National Quantum Computing Centre

Technical Report

The UK Quantum Hackathon – July 2023

Delivered by the NQCC at the University of Birmingham

National Quantum Computing Centre

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Principal authors:

Daisy Shearer, Outreach and Engagement Officer, NQCC
Abby Casey, Quantum Readiness Delivery Lead, NQCC
Natasha Oughton, Quantum Computing Policy and Ethics Lead, NQCC

Contributors:

Robert Cumming and Tim Thomas, Applied Quantum Computing ● Catherine White, BT ● Roberta Rehus, Jacobs ● Francisco Celis Andrade and Vikaran Khanna, National Grid ESO ● Kevin Fasusi, NHS ● Jan Novotny, Nomura International Plc. ● Jarrett Smalley, Rolls Royce ● Fazal Chaudry, UK Atomic Energy Authority ● Alan Mott and Salvatore Sinno, Unisys ● Max Arnott, Zaiku Group Ltd.

Reviewers:

Manav Babel, Quantum Applications Engineer, NQCC
Theodoros Kapourniotis, Analogue Quantum Applications Engineer, NQCC

Production and management team:

Simon Plant, Deputy Director of Innovation, NQCC
Soma Deshprabhu, Communications Manager, NQCC

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Executive summary

In July 2023, the National Quantum Computing Centre (NQCC) held its second UK Quantum Hackathon at the University of Birmingham as part of SparQ, its user engagement programme. Over the course of two days, ten teams of early-career researchers used quantum computing to tackle practical problems based on use cases provided by industrial end-users.

The teams had the opportunity to develop model solutions and run their code on real quantum processors and emulators, which could be accessed via the cloud. The use cases spanned multiple sectors (energy, healthcare, telecommunications, aerospace, finance) and problem domains (optimisation, machine learning and simulation). The number of end-user companies involved in the event increased from six in the 2022 UK Quantum Hackathon to ten in 2023, with the wider variety of practical use cases demonstrating a growing awareness of quantum computing and the diversity of its potential applications.

The 2023 hackathon also saw an increase in the number of companies providing access to their hardware platforms, which represented both gate-based and annealer-based quantum hardware. Different use case solutions were tested on superconducting, trapped-ion or photonic platforms, and compared with emulated results.

Within this report, all ten use cases and their solutions have been summarised by the industrial end-user mentors from each team. These technical summaries provide insights into the types of problems that could be addressed by quantum computing, as well as the current capabilities and limitations of the technology.

At the event, the teams had the opportunity to present their solutions and results to a panel of judges with expertise in quantum computing. The first, second, and third-place teams and use cases were: Rolls Royce team 'Near-term quantum linear solver algorithms'; Jacobs team '1-D Monte Carlo particle transport'; and Applied Quantum Computing team 'Vaccination centre location'.

1st place: Rolls Royce team
Use-case: Near-term quantum linear solver algorithms

2nd place: Jacobs team
Use-case: 1-D Monte Carlo Particle Transport

3rd place: Applied Quantum Computing team
Use-case: Vaccination centre location

Objectives

The UK Quantum Hackathon is part of the NQCC's SparQ programme, which enables quantum computing users to develop their skills, gain an understanding of the current and future capabilities of quantum computers, and make connections across the quantum computing ecosystem. The UK Quantum Hackathon represents a microcosm of the wider SparQ programme, as it provides an opportunity for participants to gain hands-on experience with programming quantum computers, coding and running quantum algorithms on real and emulated quantum processors, formulating computational solutions in response to practical use cases, and exploring the capabilities and limitations of current cutting-edge technology. The event also offers a valuable networking opportunity for the UK's quantum community.

Table 1 outlines the outcomes of the 2023 event against its objectives. The results clearly demonstrate the benefit to participants of attending the event. For example, end-user organisations were able to develop and explore new use cases, developers gained new skills and knowledge, technology providers tested real use cases on their platforms, and all groups had the opportunity to network and connect with the wider quantum ecosystem.

2023 objectives	2023 results
Investigate quantum solutions for industry-provided use cases across different sectors and application domains such as optimisation, simulation and machine learning.	10 use cases across 5 industrial sectors with optimisation, simulation and machine learning problems represented.
Create an active quantum computing community spanning the full value chain from quantum compute providers, through to quantum developers and end-users.	53 developers, 5 technology types used (with representation from 7 hardware platform providers on the day), 10 end-user companies and a total of 32 provider and end-user mentors to support the teams.
Enhance connectivity between quantum computing providers and end-users, enabling discussions on both opportunities and limitations of current technology.	74% of respondents mentioned networking and connecting with the user community when asked 'What were your key highlights from the hackathon?'
To increase awareness of quantum computing and potential use cases to research students and early-career scientists (Masters, PhD and Postdoctoral level).	72% of respondents said that they acquired skills and knowledge in a new area.

Table 1: The results of the UK Quantum Hackathon 2023 against objectives.

Introduction and background

The NQCC's SparQ program aims to support the discovery and development of use cases and applications for quantum computing, enhance quantum computing literacy and programming skills, and build a UK user community for quantum computing through knowledge exchange and networking.

The hackathon format is ideal for meeting these aims as it brings together a community of programmers, technology providers, and end-users, with the aim of developing their skills, investigating different use cases, and building a network of developers and end-users.

Hackathons are events that bring together individuals to solve specific problems related to a particular theme. The events offer an opportunity for a whole community to work side-by-side to tackle technology challenges, usually by developing or advancing computer programs.[1] Hackathons bring together experts from different domains, harnessing their diverse skillsets to achieve a common goal: designing the best solution to their problem within the timescale of the event.

Some researchers have pointed out the power of hackathons for community-based and inquiry-based learning for those involved, as well as the opportunity for networking with peers and potential future employers.[2]

Daisy Shearer, Outreach and Engagement Officer, NQCC.

As quantum computing develops as an emerging technology, end-users are interested in exploring potential applications relevant to their industries. Quantum hackathons provide an important launch pad for end-users to begin this exploration. In addition, a growing skills gap across the quantum computing value chain has been identified, including algorithm development for real-world use cases.[3] As part of the efforts to develop a quantum-literate workforce, several institutions and organisations have hosted quantum hackathons in recent years where participants are provided with access to quantum computing hardware to test and develop their solutions.[4-7]

Though the technology is still early in its development, quantum hackathons allow end-users, technology providers and developers to test the capabilities and limitations of quantum computing hardware and software. Many existing quantum hackathons focus on education, skills development, and networking elements, often incorporating tutorials rather than exploring industrially relevant use cases.

As a microcosm of the NQCC's SparQ programme, the hackathon enables early-stage application discovery, provides access to quantum computing resources across different hardware modalities, facilitates networking within the quantum ecosystem, and develops the skills of developers through inquiry-based learning.

Through this annual event, the NQCC brings together the quantum community in the UK, facilitating the engagement of early-career researchers with a range of stakeholders in the UK quantum computing industry. This supports the NQCC's vision of enabling the UK to solve some of the most complex and challenging problems facing society by harnessing the potential of quantum computing.

By ensuring that a broad range of industries are represented in the use cases and a wide variety of state-of-the-art quantum computing platforms are available, the NQCC's Quantum Hackathon offers a unique opportunity for participants to explore the potential of current quantum computing technology.

Additionally, the 2023 hackathon asked participants to consider the need for responsible and ethical quantum computing within the context of use case development and quantum programming, emphasising that this technology has the potential for a profound impact on society and the responsibility of the quantum computing community to ensure that the technology is used responsibly, safely, and for the benefit of society.

The NQCC's UK Quantum Hackathon 2023

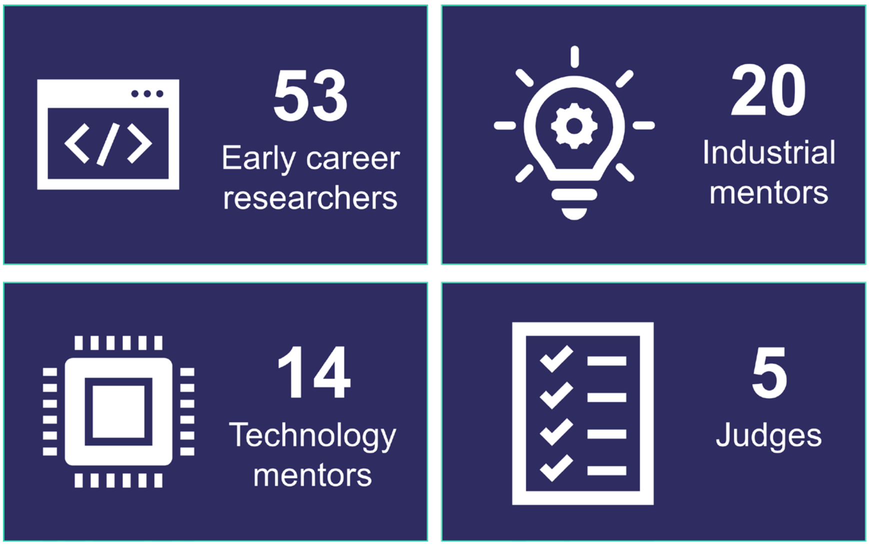


Figure 1. Overview of the number of people participating in the hackathon.

Each end-user organisation provided an industrially relevant use case problem for teams to work on, with the specific use cases and their solutions explored in more detail later in this report. Some of the participating end users had already been exploring quantum computing applications within their industry, while others were relatively new to the technology. Incorporating use cases from end-users across a variety of sectors gives stakeholders the opportunity to explore relevant problems for driving future innovation. The technical progress made by the teams during the event can be taken forward by the end-users, making a direct contribution to the development of quantum computing in the UK.

The ten end user organisations who provided teams with use cases were:

- Applied Quantum Computing
- BT
- Jacobs
- National Grid ESO
- NHS
- Nomura International Plc.
- Rolls Royce
- UK Atomic Energy Authority
- Unisys
- Zaiku Group Ltd.

The NQCC's hackathon provided access to a wide variety of emerging quantum compute resources operating in the Noisy Intermediate Scale Quantum (NISQ) regime, rather than offering access through a single platform provider. This broadens the scope of problem exploration since each use case can be matched to the most suitable quantum computing platforms for the problem type. Developers were supported by NQCC applications engineers as well as end-user and provider mentors, allowing teams to draw on a breadth of expertise. Care was taken to ensure that each team was made up of a diverse range of people and that they had a balance of skill levels. Those with more quantum computing experience and knowledge were able to support and mentor participants who were newer to quantum application development. This peer-to-peer learning, along with the fast pace of the hackathon, facilitated a dynamic environment that is ideal for skills development, knowledge exchange, creativity, and innovation.

A diverse range of quantum providers participated in the 2023 hackathon. The providers who directly supported the event were:

- AWS
- Classiq
- D-Wave
- IBM Quantum
- IonQ
- ORCA Computing
- Oxford Quantum Circuits
- Quantinuum

These providers represented a broader range of technologies than the 2022 event, giving participants access to both gate-based and annealing-based quantum computers as well as quantum emulators. Teams were allocated primary and secondary quantum hardware providers to ensure that backup options were available in the event of hardware access limitations. Access to quantum emulators allowed results from real quantum hardware to be compared to error-free emulated results, enabling participants to better understand the limitations and potential of current quantum hardware. In the weeks prior to the hackathon event itself, quantum computing providers gave training sessions to the participants to introduce them to their platforms and allow them to start exploring the tools they would be using during the hackathon.

The hackathon concluded with short presentations from the teams to a panel of quantum experts who assessed their solutions based on the following criteria:

1. Success of the solution for the given use case for the allocated resources
2. Creativity and novelty of the solution given the initial use case
3. Investigation into scaling
4. Responsible and ethical quantum computing considerations
5. Quality of the presentation: clarity
6. Quality of the presentation: engagement, length
7. Quality of answers to questions

Having experts in the quantum computing industry to judge the teams' solutions contributes to the innovative and interactive environment cultivated by the hackathon. An aspect of healthy competition also motivates participants to make the best use of their time at the hackathon.

Alongside the technical considerations of their use case, developers were also challenged to consider the wider societal context of their solution. Responsible innovation, which involves taking an anticipatory and inclusive approach to considering and responding to the potential impact of the development, is an important part of the innovation process. Since the format of the hackathon replicates at a smaller scale the process of innovation in the real world, this additional focus on responsible and ethical quantum computing (REQC) enabled developers, mentors, and use-case providers to experience all aspects of the innovation process.

To enable engagement with the REQC component, participants were introduced at the start of the hackathon to the key ideas behind responsible innovation, including its purpose, key definitions, and the AREA framework (Anticipate, Reflect, Engage, Act) endorsed by UKRI. Key considerations in the context of quantum computing were also presented, with reference to the World Economic Forum's Quantum Computing Governance principles, including technology stakeholders and core values for responsible innovation. The teams were then challenged to build societal benefit into their solutions by considering stakeholders who might be impacted, those who might have influence, and where values could be maximised.

Figure 2. The questions posed to participants to consider the societal impact of their use cases in the introductory presentation.

To support engagement, participants were invited to consider these three questions for a practice use case, submitting their answers via Mentimeter to facilitate shared understanding. The teams were then asked to consider the same questions for their own use case and incorporate their answers into their presentations, which were then appraised as part of the judging process. Integrating this REQC component into the hackathon helped to raise awareness and understanding of the importance of responsible innovation, as well as key considerations in the context of quantum computing, among developers, industry mentors, and technology providers.

References

[1] N. Taylor and L. Clarke, "Everybody's Hacking: Participation and the Mainstreaming of Hackathons," Proceedings of the 2018 CHI Conference on Human Factors in Computing Systems, 2018. doi:10.1145/3173574.3173746

[2] S. Monsef, M. Yarmohammadian, S. Javanmard, Y. Yazdi, and M. Amini-Rarani, "The role of hackathon in education: Can hackathon improve health and medical education?," Journal of Education and Health Promotion, vol. 10, no. 1, p. 334, 2021. doi:10.4103/jehp.jehp_1183_20

[3] Chow, J.; Greplová, E.; Heijman, F.; Kuchkovsky, C.; O'Halloran, D.; Pointing, J.; Shutko, G.; Williams, C. J. State of Quantum Computing: Building a Quantum Economy; World Economic Forum, 2022. https://www.weforum.org/reports/state-of-quantum-computingbuilding-a-quantum-economy

[4] Qiskit Fall Fest 2023, IBM Quantum Computing. Available at: https://qiskit.org/events/fall-fest

[5] QHack 2024 - quantum computing hackathon, QHack 2024 - Quantum computing hackathon. Available at: https://qhack.ai/

[6] Womanium // Quantum, WOMANIUM. Available at: https://womanium.org/Quantum/Hackathon

[7] Big Quantum Hackathon, QuantX. Available at: https://quantx.fr/BIG-quantum-hackathon

Use cases, teams and solutions

The teams' use cases and solutions are summarised in the following sections, as provided by their industry mentors.

The Teams

Table 1. The use case provided to each team, along with the type of problem, the end-user and their industry sector, and hardware providers that were allocated to each team.

Team #	Use case	Problem domain	End-user	Sector	Providers
1	Practical equivariant embeddings for DNA sequencing over the current NISQ devices	Machine learning	Zaiku Group Ltd.	Healthcare	AWS (OQC) AWS (Rigetti) Emulation: AWS
2	The travelling salesman problem – route optimisation in healthcare	Optimisation	NHS	Healthcare	AWS (QuEra) D-Wave Emulation: AWS
3	Explore the use of quantum computing for unit commitment to balance the electricity grid	Optimisation	National Grid ESO	Energy	ORCA Computing D-Wave Emulation: D-Wave
4	Quantum computing for nuclear fusion engineering and design with the finite element method	Simulation	UKAEA	Energy	AWS (OQC) Quantinuum Emulation: AWS
5	1-D Monte Carlo particle transport	Simulation	Jacobs	Energy	Quantinuum IBMQ Emulation: IBMQ
6	Near-term quantum linear solver algorithms	Simulation	Rolls Royce	Aerospace	Classiq (IonQ) IBMQ Emulation: Classiq (IonQ)
7	Skills constrained capacitated vehicle routing problem with time window (SC-CVRP-TW)	Optimisation	Unisys	Logistics	IBMQ D-Wave Emulation: IBMQ
8	Price prediction over different time horizons	Machine learning	Nomura International Plc.	Finance	IBMQ ORCA Computing Emulation: IBMQ
9	Generating efficient and resilient routes for unicast and multicast traffic	Optimisation	BT	Telecommuni-cations	D-Wave AWS (Rigetti) Emulation: D-Wave
10	Vaccination centre location	Optimisation	Applied Quantum Computing	Healthcare	AWS (IonQ) D-Wave Emulation: AWS

Team 1: Practical equivariant embeddings for DNA sequencing over the current NISQ devices

Author: Max Arnott
Organisation: Zaiku Group Ltd.

Problem

The team's task was to define an equivariant embedding of DNA sequences into quantum states, and to demonstrate an equivariant circuit in action that respects the symmetries of the dataset. Machine learning techniques can be effective for applications such as detecting genetic diseases and drug discovery, and we believe that a quantum approach may be advantageous in overcoming the unwieldy length of DNA sequences.

Solution

The team identified the reverse-complement symmetry of DNA sequences and defined an angle-based embedding with two features per qubit, in which the symmetry was represented on the Hilbert space via conjugation by a tensor product of Pauli-X gates. They created a synthetic dataset of eight sequences in length and defined via their representation an equivariant circuit to detect the string 'AT' within a sequence - an equivariant version of a small, typical variational ansatz. They compared this model's performance to an analogous non-equivariant model on a simulated device. Time did not permit training on a real device but the angle-based solution would have been suitable for NISQ devices.

Outcome

The equivariant model appeared to reach a lower cost than the non-equivariant counterpart given the same amount of training, which was a nice conclusion.

Time limitations meant that the team could not practise a training/validation/test data split for benchmarking. Further, the hybrid nature of training loops meant that performing the task on a real device would have taken too long. These loose ends would be a natural starting point for further investigation, along with applications of the method to real-world datasets. It would also be interesting to compare the two quantum models to a classical approach to the same task.

References

J. J. Meyer, M. Mularski, E. Gil-Fuster, A. A. Mele, F. Arzani, A. Wilms, and J. Eisert, "Exploiting symmetry in variational quantum machine learning," arXiv:2205.06217, 2022.

N. Innan and M. Al-Zafar Khan, "Classical-to-Quantum Sequence Encoding in Genomics," arXiv:2304.10786, 2023.

Team 2: The travelling salesman problem – route optimisation in healthcare

Author: Kevin Fasusi
Organisation: NHS

Problem

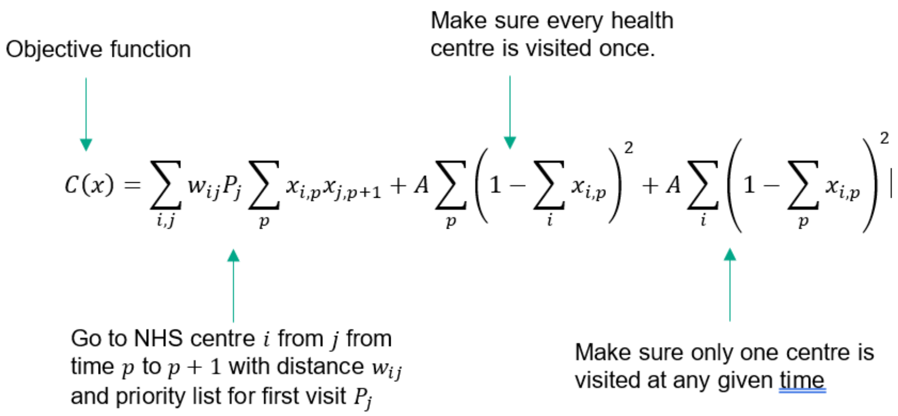
Routing and scheduling optimisation is a constant exercise when seeking cost reduction and improvement of service times in the healthcare operational environment. In addition to the transportation of patients via ambulance, NHS services also require the transportation of time-sensitive material to multiple locations. The computation of optimal routes is of value and a common classical problem. An algorithm in computer science is said to be “efficient” if it executes in polynomial time or less. Owing to the nature of routing and scheduling problems as NP-complete, the application of quantum computing for problem solving in a healthcare setting is an exciting proposition. Routing and scheduling optimisation problems are commonplace, and innovative ways to tackle these problems may offer advantages not yet realised via classical methods.

Solution

To make the problem tractable, the team used a hybrid method that combines classical compute for clustering (k-means-constrained) with quantum annealing. The clustering technique focuses on finding non-overlapping clusters, constraining the search space, and making the solution viable for existing hardware and at scale.

The team used the D-Wave solver to implement the quantum annealing. Their objective function is defined in Equation 1.

Simulated annealing in a classical setting is prone to being trapped in local minima. Finding the global minimum using classical compute is computationally intensive and takes time. Quantum annealing takes advantage of low-energy states in quantum physics to find the low-energy states of a problem, and the solutions provided by D-wave are designed for these types of problems. Once the team encoded their problem onto an initial Hamiltonian, mapping eigenstates to energies, they sought an optimal solution.



Equation 1. Objective Function for Solver, Source: Team Presentation

Outcome

Several clustering methods were attempted, and k-means-constrained proved most useful. Hospitals were clustered before using D-Wave to provide solutions for the optimal route based on the shortest path between clusters. The team had a limited number of qubits to use but were still capable of finding solutions for up to five health centres.

References

S., Jain, 2021. Solving the traveling salesman problem on the d-wave quantum computer. Frontiers in Physics, p.646.

Team 3: Explore the use of quantum computing for unit commitment to balance the electricity grid

Authors: Francisco Celis Andrade and Vikaran Khanna
Organisation: National Grid ESO

Problem

The Unit Commitment (UC) problem is a fundamental problem in the electric power industry. The objective of UC is to determine an optimal schedule for each generating unit to meet the demand for power with the minimum cost.

Given its mixed-integer programming (MIP) nature, UC solution speeds could potentially be greatly enhanced with quantum computing.

Solution

We took a simplified version of UC to the hackathon that made it a combinatorial problem in which all the optimisation variables were binary, representing whether a generator was online or offline. Modelled constraints were positive margins and minimum up/down times for generators.

Objective function – minimise costs to operate the system:

$$\min_{b_{j,t}} \sum_{t} \sum_{j} b_{j,t} \cdot c_j \cdot \overline{P}_j \cdot \Delta + u_{j,t} \cdot c_j^U$$

Subject to:

- Positive margin: $\forall t \ \sum_j b_{j,t} \cdot \overline{P}_j \geq D_t$
- Minimum nonzero time: $\forall j, \forall t \in \{L_j + 1, \ldots, |T|\} \sum_{k=t-MNZT_j+1}^{t} u_{j,k} \leq b_{j,t}$
- Minimum zero time: $\forall j, \forall t \in \{F_j + 1, \ldots, |T|\} \ b_{j,t} + \sum_{k=t-MZT_j+1}^{t} d_{j,k} \leq 1$
- Binary consistency: $\forall j, t \ b_{j,t-1} - b_{j,t} = d_{j,t} - u_{j,t}$

We worked with ORCA Computing and D-Wave to solve this problem using quantum hardware and simulators.

Outcome

The team explored the possibility of formulating UC as a quadratic unconstrained binary optimisation (QUBO). Additionally, we used D-Wave's hybrid solver to implement the constrained problem. This way, the team succeeded in solving a toy case of four generators and four time periods.

We found that:

- Formulating a QUBO problem for a simplified version of UC wasn't straightforward and the limited time available made it more challenging. We can only speculate how much harder it would be for the full Security-Constrained UC problem
- Solving constrained optimisation problems using quantum platforms allows specifying 'a-priory' Langrage multipliers for the constraints. This means that it's difficult to assess the optimality of a solution and the general applicability of an implementation without a reference solution
- While quantum computing shows great potential to solve complex optimisation problems in other sectors, there's an outstanding gap before it can be directly applicable to power system operation. We'd be keen to continue exploring how to bridge this gap.

Team 4: Quantum computing for nuclear fusion engineering and design with the finite element method

Author: Fazal Chaudry
Organisation: UK Atomic Energy Authority

Problem

The design of nuclear fusion reactors requires accurate simulations of complex phenomena to optimise design parameters and reduce the need for costly physical prototypes. Unfortunately, the computational cost of some of these complex simulations limits their applicability and benefits. The improved computational performance promised by quantum computers will be of great benefit for shortening engineering design cycles and improving the accuracy of designs.

Solution

Finite Element Analysis (FEA) is a numerical simulation technique used for fusion reactor design that solves the complex dynamics of the fusion domain using a linearised set of equations. This is equivalent to solving the equation Ax=b, where the inverse of the matrix A is used to determine the vector x given a set of initialised values of b. The Harrow-Hassidim-Loyd (HHL) algorithm was deployed to solve the equation Ax=b, as an early demonstrator of a quantum solver for linear equations. The algorithm requires a large circuit depth, due to the initialisation operations required to store the value of the vector b. Gate operations were then conducted to apply the inverse matrix A on the qubit value of vector b to solve for vector x. To solve for a single qubit circuit line, seven qubits were used as control and scratch qubits. This was implemented on the eight-qubit Lucy quantum processor provided by Oxford Quantum Circuits.

Outcome

The experiment demonstrates that it is possible to solve linear matrix operations. However, these were based on classical binary input values, and representing large vectors with a large matrix space at the binary level will require large amounts of qubits and quantum information to represent the binary data and respective quantum transformation. Therefore, it is proposed to improve the encoding of classical high-level data to quantum qubit data to improve the computational expense and complex quantum algorithms with large depths of circuits and possible larger entanglement requirements. Also, to implement one logical qubit requires approximately seven physical qubits, which will significantly increase the number of physical qubits required if error corrects are to be considered.

FEA is a widely used numerical simulation technique, and therefore this algorithm has applicability in all complex engineering sectors such as aerospace, automotive, construction and so forth. In future exploration it would be interesting to merge quantum numerical simulation techniques in neural network loss functions with optimisations to improve the training for Physics Informed Neural Networks (PINNS).

Team 5: 1-D Monte Carlo particle transport

Author: Roberta Rehus
Organisation: Jacobs

Problem

Mathematical modelling of the transport of subatomic particles in matter, such as neutrons, plays an important role in the operation of radioactive facilities. The Monte Carlo (MC) approach to simulating radiation transport provides accurate results but is computationally expensive. Quantum computing may have a role in speeding up MC simulations.

Solution

The MC method consists of sampling from specified statistical distributions to determine the collision type, direction and distance travelled by the particle. Quantum sampling may be more advantageous to classical sampling due to accuracy and speed improvements. An alternative method involved encoding the probability distribution of particle penetration as a biased quantum coin, with the probability of penetration estimated via a circuit for quantum amplitude estimation (QAE). The H1 Emulator provided by Quantinuum was used to implement these circuits, with sampling of uniform distribution achieved via circuits with a depth of one and four gates. Sampling of exponential distribution was done via a state preparation box, leading to a deeper circuit. The circuit for QAE consists of more quantum gates, corresponding to greater depth if non-optimised, and is ideal for fault-tolerant systems, while quantum sampling may be better suited for NISQ devices.

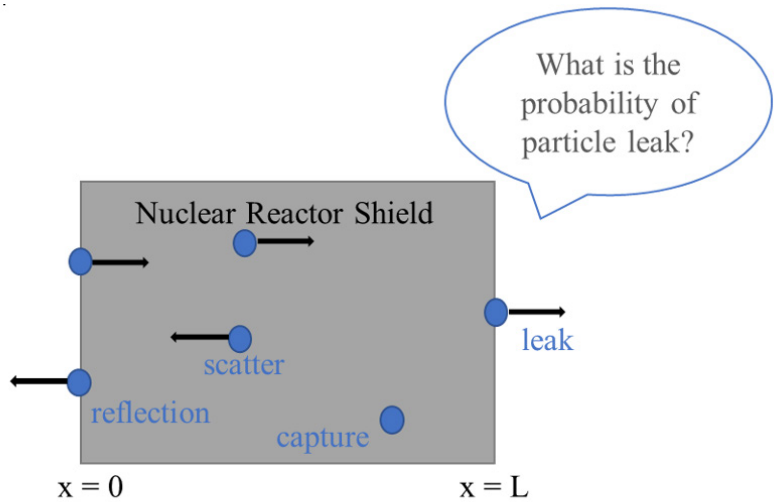


Figure 3. Example of particles travelling through a 1-D shield of length L.

Outcome

The solutions obtained via quantum sampling showed a large variation from the analytical solutions. Error correction techniques were not implemented, which could account for the difference in expected and obtained results. The use case was also a simple example with only two energy levels and limited neutron interactions (capture, scatter, leak). Future extensions could consider higher dimensions, more energy levels, as well as fission interactions. The alternative method using QAE was not fully explored, and could be better investigated in the future.

Team 6: Near-term quantum linear solver algorithms

Author: Jarrett Smalley
Organisation: Rolls Royce

Problem

Rolls Royce designs and manufactures power systems for applications such as aviation and marine propulsion. For the simulation and modelling of modern power systems, engineers utilise Computational Fluid Dynamics and Finite Element Method algorithms. These reduce to the computationally intensive task of matrix inversion for solving systems of differential equations, which can bottleneck even supercomputing throughputs. Quantum computing's dense matrix algebra indicates a potential advance for this use case.

Solution

Examples of the problem present as small instances of linear systems of equations, which may be formulated as Ax=b, presented with a matrix of equations A and a vector of constants b to solve for the vector x. Examples from sizes of 2x2 to 16x16 matrices were solved for this use case. Two different algorithms were studied to approach this, a Coherent Variational Quantum Linear Solver (CVQLS) that could be easily implemented on NISQ hardware and the Quantum Singular Value Transformation (QSVT), which is more intended for fault-tolerant systems. These were predominantly developed in Classiq to optimally compile a circuit with minimal execution time, with some bits being done in Pennylane and exported via QASM file to Classiq.

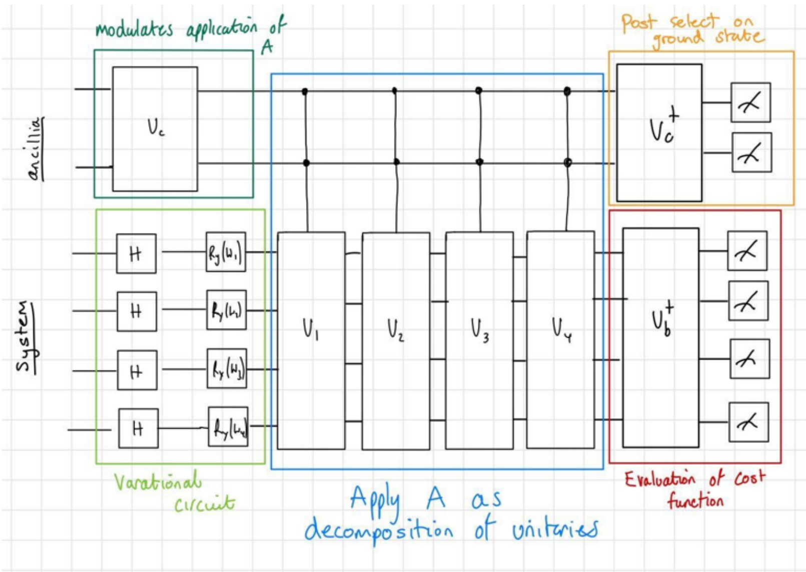


Figure 4. Circuit for the CVQLS with descriptions of the different portions

Outcome

The team performed runs of the CVQLS on the 16-qubit IBM Guadalupe device using Classiq and IBM Quantum, and on a 20-algorithmic qubit IonQ Aria device as well as the IonQ Harmony device using Classiq. Limited by the circuit size, the team was able to reach results for linear systems of up to 4x4 using the hardware devices, while simulation reached up to 16x16 matrix sizes. Besides normally not being a NISQ algorithm, the QSVT encountered issues in its hardware implementation as Pennylane's newly introduced QSVT module did not compile to QASM code, and this will be a necessary step towards implementing the QSVT in hardware. Further implementations of quantum linear solvers are expected to be developed by Rolls Royce and partners for the future development of hydrogen-based systems.

References

https://pennylane.ai/qml/demos/tutorial_coherent_vqls

https://pennylane.ai/qml/demos/tutorial_apply_qsvt/

Team 7: Skills constrained capacitated vehicle routing problem with time window (SC-CVRP-TW)

Authors: Alan Mott & Salvatore Sinno
Organisation: Unisys

Problem

A specific version of the Vehicle Routing Problem (VRP) is the Vehicle Routing Problem with Time Window and Skill Set constraints (VRP-TWSS). This involves calculating optimal routes for a fleet of vehicles where each vehicle has a particular set of skills, and each destination has a required skill and time window.

Providing a successful resolution to the optimisation of vehicle routing problems will:

- Provide cost savings in operational costs
- Reduce environmental impact by minimising journey times and distances for delivery vehicles, lowering both CO_2 emissions and traffic congestion.

Current classical solutions to these problems do not scale to the level faced by many of our customers, even with High Performance Computing (HPC).

Solution

No quantum circuit was developed as the solution was developed on D-Wave's quantum annealer. Instead, the mathematical model was implemented directly using the Constrained Quadratic Model (CQM) in D-Wave's Ocean Software Development Kit (SDK).

The solution was based on the mathematical model defined in L. Han's paper.[1] In the time available, no consistent solution was returned by D-Wave. Different solutions were considered optimal by the quantum annealer on different runs of the code. This may very well result from the high density of constraints, a problem Unisys have encountered before and outlined in our whitepaper.[2]

Outcome

During the hackathon, the team very quickly (within a few hours) encountered hardware limitations using the IBMQ platform. The team's use case was solving a small vehicle routing problem (32 nodes and 5 vehicles, or n32-k5) with time-window and skill-set constraints. Even without the time-window and skill constraints embedded in the model, the IBMQ platform did not yield results after running the model, even with a smaller model consisting of 8 nodes and 3 vehicles (n8-k3). By comparison, running the same model on the High-performance parallel linear optimisation Software (HIGHS) classical solver installed on an Orange Pi 5 returned results within minutes. Using a quantum annealer from D-Wave, results were also obtained within minutes.

References

[1] L. Han, "Metaheuristic Algorithms For The Vehicle Routing Problem With Time Window And Skill Set Constraints", Dec 2016. Available: Han-Lu-MSc-IENG-Dec-2016.pdf (dal.ca)

[2] S. Sinno, T. Gross, A. Mott, A. Sahoo, D. Honnalli, S. Thruvavakkath, B. Bhalgamiya et al., "Performance of Commercial Quantum Annealing Solvers for the Capacitated Vehicle Routing Problem,", Sep 2023. Available: 2309.05564.pdf (arxiv.org)

Team 8: Price prediction over different time horizons

Author: Jan Novotny
Organisation: Nomura International Plc.

Problem

The team was provided with a problem to predict the time series of financial data. The data are well known to be noisy with very low signal-to-noise ratio, and also have complex memory structure. The aim was to create a supervised machine-learning model that makes use of quantum resources.

Solution

The main approach to the problem was to utilise a quantum-enhanced Long Short-Term Memory (LSTM) model. The LSTM model is a neural network-based model that separately models the long and short memory, along with the process of forgetting the past. The process contains several parallel neural networks that are trained as part of the calibration. We replaced the neural networks with quantum equivalents and trained the model with IBMQ resources. The model showed promising results within the reach of currently available hardware (16-qubit processor), while we utilised a simulator for most of the analysis.

Outcome

The result was very encouraging and showed potential for how existing quantum hardware can be used to enhance existing algorithms or as a hybrid combination of classical and quantum parts. The project opened more questions to pursue in the future, such as the optimal combination, and which one dominates any existing setup, but it suggests that some form of enhancement is within reach in the short term.

Team 9: Generating efficient and resilient routes for unicast and multicast traffic

Author: Catherine White
Organisation: BT

Problem

Allocating routes for transmitting data across telecommunication networks can become computationally hard under certain conditions, such as when the network is very congested, with different demands when the data traffic allocation on each channel is broken into a small number of options (integer flow). This can occur, for example, when assigning optical channels at layer 1, and where it is required to provide resilience by planning two independent routes for each demand that is completely independent of the first route. Further complications can include requirements for multicast (one source to many sinks) traffic and constraints such as the maximum latency of a route.

Solution

The team identified that data traffic flow is a variation of the standard commodity flow satisfaction problem. The team used a Quadratic Unconstrained Binary Optimisation (QUBO) representation of the routing and demand satisfaction model, and this was run on a D-Wave quantum annealing system with 5000 qubits. A number of approaches were investigated to represent this problem using the QUBO form. For single-commodity flow problems (both unicast routes and multicast trees), the team settled on a flow continuity model that used Kirchoff's current laws at each node. Qubits represented the links of the network. The capacity of each link could be constrained using the choice of encoding the amount of flow in the link by using a binary expansion of the total capacity of each link (such that no configuration of weights could exceed the maximum capacity). This was efficient, creating a number of weighted qubits of order log C for each edge. The encoding of single-commodity flow required approximately E log2 C qubits (where E is the number of links in the original network, and C is the average capacity). However, for highly connected networks, additional qubits would be needed to overcome native Quantum Processing Unit (QPU) connectivity constraints. For the more realistic multicommodity flow problem (planning routes for different types of data), it was necessary to create multiple copies of the original qubit representation of the different commodity flows on the network coupled to represent the shared capacity constraints, with slack variables because the capacity represented an upper limit.

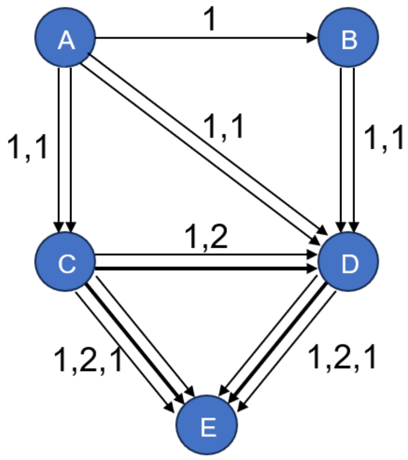


Figure 5. Example of commodity flow over a network of 5 nodes.

Outcome

The team showed that it was possible to encode a large number of different variations of the efficient routing problem. Smaller problems up to network sizes of 10 nodes were solved using the D-Wave native QPU (5000 qubits). Larger problems were run on the D-Wave Leap hybrid solver. Repeated anneals usually returned some correct solutions (with the lowest energy in the sample set), but the QUBO formulation had some technical issues that could affect the quality of the solution. Changing the weighting between the linearly independent terms (representing different constraints) often affected the probability of returning a valid solution in any given run. This was true both for the D-Wave native QPU and the hybrid solver.

The fact that very complex routing problems could be represented quite efficiently in numbers of qubits in a QUBO was very promising. However, the fact that the ground state optimum (and correct) solutions were not found a high percentage of the time was a limitation. This was not unexpected given that the annealer has some noise, and the encoding of the problem had not given any consideration to error mitigation, plus we expect larger problems to have smaller energy gaps between the ground state solution, and excited states. Whether an encoding on the current D-Wave annealer could mitigate errors (for example, by coupling qubits in redundant groups to represent single logical QUBO variables) and whether this would be efficient would be interesting to explore. The effect of varying the weightings of the different linearly independent constraint terms on the quality of the solution set was also something that needs to be explored and understood further. Ground state solutions were found, however, which are promising, especially in light of the potential to improve the annealing performance with emerging developments in quantum annealer hardware and methods. Continued increase in quantum annealer QPU size will also be helpful.

This use case was further developed by the hackathon team, leading to a paper entitled 'Optical Routing with Binary Optimisation and Quantum Annealing' where the details of this problem are explored in more depth and future work building from that conducted at the hackathon is reported.

References

E. Davies et al., "Optical Routing with Binary Optimisation and Quantum Annealing," arXiv, 2402.07600v1, 2024

Team 10: Vaccination centre location

Authors: Robert Cumming and Tim Thomas
Organisation: Applied Quantum Computing

Problem

Optimising the location of vaccination centres during a pandemic is an important means of reducing the pandemic's impact. Optimal locations will help to maximise vaccination rates in the population, thereby reducing the chances of the vaccinated individuals catching the disease and also helping reduce the rate of spread, benefiting the whole population. The real-world problem objective is to maximise vaccination take-up by considering travel times (to be minimised), clinic capacity, population size and demographics, and the proportion of the population already vaccinated. Here, we consider the simplified problem of minimising population to vaccine centre travel times. At large scale, such problems cannot be optimally solved using classical means.

Solution

The problem can be considered as a weighted-set cover problem and formulated as a QUBO, which can be translated into Ising form for running on a quantum computer.[1] The objective function, which is to be minimised, encodes the total distance from the population centres, N, (nodes) to the vaccination centre(s), V, (also nodes) and includes certain problem constraints encoded using the Lagrange multiplier method, such as the requirement that each population centre is only served by one vaccination centre.

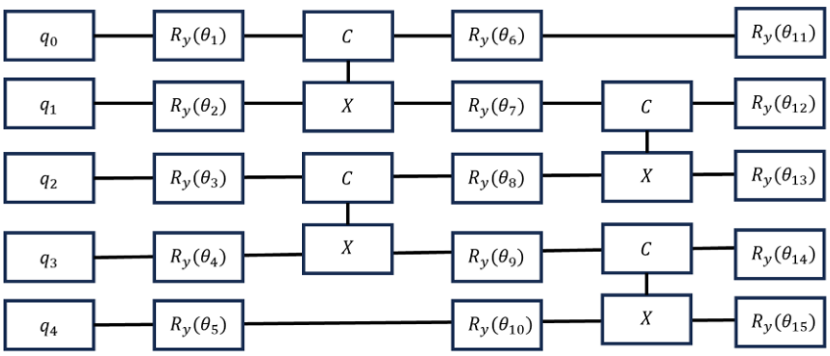


Figure 6. Example of VQE parameterised quantum circuit with 5 qubits.

Two NISQ-era hybrid algorithms were used: QAOA (Quantum Approximate Optimisation Algorithm) and VQE (Variational Quantum Eigensolver), each of which seeks to optimise a parameterised circuit.[2, 3] An example circuit to run the VQE parameterised algorithm is shown above. Two simulators were used: Amazon Braket SDK for VQE and IBM Qiskit for QAOA.

Outcome

Two small-scale instances of the problem were considered: (A) N=4, V=2 and (B) N=3, V=2, with instance (A) run using QAOA and instance (B) using VQE. Each was run using up to 20 random initial choices for the circuit parameters and was successful in very significantly improving the probability of finding the optimal configuration (the ground state) by comparison with the initial problem starting state – for example, the VQE approach was able to achieve an 89% probability of finding the ground state with the best set of initial parameters.

An important unresolved question is how the approach scales with problem size and in particular, if the time to solution on a quantum processor for a real-world problem instance can be achieved (i.e. sufficiently short), which would make this approach practically valuable.

If improved versions of this method and associated hardware developments can be achieved, this approach could be applied to a wide variety of valuable applications in healthcare and other sectors.

References

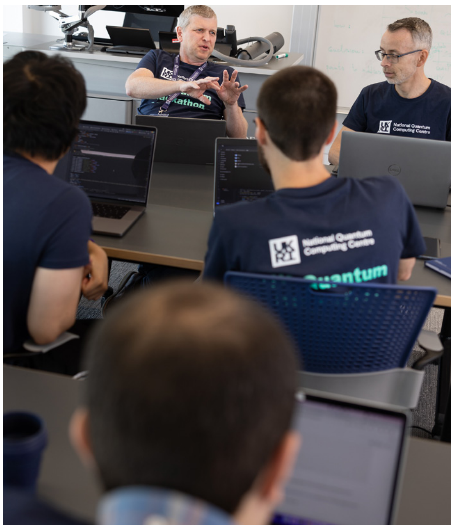
A. Lucas, "Ising formulations of many NP problems," arXiv, 1302.5843v3, 2013.
E. Farhi, J. Goldstone and S. Gutmann "A Quantum Approximate Optimization Algorithm," arXiv, 1411.4028v1, 2014.
A. Peruzzo et al., "A variational eigenvalue solver on a photonic quantum processor," Nature Communications, vol. 5, no. 4213, 2014.

Discussion

The solutions the teams developed throughout the hackathon highlight both the potential and current limitations of quantum computing technology. Taking into account the short timescale that this type of event imposes by design, some impressive progress was made on many of the real-world problems that were posed. One particular theme that emerged was the usefulness of quantum annealers in the current quantum hardware landscape. Many of the use cases fell into the domain of optimisation problems, which map well to this annealing hardware. In the case of optimisation problems, we saw many teams turn to the D-Wave hardware once they had formulated a QUBO problem. These are combinatorial optimisation problems, where a binary vector is minimised with respect to a set function, and are particularly useful when solving problems where a large number of binary decisions have to be made. Others found success in hybrid algorithms, and there were early indications of quantum advantage through emulation or small-scale toy problems that could be scaled if given more time. In their final presentations, all teams demonstrated that they had engaged with the REQC aspects of their solution development.

The event highlighted that quantum computing technology is still in its early stages. However, we have also shown that bringing people together through the hackathon process can accelerate progress on real-world problems. Many teams proposed promising next steps for future work, that could be pursued to improve the work they started during the hackathon. The fact that such a broad range of sectors and hardware options can be brought together in a single event, demonstrates both the interest and importance of quantum computing as a tool for innovation and research.

Alongside the technical outcomes that the teams produced, the hackathon was intended to provide a networking and skills development environment for participants. Feedback indicated that developers, end-users, and technology providers found the hackathon valuable as a way of connecting with the quantum computing community in the UK, as well as being able to make progress on their solutions (please see Table 1). While some end-user organisations were already heavily engaged with quantum computing applications development, others found that the hackathon provided a new perspective on both the opportunities of the technology in their sector, as well as its current limitations in terms of the progress of the technological development and the skills required to develop quantum applications.



Participants from the UK Quantum Hackathon 2023.

Conclusion

The NQCC's 2023 UK Quantum Hackathon emphasised that there is considerable interest in exploring quantum computing use cases across a variety of sectors in the UK. Building on the success of the inaugural UK Quantum Hackathon in 2022, the 2023 event involved a wider range of end-users and quantum providers. In addition to aiding the development of quantum skills and driving responsible innovation, the event provided an ideal networking space. This fostered collaborations between quantum providers and end-users, who may want to further explore the potential of quantum computing in their respective sectors. The teams demonstrated that quantum computing continues to be a promising technology for solving challenging problems. In particular, the quantum annealer showed promising results for optimisation problems across different sectors, indicating that near-term future exploration of optimisation problems may yield useful results. In the future, it would be beneficial to find a balance between a time-limited event that provides the energy to cultivate innovation, and an event with enough time for participants to make satisfying progress on their use case solutions.

The objectives for the hackathon laid out at the beginning of this report were to:

1. Investigate quantum solutions for industry-provided use case problems across different sectors and application domains such as optimisation, simulation and machine learning.
2. Create an active quantum computing community spanning the full value chain from quantum compute providers, through to quantum developers and end-users.
3. Enhance connectivity between quantum computing providers and end-users, enabling discussions on both opportunities and limitations of current technology.
4. To increase awareness of quantum computing and potential use cases to research students and early-career scientists (Masters, PhD and Postdoctoral level).

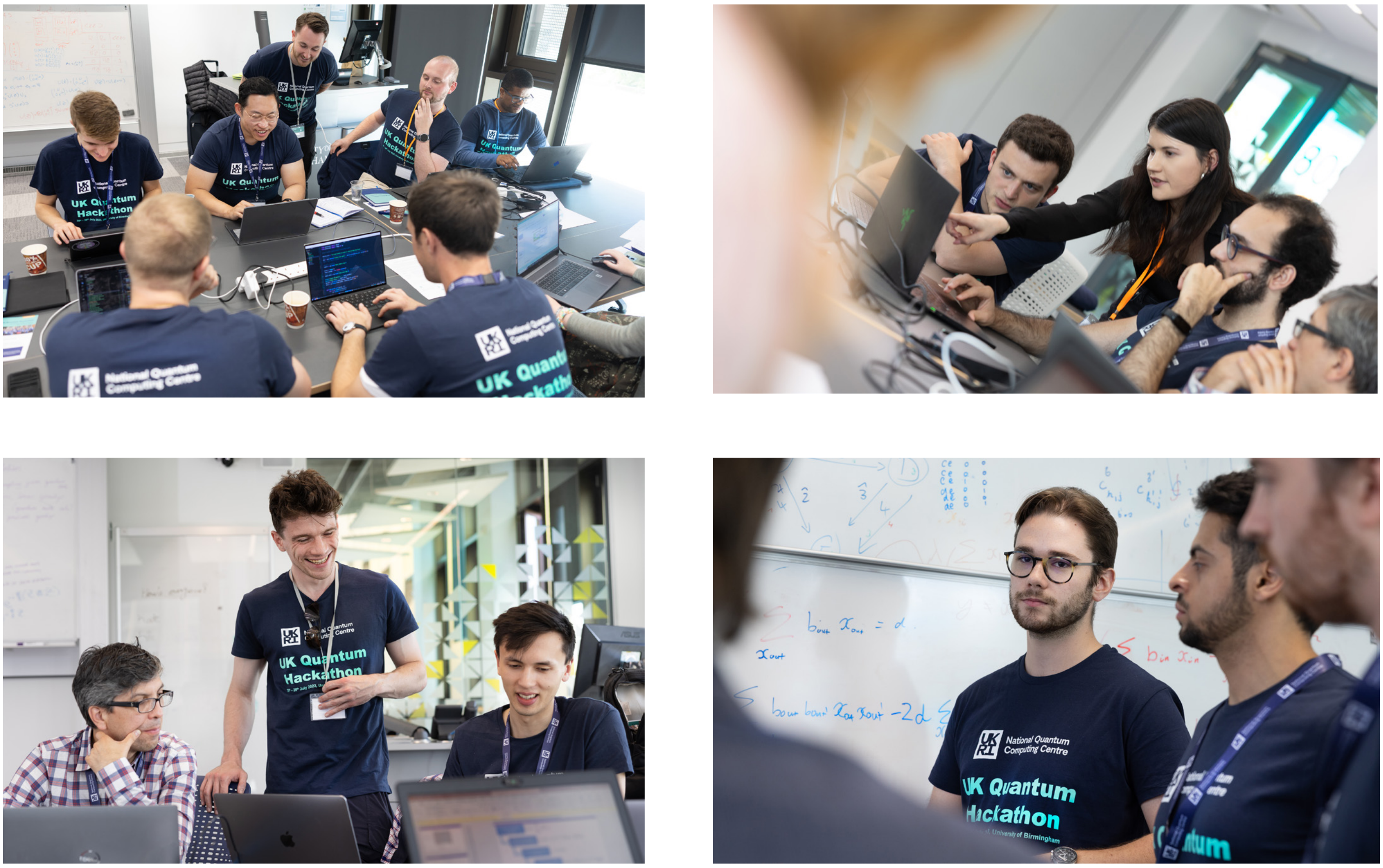
The inclusion of ten use cases across five industrial sectors, representing a range of application domains, allowed participants to explore solutions to a variety of use case problems. Many of these yielded promising results and enabled future development of their solutions after the hackathon itself. Through the results reported by each team, we have been able to test the limits of a range of quantum computing technologies for different types of problems, providing a clear idea of the opportunities and current limits of quantum computing. The nature of the event enabled the UK quantum community to come together, from technology providers through to quantum developers and end-users, and this networking aspect of the hackathon created a vibrant atmosphere that facilitated discussions and collaborations between various parties. Feedback from early-career researchers and end-users who participated in the hackathon indicated that they had acquired new skills and knowledge in quantum computing. The event enabled an exploration of the potential of quantum computing use cases in an intensive environment, which accelerated the development of the teams' solutions and highlighted some of the current limitations of the technology.

Overall, the NQCC's UK Quantum Hackathon 2023 met its objectives and delivered a vibrant event. The participants benefitted from increased knowledge and skills, new collaborations, meeting new potential employers/employees, exploring the limits of current technology, and considering the broader impact of quantum computing on society.

Glossary: Acronyms

AWS	Amazon Web Services
BT	British Telecom
CQM	Constrained Quadratic Model
CVQLS	Coherent Variational Quantum Linear Solver
EPSRC	Engineering and Physical Sciences Research Council
FEA	Finite Element Analysis
HHL	Harrow-Hassidim-Loyd algorithm
HPC	High-Performance Computing
IBMQ	IBM Quantum
LSTM	Long Short-Term Memory
MC	Monte Carlo
MIP	Mixed Integer Programming
NHS	National Health Service
NISQ	Noisy Intermediate Scale Quantum
NP	Nondeterministic polynomial time
NQCC	National Quantum Computing Centre
OQC	Oxford Quantum Circuits
PINNS	Physics-Informed Neural Networks
QAE	Quantum Amplitude Estimation
QAOA	Quantum Approximate Optimisation Algorithm
QASM	Quantum Assembly Language
QPU	Quantum Processing Unit
QSVT	Quantum Singular Value Transformation
QUBO	Quadratic Unconstrained Binary Optimisation
SDK	Software Development Kit
STFC	Science and Technology Facilities Council
UC	Unit Commitment
UKAEA	UK Atomic Energy Authority
VQE	Variational Quantum Eigensolver
VRP	Vehicle Routing Problem
VRP-TWSS	Vehicle Routing Problem with Time Window and Skill Set constraints

National Quantum Computing Centre



Participants from the UK Quantum Hackathon 2023.

UK Quantum Hackathon 2024

We are pleased to announce the dates and venue of our UK Quantum Hackathon 2024. This year the event will be held over three days starting 22nd of July 2024 at the University of Warwick. We expect over 80 hackers to particiapte in the event.

For more information, please get in touch with us:

National Quantum Computing Centre
RAL, Harwell Campus, Didcot, Oxfordshire
OX11 0QX

hackathon@nqcc.ac.uk
nqcc.ac.uk

Follow us on LinkedIn here.

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For more information, email nqccinfo@nqcc.ac.uk

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