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Leibniz Supercomputing Centre

of the Bavarian Academy of Sciences and Humanities

Quantum-Accelerated HPC: Opportunities for Astrophysics and Astronomy

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Agenda

What is Quantum Computing? What is *not* QC?

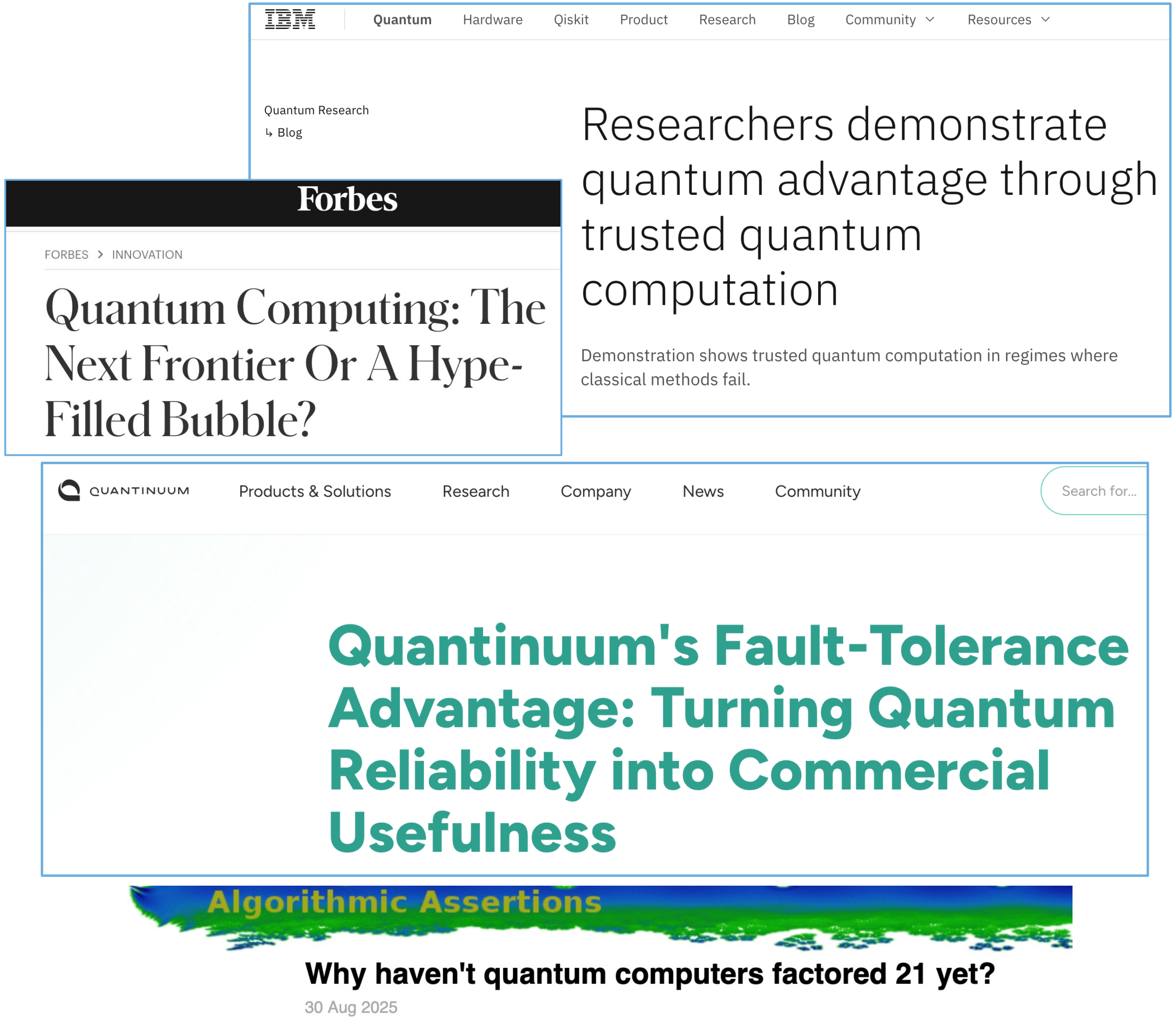
High-Performance Computing and QC (HPCQC)

Current status of QC

Applications of QC

The HPCQC ecosystem at LRZ and access opportunities

What is Quantum Computing?


IBM Quantum Hardware Qiskit Product Research Blog Community Resources

Quantum Research
↳ Blog

Researchers demonstrate quantum advantage through trusted quantum computation

Demonstration shows trusted quantum computation in regimes where classical methods fail.

Forbes

FORBES > INNOVATION

Quantum Computing: The Next Frontier Or A Hype-Filled Bubble?

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Quantinuum's Fault-Tolerance Advantage: Turning Quantum Reliability into Commercial Usefulness

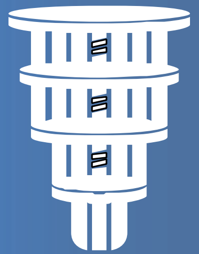
Algorithmic Assertions

Why haven't quantum computers factored 21 yet?

30 Aug 2025

Headlines range from "quantum advantage is here" to “QC is mostly hype.“ The reality lies between these extremes.

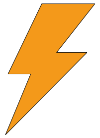
Quantum computing is a computing paradigm that exploits quantum mechanics (superposition, entanglement) ***at the abstract level*** in order to do calculations.



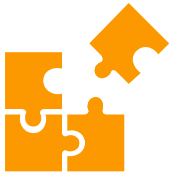
What a Quantum Computer is not

A quantum computer is not faster than a traditional one – it is just a different computing paradigm

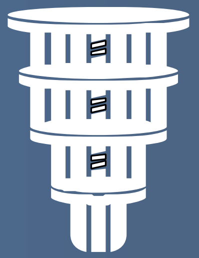
We don‘t think that their power is unlimited – there are problems which are hard also for quantum computers



Most problems can be solved on quantum computers as fast as on traditional ones



But, on some important algorithms quantum computers promise to be more powerful and scalable than traditional computers



Why is QC interesting from a HPC perspective?

Heterogeneous, accelerated HPC

Complex but non-accelerated systems (e.g., SuperMUC-NG)

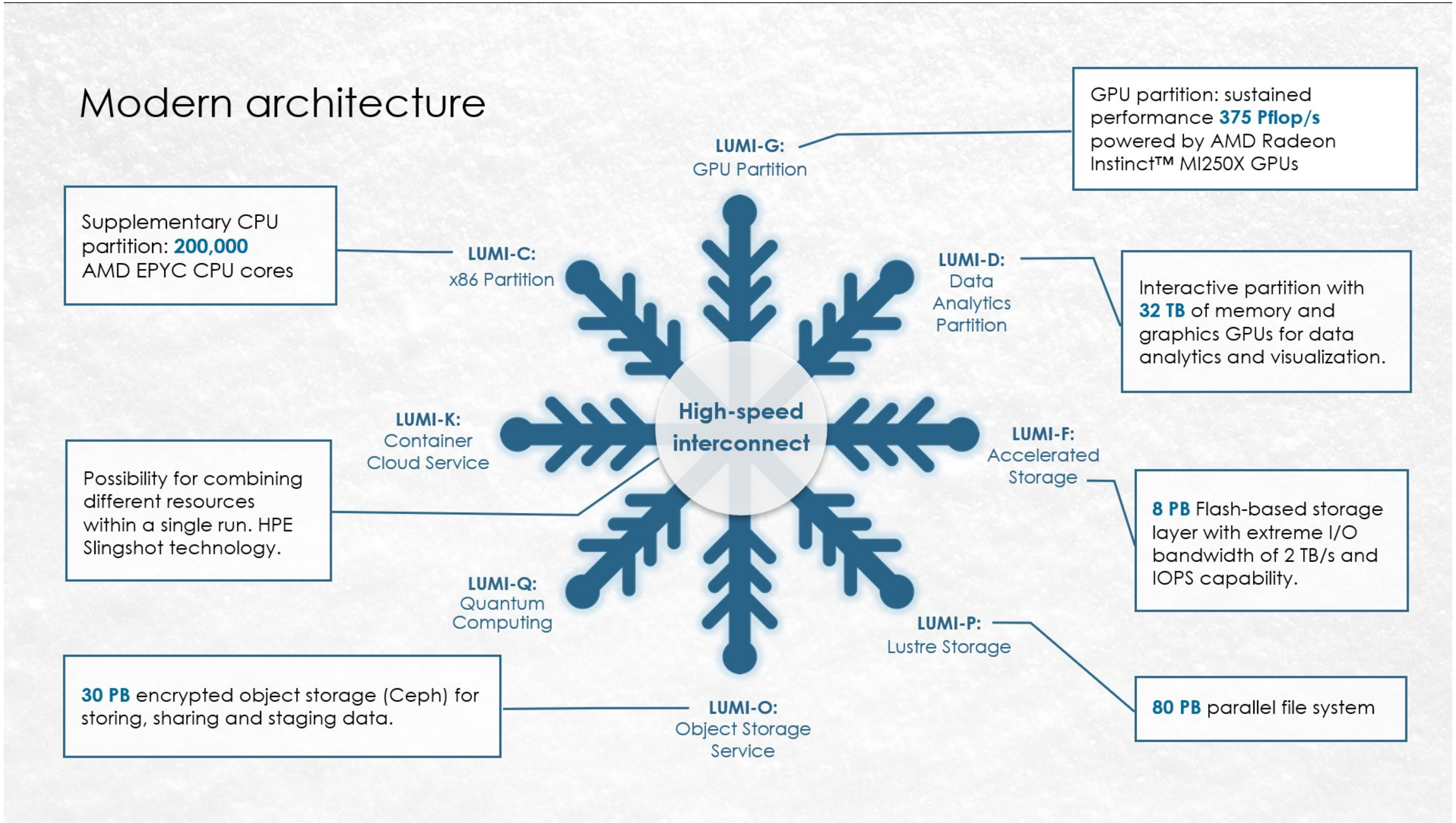
Accelerated systems: compute-intensive tasks offloaded to dedicated compute modules (e.g., GPUs)

One HPC architecture fitting most needs from the community (compute, ML, AI, HPDA, …)

Many architectures to cover different needs.

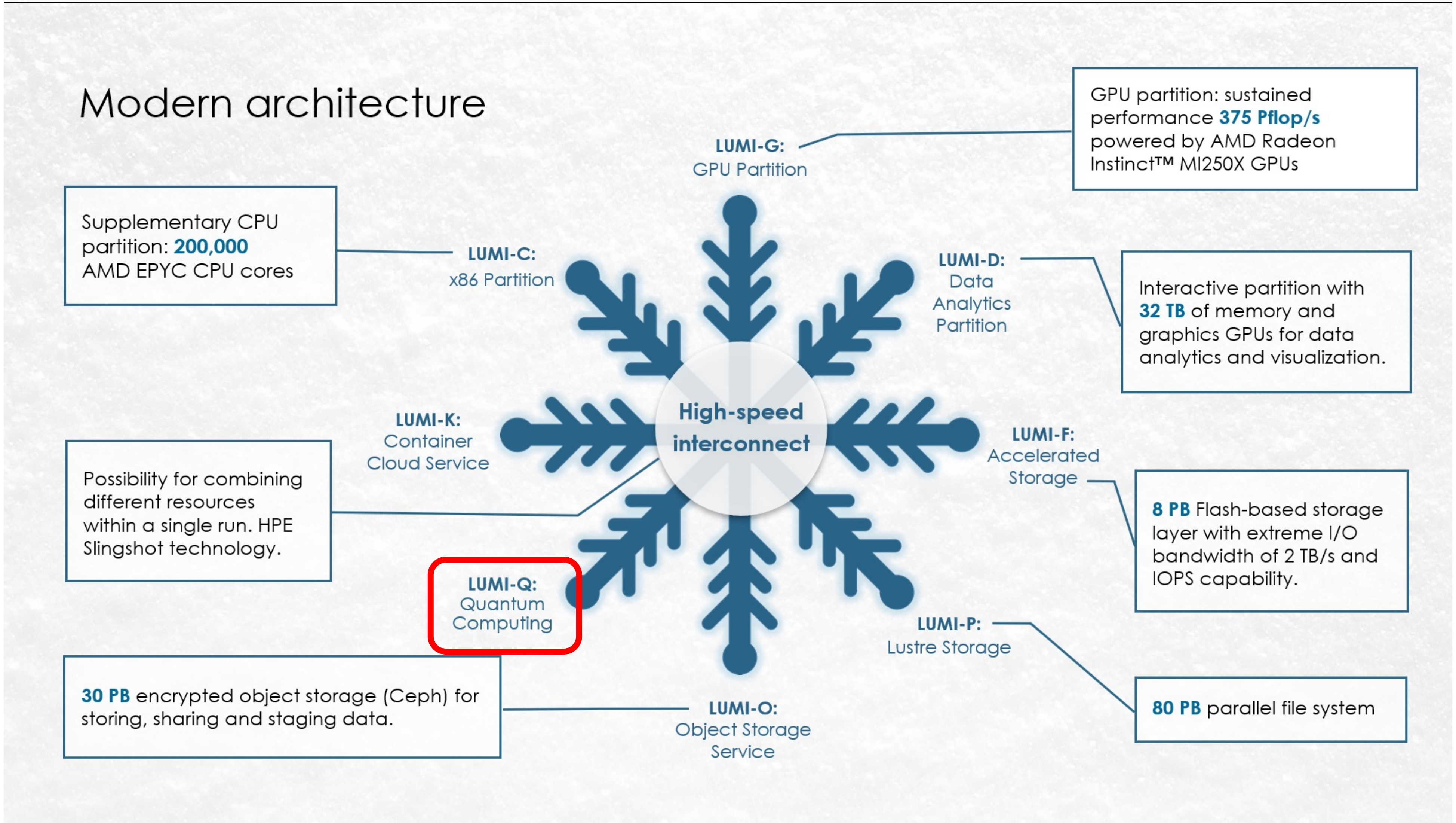
Often they are bundled in heterogenous, modular HPC systems

Modular HPC architectures: the example of LUMI @ CSC (Finland)



(credits: https://www.lumi-supercomputer.eu/)

Modular HPC architectures: the example of LUMI @ CSC (Finland)



(credits: https://www.lumi-supercomputer.eu/)

Current status of QC

Leading hardware modalities

The qubit is the fundamental unit of information in QC. Its physical realisation differs in the available hardware modalities:

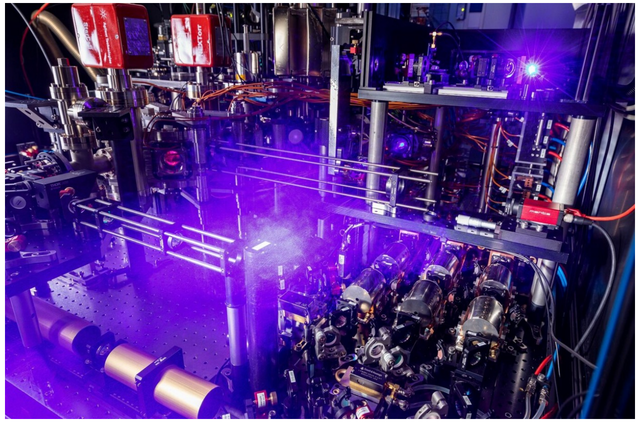
Superconducting

(Euro-Q-Exa @ LRZ, IQM)

Ion-trap

(Marmot @ LRZ, AQT)

Neutral atoms



(credits: MPQ / planqc)

Limitations of QC: NISQ (Noisy, Intermediate-Scale Quantum)

Technology limitations

- Limited number of qubits, *O*(10-100)
- Short coherence time, *O*(100μs – 1s)
- Error correction needs *O*(100) physical qubits per logical qubit
- Gate fidelities, degree of entanglement, read-out errors… all need improvements to enable scale-out and **fault-tolerant systems**

Intrinsic limitations

Quantum computers are not suited for I/O:

- Data encoding („initial conditions“) is an issue
- Specular problem: **throughput**
- The output of a quantum computation will be limited to **as many bits** as it processes qubits

Which questions can we pose, that can be addressed within these limitations with a minimal amount of information?

HPC Integration and **hybrid, variational algorithms**

QC applications in astrophysics and astronomy

In order to characterize the applications of QC, four main groups have been identified:

- Quantum simulation of quantum systems,
- Quantum optimization,
- Quantum machine learning, and
- Quantum linear systems

Simulations of neutrinos, talk by Sajad Abbar, and one example in the following

Examples in space science (image acquisition for satellites)

Examples in the talk by Farida Farsian

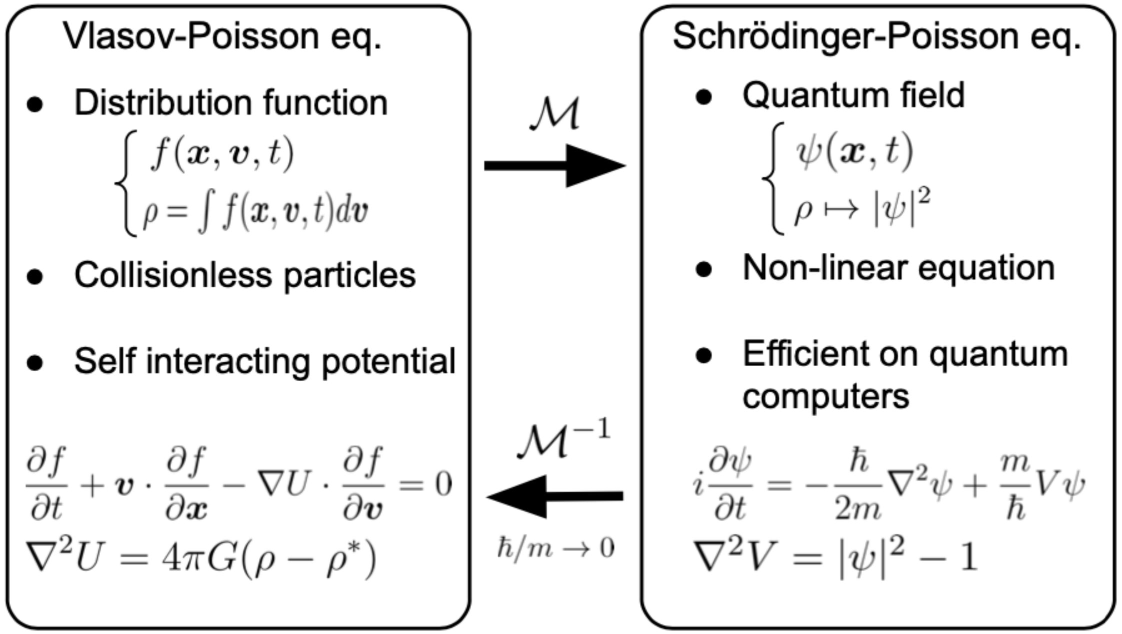
QC for fluid dynamics

Dark Matter simulation with a quantum variational time evolution algorithm (Cappelli et al., 2307.06032, https://doi.org/10.1103/PhysRevResearch.6.013282)

Study of the DM phase-space distribution function: **Vlasov-Poisson** equations.

Monte-Carlo approach to collisionless dynamics: sampling into particles
→ **DM N-Body simulations**

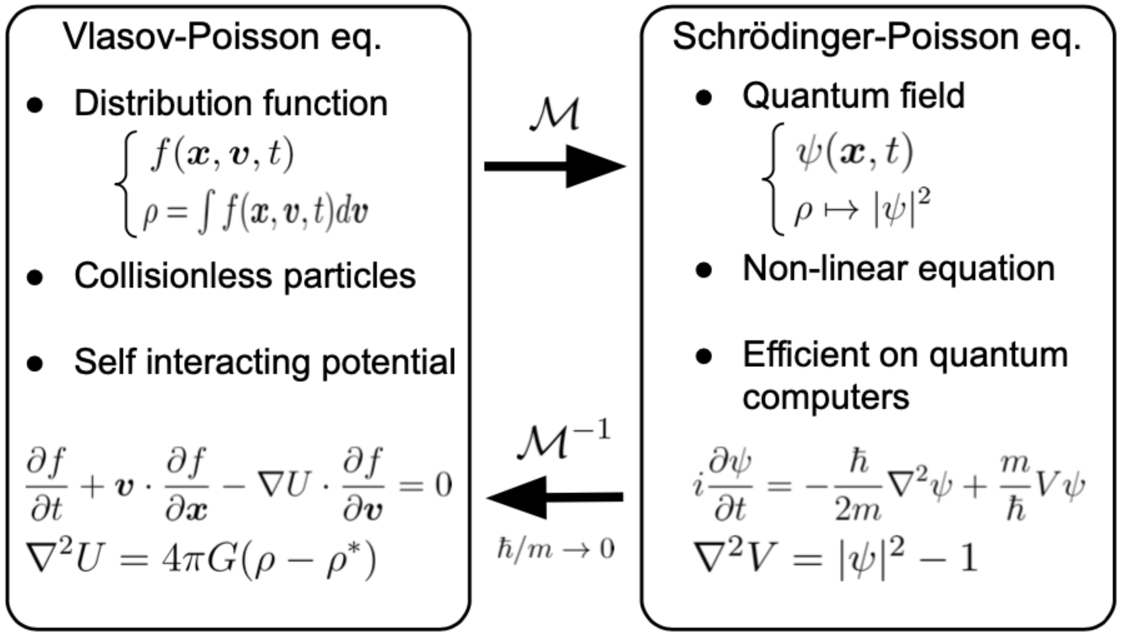
Let’s think quantum:
Vlasov-Poisson as generalisation of the evolution of a (non-relativistic) DM scalar field, described by a complex wavefunction: **Schrödinger-Poisson** equations



A similar approach has been taken e.g. by Mocz & Szasz 2021

Dark Matter simulation with a quantum variational time evolution algorithm (Cappelli et al., 2307.06032, https://doi.org/10.1103/PhysRevResearch.6.013282)

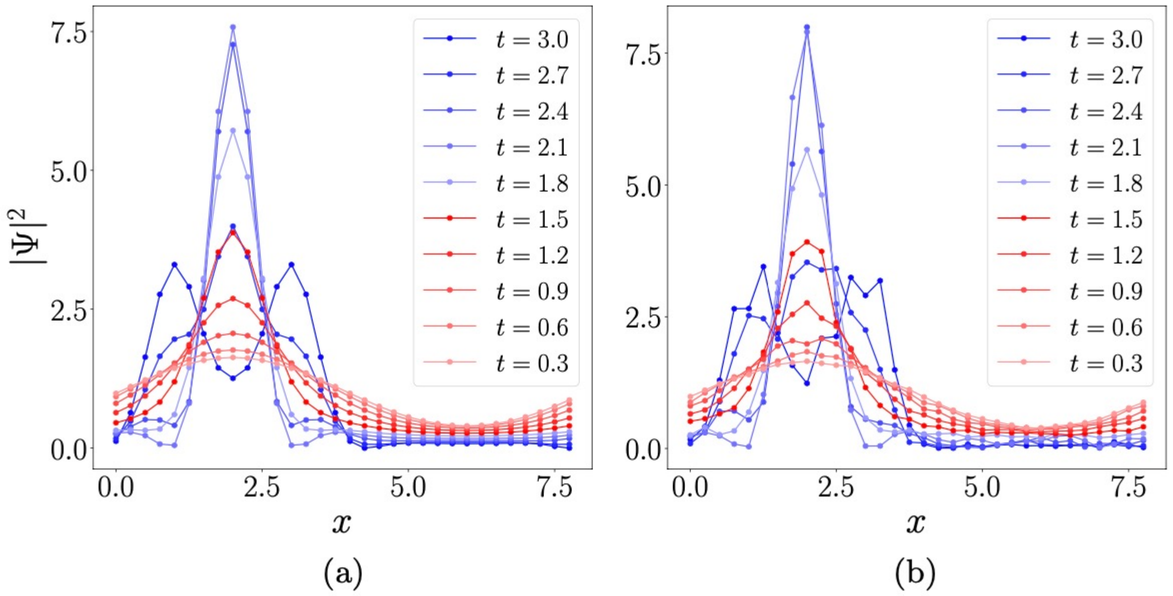
- N-body method? Quantum-friendly strategy: evolution of the wave function
- The mapping reduces the dimensionality from 6*D* +1 to 3*D* +1
- Problems when dealing with non-linear equations due to the intrinsic linearity of the QC formalism
- Solution: variational time evolution (VTE) approach



Dark Matter simulation with a quantum variational time evolution algorithm (Cappelli et al., 2307.06032, https://doi.org/10.1103/PhysRevResearch.6.013282)

- First proof of concept in the paper: 1D case, discretised on a "grid" of $2^5 = 32$ elements, ru on a 5-qubit Qiskit simulator.
- The algorithm results in circuits which are not shallow → unsuitable for NISQ hardware.
- The problem is numerically challenging for higher dimensions and realistic cases, a general method for solving it has still to be identified

$$\psi(x,0) = \sqrt{1 + 0.6\sin(\pi x/4)}$$



Time evolution of a wave function with classical methods (a) and QC implementation (b).

HPC simulation tools for quantum algorithms

Vector representation of a quantum state of a system with *n* qubits:

$$|\Phi\rangle = \alpha_{00...0}\,|00...0\rangle + \alpha_{00...1}\,|00...1\rangle + ...\alpha_{11...1}\,|11...1\rangle$$

Memory footprint of a state vector simulation of a quantum system with *n* qubits (complex double precision): 2^{n+4} bytes.

- Largest system to be simulated on my private laptop (4GB RAM): 27 qubits
- Largest system on a SuperMUC-NG node (96GB RAM): 32 qubits
- Largest system tested on the whole machine (6000 nodes): 42 qubits
- Largest system on the **Eviden Qaptiva** (6TB RAM): 38 qubits

Comparing performance of variational quantum algorithm simulations on HPC systems (De Pascale, … *LI*, … et al., LRZ and Fraunhofer IKS teams, 2025 IEEE QCE conf.)

Software simulators

- Qiskit
- Pennylane lightning
- Intel-QS
- CUDA-Q
- pyAQASM

Use Cases

- Optimisation: QAOA simulation of Max-Cut
- Optimisation: VQE simulation of the Traveling Salesman problem

HPC hardware (at LRZ)

- Multi-node HPC system:

  SuperMUC-NG Phase 1
- GPU-accelerated system: DGX-A100
- Shared-memory system (QC hardware simulator): Eviden Qaptiva 800

Considerations and lessons learnt

- Approach perpendicular to the Santa Barbara cluster: running the same circuits (via a toolchain), avoiding ”black boxes”
- The variational algorithms are mainly limited by runtime, not by memory footprint
- Parallelisation and scaling are lagging far behind astro simulations!
- Dedicated hardware and GPU acceleration provide valuable solutions

The simulators are now available on the LRZ HPC systems: our **QC Scalable Software Suite**

The QC ecosystem at LRZ and access opportunities

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 (applications through the JU portal) and German users (applications at LRZ)
- Regular user operation started in August

The Euro-Q-Exa Friendly User Pilot Phase

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

Work in different application areas:

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

Summary and final remarks

The slowdown of HPC growth is pushing towards more heterogeneity

Quantum computing is a new computing paradigm with the potential of delivering disruptive advantage on a number of important algorithms

The first interesting application areas will be the ones capable of exploiting the synergy of HPC and QC (variational algorithms)

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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Quantum-Accelerated HPC: Opportunities for Astrophysics and Astronomy

European Commission
EuroHPC Joint Undertaking
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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