National Quantum Computing Centre

SparQ

SparQ Quantum Applications Portfolio 2023–25

Quantum Computing Use Case Compendium

The NQCC works across government, industry and the research community to drive quantum readiness in the UK and support the long-term strategic goal of employing quantum computing to deliver prosperity and security for societal good.

Publication information

This is a publication from the National Quantum Computing Centre (NQCC) which is funded through UK Research and Innovation and sponsored by the Engineering and Physical Sciences Research Council (EPSRC) and the Science and Technology Facilities Council (STFC).

Acknowledgements

The authors would like to acknowledge the following valued SparQ partners for having contributed to the NQCC Quantum Computing Use Case Compendium:

Airbus, AIOI R&D Lab, Applied Quantum Computing, Avatrial, Brunel University of London, Capgemini, Centre for Molecular Medicine and Biobanking, University of Malta, Digital Catapult, D Wave, Frazer-Nash Consultancy, Hampshire Hospitals NHS foundation trust, HSBC Holdings plc, Imperial College London, Infleqtion (Cold Quanta UK), Innovate UK, Kings College London, Kuano, LTI Mindtree, Mind Foundry, Newcastle University, Orca Computing, Oxford Ionics, Paysafe, PsiQuantum, Qinetiq, Quanscient, Quantarverse, Quantinuum, Quantum Base Alpha, Quantum Software Lab, Radiation Analysis Services Ltd, Rigetti, Riverlane, Rolls Royce, Royal Brompton and Harefield Hospitals, Samsung UK, STFC Cross Cluster, STFC Hartree Centre, STFC Scientific Computing, University College London, Unisys, The Crown Estate , The Public Service Consultants, The University of Edinburgh, Zaiku Group

Principal author(s):

- Sonali Mohapatra, Quantum Innovation Sector Lead, NQCC
- Mariana Manso, Quantum Innovation Sector Lead, NQCC
- Zoe Dale, STFC Graduate Cluster Development Officer, Secondment, NQCC

Contributors:

- Rob Whiteman, Quantum Readiness Delivery Lead, NQCC
- Konstantinos Georgopoulos, Quantum Applications Lead, NQCC
- Simon Plant, Deputy Director of Innovation, NQCC
- Michael Cuthbert, Director, NQCC

Production:

Soma Deshprabhu,
Communications Manager, NQCC

Publication release:

Released on 5th June 2025

@ National Quantum Computing Centre, 2025.
All rights reserved.

Foreword

Quantum technologies are poised to transform our technology landscape – unlocking advances in scientific understanding and reshaping industrial sectors for economic and societal good.

The United Kingdom has committed to building global leadership in quantum technologies through the National Quantum Strategy and our broader innovation missions, recognising their potential to address complex challenges and deliver significant economic and societal benefits.

At the National Quantum Computing Centre (NQCC), we are proud to play a key role in realising this ambition. Our focus is on scaling quantum computing, both the technology and the user community. As part of this we are working to accelerate access to early quantum computing capabilities, develop national readiness, and foster collaboration across sectors. Furthermore, we seek out use cases and computational methods that will demonstrate the true value of quantum computation over traditional classical methods – quantum advantage.

This Quantum Computing Use Case Compendium is a reflection of that broader vision. It highlights the areas where we at the NQCC have been working with colleagues across government, academia and industry to investigate some of the most pressing computational challenges of our time – from advancing clean energy and sustainable manufacturing, to accelerating pharmaceutical discovery, optimising complex logistics, and underpinning resilient financial systems. These challenges align not only with the technical frontiers of quantum computing, but also with the UK's National Missions on Net Zero, Health, Digital and Data, and the Future of Transport.

By translating scientific promise into targeted research and development efforts, we move closer to achieving strategic advantage: creating new industries, strengthening national resilience, and driving economic growth in a rapidly changing global environment.

This work will not happen in isolation. It demands the collective efforts of academia, industry, innovators, and policymakers. Through collaboration, investment, and a shared commitment to excellence, we will ensure that quantum computing delivers meaningful and lasting benefits for the UK.

I extend my sincere thanks to our partners involved in the 19 projects featured in this publication – the STFC Cross-Cluster Team for the Proof-of-Concept (POC) projects and the Innovate UK for the Feasibility projects. Early examination of such computational use cases and mapping them onto quantum compute resources is a critical step towards independent and verifiable quantum advantage

Dr Michael Cuthbert
Director,
National Quantum Computing Centre (NQCC)

Executive Summary

This Quantum Computing Use case Compendium brings together a record of industry-led proof-of-concept (PoC) and feasibility studies conducted between 2023 and 2025. These projects, facilitated by the National Quantum Computing Centre (NQCC) through its SparQ programme, explore practical applications of quantum computing across various sectors.

Programme overview

The SparQ initiative is central to the NQCC's strategy for achieving quantum readiness. It supports the development of quantum applications, enhances skills, and fosters a collaborative quantum computing community. The programme provides access to quantum hardware, software platforms, and expert guidance, enabling organisations to explore and develop quantum solutions.

Building quantum readiness in the UK

A quantum ready economy is one that can generate and retain value from quantum computing. The SparQ programme contributes to the UK's quantum readiness by:

- **Skills development:** Training researchers and engineers through hands-on projects to develop an informed user base and an entrepreneurial supply chain.
- **Access to resources:** Providing early and assured access to evolving quantum computing hardware and software stacks and expert support.
- **Collaborative ecosystem:** Fostering partnerships between academia, industry, and government to accelerate quantum innovation, and enabling clear policy, standards and public trust frameworks.

The projects in this compendium advance readiness by:
- up-skilling more than 200 researchers and engineers through embedded teams,
- validating early access pathways; and
- leveraging public money with suitable private commitment.

Route to practical applications

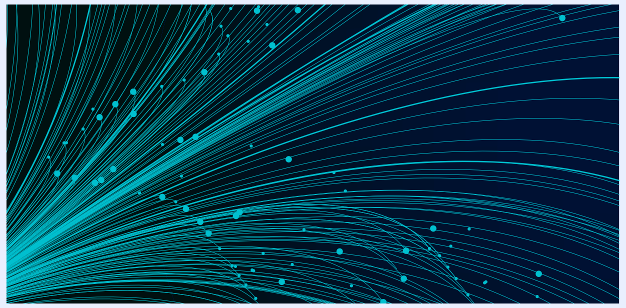
The studies follow a consistent pathway:

- **Opportunity framing** – Industrial partners define a high-value challenge
- **Application discovery and PoC** – Small-scale experiments benchmark near-term quantum algorithms or hybrid workflows
- **Feasibility and scale-up** – Larger studies stress-test the most promising approaches, quantify resource needs and identify integration points with existing tools and data pipelines
- **Readiness assessment** – Each case study includes indicators of algorithmic maturity, hardware requirements and skills needed for the next stage.

Call	NQCC funding	Matched private investment	Projects	Organisations
STFC Cross Cluster PoC (2024/25)*	£726k	≥£726k	12	28
Innovate UK Industrial Applications Feasibility (2023 25)**	£6.2m	>£2.8m	19 (NQCC core partner on 7)	61
Total	**£6.9m**	**>£3.5m**	**31**	**80+**

* Projects provided 50% match funding or over ** Match funding levels depending on organisation type

Quantum Computing Use Case Compendium



By working together on real industrial challenges, we convert scientific promise into measurable progress towards deployable quantum solutions.

Dr Rob Whiteman
Quantum Readiness Lead, NQCC

What the reader will find

- **19 case studies:** Spanning energy, advanced materials, healthcare & pharma, finance, logistics, aerospace and communications
- **Sectors addressed:** Energy & Net-Zero, Healthcare & Pharma, Advanced Materials, Financial Services, Logistics & Transport, Aerospace, Communications, and Space
- A clear outline of each industrial challenge, the quantum approach tested, early performance indicators and the next milestones on the path to quantum enabled solutions
- A glossary of key terms and a directory of the organisations involved, to help new entrants navigate the landscape.

This staged approach provides a realistic route to practical adoption, ensuring that effort is focused on problems where quantum advantage (speed, accuracy, energy-efficiency or solution quality) is most likely to matter in real-world settings.

Why this matters now

Early engagement allows UK organisations to build quantum readiness – the skills, supply chains and evidence base needed to adopt quantum computing when commercial advantage appears. The projects documented here show:

- **Near term experimentation:** Results obtained on today's available quantum computing platforms spread across modalities
- **Route to deployment:** Each study maps the (early) technical and economic steps from laboratory proof to an operational tool inside existing industrial workflows
- **Collaboration at scale:** More than 70+ companies, research institutes and public bodies have contributed expertise, data and funding.

How to use the Compendium

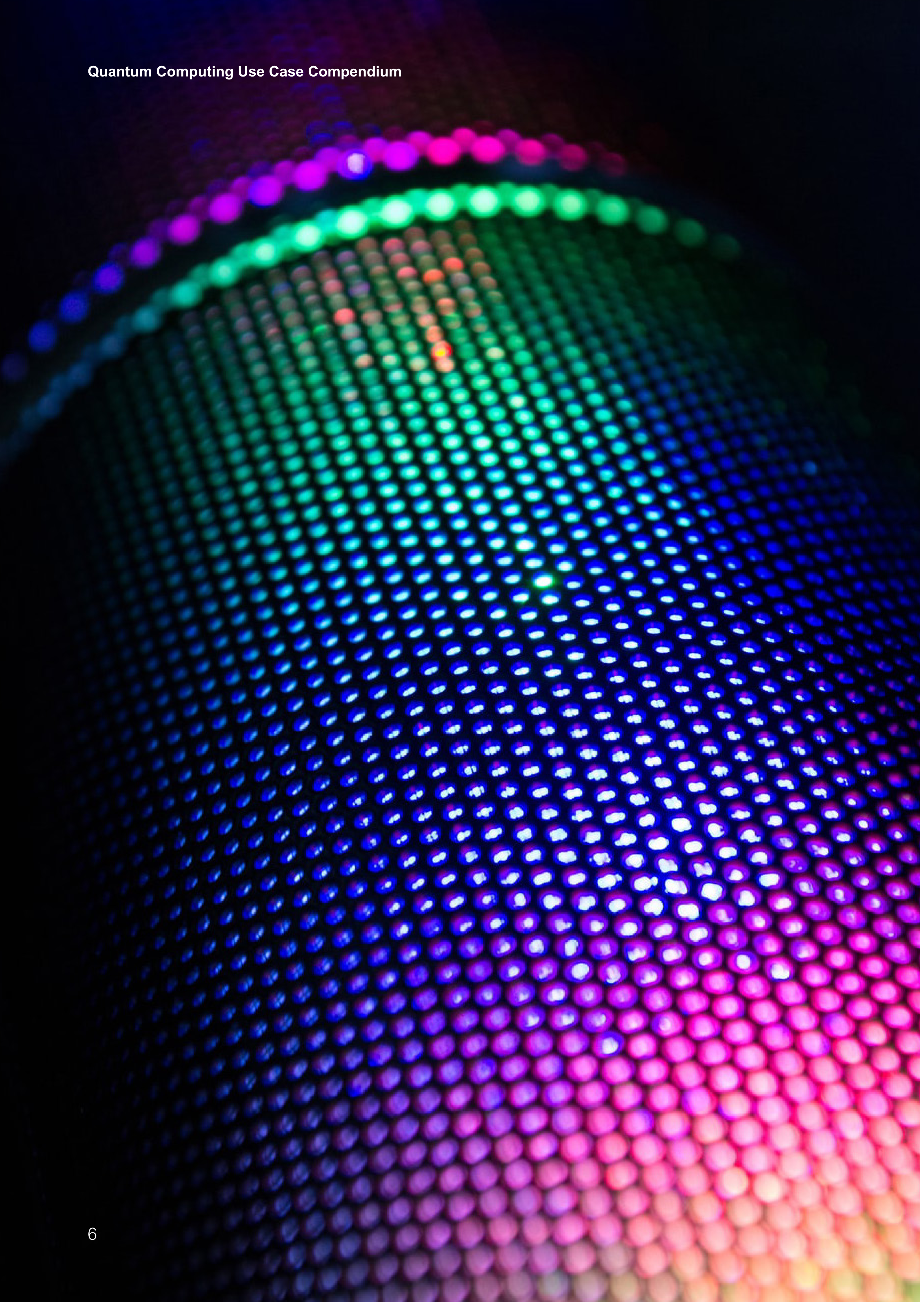
Each case study is presented in a common template that highlights:

- the industrial challenge and why it matters
- the quantum approach taken and current performance
- next technical and commercial milestones
- collaboration opportunities for new partners.

Together, they provide a state-of-practice snapshot for decision-makers assessing when and where quantum computing may enter mainstream workflows.

This executive summary is intended to orient readers quickly. Detailed technical results, partner testimonials and glossary material follow in the main document. We welcome further collaboration as the UK moves, step by pragmatic step, from early experimentation to demonstrable quantum advantage.

For more information on the SparQ programme and to access the full compendium, please visit nqcc.ac.uk.



Contents

SparQ Quantum Computing Call

SparQ

STFC Cross Cluster Proof of Concept: Use Cases 2024-25

National Quantum Computing Centre

Science and Technology Facilities Council
Innovation Clusters

> Partnering with the NQCC on the Cross Cluster Proof of Concept: SparQ Quantum Computing Call, enabled us to support innovative businesses that are exploring practical applications and use cases for quantum computing. To accelerate development of this emerging technology, the NQCC provided access to dedicated quantum expertise and resources, through its SparQ programme. In addition to advancing projects with the potential for real-world impact, the call strengthened connections between NQCC, industry and end-users, and supported cluster growth.

Dr Lee Glassbrook
Deputy Director, Innovation Clusters & Harwell Campus

SparQ

28 companies

726k funding

12 use cases

- 3 months
- Application engineer support
- Innovation sector lead support
- QC resources

Funding call overview

The National Quantum Computing Centre (NQCC), in collaboration with the Science and Technology Facilities Council (STFC), support an annual portfolio of business-led proof-of-concept projects. Funded through the NQCC's SparQ programme, the initiative aims to identify and develop early practical applications and use cases for quantum computing across the public, private, and charitable sectors.

Projects are expected to appraise hardware and software requirements, verify current quantum computing capabilities, and develop models using quantum algorithms on real or emulated quantum processors. The 2024/2025 initiative successfully supported the exploration of 12 use cases, contributing to the UK's efforts in advancing quantum readiness and fostering industry engagement in quantum technologies.

Participating organisations

AIRBUS, AIOI R&D LAB Oxford, AppliedQuantumComputing, AVATRIAL Therapeutic Discovery Architects, Brunel University of London, Capgemini, Digital Catapult, D-Wave, Frazer-Nash Consultancy, Imperial, Infleqtion, King's College London, LTIMindtree, mind Foundry, National Quantum Computing Centre, ORCA Computing, oxford ionics, PsiQuantum, Paysafe It starts here, QinetiQ, Quanscient, Quantinuum, Quantarverse, Radiation Analysis Services Ltd, Royal Brompton & Harefield NHS Foundation Trust, STFC Hartree Centre, STFC Scientific Computing, The Crown Estate, Unisys

Quantum machine learning for fraud detection in credit card transactions

The consortium explored the use of quantum machine learning (QML) techniques to detect anomalies in financial transactions, with a specific focus on identifying credit card fraud. By applying quantum restricted boltzmann machines (QRBMs), the project aimed to assess whether quantum-enhanced models could offer performance advantages over traditional machine learning approaches in detecting fraudulent activity within large, imbalanced datasets.

Lead: unisys

Partner: UKRI National Quantum Computing Centre

Observer: Paysafe It starts here

Challenges of financial fraud detection

As financial fraud, particularly credit card fraud, becomes increasingly sophisticated, detecting fraudulent transactions remains a key challenge in the financial sector. One of the primary obstacles is the significant data imbalance, with fraudulent transactions representing only a small fraction of the total amount of data. This imbalance can pose challenges for traditional machine learning models to effectively identify fraudulent transactions, often leading to false positives or missed fraud cases.

This project explored the use of quantum machine learning, specifically quantum restricted boltzmann machines (QRBMs), for detecting anomalies in financial transactions.

Exploring quantum machine learning for enhanced fraud detection

The QRBM model was trained and evaluated using a known public dataset of anonymised credit card transactions from European cardholders, a dataset commonly used in fraud detection research due to its real-world relevance.

Despite the challenging imbalance of the data, the model demonstrated competitive performance, achieving promising results with no false negatives and very few false positives.

The results were comparable to, and in some cases surpassed, those of established classical approaches. The approach successfully leveraged quantum energy-based modelling to separate complex data patterns, showing its potential for improving fraud detection performance.

Impact

The project laid the foundation for future work focused on scaling QRBMs for larger datasets and optimising their compatibility with existing quantum hardware. It also identified the potential for exploring hybrid systems that combine both classical and quantum computing to enhance fraud detection performance in the future.

Beyond performance metrics, the project offered valuable insights into the practical application of quantum computing within the finance sector. It highlighted potential opportunities and limitations, including hardware scalability, the need for model transparency, considerations for regulatory compliance in real-world environments, and the requirements for integration in practical systems.

The results showed that QRBMs are a viable candidate for future fraud detection frameworks, particularly in scenarios requiring high precision and recall. This work marked an important contribution to real-world applications of quantum computing in financial services and provided a foundation for further development of quantum machine learning models for fraud detection.

> At Unisys, we envision a future where quantum innovation transforms industries. Our work in quantum machine learning for fraud detection shows how quantum systems can drive practical impact today, setting a powerful foundation for tomorrow's financial security.

Unisys Ltd

Healthcare

Machine Learning

Using quantum machine learning to improve early detection of cancer

The project demonstrated improved classification of cancer cell types in liquid biopsies using a quantum machine learning approach compared to a classical machine learning classifier. Led by Applied Quantum Computing Ltd., the consortium comprised partners from academia, as well as public and private sectors. Initial evidence was generated supporting the application of quantum machine learning methods in cancer detection.

Lead:
AppliedQuantumComputing

Partners:
IMPERIAL
Brunel University of London
Digital Catapult
NHS Royal Brompton & Harefield NHS Foundation Trust
UKRI Science and Technology Facilities Council Scientific Computing
UKRI National Quantum Computing Centre

Non-Invasive techniques for cancer detection

Minimally- or non-invasive testing techniques are becoming increasingly important in healthcare environments for the early detection of cancer. They allow for improved patient experience and for cancers to be detected at earlier stages. One such technique is liquid biopsies, involving examining cancer-related materials, such as cancer cells or DNA, from certain bodily fluids.

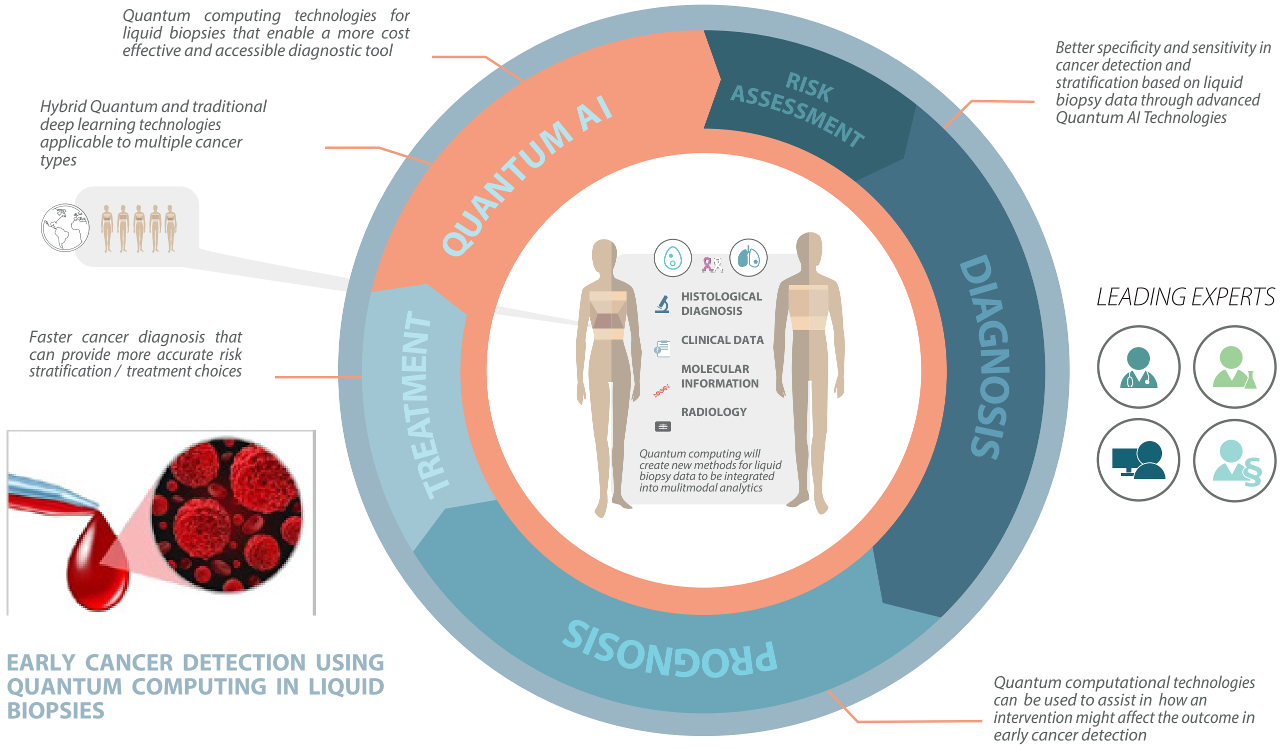
This project looked to investigate the potential for Quantum machine learning (QML) methods to analyse different types of cancer that could be found within liquid biopsies. Data of the different cancers were used to investigate this use case.

Classifying using quantum and classical machine learning methods

The labelled data from several cancer types were fed into a classical encoder for feature selection. When fed into a quantum support vector machine (QSVM), a commonly used quantum classifier within QML, interesting results were obtained.

The quantum classifier was able to successfully distinguish between cancer pairs with f1 scores (measure of predictive performance) in 3 of the 5 cases exceeding 0.9. Alongside this, feature sets were fed into a classical machine learning classifier based on a pretrained deep neural network.

Similar results were achieved in 3 of the cases but were less good than the quantum classifier in the others. The sample results were also able to be replicated on an IBM quantum computer, through access provided by the National Quantum Computing Centre (NQCC).



Impact

The benefits of this approach as an early diagnostic technique for cancer, including low cost and minimal invasiveness for the patient, made this a compelling use case. The initial proof-of-concept results achieved through this project, as compared to classical classifier results, suggest that QML or hybrid methods may be able to increase the efficiency of cancer data analysis. This would allow health providers to identify different tumour variations quicker and more easily.

Further development of this work could assist in ensuring earlier cancer diagnosis, and contribute to the field of personalised medicine, ensuring treatments are more customised to the individual patient's cancer.

> We are delighted to have had the opportunity to work on such a potentially impactful quantum project where the prize is to advance the effectiveness of cancer diagnostic techniques with possible future benefits in terms of earlier cancer detection and improved patient treatment.

Tim Thomas
CEO, Applied Quantum Computing

Quantum machine learning for clustering multi-omics data in cancer research

By comparing classical and quantum machine learning (QML) methods to cluster omics data, Infleqtion (previously ColdQuanta UK), alongside Avatrial, were able to demonstrate the advantages of QML in capturing the complexity of multi-omics data to provide cancer and disease insights.

Lead: Infleqtion

Partner: AVATRIAL Therapeutic Discovery Architects

Observer: UKRI National Quantum Computing Centre

Multi-omics approaches and machine learning

Biological molecules translate into the structure, function and dynamics of an organism and can be grouped into pools. Understanding, characterising and quantifying these pools to look at biological function is known as omics. Multi-omics approaches can be used in cancer research, combining omic datasets (proteomics, genomics, metabolomics etc.,) generated from the same patients to understand and classify the molecular and clinical features of cancers.

Clustering is an unsupervised machine learning technique that can be used to group data (including omic data) based on similarities and patterns. This can be utilised in multi-omics approaches, revealing system level and disease insights to inform treatment decisions.

The complexity problem

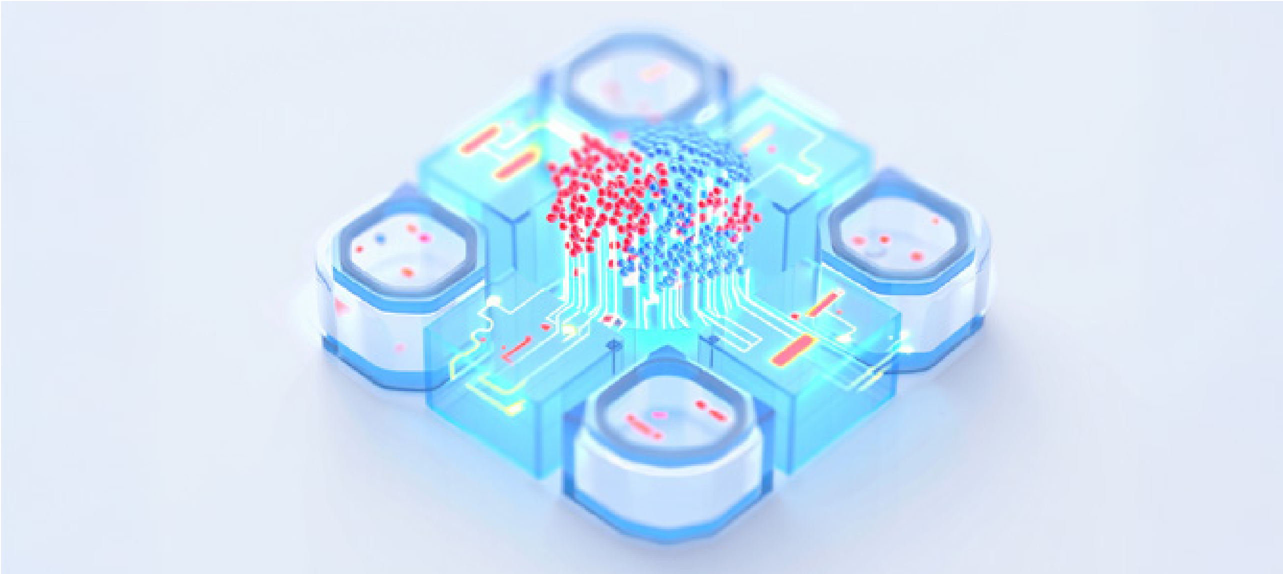
Clustering multi-omics data is a computationally expensive task, especially as the size and complexity of the data set increases. This proof-of-concept project looked to investigate the advantages of Quantum Machine Learning, over classical methods, to improve the scalability and accuracy of the complex task of multi-omics clustering.

Comparing QML and classical multi-omics clustering

The project looked at clustering integrated omics data from 10 matched normal and tumour patients using in-house data provided by Avatrial, and compared the clusters produced. To do this, different ansatzes were studied, and a novel way to perform quantum kernel alignment was developed, using the variance of the kernel matrix for an unsupervised learning task.

The project team was able to experimentally confirm that maximising the variance led to a meaningful kernel matrix that captured the underlying structure of the data set. To increase the real-world applicability of this project, the results were also tested in the presence of noise, and clustering was found to be robust up to an error rate similar to current quantum computers. Finally, the team verified the results by running simulations on an actual quantum device.

Overall, results showed that both classical and QML methods were found to effectively distinguish tumour samples from normal samples in complex multi-omics data. However, when the tumour samples only were clustered, the sub-clusters varied significantly between QML and classical. Classical showed distinct signalling pathway profiles but QML indicated consistent trans-omics pathway activity.



The proof of concept demonstrated that QML more accurately managed to capture the complexity of multivariate omic patterns.

The project team acknowledges that the small sample size limits the generalisation possible from results. There was also limited information on patient clinical outcomes and treatment regimens, hindering the ability to draw conclusive inferences about portioning of identified clusters. Data processing methods and the computational environment for classical and QML were also recognised as different, making direct approach comparisons difficult.

On balance, this project demonstrated the advantages of QML for clustering multi-omics data, applicable to use cases in cancer and disease clinical research, as well as paving the way to understanding quantum kernel-based approaches in QML more generally.

> This collaboration between Avatrial and Infleqtion shows how quantum computing can be applied to critical use cases such as cancer drug discovery. The quantum clustering method developed during this project applied on the high quality dataset resulted in meaningful clusters, paving the way towards personalised cancer treatment.
>
> Infleqtion

Energy & Sustainability

Optimisation

From batteries to wind farms: quantum optimisation solutions for the renewable sector

The project explored the potential of quantum computing to address key optimisation challenges in the UK's renewable energy sector, with a focus on offshore wind power. The successful roll-out of large-scale renewable infrastructure makes efficient and informed planning essential. Quantum optimisation offers a potential approach to tackling these challenges, particularly in areas such as asset deployment and spatial optimisation.

Lead: FRAZER-NASH CONSULTANCY

Partners: THE CROWN ESTATE, ORCA COMPUTING, UKRI National Quantum Computing Centre

Unlocking quantum potential for wind energy

Following a survey of potential applications across the renewables landscape, the consortium explored how quantum computing could be practically applied to support the deployment of offshore wind energy. Two use cases were identified as particularly promising areas for quantum optimisation.

1. Offshore deployment modelling
Determining optimal locations and configurations for new offshore wind farms is a complex spatial optimisation problem. The project explored quantum techniques to address this challenge and assess their potential for high-level deployment modelling.

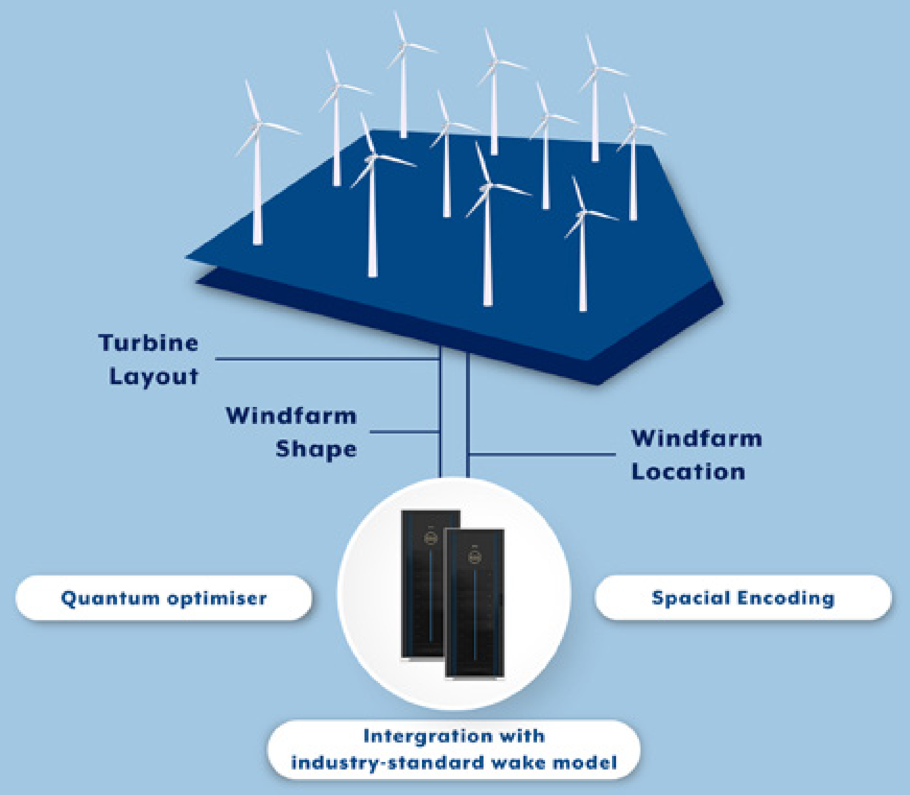
These methods may also have broader applicability in other domains involving spatial optimisation such as land use planning, facility layout, and natural resource management.

2. Wind farm layout optimisation
Optimising the layout of individual turbines within a wind farm is crucial to maximise energy production and ensure the economic viability of wind energy projects. This initiative explored a quantum-enabled approach to layout optimisation, integrating with existing industry-standard tools to model turbine interactions. The work provided an early demonstration of how quantum computing can be applied to wind farm design at a near-commercial level of detail.

Hardware implementation and technical achievements

Both optimisation use cases were implemented on ORCA PT series photonic quantum hardware. The project addressed one of the larger problems solved on this type of system, providing insights into current hardware capabilities and resource requirements for future scaling.

Quantum optimisation of offshore windfarms



Impact

The project delivered several tangible outcomes, including a demonstration that spatial and layout optimisation tasks in renewable energy can be approached using near-term quantum hardware. It also provided insight into current device performance and laid the groundwork for further feasibility studies exploring integration with existing workflows and benchmarking against classical methods.

By contributing to quantum-readiness in the UK's renewable energy sector, this work supports ongoing efforts to advance climate goals and explore solutions to large-scale energy system challenges.

> Renewable energy systems are key to tackling climate change, boosting supply security, and cutting bills. This project showed how quantum computing might address some of the sector's challenges and highlighted some exciting new possibilities, especially in quantum optimisation for offshore wind power.

Frazer Nash Consultancy

Quantum computers for simulating NMR spectra in next-generation battery materials

A new quantum computational workflow for simulating NMR spectra of battery materials was developed through a collaborative project led by Quantinuum Ltd. The development of this new quantum workflow allowed for hardware resource estimates to be calculated for large-scale NMR simulations on both current and promising future fault-tolerant devices. This work provides a stepping stone towards the application of quantum computing for next-generation battery solutions.

Lead: QUANTINUUM

Partner: UKRI Science and Technology Facilities Council Hartree Centre

Observer: UKRI National Quantum Computing Centre

NMR spectroscopy for next-generation batteries

Advanced battery technologies, and their component materials, play a vital part in clean energy solutions. They are therefore key to advancing the transition to clean energy, in line with the UK Government's commitment to net zero emissions by 2050 and the UK battery strategy.

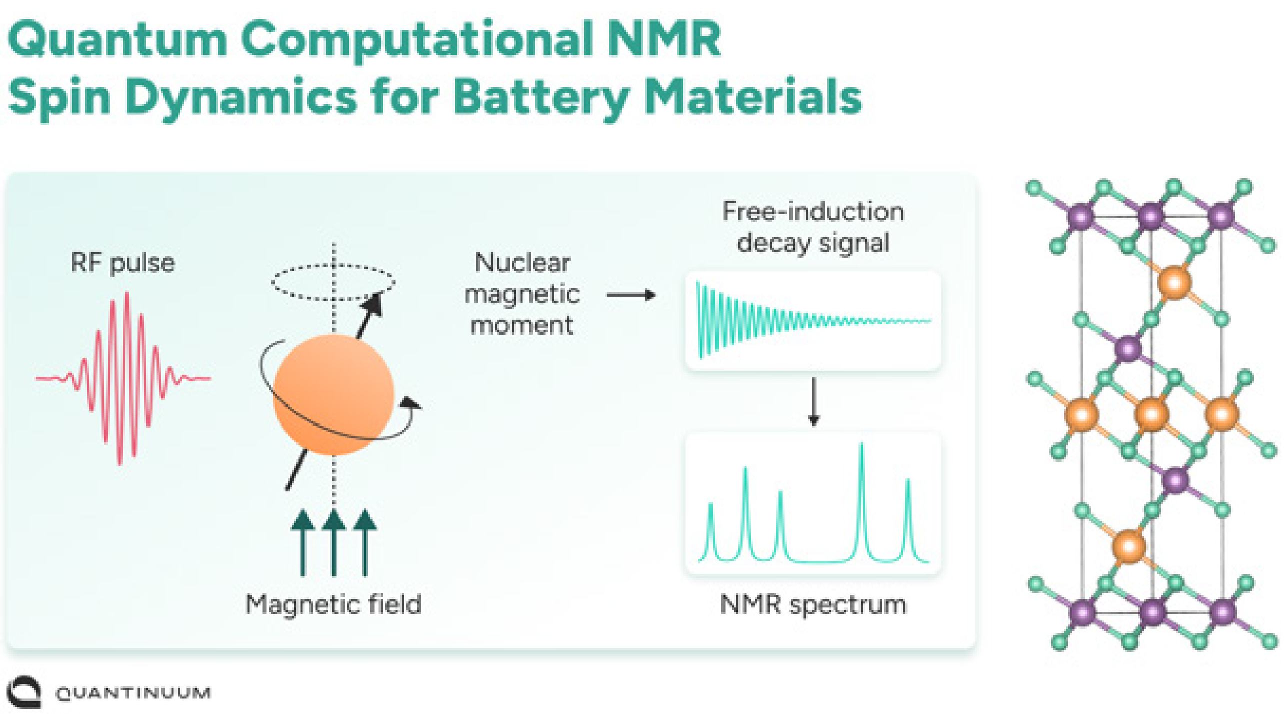
Characterising complex battery materials requires tools such as Nuclear Magnetic Resonance (NMR) spectroscopy. This relies on the quantum dynamic effects within materials and interpreting local electronic structures and atomic nuclei environments. To interpret NMR spectra, detailed theoretical models that can reliably and accurately capture electronic interactions are needed to fully characterise the material. Currently, classical models struggle to simulate the long-time spin dynamics of many, coupled atomic nuclei, especially those commonly found in batteries, such as cobalt, or other transition metals.

Developing a quantum computing workflow

The aim of this proof-of-concept project was to address these classical limitations by developing a new quantum computational workflow for simulating these materials. Through combining Quantinuum's state-of-the-art quantum computational techniques and software with established classical methods, a hybrid computational workflow was successfully created.

This was capable of simulating NMR spectra of battery materials from first principles. The workflow was then tested on lithium cobalt oxide, one of the most widely used cathode materials in lithium-ion batteries.

High-level classical ab initio calculations were used to produce NMR parameters used in the construction of quantum circuits. Following compiling and optimising, quantum hardware resource estimates for the number of qubits, gates and shots necessary for large-scale NMR simulations were calculated. This was both for current hardware and promising future fault-tolerant architectures.



Impact

The outcomes of this project underscore the potential for scalable quantum computers to solve materials science problems that are currently complex and difficult to solve with classical systems. As a result, the impact of this work could play a significant role in the UK's ability to design and optimise battery materials and develop reliable and efficient energy systems. This project was also the first to apply quantum computing to atomic nuclei with high spins in NMR simulations, showcasing how quantum computing can be applied to a large range of NMR spectroscopy applications.

It therefore provides compelling evidence that quantum computing can play a pivotal role in meeting net zero and battery targets, as well as further reaching correlated materials applications such as catalysts or rare earth metals.

> This work demonstrates how quantum computing has the potential to accelerate battery innovation by developing quantum computational workflows for the interpretation of NMR spectra to characterise novel battery materials and estimates the quantum resources for such computations. By aligning quantum resource estimates with Quantinuum's hardware roadmap, we chart a practical path to application-driven quantum simulation in materials science.
>
> Quantinuum

Quantum computing meets materials science: A novel approach to understanding metal corrosion

The consortium investigated the potential of quantum computing to advance the study of material degradation processes, focusing specifically on metal corrosion. This challenge is particularly relevant in sectors such as aerospace and materials science. The project aimed to demonstrate how combining quantum and classical computing could help solve complex chemical simulations and offer early insights into their potential use in real-world materials science.

Lead: Capgemini

Partners: AIRBUS, UKRI National Quantum Computing Centre

Observer: King's College London

Exploring corrosion at the atomic scale

Corrosion, the process by which metals degrade due to chemical reactions, particularly in the presence of oxygen, poses a significant challenge to material longevity and performance. To investigate this, the consortium applied a quantum embedding strategy developed by researchers at King's College London. This approach used cluster wavefunctions, which capture interactions within groups of particles, to divide complex chemical problems into smaller, more manageable components. These components were then distributed across classical and quantum computing resources, enabling more effective simulation of corrosion-related processes.

The project focused on modelling copper-rich alloys reacting with oxygen, a representative process in early-stage corrosion. This collaboration combined advanced quantum algorithms with industry-relevant expertise in computational chemistry.

Evaluation of the performance on quantum hardware

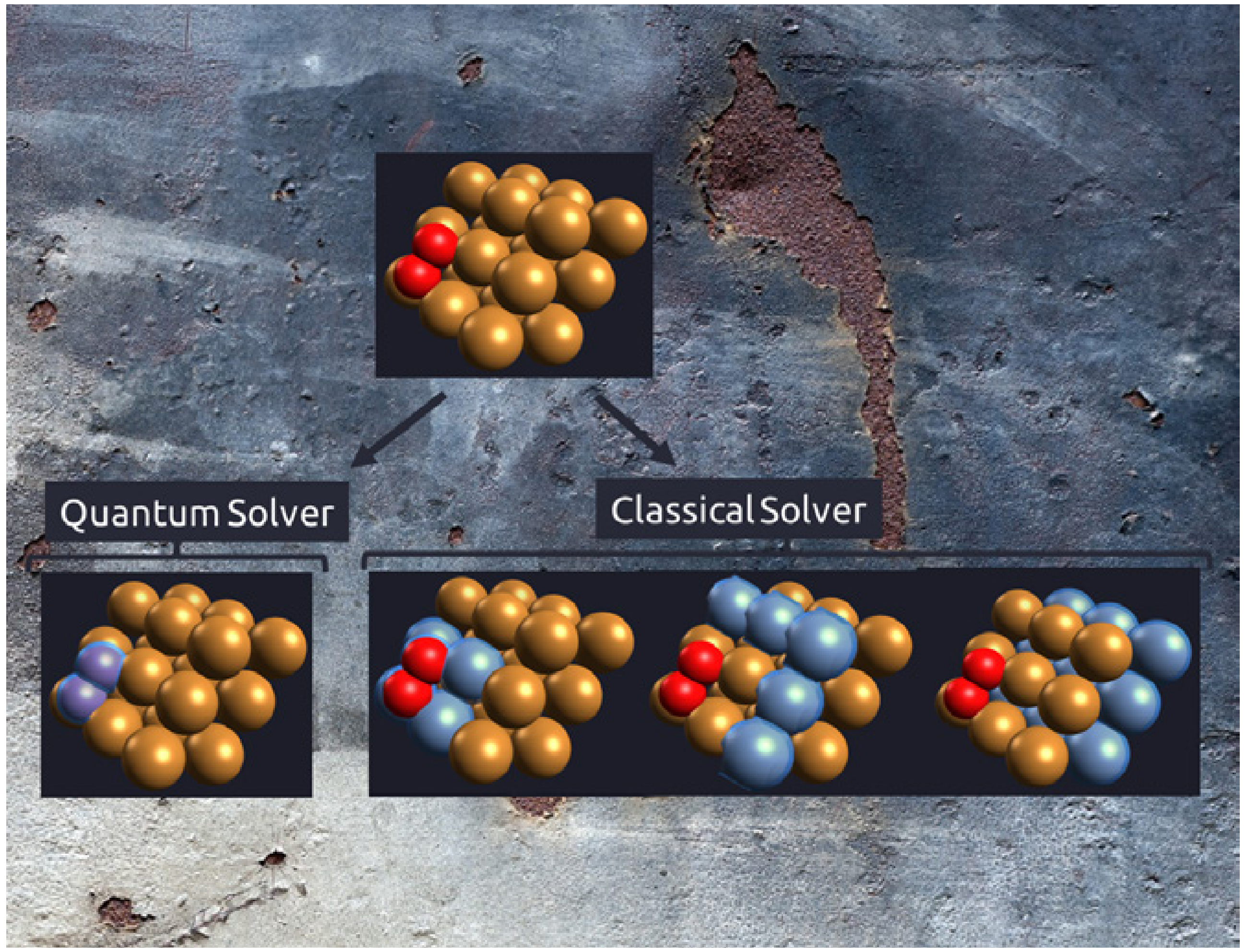
A central goal of the project was to evaluate how well this new quantum-classical method performed on current quantum devices. Multiple quantum computing platforms were used to assess variations in performance, accuracy, and convergence.

This benchmarking exercise provided initial insights into the potential limitations of current quantum systems and highlighted possible areas for algorithmic optimisation.

Impact

The findings from this project lay the groundwork for future applications of quantum computing in materials science. By improving the modelling of corrosion processes, this work could inform the development of more resilient alloys and support more effective predictive maintenance strategies across a range of industries.

As the technology continues to mature, this work represents a step toward translating theoretical quantum models into practical tools for industry.



> At Capgemini, we're pioneering application-focused quantum innovation by implementing quantum embedding strategies that break down complex material problems into manageable components. This approach allows us to distribute computational tasks between classical and quantum resources, creating a practical pathway to address real industry challenges like metal corrosion in aerospace applications.

Dr Phalgun Lolur
Scientific Quantum Development Lead, Capgemini

Quantum computer resource estimation for simulating polymers

The QREPPS (Quantum Resource Estimation as a Pipeline for Polymer Simulation) project looked to investigate what size and capabilities of a fault-tolerant quantum computer would be necessary to perform certain energy calculations on polymers. This work lays the groundwork for future quantum computing applications in smart material design.

Lead: PsiQuantum

Partners: QINETIQ, Science and Technology Facilities Council Hartree Centre

Observer: National Quantum Computing Centre

Complex materials

Current classical computers' inability to accurately model sufficiently complex molecules and materials limits the rate of innovation in multiple industries. This includes for commercially important classes of polymers – materials consisting of molecules built from large numbers of repeating units bonded together. Polymers are used in manufacturing and infrastructure, automotive, aerospace, plastics, and medical industries.

Quantum computers are expected to reach sufficient scale to achieve fault-tolerance and error correction. Once these fault-tolerant quantum computers are available, these systems promise to transform materials discovery by accurately predicting important material properties. This could include complex materials that are currently limited by expensive physical experimentation and classical computational approximations in current modelling techniques.

Quantum resource estimation for simulation

This project investigated what size and capabilities of a fault-tolerant quantum computer would be necessary to perform ground state energy calculations on a variety of commercially promising polymer candidates through resource estimation. Ground-state energy refers to the lowest energy state of an atom or molecule and is important to accurately determine as it is the starting point for any chemical reaction and is relevant to other chemical properties.

Results showed that early-generation fault-tolerant quantum computers show great promise for polymer simulation. Additionally, the project team were able to significantly reduce the required resources to run ground state energy estimations through novel pre-processing techniques developed.

Impact

This project laid the groundwork for future investigation into quantum computing for polymer simulation in fault-tolerant architectures. Further work is still needed to take the calculations beyond ground-state energies and to more complex, commercially important material properties. Both the work of this project, and its future possibilities, will aid scientists in using quantum computers to design novel, smart materials with accurate and bespoke physical and chemical properties.

> The QREPPS project explored how early fault-tolerant quantum computers could revolutionise polymer discovery by simulating ground state energies more efficiently than traditional methods. It leveraged cutting-edge FTQC quantum resource estimation automation tools, explored architecture-dependent optimisations, and lays a foundation for broader quantum applications in designing advanced materials across key industries.

PsiQuantum

Quantum computing for fluid simulations in aerospace applications

By assessing the feasibility of running Computational Fluid Dynamics (CFD) simulations on real quantum hardware, this proof-of-concept project provided evidence for the use of quantum computing to enable the next generation of aerodynamic design and optimisation in aerospace and adjacent industries.

Lead: oxford ionics

Partners: QUANSCIENT, UKRI National Quantum Computing Centre

Computational fluid dynamics (CFD)

Used across a wide range of sectors, computational fluid dynamics (CFD) is a way of numerically simulating, analysing, and predicting the flow of fluids. This includes both free fluid flow and interaction of the fluid with surfaces.

For the aerospace industry, such dynamics are essential to understand how fluids would interact with or flow around aerospace vehicles. CFD is therefore a critical tool for predicting aerodynamic performance, optimising airfoil shapes, reducing drag, improving fuel efficiency, and ensuring structural integrity.

Assessing CFD on near-term quantum hardware

Classical CFD simulations are limited by high computational demands, restricting the level of precision achievable with standard methods. This level of precision is often insufficient for the development and validation of new products. As a result, companies typically rely on costly and time-consuming physical wind tunnel tests, which slows down the pace of design exploration.

This proof-of-concept project allowed Quanscient to test the real-world performance of its proprietary quantum CFD algorithms using Oxford Ionics' emulator, which replicates the behaviour of its record-breaking quantum computers. An expert end-user offered insights to guide development toward practical aerospace applications.

Quanscient's quantum CFD algorithms offer the potential for major gains in computational efficiency over traditional methods. This project aimed to assess whether that advantage would be affected by performance losses when running the algorithms on real hardware, with a particular focus on measurement errors. The results showed that measurement errors had a negligible effect on simulation accuracy, preserving the performance advantage without sacrificing reliability. This is made possible by the measurement accuracy of Oxford Ionics' quantum hardware, which ensures the algorithm operates within required tolerances.

Impact

The findings of this project provide evidence towards a viable pathway to deploying quantum CFD simulations with real-world impact in the aerospace sector. With 23 high-fidelity qubits, the consortium has shown they would be able to simulate the airflow around the NACA0012 airfoil, an industrially recognised geometry for CFD.

By extrapolating these results, it was also predicted that at ~100 high-fidelity qubits, quantum CFD simulations could become classically intractable. Most importantly for the near-term, this project has provided tangible results that illustrate the progress being made in designing robust and efficient quantum circuits for CFD. The impact this has on algorithm development and accuracy could yield numerous benefits for the aerospace and adjacent automotive sectors, including accelerated airfoil and vehicle designs, reduced dependency on physical testing, and significant cost savings.

The evidence from this use case goes to show that quantum computing has tremendous potential for improving aerodynamic design and optimisation – impacting not just the aerospace industry, but also adjacent sectors like automotive and energy.

> Powerful quantum computers are poised to radically transform how we approach complex computational challenges like CFD – the question is no longer if, but when, we'll see this value unlocked. Oxford Ionics was thrilled to work with Quanscient, and an expert end-user, on research that took the fundamental steps required towards making this future a reality.

Dr Chris Ballance
CEO and co-founder, Oxford Ionics

Communications

Optimisation

Quantum optimisation of planning in field sensor networks for supporting disaster response operations

Radio communication networks are critical in disaster response scenarios, where reliable and rapid deployment can significantly improve coordination and aid delivery. This proof-of-concept project investigated quantum optimisation methods for placing in-field communication nodes across user-defined areas, whilst balancing maximum connectivity with minimal deployment resources.

Lead: Mind Foundry

Partner: UKRI National Quantum Computing Centre

Improving network design for rapid deployment

The project explored how network layout can be optimised to ensure effective coverage of key target areas, particularly in the aftermath of natural disasters. This includes connecting communication and sensor nodes. A primary challenge in these scenarios is maximising coverage while minimising the number of radio nodes required. Addressing this challenge can result in more efficient resource use and enable faster deployment in high-pressure situations.

The team focused on refining algorithmic solutions for where the nodes are placed. This aimed to improve on existing classical methods and investigate the potential of quantum computing techniques. The goal was to optimise network coverage, reduce the number of sensor locations and improve the overall efficiency of communication systems for disaster relief.

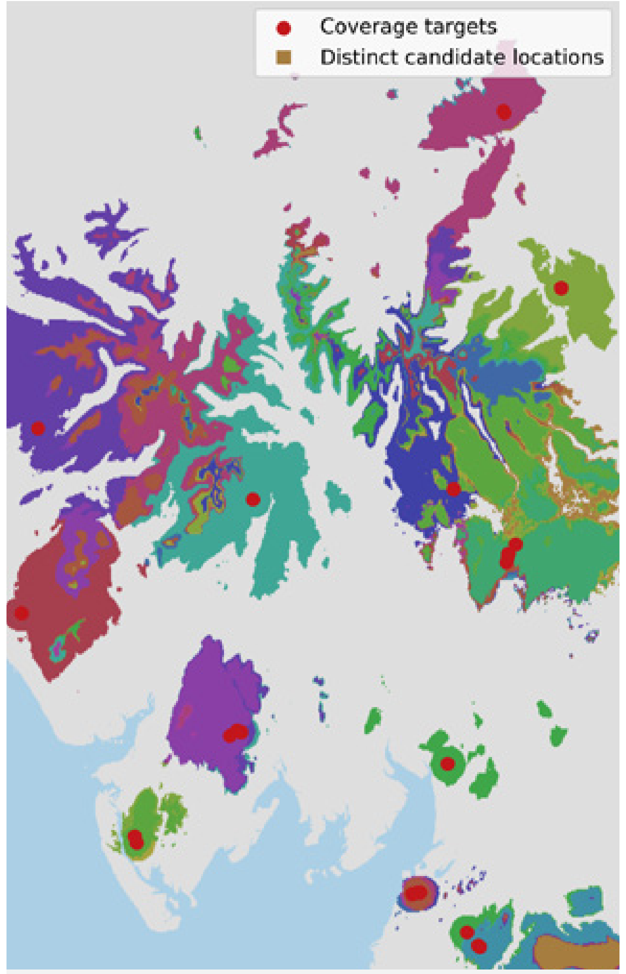
Exploring classical and quantum solutions

This project focused on advancing a classical solution using a genetic algorithm-based approach. This resulted in performance improvements, allowing the consortium to explore more complex node placement problems and the generation of higher-quality layouts. In parallel, a novel combinatorial formulation of the problem was developed, demonstrating better performance in certain disaster-relief use cases and offering a promising target for quantum optimisation techniques. Quantum annealing methods were also investigated as a potential tool for solving these combinatorial node layout problems. Comparative studies were conducted against standard combinatorial solvers, assessing the performance and applicability of quantum approaches in this domain.

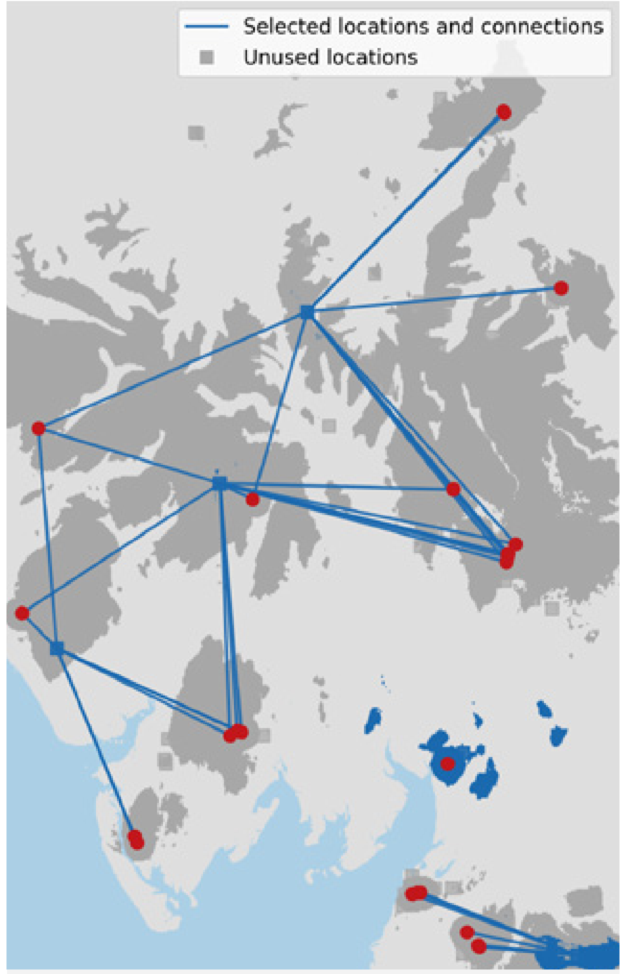
Impact

The project led to significant progress in optimising communication network placement, especially in critical disaster-relief scenarios. By refining classical algorithms and exploring the potential of quantum computing for these use cases, the work laid the foundation for tools capable of enabling faster and more informed deployment decisions.

Future work may focus on adapting the developed techniques to related optimisation problems, as well as continuing to explore the use of quantum computers for operational deployment. With further development, such methods could significantly enhance the speed and reliability of emergency response networks around the world.



Distinct candidate locations



Selected solution providing maximum coverage

Coverage as a partial max-satisfiability problem in lake_district. Maximise coverage of 24 targets by selecting 6 of 156 candidates,

> Understanding where to place temporary radio transmitters and receivers in a disaster landscape to maximise communication coverage while balancing demands like power consumption is a computationally challenging optimisation problem. By identifying graph sub-problems, we explored the applying quantum optimisation to an existing product of use to disaster response teams.

Mindfoundry

Transport

Optimisation

Developing scheduling methods for roadwork optimisation

The project aimed to simplify the complex real-world challenge of roadwork scheduling by exploring optimisation techniques using both classical and quantum computing architectures. Improving the efficiency of scheduling has the potential to reduce public disruption and enhance the management of infrastructure maintenance.

Lead: AIOI R&D LAB OXFORD

Partners: mind FOUNDRY, UKRI National Quantum Computing Centre

Roadwork optimisation

Scheduled road maintenance and works are necessary to maintain essential infrastructure and transport routes in the UK. However, they often cause significant disruption to the public, blocking routes and causing delays and increased traffic.

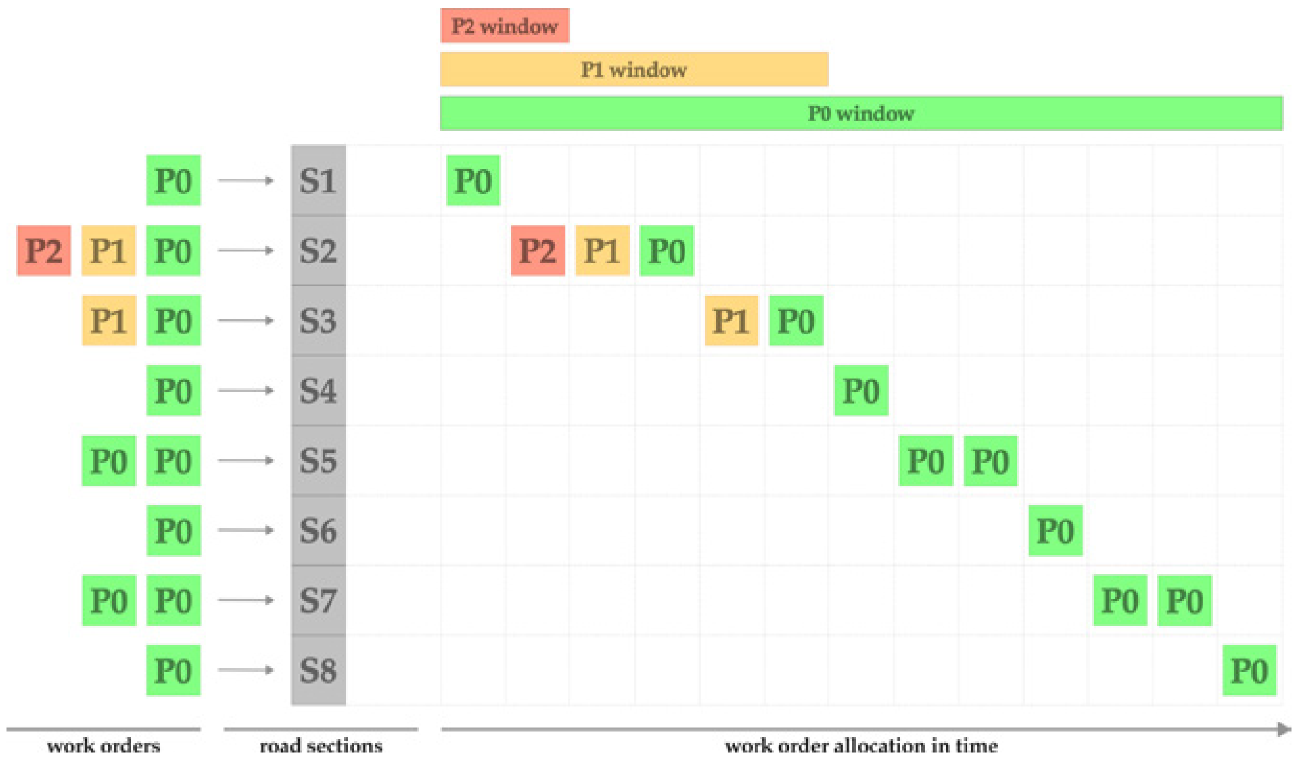
Optimising the scheduling of such roadworks reduces impacts on the public and decreases costs and time wasted for contractors delivering the work. Efficient scheduling involves figuring out the best times, and order of works, for the necessary maintenance to be carried out across the road network.

Translating and testing optimisation solutions

Quantum computers can be utilised as a tool to run optimisation algorithms. This proof-of-concept project carried out work to translate the real-world problem of roadwork scheduling into a computationally tractable form. This included analysing the performance of algorithms developed, and solutions produced, on different hardware.

Following consultation with Sir Robert McAlpine regarding the planning of maintenance on the A19 road in the UK, the team explored mathematical ways to describe the roadwork scheduling problem and set parameters.

Scheduling methods on classical and quantum hardware were then tested. This involved the consortium, including Quantum Applications Engineers from the NQCC, working to implement and test quantum optimisation algorithms on real-world quantum computers. A technical report detailing how algorithm parameters were tuned, alongside a comparison of the optimised road maintenance schedules outputted from the classical and quantum hardware, was produced. This estimated the performances of the algorithms developed.



Impact

The project outcomes showcased the feasibility of utilising near-term quantum hardware to optimise scheduling problems for small synthetic data sets. The project team were able to gain unique experience in "translating" the real-world problem in a format suitable for quantum computing.

Further development in this field, focused on tuning these algorithms and implementing them on scaled quantum computers, could help save public money and ensure roads are maintained in good condition. The solutions calculated could be eventually used by road authorities to plan and manage roadworks more effectively.

> We have developed a simplified approach to the road works scheduling problem. The problem focuses on optimally allocating a fixed number of work orders to different sections of a road under a variety of constraints and cost functions. This initial problem definition serves as a complexity baseline, with potential options for increasing the complexity.

Aioi R&D Labs Ltd

The job shop problem: quantum computing for efficient resource scheduling

The project analysed the capabilities and limitations of current quantum hardware and software to solve an industry-scale dynamic flexible job shop scheduling problem (DFJSSP). This was to provide insights to guide future applications of quantum computing for industry scheduling optimisation.

Lead: LTIMindtree

Partner: D-Wave

Observer: UKRI National Quantum Computing Centre

Efficient resource scheduling and DFJSSP

Efficient resource scheduling is critical across industries such as manufacturing, retail, logistics, healthcare, hospitality, construction, aerospace, and data centres. Effective scheduling minimises costs and reduces waste by optimising resource use while meeting constraints. In manufacturing, resources include personnel, machinery, and materials. These resources may be shared across concurrent projects, have limited use times, or be finite.

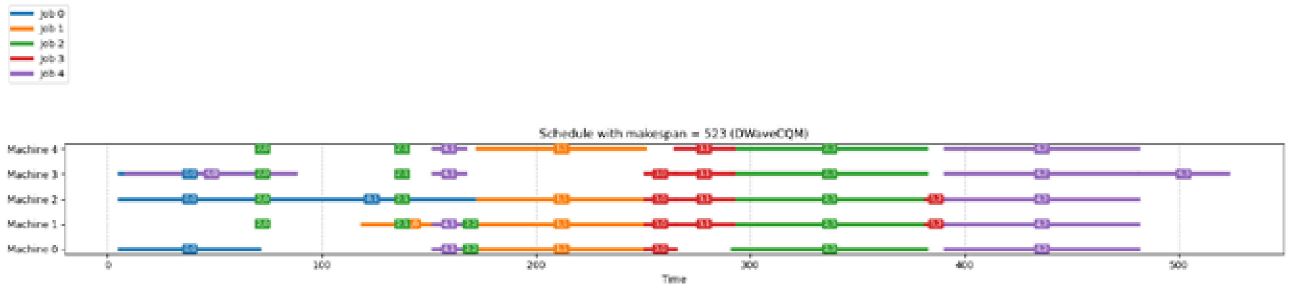
Dynamic flexible job shop scheduling problem (DFJSSP) is a complex real-world scheduling challenge relevant to the manufacturing sector. It involves scheduling a set of jobs, each consisting of multiple operations in a predefined sequence, on a set of machines with the objective to minimise completion time. Each operation requires different machines, with varying processing times. Jobs arrive dynamically over time, each with its own arrival time. Scheduling must respect manufacturing process constraints.

Testing current quantum hardware for DFJSSP

This proof-of-concept project looked to analyse the capabilities and limitations of current quantum computers to solve industry-scale DFJSSP and provide insights for future applications of quantum technology in this field.

In the initial stages of the project, DFJSSP parameters were defined, a synthetic problem generator created, and a benchmarking dataset created to feed into later work. Following this, the consortium developed a mixed-integer programming (MIP) model and mapped it to D-Wave's constrained quadratic model (CQM) solver, as well as Google's OR-Tools constraint programming model (CpM) solver. Final stages of the project involved benchmarking the two advanced solvers, evaluating their performance based on solution quality, solution type, and time to solution.

The experiments, and subsequent scaling analysis, showed that both solvers provided optimal solutions for smaller problems. While the current problem modelling showed decreased optimality as the problem size grows, finding optimal solutions for large-scale problems looks promising when the modelling is tailored to D-Wave's hardware and state-of-the-art solvers.



Impact

The results demonstrated on these models provide evidence that quantum computing could enhance large-scale scheduling problems. Industry impact from this, with regards to operational efficiency, cost reduction and innovation, would be profound due to the number of applicable industries utilising resource scheduling.

> DFJSSP involves scheduling jobs with multiple operations on various machines to minimize completion time. The results have demonstrated that quantum annealing-based approaches can be effectively utilised today to address job scheduling problems with real-world complexities in manufacturing and scaled in the near future. This work has revealed to domain consultants the immense potential and value that application-focused quantum solutions can bring to various scheduling and optimisation use cases within their respective fields.
>
> LTIMindtree Ltd

Orbital quantum computing: investigating space-hardened quantum error correction

What does it take to deploy a quantum computer to low earth orbit (LEO)? This proof of concept project demonstrated the feasibility of deploying a quantum computer in space including investigating fundamental challenges in space radiation effects and space-appropriate quantum error correction (QEC) methods.

Lead:

Partners:

National Quantum Computing Centre

Quantum computing in space

Quantum computing is not just limited to earth. There has been growing interest in deploying quantum computers to earth orbit and space; such computers could offer transformative advantages in secure communications, data processing, scientific research and defence applications. Space-bound quantum computers will still require full stack innovation to ensure efficient operation.

Current usable NISQ-era quantum computers can solve real-world problems.

However, there are still significant challenges to reach future fault-tolerant architectures, including scale-up and the development of quantum error correction (QEC) methods. QEC techniques deployed protect quantum information from noise and errors.

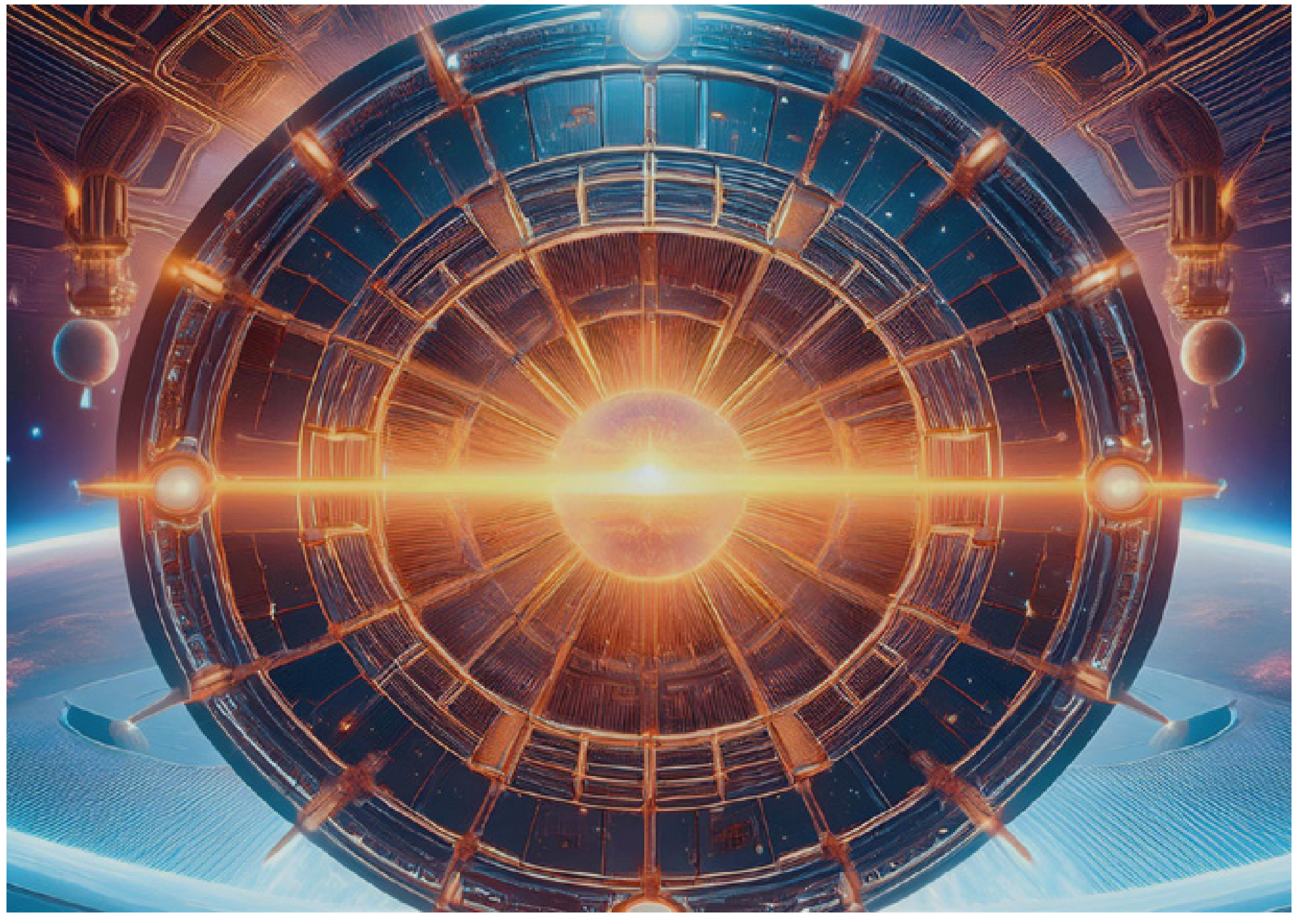
QEC in harsh space environments

QEC methods deployed in space must be tailored for the harsh space environment. This proof-of-concept project looked to address the fundamental challenges of space radiation effects on quantum systems, and the innovative QEC methods required.

The project consortium carried out a comprehensive analysis of space radiation environments, revealing that different LEO orbital parameters experience varying radiation profiles. This included differences between the radiation types experienced by sun-synchronous orbits and 45° inclined orbits. These results informed the development of space-hardened QEC protocols which demonstrated performance of 94.07% error-free operation. They also showed clear differentiation between quantum error types in simulations with 1,500,000 shots.

The team was able to deploy the protocols on current hardware, the Rigetti Ankaa-3 quantum processor, with access provided by the NQCC. This allowed the team to establish realistic benchmarks for current technology limitations.

The project took system-level radiation resilience analysis one step further and was able to identify shielding materials appropriate for quantum computing shielding in space. This included identifying high-hydrogen-content plastics outperformed traditional aluminium protection.



Impact

An introductory software framework produced by Quantaverse Ltd., integrated radiation simulation, noise modelling and quantum error correction protocols established within this project. This will allow researchers to test and optimise quantum architectures for space environments.

This work also advances Quantarverse's commercial roadmap towards deploying a quantum computing constellation, which would aim to contribute to positioning the UK at the forefront of space-hardened quantum computing. It also advances radiation-tolerant quantum hardware and error correction algorithms and acts as a stepping stone towards operational quantum computing in space. Such an achievement would have a significant impact on communications, data, research and defence in the future.

> Our space-hardened quantum error correction protocols represent a crucial step toward operational quantum computing in space. By addressing the unique challenges of the space radiation environment, we are unlocking transformative applications in secure communications, data processing, medical diagnostics and defence that will position the UK at the forefront of this revolutionary field.

Quantarverse Ltd

Quantum Computing Industrial Applications Call

SparQ

IUK Feasibility Studies in Quantum Computing Applications: Use Cases 2023–2025

National Quantum Computing Centre

Innovate UK

> The partnership between Innovate UK and the NQCC exemplifies how targeted investment in quantum computing can yield tangible industrial benefits. Together, we have created a structured, well-supported initiative where companies can safely experiment, innovate, and integrate quantum computing into their product roadmaps. This collaboration has been instrumental in laying the groundwork for a quantum-ready economy.

Mareike Schmidt
Deputy Challenge Director, Innovate UK

SparQ

61 organisations

£6.2m funding

19 projects awarded

- Core partner on 7
- 12-18 months
- Application engineer support
- Innovation Sector Lead support
- QC resources

Funding call overview

In 2023, Innovate UK, in collaboration with the National Quantum Computing Centre, launched an £8 million funding competition to support feasibility studies to explore innovative quantum computing solutions to industrial challenges. The initiative aimed to foster collaboration between UK businesses and research organisations, and to develop practical use cases that demonstrate the potential and commercial benefits of quantum computing across sectors such as manufacturing, transport, and financial services.

Projects were required to include at least one end-user partner, have total costs of up to £500,000, and have a duration of up to 18 months. This competition marked a significant step forward in advancing the UK's quantum readiness by encouraging industry-led exploration of quantum solutions beyond an initial proof-of-concept phase.

The projects included in this compendium are from the 7 projects in which NQCC was a core partner.

Participating organisations

AppliedQuantumComputing, BioGeMT, NHS Hampshire Hospitals NHS Foundation Trust, HSBC, KUANO, National Quantum Computing Centre, NATS, Newcastle University, Quantum Base Alpha, QSL Quantum Software Lab, rigetti, river lane, Rolls-Royce, SAMSUNG, The PSC, The University of Edinburgh, UCL, unisys, Zaiku Group

Quantum unsupervised learning for anti-money laundering detection

Financial fraud presents a major challenge to digital payment systems, requiring more sophisticated detection methods. This project explores how quantum machine learning can enhance fraud detection, combining quantum-inspired models with advanced data pre-processing techniques to lay the groundwork for more accurate and efficient financial security solutions.

Lead: Rigetti

Partners: HSBC, The University of Edinburgh, National Quantum Computing Centre

Fighting financial fraud in the UK

Fraudulent financial transactions affect millions of people every year. In 2023, financial crime accounted for 40% of all criminal offences in the UK, leading to total losses exceeding £2.3 billion across all sectors of the economy. Electronic payments, such as those carried out using credit or debit cards, rely on automated systems for security, often utilising machine learning algorithms to identify potentially fraudulent transactions. Such systems must simultaneously ensure the rigorous blocking of unlawful payment requests while also needing to minimise 'false flags', the mistaken flagging of legitimate unusual spending, which drives up operational costs.

Rigetti UK Limited, HSBC Holdings plc, The University of Edinburgh Quantum Software Lab (QSL), and the National Quantum Computing Centre (NQCC) partnered to prototype quantum computing methods to explore quantum machine learning's (QML) potential for enhancing fraudulent transaction detection, an area where, despite effective classical techniques, the demand for computational sophistication is substantial. The complexities introduced by the rapidly evolving technological landscape, enabling sophisticated new fraud patterns, further underscore the need for advanced detection techniques.

Enhancing machine learning detection with quantum computing in the short and medium terms

HSBC developed a quantum-inspired machine learning model using low-depth quantum circuits to encode classical data on quantum spaces, implemented via a matrix product state backend. Tensor network feature maps were used for several model implementations, including quantum support vector machine and projected quantum features. This quantum-inspired machine learning model can scale to meet the full problem scope for fraud detection using classical computing resources. HSBC benchmarked the model against champion production fraud detection models using UK retail customer data.

The QSL and the NQCC built upon this work by developing a quantum-based data pre-processing algorithm to accelerate the model training. The Quantum approximate optimization algorithm was used to implement a quantum version of feature bundling. This data pre-processing method combined complementary features, aiming to reduce the computational workload without compromising the model quality, as training time typically increases with data dimensionality. As the quantum computer is required only during the training of the anomaly detection model, the additional complexity of deploying a current noisy intermediate-scale quantum computer is avoided. Quantum feature bundling was tested with simulations and on Rigetti's hardware, yielding encouraging results with a small cost in classification accuracy.

> Identifying and developing real-world quantum applications with today's quantum computers not only helps industries become quantum ready but also deepens our understanding of how to design and build fault-tolerant quantum computers. By collaborating with industry leaders and academic experts, we can identify real-world use cases and continue to improve quantum computing capabilities with an eye towards the future.

Dr. Subodh Kulkarni
Rigetti CEO

Rigetti's team showed that quantum feature maps, based on deep quantum circuits that are costly to simulate classically, further improve fraud detection. However, executing these circuits efficiently at scale will require future quantum hardware, as current devices are limited by high error rates. In this work, the output of such deep quantum circuits was simulated for a small number of qubits using the Cirrus Tier-2 HPC Service. Machine learning models trained on the quantum-simulated output detected more fraud while minimising false positives. These improvements were observed over the same model trained on both the original inputs and data processed with shallow quantum circuits, using a sizable open-source credit card dataset of approximately 250,000 transactions. The most significant performance gains were achieved when focusing on a reduced dataset comprising the top 10% most valuable transactions. This is particularly significant, as limited data typically makes model training more challenging. The results suggest a potential path for useful applications as quantum hardware capabilities mature further.

In summary, the project showed a clear potential to deploy quantum-inspired models efficiently today with a pathway for even greater performance in the future as quantum computer hardware develops.

Addressing operational and regulatory challenges in banking and digital payments

Looking ahead, even greater enhancements in detection may be possible by leveraging deep quantum circuits executed by error-corrected quantum computers and integrated into fraud workflows. However, realising the full potential poses several challenges. Firstly, implementing low-error-rate logical quantum operations is an area of active development, and a priority highlighted in the UK's Quantum Strategy Missions. Secondly, due to the sensitive nature of financial data, regulatory complexities arise concerning its transfer to third-party quantum computing cloud services.

Rigetti and other quantum computing companies are working with their UK ecosystem partners to advance the implementation of quantum error correction, which would enable the demonstration of QML detection models with increased precision. Moreover, the project partners are engaging in regular conversations with regulatory bodies, such as the Financial Conduct Authority (FCA), to address regulatory hurdles while upholding the highest standards in protecting personal digital information.

Using quantum optimisation techniques to improve operational healthcare

This feasibility study identified specific large-scale processes in the provision of healthcare, especially in a hospital context, which could benefit from improved optimisation. Examples are large complex staff rosters and theatre planning. The consortium investigated the application of a range of quantum computing methods and was able to identify improved algorithms which improved time to solution by up to ~10,000 times by comparison with standard quantum implementations. The study also estimated further improvements in hardware and software that would be needed to make a quantum application practically implementable for a working hospital.

Lead: AppliedQuantumComputing

Partners: NHS Hampshire Hospitals NHS Foundation Trust; The PSC; UKRI National Quantum Computing Centre

Healthcare background and government priorities

Healthcare provision in the UK accounts for approximately 10% of UK GDP and is the single largest area of UK Government expenditure. The NHS faces many challenges in providing the quantity and quality of care expected by patients and it has highlighted the need to improve productivity as critical to achieving its objectives to 'reduce elective long waits and improve performance against the core diagnostic standard'.

An important potential contributor to delivering on these objectives is through applying optimisation techniques to the many large-scale processes that drive the operation of a modern hospital. Quantum computing has the potential to address these large-scale process challenges and in this feasibility study the consortium researched how such techniques could be applied to selected key processes.

Selecting key operational healthcare use cases

In collaboration with healthcare professionals from Hampshire Hospitals NHS Foundation Trust, over 20 operational processes were initially identified as potential candidates for further investigation. Following an in-depth assessment, three processes were selected for detailed specification and technical evaluation:

1. Staff rostering
2. Patient allocation to diagnostic scanners
3. Theatre planning and patient allocation.

Each one of these processes is critical to the efficient running of hospitals and a core enabler of delivering the best possible care to patients.

Evaluating quantum computing's potential

Each of the three use cases was encoded into a format suitable for generating optimised solutions using quantum computing techniques. More than ten variations of current NISQ-era algorithms, including as the variational quantum eigensolver (VQE), quantum approximate optimisation algorithm (QAOA), and quantum annealing-based methods, were examined. This included looking at quantum annealing based methods.

Initially classical simulation methods were used for the evaluation with the best methods also being subsequently tested on IBM quantum hardware. The best methods required up to 10,000 fewer quantum circuit evaluations by comparison with "plain vanilla" implementations. Current state of the art quantum computing hardware is still relatively modest in size even if it is "beyond classical simulation" and is still short of the scale required to address problems of the size relevant to the applications examined in a hospital context.

Implications from the study

The project demonstrated high potential value to the NHS for more effective use of optimisation techniques. For quantum computing methods to be valuably applied, there is a need for larger hardware to become available.

The project identified a need for further development of quantum algorithms, particularly in terms of convergence speed, to enable timely solutions suitable for routine hospital operations. However, considerable improvements were made to existing algorithms, and further material gains are anticipated through continued research and refinement. These findings support a positive outlook that quantum computing will, in time, contribute to the optimisation of hospital processes and to the broader delivery of healthcare.

> Optimising key processes in NHS hospitals is crucial to delivering timely, quality healthcare for patients. This feasibility study, supported by our collaboration partners Hampshire Hospitals and The PSC, shows a route to how quantum computing will be able to contribute to this goal in the future.

Tim Thomas
CEO, Applied Quantum Computing

A next-generation quantum computing based approach to enzyme targeted drug discovery

The project explored and developed novel quantum computing algorithms to investigate otherwise inaccessible drug design targets for enzyme inhibitors. The feasibility of applying these algorithms on currently available NISQ-era quantum computing hardware was assessed, along with identifying a pathway for their integration into drug design workflows. The study resulted in the development of new methods for active space selection, acceleration and quantum dynamics in the context of drug discovery.

Lead: KUANO

Partners: UCL, UKRI National Quantum Computing Centre

The importance of capturing quantum effects in drug discovery

A better understanding of the underlying physics and chemistry, especially at a quantum level, is of crucial importance to further advance in-silico drug design. This project considered, in particular, the interactions found in enzyme inhibitors, for which larger classes exist that are considered either entirely undruggable or where current classical methods only give insufficient information for efficient drug design. Examples include metalloenzymes, where strong correlations are important due to the presence of transition metals; systems at the transition state, which often exhibit electronically correlated wavefunctions; and covalent inhibitors, where a detailed understanding of bond formation is of crucial importance.

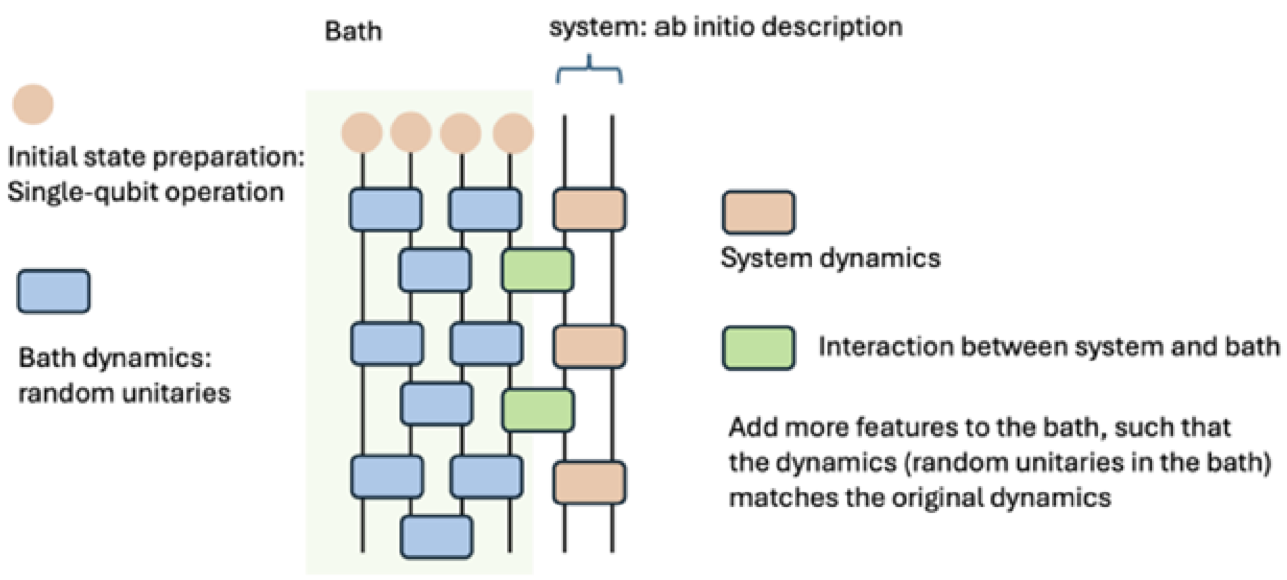
In the context of efficient drug design pipelines the project went beyond an approach that focuses primarily on improving the accuracy of the description of the quantum effects but also considered how automation can be achieved. This is crucial for any future real-world application in scalable workflows.

Optimising quantum chemistry approaches for drug design on quantum computers

The partnership pursued three inherently connected aspects of quantum chemistry for drug design:

i) How to efficiently prepare active spaces for VQE
ii) How to accelerate such calculations
iii) How to move beyond ground state calculations and consider quantum dynamics.

Selecting orbitals for optimal active spaces of multireference post-Hartree-Fock calculations is a long-standing problem already for classical approaches. The project addressed this by considering an approach based on ideas from quantum information science and develop a fully automated method to achieve preparation of the orbitals for quantum computing calculations. The project relies on a tensor-network-based approach within the framework of the quantum chemistry density matrix renormalization group (QC-DMRG).



Schematic of the full quantum system circuit. The objective is to obtain an effective description of the quantum dynamics of the distant part of the system. To achieve this, the full, large system is divided into the bath and the system.

This technology also allowed the consortium to address acceleration of quantum computing calculations by extracting the matrix product states which can be employed to prepare quantum circuits. Finally, the project explored quantum dynamics, establishing a framework for dividing a chemical system into simpler parts in order to better embed the problem on a current quantum computer. The project proposed a toy model for chemical bond formation and have provided quantum circuit models to demonstrate this process, successfully demonstrating the bond formation on a quantum device.

Advancing drug design through quantum dynamics, active space optimisation and novel acceleration methods

Cutting-edge quantum algorithms were employed to explore previously inaccessible classes of enzyme inhibitors for next-generation therapeutics. Conventional methods often struggle to elucidate and accurately describe the intricate quantum interactions within enzyme inhibitors, particularly those involving transition metals and covalent bonding. These interactions, which are fundamental to understanding drug efficacy, are frequently overlooked or inaccurately modelled by classical approaches, limiting the development of effective therapies.

This project demonstrated how quantum computing approaches can support drug discovery while identifying current limitations. The methods developed for active space selection in VQE calculations can already be applied within workflows based on classical approaches, offering immediate commercial impact. The results on quantum dynamics represent important progress beyond traditional methods that consider only the ground state of chemical systems and will enable further exploration of the physics of bond breakage and formation, crucial for both fundamental chemistry and commercial applications.

> Our collaboration with NQCC and UCL allowed us to explore how and when quantum algorithms can enable us to provide new insights into drug design relevant chemical systems and helped us to identify market fit for both the short and long term commercial opportunities.
>
> Kuano Ltd

Security-first federated quantum machine learning for genomics

The project has advanced the development of secure, privacy-preserving AI tools for healthcare by integrating quantum computing, federated learning and fully homomorphic encryption. Aimed at addressing the unique data protection and performance challenges in medical and genomic contexts, the project resulted in Sakurai.cloud – an early-stage platform that lays the groundwork for scalable, regulation-compliant AI applications in clinical and research environments.

Lead: Zaiku Group

Partners: BioGeMT, UKRI National Quantum Computing Centre

Healthcare organisations face significant challenges in identifying and trusting AI models that balance innovation, stringent security and regulatory compliance. Particularly in medical and genomic fields, the sensitivity of healthcare data demands AI solutions with superior security measures that do not compromise on performance. Addressing this challenge is crucial to unlocking advanced AI's full potential in healthcare settings, enhancing patient care, and ensuring regulatory compliance.

Technical approach and methodology

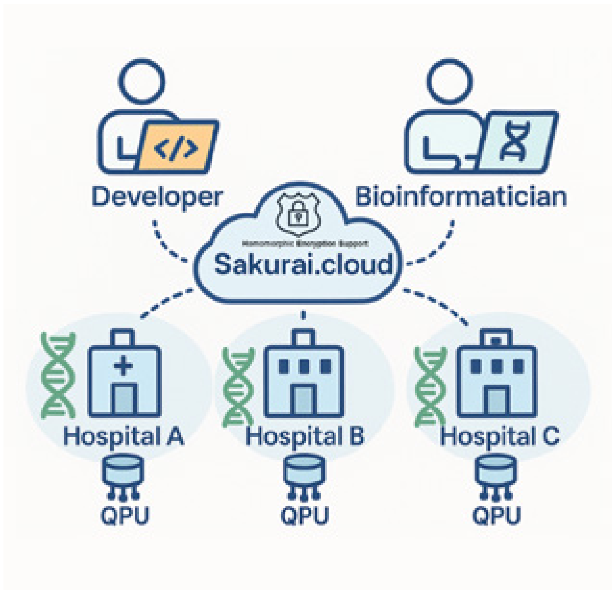
Zaiku Group led the development of Sakurai.cloud, a cloud-based platform designed to empower researchers to combine quantum computing, federated learning, and fully homomorphic encryption (FHE) in building hybrid classical quantum machine learning models for biomedical datasets.

Quantum computing is leveraged for its ability to efficiently process high dimensional biomedical data. Federated learning enables decentralised and privacy preserving model training across distributed datasets, mitigating the risks associated with data centralisation. Meanwhile, FHE safeguards against model parameter inference attacks by encrypting model parameters during training. This ensures that aggregation across participants in federated learning is performed homomorphically, that is, directly over encrypted parameters, preserving data confidentiality throughout the training process. Models featured on the Sakurai platform also undergo rigorous testing and vetting to ensure adherence to strict security, performance, and compliance standards. This meticulous curation guarantees healthcare organisations can confidently deploy these innovative AI tools.

Impact

Sakurai AI sets new benchmarks for security and performance in healthcare-focused AI solutions, offering significant benefits including:

- **Enhanced security**
  By supporting FHE, the solution provides protection against emerging quantum threats. Since the FHE scheme employed is lattice based, it inherently offers post quantum cryptographic security. This significantly enhances the trustworthiness and reliability of the system.
- **Regulatory compliance**
  Full compliance with stringent data protection regulations such as GDPR and HIPAA ensures data privacy and security.
- **Healthcare-focused innovation**
  Purpose built models tailored specifically to medical and genomic applications directly address the sector's unique needs.



Sakurai Cloud Diagram

- **Novel classical to quantum data encoding**
  Given that the use case centred on DNA sequences, which are classical data by nature, new methods were developed for encoding this information into quantum states more efficiently than existing schemes. To achieve this, a technique called Reverse Complement Embedding was introduced, leveraging the natural symmetries inherent in DNA sequences to enable more structured and resource-efficient quantum representations.

Although still at an early stage of technological maturity, the platform is strategically positioned to enable the widespread adoption of secure, high performance AI solutions in healthcare. It holds strong potential to unlock new pathways for improving patient outcomes and enhancing operational efficiency across clinical settings. Looking ahead, future developments will focus on continuous model refinement, deeper integration with other emerging quantum technologies such as sensing, and broader collaboration with healthcare providers and research institutions.

> The project has been both intellectually stimulating and technically challenging. One of the primary complexities arose from our aim to allow each client to use a quantum processing unit (QPU) of their choice. For example, one client might opt for a superconducting processor, while another might prefer a trapped ion processor. This required us to account for such variations algorithmically, not only at the level of quantum data encoding but also further upstream in the learning pipeline.
>
> Another important consideration is the availability of quantum hardware. Since existing quantum processors are not always accessible in real time, there is a risk that a client's preferred QPU might be unavailable during the training phase. To address this, we designed the system to support asynchronous federated quantum learning. This enables each client to train independently based on their own schedule, with model aggregation occurring once all clients have completed a training cycle.

Zaiku Group Ltd

The quantum accelerator for materials design (QuAMaD)

The project explored advanced quantum algorithms to reduce computational resource requirements for industrially relevant materials simulations, supporting future integration of quantum computing into commercial materials design workflows.

Lead: river lane

Partners: Rolls-Royce, SAMSUNG, UKRI National Quantum Computing Centre

Context and objective

Current approaches to materials design rely on a mix of slow and expensive experiments or classical computational approaches that require significant approximations to run on even the most powerful computational hardware. Quantum computing has the potential to enable computational materials science with drastically improved accuracy and reduced cost.

However, the current estimated computational cost of quantum algorithms for simulating industrially useful materials exceeds 1 billion physical qubits. Even the most ambitious roadmaps of leading quantum hardware companies put deployment of quantum computers of such scale beyond the horizon for most business investment cycles. To accelerate the commercial uptake of quantum computers, algorithmic improvements must drastically reduce the scale of quantum hardware required to solve industrially relevant problems.

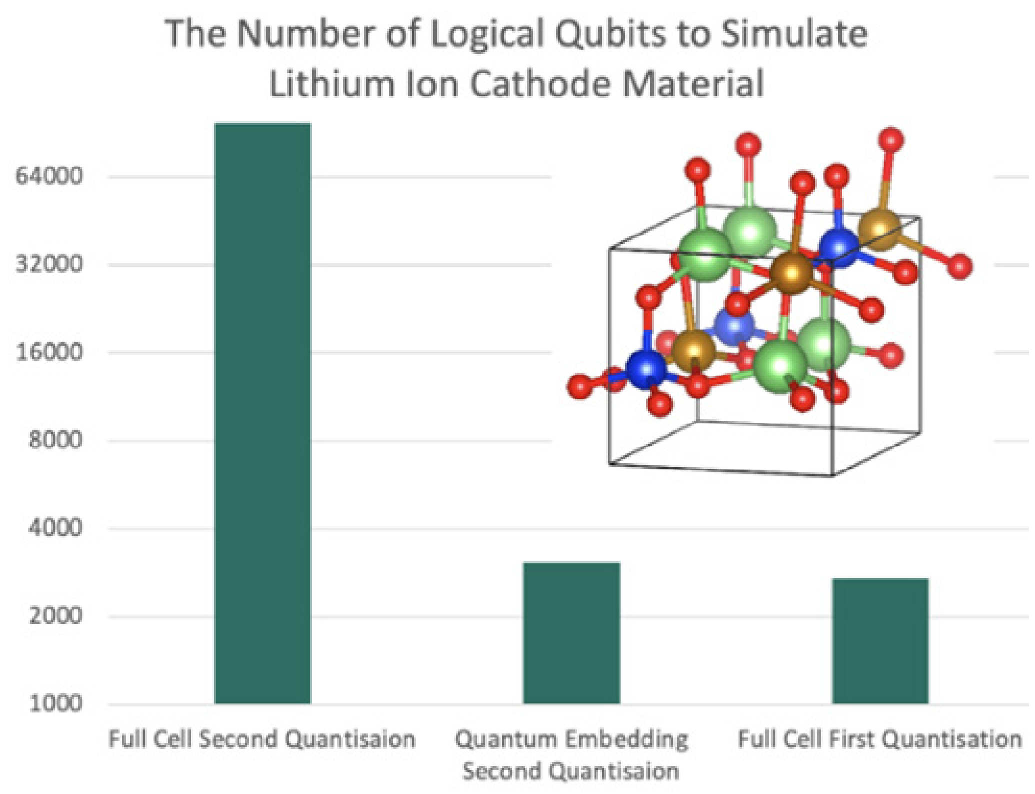
Impact

Through this project Riverlane was able to apply its quantum algorithmic expertise to reducing the quantum resource requirements of a set of commercially relevant materials simulation problems identified by the industrial partners.

Through application of state-of-the-art techniques such as projector augmented-wave methods and improved quantum embedding, required resources were drastically reduced bringing forward the time when such problems are surmountable by available hardware. For example, the computational cost for one use case in battery materials was reduced from an initial 98,000 logical qubits to just 2,700.

Linking in with the UK Quantum Missions, a particular class of problems (statistical phase estimation) have been shown to be applicable to quantum computers at the MegaQuop scale (currently targeted for 2028 as part of Quantum Mission 1).

Tools developed through this project have enabled an improved workflow of producing resource estimates for chosen use cases, as well as the development of improved embedding methods to reduce resource requirements. Industrial partners have also developed their fluency in quantum computing, as well as gaining an improved understanding of the timescale for when such devices will be business-ready.



> With internal air temperatures reaching 2000°C, beyond the melting point of the materials we use, jet engines are a hostile environment for its components. Our current state-of-the-art materials have taken many years to develop, and we continually seek improvements in their properties to deliver more efficient engines. Quantum computing has the potential to revolutionise our ability to understand and design new materials.

Leigh Lapworth
Rolls-Royce Fellow in Computational Science

Feasibility study on quantum optimisation of aircraft container loading

This feasibility study project examined how quantum computing could potentially reduce the time required for the unit load devices (ULD) loading process and improve both the gross load factor (GLF) and net load factor (NLF) for Aircraft container loading. The study assessed the integration of quantum computing elements into the current air-cargo solution by analysing and evaluating the potential of quantum optimisation for aircraft loading. It identified the strengths, weaknesses, opportunities, and threats associated with quantum optimisation and determined the resources needed to offer real-time solutions to clients using quantum computing.

Lead: Unisys

Partners: Newcastle University, National Quantum Computing Centre

Challenges of air cargo loading

Traditionally, load planning in the air cargo industry is a manual, labour-intensive task experienced planners perform using pen-and-paper methods or spreadsheets. This leads to high labour costs and often suboptimal loading configurations due to time constraints and the complexity of variables involved, such as weight distribution, the centre of gravity, and fuel efficiency.

In air cargo logistics, efficiently allocating goods within aircraft is a critical and intricate challenge. This complex task, known as the Air Cargo Load Planning and Balancing Problem, entails optimising cargo loading onto aircraft while adhering to many constraints and regulations. Proper load planning is paramount not only for economic reasons, as it directly impacts operational costs, but also for safety and compliance considerations, as imbalanced or improperly distributed cargo can pose significant risks to flight stability and overall airworthiness.

The problem encompasses various facets, including weight and balance distribution, space utilisation, load capacity, and compliance with safety regulations. Addressing these multifaceted demands requires a sophisticated combination of mathematical optimisation, heuristics, and sometimes machine learning approaches. These methods aim to provide an optimal cargo configuration that maximises space utilisation, minimises operational costs and ensures the safety and stability of the aircraft.

Exploring quantum computing for air cargo loading

To address the complex challenge of optimising air cargo loading, the team divided the problem into two distinct but connected phases. In the first phase, the project tackled the knapsack problem, which involved loading as many unit load devices (ULDs) as possible into the cargo bay without exceeding the aircraft's weight, volume, and dimensional constraints. This phase represented a classic combinatorial optimisation challenge, requiring intelligent selection strategies to maximise the payload within strict operational limits.

The second phase focused on arranging the selected ULDs within the cargo bay to ensure that the centre of gravity (CG) of the aircraft was positioned as close as possible to its geometric centre. Achieving an optimal CG is vital for ensuring flight stability, improving fuel efficiency and complying with stringent aviation safety regulations.

The project explored a range of quantum computing algorithms and hybrid quantum-classical approaches to solve these challenges. Quantum annealing was investigated as a promising technique for addressing the combinatorial complexity of the knapsack problem, utilising the inherent strengths of quantum systems to search large solution spaces more efficiently than classical methods. Hybrid approaches, combining quantum solvers with classical pre- and post-processing techniques, were also evaluated to enhance solution quality and practical usability, especially given the current limitations of quantum hardware.

Early results indicated that quantum methods showed particular promise for highly constrained, small- to medium-sized problem instances, where they achieved competitive or faster solutions compared to traditional heuristics. However, several limitations were identified, including issues of scaling, noise, and embedding complexity on current quantum devices. These findings suggest that hybrid quantum-classical systems are the most practical near-term path for applying quantum computing to air cargo loading.

Overall, this exploration provided valuable early insights into how quantum computing could complement classical optimisation techniques. While classical methods remain dominant for large-scale problems today, quantum computing offers exciting potential for enhancing real-time operational decision-making as the technology continues to evolve.

> At Unisys, we are shaping the future by exploring how quantum computing can solve real-world challenges. Our feasibility study on Quantum Optimisation of Aircraft Container Loading demonstrates that targeted, application-driven innovation is key to unlocking quantum's potential, delivering practical insights today to drive operational and environmental improvements tomorrow.
>
> Unisys Ltd

Impact

The project delivered meaningful benefits beyond the consortium, particularly in environmental sustainability, operational efficiency, regulatory compliance, and the advancement of quantum technologies. It demonstrated that optimising aircraft centre of gravity could yield measurable fuel savings — potentially around 4,000 tons over a 10,000-mile journey — contributing to broader efforts to reduce carbon emissions in the aviation sector. While these outcomes were based on modelling and proof-of-concept work, they align with the ambitions of the UK's Sixth Carbon Budget and long-term net-zero targets.

Beyond environmental impacts, the project addressed some of the operational challenges faced by the aviation industry, including disruptions from the COVID-19 pandemic and geopolitical instability. By applying quantum computing techniques to cargo loading optimisation, the work showed potential to improve supply chain resilience, operational efficiency, and fuel consumption in the long term, although further development is needed for full real-world application.

The feasibility study allowed the consortium to:

- **Assess performance**
  Determine under which conditions the quantum annealer outperformed classical HPC methods or achieved comparable results in reduced time frames.
- **Evaluate scalability**
  Understand how each approach handled increasing problem sizes and complexities.
- **Identify optimal use cases**
  Pinpoint scenarios where quantum computing provided tangible benefits over classical computing.
- **Gain insights**
  Explore the practical implications of integrating quantum solutions into existing operational workflows.

By leveraging HPC and quantum annealing, the project provided valuable insights into when and how quantum solvers could enhance the ULD loading process. This approach helped identify the strengths and current limitations of quantum computing, guiding future recommendations for reducing processing times and improving load factors effectively.

Finally, the project contributed to early-stage advances in the UK's quantum computing ecosystem, supporting the development of practical use cases while helping to inform the future direction of quantum adoption in critical industries.

Investigating the use of quantum computing and quantum machine learning to reduce carbon emissions in aviation

This project, also known as Quantum Breakthrough Innovate R&D / Project Q-BIRD, investigated the potential of quantum computing and quantum machine learning to reduce aviation-related carbon emissions by optimising flight paths. By modelling airspace through graph-based representations and evaluating both circuit-based and annealing quantum approaches, the study demonstrated the theoretical feasibility of quantum-enhanced air traffic optimisation. Additionally, it explored classical bottlenecks in air traffic management and proposed hybrid quantum-classical techniques, some of which are now under consideration for patent protection. The results support continued development and have laid the groundwork for future research and collaborative opportunities.

Lead: Quantum Base Alpha

Partners: The University of Edinburgh, QSL Quantum Software Lab, UKRI National Quantum Computing Centre

Observer: NATS

Context and objective

Quantum Base Alpha, in collaboration with academic and national research partners, investigated the potential of Quantum Computing (QC) together with Quantum Machine Learning (QML) to help solve a vital but currently intractable problem. The project's focus is to minimise the carbon emissions caused by aviation by optimising flight paths.

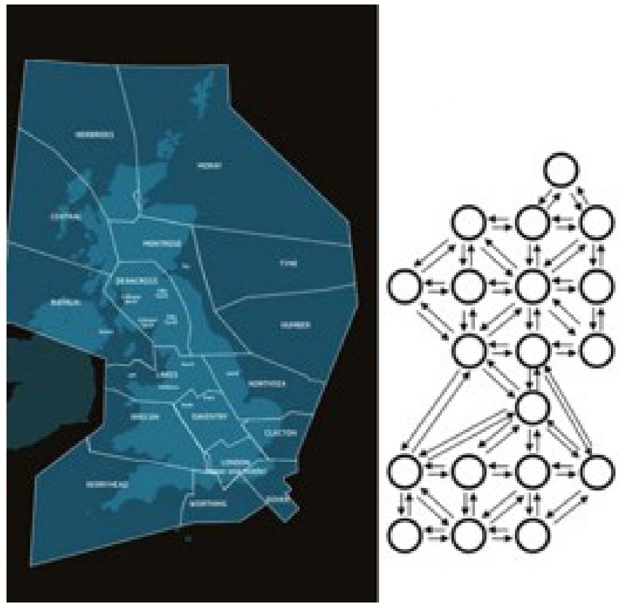
The Climate Change Committee, an independent body advising the UK Government, has reported that aviation currently produces 8% of UK Greenhouse Gas Emissions. The 7th Carbon Budget published in February 2025 concluded that major emission mitigating technological breakthroughs in aviation are unlikely to make significant differences given long development and certification lead times and the slow turnover of fleets. Hence by 2050, the legally binding target for Net Zero Carbon, it is predicted to be the highest sector with significant remaining emissions. Therefore, there is a need to improve the use of airspace, including the deployment of cutting-edge tools in Air Traffic Control. This includes the need to research and develop evolving Quantum Computing techniques alongside AI and Machine Learning.

Technical approach and methodology

Several approaches were considered and initial work was conducted on five candidate techniques including Travelling Salesperson, take-off and landing cycles, and the cruise section of flights in UK airspace. Considering real-life operational issues and priority customer needs, two strands were taken forward.

In the first, the classical aviation control system was converted into a graph-based model. The airspace representation used subregions as nodes, with connections defined by minimum centre-to-centre distances.

The project used the UK's largest supercomputer ARCHER2 to emulate a 44-qubit quantum computer, enabling error-free, extended operations. The study compared classical algorithms with an emulated circuit-based quantum computer and a quantum annealer, a non-circuit-based quantum computer optimized for problems like shortest pathfinding. The project demonstrated that quantum algorithms could determine shortest traversal paths on both a D-Wave quantum annealer and an emulated circuit-based quantum computer.



A graph representation of the simplified airspace model used with regions being represented by nodes and borders by vectors.

> Support from the NQCC, the Quantum Software Lab, and the University of Edinburgh has been crucial for SME QBA's mission to address aviation emissions – a significant contributor to global warming – by utilising the advancing potential of quantum computational technology to safeguard our sustainable future. The feasibility study recently completed is planned to evolve into further CR&D with the existing consortium being joined by Tier 1 aviation partners.
>
> Quantum Base Alpha Ltd

Despite challenges of computational time, this demonstrated that a quantum computer could theoretically find optimal airplane paths in simulated airspace. While not delivering quantum supremacy yet, it suggested further development would be worth investigation.

The second strand involved investigating existing classic computational bottlenecks for Air Traffic Management R&D. A range of techniques was implemented, some based on Grover's Search, which provided a potential quantised hybrid improvement to the identified classic optimisation problem. Subsequent IP advice recommends this can be patented with additional refinement. This work may additionally open further commercial pathways for similar applications.

Impact

Project results, where appropriate, have been disseminated at several events including the Economist Commercialising Quantum, SC24 (International Conference for High Performance Computing in Atlanta) and the Computer Insight UK (CIUK) conference in Manchester.

Further academic publications and presentations are planned but currently on hold following advice from IP lawyers, who indicated that with further refinement the algorithms may be incorporated as software within a technical process. Due to considerations of novelty and inventive step, additional public disclosure could jeopardize patentability. Nonetheless, the research has entered a pending patent application, which is encouraging.

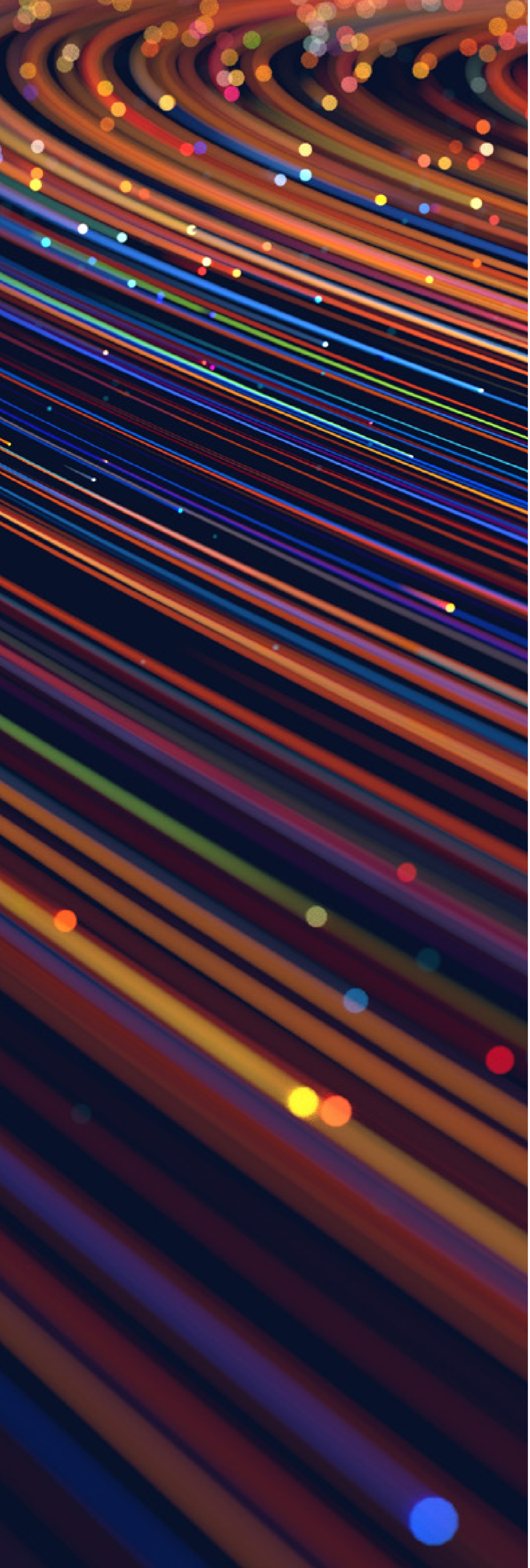
The overall project has reinforced confidence in the potential of quantum computation in this field. This has strengthened the consortium with the addition of a Tier 1 aviation partner for future collaboration. Together, efforts are underway to scope further R&D funding through SESAR (Single European Sky ATM Research), Horizon Europe 2025, and potential Innovate UK Experimental CR&D programs.

This work builds on progress made during the Fast Start (Oct 2022) and Feasibility Study (Sep 2023), supported and funded by Innovate UK and the NQCC, which were critical in catalysing and advancing the project.

Glossary

AI	Artificial Intelligence
CFD	Computational Fluid Dynamics
CG	Centre of Gravity
CIUK	Computer Insight UK
CR&D	Collaborative Research and Development
CpM	Constraint programming Model
CQM	Constrained Quadratic Model
DFJSSP	Dynamic Flexible Job Shop Scheduling Problem
FCA	Financial Conduct Authority
FHE	Fully Homomorphic Encryption
GDP	Gross Domestic Product
GDPR	General Data Protection Regulation
GLF	Gross Load Factor
HIPAA	Health Insurance Portability and Accountability Act
HPC	High-performance Computing
IP	Intellectual Property
LEO	Low Earth Orbit
MIP	Mixed-integer Programming
NISQ	Noisy Intermediate-scale Quantum
NLF	Net Load Factor
NHS	National Health Service
NMR	Nuclear Magnetic Resonance
NQCC	National Quantum Computing Centre
QRBMs	Quantum Restricted Boltzmann Machines
QAOA	Quantum Approximate Optimisation Algorithm
QC	Quantum Computing
QC-DMRG	Quantum Chemistry Density Matrix Renormalisation Group
QEC	Quantum Error Correction
QML	Quantum Machine Learning
QREPPS	Quantum Resource Estimation as a Pipeline for Polymer Simulation
QSL	Quantum Software Lab
QSVM	Quantum Support Vector Machine
R&D	Research and Development
SC24	International Conference for High Performance Computing 2024
SESAR	Single European Sky ATM Research
STFC	Science and Technology Facilities Council
UCL	University College London
UK	United Kingdom
UKRI	UK Research and Innovation
ULD	Unit Load Device
VQE	Variational Quantum Eigensolver

Notes



Disclaimer

NQCC advises that the information contained in this publication comprises general statements based on scientific research and stakeholder consultation. The reader is advised and needs to be aware that such information may be incomplete and will be superseded as research progress is made.

To the extent permitted by law, NQCC excludes all liability to any person for any consequences, including but not limited to all losses, damages, costs, expenses and any other compensation, arising directly or indirectly from using this publication (in part or in whole) and any information or material contained in it.

Contact information

National Quantum Computing Centre
Rutherford Appleton Laboratory
Harwell Campus
Didcot
Oxfordshire
OX11 0QX

Email: **nqccinfo@nqcc.ac.uk**
Website: **www.nqcc.ac.uk**
LinkedIn: **National Quantum Computing Centre (NQCC)**

© National Quantum Computing Centre, 2025.
All rights reserved.