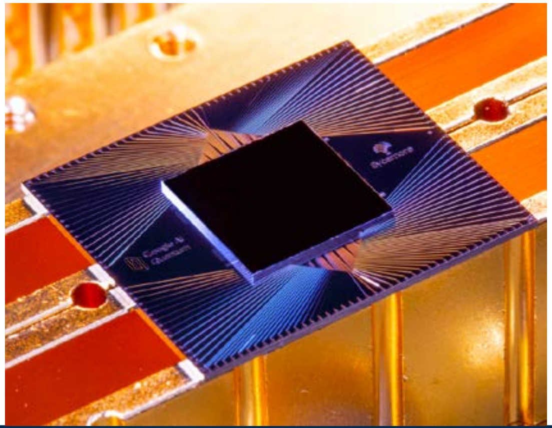
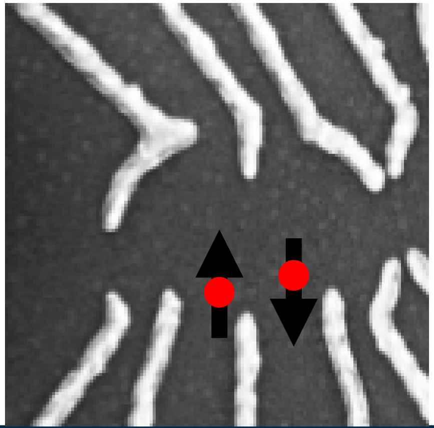


JUNIQ – JÜLICH UNIFIED INFRASTRUCTURE FOR QUANTUM COMPUTING

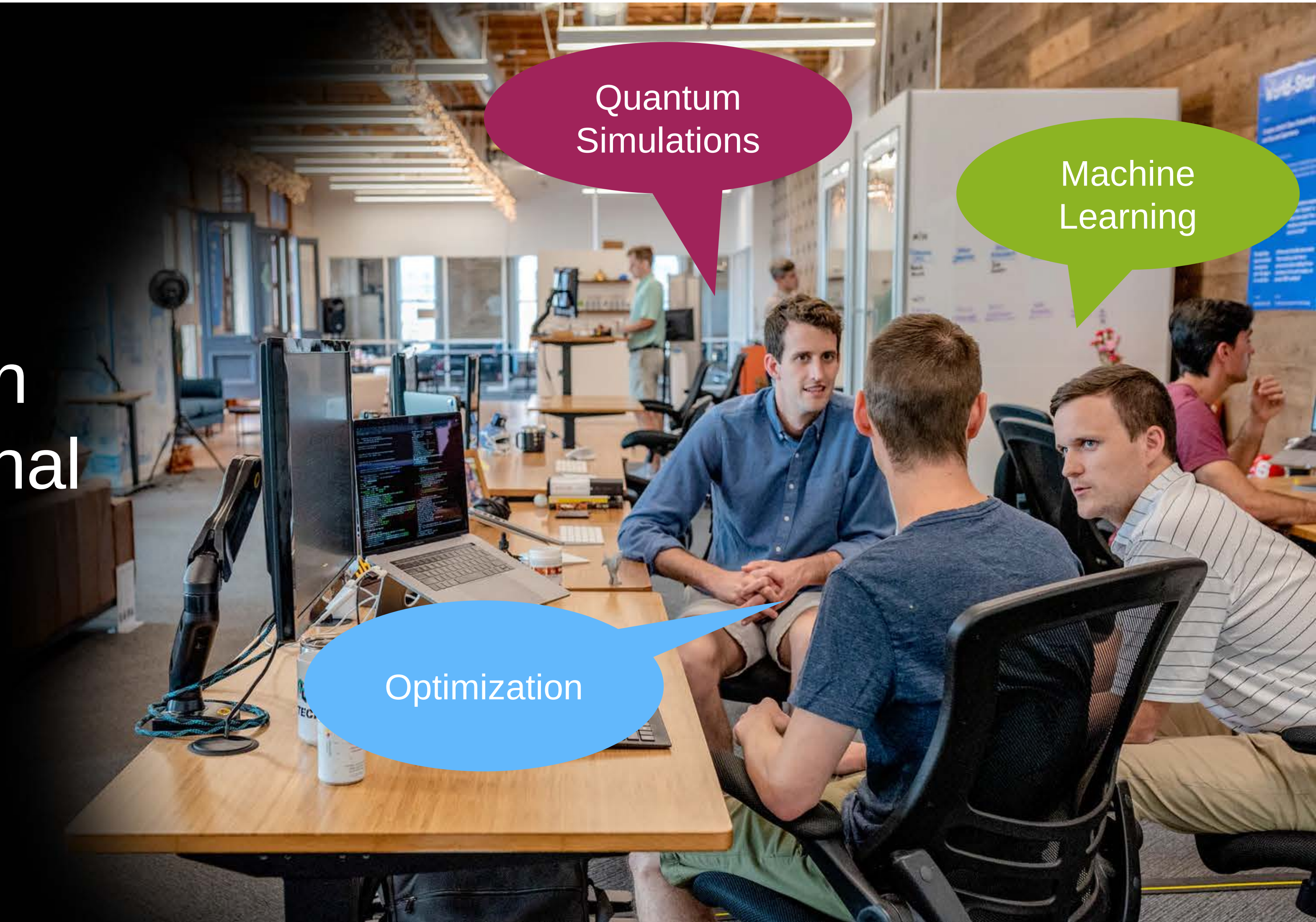
ZKI-AK SUPERCOMPUTING | SEPTEMBER 10 -11, 2020 | KRISTEL MICHIELSEN

JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

QUANTUM COMPUTING:

new, disruptive compute technology

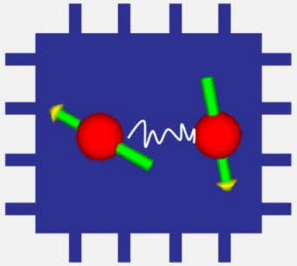
Science & Industry:
Diverse user group with various hard computational challenges to unravel complex systems



QUANTUM TECHNOLOGY READINESS LEVELS

QTRL

Quantum Technology Readiness Levels describing the maturity of Quantum Computing Technology

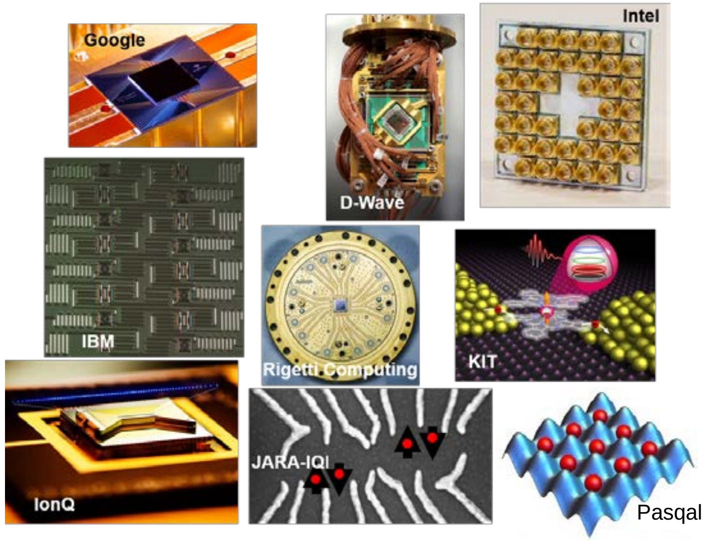


- **QTRL9** QCs (QAs) exceed power of classical computers
- **QTRL8** Scalable version of QC (QA) completed and qualified in test
- **QTRL7** Prototype QC (QA) built solving small but user-relevant problems
- **QTRL6** Components integrated in small quantum processor w/ error correction
- **QTRL5** Components integrated in small quantum processor w/o error correction
- **QTRL4** Multi-qubit system fabricated; classical devices for qubit manipulation developed
- **QTRL3** Imperfect physical qubits fabricated
- **QTRL2** Applications / technologically relevant algorithms formulated
- **QTRL1** Theoretical framework for quantum computation (annealing) formulated

D-Wave
Quantum Annealing

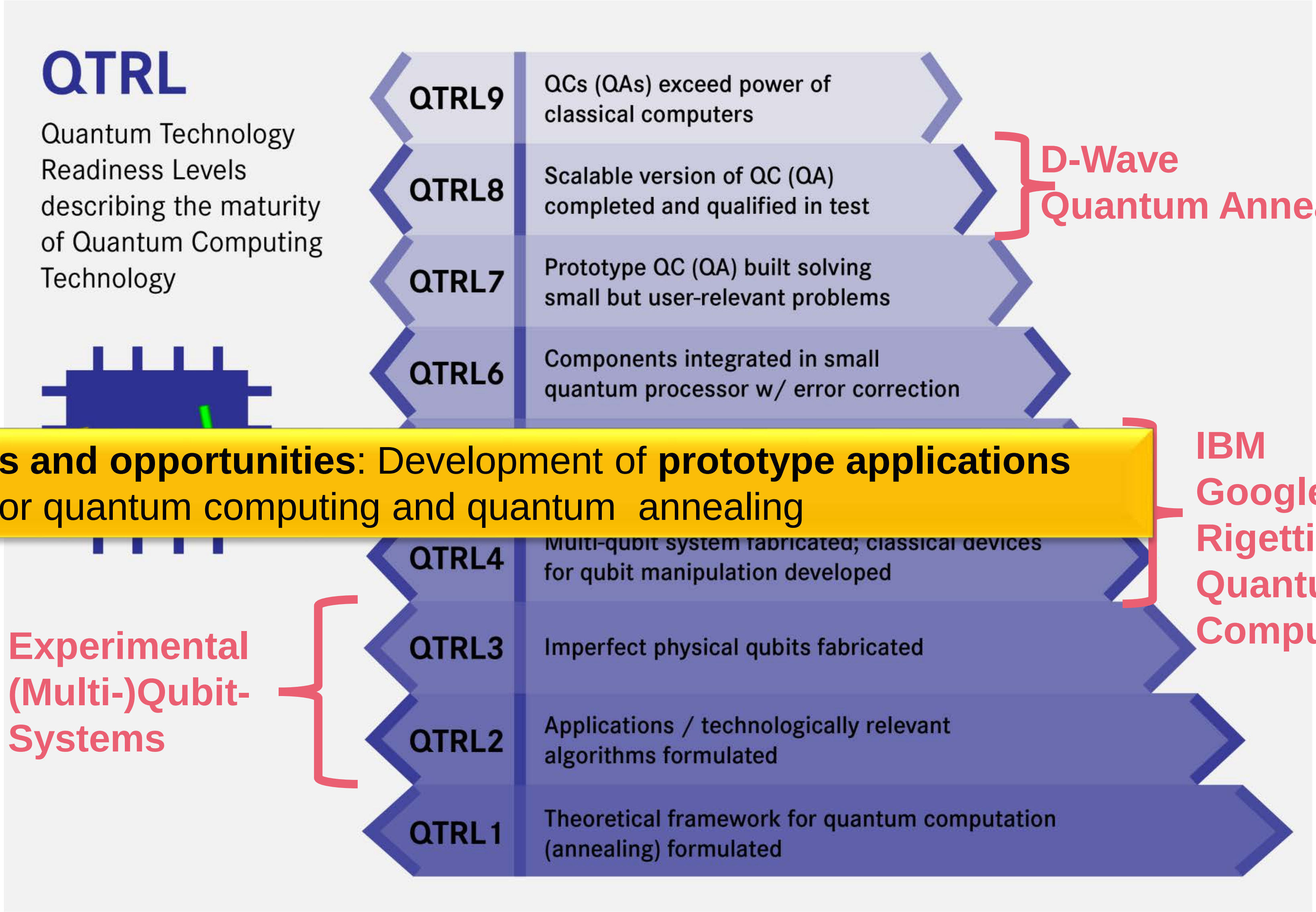
IBM
Google
Rigetti
Quantum
Computing

Experimental
(Multi-)Qubit-
Systems



(http://www.fz-juelich.de/ias/jsc/EN/Research/ModellingSimulation/QIP/QTRL/_node.html)

QUANTUM TECHNOLOGY READINESS LEVELS

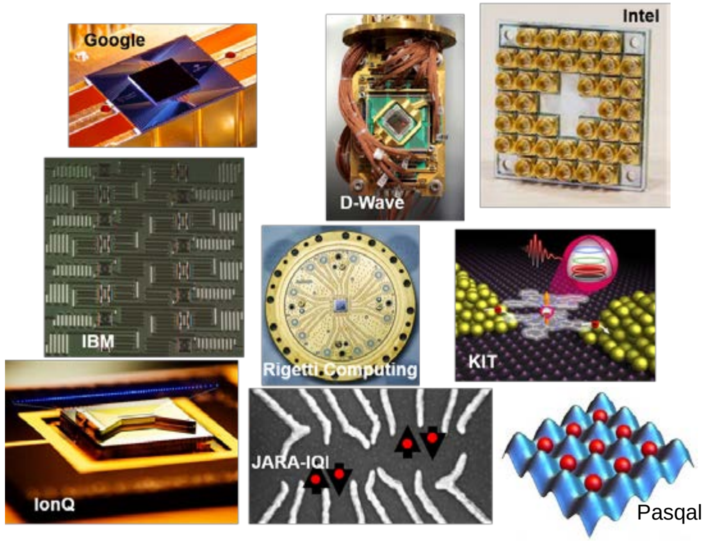


Huge challenges and opportunities: Development of **prototype applications and use cases** for quantum computing and quantum annealing

D-Wave
Quantum Annealing

IBM
Google
Rigetti
Quantum
Computing

Experimental (Multi-)Qubit-Systems



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(http://www.fz-juelich.de/ias/jsc/EN/Research/ModellingSimulation/QIP/QTRL/_node.html)

HIGH PERFORMANCE & QUANTUM COMPUTERS

linked, to solve problems optimally

High Performance Computers

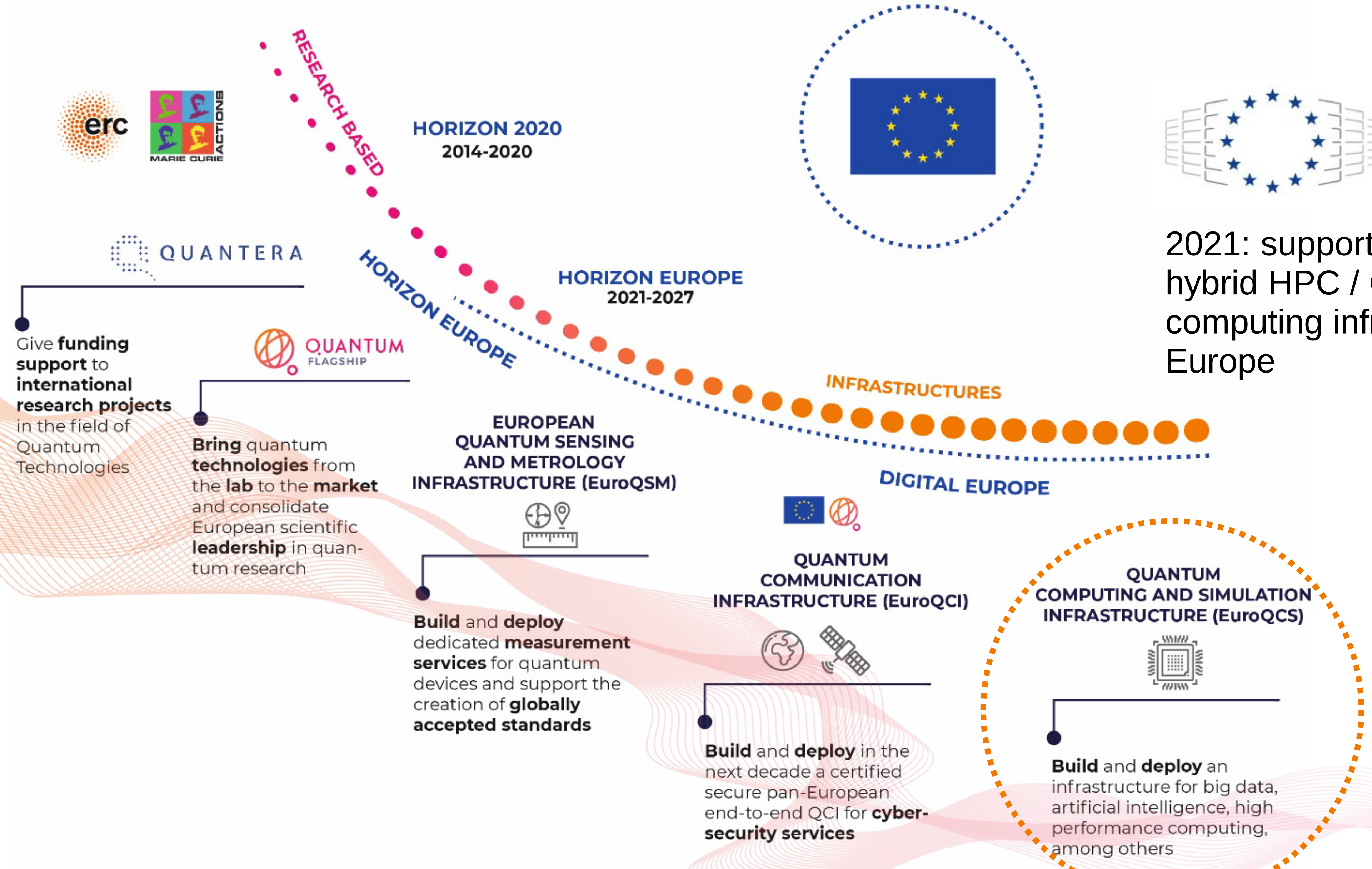
HPC simulations of quantum computing / annealing devices

Quantum Computers & Annealers

Understanding – Design – Benchmarking

(Hybrid) simulations for applications

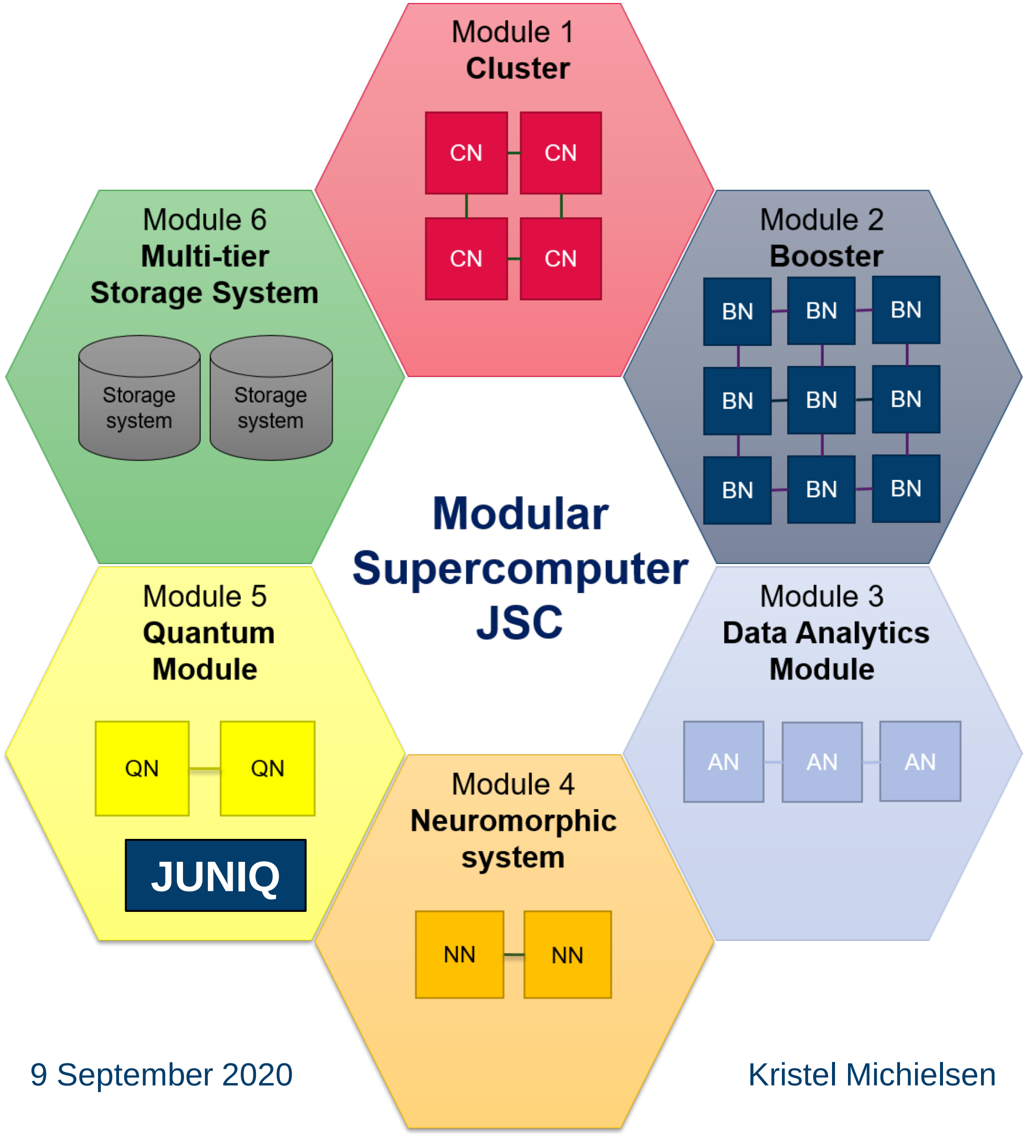
From Vision to Reality – the EU's commitment



2021: support for the first hybrid HPC / Quantum computing infrastructure in Europe

JUNIQ - Jülich UNified Infrastructure for Quantum computing

Building a European quantum computer user facility at the Jülich Supercomputing Centre



JUNIQ - Jülich UNified Infrastructure for Quantum computing

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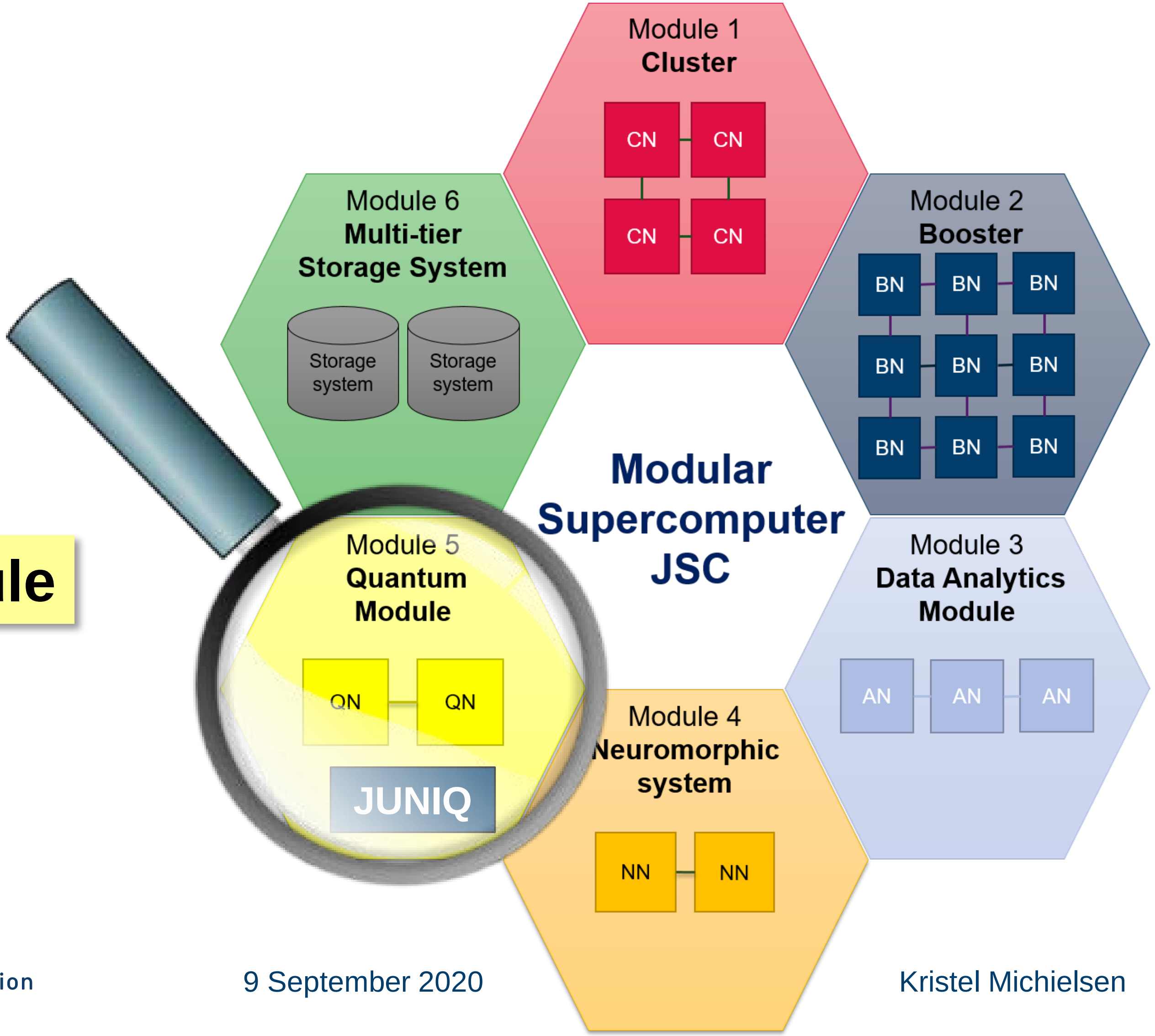
Quantum Module



Perspective:
Quantum-Classical
Hybrid Computing Models

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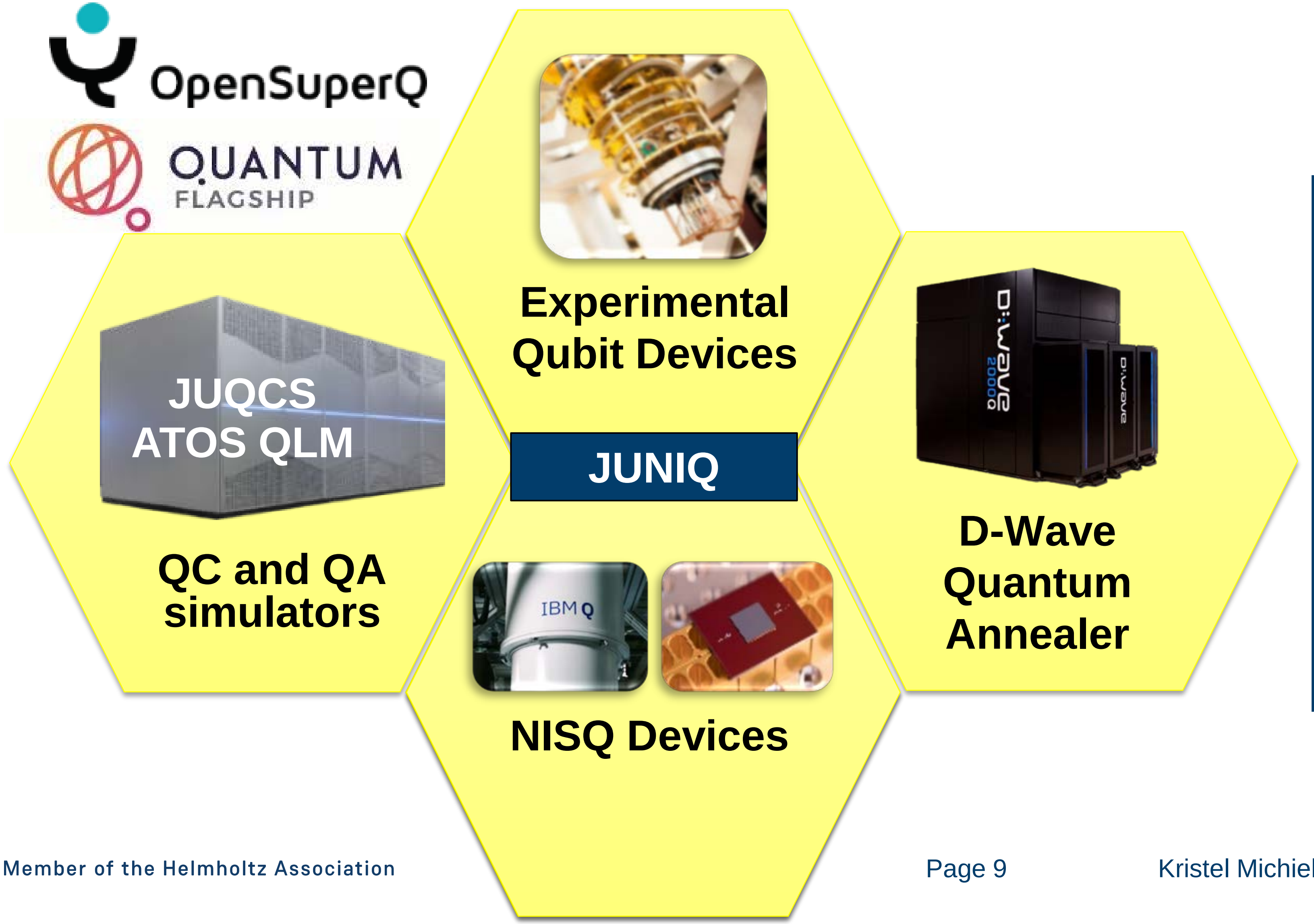
JUNIQ - Jülich UNified Infrastructure for Quantum computing

Building a European quantum computer user facility at the Jülich Supercomputing Centre

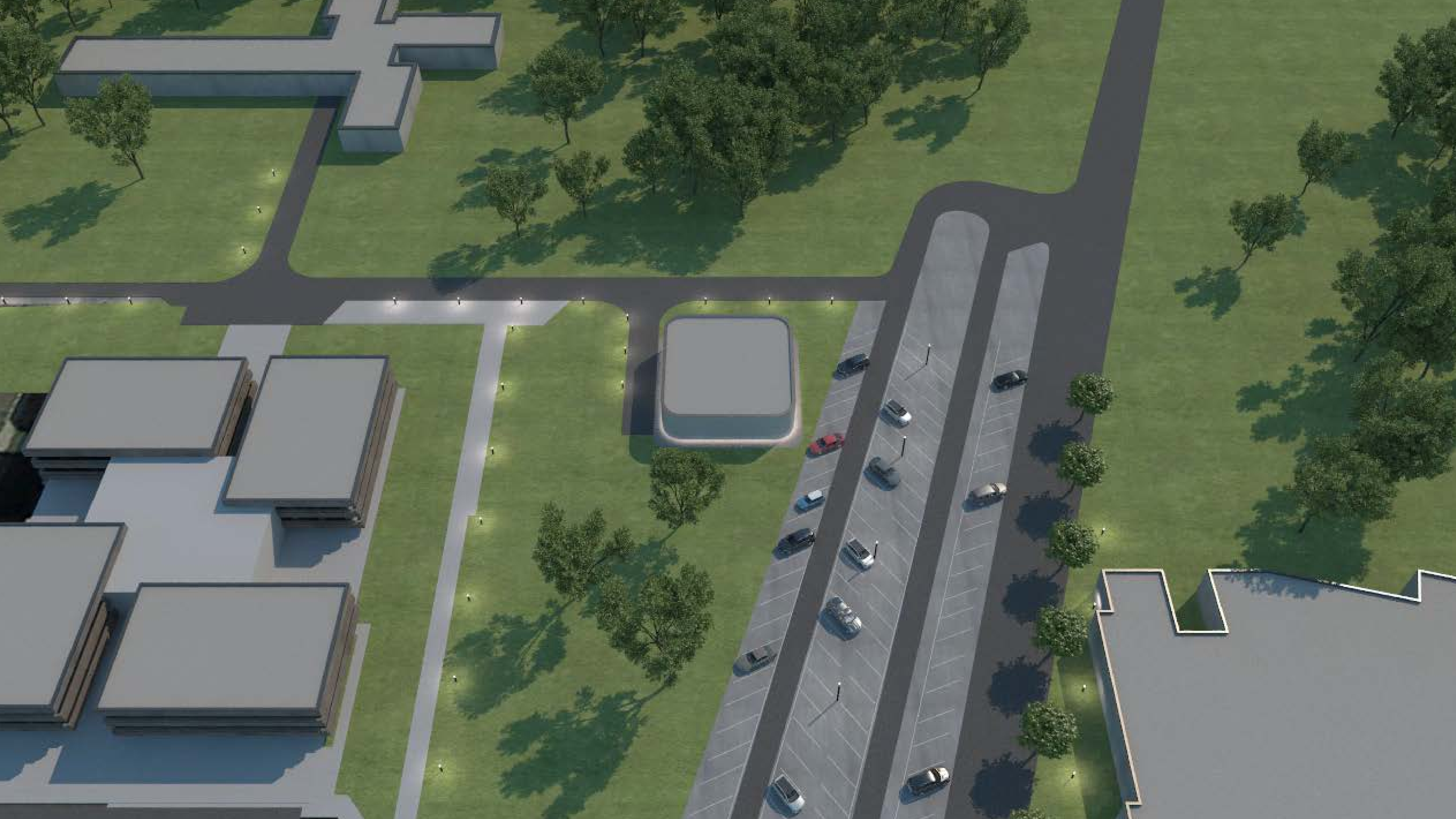
OpenSuperQ

QUANTUM FLAGSHIP

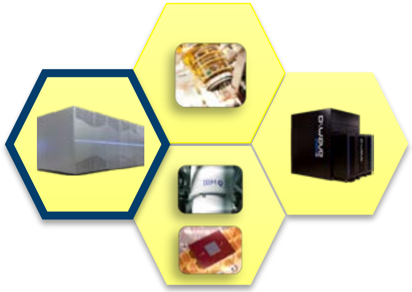


- Uniform portal for access to quantum computer simulators and quantum computer technologies at different levels of maturity
- Development of quantum algorithms, protocols, tools and prototype use cases
- User support and training in HPC and QC usage

JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE



SIMULATORS



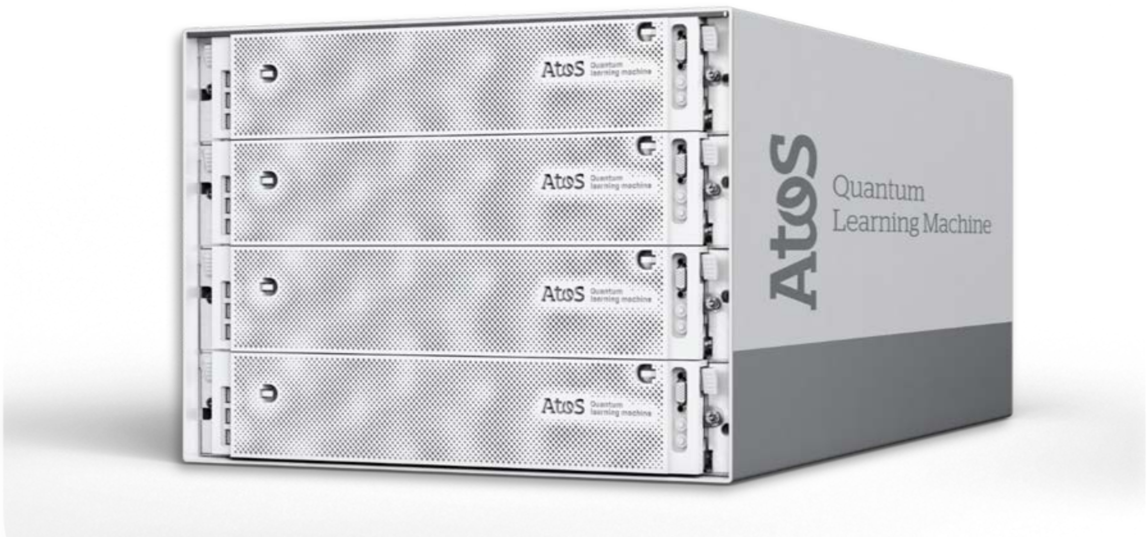
48 Qubits

K
Kobe, Japan

Sunway TaihuLight
Wuxi, China

45 Qubits

JUWELS
Jülich, Germany



30 Qubits

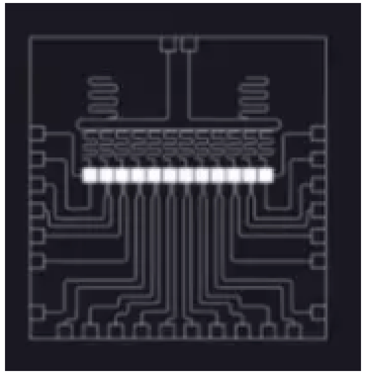
JUQCS – Jülich Universal Quantum Computer Simulator

ATOS Quantum Learning Machine QLM-30

JUQCS - BENCHMARKING

IBM QX and CAS-Alibaba quantum processors

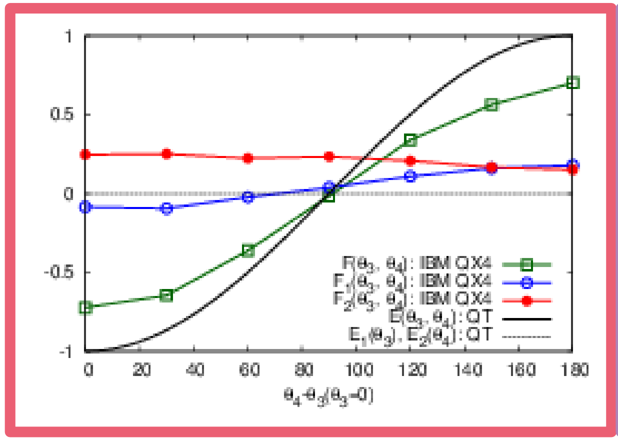
IBM QX, Yorktown Heights, USA

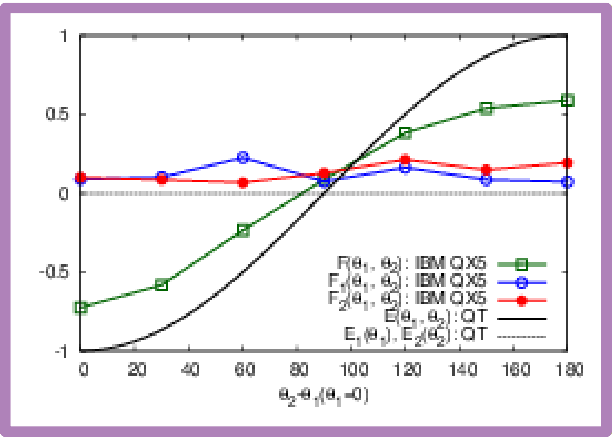


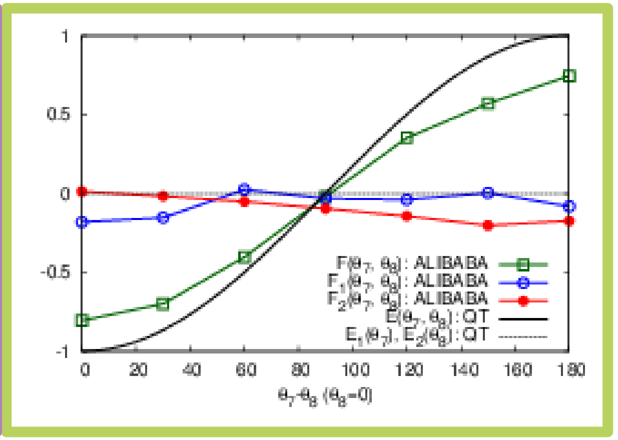
Alibaba Quantum Laboratory, China

Performance test (2018) of the quantum processors **IBM QX4** (5 qubits), **IBM QX5** (16 qubits) and **CAS-Alibaba** (11 qubits) processors

- Simple algorithms: measurement of singlet state







Conclusion: The results only qualitatively agree with quantum theory.

Deviations are not within 5 standard deviations.

K. Michielsen et al., *Simulation on and HPC simulation of quantum computers and annealers*, in Future Trends of HPC in a Disruptive Scenario, eds. Grandinetti, L. et al., Advances in Parallel Computing 34 (IOS Press, Amsterdam, 2019), pp. 101 - 119

JUQCS - BENCHMARKING

Google Sycamore quantumprocessor

QUANTUM SUPREMACY

marks the moment when a quantum computer, for the first time, outperforms state-of-the-art conventional computers for a specific task

ACHIEVED

with Google’s 53 qubit quantum processor
SYCAMORE

AND PUBLISHED

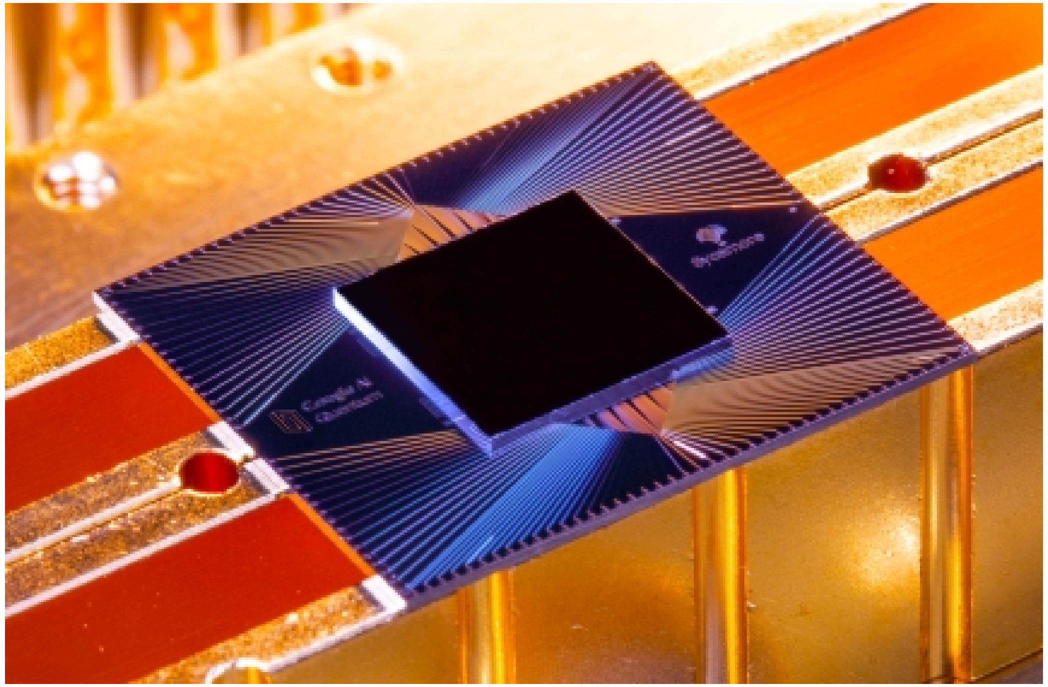
F. Arute et al., *Quantum supremacy using a programmable superconducting processor*, Nature 574, 505-510 (2019)

Quantum supremacy:
A milestone in quantum computing

JUQCS - BENCHMARKING

Google Sycamore quantumprocessor

BENCHMARKING SYCAMORE



WITH SUPERCOMPUTERS

Google clusters

SUMMIT
Oak Ridge National Laboratory

JUWELS
Jülich Supercomputing Centre

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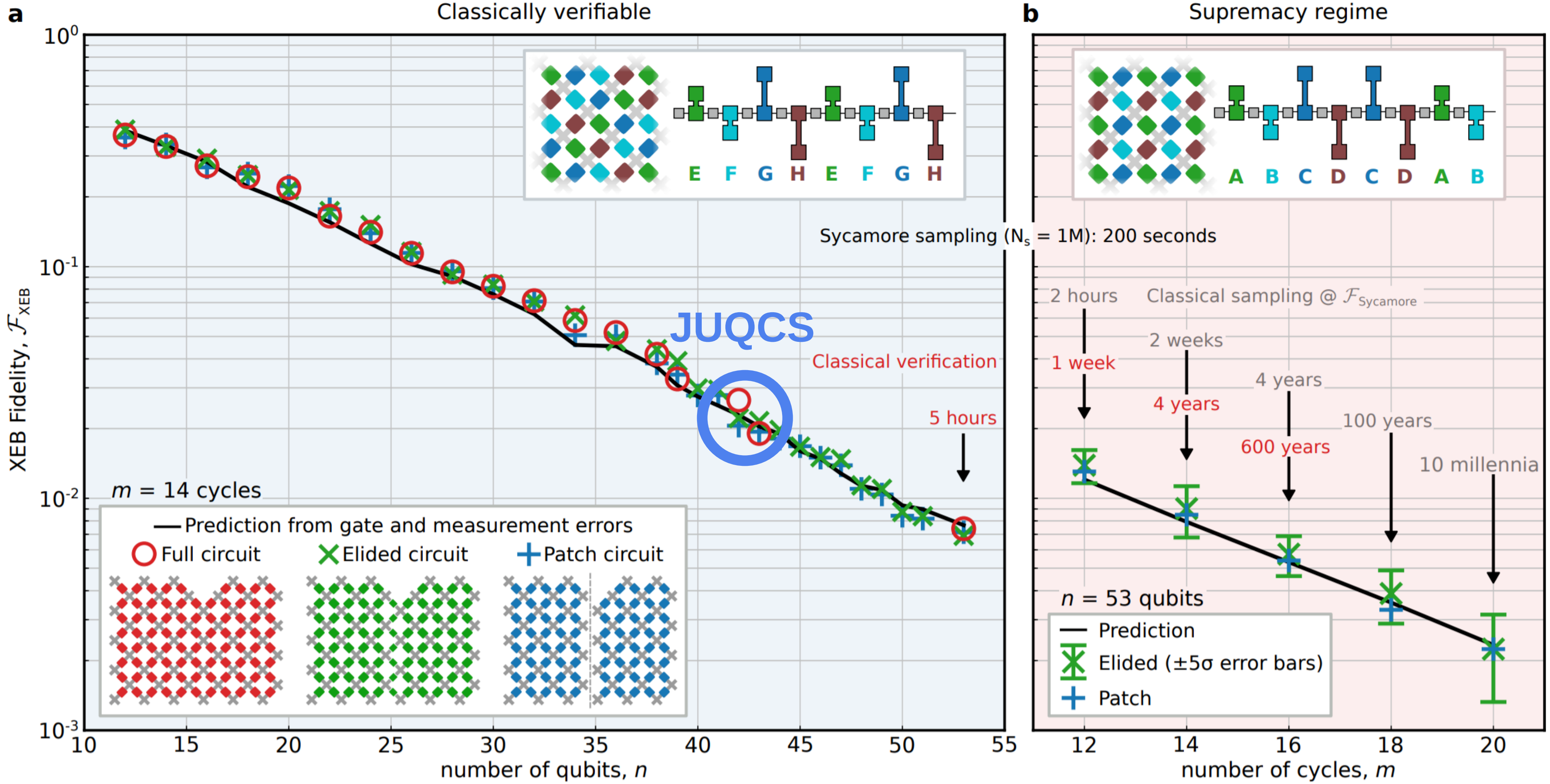
JUQCS - BENCHMARKING

Google Sycamore quantumprocessor



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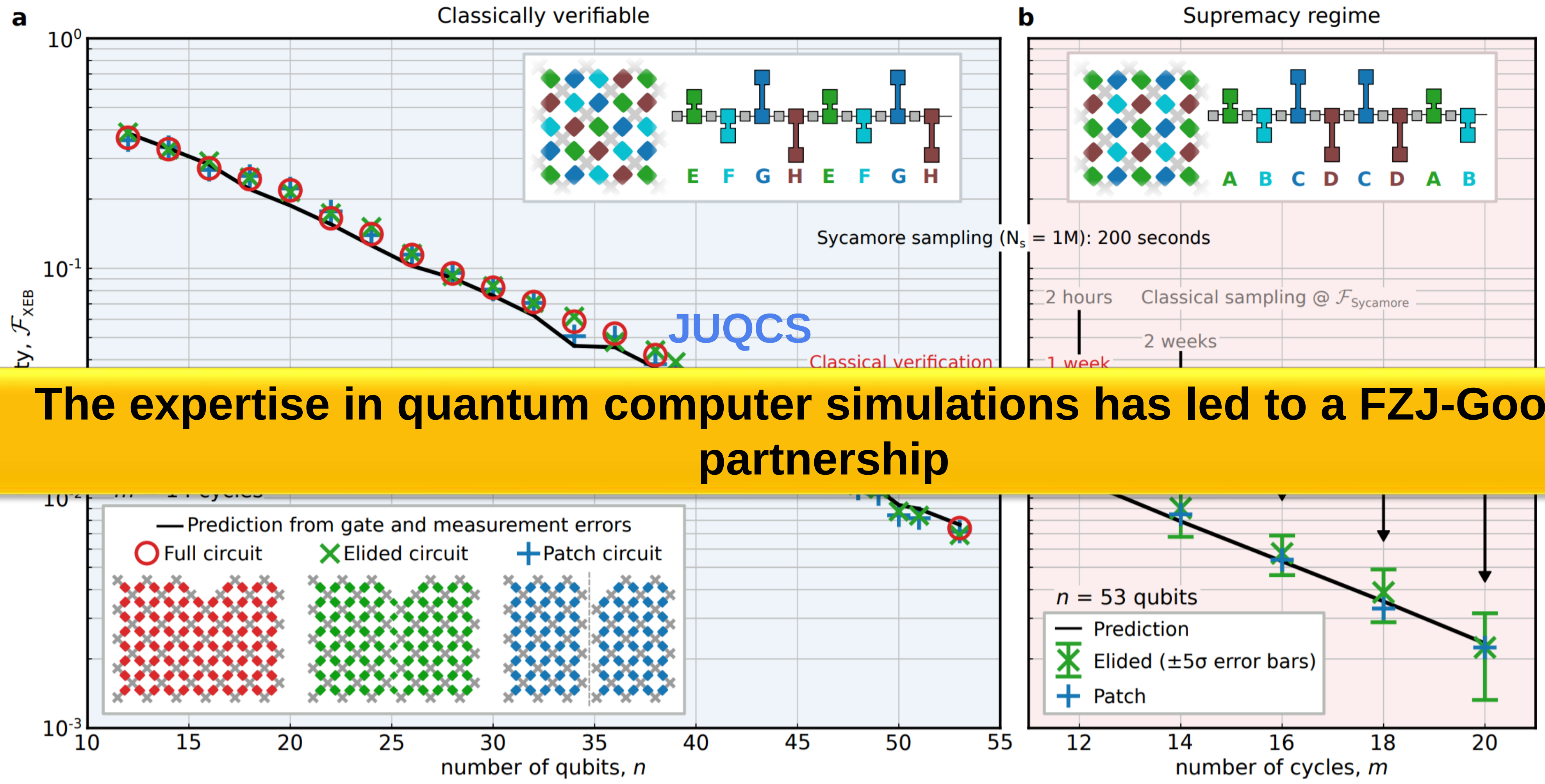
JUQCS - BENCHMARKING

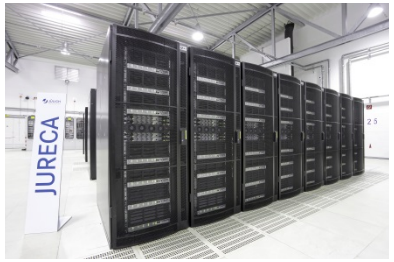
Google Sycamore quantumprocessor



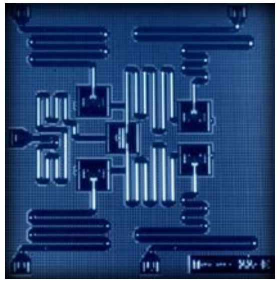
The expertise in quantum computer simulations has led to a FZJ-Google partnership

QUANTUM COMPUTER SIMULATORS

Understanding & design of quantum computers



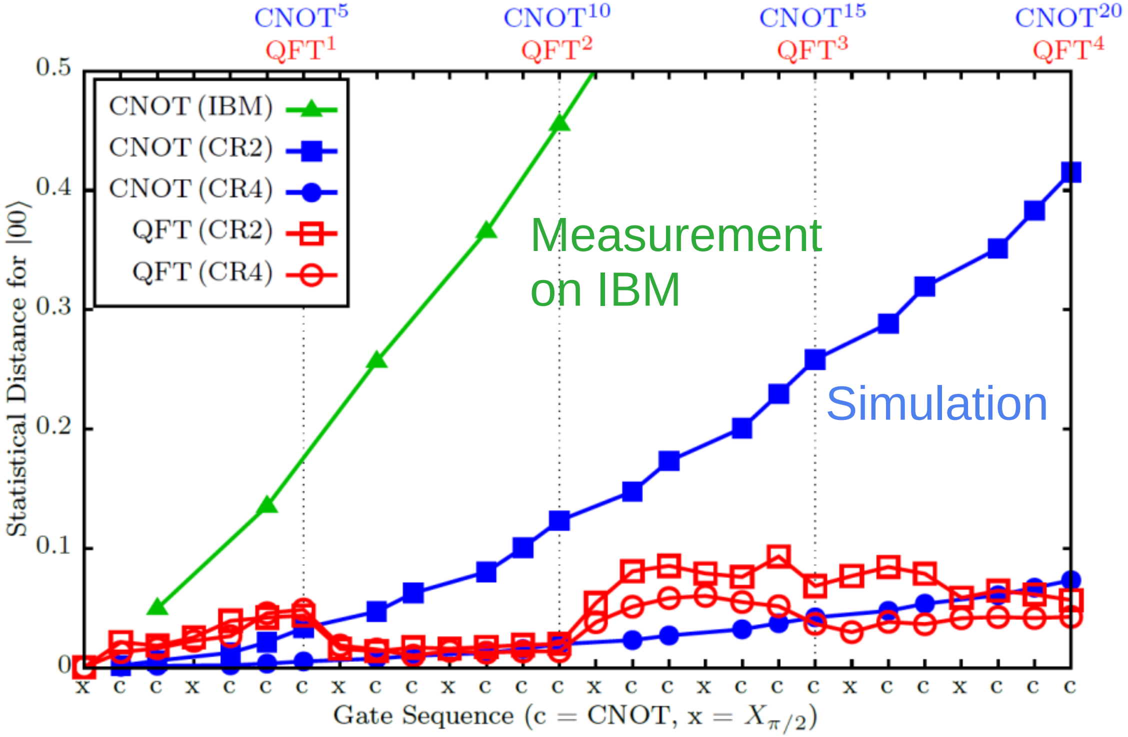
JURECA, Jülich, Germany



IBM QX, Yorktown Heights, USA

D. Willsch et al., *Gate error analysis in simulations of quantum computers with transmon qubits*, Phys. Rev. A 96, 062302 (2017)

- Simulation of the real-time dynamics of physical models of systems with two transmon qubits
- Comparison with IBM QX1 device



Gate metrics provide insights into errors of the implemented gate pulses, but this information is not enough to assess the error induced by repeatedly using the gate in quantum algorithms.

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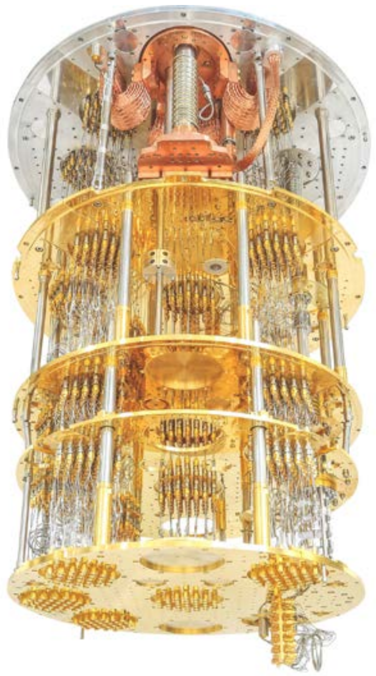
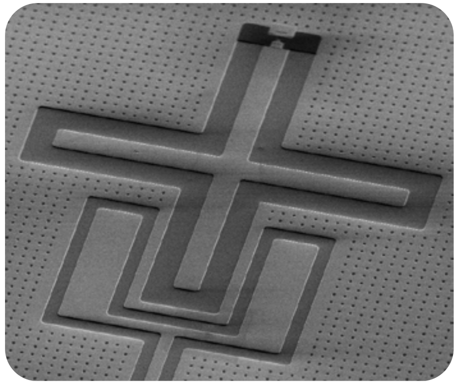
OpenSuperQ – An Open Superconductor Quantum Computer

QUANTUM FLAGSHIP

- **Main goal:** design, build and operate a quantum computer (QC) with up to 100 superconducting qubits
- **Our task (JSC - Research Group QIP):**
  - Benchmarking of the hardware using the world record holding simulator JUQCS (48 qubits) on HPCs
  - Simulation of prototype applications (e.g. ground state calculation for small molecules) on HPCs
  - Development of software code to simulate an ideal, but realistic model of the hardware on HPCs
  - Provide cloud-based access to the hardware via JUNIQ – development of a QC-PaaS



Cryostat



Superconducting transmon qubit

EURICE EUROPEAN RESEARCH AND PROJECT OFFICE GMBH

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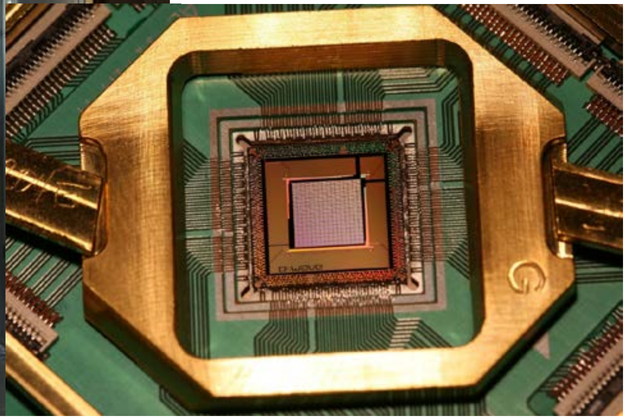
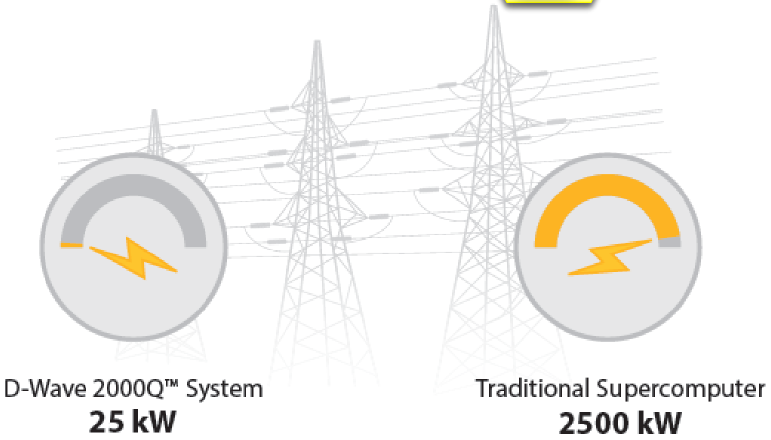
QUANTUM ANNEALER





QUANTUM ANNEALING

Prototype Applications (R&D)

- **QIP, JSC:** Kernel-based support vector machines - supervised machine learning algorithms for classification and regression problems
- **D-Wave Systems:** Simulation of quantum systems
    - Kosterlitz-Thouless phase transition in a system with **1800 Qubits** [Nature 560, 439 & 456 (2018)]
    - Phase transitions in **3D** (8 x 8 x 8) transversal Ising model [Science 361, 162 (2018)]
- **Los Alamos National Laboratory:** Nonnegative/Binary Matrix Factorization, Combinatorial Optimization, Graph Partitioning for Electronic Structure Problems, Quantum Computational Hydrology
- **NASA:** General Planning Problems (e.g., navigation, scheduling, asset allocation), Job Shop Scheduling, Graph-based Fault Detection (Electrical Power Networks), Machine Learning
- **Volkswagen:** Traffic Flow Optimization
- **Booz Allen Hamilton:** Heterogeneous Quantum Computing for Satellite Optimization
- **Recruit Communications:** Display Advertising Optimization, Hotel Reservation Optimization
- **Denso:** Autonomous Driving, Factory Optimization
- **Oak Ridge National Laboratory:** Complex Deep Learning Networks on High Performance, Neuromorphic, and Quantum Computers
- **Q^{X}Branch:** Quantum Machine Learning for Election Modelling (American Presidential Elections)
- **Airbus:** Fault Tree Analyses
- …

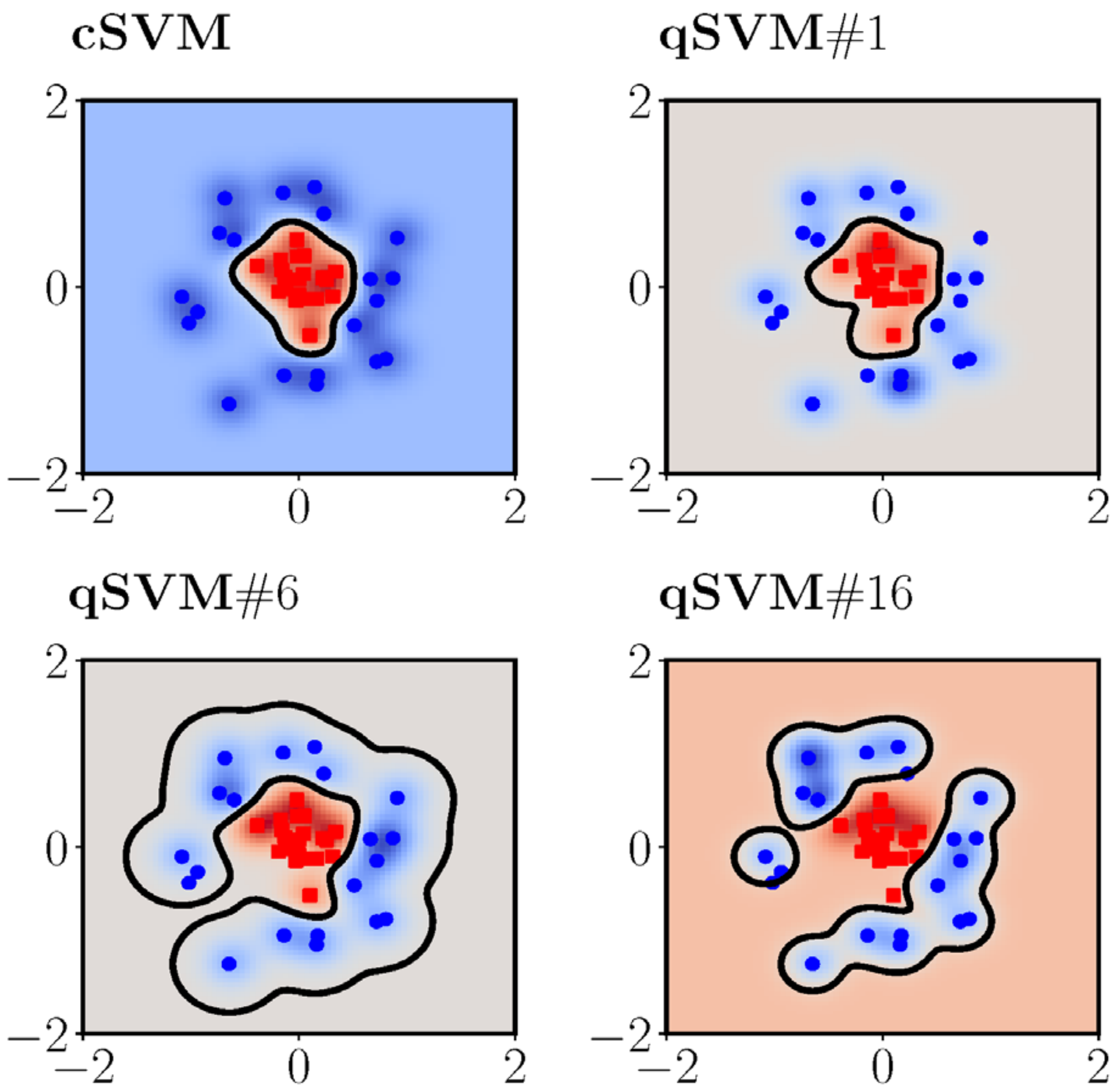
QUANTUM MACHINE LEARNING

Support Vector Machine (SVM) - Supervised machine learning algorithm for classification and regression

- **Classical SVM (cSVM):** training corresponds to a convex quadratic optimization problem, one of the rare minimization problems in machine learning having a **global minimum**
  - Global minimum for training dataset is not necessarily optimal for test dataset

- **Quantum SVM (qSVM)** on a D-Wave quantum annealer (**hybrid** workflow)
  - Quantum annealer produces various **close-to-optimal solutions** for the training data, whereby the different solutions often emphasize different features of the training data
  - Combination of these solutions to test data might solve the classification task better than cSVM

BOOSTING MACHINE LEARNING

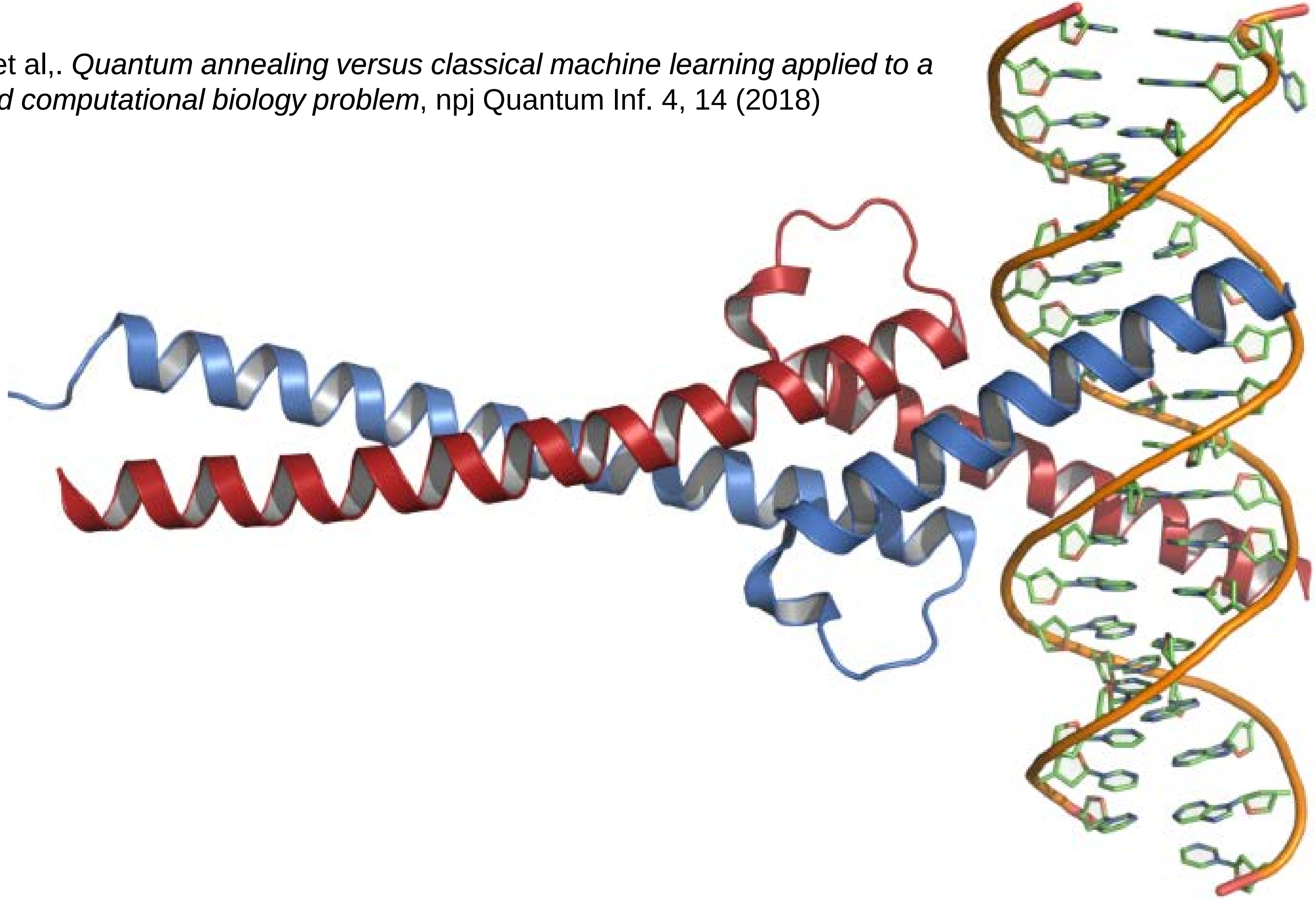


D. Willsch et al., *Support vector machines on the D-Wave quantum annealer,* Comp. Phys. Comm. 248, 107006 (2020)

TO BIND OR NOT TO BIND, THAT IS A QUESTION !

Classification task: Decide whether a certain protein binds to a certain DNA sequence

R. Y. Li et al,. *Quantum annealing versus classical machine learning applied to a simplified computational biology problem*, npj Quantum Inf. 4, 14 (2018)



1. qSVM can produce significantly stronger classifiers than cSVM for the same little training data and parameters
2. qSVM performs better or comparative to cSVM for all datasets

D. Willsch et al., *Support vector machines on the D-Wave quantum annealer,* Comp. Phys. Comm. 248, 107006 (2020)

OPTIMIZATION

M. Willsch, et al., *Benchmarking the Quantum Approximate Optimization Algorithm*, Quant. Inf. Proc. 19, 197 (2020)

Quantum Approximate Optimization Algorithm (QAOA) & quantum annealing

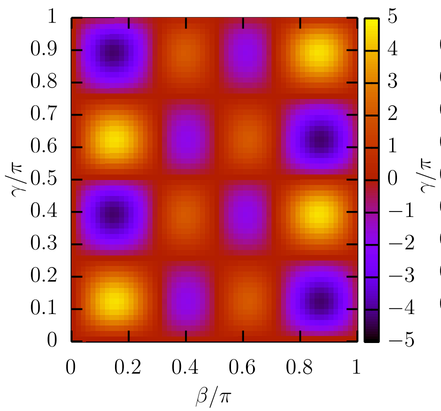
QAOA

- Variational quantum algorithm (**hybrid** algorithm)
- Relies on iteratively applying a series of parametrized unitary transformations to a quantum register, measuring its resulting state and evaluating the **energy expectation value**
  - Number of iterations $p \geq 1$
- A **classical optimization algorithm** is used to optimize the parameters β and γ of the unitary transformations
- For $p \to \infty$ and β and γ taken according to a quantum annealing scheme the solution is found

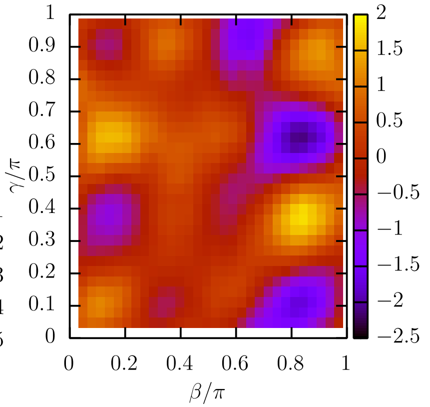
Gate-based quantum computer

Quantum annealer

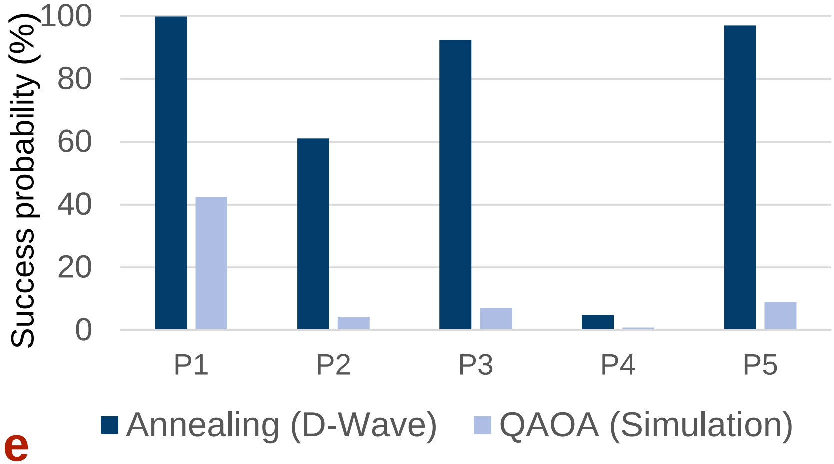
QAOA



Simulation



IBM-Q16 Melbourne (2019)



HYBRID USAGE OF HIGH PERFORMANCE & QUANTUM COMPUTERS

Quantum Computers & Annealers

High Performance Computers

Succesful development of quantum computing applications


Thank
you