Leibniz Supercomputing Centre
of the Bavarian Academy of Sciences and Humanities

External

Operating quantum hardware in an HPC environment: potential, challenges, lessons learnt

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Agenda

Thank you QCT!

Integration and HPCQC End Goals

Hardware	Quantum Computing Appliance + HPC System	Single system with integrated QC accelerator(s)
Logistics	Two environments with own policies and rules	Logistics and bureaucracy of a unified entity
Software	Two separate software stacks with “glue scripts”	Single-source programming with high-level abstractions
Algorithms	QC and classical components of (mildly) interacting workloads	Hybrid use cases leveraging computing resources
Users	Computer Science, Math, Electrical Engineering, Physics communities	Just one HPCQC community

Hardware integration

Euro-Q-Exa

- Co-funding between EuroHPC-JU, BMBTR, State of Bavaria
- Two systems: 54 qubits (IQM “Emerald”), now installed, and 150 qubits (end of 2026), superconducting, provided by IQM
- The system is currently integrated into an experimental HPC cluster at LRZ; moving to integration on SuperMUC-NG Phase 2
- Available for European users
- Q-Exa as pre-access platform, in March 2026 onboarding test users, in July/August 2026 regular user operation expected

Interim system

Q-Exa

- Inaugurated June 18, 2024
- Outcome of the Q-Exa project (with IQM, HQS and Eviden)
- 20-qubit superconducting system “IQM Garnet” (ArXiv: 2408.12433)
- First co-located hybrid quantum-HPC job run in a data center environment
- Test user operation in 2024; regular user operation started in September 2025
- Noise model deployed on our Qaptiva hardware simulator

Software integration

The Munich Quantum Software Stack

MQSS Munich Quantum Software Stack

lrz

Quantum Resource Manager

End users

Hybrid/Quantum Programming Toolkits / Libraries

Web-Portal Access

HPCQC Access with Quantum Acceleration

Cutting and Scheduling Resource Management

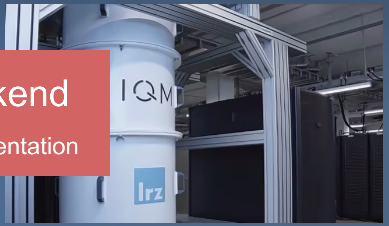
Figures of Merit and Constraints

Quantum Compiler

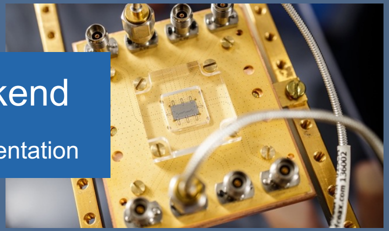
Comprehensive Toolkits
Optimizers
Verifiers
Transpilers
Mappers

QDMI Quantum Device Management Interface

Backend Implementation



Backend Implementation



Backend Implementation

Euro-Q-Exa

The Friendly User Pilot Phase

lrz

Concept borrowed from HPC

- Starting user operation with few, selected users
- No guarantee that everything runs as smooth as expected
- Users run on a system with less load
- Stress test for the system
- Tight feedback loop between LRZ consulting/support team, IQM and users

Teams and users

10 invited research teams from all over Europe

Selection based on excellence and ongoing collaborations

Initial kick-off on March 11

Four Open Mic sessions

Mailing list and Element room

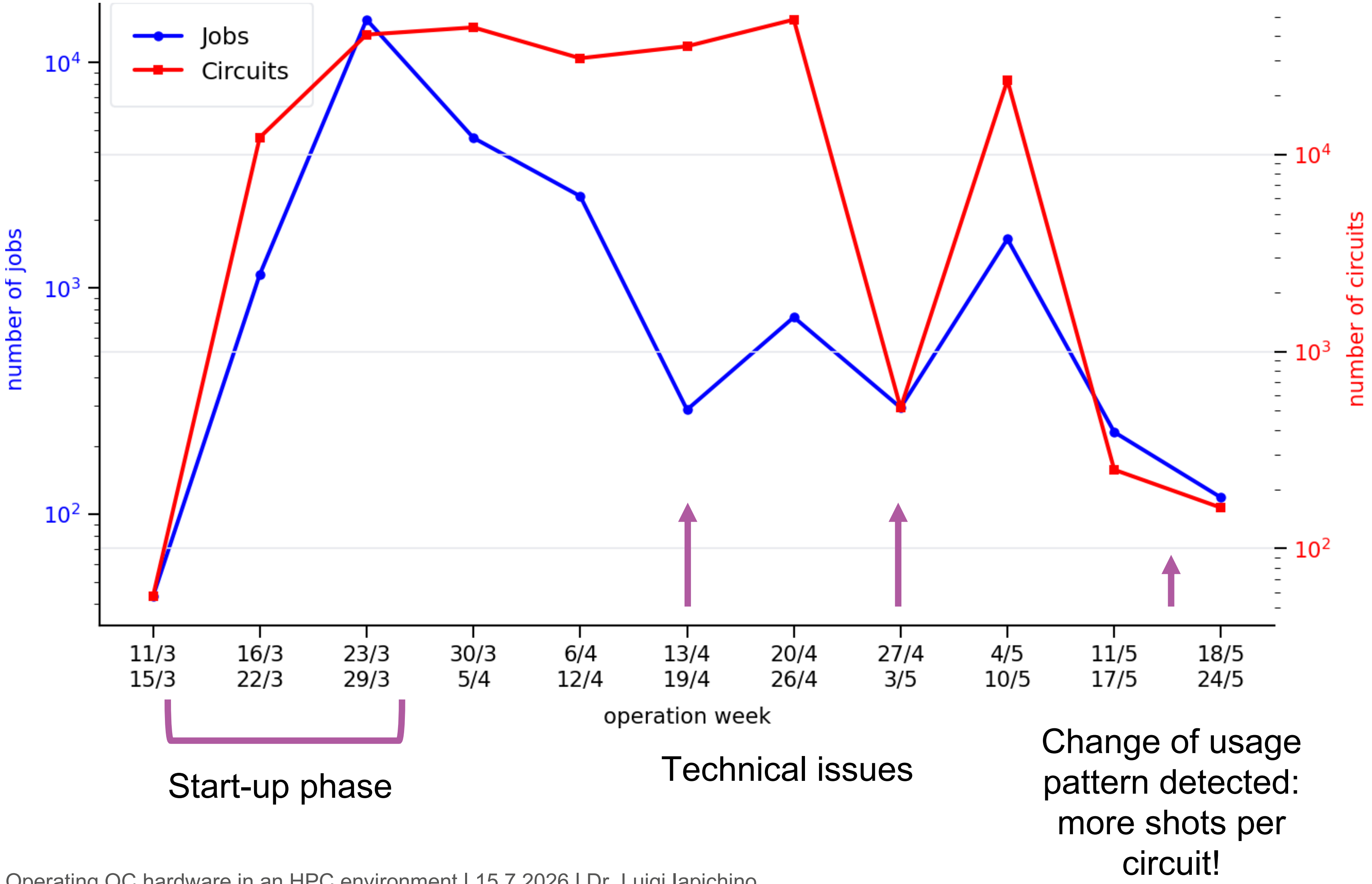
About 25 users onboarded

Work in different application areas:

- Optimisation
- Computational chemistry
- Quantum Machine Learning
- Astrophysics
- Quantum resource theory
- Many-body physics
- Error mitigation

System usage

Statistics per Operation Week



Up to 14
Number of active users per week

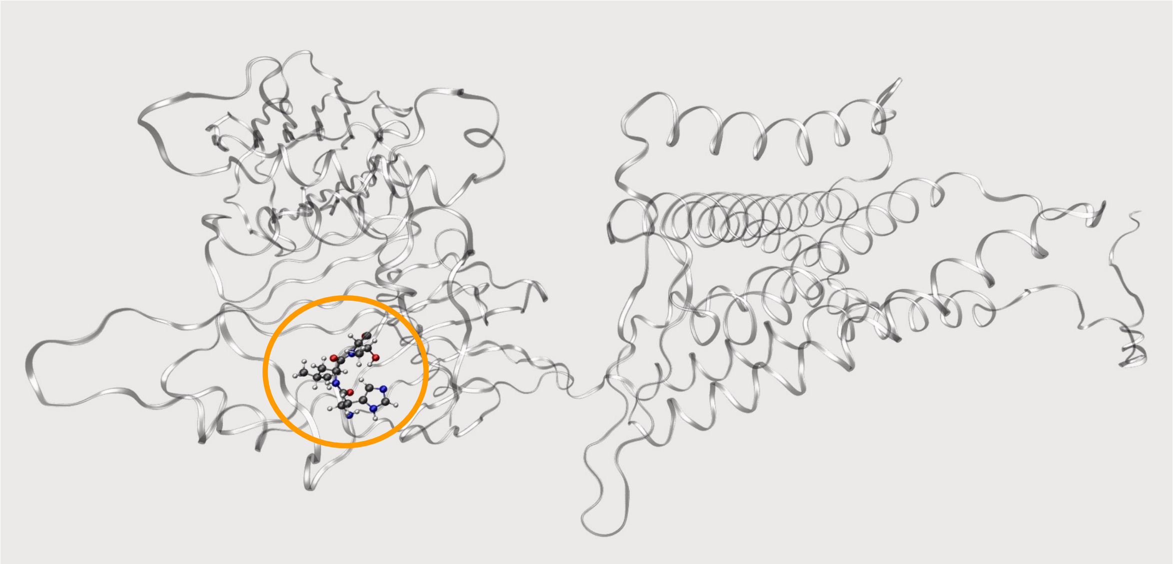
27,104
Total number of jobs

236,377
Total number of circuits (system still not heavily used)

Algorithms and HPCQC synergies in the integration: A few examples

Hybrid Quantum-GPU Biomolecular Simulation (work in progress)

- First integrated pipeline combining quantum computing, GPU-accelerated supercomputing, and classical simulation
- Developed by UCL, TUM, LMU, NVIDIA, LRZ, QMatter and IQM
- Uses Euro-Q-Exa with the LRZ BDAI cluster
- Multiscale approach: quantum modeling of active regions + classical environment
- Demonstrated on G-protein-coupled receptors (key drug target; ~1/3 of medicines act on them)
- Opens new paths for drug discovery, molecular engineering and life sciences



Full GPCR structure and the active site simulated on quantum hardware (from QMatter website)

Quantum and classical components of the algorithm

Quantum-selected Configuration Interaction (QSCI)

Idea: Diagonalize Hamiltonian in a subspace spanned by configurations sampled from the QPU

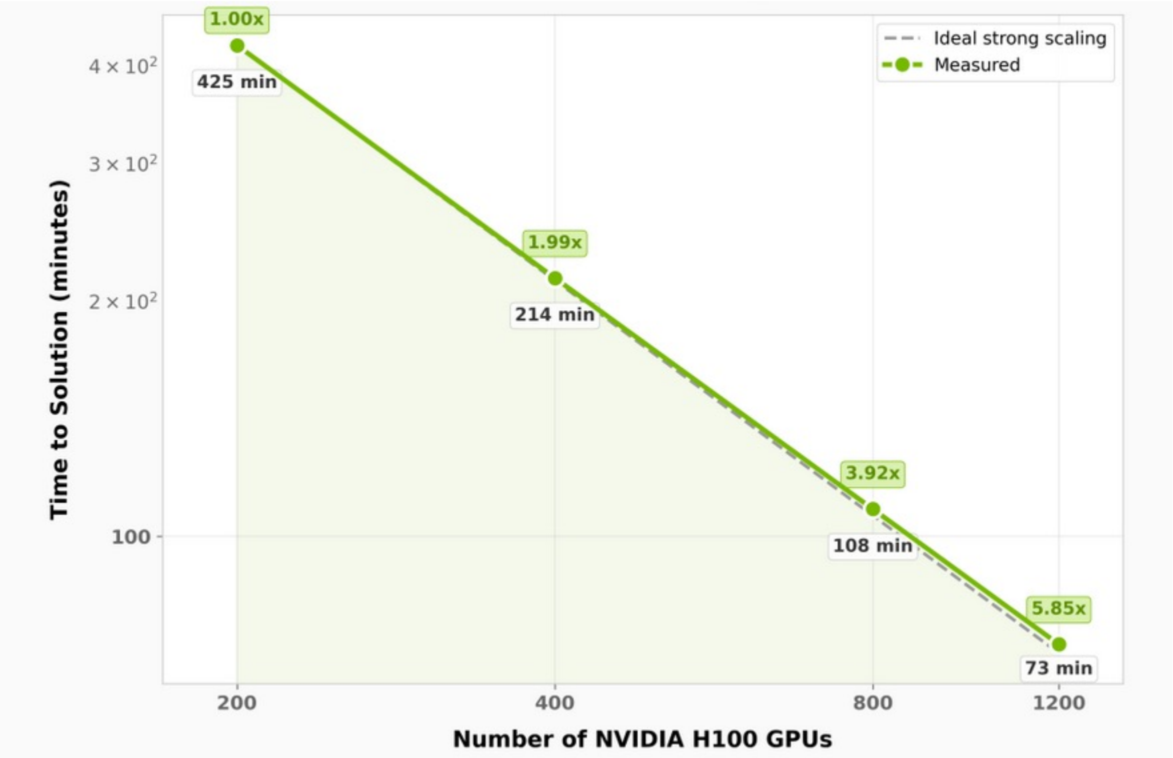
QPU $|\Psi_1\rangle, |\Psi_2\rangle, |\Psi_3\rangle, \ldots$*

Classical matrix diagonalization $\begin{pmatrix} \langle\Psi_1|H|\Psi_1\rangle & \cdots & \langle\Psi_1|H|\Psi_N\rangle \\ \vdots & \ddots & \vdots \\ \langle\Psi_N|H|\Psi_1\rangle & \cdots & \langle\Psi_N|H|\Psi_N\rangle \end{pmatrix}$

*potentially prepared with VQE

Courtesy: Alex Orlov

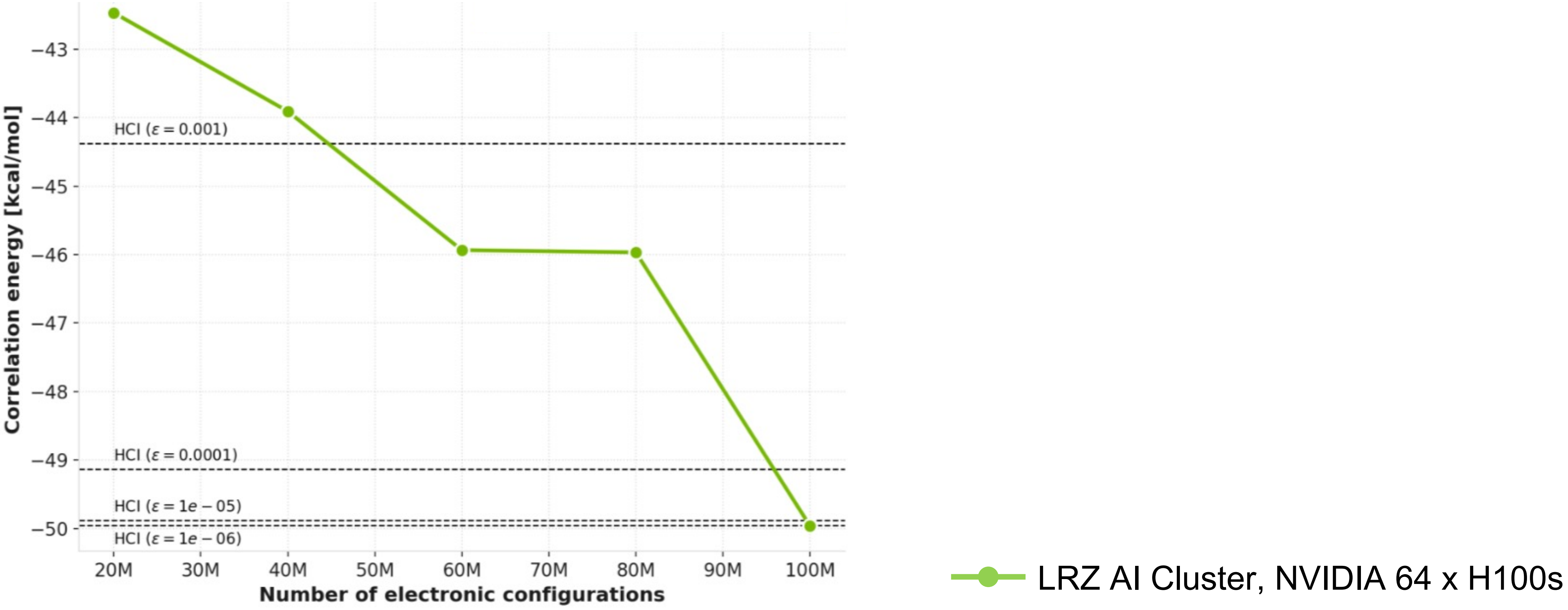
Strong scaling – 200 to 1200 NVIDIA H100s,
1 Billion Quantum Configurations



The post-processing step has an excellent GPU scaling. Less sensitive to latency and tight integration requirements.

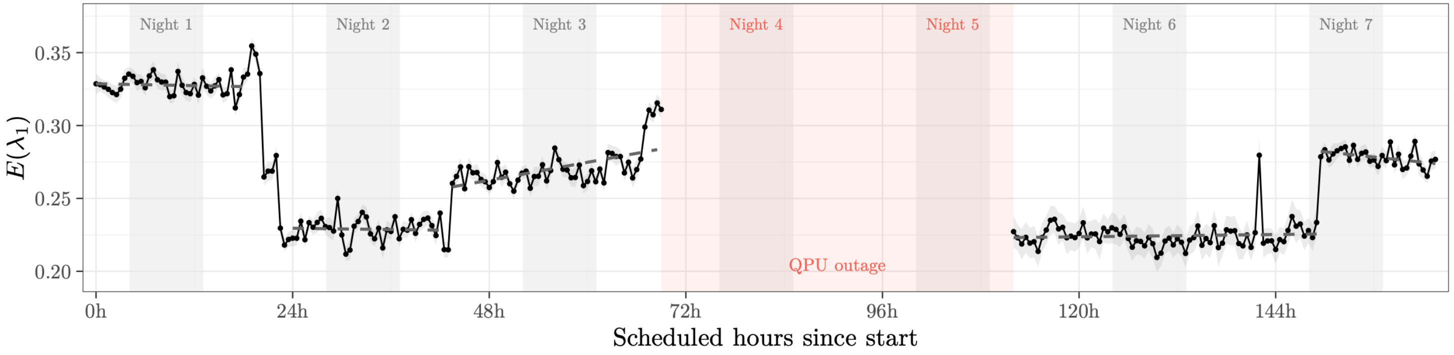
Algorithmic convergence

Energy convergence in the chosen 52-qubit active space of the GPCR system



Claim against Measurement - the use case from OTH Regensburg

Claim against Measurement: Statistical Artefacts in Quantum Error Mitigation Benchmarks[1]



Longitudinal drift experiment on Euro-Q-Exa over seven days of operation

Quantum error mitigation studies typically neglect intrinsic variations of the hardware.
Experiments demonstrate strong temporal drift effects:

- Same QEM configuration yields very different error-mitigation outcomes over time
- Effect sizes can vary by >3x depending only on execution timing
- Influence results as strongly as the QEM method itself

Establishing statistically rigorous benchmarking standards is essential for QEM and for quantum computing progress in general.

Source | Köster, Dominik / Mauerer, Wolfgang, OTH Regensburg, 2026. – Preprint on arXiv:2605.29872 [quant-ph].

What else? What comes next?

Operating Euro-Q-Exa is demanding also from a policy / legal viewpoint (export control, …)

The regular user operation starts this month, after a “Special Operation Phase” during which we reserve the system for users with non-standard needs

At European level: Quantum Access Pilot has been launched (https://access.eurohpc-ju.europa.eu/calls/61).

There’s no QC without HPC, now and in the fault-tolerant phase. New algorithms (e.g. QSCI) are moving the focus, affecting the extent of HPC computing power to be coupled with QC resources.

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EURO-Q-EXA

European Commission

EuroHPC Joint Undertaking

Federal Ministry of Research, Technology and Space

Federal Ministry for Economic Affairs and Energy

Bavarian State Ministry of Science and the Arts

Bavarian Ministry of Economic Affairs, Regional Development and Energy

MQV