JUNIQ – Jülich UNified Infrastructure for Quantum computing

HELMHOLTZ
RESEARCH FOR GRAND CHALLENGES

Integration of quantum computers in an HPC environment

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QUANTUM

For practical quantum computing …

the best of both computer technologies must be combined

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Content

Hardware integration

User requirements

Current systems at Juelich Supercomputing Centre (JSC)

What's needed from the providers?

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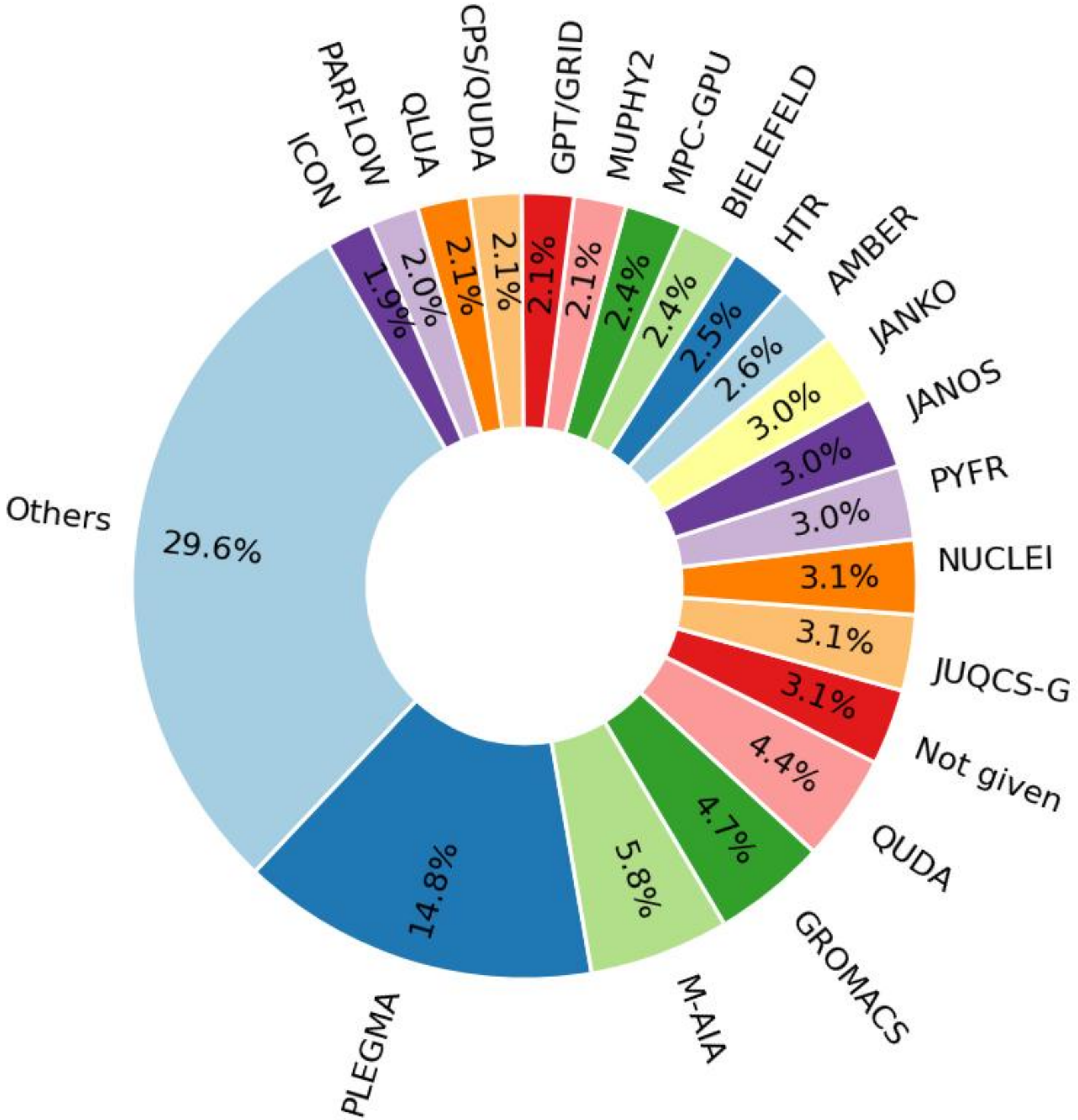
Hardware Integration

Hardware interfaces

- Electrical:
  - Typical: 3-phase connection to compressor, gas handling system
  - Usually avoid residual current device (RCD), as it is only required for protection of humans -> **less probability of unplanned outages**
- Water cooling
  - Make sure there is resilience built into your circuit. Shutdown due to over-temperature results equally in total system shutdown.
- Network connectivity
  - Normally the least demanding part: in most cases a 1Gbit/s line is more than you need
- Staff access
  - Technicians/engineers for compliance with SLAs are to be granted access

Proposals for compute frameworks at the Juelich Supercomputing Centre



Proposals for compute frameworks at the Juelich Supercomputing Centre

#	Software	Description	Typical Use Cases
1	AMBER	Molecular dynamics for biomolecules	Protein folding, drug design
2	Arbor	Neuroscience spiking network simulator	Brain modeling
3	BIELEFELD	Lattice QCD simulation framework	Quantum Chromodynamics research
4	Chroma	Lattice QCD large-scale simulations	Hadron structure, quantum physics
5	CPS/QUDA	Lattice QCD GPU library	Quantum chromodynamics on GPU
6	DynQCD	Dynamical fermion lattice QCD code	Particle physics simulations
7	GPT/GRID	Grid lattice QCD solver	Gauge field simulations
8	GROMACS	Molecular dynamics package	Biophysics, chemistry

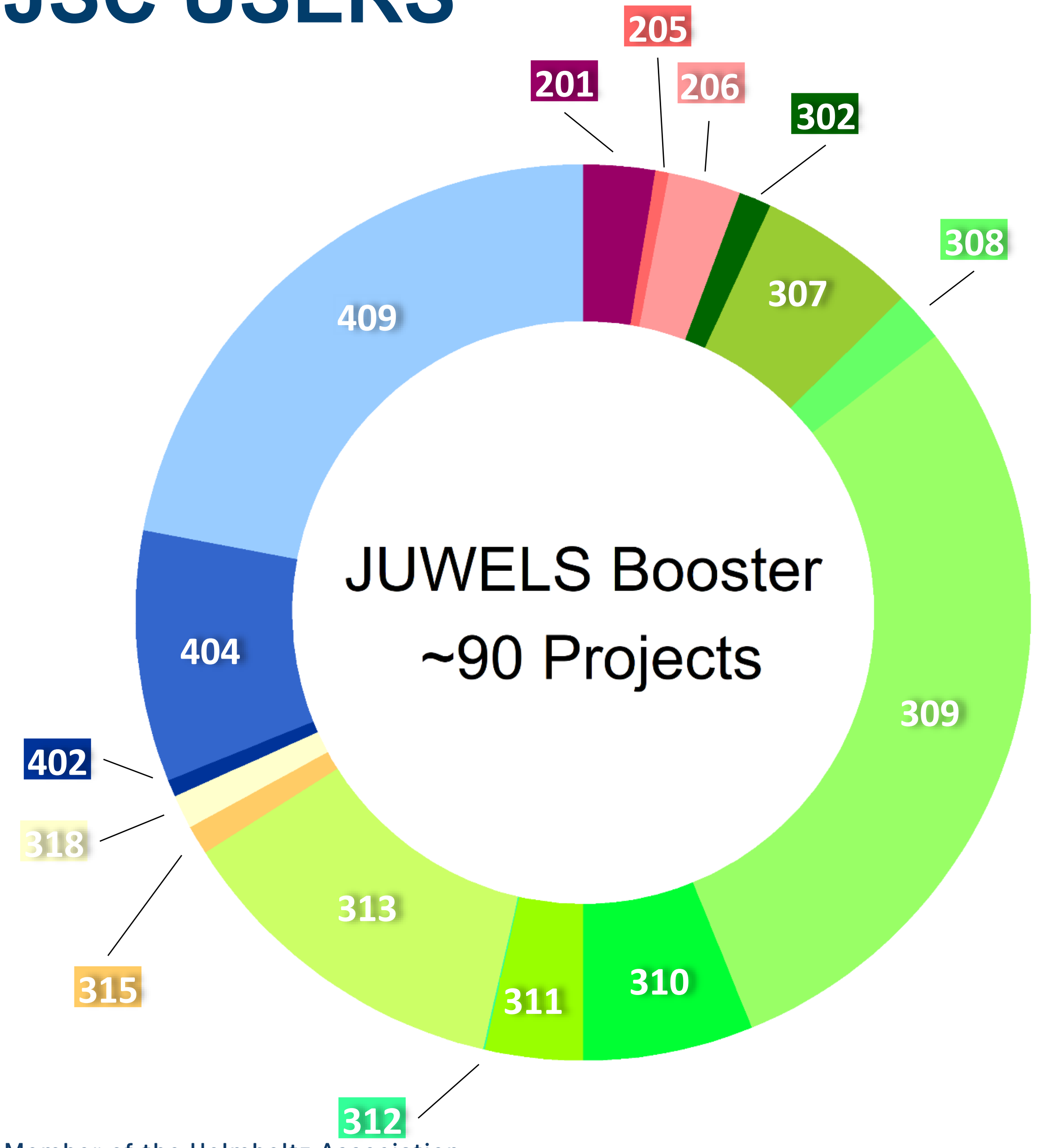
#	Software	Description	Typical Use Cases
9	HTR	Hypersonic reacting flows simulator	Aerospace, combustion research
10	ICON	Climate and weather simulation model	Weather forecasting, climate
11	JANOS	HPC framework for multiphysics	Engineering simulations
12	JANKO	HPC framework for materials science	Material simulations
13	JUQCS-G	Quantum computer simulator with GPU	Quantum algorithm prototyping
14	M-AIA	AI/ML framework for scientific computing	Machine learning workloads
15	MMoCLIP	Multimodal contrastive learning	Vision-language AI models
16	MPC-GPU	GPU-based multiphysics simulations	Fluid dynamics, robotics

Proposals for compute frameworks at the Juelich Supercomputing Centre

#	Software	Description	Typical Use Cases
17	MUPHY2	Multiphysics for complex fluids	Biophysics, plasma simulation
18	NAStJA	Lattice QCD analysis software	High-precision QCD analysis
19	NEKRS	GPU spectral element solver	Incompressible flows, CFD
20	NLP (Megatron)	Large-scale transformer NLP training	Natural language processing
21	NUCLEI	Nuclear structure and reaction model	Nuclear physics
22	PARFLOW	Parallel groundwater flow solver	Hydrology, environment modeling
23	PIConGPU	Particle-in-cell plasma simulations	Plasma physics, astrophysics
24	PLEGMA	HPC framework for quantum materials	Multiscale simulations

#	Software	Description	Typical Use Cases
25	PYFR	Python high-order CFD solver	Turbulence, aerodynamics
26	QUANTUM ESPRESSO	Plane-wave DFT electronic structure package	Materials science, quantum chemistry
27	QUDA	GPU library for lattice QCD	Lattice QCD GPU acceleration
28	SOMA	Simulation environment for neuromorphic apps	Brain-inspired computing

JSC USERS



Reseach Fields

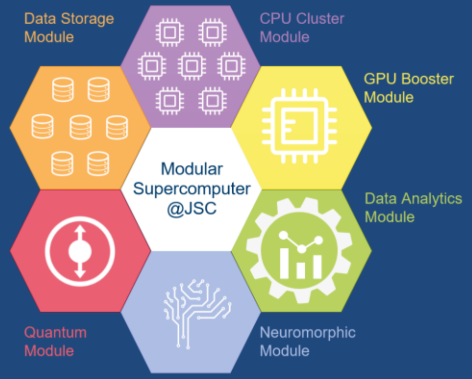
- 201 Basic Biological and Medical Research
- 205 Medicine
- 206 Neurosciences
- 302 Chemical Solid State and Surface Research
- 307 Condensed Matter Physics
- 308 Optics, Quantum Optics and Physics of Atoms, Molecules and Plasmas
- 309 Particles, Nuclei and Fields
- 310 Statistical Physics, Soft Matter, Biological Physics, Nonlinear Dynamics
- 311 Astrophysics and Astronomy
- 312 Mathematics
- 313 Atmospheric Science, Oceanography and Climate Research
- 315 Geophysics and Geodesy
- 318 Water Research
- 402 Mechanics and Constructive Mechanical Engineering
- 404 Heat Energy Technology, Thermal Machines, Fluid Mechanics
- 409 Computer Science

→ Define Benchmarks

HPC-QC integration models

Different QPU access models for different integration levels

QPU access model	Integration mode	QPU scarcity	Advantages	Disadvantages	Example	Compatibility
Cloud access	None	1 QPU / many HPC centers	No integration work required on HPC center.	**Scheduler on cloud-side impedes real HPC workloads.**	Qiskit Leap²	N/A.
HPC system-global	"Flexible"	Few (diverse) QPUs / 1 HPC center	Supports HPC workloads. **Allows QPU-sharing.**	Scheduling is tricky (HPC vs QC job timescales, resource sharing).	JÜLICH Forschungszentrum | JUNIQ QUANTUM USER FACILITY	Can support cloud access too.
HPC node-local	"Fixed"	Many QPUs / 1 HPC center	**Highest performance potential.** Delegates scheduling issues.	Assumes QPUs are widely-available resources (like GPUs). No QPU sharing.	NVIDIA CUDA QUANTUM	None.



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JUNIQ-Cloud portal

User access via JupyterHub portal

- Portal-based access in form of a QC-PaaS under European legislation
  - Based on pre-existing JupyterHub solution for HPC access,
  - Deploys on HPC or JSC cloud services,
  - Pre-configured access to QPUs,
  - Loaded with QC SW for beginner users,
  - Customizable environment for advanced users.

Qaptiva 800s

One flexible HPCQC integration approach

QSOLID ⟨HPC|QS⟩

Environment for developing & emulating quantum software, hosted at JSC.

- Serves as bridge between HPC systems and QC devices
- Bundles access to:
  - Pasqal QS (HPCQS),
  - QSolid QPU (QSolid),
  - eleQtron QPU (EPIQ),
  - IQM QPU,
  - Qaptiva emulator suite.
- Financed by QSolid project.

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JUPITER HIGH LEVEL ARCHITECTURE

JUPITER – HIGH-LEVEL AR… …TURE

- >1 ExaFLOP/s FP64 HPL
- >70 ExaFLOP/s FP8 AI
- ~6000 Nodes
- ~24000 NVIDIA Grace-Hopper
- NVIDIA Mellanox NDR
- BullSequana XH3000

- JUPITER Management Stack
  - Modular System Architecture
  - ParTec ParaStation Modulo
  - Eviden SMC xScale
- Scheduler: Slurm
- Scientific Software: EasyBuild
- Jobreporting: LLview

Parallel …pacity …apacity …/Archi…

High Capa… Backu…

- >5 PetaFLOP/s FP64 HPL
- ~1300 Nodes
- ~2600 SiPearl Rhea1
- BullSequana XH3000

- 210 PB useable SAS
- ~1,5 TB/s
- 22* IBM SSS6000

Interactive Computation and Visualization

- 23 Login Nodes
- NVIDIA Hopper/A40
- 200 Gbit/s connectivity

EU-Tech… Enabling…

…-Technology …abling Module

- 21 PB useable Flash
- ~2,5 TB/s
- 20* IBM SSS6000

C…guration

Future Call Modules

Core Configuration

Future Call Modules

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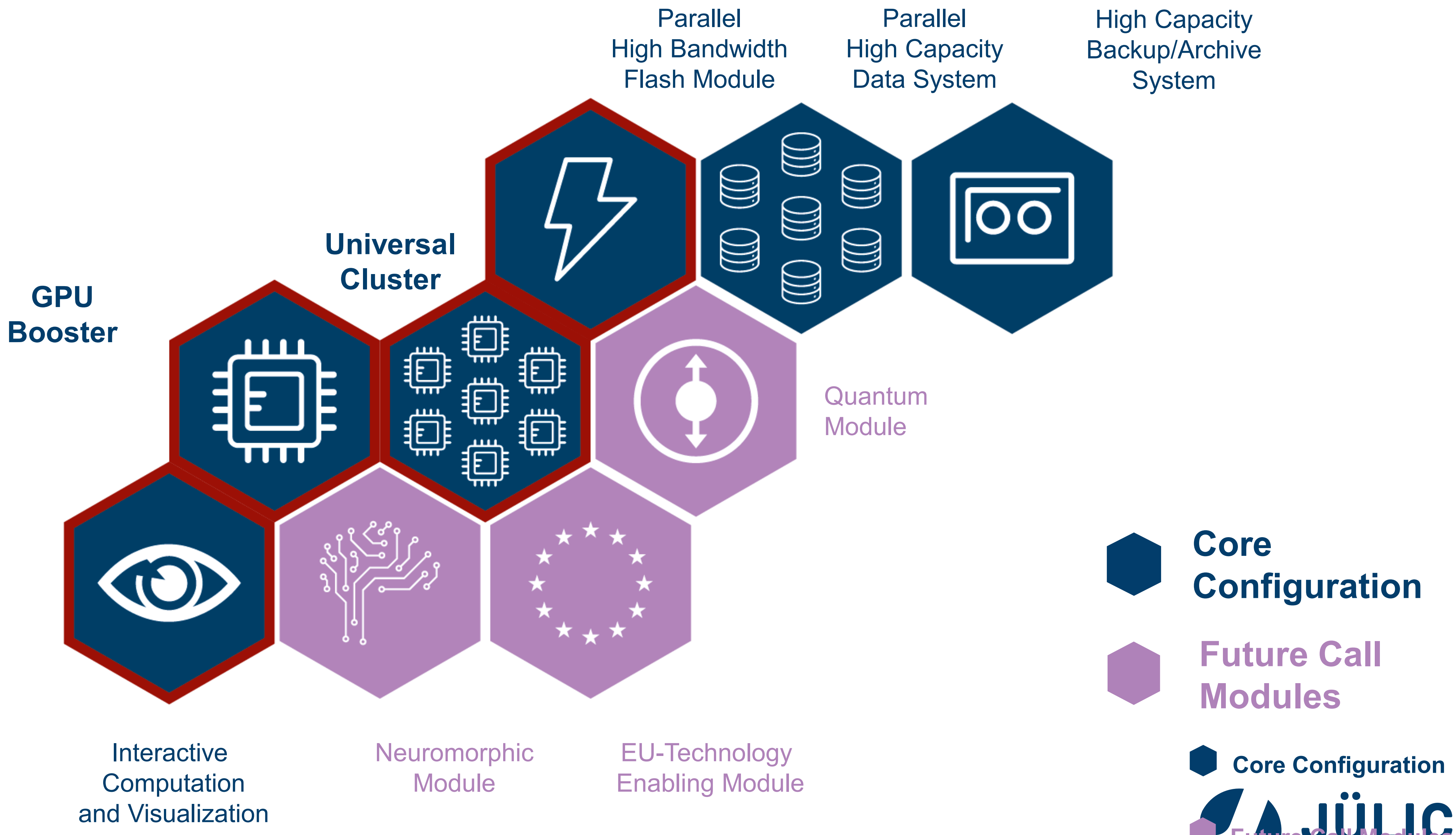
…Association

JUPITER – HIGH-LEVEL ARCHITECTURE



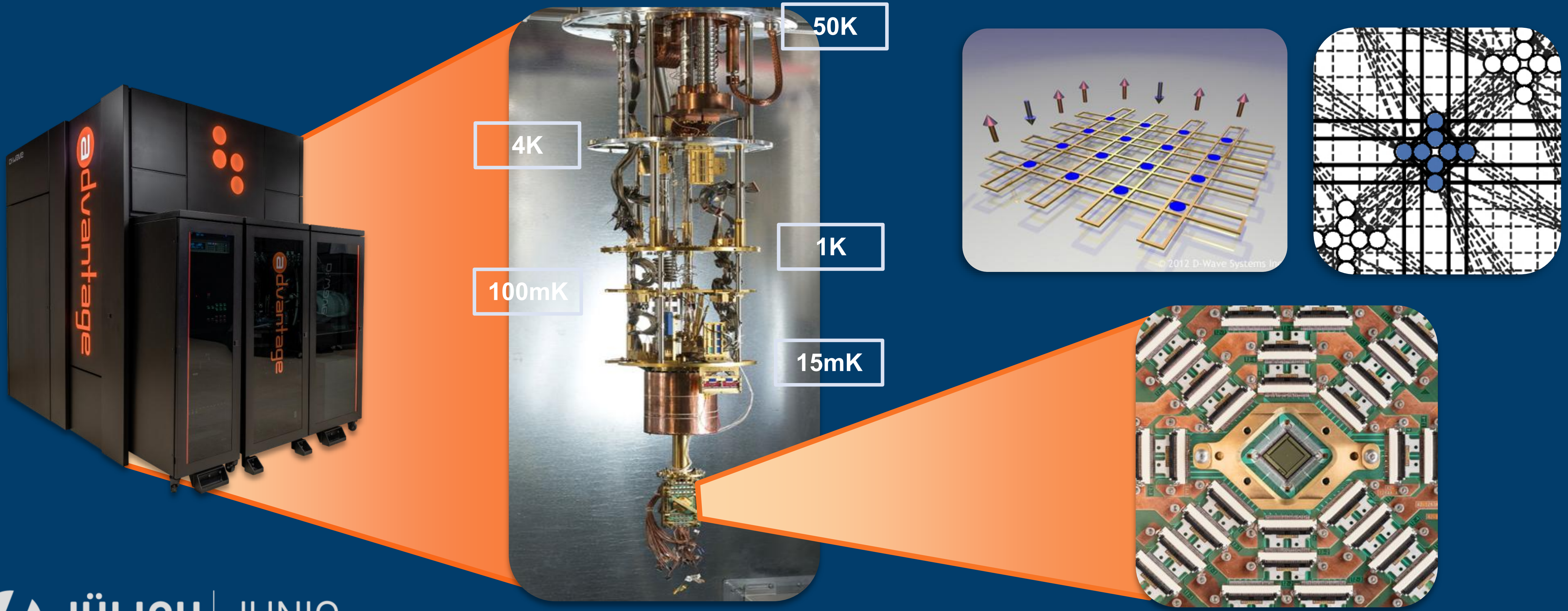
D:WAVE The Quantum Computing Company™ **Advantage**

Cooling system

25kW power consumption

Quantum Processing Unit

5640 superconducting qubits
Pegasus topology with 40.484 couplers



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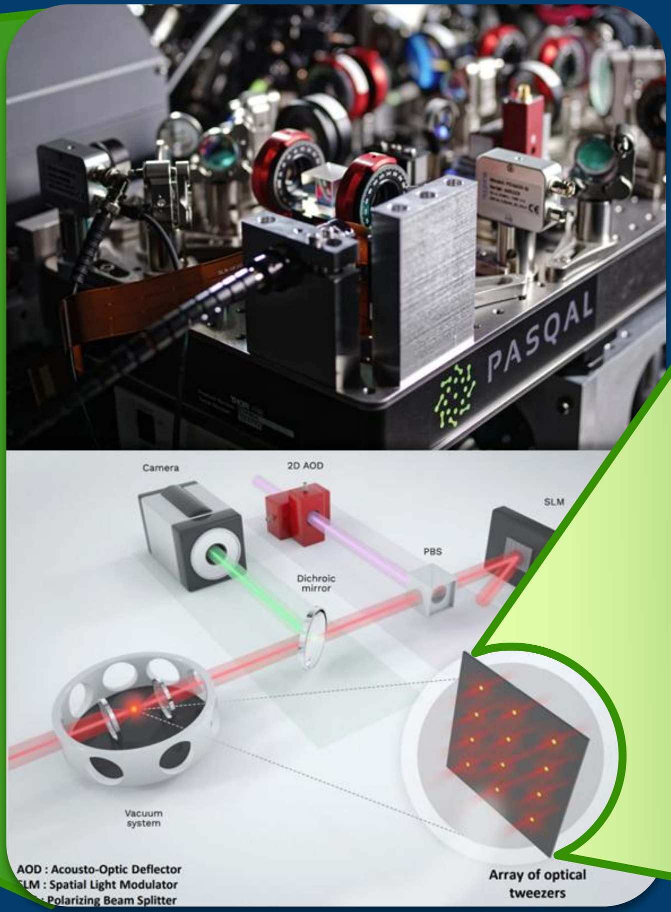
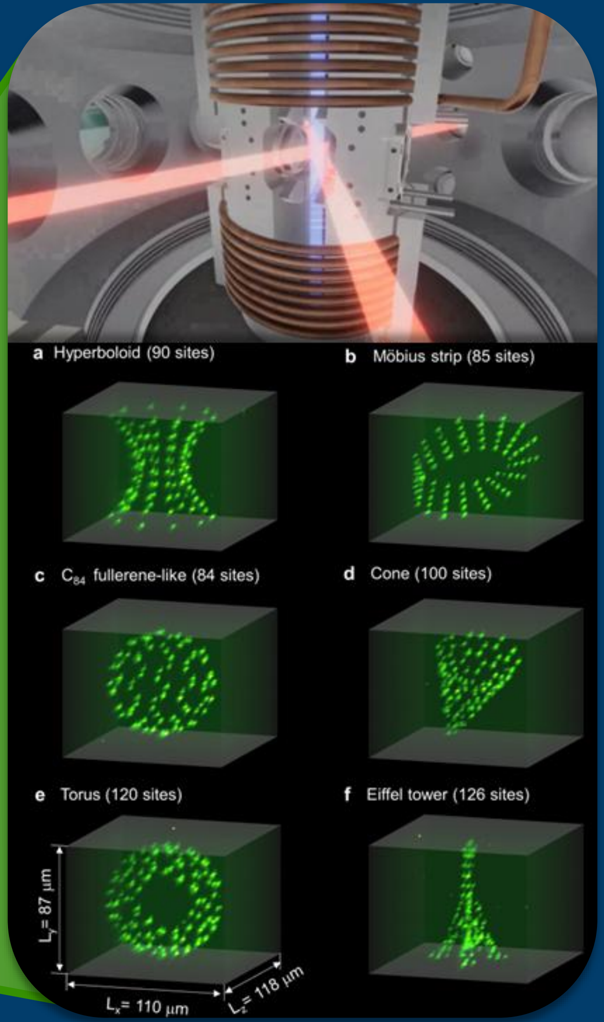
PASQAL **Fresnel**

Quantum Processing Unit

Quantum Register

100 Rydberg atoms tapped in a 3D lattice





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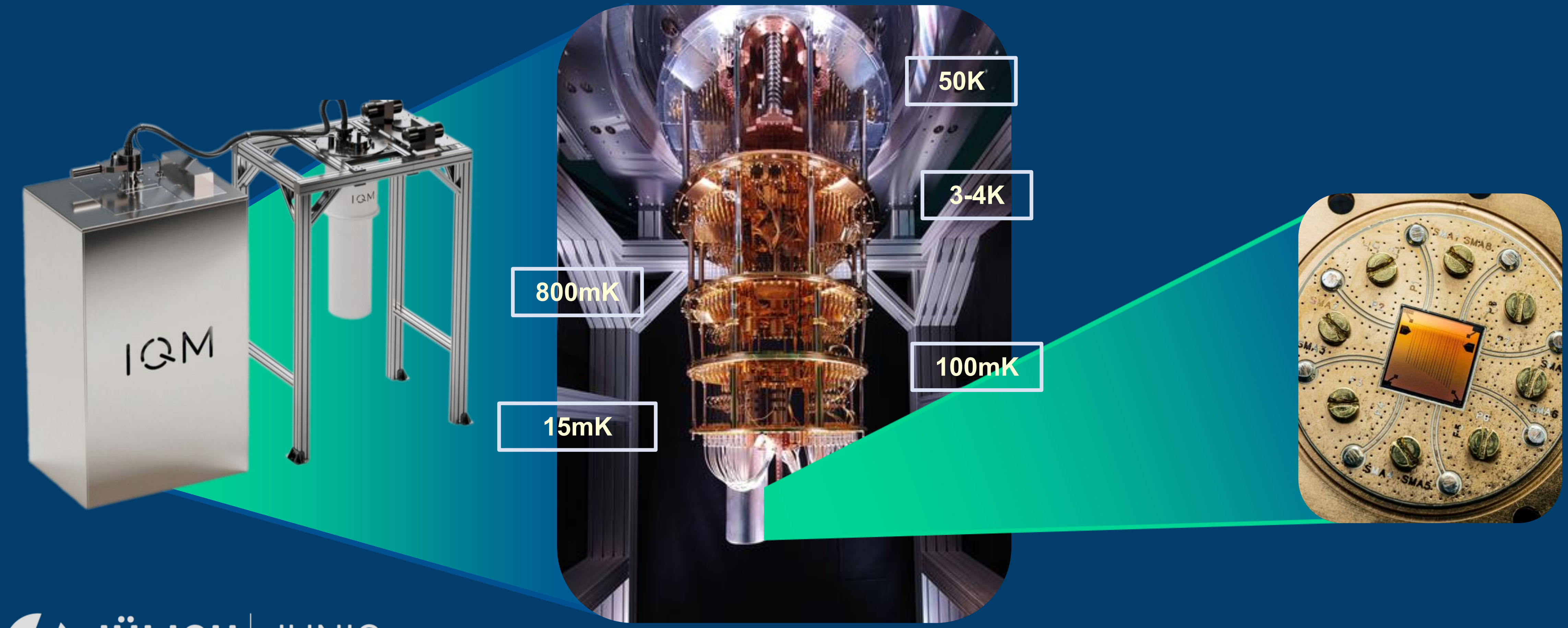
IQM Spark

Cooling system

Quantum Processing Unit

5 superconducting qubits



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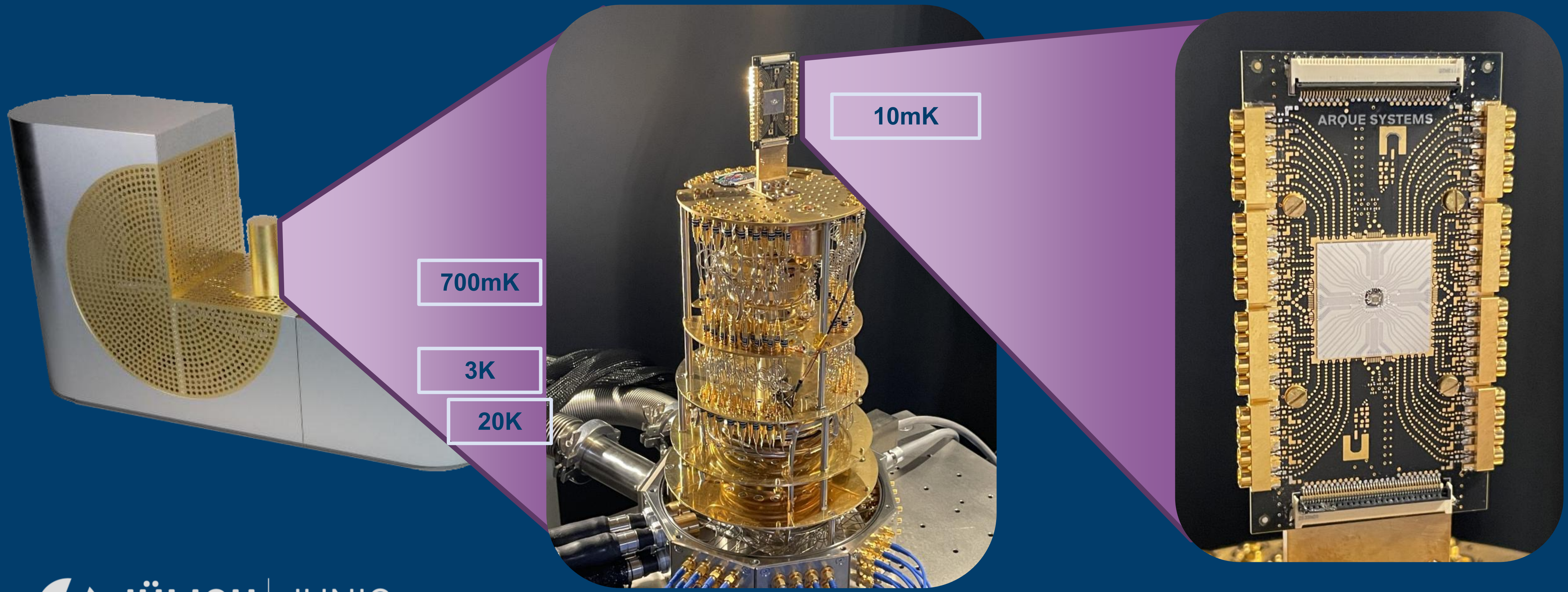
ARQUE5

ARQUE SYSTEMS

Cooling system

Quantum Processing Unit

5 electron-spin qubits



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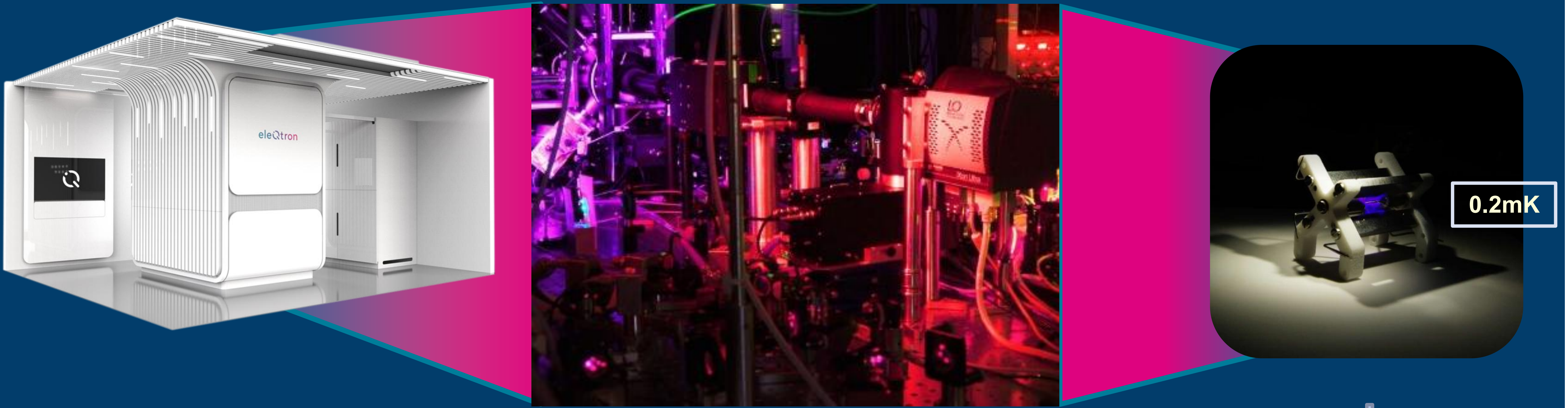
eleQtron

Quantum Processing Unit

Linear ion trap

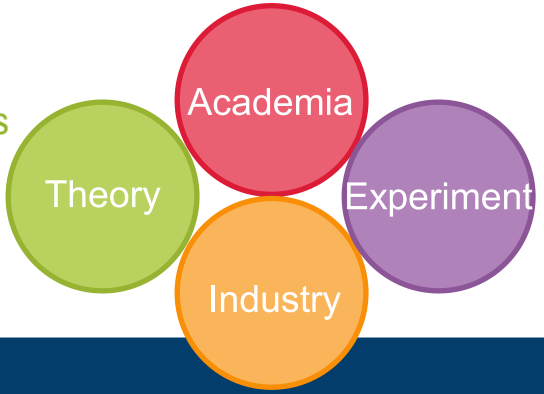
Quantum Register

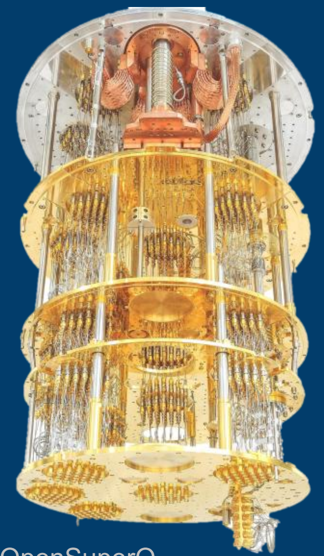
20-30 trapped ion qubits controlled with MAGIC technology



Quantum Computing

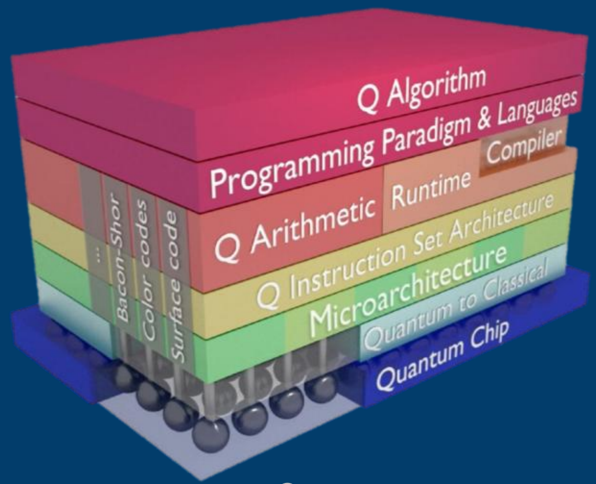
What is needed?





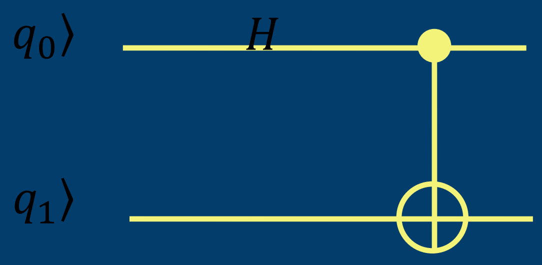
© OpenSuperQ

Quantum computer hardware
Quantum processor/chip



© QuTech

Quantum software stack
Quantum control, quantum error correction, compiler, user interfaces, …



$1\rangle_1 1\rangle_2 \rightarrow entangledstate$

Quantum algorithms
Sequence of controlled one- and two-qubit operations

Use cases & access
Quantum computer user infrastructure

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The potential of Quantum Computing

Science & Industry:

A diverse user group with various hard computational challenges to unravel complex systems

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JSC’s Quantum Computing Strategy

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Four Pillars

I. Modeling and emulation (since 2004)

II. Provision of QC systems (since 2016)

III. HPC-QC integration (since 2017)

IV. Creation of a quantum computing user infrastructure (since 2016)

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Quantum computing

... promises to solve some of our toughest problems

Drug design

Materials design

Supply chain logistics

Traffic optimization

Energy grid management

Vegetation evolution – climate change

Human brain functionality – neural networks

QML

What's needed from the suppliers?

As Supercomputing Centre Operator you want to be able to react:

- SLAs with quantum computer suppliers
- Assignment of „task severities“ to either local trained staff or suppliers' responsible staff.
- Software middleware needs to be well documented, each abstraction layer may require separate definition of access rights and responsibilities.

Questions?

Also offline:

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+49 157 74512305

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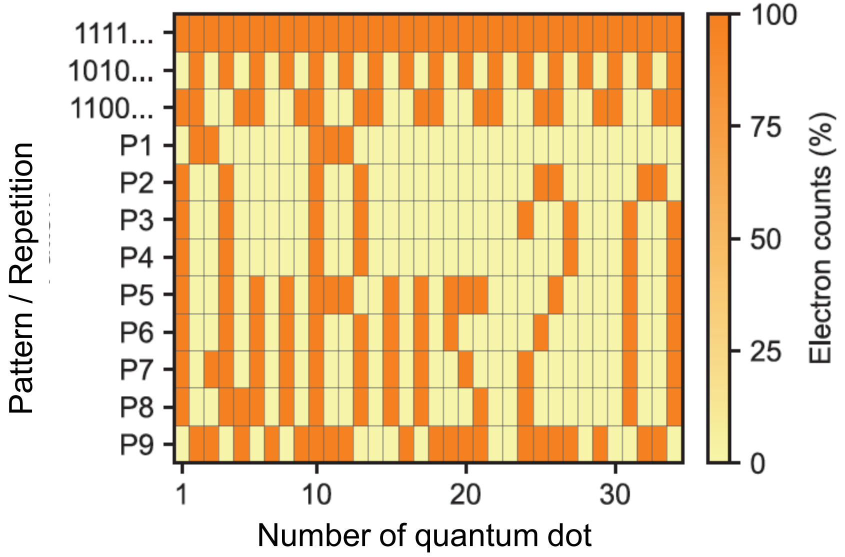
Backup slides next...

ARQUE shuttling achievements - Summary

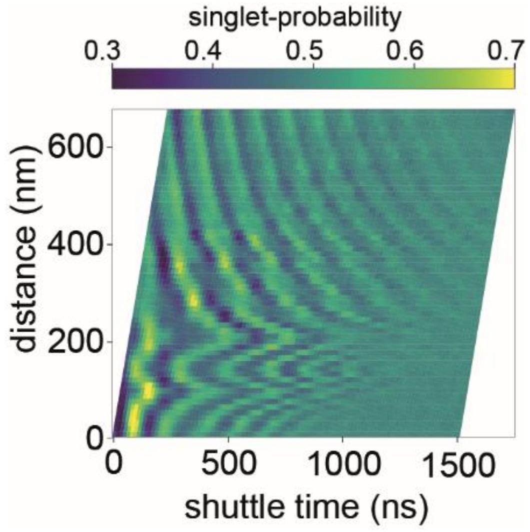
10 µm

Shuttle fidelity 99.7 % @ 18 µm
34 QDs controlled by 4+2 signals



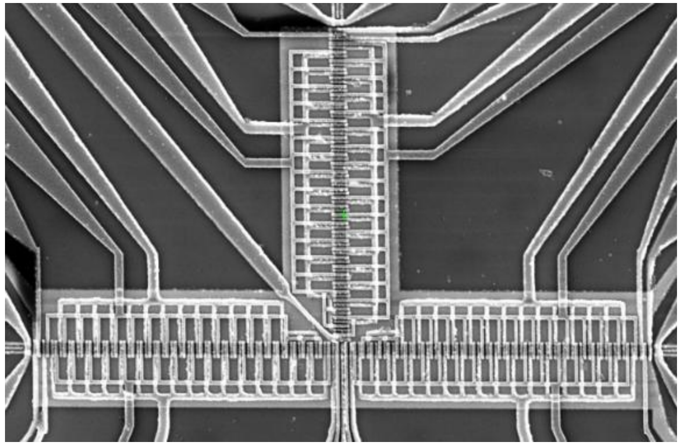
R. Xue *et al.*, Nature Commun. **15**, 2296 (2024)

spin-EPR pair shuttle & mapping of valley splitting



Struck *et al.*, Nature Commun. **15**:1325 (2024)
M. Volmer *et al.*, npj Quantum Inf. **10**, 61 (2024)

T-junction

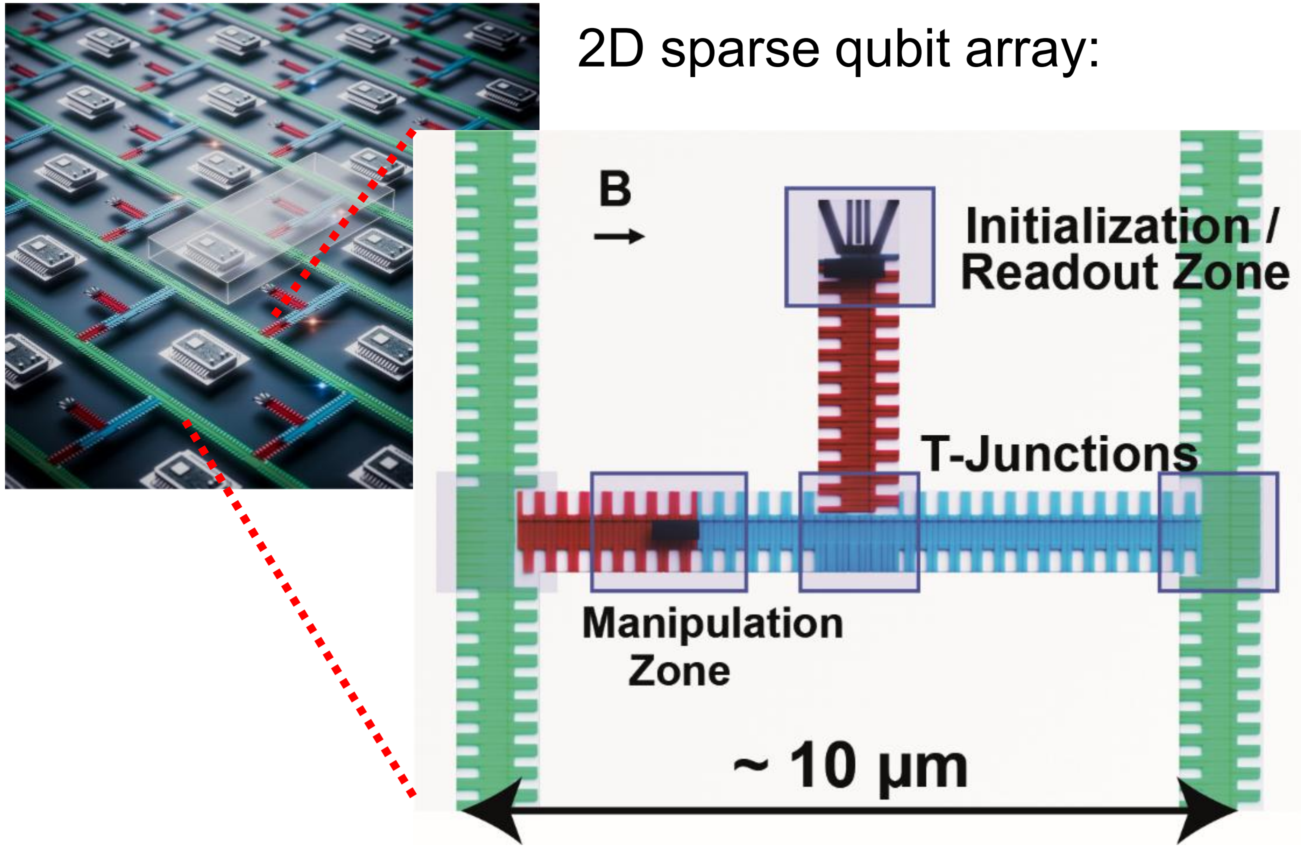


51 QDs controlled by 4+4+2 signals

Quantum computer production chain

Industry grade fabrication

2D sparse qubit array:



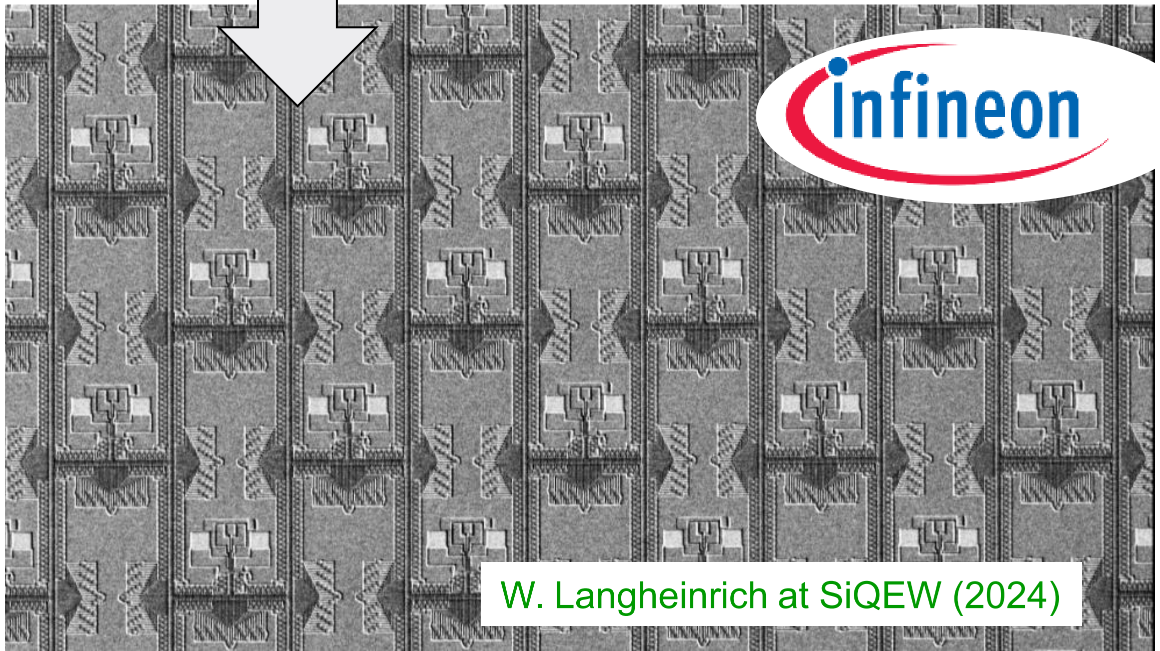
Künne & Willmes *et al.*, Nature Commun. **15**, 4977 (2024)
T. Huckemann *et al.*, IEEE Electron Device Letters **46**, 868 (2025)

Wafer

Fabrication

Characterisation

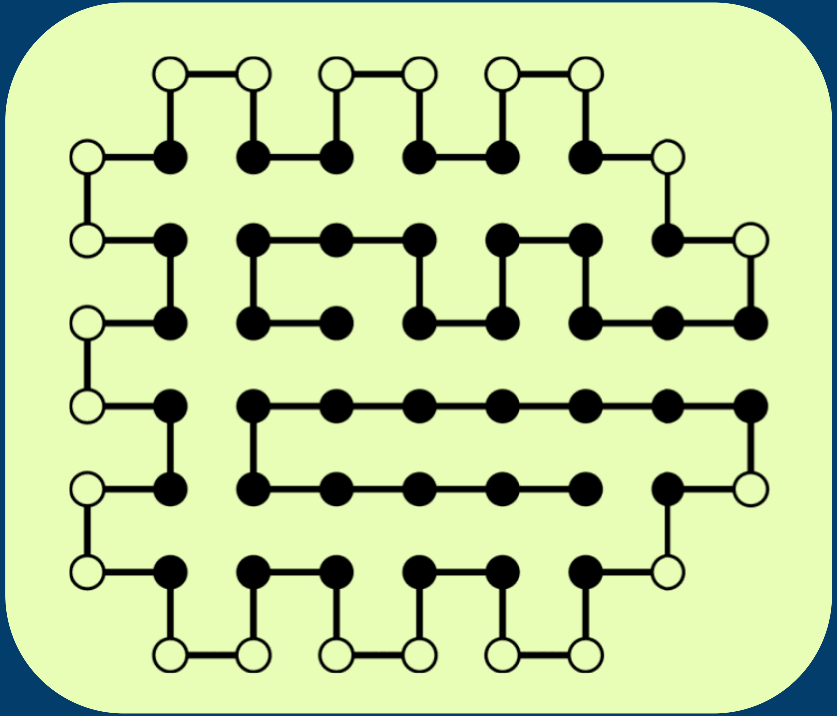
Integration



W. Langheinrich at SiQEW (2024)

Application I

Protein folding on JUNIQ’s D-Wave quantum annealer JUPSI



Example of a lowest energy structure of a chain with 64 amino acids

A. Irbäck, et al., Phys. Rev. Research 4, 043013 (2022)

- Simplified problem: two types of amino acids in protein chain, each amino acid is a ball occupying a lattice site, no surrounding medium
  □ search for the “best” arrangement
- JUPSI performs better than laptop: Success rate on
  - JUPSI: 100% for chains with up to 64 amino acids
  - Laptop: 80% for 30 amino acids and much less for 48 and 64 amino acids

"I should point out that as of today, even with such simplified models, being able to study chains of 64 amino acids using a quantum computer is a hard problem, which makes our results very satisfying!"

Dr. Sandipan Mohanty, Simulation and Data Lab Biology, JSC

Application II

Tail Assignment Problem (Hybrid Quantum – Classical Computing)

QAOA - Variational quantum algorithm (hybrid algorithm)

- Quantum algorithm to iteratively apply a series of parametrized unitary transformations to a quantum register and evaluate its energy expectation value
- Classical optimization algorithm to optimize the parameters of the unitary transformations

GPUs of JUWELS Booster
 QPUs

CPUs of JUWELS Booster

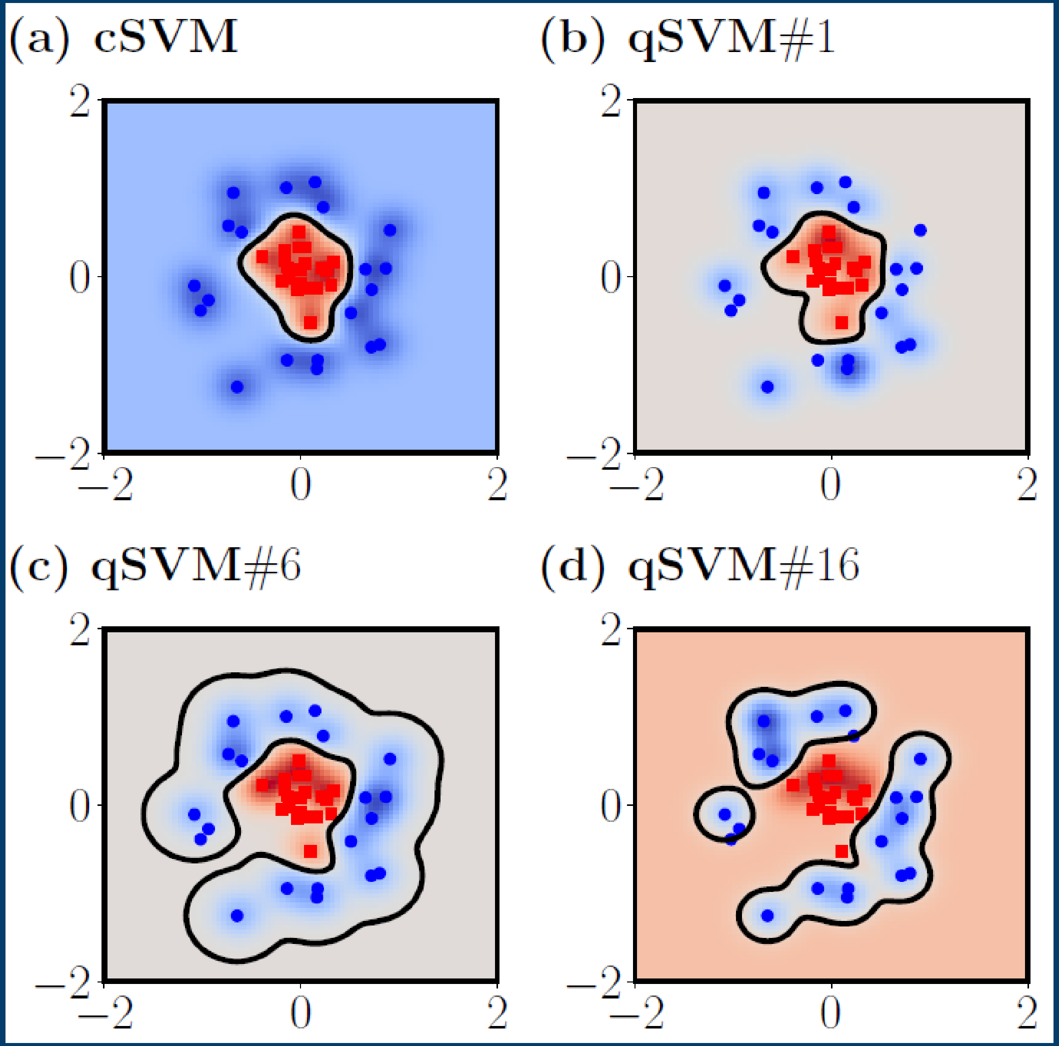
Assign aircrafts to flights – minimize overall cost respecting operational constraints

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

 problem with **40 qubits**

Application III

Machine learning on the D-Wave quantum annealer



Support Vector Machine (SVM), a supervised machine learning algorithm

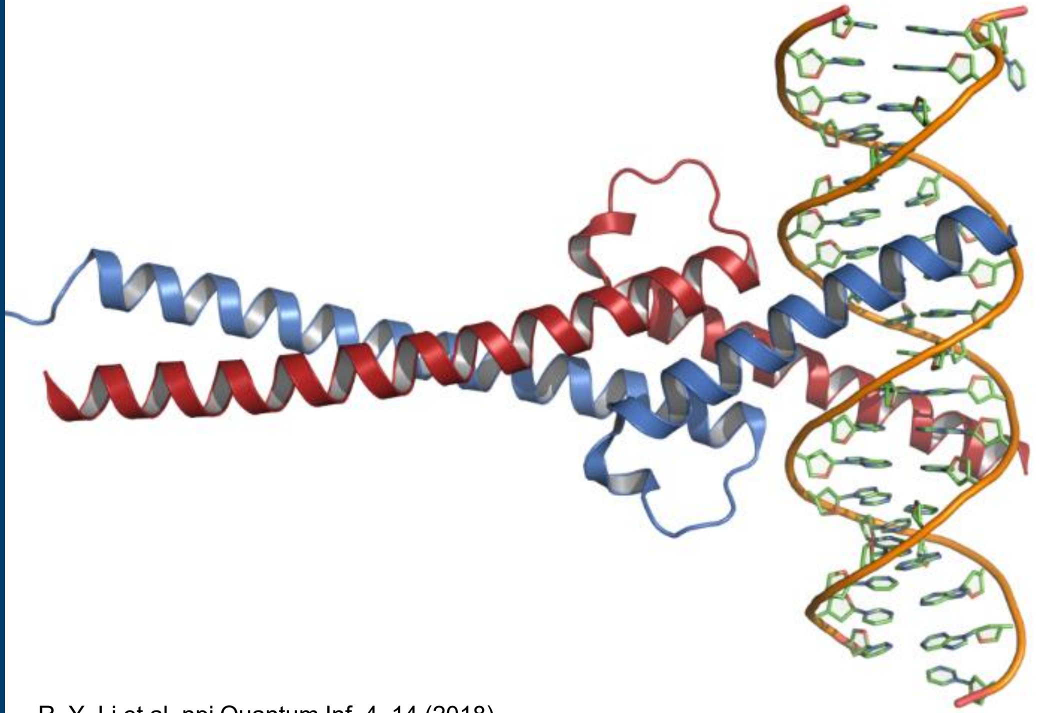
- Classical SVM (CSVM): training corresponds to a convex quadratic optimization problem, having a global minimum;
- Quantum SVM (QSVM) on a D-Wave quantum annealer: quantum annealer produces various close-to-optimal solutions for the training data, which are combined to create an optimized qSVM classifier.

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

Application IV

Classification on the D-Wave quantum annealer:

Decide whether a certain protein binds to a certain DNA sequence



R. Y. Li et al,.npj Quantum Inf. 4, 14 (2018)

Support Vector Machine (SVM), a supervised machine learning algorithm

- qSVM on a D-Wave quantum annealer (hybrid workflow) can produce significantly stronger classifiers than cSVM for the same little training data and parameters;
- qSVM performs better or comparative to cSVM for all datasets

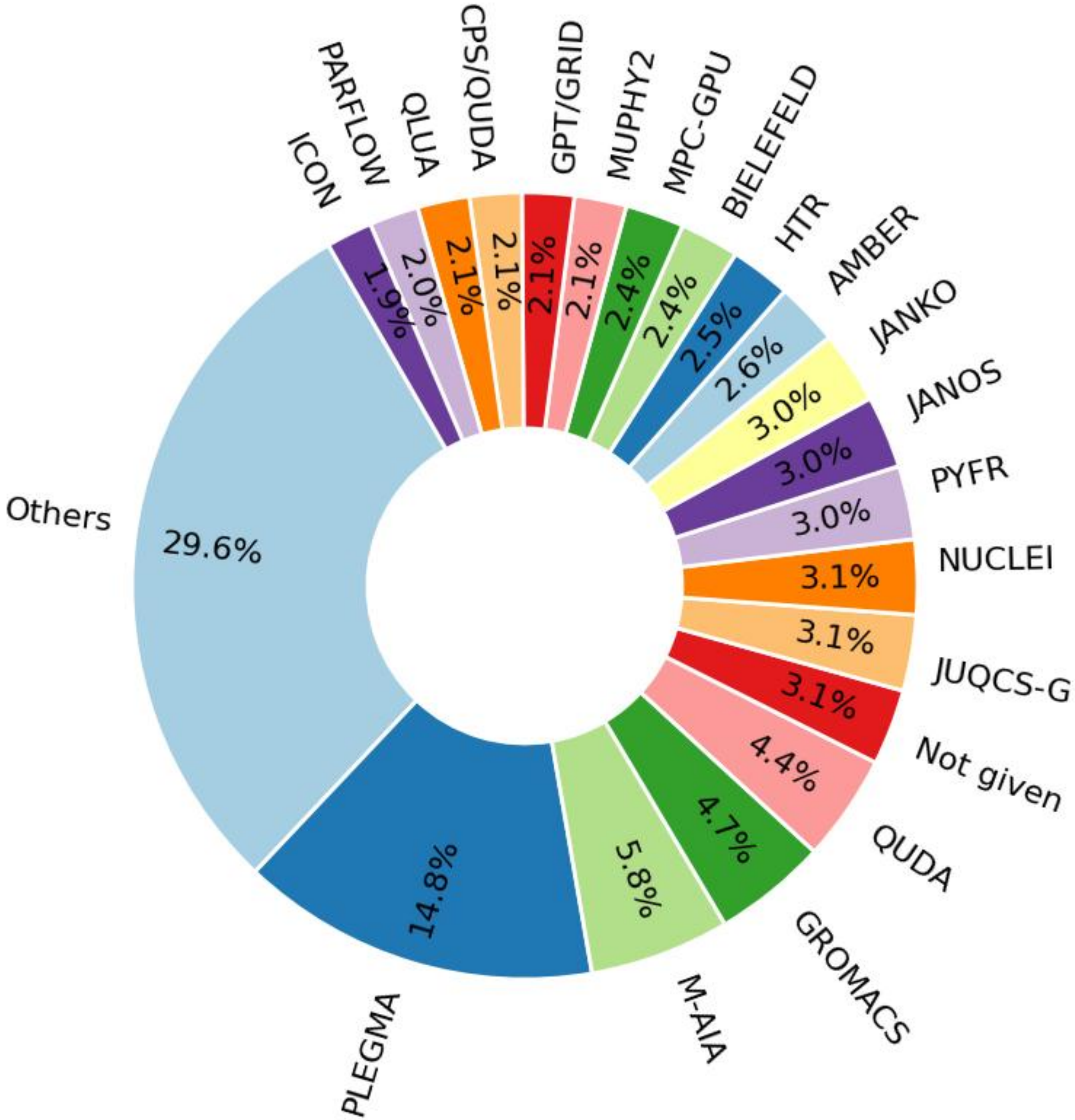
Willsch et al., Comput. Phys. Commun. 248, 107006 (2020)

Quantum computers at commercial data centers?

Question to the audience:

What types of applications are requested at your data centers?

Proposals for compute frameworks at the Juelich Supercomputing Centre



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