Efficient QUantum ALgorithms for IndusTrY

WP6 Impact Creation

D6.6 Roadmap towards Quantum Advantage

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Document description	This deliverable presents an overview of five principal technologies, developed by EQUALITY consortium. It highlights the progress made by the consortium,

[1] R: Document, report (excluding the periodic and final reports); DEM: Demonstrator, pilot, prototype, plan designs; DEC: Websites, patents filing, press & media actions, videos, etc.; DATA: Data sets, microdata, etc.; DMP: Data management plan; ETHICS: Deliverables related to ethics issues.; SECURITY: Deliverables related to security issues; OTHER: Software, technical diagram, algorithms, models, etc.

[2] PU – Public, fully open, e.g. web (Deliverables flagged as public will be automatically published in CORDIS project's page); SEN – Sensitive, limited under the conditions of the Grant Agreement; Classified R-UE/EU-R – EU RESTRICTED under the Commission Decision No2015/444; Classified C-UE/EU-C – EU CONFIDENTIAL under the Commission Decision No2015/444; Classified S-UE/EU-S – EU SECRET under the Commission Decision No2015/444

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Abstract

A quantum revolution is unfolding, and European scientists are on the lead. Now, it is time to take decisive action and transform our scientific potential into a competitive advantage. Achieving this goal will be critical to ensuring Europe's technological sovereignty in the coming decades.

EQUALITY brings together scientists, innovators, and prominent industrial players with the mission of developing cutting-edge quantum algorithms to solve strategic industrial problems. The consortium develops a set of algorithmic primitives which could be used as modules for various industry-specific workflows. These primitives include differential equation solvers, material simulation algorithms, quantum optimisers, etc.

To focus our efforts, we target eight paradigmatic industrial problems. These problems are likely to yield to early quantum advantage and pertain to the aerospace and energy storage industries. They include airfoil aerodynamics, battery and fuel cell design, space mission optimisation, etc. Our goal is to develop quantum algorithms for real industrial problems using real quantum hardware. This requires grappling with the limitations of present-day quantum hardware. Thus, we devote a large portion of our efforts to developing strategies for optimal hardware exploitation. These low-level implementations account for the effects of noise and topology and optimise algorithms to run on limited hardware.

EQUALITY builds synergies with Quantum Flagship projects and Europe's thriving ecosystem of quantum start-ups. Use cases are being tested on quantum hardware from Europe's leading vendors and HPC centres. The applications targeted have the potential of creating billions of euros for end-users and technology providers over the coming decades. With EQUALITY, we aim at playing a role in unlocking this value and placing Europe at the centre of this development. The project gathers 8 partners and has a budget of €6M over 3 years.

Consortium

The EQUALITY consortium members are listed below.

Legal Name on Grant Agreement	Short name	Country
CAPGEMINI DEUTSCHLAND GMBH	CAP	DE
DA VINCI LABS	DVL	FR
AIRBUS OPERATIONS GMBH	AOG	DE
DEUTSCHES ZENTRUM FUR LUFT - UND RAUMFAHRT EV (DLR)	DLR	DE
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Table of Contents

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List of Abbreviations

CASSCF	Complete Active Space Self-Consistent Field
CFD	Computational Fluid Dynamics
CNOT	Controlled-NOT gate
CZ	Controlled-Z gate
DFT	Density Functional Theory
DQC	Differentiable Quantum Circuits
FCI	Full Configuration Interaction
FEM	Finite-Element Modelling
FTQC	Fault-Tolerant Quantum Computer
HF	Hartree-Fock
HPC	High-Performance Computing
MVP	Minimal Viable Product
NISQ	Noisy Intermediate-Scale Quantum
NP-hard	Non-deterministic Polynomial-hard problem (complexity class)
NUFFT	Non-Uniform Fast Fourier Transform
PDE	Partial Differential Equations
PINN	Physics-Informed Neural Networks
QEM	Quantum Error Mitigation
QPE	Quantum Phase Estimation
QM/QM	Quantum Mechanical / Quantum Mechanical (embedding scheme)
QPU	Quantum Processing Unit
QUBO	Quadratic Unconstrained Binary Optimisation
SWAP	SWAP gate
TFIM	Transverse Field Ising Model
TRL	Technology Readiness Level
UCCD	Unitary Coupled Cluster Doubles
UCCSD	Unitary Coupled Cluster Singles and Doubles
VQE	Variational Quantum Eigensolver

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Executive Summary

This document is a deliverable of the EQUALITY project, funded under grant agreement number 101080142.

This deliverable, D6.6 Roadmap towards Quantum Advantage, is part of work package, WP6 Impact Creation, aimed to present the updates on the core technologies, developed within the Equality project. It highlights the main advancements to the technologies within the project, provides scientific perspective on further development, and industrial outlook on their anticipated utilisation.

This document is related to the previous deliverable **D6.5** "Market analysis, business model and upscaling" of Equality Project [1], presenting the update to the initial exploitation plan, taking into account the changes of technological and economic landscapes during the runtime of the project, as well as the to-date development course and status of the corresponding technologies.

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1 Technology - Differential Equation Solvers

1.1 Technical Overview

Solving large systems of Partial Differential Equations (PDEs) is met across different industries, Computational Fluid Dynamics being one of them. Finite-Element Modelling (FEM) methods used nowadays are highly evolved and can tackle problems of impressive size in practical time: simulations containing up to 50 million voxels at a time are routinely faced in aerodynamic industry.

However at such scale current approaches to FEM already demonstrate their limitations: with either solution quality, or runtime: today's largest models take multiple days to prepare and run for weeks after that. This typically happens with problems, where multi-scale dynamics needs to be represented realistically, like for example where the airflow meets sharp edges or non-spline surfaces, forming turbulence, etc. To advance the domain and its products further - development of new types of PDE solvers is instrumental.

Concept of Physics-Informed Neural Networks (PINNs) has been suggested [2] , and as the domain of Machine Learning has shown dramatic progress in the recent years - PINNs present substantial interest as a potential way to improve PDE solvers. Recently, researchers suggested a Quantum counterpart of PINNs in form of Differentiable Quantum Circuits (DQC) [3], [4] . Project partner Pasqal has developed the concept further within the Equality project.

The concept is based on defining a parameterised quantum circuit, structured in a special way to represent the analytical differentiation using phase shift rule. A schematic diagram is shown in Figure 1, from [5]. Initial quantum state represents an embedding of input data (parameters of equation, its initial and boundary conditions, etc), projected over a basis set of functions. The circuit is then trained (in either a supervised way - then the concept is known as Quantum Circuit Learning, or in unsupervised way - known as DQC itself), such that its output would approximate the solution of desired differential equation in the given basis. In the unsupervised case, training loss function is sophisticated, as it has to precisely account for the core properties of the solution, like conservation laws, boundary conditions, etc. Correct formulation of the loss function to a high degree defines the success of the approach.

The main benefit this approach offers is that each of the basis set functions (a Fourier Frequency, for example) is encoded using a single qubit. This defines modest demands on the quantum hardware scale and suggests better performance at simulating multi-scale phenomena.Together with the analytic nature of output, such encoding is also expected to offer better scaling to larger simulation domains. The assumption is that differentiable quantum circuits, which leverage entanglement to represent complex states, can be trained using parameter shift rules to solve problems defined by differential equations and their boundary conditions. Success in this area is expected to allow for a more efficient and accurate modelling of complex, multi-scale dynamics than is possible with classical computers.

The research within Equality project has focused on further improving the method of DQC and testing it in the industrially-relevant use-cases in the domains of Aerodynamics and Electrochemistry. Project partner Pasqal has realised the approach in its open-source software package Qadence: [6],[7], [8] and developed a production-grade API for online access to its in-house state-of-the-art realisation of the algorithms, to allow researchers experiment with the performance of the DQC routines . Together with the researchers from Airbus and DLR working on the use-cases of Computational Fluid Dynamics and Electrochemical Modelling respectively, the DQC algorithms were tested and fine-tuned to best perform for the industry-relevant context. Researchers explored different feature maps for embedding the problem structure into

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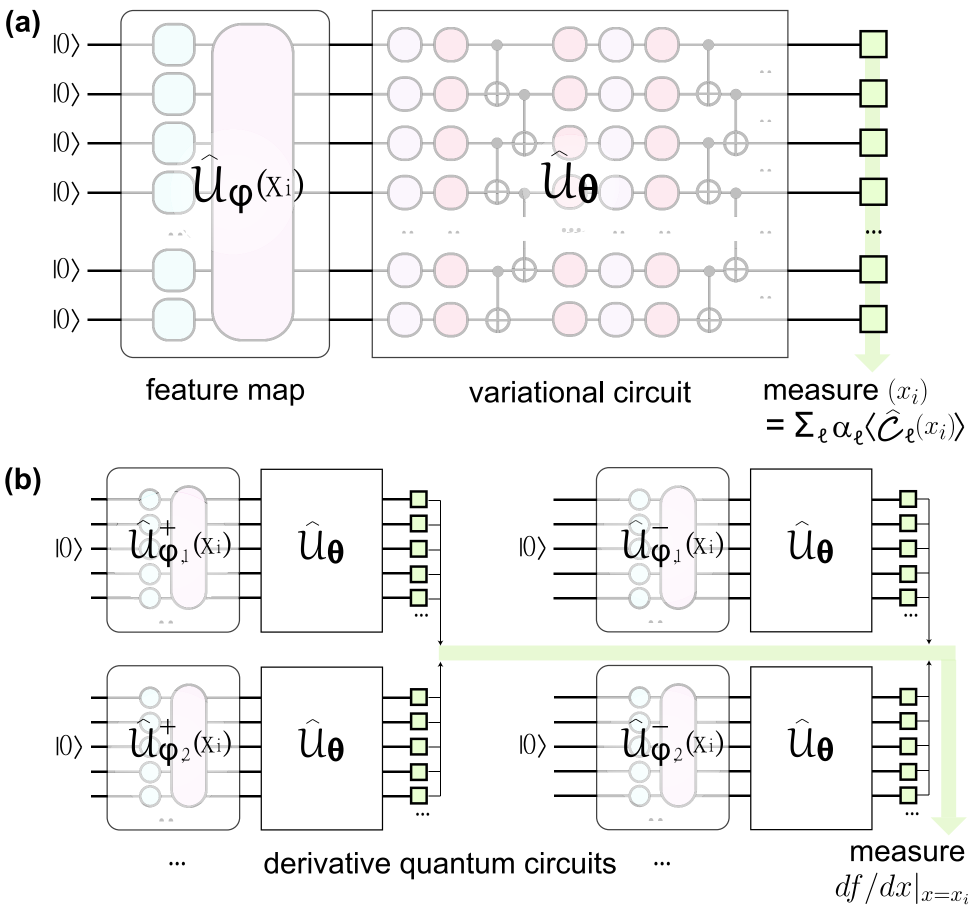

Figure 1: **Differentiable quantum circuits.** (a) Quantum circuit used for encoding the value of a function at a specific value of the variable $x = x_i$. The circuit consists of a feature map $\hat{U}_\varphi$ that encodes the x-dependence, followed by variational ansatz $\hat{U}_\theta$, and an observable-based readout for the set of operators $\hat{C}_\ell$. The measurement result is classically post-processed to provide a quantum function representation $f_\theta(x)$ as a sum of expectations. To compose the loss function circuit measurements for different points of optimisation grid $\{x_j\}_j$ are required. (b) Derivative of the sought function $f_\theta(x)$ evaluated at specific point $x = x_i$ is estimated as a sum of expectations for derivative quantum circuits. Graphics from [5], by Pasqal

quantum circuit, such as Chebyshev Polynomials or Fourier Feature Maps, and demonstrated that choice of this basis is crucial for the success of the whole approach. They also explored how the definition of loss functions, boundary conditions and other hyperparamters influences the solution quality. Most importantly, the researchers have explored performance of the algorithm for different PDEs with various ”complexity” (dimension and degree, number of terms and boundary conditions). Performance of the algorithm after fine-tuning for specific problems has been found satisfactory, and most fruitful directions for further research were identified.

From the project findings, researchers could estimate that the main potential of the algorithm lays in its ability to capture complex structure of PDE solutions with modest quantum resource, once suitable basis set is used for embedding. However, as the size and complexity of the problem grows - theoretical exploration becomes more complex, mostly due to emulating quantum computers with classical machines, and training of variational circuits. These two issues are generic for any Quantum Machine Learning approach, and are thus actively explored by the community. Transition to commercially-available hardware, especially that operating in analog mode like the QPUs of Pasqal [6], or ones using error mitigation routines, could facilitate further exploration to some extent. However, in the digital mode at least, the circuits remain too deep to expect practical advantage with near-term hardware.

Future developments of PDE solvers based on Differential Quantum Circuits is interesting as applied, problem-centered research, in synergy between fundamental developments with use-case insights. Specifically, we suggest the next steps being:

- hardware-oriented developments of algorithms, especially tailored to the analog modes of specific QPU types
- exploration of different types of feature embedding maps, better suited to certain equation types
- study of problem-specific variational ansätzen, especially ones aimed at reducing circuit depth and demands on qubit connectivity
- advances in QML foundational algorithms, allowing for more resource-efficient training

All of these would require a substantial amount of research, but would significantly approach first implementations of DQC and similar algorithms at industry-relevant scale. The pipelines explored in this project do not imply the requirement for complete fault-tolerance, which is typical for variational algorithms relying instead on close hybridisation with classical computer and evolved optimisation routines. However, the size of industrially-relevant problems in the domains of Computational Fluid Dynamics and Electrochemistry sets a very high bar in performance for emergent technologies, while classical ML approaches (such as PINNs) present a strong competitor.

1.2 Technology Adoption Roadmap and Impact

From the properties of the algorithm described above, the best problems for exploration would be the complex analytical models, where classical numerical models struggle with convergence due to large span of geometric scales and physical phenomena involved. Analytical insights into the structure of the solutions present substantial benefit to the algorithm, as does the data for reference solutions.

We suggest the most interesting use-cases for such approaches could be found in intricate multi-physical simulations. In the domain of Energy those are found in simulating batteries and fuel cells. In the domain of Aerodynamics such problems can be found in workflows of structural mechanics, thermal analysis, and materials science.

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Explored approach would benefit from findings in the adjacent domains of: hardware-efficient quantum circuits, hybrid HPC-QC techniques, foundational models in QML, as well as from deep insights into the use-case experts as presented by Equality project.

Specific realisations of DQC in Qadence [6] are depending on IP of Pasqal, and reaching best performance in analog mode would require close integration with Pasqal's Neutral Atom QPU.

By end of 2025, explored technology is at the stage of first Demonstrators applied to industrially-relevant problems, but not yet at industry-relevant scale, corresponding to the TRL 5 in European framework. The primary exploitation plan is then centered on internal growth of competence and insights, and further collaborative research. Project partners aim to apply the insights gained from this study to steer own R&D roadmaps in quantum computing. Researchers aim to continue exploring and building upon these findings, aiming to primarily use open-source tools like the Qadence library[6], to deepen the expertise and maintain a leading-edge understanding of the technology's potential.

Once matured and if deployed at scale, the technology could help alleviating computational bottlenecks in numerical modelling pipelines across different domains, resulting in significant advantages for the use-cases: more insights seized from the simulation of complex phenomena and faster time-to-solution. This would unlock countless opportunities across different domains of application. In the Aerospace and Energy domains, this would shrink development cycles and improve product performance. Potentially, quantum simulations could reduce energy footprint of PDE-solving pipelines. From the current state of technology, we could project, that to deliver results of industrial relevance, DQC or the technology stemming from its concept would rely on close hybridisation with classical PDE solvers run on HPC, finding use at the Computing Centres of the end-users, implying the "on-premise" deployment model. Overall, the technology is poised to deliver impact at scale and across domains. However, one shall hold realistic expectations about the timelines of technological readiness, which depend on many factors and pace of research in multiple domains: quantum computing Hardware, quantum Algorithms and classical ML and simulation techniques.

Due to technology being at still low TRL, and reliant on multiple advancements in aforementioned domains, it may significantly change before the MVP stage, in both performance and mode of operation. Therefore, quantitative study of the business-case is not possible at the moment. More general details of the business case could be found in the previous study of Business Models in Deliverable D6.5 of Equality project [1].

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2 Technology - Quantum Chemistry

2.1 Technical overview

The accurate description of the electronic structure of molecules and periodic systems remains even after 100 years of the birth of Quantum Mechanics a challenging task. Computational methods with a balance between accuracy and computational cost, like Density-Functional-Theory (DFT) and Hartree-Fock (HF) show limitations, especially when describing strong electron correlation. On the other hand, more sophisticated methods which go beyond a single Slater-Determinant Ansatz, like complete active space self consistent field (CASSCF) or full configuration interaction (FCI) show unfavourable factorial scaling behaviour with basis set and system size, limiting their application to relatively small systems. Quantum Computing, due to superposition and entanglement, is expected to be especially beneficial where the Hilbert-Space containing the eigenfunctions of the Hamiltonian can be explored using unitary operators acting on a trial state (often the HF state).

Achievements of EQUALITY project

For fault-tolerant quantum computers the Quantum Phase Estimation (QPE) algorithm is expected to give accurate eigenvalues of the Hamiltonian. This is especially important in cases where a classical exact diagonalisation is intractable. However for Noisy Intermediate-Scale Quantum (NISQ) devices often different variations of the Variational Quantum Eigensolver (VQE) algorithm are used to approximate the ground state energy of a system. VQE is a hybrid quantum-classical approach where a parameterised unitary operator is applied to generate a quantum mechanical state from which the expectation value of the Hamiltonian is measured and a classical optimizer proposes new parameters until convergence of energy is reached.

Often a chemically informed Ansatz like Unitary Coupled Cluster restricted to Singles and Doubles excitations (UCCSD) is used to describe the unitary operator. Pasqal implemented the paired-UCCD Ansatz, which allows only for doubly occupied or empty orbitals [9]. In order to emulate digital one- and two-qubit gates on neutral atom hardware, Pasqal developed within Equality a corresponding digital-analog emulation protocol [10] using a sequence of analogue pulses. This protocol has been tested on the hydrogen molecule (H_2) and Lithium Hydride (LiH), where for various basis sets an accuracy within the same order of magnitude as chemical accuracy (1 kcal/mole) could be reached. However where analogue implementation for some gates, e.g. CNOT/CZ is feasible within Rydberg lifetimes (100 μs), for others like SWAP and Givens SWAP this is challenging. This along side the limitations of NISQ-devices lead Pasqal to proceed exploring different algorithms than VQE for periodic and amorphous systems within Equality.

For periodic materials the focus was on Ising- and XY-type hamiltonians to explore quantum magnetism, exotic phases and non-equilibrium dynamics. Pasqal presented a feasibility study to observe E8 symmetry in materials like $CoNb_2O_6$ towards a neutral atom QPU implementation. Pasqal also paved the way for a neutral atom QPU implementation of a hybrid quantum-classical approach to simulate the Fermi-Hubbard model [11]. Furthermore Pasqal described how interacting correlated topological phases can be simulated using neutral atom QPUs.

Within the project time of Equality Pasqal also proposed a way to study amorphous materials on neutral atom QPUs using the the transverse field Ising model (TFIM)[12].

Technological development roadmap

Taking into consideration the always on interaction between Rydberg atoms and challenges of describing digital gates with analogue global pulses, it is important to explore algorithms for quantum chemistry on additional quantum computing hardware types, e.g. superconducting qubits or trapped ions. One of the recently introduced algorithms that is capable of describing static electron correlation occurring, e.g. in bond breaking or transition metal chemistry, is the sampled-based quantum diagonalisation algorithm [13]. Here experiments using up to 77 superconducting qubits are demonstrated. Thinking towards simulation of the electronic Hamiltonian for periodic materials like the perovskites examined in work package four in Equality [14], an embedding scheme allowing to treat different parts of a unit cell on different levels of theory is essential. Various Quantum-Mechanical/Quantum-Mechanical (QM/QM) embedding schemes can be explored following suggestions from classical quantum chemistry, e.g. [15, 16]. The basic underlying idea is to distribute the workload between different levels of theories. Quantum advantage is expected when Quantum Computing resources are used in areas where classical methods, due to the unfavourable scaling behaviour as for example in CASSCF methods, reach their limit. Applying embedding schemes makes it possible to apply quantum computing algorithms on the truly challenging parts where difficult electron-electron interactions need to be accurately described.

2.2 Technology Adoption Roadmap and Impact

Different industrial sectors offer opportunities for optimal use cases, such as Material Science, where accurate simulation of molecular interactions and catalytic processes, including strongly correlated systems, is essential. In the domain of energy storage and transformation where new electrode materials and electrolytes can be examined on different levels of theory to correctly describe material features. For pharmaceutical industry the process of drug discovery can be accelerated using quantum-enhanced molecular modelling. For manufacturing industries and aerospace, better quantitative modelling of corrosion processes could unlock large value in improving products.

However there is strong dependence on the hardware maturity of the quantum computers. Not only is the number of available qubits important, but also the fidelity of the gate operations, decoherence time and read out accuracy. Quantum computing will always be part of a hybrid quantum-classical workflow. Classical computing plays an important role in the storage and duplication of information, as well as in the optimisation of parameters and diagonalisation. Therefore, the overall performance of these systems depends on well-designed hybrid workflows. Another important point is the accessibility of quantum hardware platforms in connection to HPC centres for scalable deployment of hybrid quantum-classical pipelines. An aspect is the importance of middle ware, that is capable of efficiently compiling abstract quantum circuits to hardware efficient circuits.
Currently we are in the NISQ era with devices around 50 - 150 qubits with limited fidelities of the operation gates and error mitigation techniques. However some hardware provider like IBM plan to achieve a large-scale fault-tolerant quantum computer (FTQC) by 2029 [17]. Google, Quantinuum, IonQ and Pasqal plan to achieve FTQC by 2030 [18, 19, 20, 21].

According to global market forecasts, the quantum technology sector is projected to contribute up to **$1 trillion by 2035** [22]. Regional analyses, such as the South Carolina Quantum Corridor initiative, estimate an annual output increase of **$18–32 billion** and productivity gains of **5–7%** in quantum-relevant industries including chemicals, pharmaceuticals, and advanced manufacturing [23].
The socio-economic benefits of quantum technology adoption are equally significant:

- **Sustainability**: Quantum-enhanced materials design can reduce greenhouse gas emissions at gigaton scale, particularly in energy storage and catalysis applications.

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- **Competitiveness**: Early adopters of quantum workflows gain a strategic advantage in innovation cycles, IP generation, and market positioning.

These impacts underscore the importance of coordinated investment in quantum infrastructure, education, and industrial partnerships.

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3 Technology - Optimisation

3.1 Technical Overview

Combinatorial Optimisation has for long been one of the most promising domains of applications predicted for Quantum Computing to excel at. Within Equality, we have focused on one industrial use-case: Optimal Planning of Imaging Satellite mission (further referred as ”Space Mission Optimisation (SMO)” or ”Mission Planning”). The problem presents a challenge for classical solvers, and one of the constraints is time-to-solution: it is crucial to find the best possible solution within a fixed time frame. Furthermore it is desired to make the algorithm even faster to be able to account for new incoming requests of high importance. To deliver the best insights, the research was focused on 3 different optimisation techniques, both classical and quantum. All three algorithms were compared in terms of solution quality, time-to-solution and scaling of both with problem size growth, using two simulated datasets, tailored to best represent the nature of SMO problem in the actual industrial context.

3.1.1 QAOA

The first method applied to this use-case is Quantum Approximate Optimisation Algorithm, or QAOA [24], popular among application researchers in the recent years. The algorithm in its original formulation is a discrete approximation of an Annealing protocol run in finite time on a gate-based Quantum Computer. It operates with a parameterised circuit, composed of a sequence of p pairs of parameterised Unitaries (or ansätze), representing the annealing-like evolution. Each of these ansätze contains two parameters associated with the annealing schedule. Ensemble of these $2p$ parameters is optimised in a variational manner such that the end-circuit measurements deliver minimum to the target cost function (minimal energy of the cost-associated Hamiltonian) formulated as a Quadratic Unconstrained Binary Optimisation problem or QUBO.

Pasqal has developed a routine, specifically tailored to represent QAOA with the Neutral Atom QPUs [25]. It aims to make use of the gate-based mode of operation of Pasqal’s QPU. This routine was tested with the test case scenaria, converted into QUBO type of problems, on a classical simulator of quantum hardware. Conversion from SMO to QUBO was computationally straightforward. Performance of the whole pipeline was found however subpar, with even noiseless simulation being highly resource-intensive and yielding sub-optimal results for the desired QUBO problem even for smaller scale of 4 targets. This has hindered an extensive study of the method in limited time of the project, also seconded by the evolution of the community opinion about the potential of QAOA in its naive formulation to deliver industrially-relevant advantage apart from select cases, due to unfavourable scaling of circuit depth and amount of training with the problem size growth. [26]

Further potential studies of this approach could include various spin-offs of QAOA, [27], [28], [29], [30], [31] aimed to decrease the circuit depth or speed-up the training. Alternatively, a fully-analog annealing routine shall yield substantially better performance. It would require the hardware to support local addressability or equivalent, which has not yet been demonstrated in experiment - but is actively worked on.

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3.1.2 MIS

Another approach is based on the outstanding capability of Neutral Atom QPUs to sample Independent Sets of a given graph using a physical principle of Rydberg Blockade [32] [33]. Researchers of Equality explored means to make use of it for the Space Mission Optimisation (SMO) problem, and suggested the following pipeline: First, SMO problem is represented as a graph of possible transitions between different targets or positions. Then, a complementary graph is built, highlighting the impossible transitions. An independent set of such a graph would represent a *possible* mission schedule. Finding a Maximal Independent Set (MIS) of such a graph can then be associated with an optimal mission planning. The main strength of this approach lays in its reliance on the fundamental physical properties of the device in operation, allowing to sample (comparatively) fast different MIS. The main bottleneck is the graph-to-graph mapping (to embed the problem in the QPU, respecting all the constraints), which is per se another NP-hard problem.

Within Equality project researchers have explored possible realisations of such a pipeline, with different approximations and classical approaches to graph conversion. This approach, while heavily constrained by the currently available hardware, has shown its potential as promising. Its scaling behaviour was found to be better than that of the algorithms finding exact optimum, while the quality of solutions (at least for small problems with less than 100 targets) is on average better than greedy classical routines.

Project researchers would expect that with advancements of Neutral Atoms-based quantum computing hardware, as well as classical graph-based algorithms, the approach might be improved and might be found competitive for certain types of problems. This, however, would necessitate orders of magnitude in speed-up of NAQC operation cycles, and in number of qubits.

3.1.3 Custom graph algorithm

The nature of Equality project was to explore potential ways to practical advantage. To follow this mission, researchers have also designed a custom graph algorithm, fully reliant on classical computation. This allowed to explore new approaches to graph-based optimisation, compare them to fully-quantum quantum and hybrid approaches, and better chart the technological horizons of the use-case.

In a nutshell, this custom algorithm represents a smart approach to traversing a time-ordered directed acyclic graph (DAG), incorporating a series of use-case driven subroutines and design decisions motivated by the nature of the problem. Specifically, each vertex of the DAG represents a feasible attempt, while edges encode transitions respecting manoeuvering constraints. The algorithm iteratively builds and extends active trajectories from source nodes, aiming to maximise distinct target coverage while avoiding repeats. To manage combinatorial growth, researchers suggested grouping trajectories with similar near-term future into ”buckets”, with further selecting top candidates per bucket based on accumulated reward and potential gains, balancing exploration and exploitation. Iterative prune-extend cycles refine the active set until optimal or stopping conditions are met.

Within the project, performance of the algorithm was explored in terms of quality and runtime scaling on the simulated datasets, and compared to other two approaches. Suggested custom algorithm was found competitive against a baseline greedy solver, producing higher quality solutions while maintaining competitive performance as complexity increased. With growing problem sizes, time-to-solution was found scaling more favourably than optimal solvers, but expectably inferiour to a greedy one. However, it was discovered than longer runtimes did

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not provide for better solutions, often reflecting exploration of unproductive branches, hinting on further potential for improvement. Pruning was found an effective way to control exploration trajectory growth for moderate sizes but showed diminishing impact on highly branching graphs, highlighting trade-offs between aggressive pruning and solution quality. Overall, the algorithm has demonstrated yet another interesting approach for resolution of SMO, not relying on progress of Quantum Technology. It could present an interesting way for further adaptation and improvement of current operational solvers.

3.2 Technology Adoption Roadmap and Impact

Within Equality project, three approaches to optimisation were tested: quantum (QAOA), hybrid-quantum (MIS), and alternative classical.

From the experiences with this project and adjacent ones, we could confirm that while quantum optimisation still keeps its aspiring promises, most of purely-quantum techniques known today require substantial evolution to present commercial advantage. Industrial advantage of quantum computing for optimisation depends on active developments of: smart hybrid routines tailored for both hardware and problems, quantum computers with large numbers of densely-interconnected and noise-mitigated qubits. If this advantage is to arise within the NISQ era, it would likely be within a narrower domain of application than what was anticipated before.

To approach this bar of utility closer to our days, two approaches are suggested: hybridisation - incorporation of quantum solvers as sub-routines into classical optimisation pipelines, in contrast of relying fully on quantum algorithm start-to-end; and hardware-oriented algorithms - like the MIS explored in this work. At the moment, most of such are still not competitive against state-of-the-art classical optimisation solvers, but there still remains large margin to evolve and improve those techniques on the algorithmic side. Thus, it would likely seize commercial advantage with smaller requirements on quantum hardware (hence- earlier) than fully-quantum routines.

Finally, the domain of classical algorithms - despite its long history - still offers some fruits, with continuous development of use-case-specific heuristics. Quantum-inspired techniques present an interesting venue here, however - not the only one. In context of quantum technologies (as core of this project), it serves a good lesson that when projecting the scaling and potential advantage of Quantum routines, one shall account for potential improvements of its classical competitors, that may substantially evolve within the same timeframe.

Algorithms studied in this work were oriented at resolution of Space Mission Planning problem, which is a type of Time Dependent Travelling Salesman Problem with Time Windows (TD TSP TW). Within suggested pipelines the problem was reformulated to more common formats (like QUBO or MIS), which opened opportunities to apply same findings to a variety of other use-cases.

From the results of this projects, one would expect that in the mid-term perspective quantum and quantum-hybrid optimisation algorithms would perform best at solving graph-based optimisation problems with the following properties: limited spatial connectivity (planar graphs), especially the graphs with bounded degree below that of the suggested quantum hardware; planar graphs; problems where long-distance indirect (via-intermediate) correlations is important and branch the tree of possible solutions too fast (e.g. - the MIS itself).

Industrial impact of technologies explored in this project is mostly foundational - creating the basis and laying the way for the next generations of quantum, quantum-hybrid and quantum-inspired algorithms. Projecting to the first examples of practically-relevant quantum optimisers,

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we would expect those to be highly tailored to the use-case. Therefore, the first fruits of this technology would be a dramatic raise of interest - and consequentially funding and research - in the domain. Finally, in the times when such technologies mature to be universally-relevant (better than HPC-driven state-of-the-art optimisers), the impact of actual commercial deployment at scale would be seen shortly, and is expected to pay back long years of investment within a decade.

All in all, the present state of technology does not allow for any more precise quantitative assessments of business use-cases, better than in the previous Deliverable D6.5.

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4 Technology - Quantum Machine Learning techniques

4.1 Technical Overview

Modern approaches to quantum machine learning (QML) uses quantum circuits (programs) to solve a broad spectrum of tasks, such as supervised and unsupervised learning. Two broad ideas dominate. The first is the so-called quantum kernels approach: the learning model is built around a similarity measure which is aimed at extracting the most salient features of data. In particular, data points are mapped through quantum "feature mapping", after which similarities are estimated. From this matrix of similarities a classical optimisation process finds the best classifier. One of the works which emerged from this project clarifies what these "quantum kernels" can cover and where their limits are. In broad strokes, we show that the mainstream approaches to construct quantum kernel called embedding quantum kernel, already spans very large, useful model families (e.g., common shift-invariant kernels and a broader "composition" class). In other words, the current study covers many important classes of kernels. However we have also identified limitations of the conventional approach, and identified abstract mathematical conditions which - if they can be met, and this is still an open question - would open doors to completely new ways of doing machine learning. This is explored in the paper [34].

The second main idea for QML is that of trainable quantum circuits (sometimes called variational or PQC models). These look more like neural nets: data is fed into a quantum circuit, which is then modified in the training until good prediction on the training set is achieved. One of the bottlenecks in running such models in the near term is the circuit depth: today's hardware prefers short, shallow circuits. In this project we also devised a new class of methods to run deeper circuits such as for QML on shallower machines. In [35], we introduced a "divide and chop" which allows one to reconstruct outputs of a deeper circuit by recombining outcomes from many runs of shallower circuits especially well suited for variational methods such as QML with trainable circuits. We have also improved on this with a more general idea of a multiple-basis representation (MBR) representation of quantum states, where we computationally combine results from several simple circuits chosen in complementary "bases." This method allows us to represent a express richer models through the stitching of shallower computations. This approach trades quantum depth for a smart hybrid structure, and which enables the running of quantum models on more restricted hardware. We have also bounded when this is feasible and showed links to known, efficiently simulable families, which helps target where real quantum help is needed. Another open question in using quantum circuits as trainable models is the inductive bias: that is, understanding what function families these models naturally represent. In our last deliverable [36] we have investigated this in the context of a concrete application. We studied Synthetic Aperture Radar processing and identified a point in the pipeline where a PQC naturally fits: replacing a costly classical step (Stolt interpolation + ground-range FFT) with a non-uniform Fourier transform-like stage. This approach is known in the classical literature but is expensive. In our analysis of quantum models we have shown that certain quantum models naturally perform operations related to the non-uniform Fourier transform, motivating building SAR-aware classifiers with quantum data re-uploading subroutine. This gives a real workflow where a quantum subroutine could matter as data sizes and accuracy demands grow.

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4.2 Technology Adoption Roadmap and Impact

Our results outline a practical roadmap. We start by letting the models lead: the kernel study [34] narrows attention to composition-style and other promising families, turning “what might work?” into concrete design targets. With model classes in hand, we fit them to today’s machines using two complementary depth-management tools, which allow for real-world testing. Finally, we prove value in a real workflow: the SAR pipeline [36] offers a clean insertion point (the NUFFT-like stage) to benchmark end-to-end accuracy, latency, and cost. Iterating this loop - choose the right model family, compress depth with divide-and-chop + MBR, validate in SAR - provides the shortest, most defensible path from NISQ hardware to demonstrable QML advantage.

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5 Technology 5 - Efficient Hardware utilisation (Circuit tailoring techniques

5.1 Technical Overview

To bring Quantum Computing to industrial utility sooner, it is essential to wisely use the near-term quantum hardware, circumventing or embracing its different limitations. This is why researchers of EQUALITY consortium have explored several approaches to reduce circuit complexity and optimise execution for specific hardware architectures.

This chapter mentions the developments and potentials of four different techniques of two different classes, so for clarity we structure the chapter by technology, each including its own descriptions, outlook and impact.

5.1.1 Logic-based methods for circuit optimisation

This section unites two techniques based on the concept of ZX-calculus.

Extending ZX-calculus to model probabilistic channels

ZX-calculus [37] is graphical language grounded in monoidal category theory and used in quantum computing to represent and reason about quantum processes using diagrams instead of complex algebra. It simplifies quantum circuits into networks of coloured nodes (called ”spiders”) connected by lines, where each colour and connection carries a specific mathematical meaning. An example can be seen in Figure 2. This visual approach allows researchers to manipulate and optimise quantum circuits more intuitively, often revealing simplifications or equivalences that are hard to spot using traditional matrix-based methods.

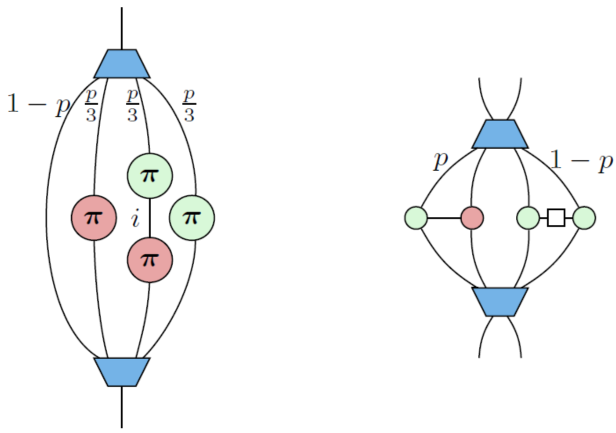

Figure 2: Left: Diagrammatic representation of the depolarising channel. Right: Diagrammatic representation of a mixture of two-qubit gates. [38]

This work extends the ZX framework by enriching it with algebraic operations [38] — specifically, probabilistic choices — via convex algebras derived from the finite distribution monad. This enrichment allows ZX-diagrams to express probabilistic mixtures and noise, making them suitable for reasoning about quantum error mitigation (QEM).

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This enriched framework introduces new rewrite rules and semantics that allow for:

- Diagrammatic reasoning about noise in quantum systems.
- Formal modelling of QEM techniques, such as symmetry verification.
- Probabilistic circuit optimisation, where circuit fragments are treated as probabilistic mixtures.

Current performance shows that enriched ZX-diagrams can model realistic noise scenarios and facilitate design of more robust QEM protocols. The framework remains compatible with existing ZX tools and could be integrated into quantum compilers.

Further development of this technique could focus on establishing completeness results and automating simplification procedures to enhance usability and formal robustness. Expanding the framework to support other monads — such as the powerset monad [39] — would enable reasoning about nondeterministic or hybrid quantum systems, broadening its applicability. Bringing enriched ZX-based simulators and compilers that incorporate noise-aware optimisation to production would, facilitate practical circuit design. Finally, applying enriched diagrams to real quantum hardware could inform and improve quantum error mitigation strategies, making them more effective on near-term devices.

Hardware-aware compilation for ion traps using global gates

Quantum computers based on trapped ions offer unique hardware capabilities to realise all-to-all qubit connectivity and access to powerful multi-qubit entangling operations known as global gates — specifically, Global Mølmer-Sørensen (GMS) gates. [40] These gates execute multiple two-qubit interactions simultaneously, making them more efficient than sequential entangling operations. However, they are also more costly in terms of runtime and fidelity. To exploit this hardware feature, researchers of EQUALITY project suggested a compilation algorithm that transforms arbitrary quantum circuits into ones optimised for ion trap platforms

Specifically, researchers demonstrate a ZX-calculus-based synthesis algorithm [41] compiling quantum circuits into a set of gates native for trapped ions hardware: single-qubit rotations and GMS gates. The algorithm introduces two key innovations: (1) a linear programming approach to extract layers of CNOT gates that can be compiled into a single GMS gate, and (2) peephole optimisation rewrites that group entangling gates and reduce single-qubit gate overhead. These techniques are integrated into the PyZX framework [42] and benchmarked against Qiskit [43] and a naive compilation strategy, taking as an example specifications of IonQ Forte [44] . Devised ZX-based compiler has shown to significantly reduce circuit runtime and number of entangling gates across a wide range of benchmark circuits (QASMBench[45], MQT Bench[46], and quantum chemistry workloads[47]). The approach is particularly effective for circuits with commuting CNOT layers or fanout structures, which are well-suited for GMS compilation

Future work could explore more flexible circuit extraction strategies within the ZX-calculus, potentially enabling new hardware-specific compilation techniques [48]. Investigating support for variable coupling strengths in GMS gates—such as those offered by EASE gates [49] —could further reduce gate counts and improve fidelity. Additionally, integrating phase gadget extraction [47] into the compilation pipeline may allow for more efficient use of global entangling operations. These enhancements would broaden the applicability of the compiler and improve performance on next-generation ion trap devices.

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5.1.2 Divide-and-conquer strategies for circuit reduction

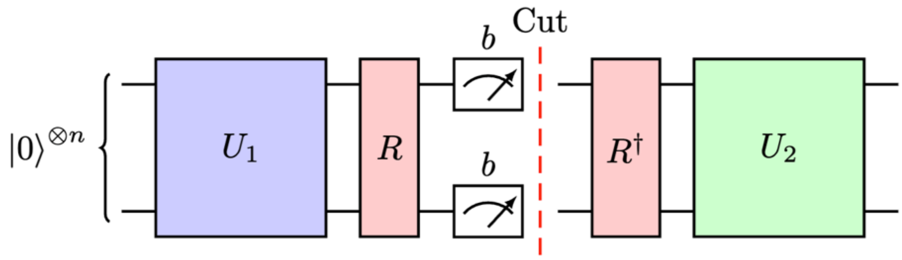

Figure 3: Schematic representation of Divide-and-Conquer approach to circuit tailoring. [35]

Reduce & Chop circuit cutting

Quantum Computers available nowadays are still constrained by limited qubit counts and lower fidelities, allowing to effectively run only shallow circuits, thus restricting the complexity of algorithms they can execute. To alleviate this, researchers of Equality introduced a novel approach — Reduce & Chop [35] — to approximate deeper quantum circuits with series of shallower ones. Inspired by Feynman's simulation approach[50, 51], new method cuts a quantum circuit into two shorter parts to be run in sequence, such that the measurement results of the first one define the input state of the second. Done naively, this would lead to exponential overheads in measurement, or loss of quantum information. To improve this, the researchers suggest a key concept - *Computational Basis Rank* (CB-rank), quantifying the complexity of the intermediate quantum state. To increase efficiency of cutting, CB-rank at cut shall be decreased. For that, researchers propose adding a shallow variational circuit, known as a Reducer R , trained to lower CB-rank so the classical stitching overhead becomes tractable in relevant cases, enabling practical execution on near-term devices. A schematic representation of the approach is shown in Figure 3.

Within this project runtime, researchers developed and refined Reduce & Chop framework, focusing on optimal design of the the variational circuit minimising CB-rank while preserving computational fidelity. This involved:

- Design and testing of reducer circuits tailored to specific problem instances [52]
- Development of a custom optimisation routine, balancing expressivity and depth of the reducer
- Benchmarking performance of the approach at different types of quantum circuits

These benchmarks demonstrated that the method can find efficient approximations of deeper circuits by a series of shallower ones, significantly reducing hardware resource requirements. Current performance metrics indicate that for select problems (e.g., small-scale quantum machine learning tasks), Reduce & Chop achieves up to 60 % reduction in depth, while maintaining accuracy within 5–10% of full-depth simulations, making it a viable solution to reduce hardware requirements, so crucial in the NISQ era.

The future work will focus on:

- Extending the method to multi-qubit entangled states and dynamic circuit chopping [53]
- Integrating error mitigation techniques to improve robustness on noisy hardware [54]

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- Automating CB-rank estimation and circuit partitioning for general quantum algorithms
- Collaborating with hardware teams to deploy reducechop on real quantum devices and validate scalability

This approach opens promising avenues for maximising the utility of near-term quantum hardware for some problems. Sooner utilisation of NISQ hardware would approach the ROI of Quantum Computing domain overall, and increase the developmental momentum.

Best way to deliver this impact across domain would be integrating developments described here in popular mid-ware packages or quantum compilers.

Multiple-Basis Representation

Among multiple applications of Quantum Computers, the most natural one is simulating Quantum Physical phenomena. While Quantum Computers can do it substantially more efficiently, than classical ones, this advantage comes at scale. With current NISQ hardware we are just approaching the edge of first practical advantage demonstrations, making every improvement in efficiency - like simulating larger systems with smaller circuits - count. This work aims to improve on solving core problems in the domain by answering the question ”How could one encode quantum states more efficiently on today's imperfect hardware?”

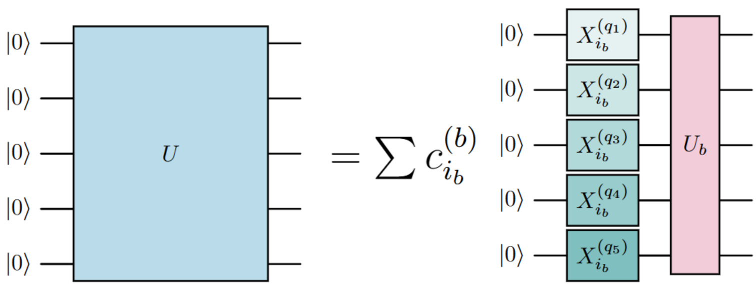

Figure 4: Motivation for the MBR is to describe states using superpositions of more easily implementable quantum circuits. [55]

Within Equality project, researchers suggested a new hybrid, efficient quantum-classical representation of quantum states, the multiple-basis representation (MBR)[55]. This representation consists in a linear combination of states that are sparse in some given and different bases, specified by shallow quantum circuits, as sketched in Figure 4. This representation could enable more meaningful computations on NISQ machines by restricting the computation to depth-limited circuits.

When encoding a quantum state onto a quantum computer, instead of relying on a single basis, new method suggests representing a quantum state as a linear combination of sparse states across multiple bases, each defined by low-depth quantum circuits. Each of these bases shall capture distinct, non-redundant information about the global state. To ensure minimal overlap and maximal expressivity, such bases are best chosen to be mutually unbiased.[56] The strength of MBR lies in using only a polynomial number of classical parameters and quantum circuits, which makes it especially useful for near-term quantum devices. Importantly, suggested Multiple-Basis Representations enable the computation of real physical quantities, such as energies, through classical post-processing of quantum measurements, offering a scalable and hardware-friendly approach to quantum simulation.

Within EQUALITY project the researchers have formalised the structure of the MBR, defined sub-classes based on classical tractability and circuit depth, and demonstrated that MBR generalises existing representations such as Matrix Product States (MPS) [57] and Stabilizer States [58]. This generalisation allows MBR to capture a broader class of quantum states, including those that are difficult to simulate using traditional tensor network methods.

Through numerical simulations, the researchers applied MBR to approximate ground states of many-body Hamiltonians, such as the transverse-field Ising model on 2D lattices. Here MBR could outperform MPS simulations for problems with long-range correlations, where tensor network methods driving MPS typically struggle. Furthermore, the project integrated MBR with the own Reduce & Chop method [35], further reducing hardware demand of the simulations. Lastly, the team developed a Tomography protocol for reconstructing unknown quantum states using MBR, supported by rigorous bounds on sampling and overlap estimation.

This work could open the path of simultaneous use of several hardware-friendly bases, a natural description of hybrid computational methods accessible for near-term hardware. Application of MBR approach to problems like approximating ground states of complex Hamiltonians could make near-term quantum simulations more expressive and resource-efficient, opening new possibilities for quantum-enhanced classical computation. Its adoption could significantly impact fields such as quantum chemistry, condensed matter physics [59], and quantum algorithm design [60].

5.1.3 Boolean Satisfiability-based routing of quantum circuit

For many NISQ realisations of quantum computers limited connectivity presents a serious bottleneck on the way to practical advantage. This is why it is important to optimise Quantum Circuits not only for certain hardware gateset, but also for a given topology. Finding such a mapping between abstract logical qubits and specific hardware qubits in a given machine is known as Routing.

Researchers of EQUALITY project have suggested a routine to find such a routing in optimal way for a class of Quantum Circuits known as Clifford circuits using Boolean Satisfiability (SAT) solvers [61] .

Clifford circuits, composed of gates like Hadamard, phase, and CNOT, play a central role in quantum information. Despite being classically simulable, they are foundational in quantum error correction (QEC) routines, quantum cryptography, and communication. The method leverages the Stabiliser formalism[62] and Tableau representations [63] to model quantum states and gate transformations, enabling optimal compilation of circuits for Quantum Processors with fixed topology.

Development of this approach resulted in a Python-based tool *QRONOS* (Quantum ROuting aNd Optimisation Software) **[64]**, which encodes the routing and optimisation of Clifford circuits [65] as SAT problems.

Within the project, researchers tested QRONOS on planar layouts, typical for today's devices, and found it effective, achieving significant gate count reductions while preserving circuit functionality. Another important aspect is that the tool was from start developed as a software, oriented at expert users. It incorporates a set of features, accommodating for different backends (like support for various SAT solvers: Z3[66], KISSAT, PySAT [67] and a potential to run on multiprocessing systems, with more features to be disclosed later). This has substantially grown the result in maturity and shortened the path from RD to practical impact of the technology.

Despite QRONOS currently targets only Clifford circuits, its integration into hybrid quantum-

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classical workflows and Quantum Error-Correction schemes could bring improvement to the overall compilation routines, thanks to its modularity and extensibility, making it adaptable for future hardware and algorithmic developments.

At the moment of editing, the software is not yet publicly available, so the technical details remain confidential, but the authors encourage scientific collaborations. Interested readers could contact Dr. Linus Scholz via name.surname(at) dlr. de

5.2 Technology Adoption Roadmap and Impact

Mid-ware comprises an essential step towards utility of quantum computation. Not only now, but at every stage of hardware maturity, end-users would wish to ”get more with less” : increase the size of quantum systems simulated, improve fidelity of end-results or try even longer routines. From the recent technological roadmaps we could witness, that the gap between ”hardware capabilities” and ”software requirements” is in often cases shrunk faster from the software side, albeit still presenting a challenge. This, together with desire to bring the ROI of rather expensive Quantum Computing technologies sooner, points at the Mid-Ware as one of the most potential elements in the stack, in terms of commercial impact. It is only confirmed by a soaring number of mid-ware toolkits, providers and start-ups in the recent few years.

A strong utilisation aspect of the technologies mentioned here is that they are either hardware-agnostic - hence, applicable to all types of quantum hardware equally, or hardware-centered - allowing to squeeze maximal performance of the very specific properties of hardware.

This defines the utilisation and commercialisation strategies for the tools: the hardware-centered routines like [41] could better suit the firmware stacks of the QPU providers, as they could leverage the unique insights into their machines. Hardware-agnostic approaches like [35] in their turn are best incorporated in the software toolkits, like compilers or dedicated optimisation tools.

Technologies presented here have relatively short time-to-market (once core science is in place, developing it into a software product is a tangible engineering job, as shown by a successful example of [68] and multiple startups like [69], [70]). Impact of such tools is often scaled across the domain relatively fast.

Main market for such solutions currently is the Quantum Computing provision itself: integrators completing full-stack solutions for the customers, and Research and Development community, developing and benchmarking quantum solutions in academic as well as in industrial contexts.

For quantum mid-ware one could observe different approaches to protecting the IP and its subsequent commercialisation. As most approaches are still at low TRL and the market is relatively small, one of the common strategies is to publish core scientific routines in peer-reviewed journals, reinforcing oneself a reputation and network. Then, the commercial strategy and UVP is heavily reliant on the know-how and expertise of the group of developers, previously proven by public materials. This strategy can be successful at the mid-term, while the core customers are developers of adjascent techniques. For long-term we would expect it shifting, mimicking the approaches found nowadays in classical software development markets.

We believe all technologies mentioned here will, or already did, bring significant and sustainable impact for the industrial applications of quantum computing, solidifying the role of the EQUALITY project in the ecosystem.

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