Perspectives of Quantum Computing at the Jülich Supercomputing Centre

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The strategy of the Jülich Supercomputing Centre to apply quantum computers in the Jülich Quantum Computing Infrastructure JUNIQ is presented. Following the JUNIQ quantum computer emulator JUQCS, the D-Wave quantum annealer JUPSI and the soon-to-be-implemented Pasqal quantum simulator JURY, pilot systems based on gates as well as early-stage experimental systems, on their stony path to become universal, will be included. The integration strategy of JUNIQ into the HPC environment of the Jülich Supercomputing Centre (JSC) is outlined. An exemplary application is presented that was implemented on the emulator JUQCS, which emulates an ideal gate-based quantum computer, and enables comparison with the D-Wave quantum annealer JUPSI. Long-term perspectives are highlighted.

1 Introduction

Forty years have passed since Richard Feynman's landmark visions on quantum computing were published[a;1,2]. Today, many scientists are convinced that we are on the threshold of the practical exploitation of quantum effects in scientific and technical computing. Indeed, in early 2022, the Jülich Supercomputing Centre (JSC) could put into operation a special variant of a quantum computer, a so-called quantum annealer (QA), manufactured by the Canadian company D-Wave Systems Inc. ("D-Wave"), a system with 5640 qubits called "D-Wave Advantage" and nicknamed JUPSI[3,4], see Fig. 1.

Figure 1. D-Wave Advantage System JUPSI – JUelich Pioneer for Spin Interference.

[a]... "because nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy. ... Can you do it with a new kind of computer – a quantum computer? ... Now it turns out, as far as I can tell, that you can simulate this with a quantum system, with quantum computer elements. ... For example, the spin waves in a spin lattice ... imitating Bose-particles in the field theory. I therefore believe it's true that with a suitable class of quantum machines you could imitate any quantum system, including the physical world. But I don't know whether the general theory of this intersimulation of quantum systems has ever been worked out ... Now, what kind of physics are we going to imitate? ... the physical world is quantum mechanical, and therefore the proper problem is the simulation of quantum physics." Indeed, as early as 1959, he had spoken of digital computing with quantum systems in an address at Caltech, with the famous headline "There's Plenty of Room at the Bottom!"

A QA is probably closest to Feynman's original vision of quantum computing, as suggested by the quote given in footnote a. A quantum spin array is assigned couplings that encode the problem to be solved. From an initial Hamiltonian, which in the z-basis generates a complete superposition state from a superposition of all the possible 2^L basis states, L being the number of qubits, which as a result of a magnetic field in the x-direction takes the lowest energy state of this operator, the system is adiabatically transferred into the problem Hamiltonian; the quantum spins should remain in the lowest energy state – more precisely, the spin-system at all times takes the lowest eigenstate of the slowly-varying Hamiltonian, and thus, at the end of the process, we know with high probability that the system is in the ground state, and that the measurement of the qubits (spins) at this point of the process should not introduce any more perturbations in the ideal world. This certainty is based on the famous adiabatic theorem of Born and Fock[5].

A QA performs a continuous physical process, *i.e.* the time course of the system is continuous. In this sense, a QA can be considered an *analog* quantum computer.

This is contrasted with the *digital* quantum computer, usually called a *gate-based* or *gate-level* quantum computer (GBQC). A GBQC is also constructed from arrays of spins that are, in contrast to the QA, controllably coupled together. The same universal spin Hamiltonian that allows the QA to be modelled is also used for the GBQC as a description model. The GBQC can manipulate single qubits as well as gates of two or three qubits in such a way that quantum states of the involved qubits can be specifically transformed and influenced. This allows quantum circuits and quantum algorithms to be executed. Usually the qubits are brought into the superposition of 2^N states at the beginning of the operation, this is done here by local Hadamard transformations, leading to a state coherently superposed of all eigenstates. Using 1-qubit and 2-qubit operations (*e.g.*, a CNOT) one can tinker entangled states representing non-local correlations. The trick is to use such manipulations to get the system into the specific eigenstate at the end of the algorithm, that is supposed to solve the posed problem. Given this situation, one then knows with certainty that one will get an unambiguous result, since the measurement, just as in the case of the QA, no longer introduces perturbations. However, on the one hand, only a few algorithms are known that lead to such a maximum amplitude amplification, but fortunately there are some important ones that amplify only a few amplitudes, *i.e.*, suppress most of them, – Shor's algorithm is of this type – and thus allow for a statistical determination of the solution. On the other hand, the qubit and gate manipulations of today's GBQC are not yet at a level of fidelity that leads to generally useful results – here quantum error correction promises a way out[6].

The currently existing digital quantum computing systems (*e.g.*, from IBM, Google, Rigetti Computing, IonQ, AQT, IQM or eleQtron) are all at such a prototype stage, as they do not meet the precision requirements for a universal GBQC. Preskill has given this stage of development the somewhat euphemistic name NISQ, the Noisy Intermediate-Scale Quantum era[7], in the hope that it is already possible to perform useful operations on such systems, *e.g.* for simulations in physical chemistry. Furthermore, there are systems that are in a deliberately chosen preliminary stage to universal GBQC, such as the so-called quantum simulator (QS) of Pasqal[8], which is on its path to become a fully digital system in a few years.

In this sense, the JSC bases its strategy for quantum computing on three pillars: The first pillar is based on the classification of quantum computers as "analog" or "digital" systems and their intermediate stages explained here, aiming at the provision of all these variants. The goal is to use systems with a high enough technological maturity as pilot production systems. For this purpose, we have introduced a classification scheme that follows the NASA technology classification[9], but in terms of Quantum Technology Readiness Levels (QTRL)[10]. Pilot production systems should show a QTRL of eight and above (QTRL8 to QTRL9). We also will implement or grant access to systems with a technological maturity of five to seven (QTRL5 to QTRL7) – this includes NISQ systems – that are considered as important test machines, and systems in an early development stage with QTRL of 3 to 4 by remote access to the respective lab for performing hardware-software co-design.

The second pillar of JSC's strategy is the tightest possible integration of breakthrough computing technologies into JSC's world-leading high performance computing (HPC) systems. For more than ten years, JSC has pursued the technical interconnection and deep integration of mutually autonomous supercomputer systems. Corresponding hardware and software have been developed in the DEEP projects funded by the European Commission and European High-Performance Computing Joint Undertaking (EuroHPC JU) since 2012[11]. The resulting concept of hardware modularity called Modular Supercomputing Architecture (MSA) allows functional parallelism at the system level[12]. The MSA concept, realised in software by ParTec's ParaStation Modulo middleware suite[13], is the perfect platform to integrate quantum computing into an HPC environment. By coordinating HPCQS[14], JSC is researching with European science, engineering and industry partners to extend the MSA integration technology to include quantum computing.

The third pillar of JSC's quantum computing strategy is the creation of a world-leading quantum computer user infrastructure. This includes the technical provision of the quantum computing systems (integrated into the HPC environment) – *nota bene* under European legislation –, the deployment of the systems via peer-reviewed calls for proposals – a rolling call for JUPSI is already running – the support of the users in simulation labs, algorithm development groups and cooperative research. These activities are carried out in the *Jülich UNified Infrastructure for Quantum computing* (JUNIQ)[15]. JUNIQ is the first infrastructure of its kind worldwide. And there is already a next level of infrastructure building under way: based on HPCQS[14], the JSC brings the principle of JUNIQ to the European level.

At JSC, we believe that our strategy will enable the earliest possible integration of breakthrough quantum computational technologies into an HPC environment. This is necessary insofar as the currently most promising algorithms for solving optimisation problems (*e.g.* the Quantum Approximate Optimisation Algorithm – QAOA) and finding solutions to eigenvalue problems in chemistry (*e.g.* the Variational Quantum Eigensolver – VQE) require the tightest coupling of classical with quantum algorithms.

This text is structured as follows: After a description of the existing and planned systems in Sec. 2 that JUNIQ aims integrating into its portfolio following our QTRL definition, a short report on an exemplary application on JUPSI as well as on JUQCS, the Jülich Universal Quantum Simulator, is given in Sec. 4. Then, the long-term perspectives of JUNIQ are outlined, followed by a summary and outlook in Sec. 6.

2 Existing and Planned Systems of JUNIQ

In planning its quantum computers, JSC focuses on both the applicability of the technology in practical computer simulations and the availability of systems at various maturity levels to bring the technology to users in a progressing manner as early as possible. Such planning requires the definition of a classification scheme of the technological maturity of the systems as a basis.

2.1 Quantum Technology Readiness Levels – QTRL

The QTRL scale is a metric introduced by the authors in 2017 to describe the maturity of quantum computing technology, see Fig. 2. The scale consists of nine technology readiness levels (QTRLs), with QTRL1 denoting the lowest and QTRL9 the highest. For simplicity, we evaluate both variants, analog (adiabatic/annealer) and digital (gate-based quantum computers), in one scheme, but also emphasise that the lack of error correction still pushes gate-based systems to a lower QTRL today.

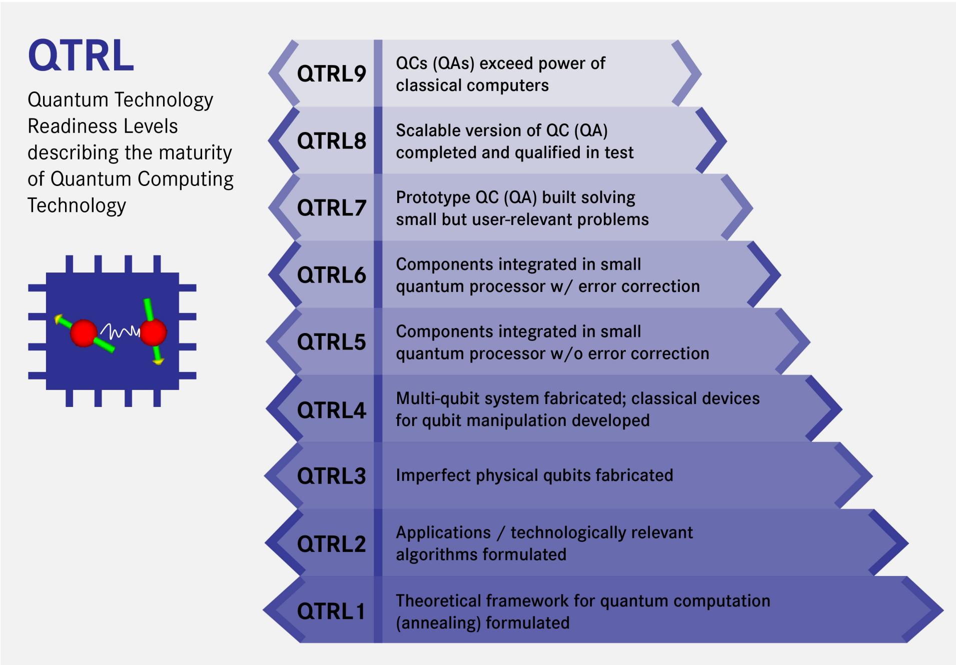

Figure 2. Definition of Quantum Technology Readiness Levels – QTRL.

1. A quantum computing technology is at QTRL of 1 when the theoretical framework for quantum computing has been formulated. Such theoretical studies of the basic properties of the quantum computing devices are moved towards applied research and development.

2. The quantum technology reaches QTRL of 2 once the basic device principles have been studied and applications or computationally relevant algorithms are formulated. QTRL2 quantum computing technology is speculative, as there are little to no experimental results yet supporting the theoretical studies.

3. Fabricated imperfect physical qubits, the basic building blocks of quantum computing devices, are defined to be at QTRL of 3. At this stage, laboratory studies aim to validate theoretical predictions of qubit properties. Theoretical and laboratory studies are required to determine whether these basic elements of the quantum computing technology are ready to proceed further through the development process.

4. At QTRL4, multi-qubit systems are fabricated and classical devices for qubit manipulation are developed. Both technical components of the quantum computer are tested together.

5. QTRL5 quantum computing technology comprises components integrated in a small quantum processor without error correction. At QTRL5, quantum computing devices are undergoing rigorous testing including running of various algorithms for benchmarking, still without error correction.

6. Components integrated in a small quantum processor with error correction are at a QTRL of 6. Rigorous testing and running algorithms is still the most important task for the QTRL6 quantum computing technology.

7. QTRL7 quantum computing technology is a prototype quantum computer (or annealer) solving small problems already relevant for applications. The prototype is demonstrated in a user environment.

8. A scalable version of a quantum computer (annealer) completed and qualified through test and demonstration is considered to be at QTRL8.

9. Once quantum computers or annealers exceed the computational power of classical computers for general (specific) problems the quantum computing technology is labelled with QTRL9 in our QTRL scheme.

We emphasise again that the scheme presented here includes QAs, QSs as well as GBQCs. This is for simplicity of classification, but it is not intended to compare the competitive aspects and prospects of the different approaches. It is obvious that quantum annealing, as the less complicated but presumably also less widely applicable technology, has already reached a higher level of maturity today. This is also a consequence of the fact that a GBQC requires high qubit fidelity to allow for efficient error correction. The lower the fidelity, the larger is the number of qubits required. At fidelity of $> 99.9\%$ the estimates range between 1,000 and 10,000 qubits per logical qubit. This reduces to a more reasonable estimate of 100 to 1,000 qubits per logical qubit for a fidelity of $> 99.99\%$, which could enable the realisation of a few logical qubits in the next years. A large number of logical error-corrected qubits required for true quantum supremacy seems not yet within reach, however.

2.2 The Jülich Universal Quantum Computing Simulator JUQCS – World's Most Capable Quantum Emulator

Most quantum computing systems can be described by a universal spin model Hamiltonian[16]:

$$H_{\text{universal}}(t) = -\sum_{j=1}^{L}\sum_{k=1}^{L}\sum_{\alpha=x,y,z} J_{j,k,\alpha}(t)\sigma_j^\alpha\sigma_k^\alpha - \sum_{j=1}^{L}\sum_{\alpha=x,y,z} h_{j,\alpha}(t)\sigma_j^\alpha, \qquad (1)$$

where σ^α, $\alpha = x, y, z$ are the Pauli matrices, $J_{j,k,\alpha}(t)$ is the strength of the interactions between the α-components of spins j and k, $h_{j,\alpha}(t)$ stands for a potentially time-dependent (external) field. The spin model can be adapted to most variants of today's and planned quantum computers like GBQCs, QSs and QAs for all varieties of technological realisation. The quantum dynamics of the model is controlled and/or probed by the static and/or time-dependent external fields $h_{j,\alpha}(t)$. Depending on the physical system, also the exchange parameters $J_{j,k,\alpha}(t)$ can be controlled.

The quantum computer emulator suite JUQCS[17,18], developed within a collaboration between JSC and the University of Groningen, simulates the execution of a quantum circuit on an ideal GBQC – a pen-&-paper quantum computer, including the quantum depolarising channel error model. The quantum computer emulator comes in two flavours: (i) A hybrid MPI/ OpenMP/GPU version simulating the ideal GBQC to machine-precision (JUQCS-E and JUQCS-G), and (ii) a hybrid MPI/OpenMP version that performs the same task with reduced precision but enabling the emulation of three more qubits relative to version (i) (JUQCS-A).

JUQCS runs on various kinds of hardware ranging from PCs to high-end supercomputers with distributed and/or shared memory and with CPUs and/or GPUs, easily ports to different software environments, and can be used to benchmark supercomputers[19]. In the course of its development, JUQCS has set a series of world records of simulating the largest ideal GBQC[20]. Currently, this is a 48-qubit GBQC simulated on the Japanese K computer and on the Chinese Sunway TaihuLight.

JUQCS allows us to run quantum computing algorithms on an ideal (!) GBQC with up to 43 qubits by means of JUWELS. In this way, we are able to validate quantum computing codes[17–19,21–23] and test the intrinsic scalability of algorithms not hindered by the shortcomings of current real GBQCs.

An interesting usage model for JUQCS is to leverage the modular capabilities of JUWELS, the leading HPC system at JSC. JUWELS consists of a CPU cluster, the JUWELS Cluster, and a GPU cluster, the JUWELS Booster. When the classical optimisation part of a hybrid classical-quantum computing code such as QAOA is running on JUWELS Cluster, JUWELS Booster can act as an emulator of an ideal GBQC realised by JUQCS. In this way JUQCS allows us to run real HPC-quantum computing codes on an ideal GBQC with up to 43 qubits on JUWELS.

In addition to the JUQCS suite, the JSC and University of Groningen team also developed software to simulate physical models respecting the real physical implementation of a quantum computer, including multi-level spin systems, as no real system strictly is a 2-level system[18,24]. For this purpose, the time-dependent Schrödinger equation for a time-dependent Hamiltonian describing the quantum computer hardware and its control has to be solved. This software is also suitable to simulate quantum-spin systems that are coupled to a heath bath, enabling to study the effect of the environment on the operation of a quantum computer.

2.3 D-Wave Advantage System JUPSI – A Quantum Annealer

JUPSI, the Jülich Advantage$^{\text{TM}}$ quantum system of D-Wave has started operation within JUNIQ at JSC in January 2022[25]. A rolling call for quantum computer time proposals has started as early as in February 2022[15].
JUPSI, see Fig. 1, comprises the following components:

- The quantum processing unit (QPU)
- The QPU control system
- The QPU I/O system
- The cryogenic dilution refrigerator system
- The magnetic shielding system
- The radio-frequency (RF)-shielded enclosure

The D-Wave Advantage QPU is a lattice of tiny metal loops, each of which acts either as a qubit or as a coupler. Below their critical temperature, these loops become superconductors and exhibit quantum-mechanical effects. The system is operated at a temperature below 15 mK. The QPU of the Advantage system provides 5,640 qubits and 40,484 couplers. In order to reach this scale, the chip can make use of 1,030,000 Josephson junctions.

The qubits of the Advantage QPU are interconnected in a topology known as *Pegasus*. In the Pegasus graph each qubit is connected with 15 other qubits except for the qubits at the edges.

As mentioned, the QPU must be kept at a temperature near absolute zero and isolated from the surrounding environment in order to behave quantum mechanically. The system meets these requirements by

- operating the QPU at temperatures below 15 mK. These cryogenic temperatures are achieved using a closed-loop cryogenic dilution refrigerator system;
- shielding the QPU from electromagnetic interference, achieved using a radio frequency (RF)-shielded enclosure and a magnetic shielding subsystem.

The RF-shielded enclosure (an electromagnetic-tight box) houses the cryostat, the QPU, the I/O system, the rest of the QPU control system, and most of the magnetic shielding system.

The cryogenic dilution refrigerator system includes a cryostat, a nitrogen cold trap, and equipment racks. The cryostat, which is surrounded by a magnetic shielding system, is mounted within the RF-shielded enclosure; the cold trap and equipment racks sit outside of it. Communication between the equipment racks and the cryostat occurs through flexible hoses and cabling. The dilution refrigerator has an internal fluid path through which helium flows in a closed cycle. The cycle includes the cold-trap dewar, where impurities that might cause blockages in the circulation path are removed. The cold-trap dewar is maintained at a cryogenic temperature by immersion in a liquid nitrogen dewar. The refrigeration system's nitrogen cold trap sits outside the RF-shielded enclosure and has flexible connections to the pumping control rack.

The server rack contains the data processing, system control, monitoring, network, and backup power resources for the system. The data processing resources provide the web user interface, web services, and the underlying communications infrastructure for users to interact with the D-Wave system. Control and monitoring servers run applications that control the system and provide remote monitoring capability. The monitoring server tracks diagnostic information from the various subsystems and alerts D-Wave support personnel if it detects abnormal events. The contents of the server rack connect flexibly to the refrigerator's instrumentation rack and to feed-through connections in the RF-shielded enclosure wall.

The gas handling control rack contains gas manifolds and pumps that circulate the helium and also contains pumps and specialised equipment used only during system service.

The pumping control rack houses the compressor for the cooling, additional pumps that circulate the helium and a control cabinet that houses the electrical and pneumatic control subsystems. This part consumes most of the required power of 25 kW.

The universal spin model Hamiltonian of Eq. 1 becomes much simpler when it is reduced to describe a D-Wave QA:

$$H_{\text{annealer}}(t) = -A(t)\sum_{j=1}^{L}\sigma_j^x - B(t)\left(\sum_{j=1}^{L}\sum_{k=1}^{L}J_{j,k}\sigma_j^z\sigma_k^z + \sum_{j=1}^{L}h_j\sigma_j^z\right). \tag{2}$$

Note that two new functions $A(t)$ and $B(t)$ have been introduced. They vary in opposite directions between zero and one during the annealing process. This allows to start the process governed by the first part of the Hamiltonian, which introduces the necessary quantum fluctuations in the ground state of the system, and further on to move the system adiabatically to the Hamiltonian of interest describing the problem to solve. The adiabatic theorem tells us that the system stays in the ground state, when the process is carried out slow enough. At the end of the process the system is in the ground state of the problem Hamiltonian, equivalent to the minimum energy of the spin model Hamiltonian [b]. In a sense one can compare the adiabatic process of the QA with the amplitude amplification in GBQC: at the end, the systems should be in a state where measurement is as unambiguous as possible.

2.4 Pasqal's Fresnel Analog Quantum Computer – A Quantum Simulator

The third system to be installed in JUNIQ – taking JUQCS on JUWELS as an ideal GBQC and validation basis as number one – is a QS with more than 100 Rydberg atoms. With preliminary working name JURY, the system will be manufactured by the French company Pasqal[8]. JURY, funded through the EuroHPC JU project HPCQS[14] in fact is a twin of a system located at CEA, Paris. JURY will be hosted by JUNIQ with installation in 2023, and will be tightly integrated with the JUWELS MSA at JSC. The QS technology grew

[b] This idealised process of course only works for ideal systems that are not affected by noise or other disturbing effects.

from 49 qubits in 2018 to more than 100 as of today and will presumably reach 1000 qubits in 2023.

The QPU of JURY is based on a configurable 2D or also 3D array of single neutral rubidium atoms. The array can be seen as a register, where each single atom plays the role of a qubit. Laser light is used to assemble and read out registers made of more than a hundred of qubits and to perform fully programmable quantum processing. In addition, electronic controls are applied to tune the light properties, apply instructions arising from the quantum software stack and extract information through atomic detection.

Figure 3. Pasqal quantum simulator. Picture credits: Pasqal.

A QS can, for example, be used to solve chemistry calculations for drug discovery, as well as for very hard optimisation problems like the maximum independent set (MIS) problem arising in a manifold of application fields. The MIS problem can be tackled by using an ensemble of interacting cold neutral atoms as the quantum resource, thus realising Feynman's dream of simulating a quantum system by another, more easy to handle quantum system.

2.5 JUNIQ's Plans for Gate-Based Quantum Computers – We are in the NISQ Era

In JSC's strategy, gate-based systems will complement the emulator JUQCS, D-Wave's QA JUPSI and Pasqal's forthcoming QS JURY such that all varieties, from an analog system (QA) to an analog-digital hybrid system (QS) to a fully digital system (GBQC [NISQ]), will be represented and provided in JUNIQ.

Not surprisingly, GBQCs still remain *in status nascendi* with QTRL $\leq$ 5. This is because such systems require individual control over qubits as well as their interactions, preferably with full connectivity. Furthermore, qubits and gates must fulfil quality criteria such as a high fidelity of qubits and gates as well as good crosstalk and readout properties in order to be able to perform reliable quantum computations. It is generally assumed that a fidelity of 99.99% is required for efficient error correction. As a consequence, all technologies used so far are limited in terms of scalability, which is also due to their analog control technology.

JUNIQ intends to offer three generations of GBQCs. This approach includes more than one prototype production system on-site based on different building principles with QTRL5 – we plan to connect such a system to the exascale supercomputer – and soon hopefully higher (as well as remote access to more such systems), remote access to experimental systems in the lab with QTRL4, and remote access to devices at QTRL3 for testing single qubits and their connections.

In Tab. 1, we present an overview over the development of quantum computer technologies including the Pasqal QS and the D-Wave QA. The most advanced technologies are cold neutral atoms (Pasqal), ion traps (eleQtron, AQT, IonQ), and superconducting qubits (IQM, as well as US companies like IBM, Rigetti Computing, Google). The characteristics of the different approaches are taken into account when selecting potential systems for JUNIQ and assessing their QTRL.

	Cold neutral atoms	**Super-conducting qubits**	**Ion traps**	**Silicon pho-tonics**	**Micro-wave pho-tonics**	**Quant-um dots in silicon**	**Nitro-gen va-cancy centres in dia-mond**	**Topol-ogical qubits**	**Quant-um anneal-ing**
Qubit	Trapped cold atoms	Joseph-son effect	Trapped ions	Single photons	Photons, super-con-ductiv-ity	Electron spins in semi-conduc-tors	Atomic nucleus spins	Anion pair, quasi-particles	Joseph-son effect
# qubits demon-strated	196 Pasqal	127 IBM	32 IonQ	A few	1	49 Intel	6 QDTI	0	5640 D-Wave
States	Atomic energy levels	Phase, energy, current direc-tion	Ion energy levels	Polarisat-ion	Polarisat-ion	Electron spin direct-ion	Energy level of cavity	Anyon direc-tion	Current direc-tion
Gates	Laser	Micro-waves, Joseph-son	Laser	Polaris-ing and dichroic filters	Micro-waves	Micro-waves	Laser	2D anyon inver-sion	Gates an-nounced
PROS	Scalabil-ity, 3D connec-tivity, perfor-mance	Availab-ility	Fidelity, Availab-ility	Room temper-ature	Perform-ance	Scalab-ility	Theo. Perform-ance	Theo. Perform-ance	In pro-duction
CONS	No digital unit so far	Weak scala-bility	Weak scala-bility	Perfor-mance t.b.d.	No 2-qubits yet	Noise	Theoret-ical	Not existing yet	Not univer-sal
QTRL	5	5	5	3	2	3	2	1	8

Table 1. Overview of quantum computing technologies.

2.5.1 eleQtron – A German Ion Trap NISQ GBQC Development

eleQtron, a spin-off of the University of Siegen, is planning to build an ion trap GBQC based on up to 320 $^{171}Yb^{+}$ ions. This is microwave-controlled ion trap technology. In this respect, it differs from systems with laser-based control, for example, and promises easier scalability. A prototype of an 8-qubit NISQ GBQC of this type already exists[26,27]. Features of the eleQtron technology are:

- The qubit control of eleQtron works with microwaves, therefore lasers are not needed for qubit manipulation.
- Operation is possible at room temperature.
- A vibration-damped base is not needed.
- eleQtron has a prototype of 8 qubits today; the company expects 20 to 30 qubits in less than 2 years and 50 to 60 in less than 3 years.
- The qubits are represented by Ytterbium ions.
- The qubit connectivity is all-to-all.
- The one-qubit gate fidelity is 99.9%, the two-qubit gate fidelity is 99.8%.
- The cross talk properties of eleQtron qubits are $< 10^{-4}$ in the Rabi regime and $< 10^{-8}$ in intensity.

With regard to alternative technologies, elecQtron offers a GBQC with proven qubit gates in the best quality currently available.

2.5.2 AQT – An Ion Trap NISQ GBQC from Austria

AQT is a spin-off company from the well known quantum computing group of Innsbruck university. AQT's quantum computer hardware is based on ion trap qubits[28]. AQT differs from eleQtron in that it uses laser-controlled qubits instead of microwaves. Recently, AQT unveiled a quantum computer demonstrator in two 19-inch racks based on $^{40}Ca^{+}$ qubits in a linear Paul trap, evolving from a laboratory-based proof-of-concept experiment to robust, integrated hardware for quantum information processing. It has been shown that the demonstrator can generate maximally entangled Greenberger-Horne-Zeilinger (GHZ) states with up to 24 qubits[29] and that as many as 50 ions can be trapped and cooled. Features of AQT's technology are:

- The qubit control of AQT works with lasers, which allow for faster operation than microwaves.
- Operation is possible at room temperature.
- A vibration-damped base is not needed.
- AQT has a prototype of 24 qubits today; the company expects a mid-term upgrade with 50 qubits and hopes that a quantum computer with more that 100 qubits is feasible based on the given architecture.

- The qubits are represented by calcium ions.
- The qubit connectivity is all-to-all.
- The one-qubit gate fidelity is 99,86%, the two-qubit gate fidelity is 97–99%.
- The resonant crosstalk properties of AQT qubits are $< 1\%$ and the non-resonant crosstalk $< 1.25 \times 10^{-4}$.

Among the ion-trap systems, AQT offers a gate-based system with fastest operation.

2.5.3 IQM – Superconducting NISQ GBQC from Finland

At the end of 2021, IQM installed its first quantum computer with five superconducting qubits. In 2023, IQM plans to deliver a 20-qubit GBQC to supercomputer centres to enable experiments with NISQ algorithms. In 2025, IQM aims to deliver a first commercial 1,000-qubit GBQC called "Prometheus", which IQM expects to achieve superior performance to solve real-world industrial problems. IQM is coordinating the two-year Horizon 2020 project of the very same name, Prometheus, which includes the development of this commercial GBQC. The processors developed in this project could then meet the scale required to run commercially viable quantum algorithms. The processor size also seems sufficient for the implementation of quantum accelerators, *i.e.*, quantum processors installed in large supercomputer centres.

Recently, IQM described its unimon qubit, a superconducting-qubit type, which combines the desired properties of high non-linearity, full insensitivity to DC charge noise, insensitivity to flux noise, and a simple structure consisting only of a single Josephson junction in a resonator[30]. According to IQM the unimon qubit might have the potential to break the 99.99% fidelity limit required for efficient quantum error correction and might achieve possible quantum advantage with noisy systems.

- The qubit control of IQM works with voltage pulses.
- Operation needs cryogenic temperatures.
- Probably, a vibration-damped base is required.
- IQM has announced to operate a prototype with 5 qubits today; the company expects 20 qubits in 2023 and 1000 qubits within 3 years.
- The qubits are represented by superconducting Josephson junctions, named unimon.
- The qubit connectivity is not known.
- The expectation of IQM is that the one-qubit gate fidelity reaches 99.99%.
- The cross talk properties of IQM qubits are not available.

With the target of a qubit fidelity of 99.99% IQM could become a promising candidate for first error corrected quantum computing. Given the required step in scale of more than a factor of 200, it remains to be seen if this goal can be achieved in a time frame of less than three years.

2.5.4 OpenSuperQ, DAQC and Qsolid Quantum Computers

JUNIQ's tasks also include access to quantum computer systems in early stages of development. These systems are mostly laboratory systems or prototype systems. Within this setting, JUNIQ will provide cloud access to experimental quantum computers developed in European and national research projects. The first experimental GBQC that can be accessed by the end of 2022 is a superconducting GBQC with 10 qubits from the quantum flagship project OpenSuperQ[31] launched in 2018.

The digital-analogue quantum computer (DAQC) of IQM that is being built in the eponymous BMBF (Federal Ministry of Education and Research) project DAQC combines the advantages of an analog quantum computer that is not very prone to errors with the flexibility of digital circuits. The DAQC is to be paired with supercomputers and will take over the task of a computing accelerator. Access to the DAQC with 54 superconducting qubits is planned for 2024.

The BMBF project QSolid[32] will develop an integrated, fully HPC-embedded quantum computing demonstration system based on cryogenic superconducting quantum processors integrated in a fully developed hardware system with control, readout and infrastructure down to the specific, optimised firmware and software. The demonstrator will house several processors. In the first phase of the project, QSolid will research high-quality components and demonstrate the technology of the medium-term device, a 10-qubit system in ladder geometry. JUNIQ cloud access to this system is planned for 2024. Based on the lessons learned from this system, three processors based on the same components and technologies will be developed. The goal is to build a GBQC with at least 30 superconducting qubits.

3 Integration Strategy

A central concern of JUNIQ is to integrate the locally installed quantum computers as closely as possible into the HPC environment of the JSC. This is done with respect to running hybrid programs, where parts are carried out on large HPC systems and other parts (will) require the functionality of quantum computers or QAs and QSs. Although this type of use, which is functional parallelism at the highest level of integration, is still in its infancy today, it is nevertheless to be expected that almost all practical applications of quantum computing will be based on this approach. Therefore, developing hardware and software systems as quickly as possible for tightly coupled low-latency use is a priority.

JUNIQ employs the concept of the MSA for the integration. It allows to enable the lowest latency integration of the QA, the imminent QS and the coming GBQCs [c]. Modular operation requires joint scheduling that will ensure an efficient exploitation of available resources.

The quantum computers are used as modules in the MSA, closely coupled with other specific modules such as the general purpose CPU and GPU acceleration systems or a tiered common high speed storage. The low-latency connection to other modules is

[c] Tight integration through the MSA will overcome the latency limitations of the cloud service-based approaches favoured so far by major manufacturers[33]. The danger of the strict cloud approach, however, lies not only in the latency limitation, but rather in the tendency of hyper-scalers to move towards the monopolisation of quantum computing and thus of hybrid HPC-QC services, to the detriment of science and subsequently industry.

achieved via an ultra-high-speed network like the one of Mellanox, but also alternatives exist.

The MSA integration will be enabled by extending ParaStation Modulo™ with an execution environment for hybrid HPC-quantum computing simulations and workflows on modular supercomputers. A portal solution provides convenient and flexible access via a web browser enabling a production-level JupyterHub Portal[34] (HPC-PaaS and QC-PaaS).

JUNIQ and HPCQS work on the integration of the QPU's system software and its front-end software system into the full management stack of the modular supercomputer including user and software management, storage access, and provisioning.

JUNIQ provides a full hybrid software stack including compilers, technical libraries and tools, that will allow users to translate use cases into quantum programs without having to deal with low-level instructions.

4 Exemplary Application: Simplified Tail Assignment Problem

To give a representative impression of the work being carried out at JSC as part of JUNIQ, we consider computational results for the simplified tail assignment problem, a potential application for both QAs and GBQCs investigated as part of the European Quantum Flagship's OpenSuperQ project[35,36] and of JUNIQ[18]. These considerations demonstrate the different degrees of maturity of QAs and GBQCs as well as the importance of the intrinsic scalability of quantum algorithms per se.

Airlines are faced with one of the largest and most challenging planning problems required to be solved regularly. For example, an airline might need to plan and operate over 1000 flights per day to over 150 cities in over 70 countries, using hundreds of aircraft of different types. The most significant expenses for an airline often consist of costs associated with aircraft and flight crew. Obtaining optimised plans for crew and aircraft while respecting regulations imposed by aviation authorities, airlines and unions is thus crucial and non-trivial. The problem called tail assignment (TAP) describes a mathematical optimisation model with constraints that when solved can provide airlines with efficient plans for how to use their aircraft. In the TAP, the task is to assign a set of airplane flights between airports to a set of routes, which are sets of flights operated in sequence by the same airplanes. The name "tail assignment" comes from the fact that each aircraft is identified by the registration number on its tail fin, its tail number. Quantum computers may provide new methods to help solving the TAP in the future.

In order to simplify the optimisation problem for studying it with real quantum computing devices Vikstål *et al.* and Willsch *et al.* considered the simplified TAP for which each flight has to be covered exactly once (no overlapping routes) and for which all flight costs are equal to zero[18,35,36]. This simplified version of the TAP is an exact cover problem, which in matrix form reads

$$\min_{x_r=0,1} \sum_{f=0}^{F-1} \left(\sum_{r=0}^{R-1} A_{rf} x_r - 1 \right)^2 , \tag{3}$$

where $r = 0, \ldots, R-1$ enumerates all routes, $f = 0, \ldots, F-1$ enumerates the flights, $x_r \in \{0,1\}$ are the Boolean problem variables with $x_r = 1$ if route r is to be selected, $A_{rf} \in \{0,1\}$ are the elements of the constraint matrix A with $A_{rf} = 1$ if flight f is contained in route r. The QUBO and Ising formulations of the exact cover problem are given in Ref. 36.

On the D-Wave QA, Willsch *et al.* studied exact cover problems corresponding to a series of realistic airline problem instances obtained by random sampling from a real-world data set with up to $N = 40$ routes, each of which contains several out of 472 flights[36]. The exact cover problem is to find a selection of the N routes to carry out the 472 flights between the airports so that the routes do not overlap. On a quantum computer, each route is represented by a qubit. If a route is to be selected, the corresponding qubit ends up in the state $|1\rangle$ when measured. By construction, the ground state of each problem instance, an N-qubit problem, is unique and contains 9 qubits in state $|1\rangle$. This means that the solution consists of nine routes. Each route is assigned to an aircraft. All other states represent invalid solutions, in the sense that not all 472 flights are covered exactly once. For 40 routes the number of possible selections is $2^{40} \approx 10^{12}$. For 120 routes, corresponding to a 120 qubit-problem, the number of selections already grows to 10^{36}.

The particular problem instance for $N = 40$, illustrated in Fig. 4, translates into a quantum optimisation problem with 40 qubits that is almost fully connected (711 of 780 couplers $J_{i,j}$ are non-zero). Hence, solving this problem requires couplers that do not physically exist on the QPU of the D-Wave annealers DW2000Q and JUPSI, the Advantage 5.1 system. The 2000+ (5000+) physical qubits of the DW2000Q QPU (JUPSI) are connected in a Chimera (Pegasus) topology to 6 (15) other physical qubits on average. Hence, in order to solve the problem it has to be embedded on the D-Wave QPU. With the embedding, the effective connectivity between the qubits is increased by combining several physical qubits into a logical qubit. The physical qubits that form a logical qubit are called a chain. In order to ensure that the physical qubits within a chain operate as a single logical qubit, the couplers $J_{i,j}$ between the physical qubits are set to a reasonably large, negative value called the chain strength. The relative chain strength is defined as the ratio of the chain strength and the maximum strength, which is the maximum absolute value of all h_i and $J_{i,j}$, and thus takes values between zero and one.

Embeddings, mappings from each logical qubit to a chain of physical qubits, are not unique and may considerably affect the quality of the solution. Therefore, in benchmarking studies it is important to investigate different embeddings and relative chain strengths.

Fig. 5 shows results for exact cover problems that correspond to the simplified TAP with 472 flights described above, with 30, 36 and 40 routes (*i.e.*, logical qubits), respectively[36]. Because these problems have a unique ground state the success rate can be calculated. It is obtained by counting the number of samples with energy zero. For each problem 10 different embeddings were generated and the success rate was evaluated as a function of the relative chain strength. It can be seen that the results obtained on the D-Wave Advantage system are generally much better than those obtained on the D-Wave 2000Q, especially for the larger problems. The reason for this is that the problems are almost fully connected, which makes them more suitable to be embedded on the Pegasus topology of the QPU of the Advantage system.

In order to assess the performance of both QAs for larger but more sparsely connected problem instances Willsch *et al.* studied exact cover problems with 50 to 120 logical qubits[36]. For each problem size, they considered six problem instances. The exact cover problems correspond to a simplified TAP as described above, but with 535 flights. Also for these problems the ground state is unique and known. It has 40 qubits in the state $|1\rangle$.

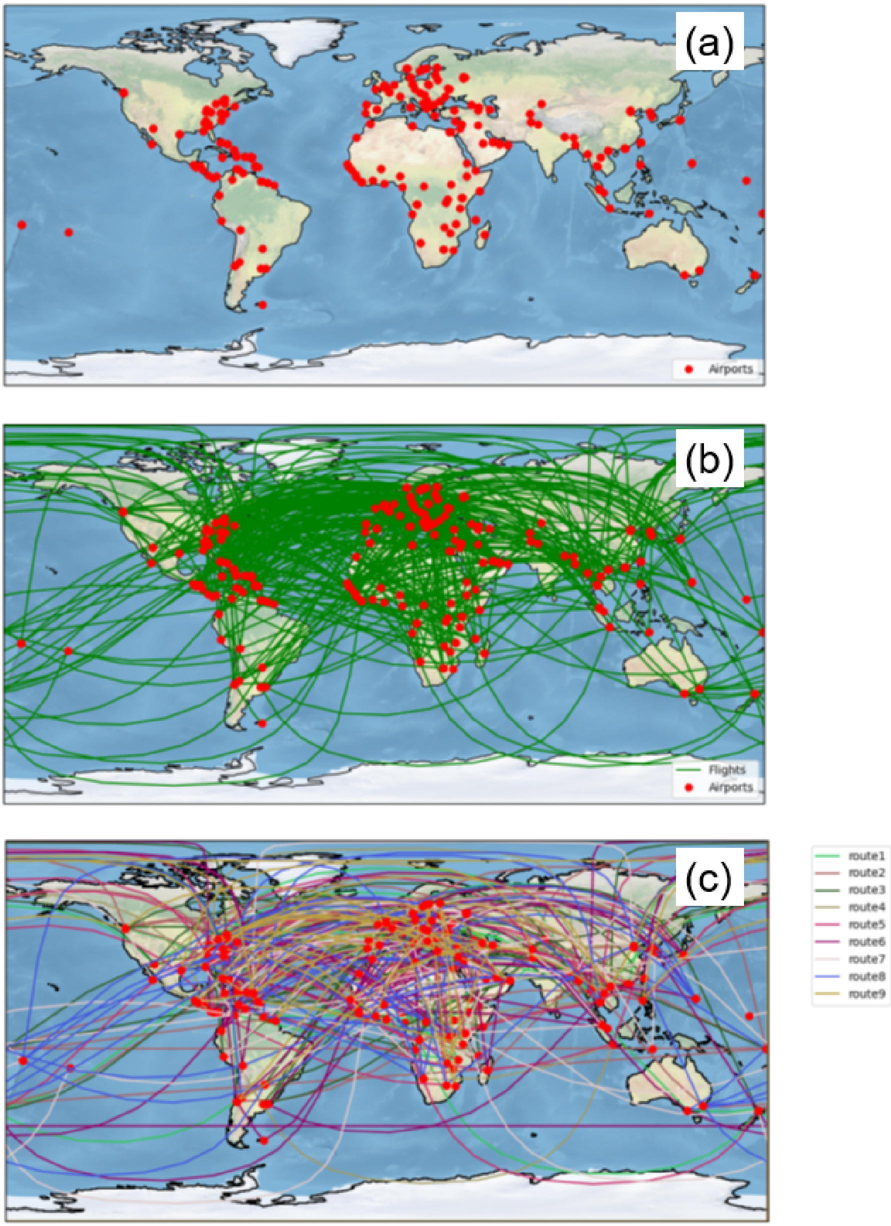

Figure 4. Problem instance of a TAP. (a) airports that are involved; (b) the 472 flights between the airports that have to be performed; (c) unique solution with 9 routes covering the 472 flights exactly once.

The success rates as a function of the relative chain strength are shown in Fig. 6. It is seen that in general for these larger problems the success rates are smaller and that the

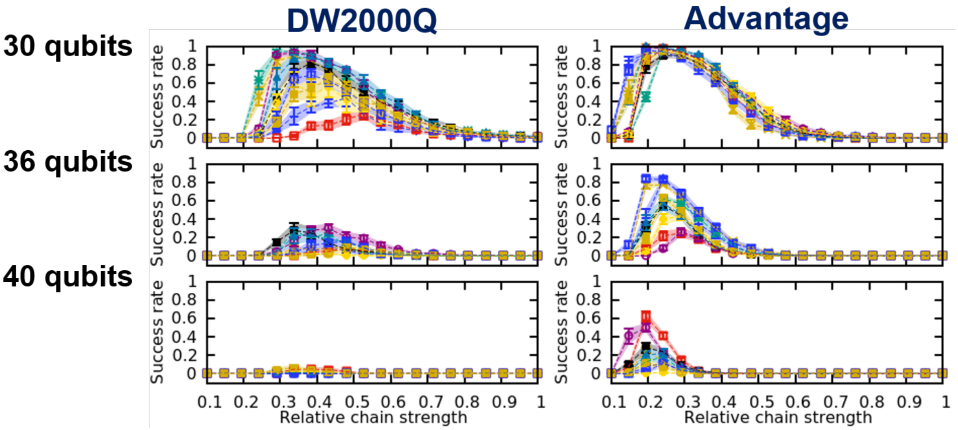

Figure 5. Success rates as a function of the relative chain strength for exact cover problems with 30, 36 and 40 logical qubits that have 90% of nonzero couplers, solved on a D-Wave 2000Q (DW_2000Q_VFYC_6) and an Advantage system (Advantage_system1.1) with the default annealing time 20μs. The scan of the relative chain strength is repeated for 10 different, randomly generated embeddings (represented by different colours) and with 10 repetitions each to gather statistics. Markers indicate the corresponding standard deviation above and below the mean. Filled areas between the markers are guides to the eye.

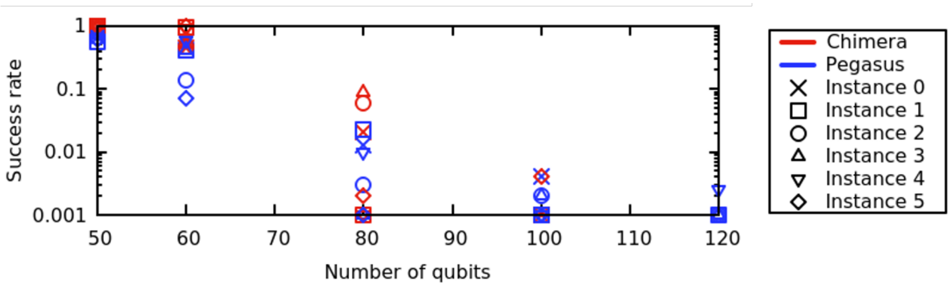

Figure 6. Success rates a function of the relative chain strength for exact cover problems with 50-120 logical qubits that have 20% of nonzero couplers, solved on a D-Wave 2000Q (DW _2000Q_VFYC_6) and an Advantage system (Advantage_system1.1). Different markers indicate different problem instances. The annealing times and the number of reads have been varied from 20μs to 2000μs and from 400 to 1000, respectively, in order to find a solution within the maximum run time of the systems (for more details, see Ref. 36).

D-Wave 2000Q is not able to solve the largest problems anymore.

For cross-platform benchmarking purposes, Willsch *et al.* also solved the simplified TAP with 40 qubits by means of QAOA and the approximate quantum annealing algorithm (AQA) for GBQCs. For this purpose they used JUQCS on JUWELS Booster. In this case JUWELS plays the role of an ideal QPU of a GBQC with all-to-all connectivity. Results of this study can be found in Ref. 18 and in this volume. The overall result of the cross-platform benchmarking study is that for this type of problems the D-Wave QA outperforms the ideal GBQC running QAOA in terms of the success rate for finding a solution.

5 Future of JUNIQ – A Visionary Roadmap

The currently observed and enjoyed acceptance of both its simulation service JUQCS and the D-Wave QA speaks strongly for JUNIQ's chosen strategy of bringing users as close as possible to the resources and as early as possible. While it is clear that active use of the systems in HPC production tasks cannot yet take place, we expect that the modular connection of the systems will happen in the next future, especially through the positive pressure of the HPCQS project and other activities at JSC, which are currently still under NDA and cannot yet be described here.

In mid-2022, JUNIQ plans to offer cloud access to the OpenSuperQ system at FZJ/PGI, and a Pasqal quantum simulator will be installed in the JUNIQ building in mid-2023. Cloud access to the digital-analog IQM DAQC system will be available in mid-2024.

As Fig. 7 demonstrates, it is intended to go into an upgrade of JUNIQ by the end of 2024 (a project called JUNIQ-Upgrade). Besides an upgrade of the D-Wave QA, the installation of a strong GBQC is planned, which will be connected directly with the coming exascale supercomputer JUPITER for execution of hybrid HPC-QC simulations

As the core of the Jülich HPCQS coordination activities, JUNIQ will thus be able to set the tone for the chosen European path towards an integrated and federated EuroQCS (European Quantum Computing and Simulation) infrastructure[33]. This will be done in parallel and in coordination with the expansion of the federation of European HPC systems. It is expected that EuroHPC JU will want to establish quantum computing systems at all pre-exascale and exascale systems, and possibly also at midrange sites.

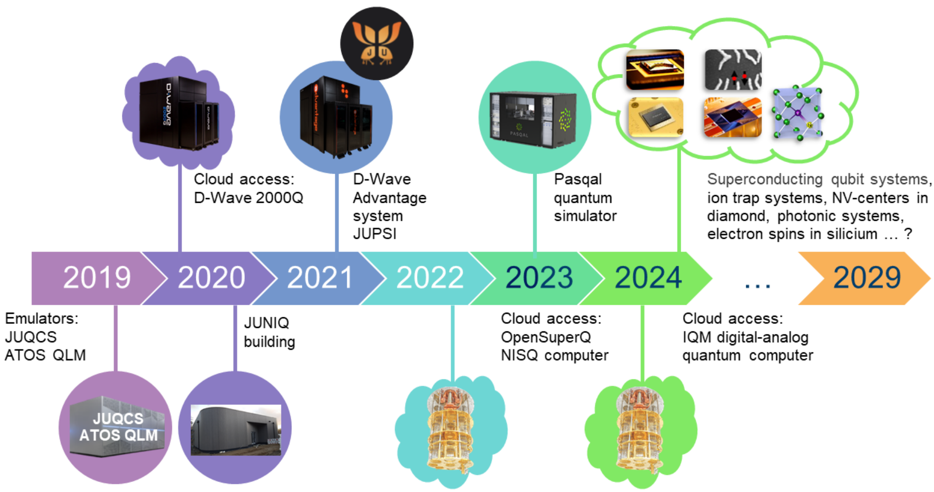

Figure 7. Roadmap JUNIQ.

6 Summary and Outlook

JUNIQ is a manufacturer-independent, comprehensive quantum computing user facility integrated in the Jülich Supercomputing Centre, with peer-reviewed access for European users from academia and industry. As such JUNIQ is a first step towards EuroQCS.

JUNIQ will offer four categories of computing systems that emulate or directly exploit quantum effects: the existing quantum computing emulator JUQCS can emulate ideal "pen-&-paper" quantum computers with up to 43 qubits on JUWELS, and the D-Wave quantum annealer JUPSI, which is in operation since begin of 2022, allows to treat optimisation problems, classification problems, and quantum simulations on more than 5000 qubits.

We have presented the tail assignment problem as an exemplary application to understand the ideal GBQC by means of the emulator JUQCS and to compare to the annealer.

The Pasqal quantum simulator JURY, to be implemented in the JUNIQ building in mid-2023, will enable the simulation of quantum spin systems and the Heisenberg model, as well as the QAOA and VQE algorithms. We have also presented three variants of gate-based quantum systems that are candidates in JUNIQ and have achieved a QTRL of 5. In addition, access will be provided to early stage experimental systems.

We have presented JUNIQ's unique integration strategy, where quantum computers become modules of the JSC HPC environment to realise functional parallelism at the highest parallel system level.

JUNIQ is the first infrastructure of its kind in the world to offer computing time on multiple systems on the basis of a call for user project submissions, in the same way as for HPC, with the difference that it is a rolling call for which submissions can be made at any time. Administrative support for the allocation is already provided by the Office for Computing Time Allocation at JSC, which carries out these tasks for the John-von-Neumann Institute and the Gauss Centre for Supercomputing (GCS).

We can expect the demand for hybrid QC-HPC computing to grow strongly in the next few years, as it is this type of application that allows the first productive use of quantum computers. With the realisation of the modular integration of quantum computers in JUNIQ into the HPC environment of the JSC, the allocation of QPU computing time is to be joined with the allocation processes of the NIC and GCS, in the same way as GPU resources have been put forward some years ago. There is a well-founded expectation that quantum computers can already play an important role in connection with the upcoming exascale supercomputer JUPITER.

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References

1. R. P. Feynman, *There's Plenty of Room at the Bottom*, Engineering and Science **23**, 22–36, 1960.
2. R. P. Feynman, *Simulating Physics with Computers*, Int. J. Theor. Phys. **21**, 467–488, 1982, doi:10.1007/BF02650179.
3. `https://www.dwavesys.com/resources/white-paper/the-d-wave-advantage-system-an-overview/`
4. `https://www.fz-juelich.de/en/ias/jsc/systems/quantum-computing/juniq-facility/juniq/d-wave-advantagetm-system-jupsi`
5. M. Born, V. Fock, *Beweis des Adiabatensatzes*, Z. Physik **51**, 165–180, 1928, doi:10.1007/BF01343193.
6. M. A. Nielsen and I. L. Chuang, *Quantum Computation and Quantum Information*, Cambridge University Press, 2000.
7. J. Preskill, *Quantum Computing in the NISQ era and beyond*, Quantum **2**, 79, 2018, doi:10.22331/q-2018-08-06-79.
8. `https://pasqal.io/`
9. `https://www.nasa.gov/directorates/heo/scan/engineering/technology/technology_readiness_level`
10. `https://www.fz-juelich.de/en/ias/jsc/about-us/structure/research-groups/qip/technology-readiness-level-of-quantum-computing-technology-qtrl`
11. `https://www.deep-projects.eu/`
12. G. Hager and G. Wellein, *Introduction to High Performance Computing for Scientists and Engineers*, Chapman and Hall / CRC computational science series, CRC Press, 2011.
13. A. Kreuzer, E. Suarez, N. Eicker, and Th. Lippert (ed.) *Porting applications to a Modular Supercomputer – Experiences from the DEEP-EST project*, Forschungszentrum Jülich GmbH, Zentralbibliothek, Verlag, 2021.
14. `https://www.hpcqs.eu/`
15. `https://www.fz-juelich.de/en/ias/jsc/systems/quantum-computing/juniq-facility`
16. H. De Raedt et al., *Quantum Computer Emulator*, Comput. Phys. Commun. **132**, 1–20, 2000.
17. K. De Raedt et al., *Massively Parallel Quantum Computer Simulator* Comput. Phys. Commun. **176**, 121–136, 2007, doi:10.1016/j.cpc.2006.08.007.
    H. De Raedt et al., *Massively parallel quantum computer simulator, eleven years later*, Comput. Phys. Commun. **237**, 47–61, 2019, doi:10.1016/j.cpc.2018.11.005.
18. D. Willsch et al., *GPU-accelerated simulations of quantum annealing and the quantum approximate optimization algorithm*, Comput. Phys. Commun. **278**, 108411, 2022, doi:10.1016/j.cpc.2022.108411.
19. D. Willsch et al., *Benchmarking supercomputers with the Jülich Universal Quantum Computer Simulator*, NIC Symposium 2020, Publication Series of the John von Neumann Institute for Computing (NIC), NIC Series 50, 255–264, 2020.
20. `https://www.hpcwire.com/2010/06/28/quantum_computer`

_simulation_new_world_record_on_jugene/
https://www.hpcwire.com/2017/12/18/world-record-quantum-computer-46-qubits-simulated/
https://www.aachener-zeitung.de/lokales/juelich/juelicher-forscher-team-haelt-weltrekord-im-simulieren-eines-quantencomputers_aid-24383883

21. M. Willsch et al., *Benchmarking the quantum approximate optimization algorithm*, Quant. Inf. Proc. **19**, 197, 2020, doi:10.1007/s11128-020-02692-8.
22. F. Arute et al., *Quantum supremacy using a programmable superconducting processor*, Nature **574**, 505–510, 2019, doi:10.1038/s41586-019-1666-5.
23. M. S. Jattana et al., *Assessment of the variational quantum eigensolver: application to the Heisenberg model*, Front. Phys., doi: 10.3389/fphy.2022.907160.
24. H. De Raedt and K. Michielsen, *Computational Methods for Simulating Quantum Computers*, Handbook of Theoretical and Computational Nanotechnology, Vol. 3: Quantum and molecular computing, quantum simulations, Chapter 1, M. Rieth and W. Schommers eds., American Scientific Publisher, Los Angeles, 248, 2006.
    D. Willsch et al., *Gate-error analysis in simulations of quantum computers with transmon qubits*, Phys. Rev. A **96**, 062302, 2017.
    M. Willsch et al., *Real-time simulation of flux qubits used for quantum annealing*, Phys. Rev. A **101**, 012327, 2020.
    H. Lagemann et al., *Numerical analysis of effective models for flux-tunable transmon systems*, arXiv:2201.02402.
25. https://www.hpcwire.com/off-the-wire/europes-first-quantum-computer-with-more-than-5k-qubits-launched-at-julich/
    https://www.youtube.com/watch?v=oeFBhBMv0fk
26. C. Piltz et al., *A trapped-ion-based quantum byte with* 10^{-5} *next-neighbour cross-talk*, Nat. Commun. **5**, 4679, 2014, doi:10.1038/ncomms5679.
27. https://www.eleqtron.com/en/
28. I. Pogorelov et al., *Compact Ion-Trap Quantum Computing Demonstrator*, PRX QUANTUM **2**, 020343, 2021, doi:10.1103/PRXQuantum.2.020343.
29. D. M. Greenberger et al., *Going Beyond Bell's Theorem.* In: M. Kafatos (eds), Bell's Theorem, Quantum Theory and Conceptions of the Universe, Fundamental Theories of Physics, vol. 37, Springer, Dordrecht, 69–72, 1989, doi:10.1007/978-94-017-0849-4_10.
30. E. Hyyppä et al., *Unimon qubit*, arXiv:2203.05896.
31. https://opensuperq.eu/
32. https://www.q-solid.de/
33. https://qt.eu/about-quantum-flagship/newsroom/european-quantum-computing-simulation/
34. https://jupyter-jsc.fz-juelich.de/hub/login
35. P. Vikstål et al., *Applying the Quantum Approximate Optimization Algorithm to the Tail Assignment Problem*, Phys. Rev. Appl. **14**, 034009, 2020, doi:10.1103/PhysRevApplied.14.034009.
36. D. Willsch et al., *Benchmarking Advantage and D-Wave 2000Q quantum annealers with exact cover problems*, Quantum Inf. Process. **21**, 141, 2022, doi:10.1007/s11128-022-03476-y.