** (Inari), **Laurent Querella** (QClavis), **Tiago Santiago do Espírito Santo** (Venturus), **Laura Scherzberg** (University of Coimbra), **Jeremy Pardo** (Inari), **Matthew Robertson** (Inari), **Valentin Senicourt** (SandboxAQ), **Gregory Shutko** (QCentroid), **Douglas Silva Domingues** (University San Paolo), **Rafael Sotelo** (Quantum South), **Jon Stokes** (McMaster University), **Maëlle Toy-Riont--Le Dos** (Reply), **Erik VanIngen** (FAO), **Ruthwika Vemulapalli** (G.Narayanamma Institute of Technology and Sciences), **Brian Ventura** (Quandela), **Ronin Wu** (QunaSys), **Jonathan Wurtz** (QuEra), **Yi Yin** (Wolfram), **Lennig Pedron** (Trust Valley), **Josua Rochat** (Trust Valley), **Philipp Kammerlander** (Open Quantum Institute), **Catherine Lefebvre** (GESDA-Open Quantum Institute).