Cambridge Quantum

SHIFT THE PARADIGM WITH Quantum Algorithms

(qa)^CQ

COMPUTER PROGRAMMING IS AN ART FORM, like the creation of poetry or music.

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Computer Scientist and Mathematician

Introduction to quantum algorithms

The fundamental ability of quantum mechanics to solve some well-defined computational problems substantially more quickly than can possibly be done on a conventional 'classical' computer was the original motivation behind the conceptualisation of the quantum computer. We are the heirs to this original vision, and our goal is to realise a definitive and unequivocal quantum computational advantage as soon as possible – this motivates everything we do.

Although we are ultimately interested in all quantum algorithms, at present we have identified three problems which show particular promise for early quantum advantage:

1. Monte Carlo estimation
2. Optimisation
3. Solving Partial Differential Equations (PDEs)

	Monte Carlo Estimation	Optimisation	Solving PDEs
Classical Challenge	Computationally resource-intensive, especially when seeking high levels of precision	Classically intractable, exponentially scaling problems where marginally better solutions can result in significant savings	Computationally resource-intensive leading to system and problem simplification
Quantum Promise	Well-known theoretical quantum speedups	Novel quantum heuristics display advantage	Quantum-inspired and pure-quantum approaches can provide exponential speedups
Practical Implementations	Practical realisation on today's NISQ-devices through proprietary Cambridge Quantum algorithms	Practical realisation and favourable resource scaling through proprietary Cambridge Quantum algorithms	Methods pioneered by Cambridge Quantum researchers can accurately simulate both simple and complex, turbulent systems
Industrial Applications	Applied to real-world risk modeling and financial use cases	Optimisation of manufacturing plan design, supply chains, and logistics networks, transportation routes	Widely applicable for some of industry's most prized challenges such as fluid dynamics, Li-ion transport in battery cells, and reservoir modeling

Our work

Quantum computing requires a paradigm shift in thinking and approach to problem-solving starting from fundamental research, innovation, and cross-functional collaboration. Our goal is to bring this research to market, demonstrate business impact, and realise long-term value creation for our partners and clients by deploying quantum algorithms to solve real, industrial problems.

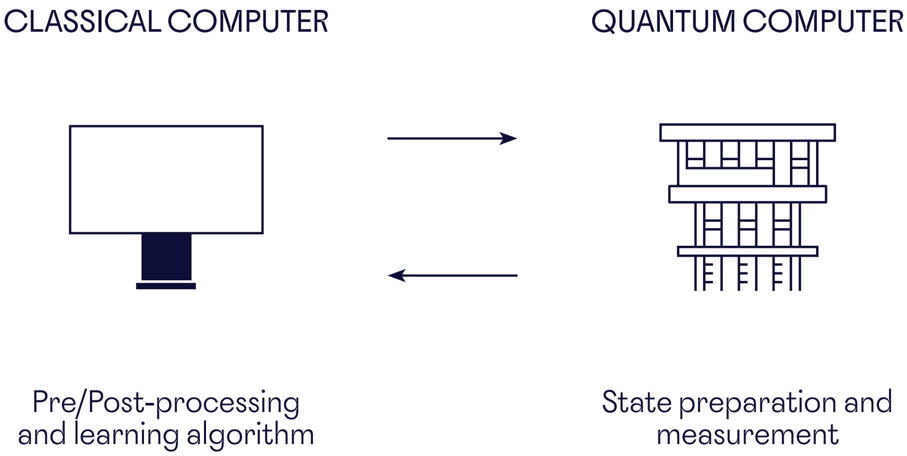
Novel science, applied research with industry partners, and real-world deployment

Our approach

We take a broad approach, from novel quantum algorithm design, to partnering with clients to tailor our best-in-class quantum solutions to problems relevant to their business through to generalising, optimising and efficiently implementing our state-of-the-art quantum algorithms with a view to productisation and real-world deployment.

CAMBRIDGE QUANTUM’S APPROACH

Blue Sky Science ⟷ Applied Research ⟷ Productisation and Deployment



We are obssessed with creating the best performing quantum algorithms for near-term quantum computers

Our outlook

Our over-arching philosophy in all of this is that 'time is of the essence' – quantum coherence is a precious commodity, a near-term quantum algorithm can be thought of as a clock ticking down to decoherence, and if we are to realise a useful quantum advantage then we must make the most of this narrow window of opportunity, we simply cannot afford to waste a single quantum operation. Thus, our research usually involves a forensic deconstruction of any quantum algorithm – identifying exactly where the quantum advantage lies, and ruthlessly eliminating all else. This involves 'handing off' any operations that can be computed classically to the classical computer.

To further expedite our path to quantum advantage, we couple all of our algorithm design and discovery efforts with that of our compilation and error mitigation work – running all of our circuits on our open source software development platform – TKET. Our TKET tool-set provides state-of-the-art circuit compilation across architectures and is integrated with our QERMIT error mitigation tool – enabling us to extract maximal value from Noisy-Intermediate-Scale-Quantum (NISQ) hardware.

MONTE CARLO ESTIMATION

Monte Carlo estimation is, at heart, a very simple algorithm consisting of three steps. Firstly it samples from some probability distribution to generate input values. Secondly, it performs some deterministic computation on the input values and, lastly, averages the results.

What is Monte Carlo estimation?

Monte Carlo estimation is, at heart, a very simple algorithm with three steps:

1. Sample from some probability distribution to generate some input values
2. Perform some deterministic computation on the input values
3. Average the results

Where is it used?

If we cannot mathematically compute some expectation, then we just sample and average – the core concept of Monte Carlo estimation.

For example, a roll of a (fair) dice is an example of sampling from a uniform distribution between 1 ... 6. In a Monte Carlo estimation, we simply roll the dice a number of times, and average the outcomes to obtain the expected value of a dice roll – in fact, the name 'Monte Carlo' itself comes from the dice games of the famous Casino. The more times you roll the dice, the more precise your expectation value will be.

Elaborations of the same essential process are incredibly widespread in myriad business, financial and scientific applications: whenever a decision must be made in the face of uncertainty, the chances are that Monte Carlo estimation is being deployed under the hood, to make the best possible choice.

Broadly speaking, Monte Carlo estimation can inform us of our current risk exposure and can help forecast likely future events – allowing us to optimise plans and analytically drive decision-making.

Classical limitations – and quantum solution

Unfortunately, Monte Carlo estimation is an incredibly resource-heavy computational process – especially when seeking precise expectation values. Classically, in order to increase precision levels by an order of magnitude, one must perform 100x as many Monte Carlo simulations.

This is where quantum computing comes in. There is a guaranteed quadratic quantum advantage in principle. Our Fourier QMCI algorithm[1] means that this advantage will be realised in practice in the very near future.

1 Dr. Steven Herbert
https://arxiv.org/abs/2105.09100
2021

Solving practical challenges

However, until recently there were numerous gaps and inefficiencies in how to do this in practice. Let's take a look at how we have resolved all of these.

State preparation

To perform Quantum Monte Carlo Integration, one cannot simply sample from a probability distribution but must instead prepare a quantum state that encodes the samples. We have shown how such a state can always be constructed without additional circuit complexity[2] – before this paper it was only conjectured that this was possible.

Expensive arithmetic quantum sub-circuits

At the heart of our approach to quantum Monte Carlo integration is our Fourier QMCI algorithm[3]. Fourier QMCI resolves the problem of needing to perform expensive quantum arithmetic on quantum computers by decomposing any function into a sum of functions that can be efficiently computed on today's devices.

Noise resilience

Quantum Amplitude Estimation (QAE) can be used in place of classical averaging which gives rise to the quadratic advantage. However, it assumes a noiseless model of quantum computer – unrealistic for near-term hardware. We have developed a Noise-Aware QAE algorithm which allows us to adjust the amplitude estimate to account for the inclement noise[4], and still obtain a quantum advantage if the noise is sufficiently mitigated.

Implementation for current hardware

We have conceived a novel approach to Quantum Amplitude Estimation to Monte Carlo Integration[5] which approximates the QAE sub-circuits to tolerate noise levels prevalent in today's devices.

2 Dr. Steven Herbert *https://arxiv.org/abs/2109.04842* 2021.

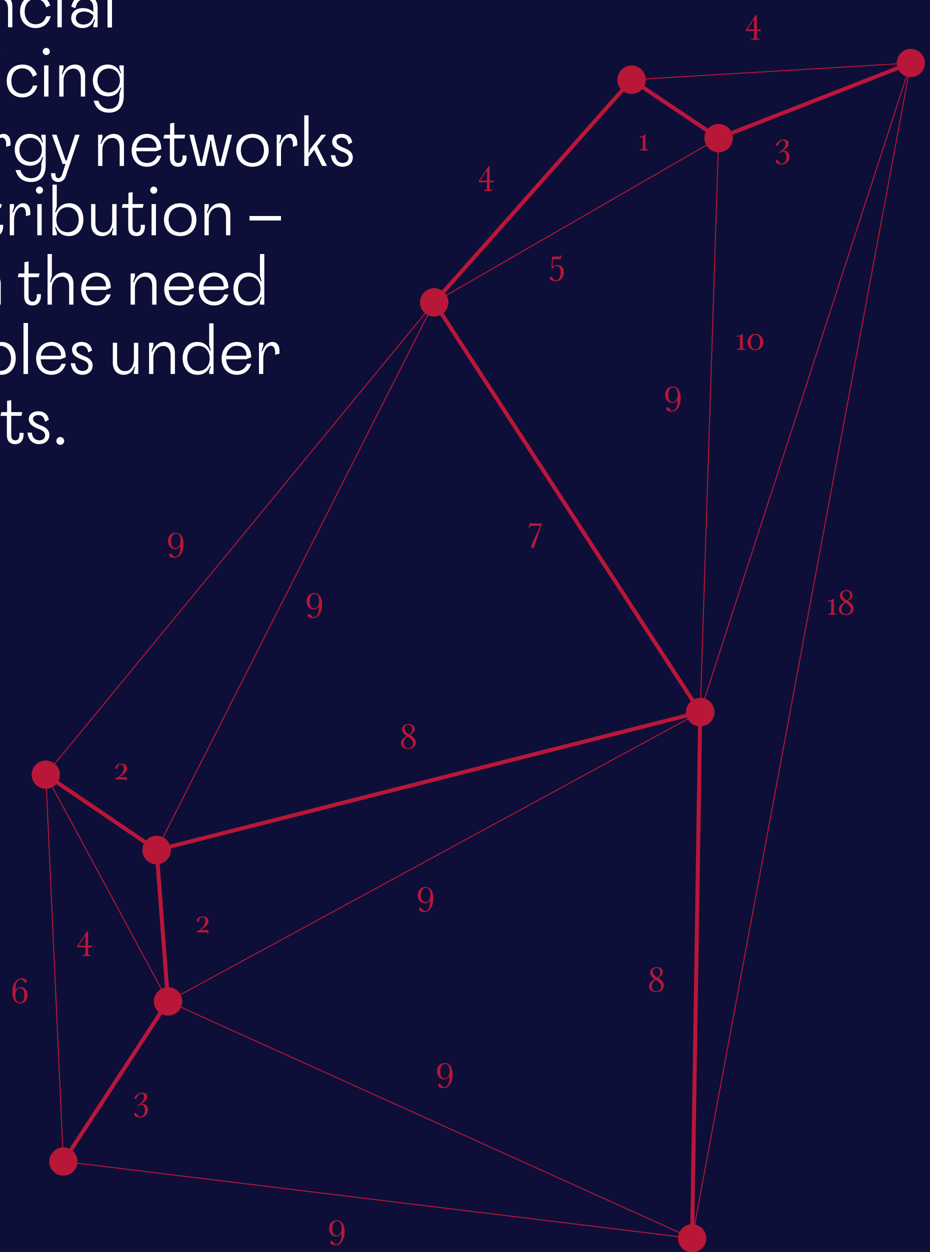
3 Dr. Steven Herbert *https://arxiv.org/abs/2105.09100* 2021

4 Herbert et al *https://arxiv.org/abs/2109.04840* 2021.

5 Plekhanov et al *https://arxiv.org/abs/2109.03687* 2021.

OPTIMISATION

Another example of a computationally hard task is combinatorial optimisation. Such optimisation problems are found at the heart of virtually every industry and sector. From logistics and supply chains to chemical processes and materials design, from financial portfolios and pricing strategies to energy networks and resource distribution – these all deal with the need to optimise variables under certain constraints.



Combinatorial optimisation

6 Amaro et al
https://arxiv.org/abs/2106.10055
2021.

7 Benedetti et al
https://journals.aps.org/prresearch/abstract/10.1103/PhysRevResearch.3.033083
2021

8 Amaro et al
https://arxiv.org/abs/2109.03745
2021.

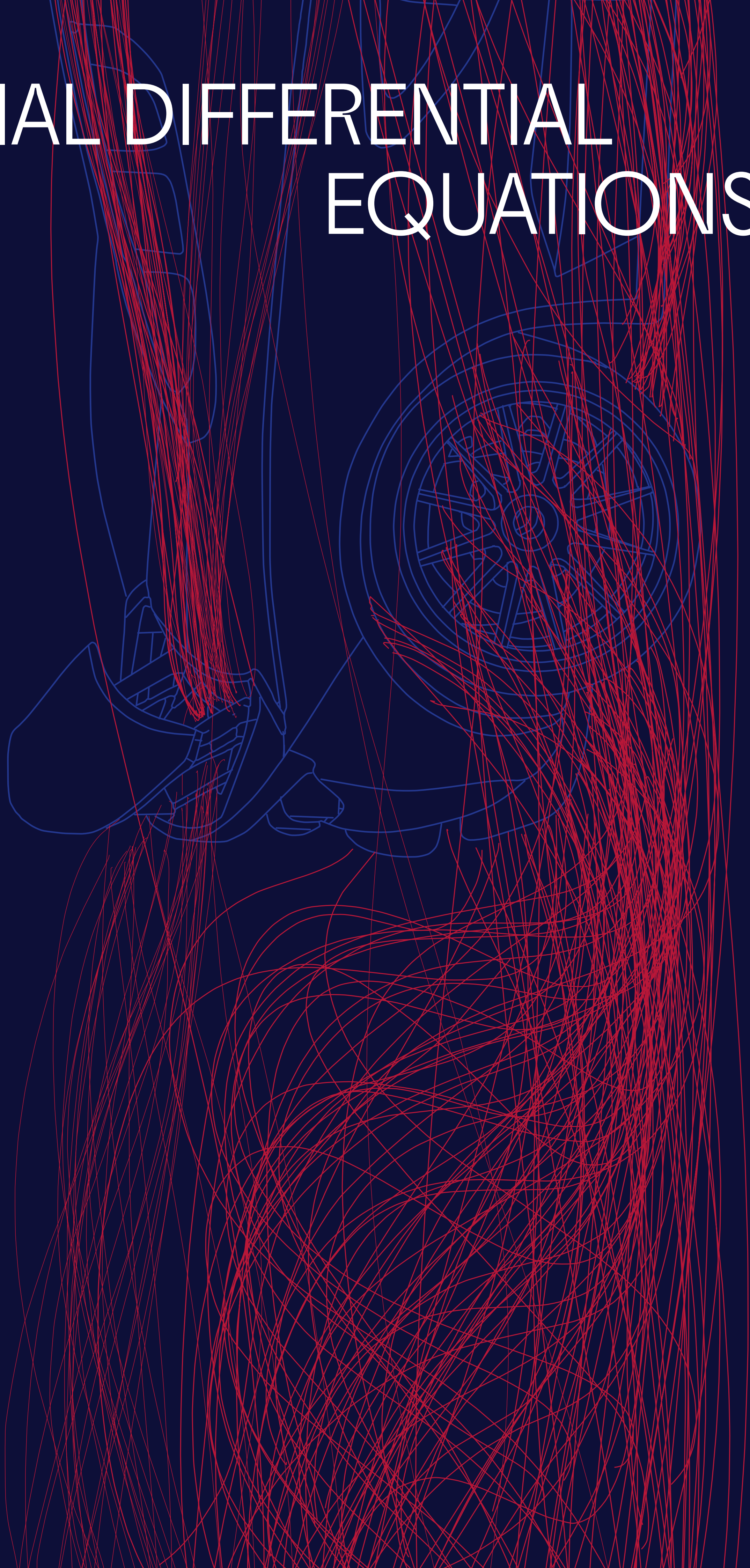
The major challenge associated with combinatorial optimisation is that problem sizes scale exponentially – and even factorially – with the number of independent variables. For example, the well-known Traveling Salesman Problem – where one determines the shortest possible route via multiple cities – is notoriously difficult: even with just ten cities there are 362,880 possible combinations. By the time you have 25 cities, there are 620,448,401,733,239,439,360,000 (6.20×10^{23}) possible combinations. Solving combinatorial and discrete optimisation problems is hard (and often intractable) for classical computers and so today, practitioners commonly employ heuristics to yield approximate solutions.

We focus on combinatorial and discrete optimisation problems. The exponential scaling of the solution space makes these problems computationally intractable. Therefore, solving them requires the use of heuristics – both on classical and quantum computers. In industry, many of these combinatorial optimisation problems are directly tied to the economics of business operations. Due to the huge impact of good quality solutions in industry, better heuristics could translate to significant resource and economic savings.

Our team develops quantum-based heuristics enabling fast and accurate convergence to optimal solutions on real quantum computers (Filtering Variational Quantum Eigensolver (F-VQE))[6]. We have innovated methods, such as casual cones[7], to scale up those heuristics, paving the way for solving problems of realistic sizes and practical relevance on quantum computers with limited quantum resources. Using these methods, the team was able to perform some of the largest combinatorial optimisation experiments on gate-based quantum computers with up to 23 qubits[8].

In addition, we develop meta-heuristics for optimisation problems where the cost function itself is either too expensive to evaluate or requires averaging over uncertain factors. Quantum machine learning methods such as variational inference can be used as a meta-heuristic to guide a classical model or optimisation procedure, while Quantum Monte Carlo estimation can be used to speed up cost function evaluation over uncertain factors.

PARTIAL DIFFERENTIAL EQUATIONS



Partial Differential Equations the backbone of science and technology

Another highly promising application of quantum computing is in solving partial differential equations (PDEs). PDEs, in essence, describe the relationships and interdependencies between variables – and how a change in one variable may impact another. Essentially, all fundamental laws of physics are expressed in terms of PDEs. As such, PDEs are ubiquitous in all areas of science and technology and are applicable to a wide set of problems including fluid dynamics, electrodynamics, electrostatics, heat transfer, elasticity, and many others.

Solving PDEs is often extremely computationally expensive and requires large HPC clusters. This often leads to the simplification of PDEs, for example, solving them on small subsets of larger systems. This computational limitation is often manifested in the small number of grid points that can be simulated using Finite Difference Methods. Here at Cambridge Quantum we have pioneered the use of quantum methods based on parameterised quantum circuits (PQCs).

Quantum methods for simulating complex, turbulent systems

Quantum algorithms are known to provide an exponential speedup in solving linear PDEs. For nonlinear PDEs, quantum approaches based on parameterised quantum circuits can be exponentially more efficient than classical approaches, potentially also for turbulent systems[9].

Quantum approaches hold two advantages:

1. they can offer exponential compression and scaling in the number of grid points that can be simulated
2. they can greatly reduce the number of parameters required to solve nonlinear PDEs.

Researchers at Cambridge Quantum have shown how these quantum methods can solve the nonlinear Schrödinger equation exponentially more efficiently than classical MPS methods[10] – using only 13 qubits – requiring only half as many parameters. It follows that quantum approaches would be well suited for tackling many types of PDE problems and today we apply such approaches to tackle industry's most prized challenges – including the simulation of lithium-ion battery cells and full waveform inversion for seismic imaging.

9 Gourianov et al *https://arxiv.org/abs/2106.05782* 2021.

10 Lubasch et al *https://arxiv.org/abs/1907.09032* 2019

Applications of quantum algorithms

Finance	– Pricing of exotic (path-dependent) options – Other derivatives, including TARF – VAR/CVAR calculations – CVA/XVA/other risk-adjusted derivative pricing – Portfolio optimisation with discrete allocations
Pharmaceuticals and Healthcare	– Meta-heuristics for faster biomarker discovery in drug development based on quantum circuit Born machines – Allocation of healthcare resources e.g. scheduling of medical staff, organ donor matching, radiation plans
Energy	– Solving Burgers and Navier-stokes equations with quantum PDE solvers – Seismic imaging using a quantum PDE solver for the wave equation – Residual statics estimation with quantum optimisation heuristics
Logisitics and Manufacturing	– Cargo loading optimisation with the quantum and / or quantum enhanced optimisation – Manufacturing process optimisation in plants and factories – Route and scheduling optimisation – Supply chain optimisation
Materials and Chemistry	– Multi-scale simulations of batteries – Process and yield optimisation in production – Simulating heat transfer, mass transfer and convection in chemical production

MANUFACTURING

Nippon Steel Corp.
Manufacturing process in optimisation in steel plants

Cambridge Quantum has pioneered a quantum-based heuristic for combinatorial optimisation using NISQ devices[11]. Together with Nippon Steel Corp. our team applied this algorithm to optimise a manufacturing process typical in a steel plant[12].

11 Amaro et al *https://arxiv.org/abs/2106.10055* 2021.

12 Kirsopp et al *https://arxiv.org/abs/2110.08163* 2021

TRANSPORTATION

A Global Top 3 Railway Service Provider
Train timetabling

Cambridge Quantum and one of the world's largest railway service providers, develop mathematical models and innovative quantum algorithms to pave the way to faster and greener transportation networks.

MATERIAL SIMULATION AND CHEMISTRY

German Aerospace Center (DLR)
Multiscale battery simulation

Cambridge Quantum and DLR research better simulation models for battery development to aid future energy utilisation. Cambridge Quantum's quantum algorithms are enabling the simulation of lithium-ion battery cells.

WHY GET STARTED WITH QA TODAY?

The computational advantages offered – typically 'quadratic' or 'exponential' – are rooted in the theory of computational complexity, and arise from the fundamental possibility of quantum states to exist, and therefore compute, in superposition. This theoretical advantage will be seen in practice in the foreseeable future, and organisations who engage early will be best-placed to reap the benefits.

With an explosion of pedagogical material and open-source software, there has never been a better time for researchers and other technically-minded people to take the plunge, and explore the advantages that quantum computing can bring in the problems that they face day-to-day.

CONTACT US

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Cambridge Quantum

We set out our vision to positively transform the world using the power of quantum computing back in 2014. Today, we are recognised as one of the foremost quantum computing companies, delivering science-led, enterprise-driven solutions to tackle hard problems across a diverse range of industries.

Cambridge Quantum designs, engineers and deploys algorithms and enterprise application libraries, translating cutting-edge research into industry leading technologies through a product-centric focus. TKET, our hardware-agnostic software development platform, and other technologies are currently utilised by an expansive and ever-growing user base.

The team at Cambridge Quantum has been developing the theoretical foundations of quantum computing for over 25 years, forging ahead with breakthroughs in the fields of quantum chemistry, quantum artificial intelligence, quantum cybersecurity and quantum algorithms.

At present, we have the deepest roster of researchers, developers and engineers, working to democratise quantum computation and realise the benefits for the greatest possible number of people.

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