



White Paper 2025

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 focuses on accelerating applications for humanity. OQI supports the development of use cases that could contribute to the achievement of the United Nations Sustainable Development Goals (SDGs) and subsequent frameworks. This effort contributes to building a global community of practice to explore potential applications of the technology that will positively impact our society and our planet while the technology gains maturity and access expands globally.

OQI has developed a rigorous framework to explore the potential of quantum computing to address global challenges [2]. Through technical and project management support, OQI supports the progress of use cases from ideation to proof-of-concept, which may lead to implementation on today's quantum devices (simulator and quantum processors) available on the cloud. As part of the support it provides, OQI offers a neutral platform for collaboration between quantum experts, subject matter experts UN agencies and large NGOs from all around the world.

OQI's use case portfolio contains a growing number of use cases at various phases of their development. A map of the global participation to OQI use cases is illustrated in Figure 1.

These use cases primarily address SDG 2 (Zero Hunger), SDG 3 (Good Health and Well-Being), 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, optimisation, machine learning and linear systems of equations, leveraging existing quantum approaches and exploring how they could be applied to problems relevant to the SDGs. 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.

The 2025 OQI Use Case White Paper first presents a full overview of the OQI portfolio in Part I, featuring quantum computing use cases relevant to the SDGs that have been supported by OQI over the past three years. The portfolio includes use cases that were initiated during the incubation phase of OQI, while the majority started their journey during the OQI pilot. Second, the 2025 Use Case White Paper provides a deep dive in Part II into 7 new use cases developed by experts from 10 countries, who have started or refined their work with OQI support since the pub-

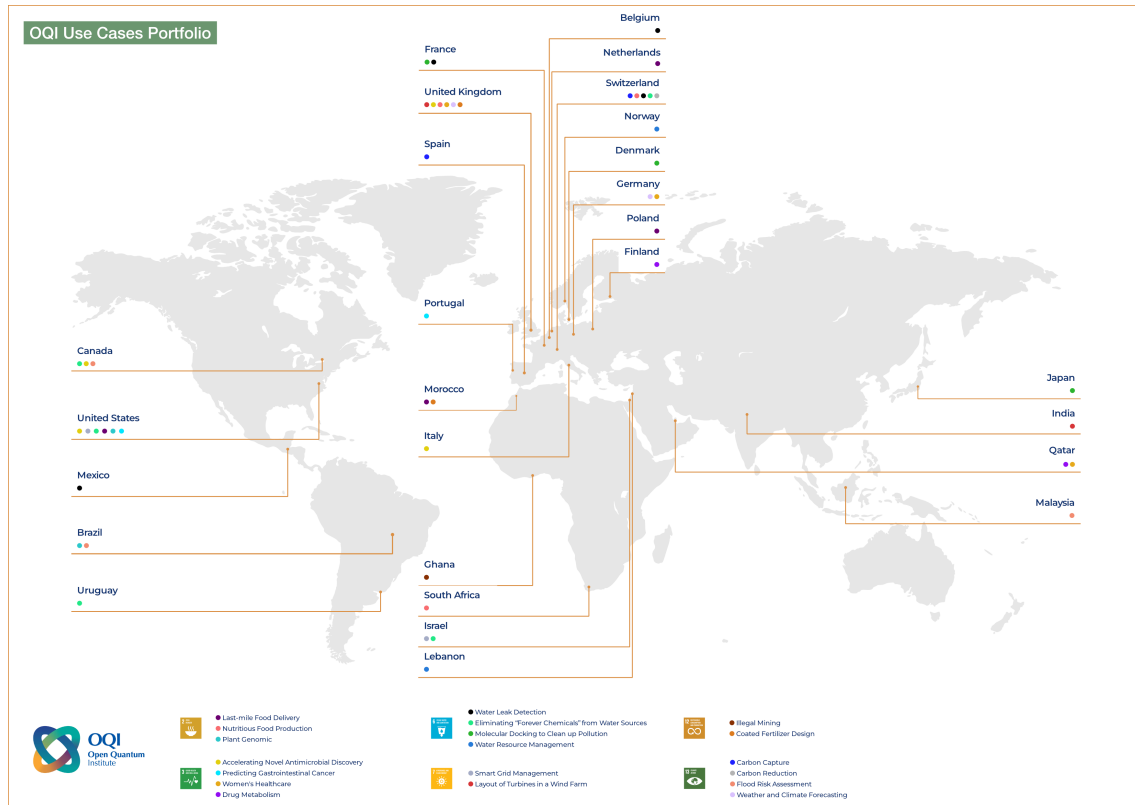


Figure 1: Use cases developed by teams across the globe to explore the potential of quantum computing to accelerate the UN Sustainable Development Goals (SDGs), with the support of OQI.

lication of the 2024 Edition [3]. For all these use cases, advancement will continue, deepening both the scientific methodology as well as the anticipated societal impact, under guidance of the OQI Scientific and Impact Committees.

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I. OQI Portfolio



OPTIMISATION

Last-Mile Food Delivery



Quantum computing optimisation of the food supply chain, in particular in the route planning of food delivery in underserved regions impacted by climate change or other crises.

COQIT, HASSAN II UNIVERSITY OF CASABLANCA, INDIAN INSTITUTE OF TECHNOLOGY, QUANTUM AI FOUNDATION, TECHNICAL UNIVERSITY OF DELFT, UNIVERSITY OF MUMBAI, YALE UNIVERSITY | WORLD FOOD PROGRAM (WFP)



MACHINE LEARNING

Plant Genomics



Quantum computing solution to improve wheat, corn and soy yield by targeted gene editing.

INARI, QUERA, VENTURUS | FOOD AND AGRICULTURE ORGANIZATION (FAO)



OPTIMISATION

Sustainable Food Production



Improving sustainability of global food systems by making them more resilient to climate change through a quantum optimisation solution to produce more nutritious food locally in less land.

ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE (EPFL), NATIONAL INSTITUTE FOR THEORETICAL AND COMPUTATIONAL SCIENCE (NITHECS), QUANTUM BASEL | GLOBAL ALLIANCE FOR IMPROVED NUTRITION (GAIN)



MACHINE LEARNING

Accelerating Novel Antimicrobial Discovery



Quantum machine learning solution to accelerate the antimicrobial discovery and lower resistance to drugs.

MCMMASTER UNIVERSITY, QBRAID, UNIVERSITÀ DEGLI STUDI DI CAGLIARI | GLOBAL ANTIBIOTIC RESEARCH AND DEVELOPMENT PARTNERSHIP (GARDP)



MACHINE LEARNING

Predicting Gastrointestinal Cancer



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

UNIVERSITY OF COIMBRA, CENTRE FOR SOCIAL STUDIES | INTERNATIONAL AGENCY FOR RESEARCH ON CANCER (IARC)



QUANTUM SIMULATION

Women's Healthcare



Quantum simulation of the molecular interaction of the biological targets and drugs involved in the treatment of endometriosis, perimenopause, and menopause.

QATAR UNIVERSITY, UNIVERSAL QUANTUM





QUANTUM SIMULATION

Drug Metabolism Design



Quantum simulation of electronic structures to understand metabolic processes of enzymes to reduce adverse drug reactions.

ALGORITHMIQ, QATAR UNIVERSITY



QUANTUM SIMULATION

Eliminating 'Forever chemicals' from Water Sources



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

QUANTUM SOUTH, SANDBOXAQ | UNHABITAT



MACHINE LEARNING

Molecular Docking to Clean Up Pollution



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

QUANDELA, QUNASYS | WORLD HEALTH ORGANIZATION (WHO)



OPTIMISATION

Water Leak Detection



Quantum optimisation solution to optimally position sensors and detect water leaks in urban water systems.

PASQAL, QCLAVIS.IO, REPLY | UNHABITAT



LINEAR SYSTEMS OF EQUATIONS & PDEs

Water Resource Management



Quantum fluid dynamics solution to model aquifer systems, prevent and monitor contaminant breakthrough and assess impact of climate change on water reservoirs.

AMERICAN UNIVERSITY OF BEIRUT, NORWEGIAN COMPUTING CENTER, | UNHABITAT



OPTIMISATION

Layout of Turbines in a Wind Farm



Quantum optimisation solution to efficiently layout turbines in a wind farm and maximise the power produced.

G. NARAYANAMMA INSTITUTE OF TECHNOLOGY, UNIVERSITY OF PLYMOUTH | INTERNATIONAL ATOMIC ENERGY AGENCY (IAEA)





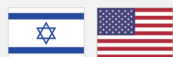
OPTIMISATION

Smart Grid Management



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

CLASSIQ, WOLFRAM | INTERNATIONAL ATOMIC ENERGY AGENCY (IAEA)



QUANTUM SIMULATION

Coated Fertiliser Design



Quantum simulation to optimise the nutrient release from coated fertilisers for sustainable agriculture.

MOHAMMED VI POLYTECHNIC UNIVERSITY (UM6P), UNIVERSITY OF NOTTINGHAM | FOOD AND AGRICULTURE ORGANIZATION (FAO)



MACHINE LEARNING

Illegal Mining



Quantum machine learning solution for monitoring illegal mining through satellite imagery and promoting environmental conservation, particularly in Ghana.

UNIVERSITY OF ENERGY AND NATURAL RESOURCES, UNIVERSITY OF EDUCATION, WINNEBA (GHANA) | UNITED NATIONS INTERREGIONAL CRIME AND JUSTICE RESEARCH INSTITUTE (UNICRI)



MACHINE LEARNING

Carbon Capture



Quantum machine learning solution to improve efficiency of catalysts involved in the chemical process of carbon capture.

QCENTROID, ETH ZURICH



QUANTUM SIMULATION

Carbon Reduction



Quantum Computing simulation to reduce carbon dioxide (CO₂) in the atmosphere by improving catalysis process responsible for the fixation of carbon on the surface of materials.

ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE (EPFL), ETH ZURICH, | UNITED NATIONS FRAMEWORK CONVENTION ON CLIMATE CHANGE (UNFCCC)



MACHINE LEARNING

Flood Risk Assessment



Quantum machine learning solution to provide better accuracy in flood prediction and improve prevention mechanisms in regions at risk, particularly Malaysia.

MALAYSIA QUANTUM INFORMATION INITIATIVE, NATURAL RESOURCES CANADA, UNIVERSITI TEKNOLOGI PETRONAS, UNIVERSITY OF CALGARY, QUATI | WORLD METEOROLOGICAL ORGANIZATION (WMO)





LINEAR SYSTEMS OF EQUATIONS & PDEs

Weather and Climate Forecasting



Quantum fluid dynamics simulation to
improve the reliability of weather and climate
forecasts.


EUROPEAN CENTRE FOR MEDIUM-RANGE WEATHER FORECASTS (ECMWF),
PLANQC, UNIVERSITY OF OXFORD | WORLD METEOROLOGICAL
ORGANIZATION (WMO)



II. Deep Dive into 2025 Use Cases



1 SDG 3 – Good Health and Well-Being


1.1 Drug Metabolism Design

 QUANTUM SIMULATION

Quantum simulation of electronic structures to understand metabolic processes of enzymes to reduce adverse drug reactions.

ALGORITHMIQ, QATAR UNIVERSITY





Context

While drugs are designed to improve health, they can also harm it. Adverse Drug Reactions (ADRs), defined by the WHO as harmful unintended responses to drugs at normal doses, are the sixth leading cause of death worldwide, affecting children and elderly patients more significantly. [1]. These unintended reactions are responsible for up to 30% of hospital admissions in the United States [2], incurring an annual direct healthcare cost of approximately \$30.1 billion. ADRs also bring their fair share of indirect economic impacts, including decreased productivity and reduced quality of life for both patients and caregivers. The effects are exacerbated in vulnerable communities. It was highlighted that HIV infection was associated with an increased risk of ADR-related hospital admission in Sub-Saharan Africa [3]. Overall, the societal cost of ADRs is estimated at around \$75 billion annually in the United States [4].

Furthermore, ADRs are a major impediment in pharmaceutical research and development, accounting for nearly one-third of drug development failures due to toxicity, thus driving up both development timelines and medication costs. The majority of pharmaceutical compounds undergo a critical biotransformation process in the liver, known as drug metabolism, to facilitate their elimination from the human body [5]. At its fundamental level, this process typically entails the conversion of an active drug molecule into a pharmacologically inactive metabolite, which is then naturally eliminated by the body. Accordingly, drug metabolism is generally considered a detoxification mechanism that mitigates drug accumulation and prevents the manifestation of toxic effects.

The ability to accurately predict the rates and understand the reaction mechanism at the atomistic level of drug metabolism is crucial in the drug discovery and drug design process in order to reduce ADRs and directly contribute to SDG 3 (Good Health and Well Being).

Computational Challenges

One of the most crucial enzyme families involved in the metabolism process is cytochrome P450 (CYP), responsible for metabolising over 70% of pharmaceutical compounds [6, 7, 8]. The CYP enzymes catalyse the reaction that converts a drug from a hydrophobic to a hydrophilic derivative. The rate at which this reaction happens directly impacts drug efficacy and potential toxicity, making its accurate prediction essential for drug discovery and development. Even more so, the metabolism process can inadvertently result in bioactivation, which can subsequently trigger cellular toxicity, immune responses, or mutagenic events. A deep understanding of the involved mechanisms is hence crucial. Important examples of bioactivation include mechanism-based inactivation of CYP enzymes, which can lead to permanent enzyme inactivation. This process is metabolically driven and irreversible, requiring new protein synthesis for functional recovery. It can result in significant drug-drug interactions and auto-inhibition of clearance effects that are often not detected until late in drug development [9].

Classical computational chemistry has played a pivotal role in simulating metabolic transformations, gaining insight into the reaction mechanisms, and determining the respective reaction rates [10]. In the context of ADRs this is particularly insightful for metabolic transformations facilitated by CYP. Deciphering the reactivity, selectivity, and underlying mechanisms of these molecules has remained a longstanding focus in enzymology and computational biochemistry [6, 10, 11].

Over the past two decades, hybrid quantum mechanics/molecular mechanics (QM / MM) approaches have become indispensable for elucidating CYP catalytic mechanisms. These multiscale methods combine the electronic resolution of quantum chemistry with the structural context provided by molecular mechanics, enabling the simulation of enzymatic reactions within a realistic biological framework.

Despite the predictive power of QM/MM techniques, several computational challenges persist. Accurate descriptions of transition metal centres, dynamic enzyme conformational states, and long-range electrostatics often require approximations that limit precision. Moreover, the computational cost of high-level quantum methods scales poorly with system size, making them difficult to apply routinely to full enzymatic systems [10]. Overall, to accurately model the electronic properties of metabolic reactions, computational simulations must account for quantum mechanical electron interactions. Traditional computational approaches (Density Functional Theory, Coupled Cluster, Complete Active Space Self-Consistent Field (CASSCF)) face several limitations, including high computational costs, limited accuracy and inefficiency in reaction rate calculations.

Specifically, classical yet exact simulations, such as CASSCF-based models, scale exponentially in computational cost in terms of active space sizes, which refer to the number of electrons and molecular orbitals that are used for accurately describing a molecule's chemical behaviour. In such simulations, the size of this space determines how many electron interactions need to be explicitly calculated. This imposes limits of computational feasibility: a simulation performed on classical supercomputers today can only accommodate up to 24 molecular orbitals [12]. However, adequate modelling of the active site of CYP enzymes requires active spaces of more than 50 molecular orbitals [13]. By fixing the simulations to reduced basis set representations rather than the full representation of the molecule, it also introduces systematic errors [14].

Potential Impact of a Quantum Solution

In light of the classical limitations, quantum computing has emerged as a promising frontier as it offers the potential to simulate strongly correlated electronic states with chemical accuracy, thereby overcoming some of the fundamental bottlenecks of classical methods as outlined above.

Furthermore, quantum algorithms can interface with hybrid quantum-classical pipelines to enhance site-of-metabolism prediction, conformational sampling, and reactivity mapping, thereby opening new frontiers in the predictive modelling of drug metabolism and facilitating the design of safer drug compounds and ADR mitigation. Quantum computing could offer to model drug metabolism pathways via variational quantum algorithms (VQAs) with adaptive multiwavelet representations, which could significantly enhance computational accuracy and efficiency beyond classical methods [14, 15] and provide a more scalable path for quantum electronic structure simulations.

In this context, quantum simulations of electronic structure have the potential to outperform classical methods in several ways. Firstly, by increasing the accuracy by eliminating basis set incompleteness errors. Secondly, by improving metabolic modelling through a focused computational simulation of CYP-mediated activation, it becomes possible to account for the full orbital correlation space of both the active site and the metabolite. This means that more than 50 orbitals could be considered, implying the use of approximately 100 qubits to perform the simulation on a quantum computer. Quantum simulations could offer deeper insights into drug metabolism [10, 13], optimising bioavailability and reducing toxicity risks associated with ADRs. In the future as the technology progresses, Quantum Phase Estimation (QPE) could be envisioned to be implemented on fault-tolerant quantum hardware to gain more accuracy of the molecular energy levels [16].

Being able to better understand metabolic processes involving CYP enzymes thanks to new quantum computing methods could eventually lead to more efficient and safer drug development cycles and thus ultimately to improved health and well-being globally.

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1.2 Women's Health




QUANTUM SIMULATION

Quantum simulation of the molecular interaction of the biological targets and drugs involved in the treatment of endometriosis, perimenopause, and menopause.

QATAR UNIVERSITY, UNIVERSAL QUANTUM



Context

Reproductive and gender-related health remains an underfunded and under-researched area [1], leading to significant disparities in healthcare outcomes. Conditions such as endometriosis, a chronic condition where tissue similar to the uterine lining grows outside the uterus [2], face delayed diagnoses and limited treatment options. Demographic disparities in access to care, diagnosis, treatment and management exacerbate these issues, particularly in underserved regions. On the other hand, endometriosis and its treatment increase the risk of pregnancy complications, including placenta previa, preterm birth, intrauterine growth restriction, and miscarriage [3]. Hence, there is an urgent need to address these conditions in health policies, provider training, and fair access to evidence-based care. Further, inadequate access to healthcare services, cultural factors, and other factors delay diagnosis and management for up to 10 years [4, 5], but the data varies widely depending on region and demographics. As a result there are far-reaching consequences, including reduced workforce participation due to untreated health issues and increased strain on healthcare systems from prolonged diagnostic and treatment pathways. Recognising endometriosis's impact on reproductive health and well-being, the World Health Organisation (WHO) drives global action to develop effective prevention, diagnosis and treatment models, particularly for underserved populations in low- and middle-income countries [2].

Specifically, endometriosis affects approximately 10% of people of reproductive age who can develop the condition globally, or around 190 million individuals [2]. These statistics underestimate the reality, as the condition is still under detected due to limited access and availability of health workforce in underserved geographies. Endometriosis can decrease quality of life due to severe pain, fatigue, depression, anxiety, and infertility. According to a report from the All Party Parliamentary Group on Endometriosis in the UK, 95% of people living with endometriosis said it has impacted their wellbeing in a negative manner, and 35% had a reduced income due to the condition [6].

Endometriosis tends to relapse and affect fertility; therefore, protecting reproduc-

tive and endocrine functions and preventing recurrence are priorities [7]. The origin and development of endometriosis are unclear. Sampson's retrograde menstruation suggests menstrual debris moves to the peritoneal cavity via the fallopian tube with reverse peristalsis, but this is common in healthy people with a uterus and doesn't always cause endometriosis. Endometriosis is multifactorial. The immune microenvironment in ectopic endometrium is altered, with immune surveillance abnormalities allowing tissue implantation without immune clearance. Ectopic tissue causes oxidative stress, inflammation, and macrophage activation, resulting in the production of growth, angiogenic, and inflammatory factors. Outcomes include inflammation, pain, gastrointestinal issues, urinary symptoms, and infertility [8].

A 2022 study from the National Library of Medicine indicated that "endometriosis was significantly associated with a higher burden of infertility, chronic comorbidities, utilisation of healthcare services, pain medications, and antidepressants, and, overall 1.75-fold higher direct medical costs" [9]. This demonstrates the wider implications for healthcare systems and the severity of the condition for the overall health of those affected.

People in low- and middle-income countries are particularly affected, as limited healthcare access and resources further widen the disparities in outcomes. Yet access to treatment remains a prevailing concern, even in developed countries. Development of therapeutics that can be self-administered — for example, the recommendation to prescribe Relugolix CT as a once a day tablet [10] in the UK represents a step change in availability of treatment for endometriosis sufferers — and that can be distributed in ambient conditions with long shelf stability would have a marked impact on reproductive and gender-related health worldwide, by offering both improved treatments accessible without a formal diagnosis, and reducing barriers to treatment access, particularly in geographic locales lacking in infrastructure. Addressing these disparities is critical to achieving equitable healthcare and improving societal well-being. Aligning with UN Sustainable Development Goals (SDGs), particularly SDG 3 (Good Health and Well-being), SDG 5 (Gender Equality), and SDG 10 (Reduced Inequalities), this use case seeks to reduce inequalities while addressing economic impacts, such as lowering healthcare burdens and enabling greater healthy workforce participation.

Computational Challenges

There is ongoing effort in improving gender-related healthcare and treatment for endometriosis. Developing novel effective drugs requires understanding complex molecular interactions, optimising drug candidates, and ensuring efficient binding to biological targets. Endometriosis, in particular, is a complex condition with multimodal interactions that requires additional precision in simulations to help capture the underlying biological reality.

Classical computer-assisted drug discovery methods are fundamental to identifying and optimising drug candidates. Techniques like molecular docking and molecular dynamics are used to simulate the interactions between small molecules (ligands) and

biological targets (proteins) [11, 12]. These methods rely on scoring functions and force fields to approximate molecular interactions and binding affinities. Force fields are parametrised based on limited datasets derived from computational chemistry methods like Density Functional Theory (DFT) and Coupled Cluster (CC). DFT and CC methods are used to calculate the electronic structure of molecules, which is critical for understanding properties such as binding affinity and reactivity. However, these methods scale poorly with system size, making it impractical to apply DFT and CC techniques directly to screening large databases of biomolecular systems [13].

A trade-off exists for computational chemistry: quantum mechanical simulations run on classical supercomputers provide high accuracy but scale poorly to large systems on classical computers; conversely, classical approximations are computationally efficient and scalable, yet suffer from limited accuracy and poor generalisability to complex systems. The larger the molecular systems — like proteins in solution — the more pronounced the limitations for simulations are. This is particularly relevant for simulations of chemical interactions involved in diseases such as endometriosis, given the need to simulate dynamics of multiple proteins, endocrine system responses, and inflammatory markers.

In recent years there has been growing interest in the use of ‘machine-learned interatomic potentials’ as a possible technique to overcome some of the limitations of force field approximations, where a machine learning approach (typically neural network based approach) is used to learn from databases of DFT results [14, 15]. Machine-learned interatomic potentials rely on a vast quantity of high-fidelity *ab initio* data for their training, and can have excellent performance, approximating the accuracy of full state simulation methods such as the CC [16]. However, with the scarcity of training data for complex molecules with non-standard interactions on compounds with metallic centres, machine-learned interatomic potentials result in poor accuracy on unseen instances, and exhibit poor extrapolation behaviour [17], [18]. Enhancing the quality and availability of high quality quantum mechanical simulation based data would significantly enhance the ability of machine-learned interatomic potentials methods to generalise to novel problem instances, and represents a significant opportunity for simulations driven by quantum computation to address this deficit.

Potential Impact of a Quantum Solution

This use case seeks to combine the benefits of well-established classical computational workflows with the strengths of quantum computing in molecular simulations to provide high-fidelity quantum mechanical simulation data as an input into a large, tailored database for drug design that would otherwise be infeasible for classical simulations.

While fully transformative applications will require fault-tolerant quantum computing (FTQC), meaningful advancements could be made now through proof-of-principle demonstrations using near-term quantum devices, using Variational Quan-

tum Eigensolvers. These efforts focus on tackling limitations of existing classical computational workflows by providing more accurate electronic structure calculations for small-to-medium-sized molecules via quantum simulation. By focusing on high-accuracy quantum mechanical calculations for key subsystems, quantum computing could improve the overall quality of the computational pipeline by bridging the gap between small-scale quantum simulations and large-scale classical approximations [11, 12, 13].

By increasing the accuracy of foundational datasets the generalisation performance and accuracy of machine-learned interatomic potentials is expected to improve, this would in turn enhance the predictive power for large-scale simulations of complex systems, including drug-receptor interactions [19, 20].

The refined data produced by the quantum simulations could help address classical computational bottlenecks and improve the overall reliability of classical drug discovery workflows. By refining machine-learned interatomic potential performance through data obtained from quantum simulations, better approximations of binding affinities, solvation effects, molecular flexibility and drug-receptor interactions for complex molecules may be possible – leading to new and novel treatments for complex conditions such as endometriosis.

Complex, multi-dimensional datasets encompassing biomarkers, genetics, and comorbidities will be required for designing effective endometriosis treatments, and the application of quantum computing to build such datasets may act as a significant accelerator to enhance diagnostic precision, improve the understanding of disease mechanisms, and accelerate drug discovery processes.

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2 SDG 6 – Clean Water and Sanitation


2.1 Water Resource Management





LINEAR SYSTEMS OF EQUATIONS & PDEs

Quantum fluid dynamics solution to model aquifer systems, prevent and monitor contaminant breakthrough and assess impact of climate change on water reservoirs.

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Context

Groundwater refers to water stored beneath the Earth's surface in the pore spaces of soil and rock formations, within geological structures called aquifers [1]. While water covers much of our planet, only a small fraction is freshwater, with approximately 99 percent of all liquid freshwater on Earth existing as groundwater. Today, groundwater supplies about half of the global domestic water use. In most rural communities without centralised distribution systems, it serves as the main source of drinking water, contributing to roughly one-quarter of the water used for agricultural irrigation. It is essential for reducing poverty, securing food and water (SDGs 1, 2, 6), promoting decent work and economic growth (SDG 8), reducing inequalities (SDG 10), and strengthening societal and ecological resilience to climate change (SDGs 13, 15) [1].

Yet groundwater is increasingly under threat. Water stress levels — the ratios of water demand to renewable supply — have increased globally. For instance, high water stress levels are observed in Southern and Central Asia, Northern Africa and Western Asia [2]. In semi-arid developing regions, water scarcity affects approximately 500 million people. This is the case in particular for the Middle East and North Africa (MENA) region, which is characterised by intense precipitation and flood potential on roughly 120 days each year, followed by growing water shortages during the remaining months [3, 4]. At the same time, rapid urbanisation fuelled by growing population is increasing demand for groundwater, while reducing its recharge capacity through the use of impermeable surfaces like asphalt and concrete for the construction of roads and buildings [2, 4, 5]. Effective management and protection of groundwater quality and quantity at the source, including wells, springs, and aquifers, is therefore essential to achieving SDG 6 (Clean Water and Sanitation) [6]. Continuous groundwater monitoring and contextualising hydrological data within relevant societal and environmental issues are both essential, and they rely on thorough hydrogeological characterisation. Therefore, understanding

water flow and management, through numerical flow and transport models remains one of today's most effective decision-support tool. These models help assessing, quantifying, and predicting how natural systems respond to internal and external changes [1, 4]. They provide a scientific basis for water-related policies and guidelines, particularly when they accurately represent aquifer behaviour, forecast water quality and quantity, and provide recommendations with minimal uncertainty [7].

Computational Challenges

Conventional computational techniques model groundwater flow as an optimisation problem, namely using the inverse simulation of Darcy's flow equation. Given observed data for pressures and flow rates at different positions, the goal is to estimate unknown parameters, such as the permeability distribution – essentially describing how easily groundwater flows or permeates through the various subsurface layers of interest – or source and sink terms, which are variables that add or remove water from the domain (like rainfall or well pumps respectively), or even boundary conditions [8, 9, 10]. Methods for solving this optimisation problem include quadratic, differential dynamic, non-linear, mixed integer, stochastic programming, and non-gradient-based search algorithms [11]. The inverse simulation of Darcy's flow equation can be solved for steady states or for transient states. A steady state implies that key variables, like groundwater flow and recharge rates, remain constant. On the other hand, a transient state implies a change over time of groundwater variables, which is needed for more accurate and realistic flow and transport simulations.

By solving Darcy's flow equation, the configuration for the permeability distribution and other initially unknown parameters is obtained. Then, in a second step, using these obtained parameters, the corresponding flow equation is solved using numerical discretisation methods, in 1, 2 or 3D, depending on the adopted model. These flow and transport parameters can be solved using the advection-diffusion equation, which describes how contaminants move through groundwater and the subsurface layers, and how easily they disperse or concentrate given the information fed in from the Darcy's flow equations [12]. Finally, the solution is validated by comparing its predictions for pressure and flows with measured data. The validated data can be further used to refine the aquifer model, by tuning approximated variables, and calibrated transport parameters. A karst aquifer model represents a system of fissures, caves, sinkholes and overall subsurface eco-system that transports water from ground level to the subsurface.

A karst system is a type of aquifer that is particularly at risk of contamination due to its unique geological structure, which includes highly permeable conduits, fractures, and sinkholes that allow rapid transport of water and pollutants. Its explicit geometry and geology is usually not known, hence flow rates and permeability rates can quickly change over small spaces of the subsystem. Given these uncertainties, models can be validated through the use of tracer tests — in which scientists can add harmless substances to the water and track their dispersion and flow rates through the system. These manual validations help to more accurately represent the complex aquifer and model its groundwater flow [8, 13].

As such, when moving from 1D, to 2D, to 3D, the complexity of the model is not only increased in number of grid points that need to be simulated, but the shape and geology of the model add additional layers of complexity and an increased number of unknown parameters that need to be accounted for. A major difficulty with conventional computational approaches is that complex multi-layered systems, such as those in groundwater flow of aquifer systems, have non-unique solutions, which lead to multiple model realisations being needed to reliably estimate flow and transport parameters. The uncertainties related to the simulation pose a challenge in using the results for assisting decision and policy making around water management efficiently. It is thus necessary to reduce prediction uncertainties and ensure the model reliably reproduces observed data.

The more complex the subsurface fissured aquifer is, the longer the computation times are for the optimisation step, as well as the time needed for simulations, whether solved in 2D or 3D. The computational complexity of flow and transport simulations thus depends primarily on the spatial dimension and the resolution of the aquifer model. The closer the simulation approximates physical and geological reality, the greater the computational demands required to model the aquifer's fractal structure and permeability at increasingly finer scales.

This is especially critical for modelling scenarios involving contaminant breakthroughs, where sharp changes in concentration over time and space require fine temporal and spatial discretisation to accurately track when and how the contaminant arrives at monitoring points. This type of modelling could be especially important to address the fate of "forever pollutants", such as per- and polyfluoroalkyl substances (PFAS), for example. Such information is crucial to support effective mitigation of water scarcity, and could offer a new approach to reformed policy in relation to urban planning.

Potential Impact of a Quantum Solution

As the sophistication of the mathematical models is enhanced, for example, by using non-linear Navier-Stokes equations instead of linear advection-diffusion, and the aquifer model's resolution is increased, computational demands become challenging enough that alternative computational approaches are needed. The Navier-Stokes equations are non-linear equations that solve the full fluid dynamics, taking into account fluid turbulence as well as other terms. Whilst the advection-diffusion equation is good enough to approximate porous aquifer systems with slow, or laminar flow using the precomputed flow from Darcy's equations, the Navier-Stokes equations improve this approximation for karst systems, by increasing the complexity and computing the flow, taking into account turbulent structures that can occur in water flow in fissured and fractured cave systems. Such an increase in complexity and computational resources is not necessary for porous aquifers, thus Navier-Stokes is only invoked when the karst systems become complex enough and has fast, turbulent flow affecting the speed and dispersion parameters of the model. [14]

Simulation of transport phenomena, such as through the advection-diffusion equa-

tion has gathered increasing interest in the quantum computing community in recent years [15, 16, 17, 18]. The motivation for looking into quantum computing approaches to solve partial differential equations with finer resolutions for aquifer models lies in the capability of quantum states to encode significantly more grid points than classical memories of comparable sizes, and potentially achieving a speed-up for high complexity cases. A promising future direction also aims at incorporating non-linearities into quantum circuits, and thus being able to study complex non-linear systems like those represented by the Navier-Stokes equations [19, 20].

For instance, simulation of Quantum Imaginary Time Evolution (QITE) via Trotterisation presents lower infidelity than variational quantum time evolution and adaptive variational quantum dynamics simulation [16], meaning QITE is a promising method for finding higher accuracy results and tackling intractable simulations on classical supercomputers. While current quantum computer restrictions limit the possibility of implementing QITE presently, this method could eventually be well-suited to be implemented on future fault-tolerant quantum computers (FTQC). In the short term, one of the other variational algorithms could be implemented on today's quantum computers (NISQ devices).

This use case aims to use and refine the approach to explore more complex advection-diffusion equations for transport in fissured aquifers. A quantum computing approach would allow to tackle more complex 2D and 3D substructures, such as conduits and permeability variations that are central to the study of real subsurface aquifer systems. An improvement in modelling finer scale aquifer systems would lead to benefits in identifying and tracing contaminant plumes, defining protection zones of wells and springs in groundwater catchments areas, and overall increasing mitigation and prevention strategies around vulnerable aquifer systems.

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3 SDG 12 – Responsible Consumption and Production

3.1 Coated Fertiliser Design



QUANTUM SIMULATION

Quantum simulation to optimise the nutrient release from coated fertilisers for sustainable agriculture.

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Context

Agriculture is the main pillar of global food security. Statistics from the the Food and Agriculture Organization (FAO) show that in 2023 agricultural land covered almost 5 billion hectares, corresponding to nearly 40% of the Earth's land surface [1]. The expansion of agricultural area, specifically cropland in the past 20 years, mostly occurred in Africa, South America, and Southeast Asia. The global population is projected to reach 8.5 billion by 2030 [2], underscoring the need to increase food production, while facing limited access to land and water resources, whilst also balancing the need to preserve natural ecosystems and biodiversity.

Modern agriculture relies heavily on mineral fertilisers to achieve current (and future) levels of food production, guaranteeing the supply of necessary plant nutrients. These are typically provided in highly soluble forms and are easily absorbed through plant roots or leaves. In 2023 alone, global use of inorganic fertilisers — nitrogen-based (N), phosphate-based (P_2O_5), and potassium-based (K_2O) fertilisers — reached approximately 190 million tonnes [3, 4]. The consumption of fertilisers continues to increase globally: Africa's agricultural use of inorganic fertilisers increased by 65% between 2002 and 2023, while the Americas saw a 48% increase, Asia 38%, and Europe 8% [4].

The high solubility of these fertilisers often results in significant nutrient losses through leaching, run-off, and volatilisation. These inefficiencies result in increased use of fertiliser to compensate for what is lost, with a substantial impact on farmers' operational costs as well as environmental and health consequences [5]. Nitrate contamination of groundwater poses serious health risks, including increased risks of cancers and thyroid disorders, particularly for pregnant women and infants [6]. Surface water pollution leads to eutrophication — an excess of nutrients, especially nitrogen and phosphorus — which causes excessive growth of algae and other plants

and leads to devastation of aquatic ecosystems and fisheries [7]. Beyond affecting water quality, use of mineral fertilisers in agriculture contributes to an estimated 700 million tonnes CO₂-equivalent per year, mainly from nitrous oxide and CO₂ emissions [8, 9, 10].

Addressing the efficient use of fertiliser is therefore critical and directly aligned with the United Nations' Sustainable Development Goals (SDGs) for responsible consumption and production (SDG 12), which targets eradicating hunger (SDG 2), and specifically SDG indicator 2.4.1 on productive and sustainable agriculture [11, 12]. Agriculture accounts for 70% of global freshwater withdrawals, and nutrient pollution threatens water security for billions [13]. In South Asia and Sub-Saharan Africa, contaminated groundwater forces the displacement of communities for safe water, facing additional health risks [14]. In addition, at the planet level, fertiliser pollution has created more than 500 coastal dead zones, devastating fisheries that feed 3.3 billion people [15].

One practical solution that has been often tried in efforts to enhance the efficiency of fertilisers is the use of polymer-coated fertilisers. This is a controlled-release fertiliser component, in which a fertiliser is encapsulated by a plastic polymer, which spreads the typical release of nutrients into the soil over an extended period of time. The specific design of specialised coatings enables a gradual release of nutrients in sync with plant demand to improve crop yields, while it contributes to reducing nutrient losses and lowering environmental footprints [16, 17, 18, 19].

By delivering nutrients more precisely, coated fertilisers support a shift toward more scalable, sustainable, and resilient agricultural practices, contributing to improve both small-holder food security and global agricultural sustainability. The challenge is to devise coating methods that optimise production and lead to maximising use efficiency in agricultural fields.

Computational Challenges

The mechanism for nitrogen release from polymer-coated urea, where urea granules are a common nitrogen fertiliser, starts with water absorbed inside the coating through the pores of the polymer. The water dissolves the urea, after which the dissolved nitrogen diffuses through the polymer into the surrounding soil. Diffusion refers to the movement of nitrogen, from a region of high concentration inside the coating, to the lower concentration environment of the soil. Temperature is a key factor influencing this process: higher temperatures accelerate diffusion by causing the polymer coating to expand, thereby enlarging the pores and facilitating nitrogen movement. Once released from the polymer, the uncoated urea quickly dissolves in soil water and is hydrolysed by the enzyme urease into ammonia or ammonium, which is subsequently converted into nitrate forms that are readily available for plant uptake [20, 21, 22].

No standardised method exists to reliably determine the nutrient release process, and it is generally studied from a macroscopic perspective [20]. Current models

typically employ classical approaches, such as diffusion-based models (e.g., Fick's law) [23], which are limited by the fact that they only represent nutrient transport, while neglecting water flow [24], empirical kinetic equations (e.g., Higuchi, Korsmeyer–Peppas) [25], or numerical solvers, like finite element methods [26, 27]. However, these models often rely on idealised conditions and empirical fitting, largely due to the limited availability of critical physical parameters like diffusivity and permeability [24].

Beyond the macroscopic process, the controlled release relies on finely tuned interactions between nutrient molecules and the surrounding polymer matrix. Such interactions include hydrogen bonding, ionic coordination, ion exchange, and polymer swelling, all of which play a critical role in controlling how and when nutrients diffuse into the soil [17]. Current computer simulations of nutrient release are limited in capturing the full dynamics at the molecular level. Accurate modelling of these molecular processes requires effective calculation of the binding energy between a urea molecule and individual monomers or small polymer oligomers [20, 21, 26].

Potential Impact of a Quantum Solution

To date, polymer–urea–water interactions have been modelled using molecular dynamics simulations or density functional theory (DFT) calculations performed on classical supercomputers. Realistic simulations must capture hundreds to thousands of atoms — including nutrient species, polymer chains, and water molecules — interacting in a highly coupled and dynamic manner [28]. Such simulations are computationally demanding, with a bottleneck of the classical approach being the lack of accuracy of the energy assignment to the structures, and the large number of configurations to study [28]. To manage these costs, researchers typically employ approximations and dimensional reduction methods, which can induce large errors and compromise the validity of the results.

In addition, while polymer-coated urea significantly reduces nitrogen pollution compared to conventional fertilisers, its polymer coating introduces environmental risks. As the coating degrades, it can fragment into microplastic, and eventually break-down into smaller nanoparticles that accumulate in soils and waterways. The design of new materials capable of environmentally safe degradation could be accelerated through computational modelling. Similarly, such simulations remain computationally demanding due to the wide range of chemical structures to survey and the limited accuracy of electronic energies obtained with classical methods [29, 30].

Quantum computing is a natural tool for simulating chemical systems and could offer a potential path to overcome some of the classical limitations by simulating key aspects of the chemical interactions involved in nutrient release from polymer-coated fertilisers, as well as in accelerating the design of new polymers. Quantum computers also offer the possibility of capturing the interactions of larger, more complete systems at scales which are intractable to classical computers. In the short-term, quantum algorithms such as adaptive variational quantum eigensolver algorithms could be considered, while in the long-term, quantum phase estimation

(QPE) algorithms could contribute to a solution by using fault-tolerant quantum (FTQC) computers [31].

Accuracy gained with quantum computing approaches would support deriving a complete mechanism of the chemical processes for i) nutrient-polymer interaction, and ii) design of safer polymer. Ultimately, this exploratory work could support the research of smarter, environmentally responsible use of fertilisers.

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3.2 Illegal Mining



MACHINE LEARNING

Quantum machine learning solution for monitoring illegal mining through satellite imagery and promoting environmental conservation, particularly in Ghana.

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Context

As the world digitalises and electrifies, demand for precious and “critical” minerals (gold, cobalt, nickel, copper, rare earths, and others) has risen sharply to feed technologies such as batteries, electronics, and renewable-energy systems. This surge in demand has increased market value and created incentives for both legitimate and illicit extraction [1]. This has fuelled a worldwide rise in illegal mining, the illicit extraction of precious metals and minerals from soil and water surfaces through unregulated artisanal small-scale mining. Illegal mining operates in complex supply-chain networks, exploiting governance gaps and poor traceability [2]. While illegal mining affects regions worldwide, from Latin America and the Caribbean to Southeast Asia, it’s particularly severe in Ghana, where it’s known locally as “galamsey” [3].

Illegal mining poses a serious threat to both the environment and public health [4]. In the gold extraction process, miners frequently rely on strong, often banned or hazardous chemicals, such as mercury and cyanide, to separate minerals from ore. If these substances are not adequately contained, they leach into aquifers and surface waters. Once released, they mobilise heavy metals such as mercury, arsenic, and lead, which significantly increase water turbidity and degrade water quality beyond safe consumption thresholds. This contamination spreads through river systems, threatening not only aquatic biodiversity but also drinking water sources for the surrounding communities [1, 5].

Studies indicate that some major rivers in Ghana, such as the Pra, Ankobra, and Offin, have dangerously high levels of contaminants, making them unsafe for human use [6]. This contamination has a direct impact on public health, resulting in an increase in waterborne diseases, heavy metal poisoning, and the loss of biodiversity in aquatic ecosystems [7]. In addition, the practice of illegal mining is often associated with organised crime groups that amplify the risks of crime, human rights abuses, and corruption in affected regions [1]. This, in turn, slows the achievement of SDG 12 (Responsible Consumption and Production) and its target 12.4, which seeks to minimise the impacts of chemicals and waste release on human health and the environment. Illegal mining is a key global concern, which prompted responses from the

international community to curb the practice, including studies [1], a formalisation framework and global data platform [8], and enforcement operations [9].

Addressing the crisis of illegal mining in Ghana and around the world requires monitoring systems that can identify illegal sites and mitigate the societal and environmental impacts of this practice.

Computational Challenges

Detecting and monitoring the environmental impacts of illegal mining can be assisted by the computational analysis of images, from satellite imagery as well as ground-level environmental datasets. Various computational approaches can be used to predict heavy metal contamination levels in bodies of water from satellite or spectral imagery, which utilises multiple bands across the electromagnetic spectrum, combined with machine learning methods, such as deep-learning methods, which rely on classical neural networks (NNs). The models can be trained in supervised, semi-supervised, or self/unsupervised regimes, depending on whether the images for training are labelled or not. A recent comprehensive survey [10] highlights the effectiveness of high-dimensional satellite data in remote sensing applications, environmental monitoring for lake contaminants, and even food contamination. A number of the methods reported rely on machine learning models trained on hyperspectral images with four bands (RGB and near-infrared (NIR)).

Challenges and bottlenecks mostly stem from the data pre-processing steps [11]. In this domain, raw spectral geospatial images typically require atmospheric corrections, spectral cross-channel calibration, and temporal alignment. The images are also often at different resolutions, requiring different labelling metrics.

Furthermore, limited and potentially imbalanced datasets also pose a challenge to training [12], as unbalanced classes of data would require further attention and pre-processing. For this use case, non-contaminated water sources are likely to vastly outnumber contaminated ones, requiring careful attention and pre-processing to avoid class imbalance. Without careful pre-processing, the machine learning model would be skewed by incorrect information to learn from. Another issue is the strong spatio-temporal autocorrelation that could inflate learning errors if images are not correctly grouped by site/time. These issues affect any downstream model in terms of learnability and performance.

Potential Impact of a Quantum Solution

Quantum computing could offer improved performance when dealing with those high-complexity and high-dimensional datasets. In particular, Quantum Neural Networks (QNNs) could be used to tackle this problem in terms of effective dimension, a property that reflects the expressivity and trainability of a model, compared to classical neural network methods [13]. QNNs could be capable in this case of modelling non-linear and complex environmental relationships, such as interactions

between mining activities and heavy metal dispersion in the environment.

The high dimensionality of the images themselves is a bottleneck in the use of NNs, such that high-performance computing (HPC) resources are often needed to load, pre-process, carry out layers of operations, and store the results of the model [14]. Geo-spatial images are sought out for the details and number of features they can provide. These high-volume and computationally expensive operations, which often require parallel processing, can be partially addressed by reducing the dimensionality of the dataset. This can be achieved through a number of feature reduction techniques to compress the dataset into a more manageable size [15]. Though of course, while reducing the dataset size decreases the computational resources required for training, it also respectively lowers the prediction accuracy of the model.

In this context, quantum machine learning offers an alternative path. If data must be compressed to its original size, one can hypothesise that quantum computers, given the same compressed features and parameter budget, may perform as well as, or better than, current classical baselines in extracting information and learning from reduced datasets. More broadly, and given the same inputs and matched parameter budget, a quantum machine learning approach with an appropriate feature map could, in principle, yield generalisation gains over classical approaches [16]. Within this hypothesis, with a large and well-curated dataset, modern machine learning methods remain the state of the art.

Finally, developing a more accurate model for predicting sites of illegal mining could strengthen response and mitigation strategies for environmental protection and safety. This is especially critical for safeguarding land and water resources that local communities rely on, as seen in Ghana.

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4 SDG 13 – Climate Action

4.1 Weather and Climate Forecasting



 LINEAR SYSTEMS OF EQUATIONS & PDEs

Quantum fluid dynamics simulation to improve the reliability of weather and climate forecasts.

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Context

The World Meteorological Organization (WMO) reported in its *State of the Climate 2024* [1] that the global mean near-surface temperature reached a record high, making 2024 the warmest year on record. It also marked the first time that each of the ten preceding years ranked individually among the warmest on record. Rising mean surface temperatures are associated with the increasing severity of extreme weather events [2], which in 2024 alone displaced more than 800,000 people and left them homeless [1]. While developing countries are the most severely affected by climate change and extreme weather events, it affects all countries around the globe. For example, the estimated cost of extreme weather events in the U.S. amounted to \$180 billion [3], and major flooding in eastern Spain led to over 200 deaths [4]. In 2025, over 800 people have died and more than 63,000 have been displaced in the Pakistan Monsoon Floods. [5].

Included in the United Nations' 2030 Agenda is the Sustainable Development Goal (SDG) 13 (Climate Action), which aims to strengthen resilience and adaptive capacity to climate-related hazards and natural disasters, integrate climate change measures into national policies, strategies and planning [6]. Early warning systems, which seek to predict possible catastrophic events and help minimise their impact, can play an important role in achieving this SDG Target. According to the WMO, early warning systems “have proved to be efficient systems that governments can use to move communities out of harm’s way before a disaster or manage the event in situ” [1]. However, for early warning systems to be effective, reliable and interpretable predictions are required. In particular, predictions based on physical models may become increasingly important if predictions based on historical weather data lose reliability as a result of climate change.

Climate change also significantly impacts other areas of societal, economic, and human development, slowing the achievements of other SDGs, including SDG 2 (Zero

Hunger), SDG 7 (Affordable & Clean Energy), and SDG 15 (Life on Land). For instance, increasing climate-based events, such as droughts and floods, are putting pressure on food security, deepening hunger for more than 735 million people across the world, and degrading hectares of land at a rapid pace [7]. Climate change also intensifies weather variability, making it harder to reliably integrate weather-dependent technologies, like solar and wind, into existing energy systems [7].

To effectively and reliably predict climate-related hazards and natural disasters, as well as build resilience across these domains, it is essential to understand local and global changes in climate and weather patterns over medium to long timescales.

Computational Challenges

Early warning systems for extreme weather events require very accurate and reliable weather forecasts. Similarly, developing climate risk and hazard mitigation strategies relies on robust climate predictions over several decades. These problems can, in part, be addressed by enhanced computational models for weather and climate forecasts.

Weather and climate predictions are performed using numerical Earth system models that represent main components, including the atmosphere, ocean, land surface, sea ice, ice on land, and ocean waves [8]. Earth systems are either represented by physical models or machine learning models [9].

The physical models are, for the most part, two- or three-dimensional fluid dynamics solvers. Physical models of the atmosphere and ocean typically discretise and solve the relevant governing equations with numerical discretisation methods, such as finite volumes or finite elements.

The machine learning models are large-scale deep learning solutions that need the most computing power during training. Similarly, performing inference at high resolution can be computationally demanding. With more available computational power, the resolution and complexity of both physical and machine learning models can be increased, and predictions can be improved. Machine learning models make use of graph neural networks [10], Fourier neural operators [11, 12] or transformer networks [13].

These models are computationally demanding and, to run the models at cutting-edge resolution, they are ported to some of the largest supercomputers available to the public [2, 14]. Leading global weather/climate models typically have a spatial resolution of 10 to 100 kilometres, which is insufficient to explicitly represent the relevant physical processes underlying the time evolution of weather and climate models [15]. Higher spatial resolution raises the computational requirements, leading to an increased cost and making practical implementation highly challenging [2].

An additional bottleneck is that these models produce large amounts of data that need to be accessed and processed. For instance, the DYAMOND (DYnamics of the Atmospheric general circulation Modeled On Non-hydrostatic Domains) configura-

tion of the ICON (ICOsaedral Nonhydrostatic) Earth system model is a specific, high-resolution setup to address large-scale storm-resolving atmospheric models. It produces 164GB per simulated day at a 5km resolution [16], and typical operational weather forecasts run hundreds of simulated days per wall clock (real-time) day [15].

Potential Impact of a Quantum Solution

Quantum and quantum-inspired algorithms could provide a solution to the bottlenecks mentioned above. This use case proposes to use quantum-inspired tensor network algorithms to enhance weather and climate prediction models.

In a first step that can be taken today, quantum-inspired tensor network algorithms running on classical hardware have the potential to outperform existing classical approaches, for specific problems which are matrix-operation intensive, in terms of accuracy and speed, by representing vector fields and matrix-vector operations in an extremely compressed format.

In a second step, tensor networks could be converted into quantum circuits on fault-tolerant quantum computers envisioned for the future. and thus port the classical algorithm to a quantum computer in a natural manner [17]. In combination with techniques for representing non-linear cost functions on quantum computers [18], a tensor network algorithm could subsequently be rewritten as a variational quantum algorithm on a quantum computer.

Focusing on the short-term solution, tensor network methods as quantum-inspired algorithms are known to be a powerful tool in theoretical quantum physics for simulating quantum many-body systems on classical hardware. This approach has enabled the simulation of physical systems that are otherwise intractable by removing unrealised correlations (entanglement) from the model [19]. More recent results [20, 21] show that this approach could be transferred to fluid flows, where correlations between different length scales take the role of entanglement. Just like when simulating quantum systems, it is believed that tensor networks can significantly reduce the number of degrees of freedom required to describe flow problems, therefore potentially giving rise to fluid dynamics simulations with higher resolution. Applied in the context of weather and climate forecasting, it has the potential to provide improved precision of simulations.

Operations that are ubiquitous in fluid dynamics simulations, such as addition, pointwise multiplication, and solutions to linear systems of equations on flow fields, can all be carried out efficiently in tensor network format [20, 21]. In addition, climate and weather models often use Fourier Transforms as a subroutine during simulations. These Fourier Transforms can also be carried out in tensor network format and, in some cases, very efficiently and with a potential speed-up over the Fast Fourier Transform [22].

To summarise, the main expected benefit for quantum-inspired tensor network algorithms would be a significant speed-up of weather and climate predictions on fine grids, which would lead to improved accuracy by enabling simulations at currently

intractable resolutions.

Looking into the future, these benefits could be further enhanced by fully quantum algorithms, which could tackle exponentially larger system sizes that not even conventional supercomputing (HPC) systems could simulate. Thanks to the possibility of encoding high-resolution grids in quantum hardware and additional quantum algorithms that could lead to benefits in a number of subroutines, including but not limited to the Quantum Fourier Transform [22], tensor network-based quantum algorithms may one day be able to give new insights into climate and weather patterns over new timescales.

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4.2 Flood Prediction

 MACHINE LEARNING

Quantum machine learning solution to provide better accuracy in flood prediction and improve prevention mechanisms in regions at risk, particularly Malaysia.

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Context

Floods have been regarded as one of the most common natural disasters happening worldwide. The Emergency Events Database (EM-DAT) published by The International Journal of Disaster Risk Reduction reported that floods account for over 20% of the "natural" disaster hazards [1], including hurricanes, landslides and so forth. Furthermore, 70% of the people at risk of extreme floods, those of 1-in-100 year occurrence, are based in South and East Asia [2]. For instance, the World Bank and Bank Negara Malaysia reported a hypothetical 1-in-20-year flood could cost Malaysia up to 4.1% of its GDP in 2030 and cause up to a 2.2% increase in the unemployment rate [3]. According to UNDRR's Global Assessment Report on Disaster Risk Reduction (GAR), water-related hazards accounted for annual losses of USD 388 billion globally, with projections to rise to 407-439 billion in annual losses by 2050 due to climate change and rapid urbanisation. [4]

Besides socio-economic aspects, flood events cause unwanted tragedies and continuously endanger human lives. Over the past three decades, the world has witnessed over 218,000 fatalities globally due to floods. Just last year, Chad and Niger recorded 576 and 396 fatalities, respectively, due to floods, and were ranked in the top 10 countries for hazard mortality rates in 2024 [5].

Rising global temperatures driven by climate change are exerting long-term impacts on regional rainfall patterns [6]. Glaciers are retreating at unprecedented rates, with 2023/2024 marking the 37th consecutive year of shrinkage among reference glaciers [7]. Melting glaciers contribute to sea level rise, while warmer air holds more moisture, increasing evaporation and cloud formation. This amplifies the intensity, duration, and frequency of precipitation, driving more extreme weather events and floods, particularly in vulnerable regions [8]. Data from the EM-DAT database (1975–2022) show that, although the number of flood events has risen, fatalities per event have declined, reflecting the effectiveness of existing prevention and mitigation efforts [9]. This underscores the critical need to sustain and continuously enhance flood forecasting, mitigation, and resilience strategies across scales to anticipate and counter escalating flood risks under climate change.

Computational Challenges

In 2003, the World Meteorological Organization listed weaknesses of flood forecasting systems [10] with two main concerns: (i) the incompatibility of meteorological and hydrological data in the integration of a flood forecasting system, and (ii) the fact that flood forecasting alerts are not risk qualified. Since then, various numerical weather prediction models have been studied, and one of the commonly adopted models is the Weather Research & Forecasting (WRF) model [11].

The WRF model discretises the three-dimensional atmospheric space into smaller grid cells and attempts to solve the dynamical evolution of each grid cell based on the initial conditions provided by the input data. However, because climate and weather behave as a coupled non-linear chaotic system [12], reliable long-term prediction and forecasting remain unfeasible. Although the ‘intrinsic limit of predictability’ is often considered to be around two weeks [13], studies such as [14] have demonstrated that the current operational European Centre for Medium-Range Weather Forecasts (ECMWF) ensemble forecasting system can retain significant predictive skill for up to 23 days. In fact, the ECMWF ensemble forecasting method shows that ensemble forecasting [15] is useful to counter the chaotic effects of weather forecasting.

Ensemble methods may improve forecasting accuracy but remain computationally demanding. To overcome this, machine learning approaches have been explored to reduce resource requirements. For instance, accurate spatial flood prediction with a machine learning model [16] was recently validated using data from Hurricane Nicholas (2021) near Galveston Bay, Texas (USA), combining real-world observations with simulated data from numerical models. Similar work applied a hybrid convolutional neural network (CNN) to predict floods in the Mahanadi river basin in India [17]. While the hybrid CNN outperforms alternative machine learning methods, its performance could be further enhanced by incorporating longer time series data, additional weather variables such as temperature and evaporation, as well as advanced optimisation techniques.

Flood data are highly complex. In order to effectively convey flood risk information, several types of flood maps were developed for the purpose of management, governance, and public services. Three types of flood maps are commonly used, namely the flood inundation map, flood hazard map, and flood risk map. The flood inundation map records the historical flooding area; the flood hazard map shows the extent of flood events in scenarios with different probabilities; the flood risk map combines the flood hazard map with socio-economic, human health, and environmental consequences associated with floods [18]. This type of information can be used to both train the machine learning methods and to inform local possible prevention and mitigation strategies.

Multi-scale approach necessarily requires the generalisation of larger hydro-meteorological models from the current open-source projects done by the Intergovernmental Panel on Climate Change and the Coupled Model Intercomparison Project, which should also be able to process the ever-increasing multi-scale datasets from international organisations, such as the National Aeronautics and Space Administration, the European Space Agency, and the United States Geological Survey [19].

Potential Impact of a Quantum Solution

Hydrodynamical models, based on the fundamental principles of physics and fluid dynamics, are computationally very demanding. Solving these partial differential equations that describe the dynamics of large-scale flood models is both computationally expensive and with limited scalability [13]. This often forces a compromise between the accuracy and speed of the computation. On a purely data-driven approach, classical machine learning methods can tackle and reduce this computational cost, yet they are limited by input data [16]. Despite demonstrating considerable success in pattern recognition and time-series forecasting in various fields [20], machine learning methods lack representation of physical principles, which can lead to physically inconsistent results.

Quantum computing could offer promising avenues for leveraging quantum-classical machine learning architectures for climate modelling and flood forecasting. In this use case, two classes of quantum-classical architectures are explored. The first one is using time series data to train machine learning models, particularly in flood risk forecasting, recurrent neural network models, such as quantum-train long short-term memory [21]. This has been demonstrated as a potential quantum use case to predict the future river water level within a certain time step, or to estimate the likelihood of flood events. Other climate time series data, such as air quality [22], can also be used. In the quantum long short-term memory paradigm, classical neural networks are substituted and optimised by parametrised quantum circuits, which have been previously identified to have strong expressivity and can, in theory, represent highly non-linear distributions well [23]. Quantum machine learning method has the potential to efficiently learn and generalise from a smaller, complex, and multi-scale dataset, like the ones available for flood prediction [24].

The second class of quantum machine learning architecture is based on quantum convolutional neural networks (QCNNs). Much work has already been done on testing and experimenting with quantum QCNNs, whilst comparing the methods to the classical performance of CNNs [25, 26, 27], and finding competitive or promising results offering a new avenue for climate modelling. It shows promise to bring more accuracy to predicting climate-related outcomes compared to their classical counterparts [28]. While there is no clear empirical evidence of a quantum advantage, quantum neural networks could offer some advantage in terms of learning accuracy.

Increasing the accuracy and reliability of a flood model would directly contribute to enhancing tools for prediction and prevention when it comes to fighting climate change and its effects. It would mean improving the mitigation strategies that governments could put in place for these natural disasters, and it would translate into saving lives in most affected areas.

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