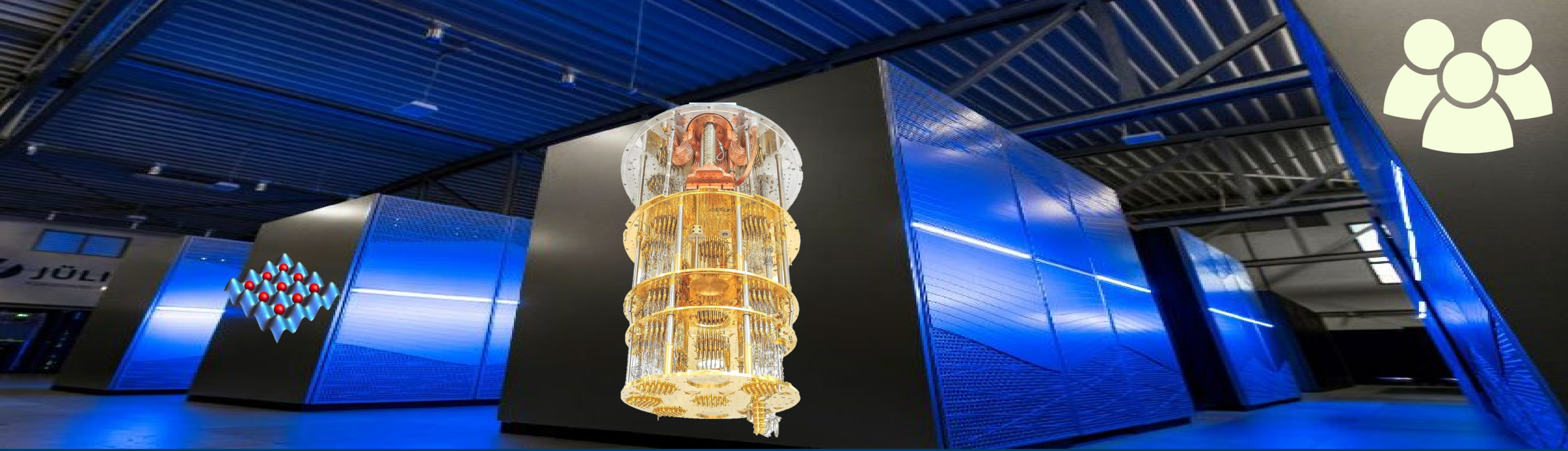


Integrating quantum computers in HPC infrastructures

IEEE Cluster 2022 | Heidelberg, Germany | September 8, 2022 | KRISTEL MICHIELSEN

Member of the Helmholtz Association

JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

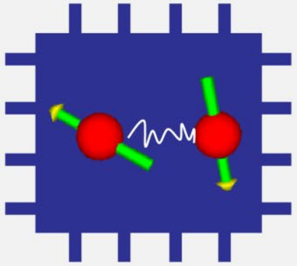
The potential of quantum computing

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

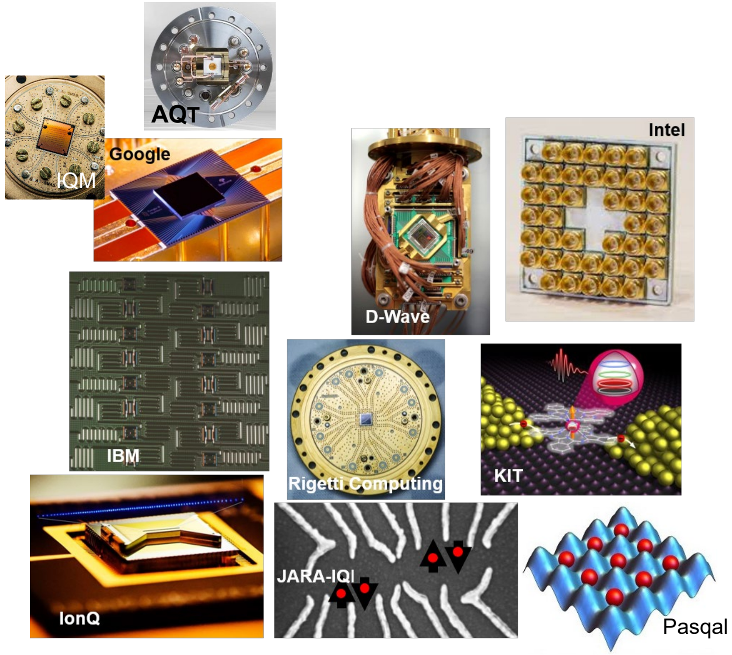
Quantum Technology Readiness Levels

QTRL

Quantum Technology Readiness Levels describing the maturity of Quantum Computing Technology

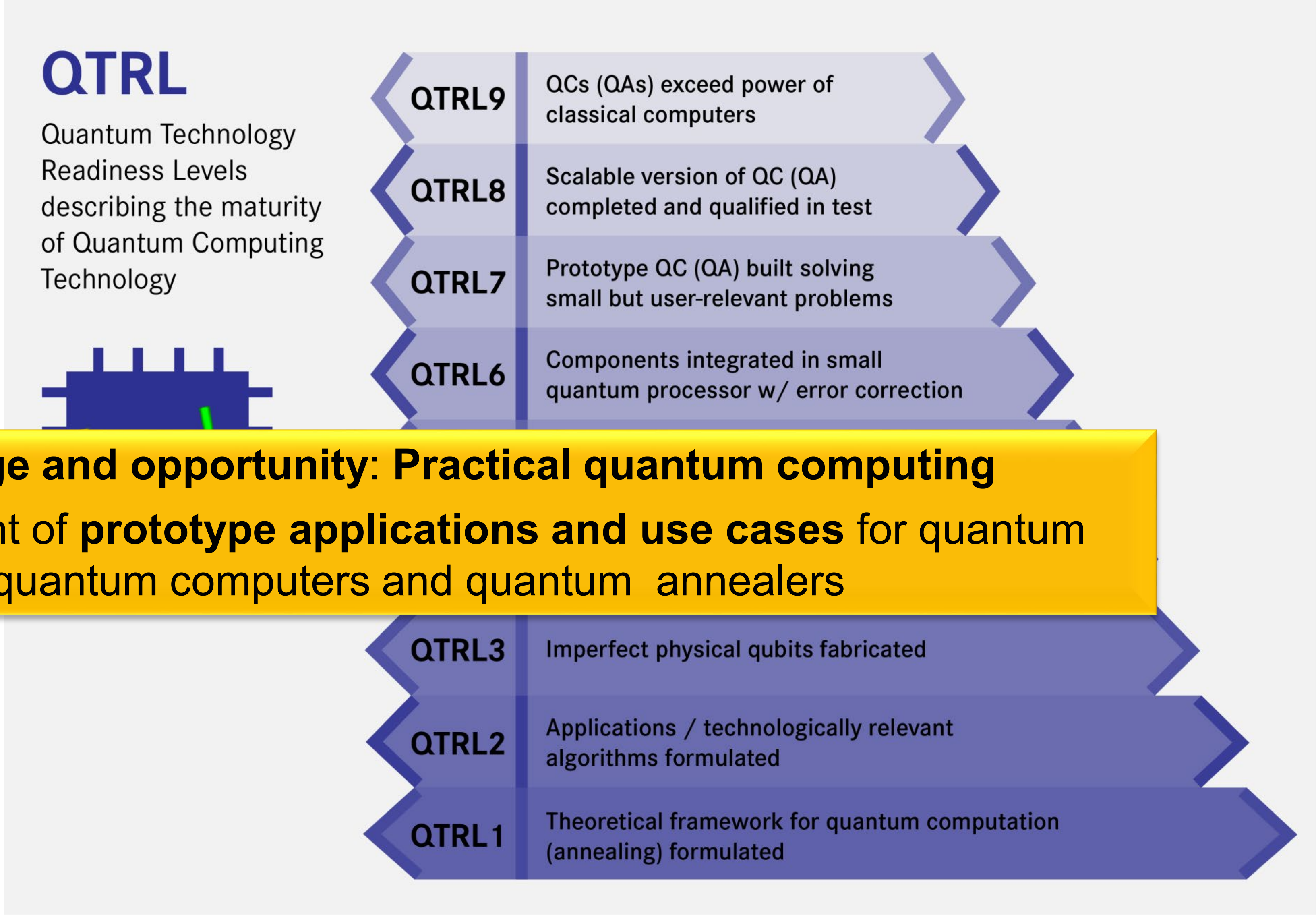


- **QTRL9** QCs (QAs) exceed power of classical computers
- **QTRL8** Scalable version of QC (QA) completed and qualified in test
- **QTRL7** Prototype QC (QA) built solving small but user-relevant problems
- **QTRL6** Components integrated in small quantum processor w/ error correction
- **QTRL5** Components 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



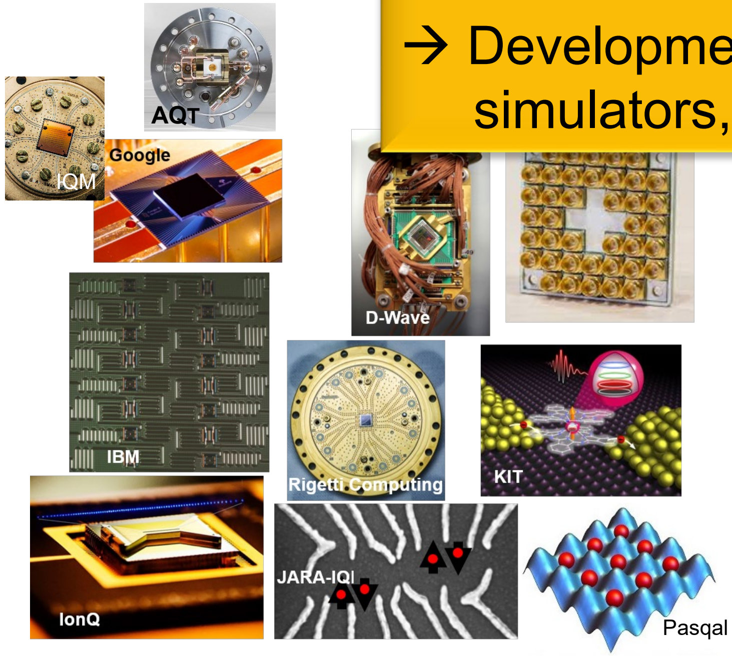
© Kristel Michielsen, Thomas Lippert – Forschungszentrum Jülich
(http://www.fz-juelich.de/ias/jsc/EN/Research/ModellingSimulation/QIP/QTRL/_node.html)

Quantum Technology Readiness Levels



Huge challenge and opportunity: **Practical quantum computing**

→ Development of **prototype applications and use cases** for quantum simulators, quantum computers and quantum annealers



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High performance & Quantum Computers

linked, to solve problems optimally

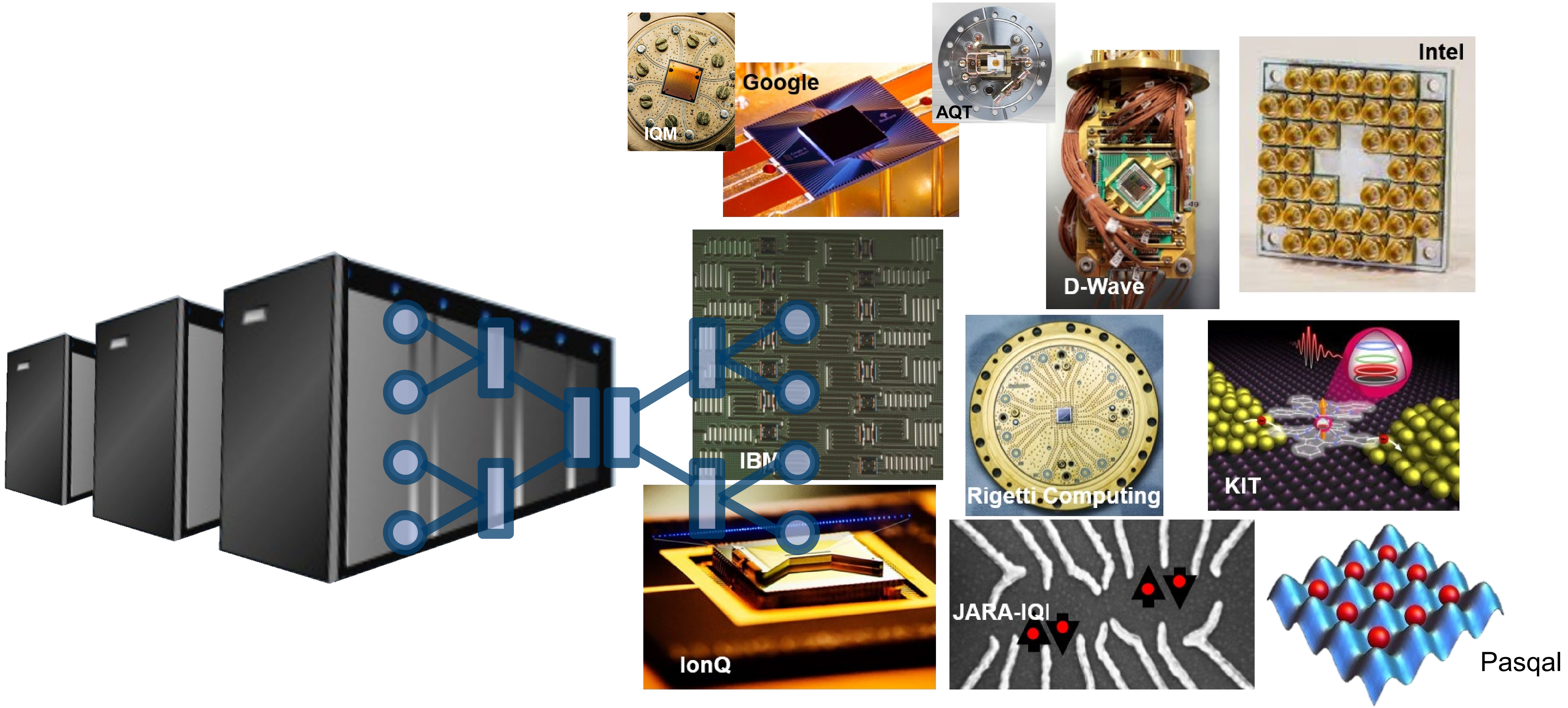
High Performance Computers

HPC simulations of quantum computing / annealing devices

Quantum Computers & Annealers

Understanding – Design – Benchmarking

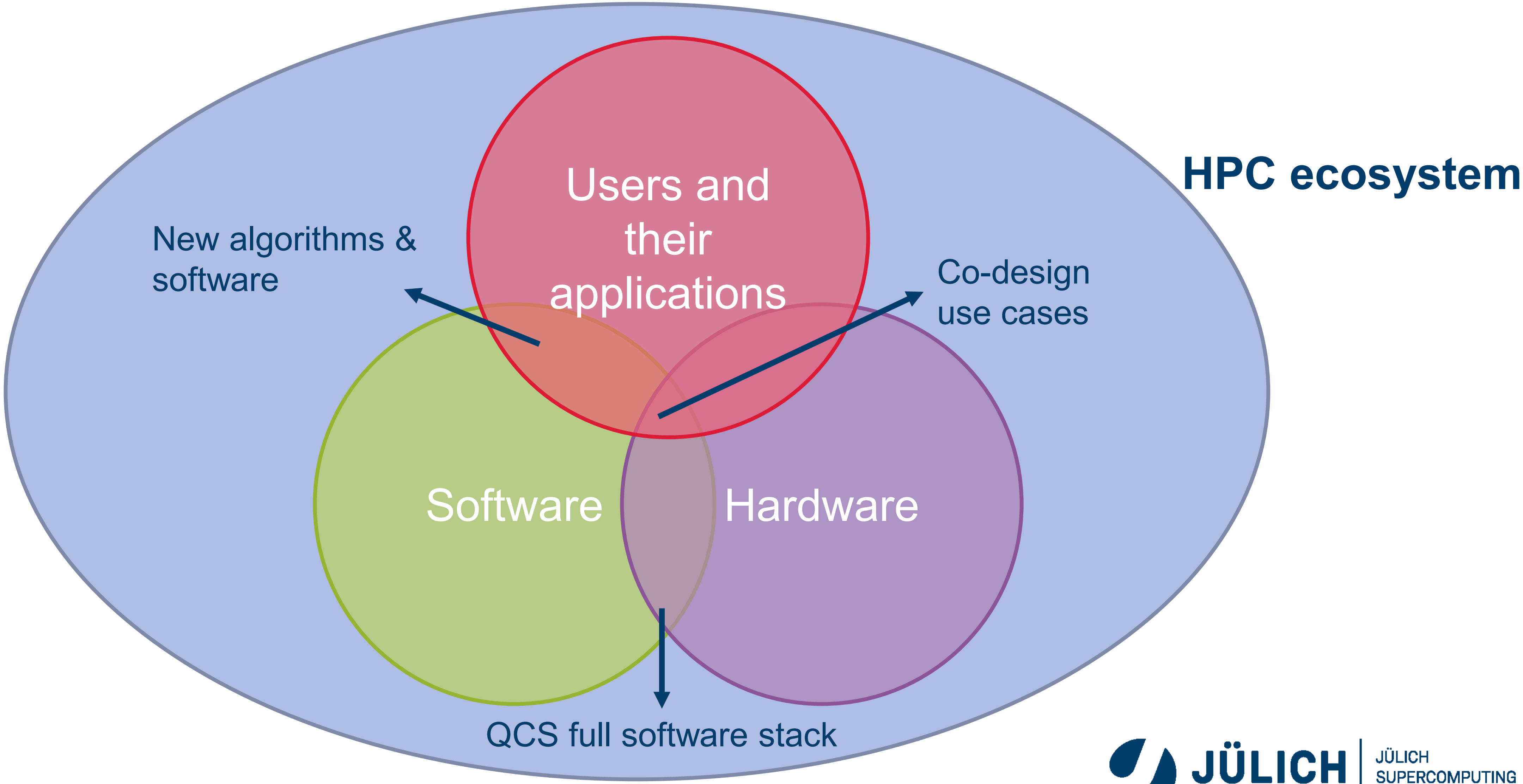
(Hybrid) simulations for applications



HPC systems

Quantum computers and simulators (QCS)

HPC-QCS integration

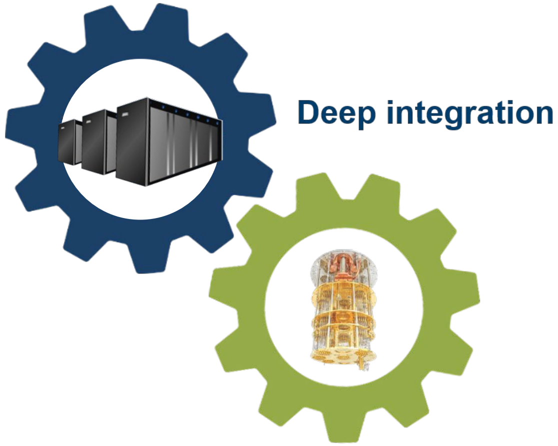


Hybrid quantum-classical computing systems

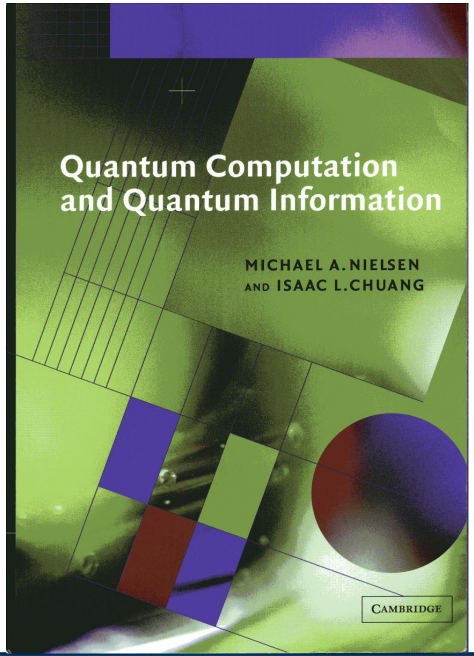
for the realization of the full potential of quantum computing

- **Hybrid quantum-classical algorithms**
  - Variational Quantum Eigensolver – **VQE**: quantum chemistry
  - Quantum Approximate Optimization Algorithm – **QAOA**: optimization
  - Quantum Support Vector Machine – **qSVM**: classification and clustering
  - Classic workflows with potential quantum content?
- **Hybrid quantum-classical hardware**

Proper benchmarking & implementation on real devices



Latencies & execution times



GATE-BASED QUANTUM COMPUTER EMULATION: PEN-AND-PAPER (PAP) VERSION

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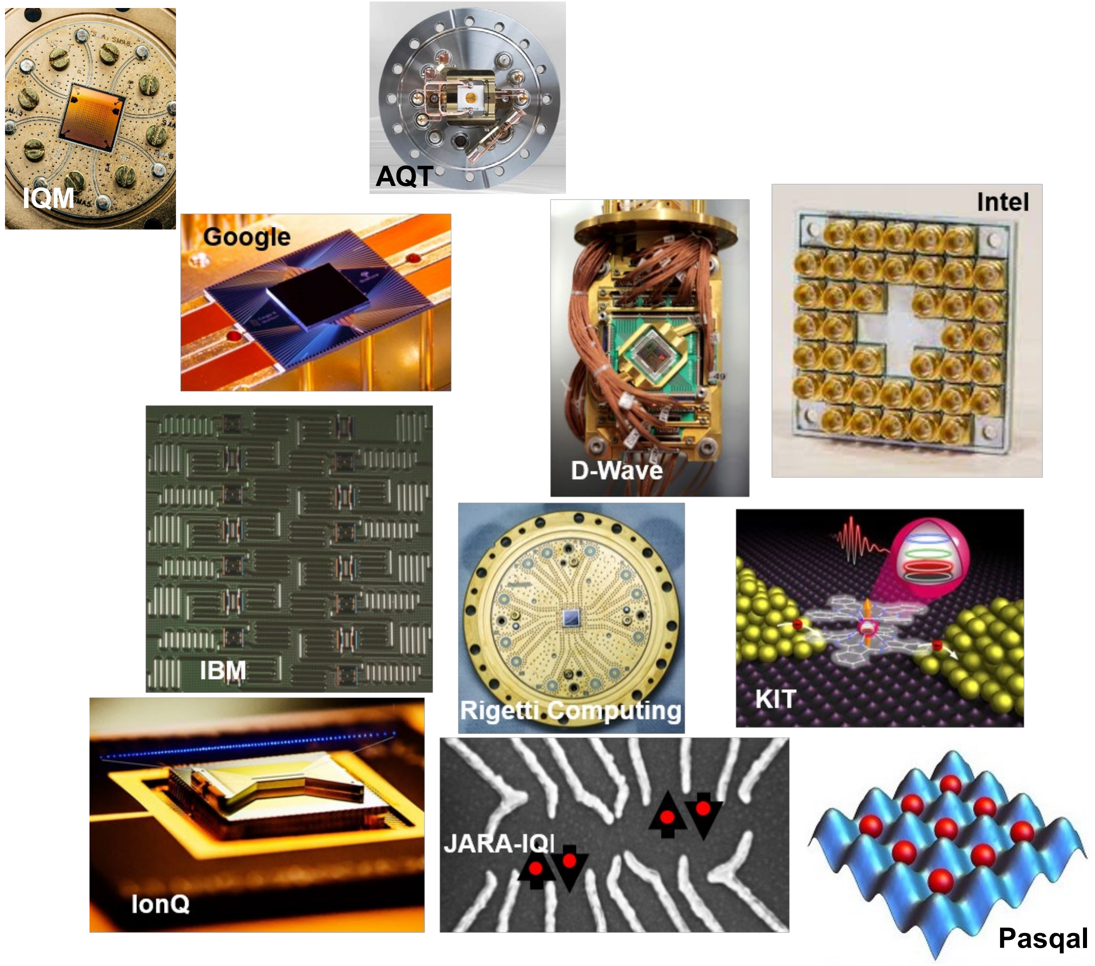
JÜLICH SUPERCOMPUTING CENTRE

Quantum computers

It is important to have theoretical tools to:

- validate **designs** of physically realizable quantum processors
- investigate the **implementation and performance of quantum algorithms** on physically realizable quantum computers



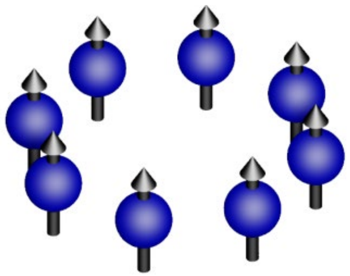
Quantum Computer & Quantum algorithm

- **Quantum computer**
  - System with 1 qubit ≡ system with 1 spin-1/2 particle

$$|\psi\rangle = a_0|0\rangle + a_1|1\rangle \quad ; \quad |a_0|^2 + |a_1|^2 = 1 \quad (a_0, a_1 \in \mathbb{C})$$

  - System with $\boldsymbol{N}$ **qubits** ≡ system with N spin-1/2 particles

$$|\psi\rangle = a(0\cdots 00)|0\rangle_{N-1}\cdots|0\rangle_1|0\rangle_0 + \cdots + a(1\cdots 11)|1\rangle_{N-1}\cdots|1\rangle_1|1\rangle_0$$



→ $|\boldsymbol{\psi}\rangle$ can be represented as a **vector of length 2^N**, containing all **complex amplitudes $\boldsymbol{a}$**

- **Quantum algorithm = sequence of quantum gates** (elementary operations) that are described by a unitary (sparse) matrix and change the state $|\psi\rangle$ of the quantum processor

2007 – 2017: Jülich UNIVERSAL Quantum Computer Simulator (JUQCS – E)

K. De Raedt, K. Michielsen, H. De Raedt, B. Trieu, G. Arnold, M. Richter, Th. Lippert, H. Watanabe, N. Ito, *Massively Parallel Quantum Computer Simulator*, Comput. Phys. Commun.176, 121 - 136 (2007)

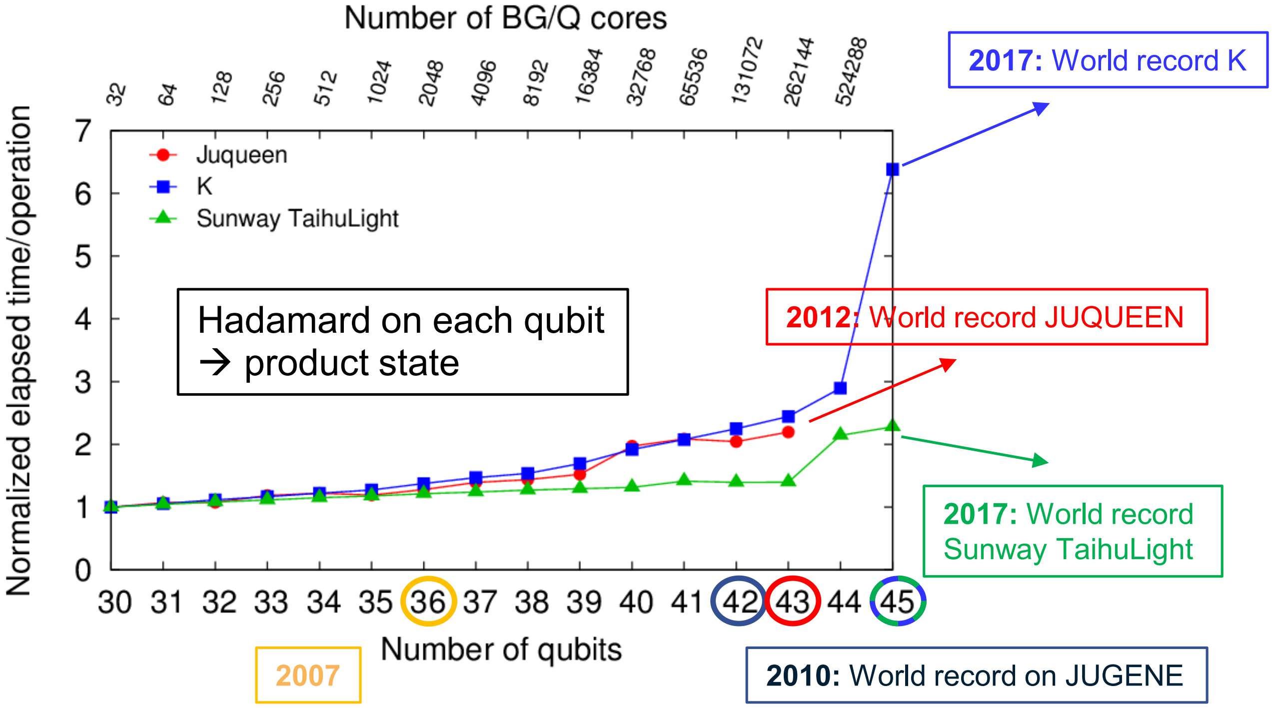
JUQUEEN Jülich, Germany


K, Kobe, Japan


Sunway TaihuLight, Wuxi, China

- N qubits → $|\psi\rangle$ is a superposition of 2^N basis states
- Represent a quantum state with 16 bytes → N qubits requires at least 2^{N+4} bytes of memory

N	Memory
24	256 MB
36	1 TB
45	0.5 PB
46	1 PB



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2007 – 2017: Jülich UNIVERSAL Quantum Computer Simulator (JUQCS – E)

K. De Raedt, K. Michielsen, H. De Raedt, B. Trieu, G. Arnold, M. Richter, Th. Lippert, H. Watanabe, N. Ito, *Massively Parallel Quantum Computer Simulator*, Comput. Phys. Commun.176, 121 - 136 (2007)

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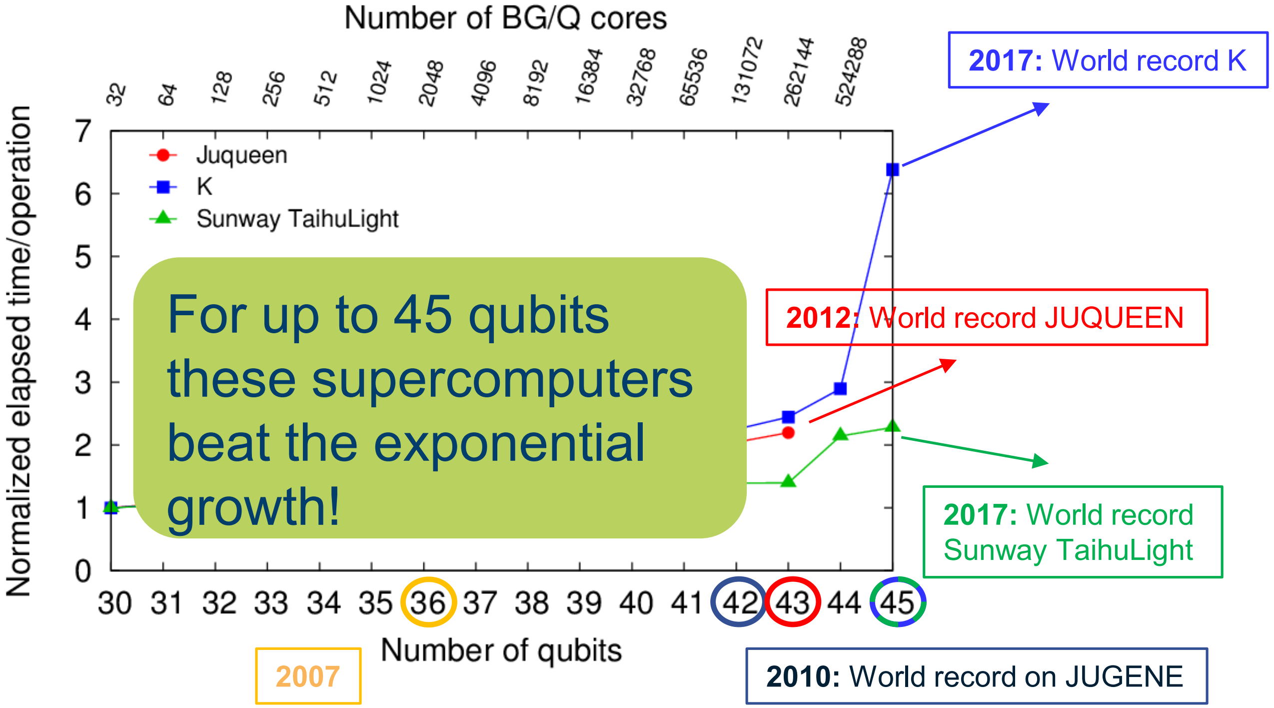


2018 – 2019: Jülich Universal Quantum Computer Simulator (JUQCS – A)

H. De Raedt, F. Jin, D. Willsch, M. Nocon, N. Yoshioka, N.Ito, S. Yuan, K. Michielsen, *Massively parallel quantum computer simulator, eleven years later*, Comput. Phys. Commun. 237, 47-61 (2019)

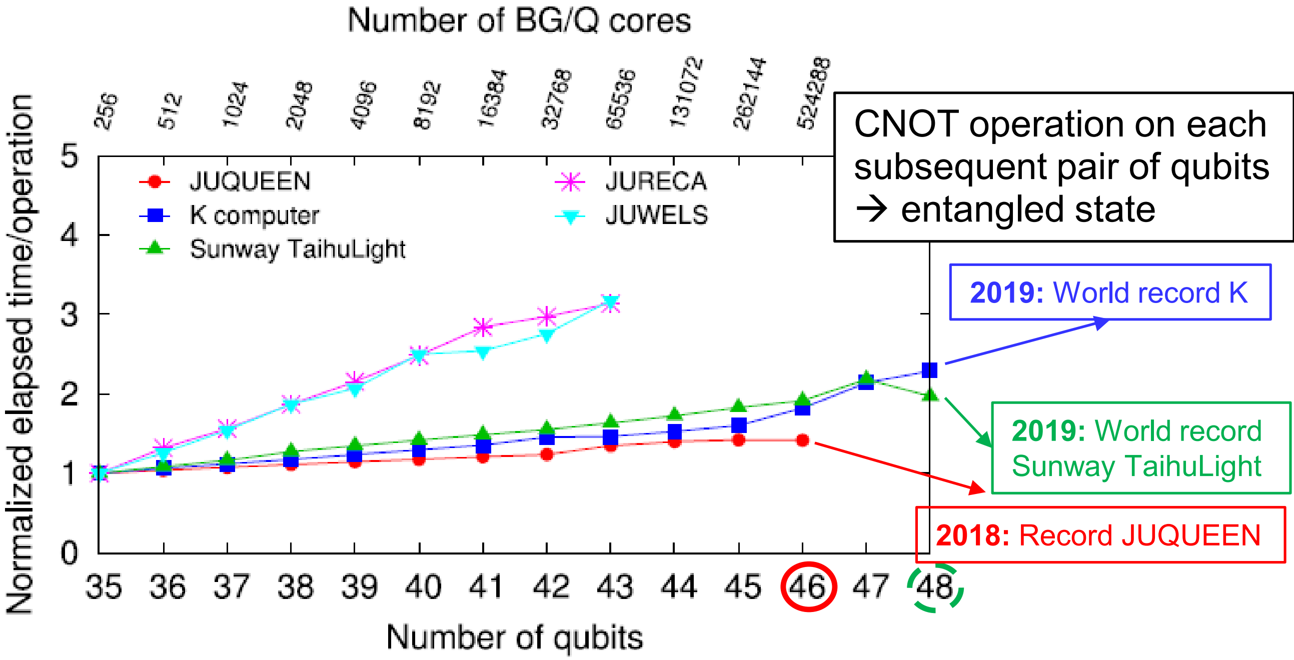
JUWELS, Jülich, Germany


K, Kobe, Japan


Sunway TaihuLight, Wuxi, China

- N qubits → $|\psi\rangle$ is a superposition of 2^N basis states
- Represent a quantum state with 2 bytes → N qubits requires at least 2^{N+1} bytes of memory → new world record

N	Memory
27	256 MB
39	1 TB
48	0.5 PB
49	1 PB



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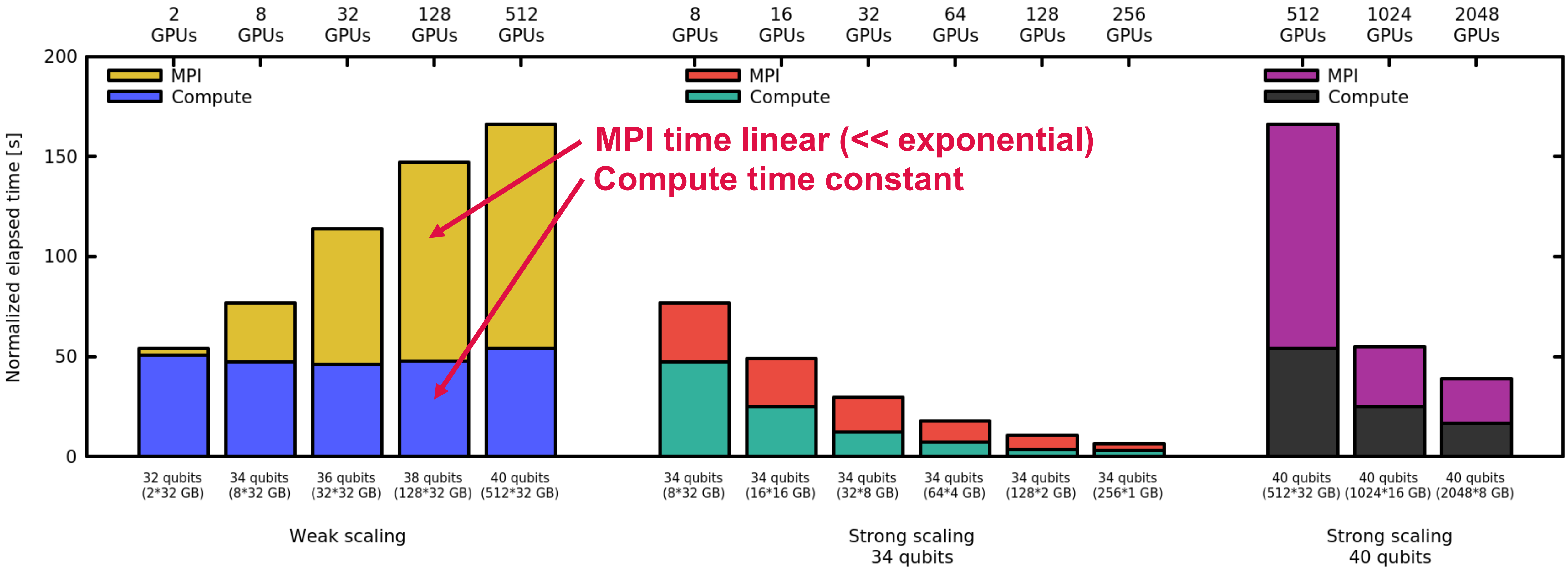
JÜLICH SUPERCOMPUTING CENTRE

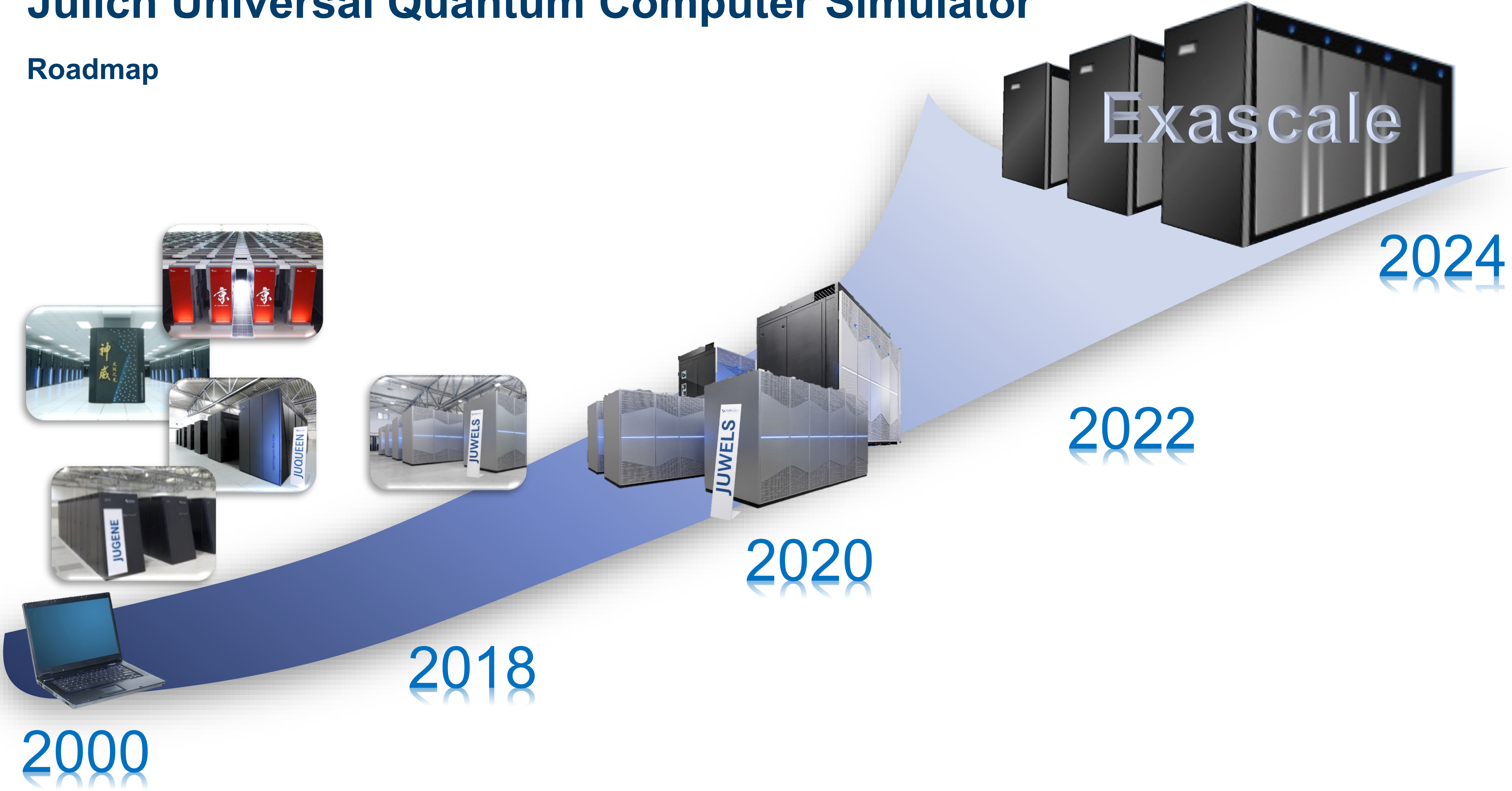
2020 – 2022: JUQCS – G

Weak and strong scaling result



Jülich Universal Quantum Computer Simulator

Roadmap



OPTIMIZATION: QAOA

Tail Assignment Problem

- Airlines: 1000 flights per day to over 150 cities in over 70 countries, using hundreds of aircraft of different types
- Costs associated with aircraft and flight crew are the most significant costs
- Tail assignment problem: describes a mathematical optimization model that when solved can provide airlines with efficient plans for how to use their aircraft

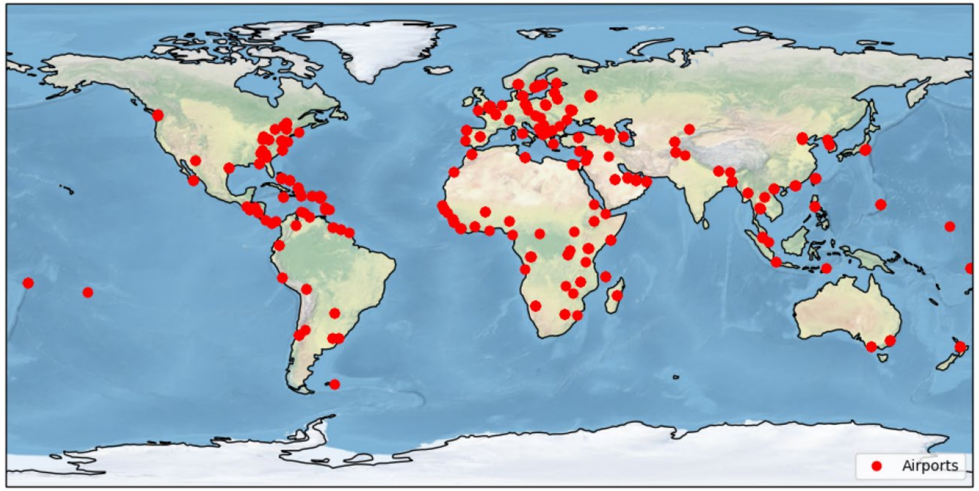
Tail Assignment

Reduced problem instances

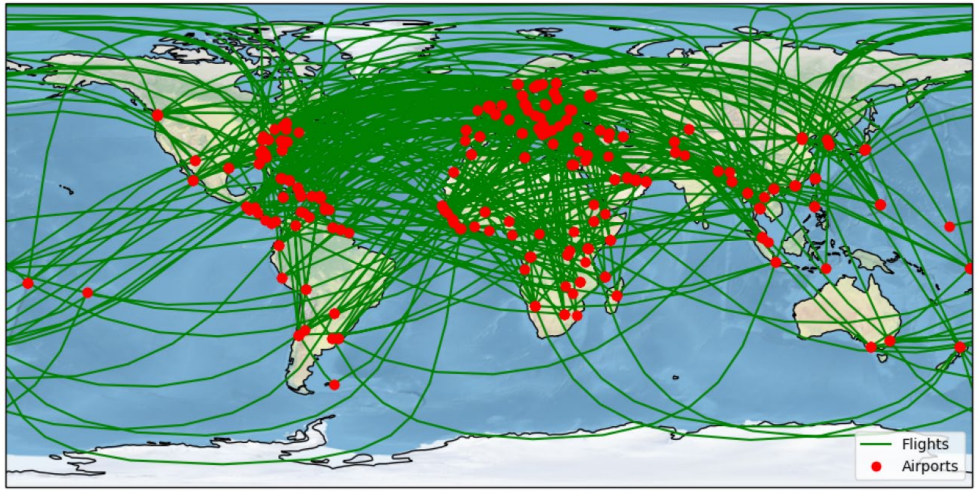
- Exact-cover problems: series of realistic problem instances obtained by random sampling from a real-world data set with up to 40 routes
- Example: Given are 40 routes, each of which contains several out of 472 flights. Find routes to carry out 472 flights between airports so that routes not overlap
  → problem with **40 qubits (routes)**
  - The problem instance has the unique **ground state (solution)** $|0000000001010010011001000001000000000110\rangle$
  - The ground state contains nine 1's → 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

Tail Assignment

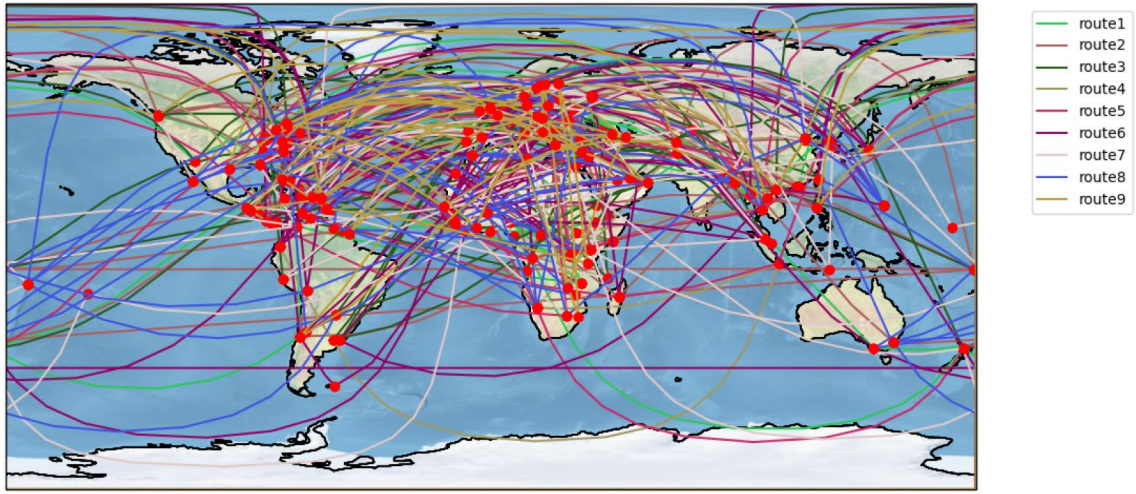
40-qubit problem



Airports



472 flights between the airports that have to be performed



Unique solution with 9 routes covering the 472 flights exactly once

Tail assignment: Quantum Approximate Optimization Algorithm

Jülich Universal Quantum Computer Simulator – JUQCS - G

Variational quantum algorithm
(hybrid algorithm)

a) **Quantum algorithm** to iteratively apply a series of parametrized unitary transformations to a quantum register and evaluate its **energy expectation value**

b) **Classical optimization algorithm** to optimize the parameters of the unitary transformations

GPUs of JUWELS Booster
→ QPUs

CPUs of JUWELS Booster

JUQCS

De Raedt et al., CPC **176**, 121 (2007)

De Raedt et al., CPC **237**, 47 (2019)

Simplified tail assignment problem

Assign aircrafts to flights – minimize overall cost respecting operational constraints

- Simplified problem: Find routes to carry out 472 flights between airports so that routes not overlap

→ problem with 40 qubits

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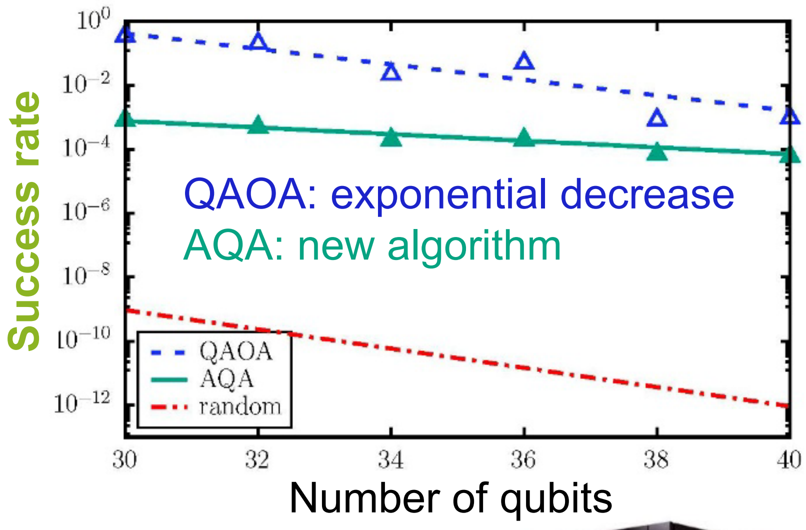
Simplified Tail Assignment Problem

Benchmarking and Algorithm Development



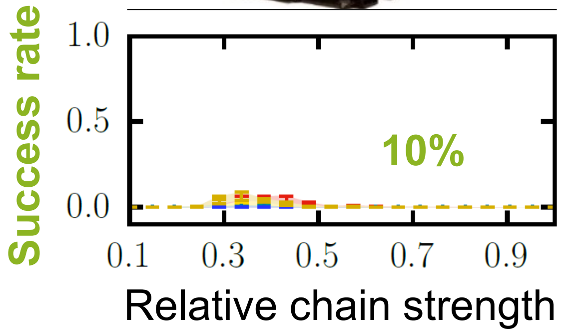
JUQCS on JUWELS @JSC

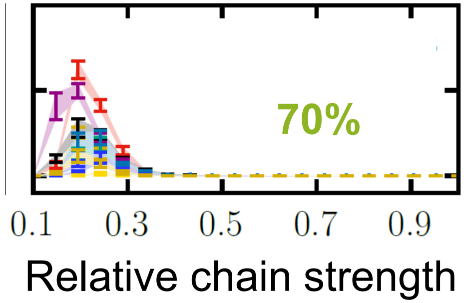
→ **Ideal digital QPU**

Quantum annealer

2000+ qubits

5000+ qubits





Willsch *et al.*, Quant. Inf. Proc. 19, 197 (2020)

Willsch *et al.*, Quant. Inf. Proc. 21, 141 (2022)

Willsch *et al.*, Comput. Phys. Commun. 278, 108411 (2022)

https://www.youtube.com/watch?v=zqRcT62cEsE

CLASSIFICATION: qSVM

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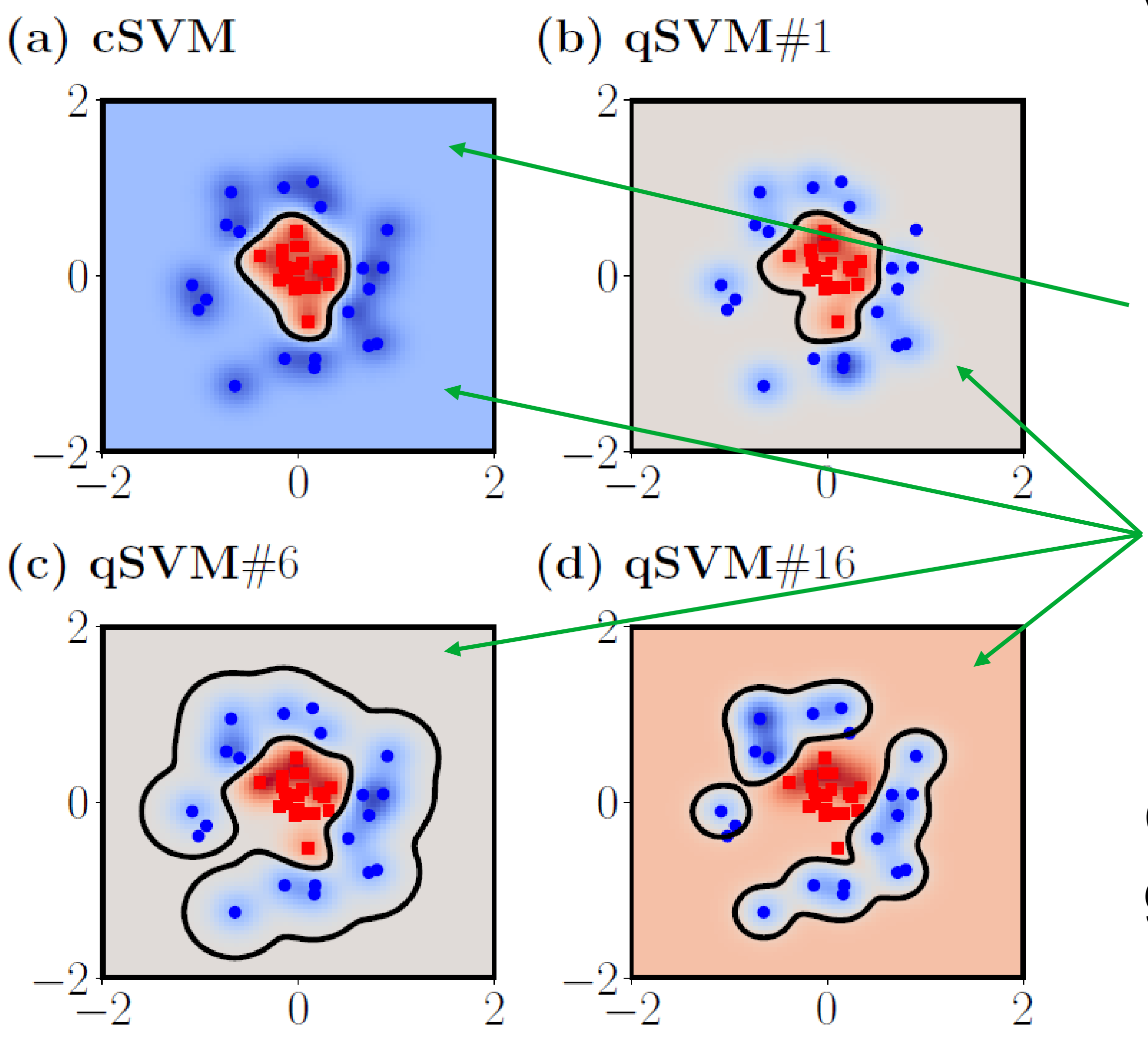
JÜLICH SUPERCOMPUTING CENTRE

Toy Model Data

Willsch *et al.*, Comput. Phys. Commun. 248, 107006 (2020)



Visualization of the classifiers

- Classical SVM (**cSVM**): global minimum, but only for training data
- Quantum SVM (**qSVM**): additional higher-energy classifiers from ensemble of solutions

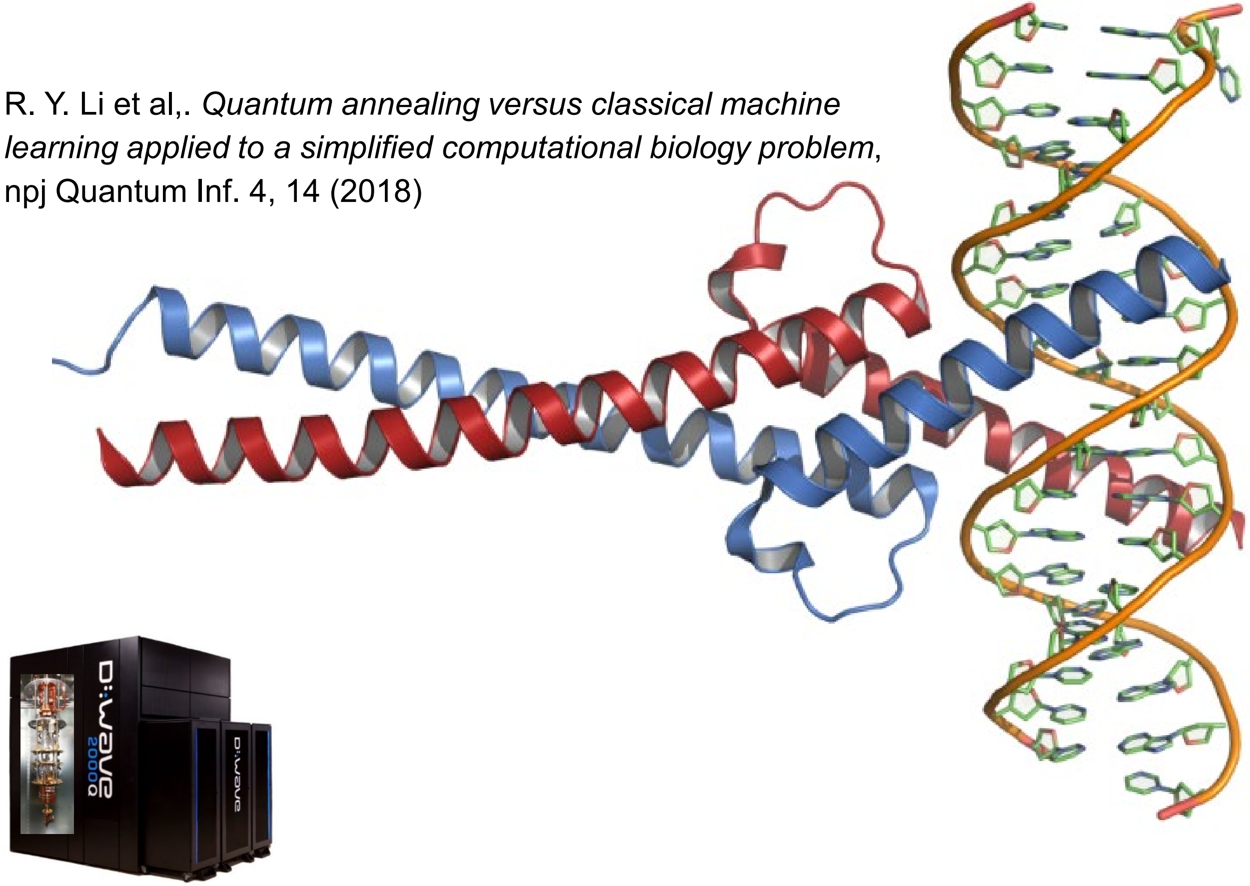
Combination of qSVM classifiers might generalize better to unseen data

PROTEIN-DNA BINDING

Classification (machine learning)

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

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 on a D-Wave quantum annealer (hybrid workflow) 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

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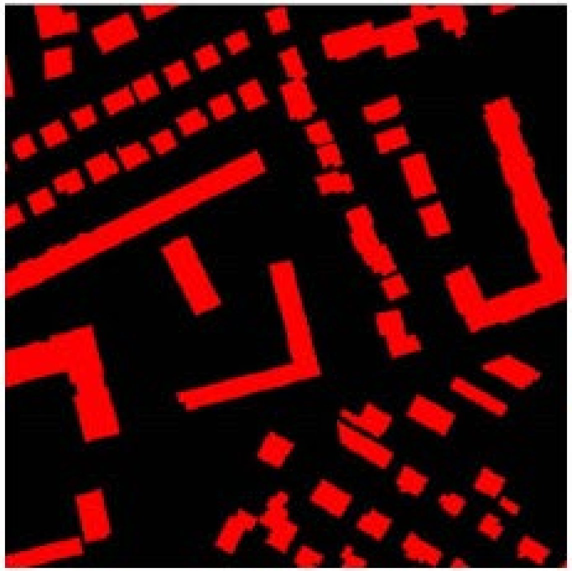
Machine Learning for Earth Observation

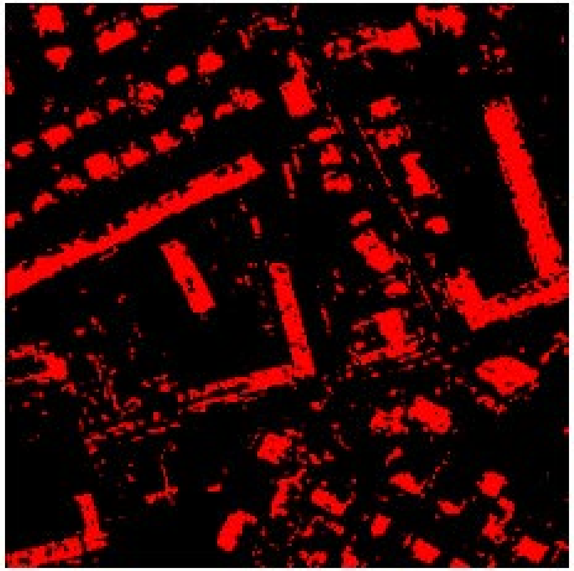
Classification of Remote Sensing Multispectral Images with Quantum SVM

False color

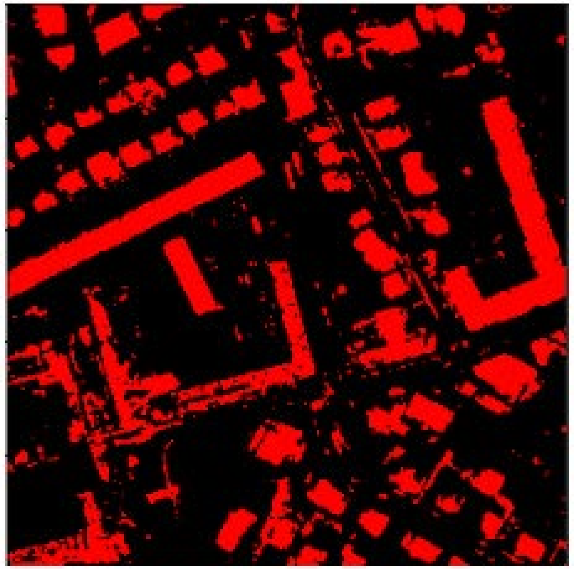
Ground truth



Classical SVM



Quantum SVM



A. Delilbasic *et al.*, https://doi.org/10.1109/IGARSS47720.2021.9554802

G. Cavallaro *et al.*, https://doi.org/10.1109/IGARSS39084.2020.9323544

esa AIDAS AI Data Analytics and Scalable Simulations

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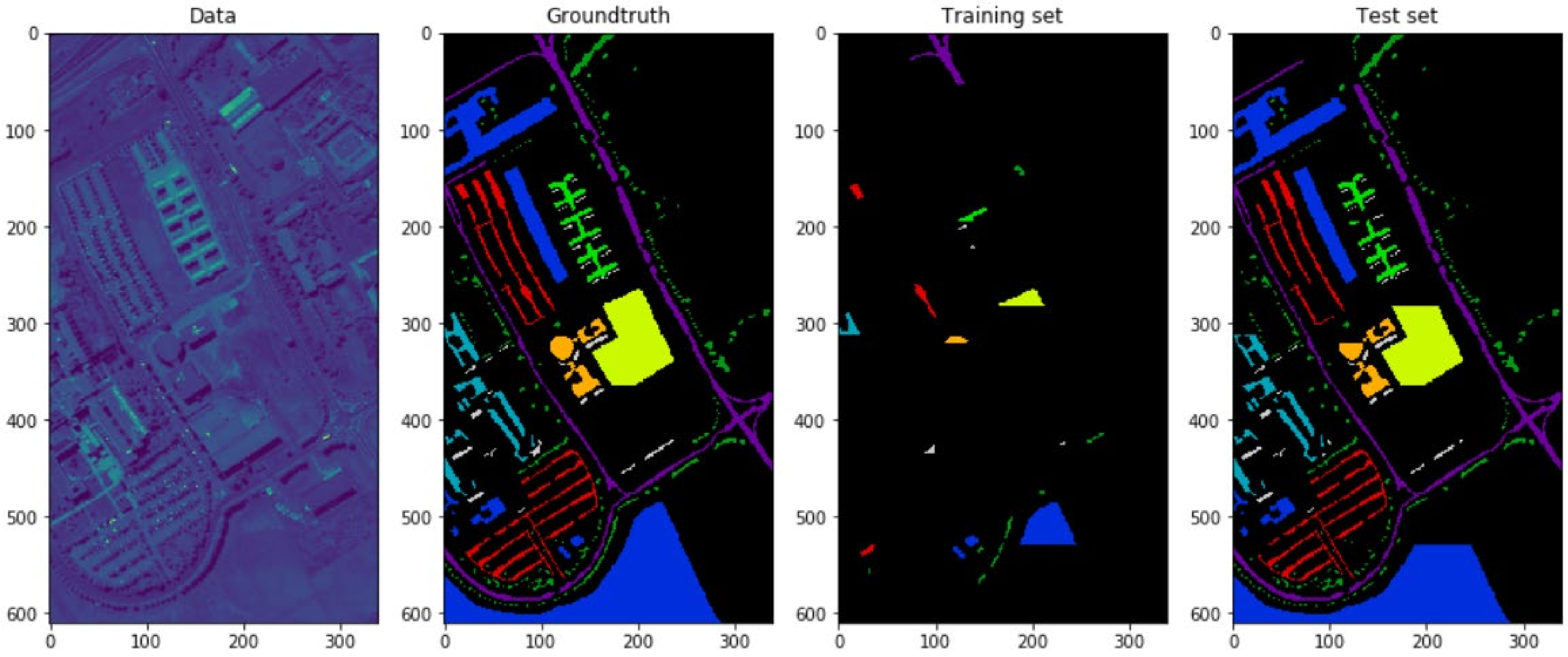
Machine Learning for Earth Observation

In progress: Multiclass Classification



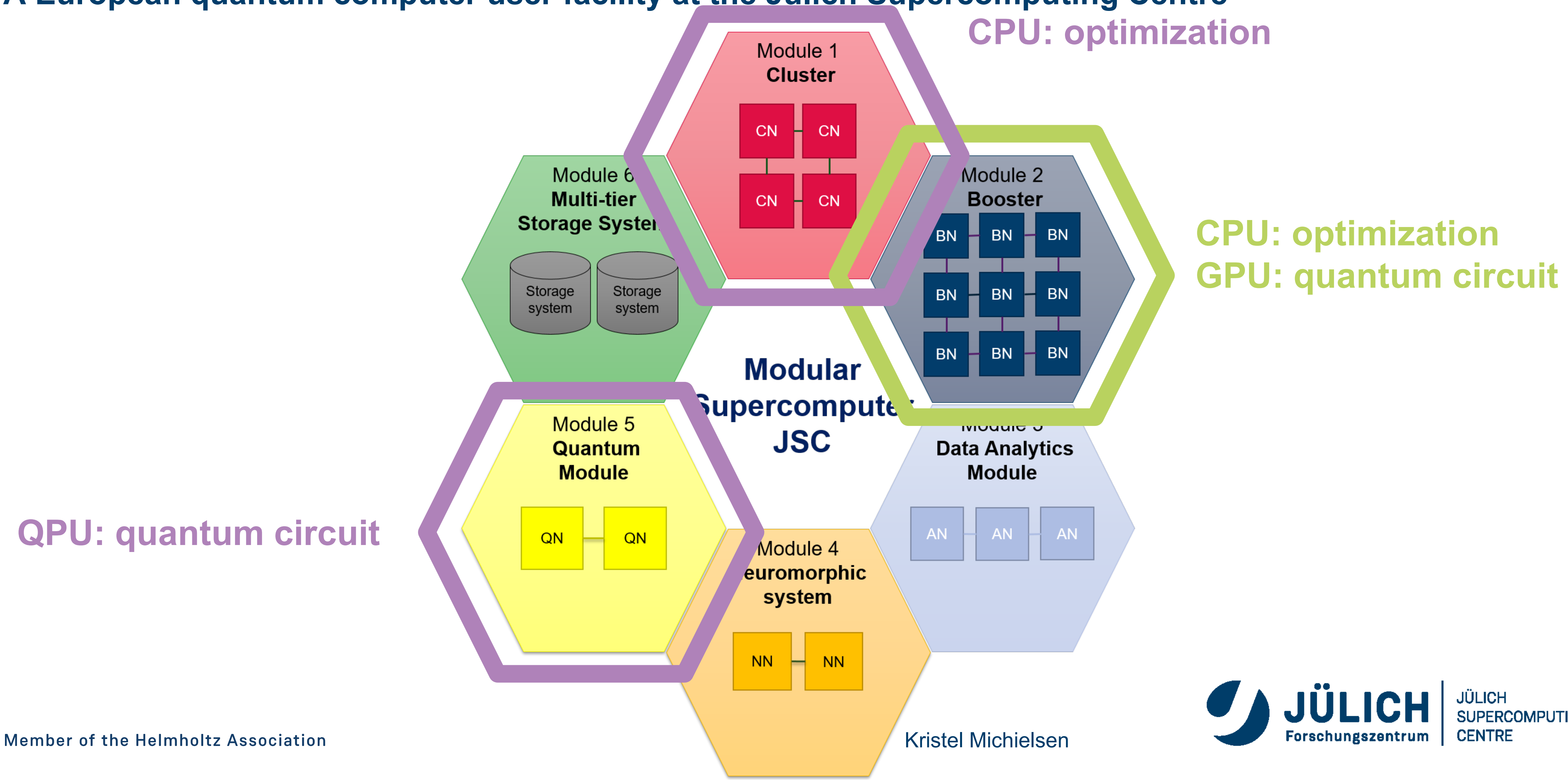
A. Delilbasic *et al.*, https://doi.org/10.1109/IGARSS47720.2021.9554802

G. Cavallaro *et al.*, https://doi.org/10.1109/IGARSS39084.2020.9323544

MODULAR SUPERCOMPUTING ARCHITECTURE

JUNIQ – Jülich UNified Infrastructure for Quantum computing

A European quantum computer user facility at the Jülich Supercomputing Centre



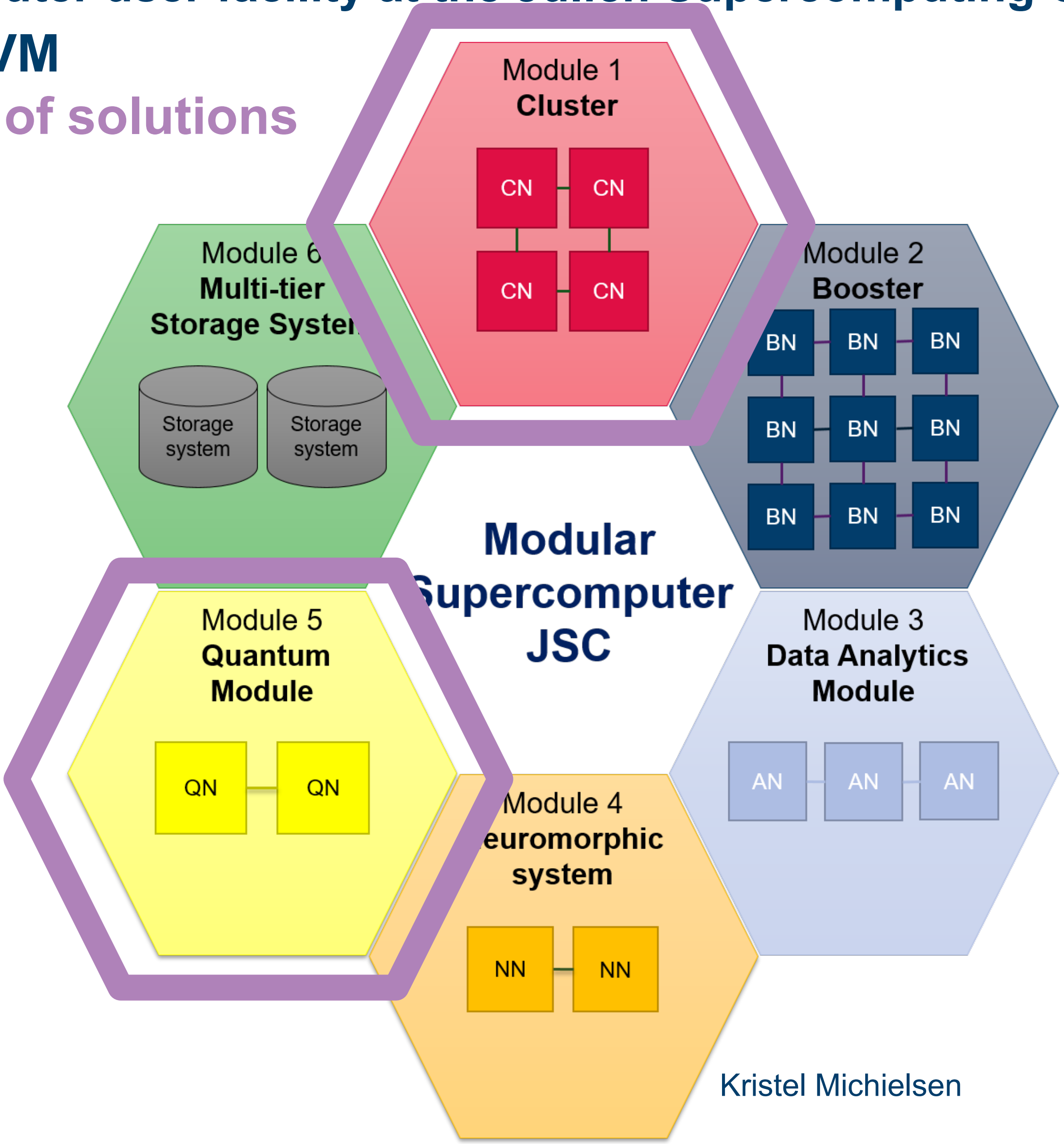
Kristel Michielsen

JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

JUNIQ – Jülich UNified Infrastructure for Quantum computing

A European quantum computer user facility at the Jülich Supercomputing Centre

qSVM
Combination of solutions

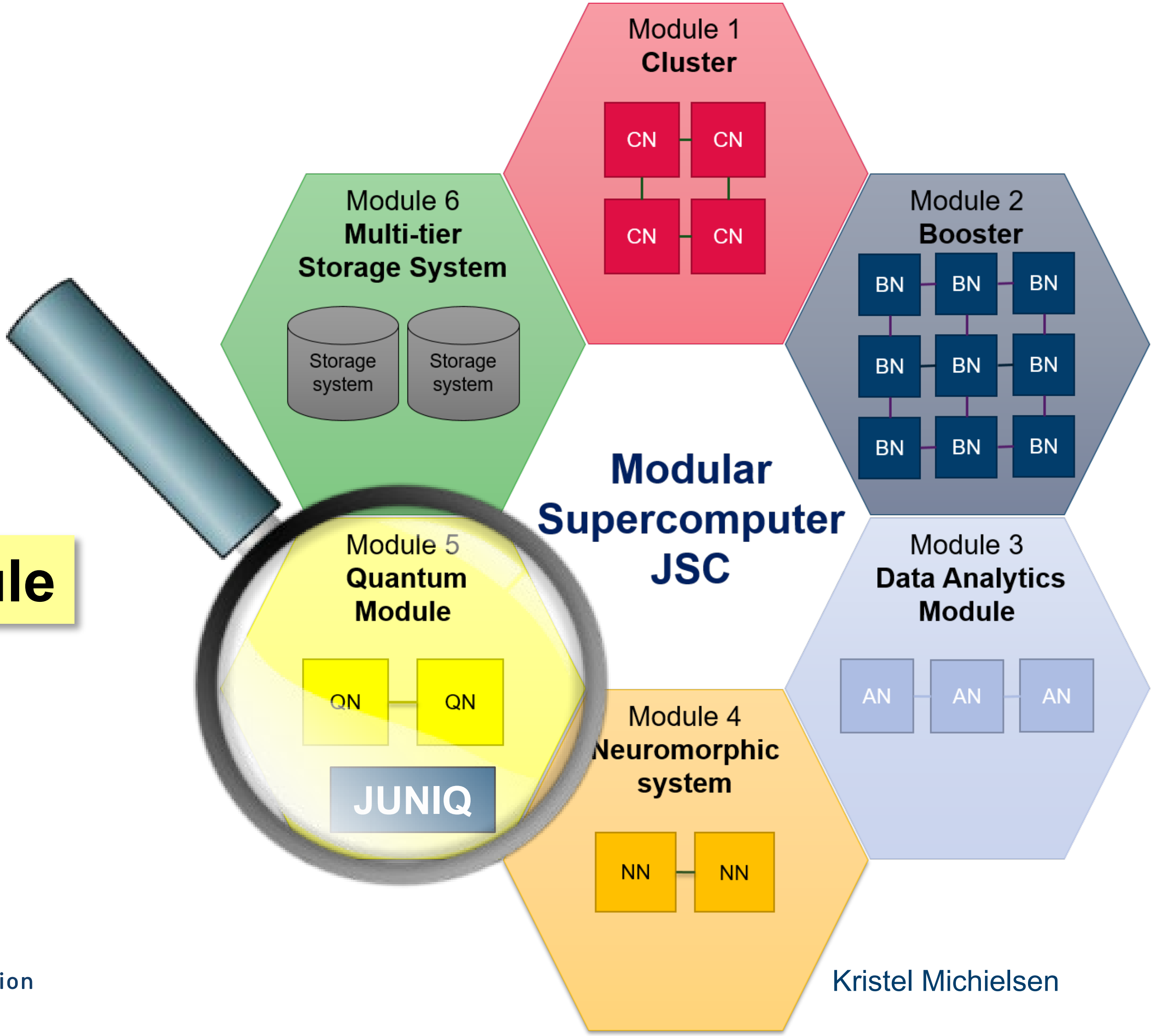


qSVM
Quantenannealer:
solutions for trainingdata

JUNIQ - Jülich UNified Infrastructure for Quantum computing

A European quantum computer user facility at the Jülich Supercomputing Centre

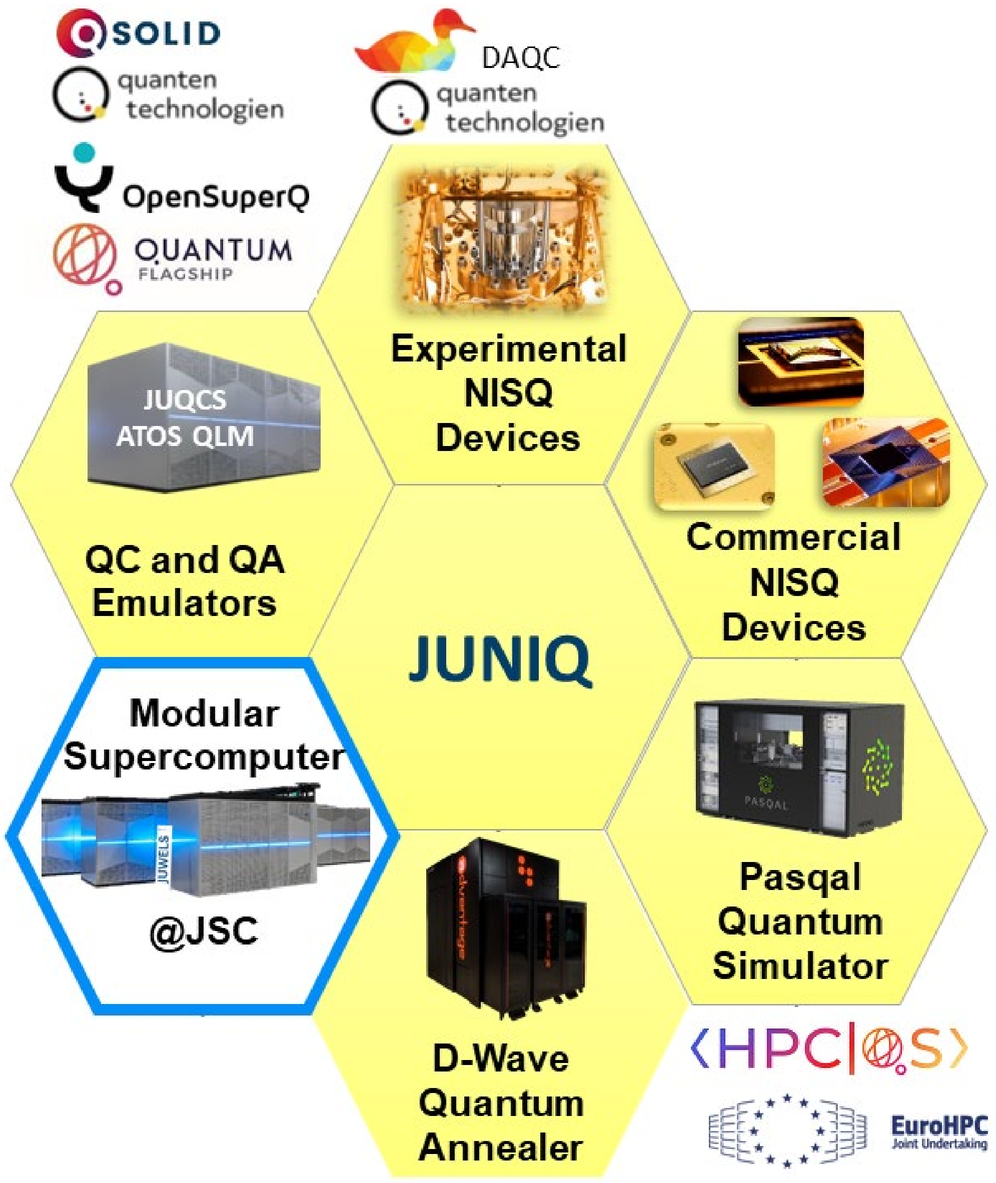
Quantum Module



Plan: Seamless QC-HPC integration

Perspective:
Quantum-Classical
Hybrid Computing Models

JUNIQ - Jülich UNified Infrastructure for Quantum computing



1. QC user facility for science and industry
2. Installation, operation and provision of QCs
3. Unified portal for access to QC emulators and to QC devices at different levels of technological maturity (QC-PaaS)
4. Development of algorithms and prototype applications
5. Services, training and user support
6. Modular quantum-HPC hybrid computing

Website: https://www.fz-juelich.de/ias/jsc/juniq

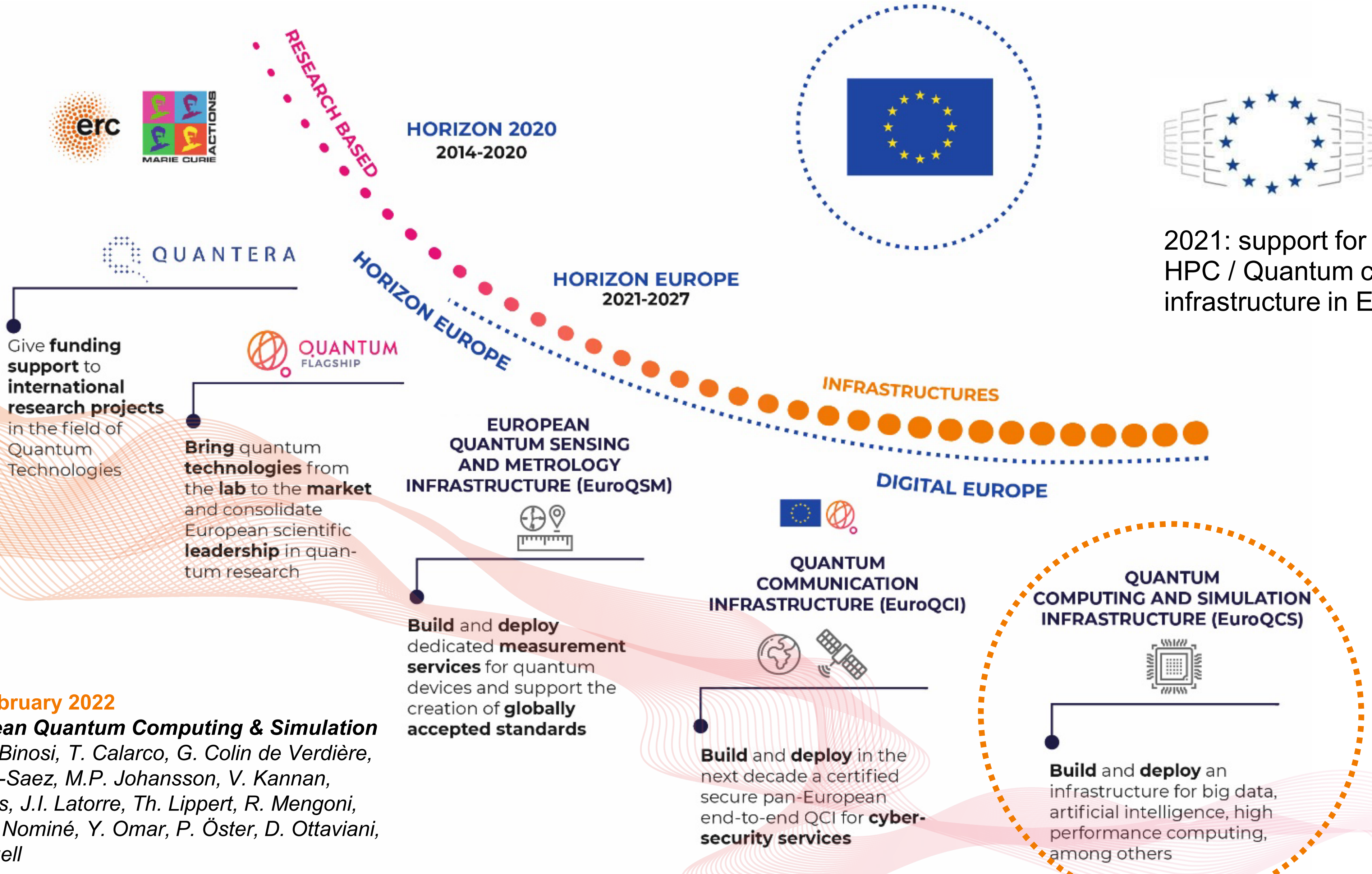
Rolling call for the submission of project proposals

JÜLICH Forschungszentrum | JUNIQ QUANTUM USER FACILITY

is a manufacturer-independent, comprehensive quantum computing user facility integrated in the Jülich Supercomputing Centre, with easy and affordable, peer-reviewed access

EuroQCS

From Vision to Reality – the EU's commitment



EuroHPC Joint Undertaking

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

White paper, 2 February 2022

EuroQCS: European Quantum Computing & Simulation Infrastructure, *D. Binosi, T. Calarco, G. Colin de Verdière, S. Corni, A. Garcia-Saez, M.P. Johansson, V. Kannan, N. Katz, I. Kerenidis, J.I. Latorre, Th. Lippert, R. Mengoni, K. Michielsen, J.P. Nominé, Y. Omar, P. Öster, D. Ottaviani, M. Schulz, L. Tarruell*

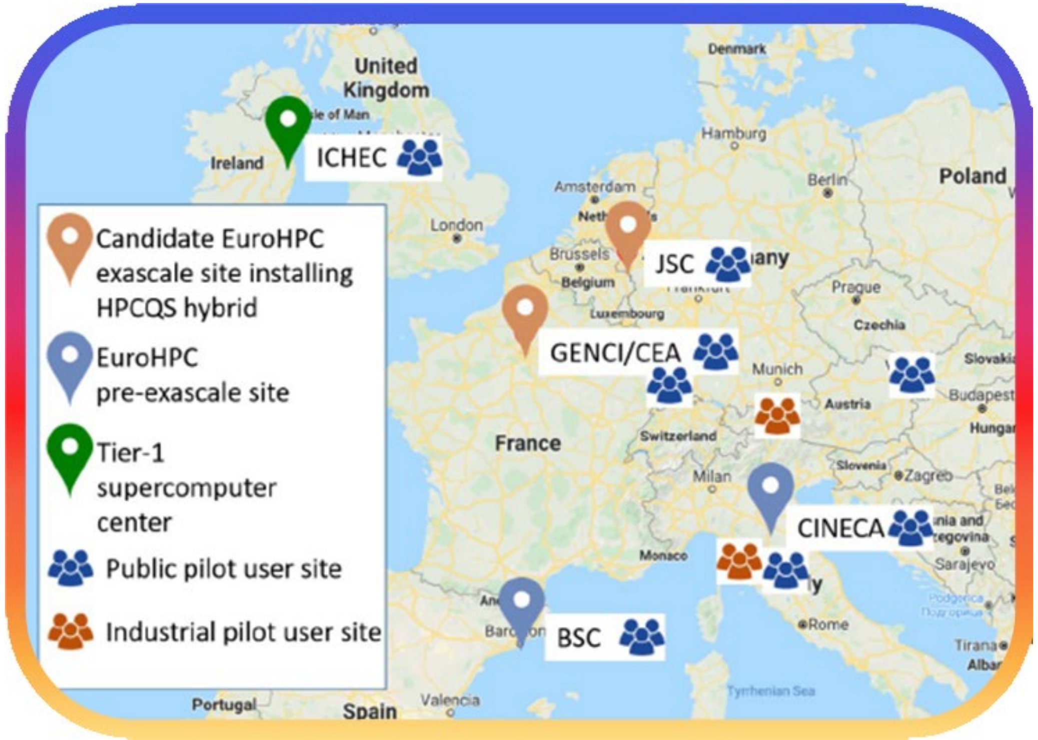
⟨HPC|QS⟩

High Performance Computer and Quantum Simulator hybrid

This project has received funding from the European High-Performance Computing Joint Undertaking (JU) under grant agreement No 101018180.
The JU receives support from the European Union’s Horizon 2020 research and innovation programme and Germany, France, Italy, Ireland,

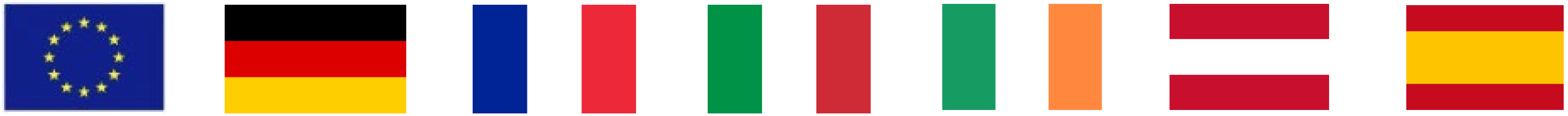
Duration and Partners

- December 1st 2021 - November 30th, 2025
- Coordinator: Forschungszentrum Jülich GmbH
- 15 partners + 3 linked 3rd parties from 6 countries



Financials

- Topic: EuroHPC-2020-01-b -Pilot on quantum simulator
- Total Cost: 12,000,000 €
- EU Contribution: 6,000,000 €
- Funding from German, French, Italian, Irish, Austrian and Spanish national funding institutions



⟨HPC|QS⟩

Work Plan

WP1

Project management and scientific coordination

WP2

Quantum simulator pilot and HPC integration

WP3

Infrastructure software

WP4

Programming technologies and technical libraries

WP5

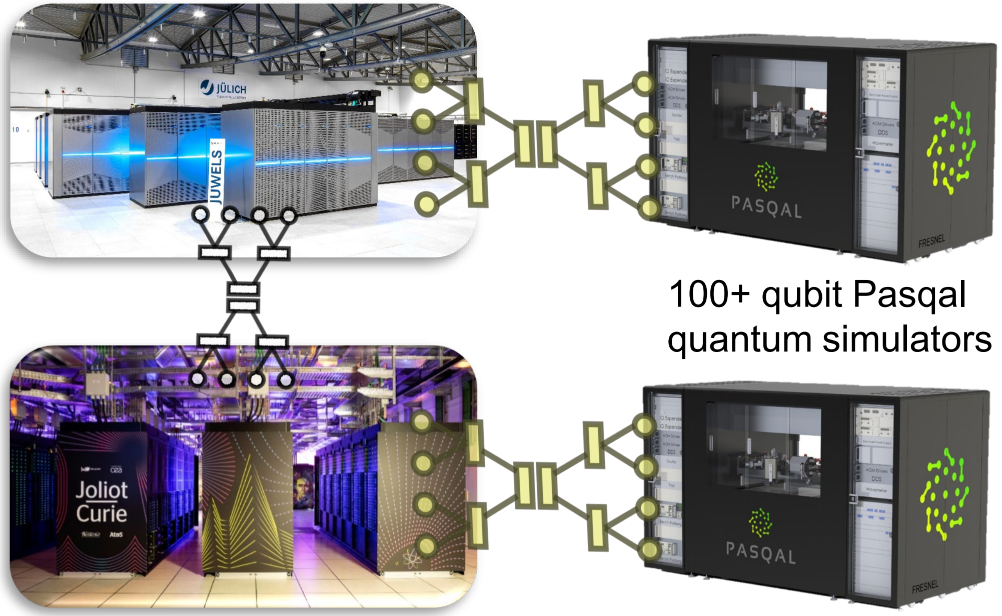
Demonstrators, training and user engagement

WP6

Dissemination, communication and exploitation

Project Aim

- Prepare Europe for the use and federal operation of quantum computers (QC) and simulators (QS)
- Develop, deploy and coordinate a European federated infrastructure integrating a QS of 100+ interacting quantum units in the HPC systems of the supercomputer centres FZJ/JSC and GENCI/CEA
- Provide cloud access for European users, on a non-commercial basis



100+ qubit Pasqal quantum simulators

Public Procurement of Innovative solutions

⟨HPC|QS⟩

HPC-QS Integration – Main Technical Components

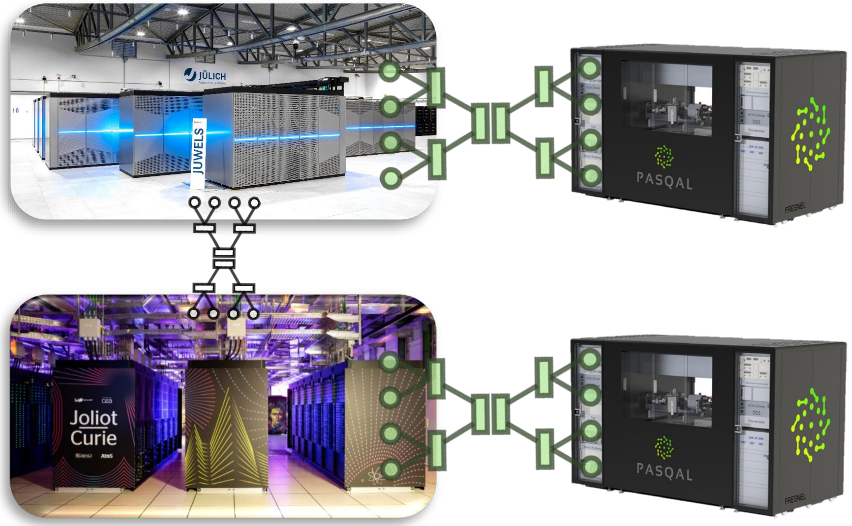
- **Quantum Learning Machine QLM**® by ATOS
  - Programming environment
  - Access to quantum computing backends the quantum simulator

- **Modular Supercomputing Architecture**
  - For lowest latency integration of the quantum simulator
  - Developed in the series of EU-funded DEEP Projects
  - Based on ParTec’s **ParaStation Modulo**® middleware suite

ParaStation MODULO

ParTec Modular Supercomputing

⟨HPC|QS⟩



is an open and evolutionary pan-European hybrid HPC/quantum infrastructure that aims at expanding in the future by including a diversity of quantum computing platforms at different technology readiness levels and by allowing the integration of other European quantum nodes

EuroQCS

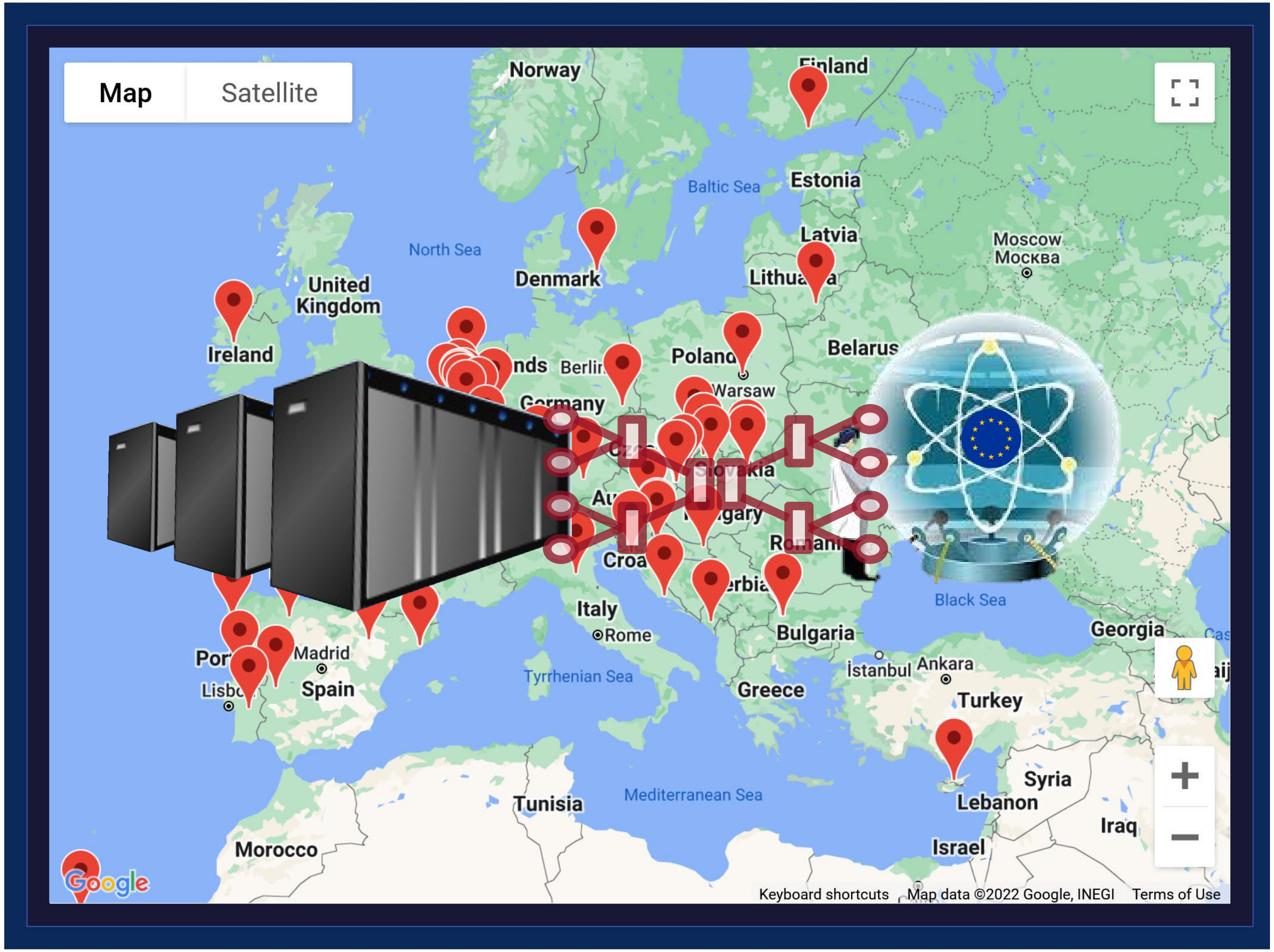
JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

EuroHPC JU call EUROHPC-2022-CEI-QC-01

Call for EoI for the hosting and operation of European quantum computers integrated in HPC supercomputers

- The selected hosting entities will operate the QCs on behalf of the EuroHPC JU
- The QCs will be integrated in existing supercomputers operated by the hosting entities
- The QCs should have at least 10 qubits, with a 2-qubit gate error rate of less than 1% and allow for a maximum circuit depth and number of entangled qubits by the installation date
- The selection will aim at ensuring a level of diversity in the technologies and architectures of the different QCs to be acquired to give users access to as many different quantum technologies as possible

EuroQCS


Map
Satellite
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Finland
Estonia
Baltic Sea
Latvia
North Sea
Denmark
Moscow
Москва
United Kingdom
Ireland
Belarus
Poland
Warsaw
Germany
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Rome
Tyrrhenian Sea
Bulgaria
Black Sea
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Madrid
Spain
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Thank you