Quantum Autumn School 2023

HPC+QC integration

Mikael Johansson

CSC – IT Center for Science

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ICT Solutions for Brilliant Minds

What is a quantum computer?

A quantum computer is a device, that *directly* exploits quantum mechanical phenomena to perform a calculation

Superposition, entanglement, wavefunction phase

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What is a quantum computer *not*?

A quantum computer is *not* a super-fast version of a classical computer —
It is *different*

Speeds up *some* types of calculations, others not at all

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Why are we as HPC centres interested in quantum computing?

Quantum computers will not replace supercomputers

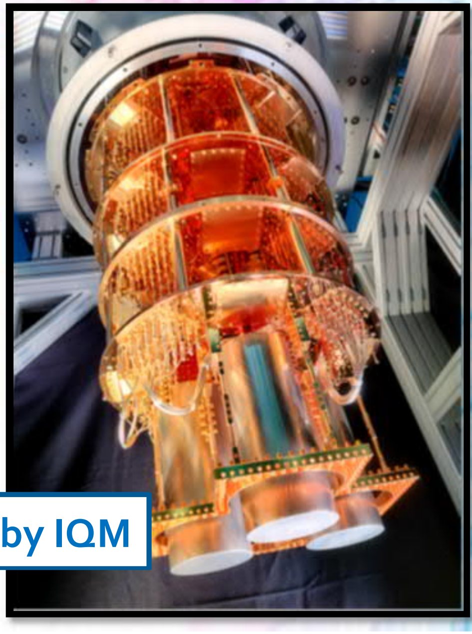
- Instead, the two will merge
- Important to stimulate **co-creation** between the HPC and QC communities

Our end-users will need early-access to HPC+QC in order to make their workflows quantum-ready

- The **transition from classical CPUs/GPUs to quantum QPUs** requires fundamental rethinking of problems and algorithms
- Requires time, resources, and support

HPC centres serve as natural starting points

- All the necessary basic services already in place:
  - User authentication and administration
  - Resource allocation and control
  - Storage, high-speed network, classical resources, …
- **End-users!**



Quantum computer by IQM

Question: What can you do with a small amount of *real* qubits?

Answer: Learn how to use *real* quantum computers

Quantum computers are very different from traditional quantum computers

- Completely different programming paradigm
- Quantum computers different from each other: different quantum computers give different answers for the same program
  - Even on the same quantum computer, two runs are *supposed* to give different results
- Quantum computers compute *wrong* most of the time

Experienced HPC users will see a large change in thinking and approach to computing

- **A quantum computer is a device for experiments**
- The cosy and comfortable feeling of absolute reproducibility is out of the window
- Need to be critical towards results in a completely new way
- Need to get a **feel and know-how for how to perform successful calculations** (experiments!) on QCs

Is a small QC setup enough to bridge the gap between users and QC?

Answer: No (Betteridge's law)

We have to provide the end-users with the prospect of quantum advantage!

- Can we do that at this stage?
- For the end-user who is interested in using QC as a tool for his/her science/R&D, quantum advantage is not obvious
- "Why invest resources on quantum computing when it doesn't give immediate returns?"

What *is* quantum advantage?

#1. Wall-time quantum advantage

Definition: Quantum computers help solve problems faster than classical binary HPC alone

- The "usual" definition of quantum advantage
- Still some time away, needs massive quantum algorithm/software development

#2. Green quantum advantage

Definition: Using quantum computers leads to a higher solved-problems/Watt ratio

- Does *not* need QPUs that outperform HPC in speed (#1)
- Solving something slower, but using less energy is an advantage
- Note: need to account for the *total* energy consumption for solving a given problem, including classical (pre/post) processing

#3. Quantum quality advantage

Definition: QC provides more accurate/better quality predictions

- Due to solving a given problem in a *different* manner
- Also possible at moderate qubit counts, before QPUs as such outperform HPC

#4. Quantum control advantage

Definition: QCs provide higher control of quantum systems

- Quantum computers provide a highly controllable environment for manipulating quantum objects
- Enables the study of, *e.g.*, fundamental physics and chemistry at a new level of accuracy

#5. Other quantum advantage

Definition: QC provides some other advantage to the user involved

- **Academic carrot:** scientific publications and project funding
- **Industrial carrot:** competence development and early IP creation, PR value not to be underestimated

Timeline of quantum advantage

#1 Wall-time quantum advantage	10 units of time
#2 Green quantum advantage	5 units of time
#3 Quantum quality advantage	3 units of time
#4 Quantum control advantage	NOW!
#5 Other quantum advantage	NOW!

‘

Non-computing applications

What is the role of HPC here?

- Need to create **added value of HPC**: classical software stack, ideally needing true HPC resources, supporting the "quantum lab" concept


Home / Chemistry / Analytical Chemistry

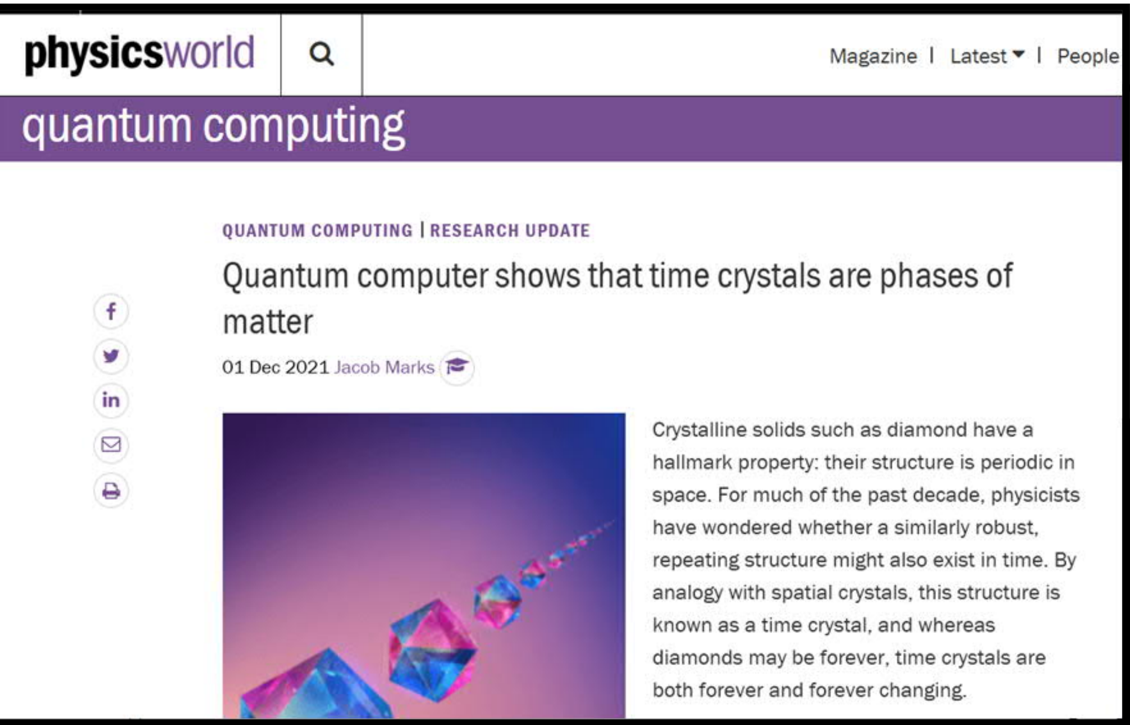
PHYS.ORG

AUGUST 28, 2023

Editors' notes

Scientists use quantum device to slow down simulated chemical reaction 100 billion times

by University of Sydney


physicsworld

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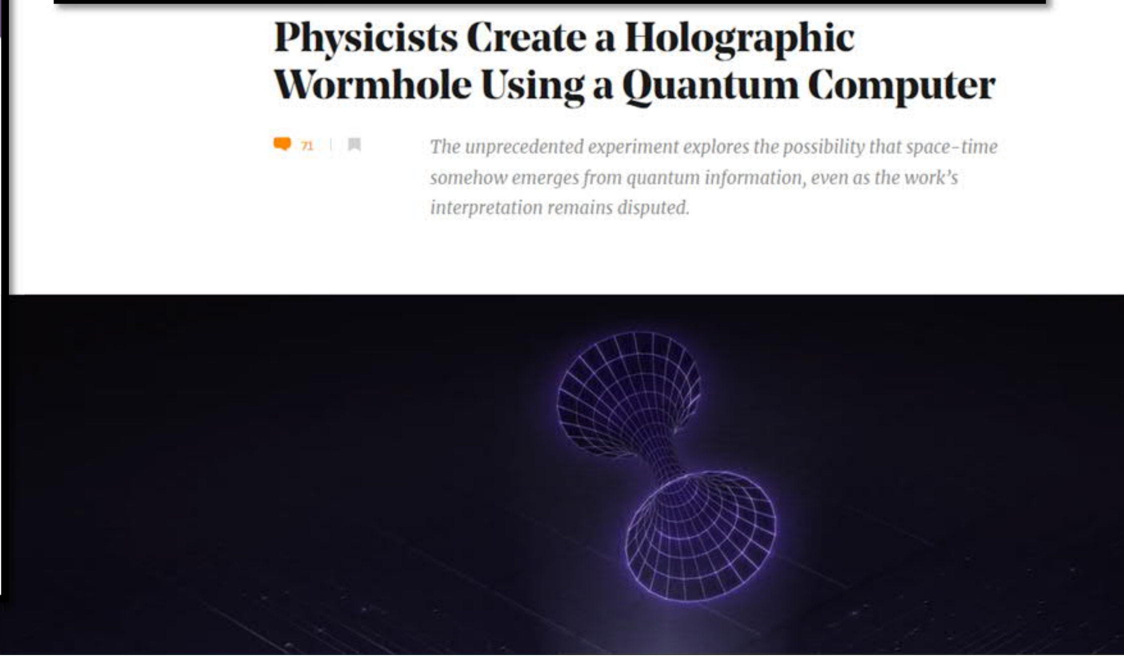
quantum computing

QUANTUM COMPUTING | RESEARCH UPDATE

Quantum computer shows that time crystals are phases of matter

01 Dec 2021 Jacob Marks

Crystalline solids such as diamond have a hallmark property: their structure is periodic in space. For much of the past decade, physicists have wondered whether a similarly robust, repeating structure might also exist in time. By analogy with spatial crystals, this structure is known as a time crystal, and whereas diamonds may be forever, time crystals are both forever and forever changing.


Physicists Create a Holographic Wormhole Using a Quantum Computer

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The unprecedented experiment explores the possibility that space-time somehow emerges from quantum information, even as the work's interpretation remains disputed.

Valuable HPC tasks for quantum computing?

Compilation and transpilation

- With increasing number of qubits, optimal compilation of quantum circuits becomes complex
- Need to get as shallow and as error-resistant circuits as possible
- Qubits not identical: increases complexity of routing
- Approximate compilation: mathematically *almost* equivalent (cf "-ffast-math", "-fp-model=fast")

Error mitigation / error suppression

- (Machine) Learn the error characteristics of the QC
  - Filter out noise in post-processing
  - Pulse optimisation

(Co)-desing of HPC+QC integration

- HPC centres know how to do HPC
- Provide insight for QC hardware/software providers on what needs to be considered for QC to fit into HPC efficiently, and *vice versa*

Simulators / emulators

Evidence for the utility of quantum computing before fault tolerance

Youngseok Kim, Andrew Eddins, Sajant Anand, Ken Xuan Wei, Ewout van den Berg, Sami Rosenblatt, Hasan Nayfeh, Yantao Wu, Michael Zaletel, Kristan Temme & Abhinav Kandala

Nature **618**, 500–505 (2023) | Cite this article

The corresponding quantum wall-clock run time was approximately 4 h for Fig. 4a and 9.5 h for Fig. 4b, but this is also far from a fundamental limit, being at present dominated by classical processing delays that stand to be largely eliminated through conceptually straightforward optimizations. Indeed, the estimated device run time for the error-mitigated expectation values using 614,400 samples (2,400 circuit instances for each gain factor and readout error mitigation, with 64 shots per instance) at a conservative sampling rate of 2 kHz is only 5 min 7 s

Three different ways of connecting HPC and QC

HPC and quantum computing

- In the future, quantum computers, QPUs, can accelerate HPC workflows

→ **quantum computing resources and HPC resources have to be coupled**

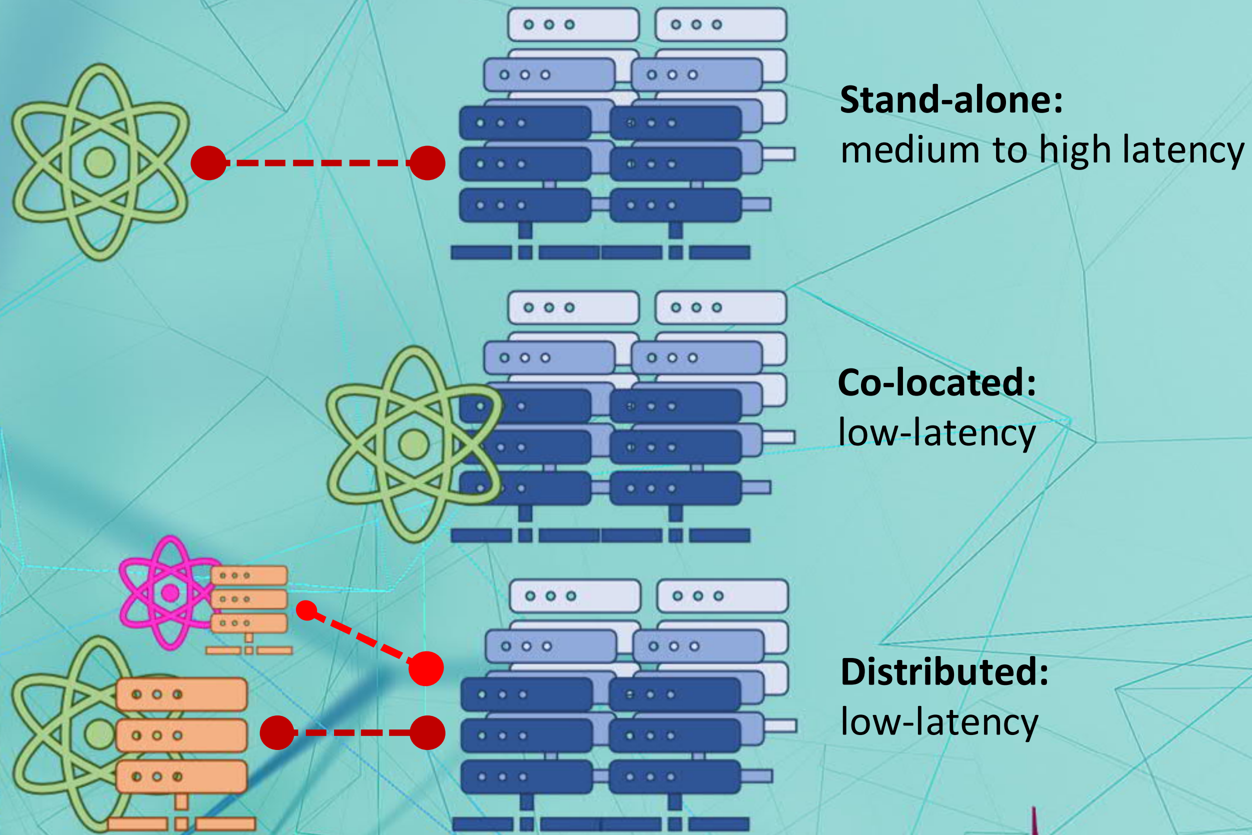
- Coupling HPC and QC resources is already taking place in several European HPC centres: **also NordIQuEst has already run its first quantum jobs!**
- Expected that the demand for QC resources will become “standard” among users of *most* HPC centres
- Here, a look at three different ways of connecting QC with an HPC centre
- In all, the HPC centre provides the “basic” services: **identity management, resource allocation, HPC capacity, storage solutions, …**

3 different ways of connecting HPC+QC

3 main ways to connect quantum and classical computers:

- **Stand-alone**, cloud access
- **Co-located** in the same premises
- **Distributed**, with QPU and HPC resources physically distant

Come with different levels of complexity for software stack



"Quantum Computing – A European Perspective" *PRACE* (2021)
DOI: 10.5281/zenodo.5547407

Latency and hybrid algorithms

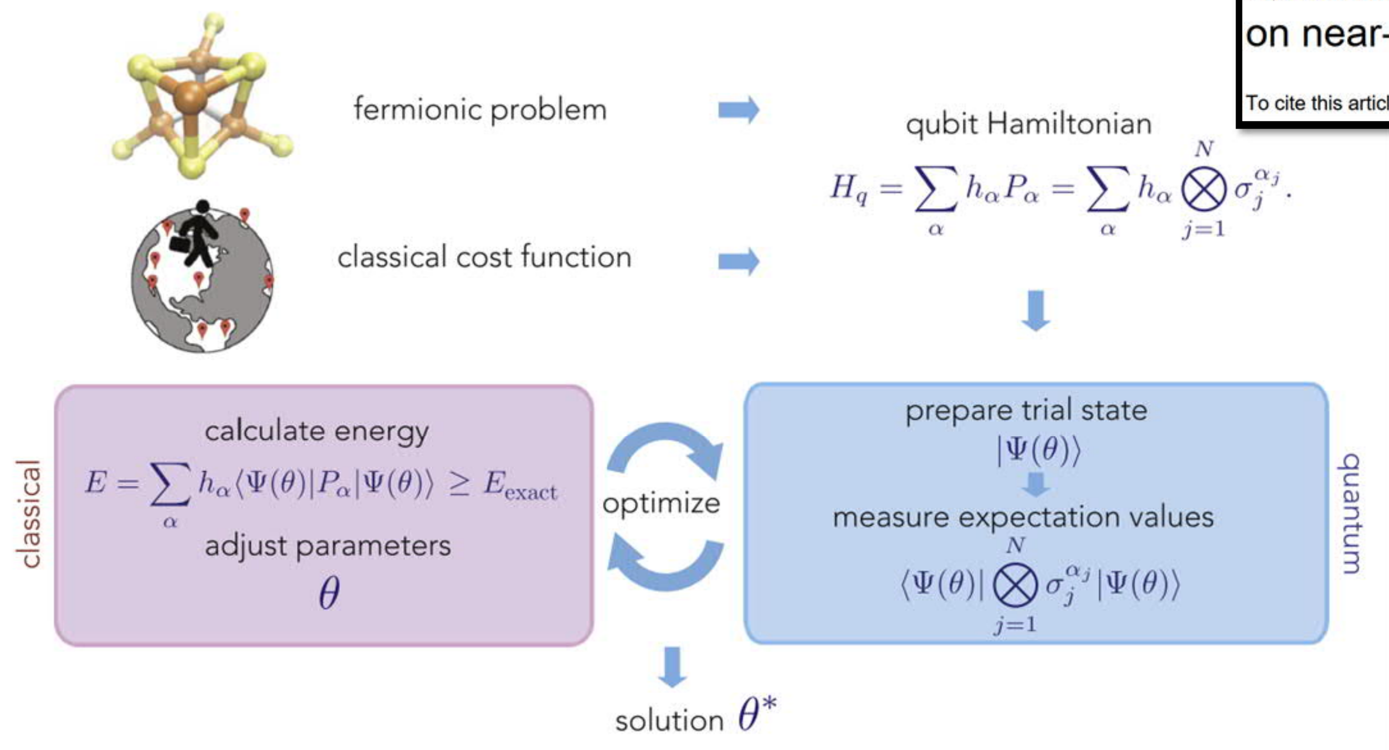


Figure 3. Variational quantum eigensolver method. The trial states, which depend on a few classical parameters $\boldsymbol{\theta}$, are created on the quantum device and used for measuring the expectation values needed. These are combined on a classical computer to calculate the energy $E_q(\boldsymbol{\theta})$, i.e. the cost function, and find new parameters $\boldsymbol{\theta}$ to minimize it. The new $\boldsymbol{\theta}$ parameters are then fed back into the algorithm. The parameters $\boldsymbol{\theta}^*$ of the solution are obtained when the minimal energy is reached.

Quantum optimization using variational algorithms on near-term quantum devices

To cite this article: Nikolaj Moll *et al* 2018 *Quantum Sci. Technol.* **3** 030503

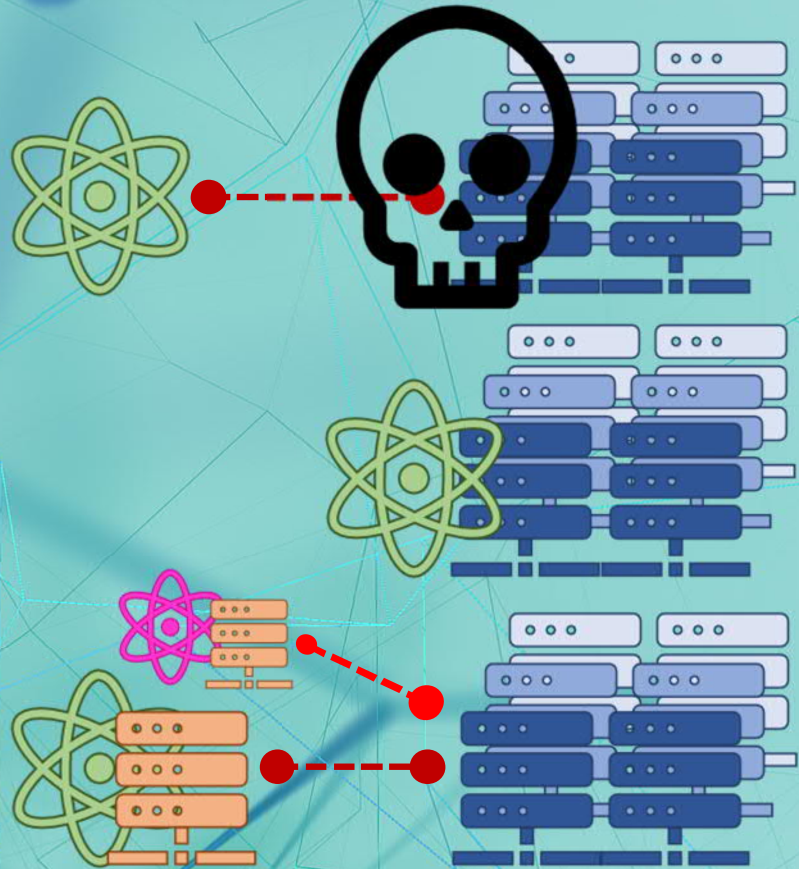
DOI: 10.1088/2058-9565/aab822

- When the quantum block *and* the classical block are fast, communication has to be even faster to avoid bottlenecks!
- **With present QPUs, decoherence *forces* the quantum block to be fast!**

Latency and hybrid algorithms

For quick loops, stand-alone creates too much overhead

- A classical processing unit needs to physically close, to **keep feeding the QPU with new input**
- **This is, however, not an HPC task**, a powerful server is more than enough



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Latency and hybrid algorithms

When QPUs mature to provide actual quantum advantage, run times of the quantum block will increase

For example Quantum Approximate Optimization Algorithms (QAOAs) are expected to require circuit depths well beyond what is presently possible

When they *do* become possible, latency becomes less important

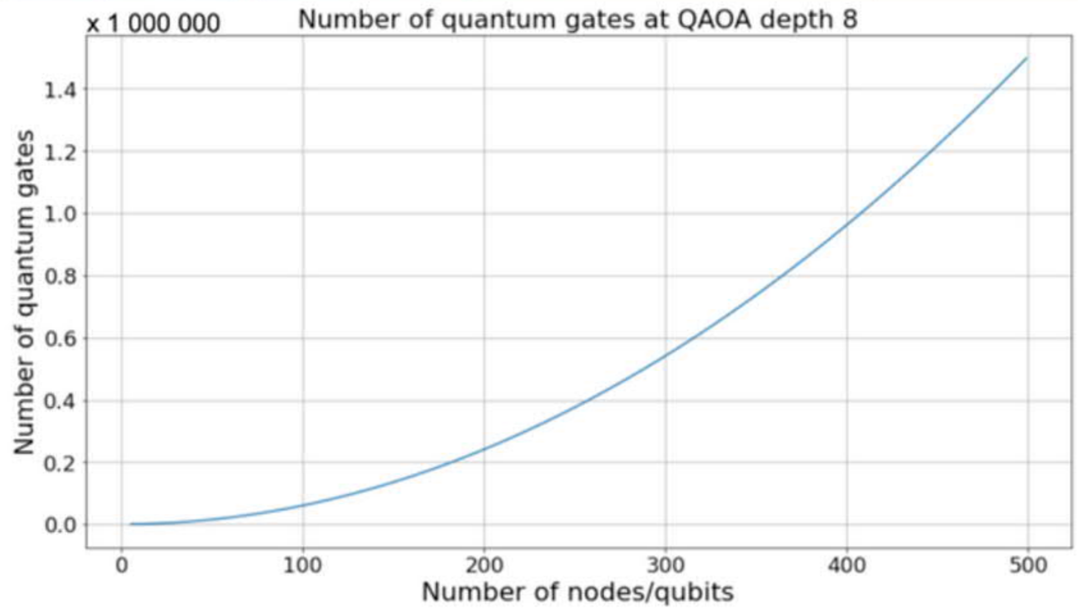
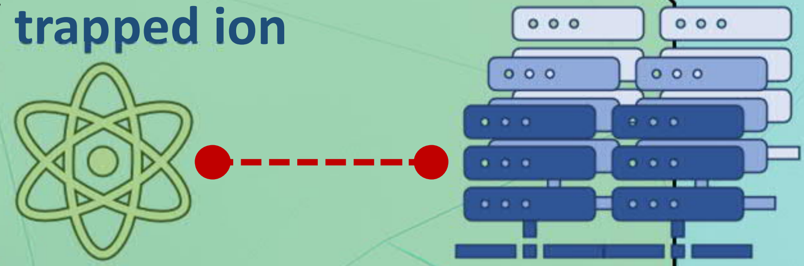


Figure 3. Achieving quantum advantage is likely to require about 500 qubits, rapidly increasing the circuit depth to millions of gates.

https://www.csc.fi/en/-/emulated-quantum-noise

Execution times of algorithms

Execution times of gate operations: superconducting / trapped ion



- 1-qubit gates: 20-25 ns / 15 µs
- 2-qubit gates: 15-300 ns / 66-200 µs

➡ **Execution time of 1,000,000 gates**

- Assuming average of 100 ns/gate: 100,000,000 ns = **100 ms**

This is for just *one* execution of the quantum circuit!

- usually one repeats the run 100-10,000 times for statistically relevant results

Signal in fibre travels at around 200,000 km/s -> around the Earth in 200 ms

➡ **The classical server does not need to be *very* close**

Values kindly provided by Cornelius Hempel / PSI.CH

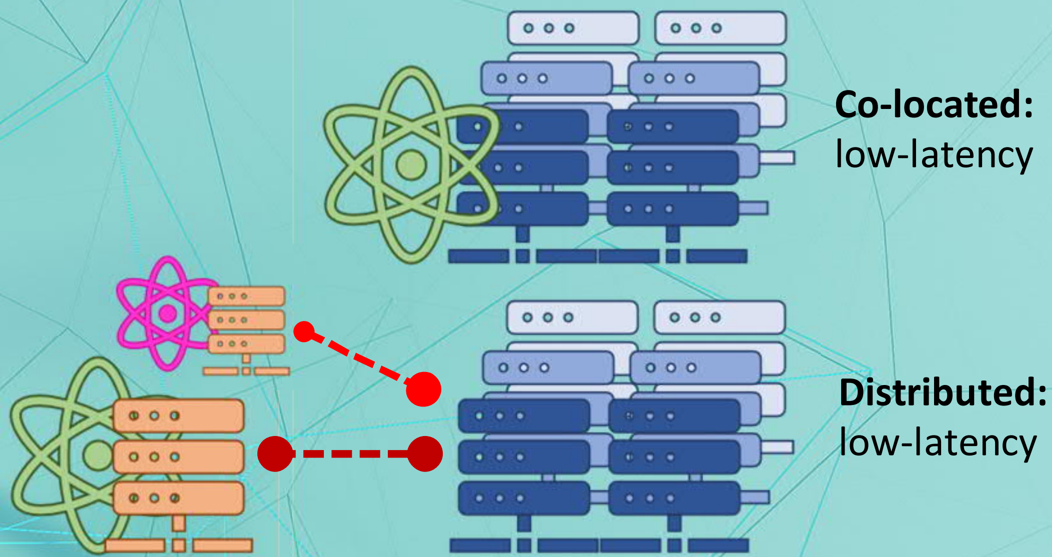
Co-located and distributed

- Low-latency *can* be important also in the future, when QCs mature
- A separate server or HPC node can take care of the classical computing that requires low-latency
- Straightforward approach: **co-location**

  server = HPC node
- More involved: **distributed**

NordIQuEst

LUMI-Q



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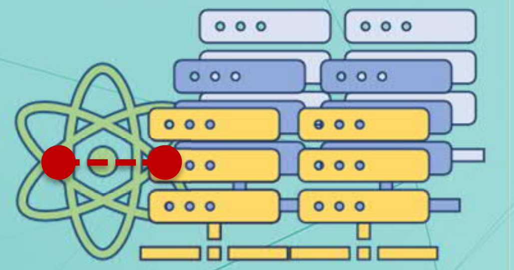

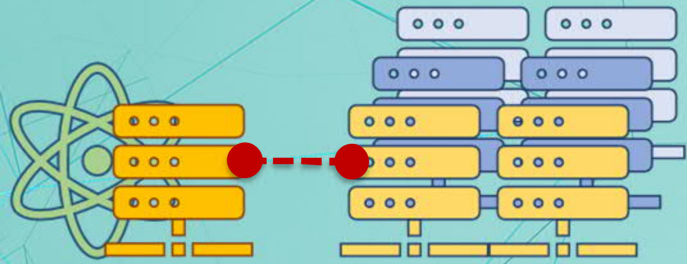

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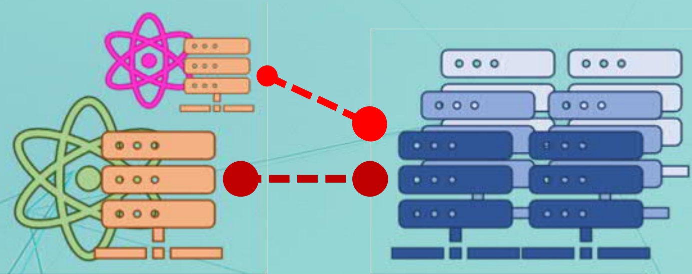
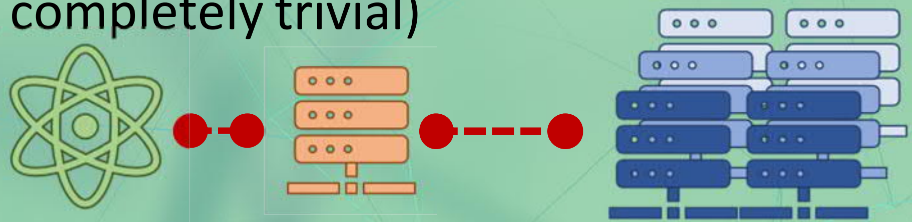
Co-located and distributed



- The **software stack** for a distributed approach requires somewhat more work than the co-located approach
  - Need to take care of one additional communication step between classical and HPC (not completely trivial)



  - User authentication needs to be done twice (rather trivial)
  - Need personnel at more than one physical location

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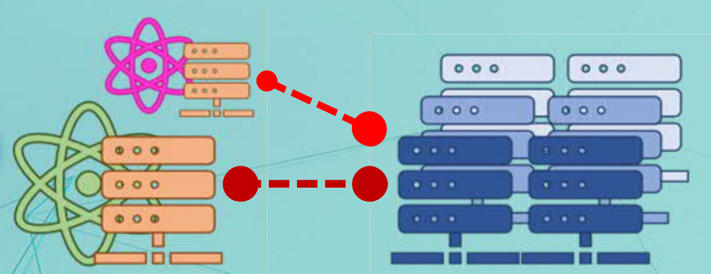
Why make distributed work?



- With the **software stack** in place, ***easy to add additional QC resources***
  - Needs only location of a classical server next to the QPU (+internet)
  - **Increases diversity and inclusiveness**
  - Users can access several QPUs from the same computing environment
  - Facilitates **time-sharing** of QPU resources
- QC and HPC can be optimally located, separately
  - HPC in large data centres with sufficient and affordable electric power
  - QC in shielded environments: temperature, vibrations, other noise sources

Article | Published: 16 June 2021

Correlated charge noise and relaxation errors in superconducting qubits

C. D. Wilen, S. Abdullah, N. A. Kurinsky, C. Stanford, L. Cardani, G. D'Imperio, C. Tomei, L. Faoro, L. Ioffe, C. H. Liu, A. Opremcak, B. G. Christensen, J. L. DuBois & R. McDermott

Nature **594**, 369–373 (2021) | Cite this article

across the millimetre-scale chip. The resulting correlated errors are explained in terms of the charging event and phonon-mediated quasiparticle generation associated with absorption of γ-rays and cosmic-ray muons in the qubit substrate. Robust quantum error correction will require the development of mitigation strategies to protect multiqubit arrays from correlated errors due to particle impacts.

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LUMI-Q

Inclusive

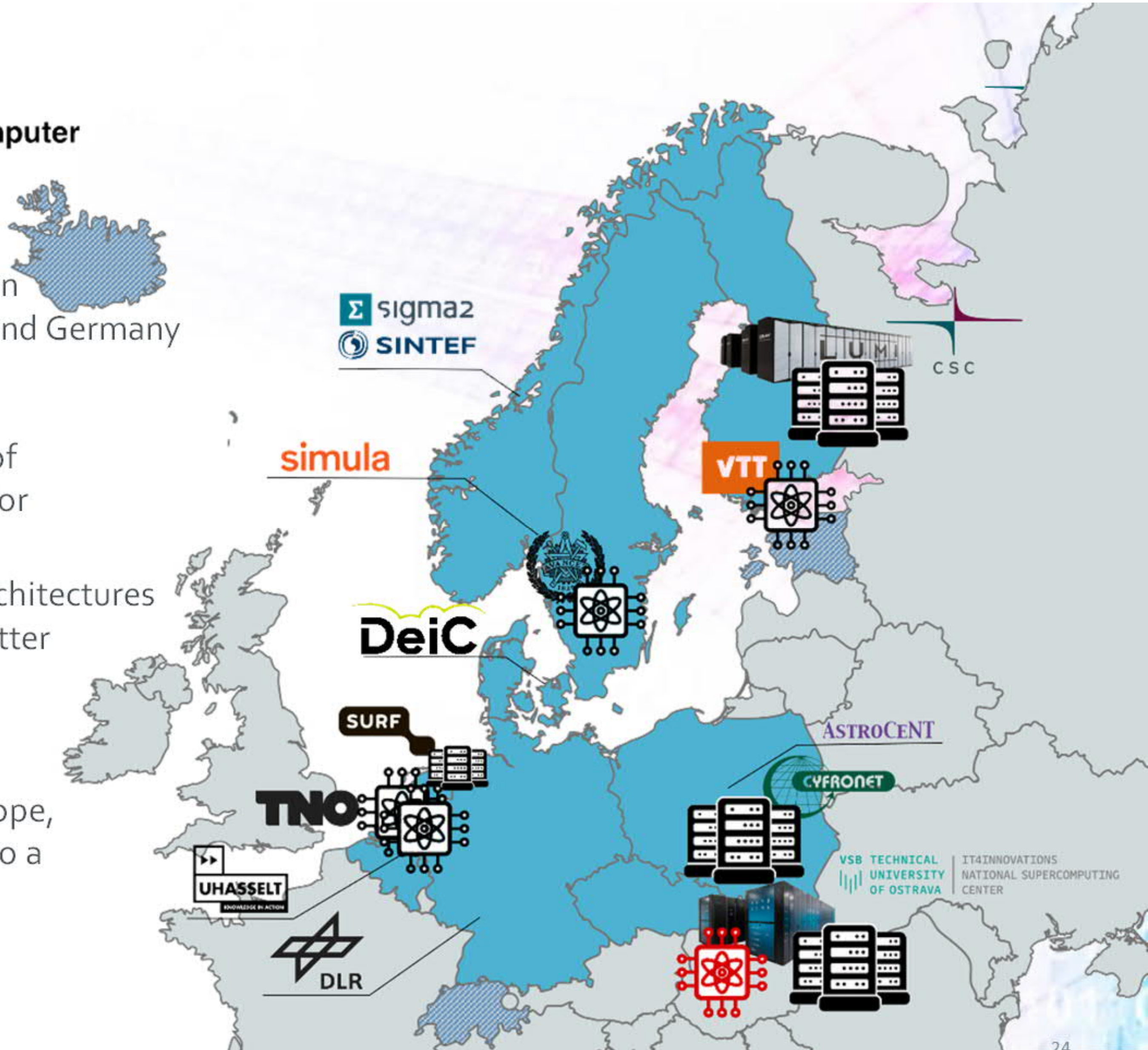
- Builds on the 10-country pan-European LUMI consortium + The Netherlands and Germany

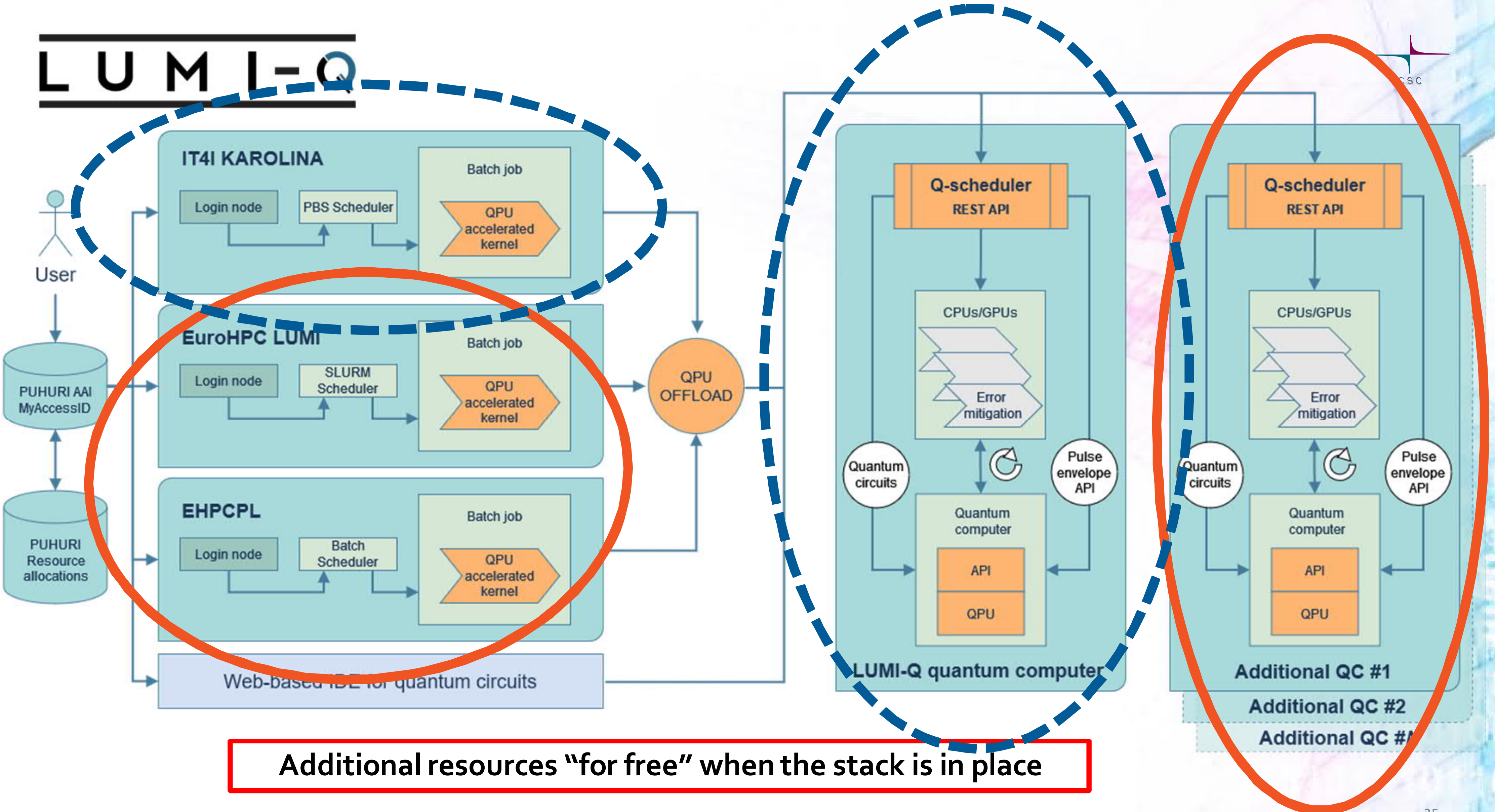
Diverse

- Getting several QCs to the fingertips of researchers and developers is crucial for catalysing software development.
- Different problems will fit different architectures **and software stack infrastructure** better

Accessible

- By being available through several platforms distributed throughout Europe, LUMI-Q provides a familiar interface to a uniquely large user base





Additional resources "for free" when the stack is in place

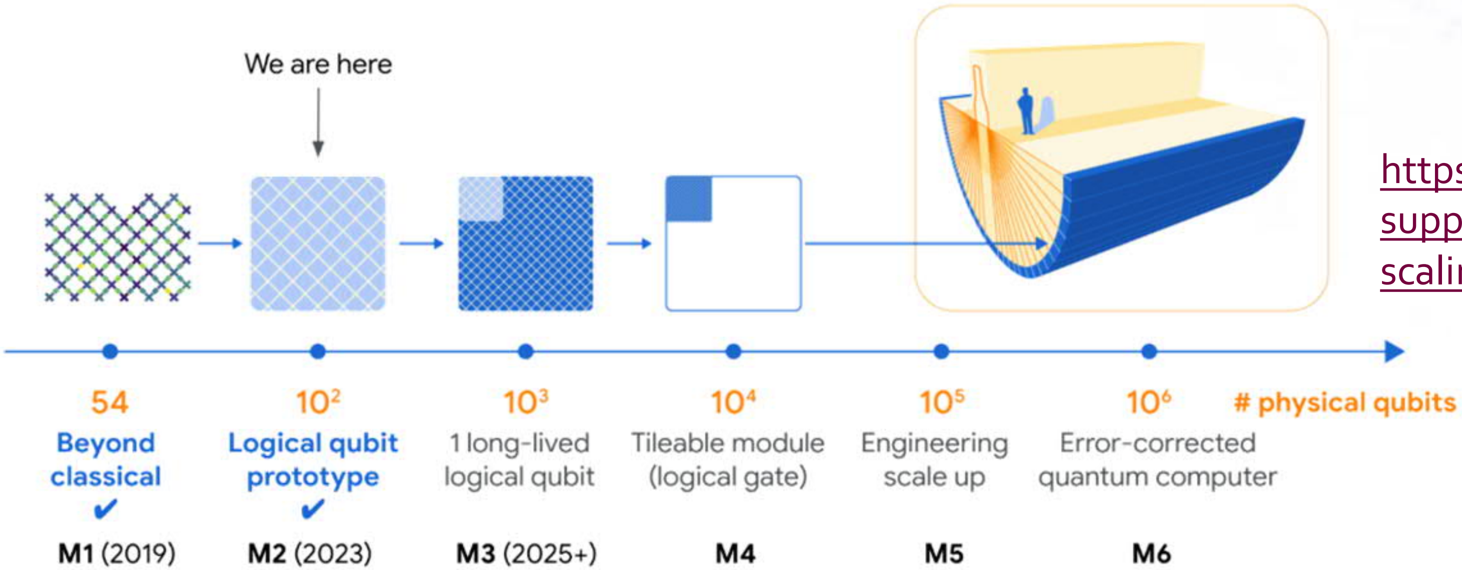
Error mitigation

Why error mitigation?

Quantum computers compute wrong most of the time

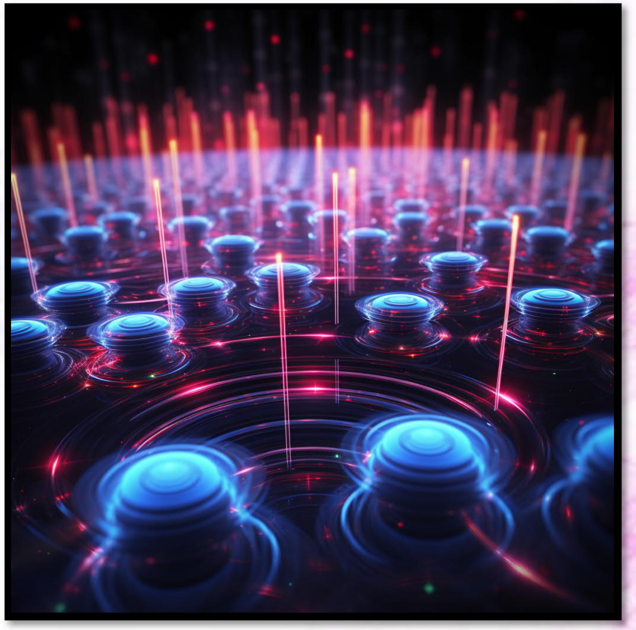
- The ultimate goal is to produce **logical qubits** out of several (hundreds) physical qubits
- **We are very far from this!**

Quantum error correction	–	Enabled	At scale
# Physical qubits	10 – 100	100 – 1000	$10^4 – 10^6$
# Logical qubits	–	1	10 – 1000+
Logical error	10^{-3}	$10^{-2} – 10^{-6}$	$10^{-6} – 10^{-12}$



https://blog.research.google/2023/02/suppressing-quantum-errors-by-scaling.html

Why error mitigation?



Need to learn how to cope with the NISQ era

- NISQ = Noisy Intermediate Scale Quantum
- In other words: **deal with the noise**
- **Noise mitigation, error suppression, error mitigation, ...**
- Algorithm design!

Error mitigation / suppression

- (Machine) Learn the error characteristics of the QC
  - Correct for noise in post-processing

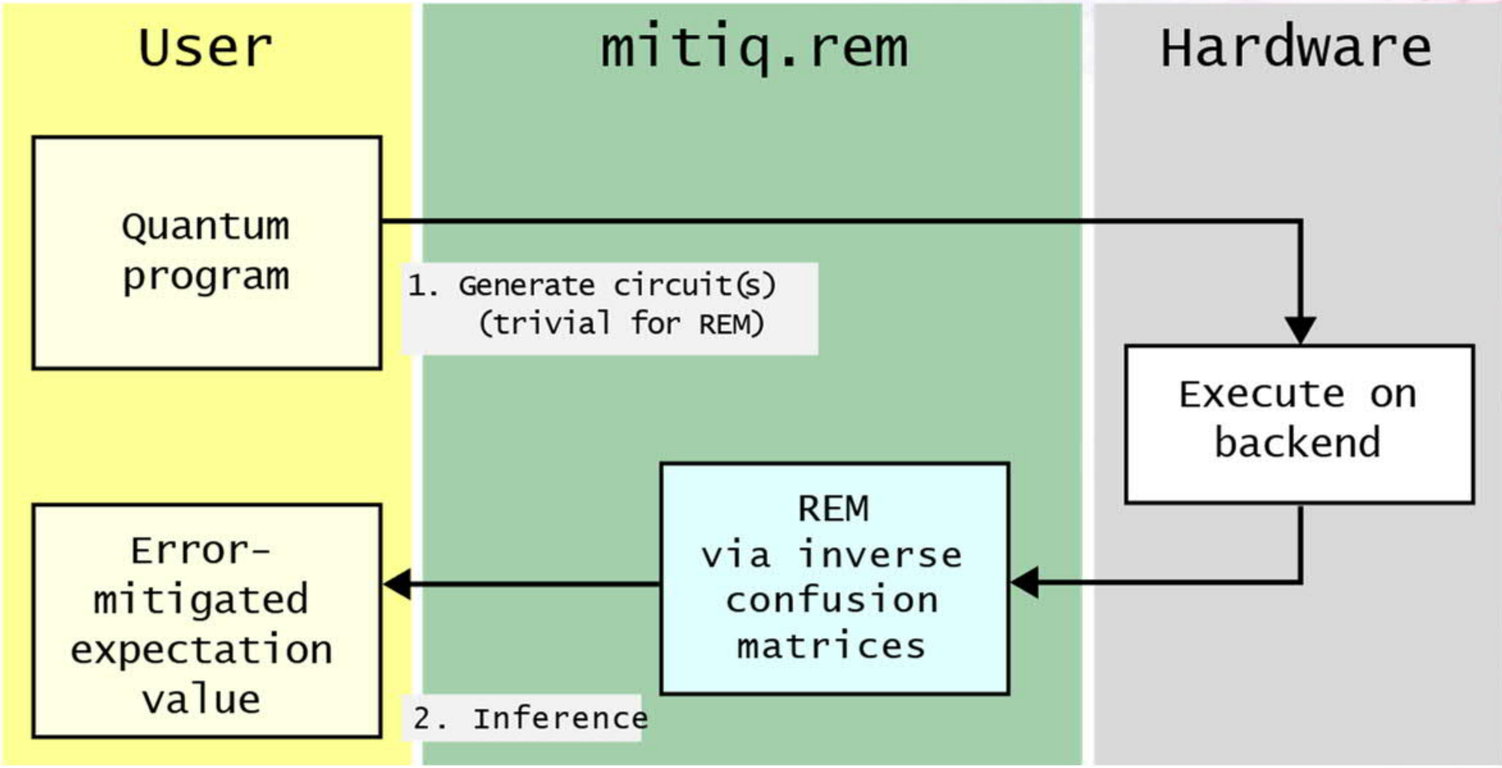
Example: readout error mitigation

- Needs characterisation of the errors inherent in the quantum computer, especially readout error
- **Error type**: qubit measurement *should* return zero, but returns one (and *vice versa*)
- The characterisation scales exponentially with qubit count... $O(2^n)$
- Otherwise simple to implement and use, for example, no modifications to the circuit necessary

Readout error mitigation (REM) with confusion matrix

Using the mitiq library

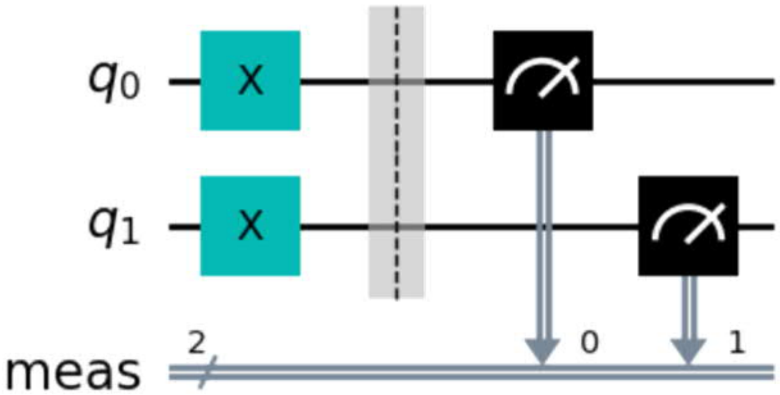
- https://mitiq.readthedocs.io

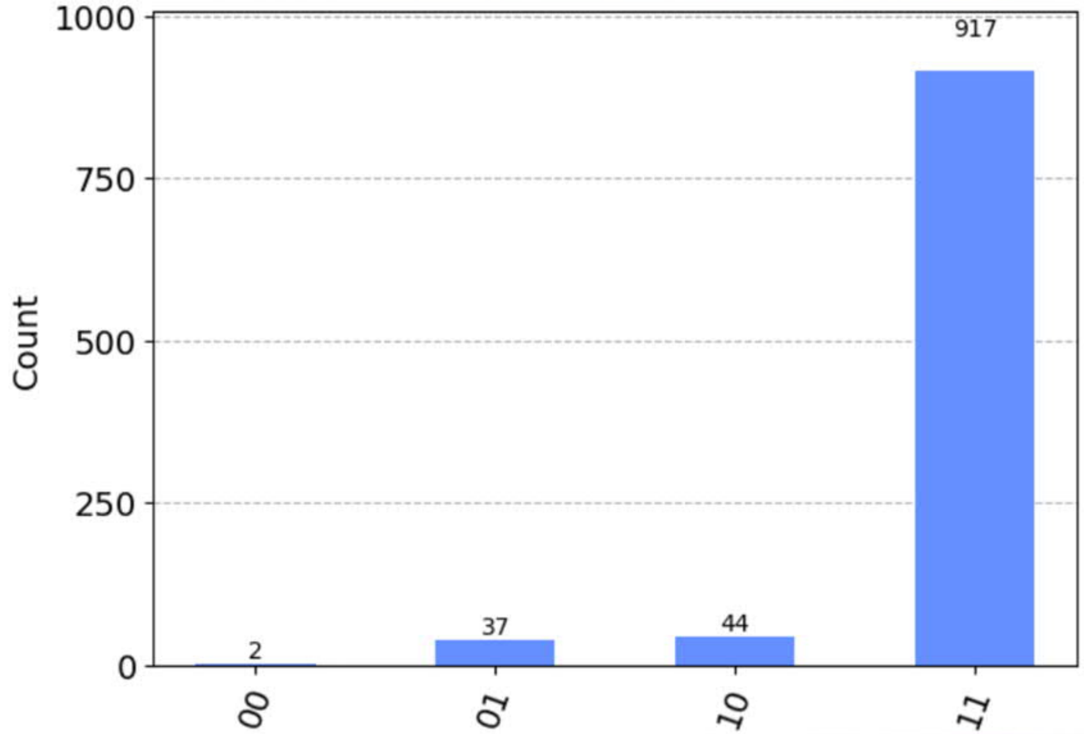


Readout error mitigation basics

Learn how the quantum computer readout goes wrong

- Need to sample how the output of the quantum computer differs from what it *should* output
- Example for two qubits (ran on Helmi last night):
- *What errors are included?*





Readout error mitigation basics

Learn how the quantum computer readout goes wrong

- For simplicity, let's assume that our QC is much worse than Helmi, and the readout error is 25%
- The **confusion matrix (error matrix)** would then look like this:

$$A = \begin{bmatrix} P(00|00) & P(00|01) & P(00|10) & P(00|11) \\ P(01|00) & P(01|01) & P(01|10) & P(01|11) \\ P(10|00) & P(10|01) & P(10|10) & P(10|11) \\ P(11|00) & P(11|01) & P(11|10) & P(11|11) \end{bmatrix} = \begin{bmatrix} 0.75 \times 0.75 = 0.5625 & 0.1875 & 0.1875 & 0.0625 \\ 0.75 \times 0.25 = 0.1875 & 0.5625 & 0.0625 & 0.1875 \\ 0.75 \times 0.25 = 0.1875 & 0.0625 & 0.5625 & 0.1875 \\ 0.25 \times 0.25 = 0.0625 & 0.1875 & 0.1875 & 0.5625 \end{bmatrix}$$

- $P(ab\,|\,ij)$ denotes the probability of measuring *ab* when one should get *ij*
  - With no error, we would have the identity matrix with just ones on the diagonal and zeros off-diagonal

- The pseudoinverse $A^{+} = A^{T}(AA^{T})^{-1}$

$$\begin{bmatrix} 2.25 & -0.75 & -0.75 & 0.25 \\ -0.75 & 2.25 & 0.25 & -0.75 \\ -0.75 & 0.25 & 2.25 & -0.75 \\ 0.25 & -0.75 & -0.75 & 2.25 \end{bmatrix}$$

https://www.emathhelp.net/en/calculators/linear-algebra/pseudoinverse-calculator/

Readout error mitigation basics

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- The error mitigated output would then be obtained by $m_{\mathrm{REM}} = A^+ m$ where m is the measured output vector:

$$m_{\mathrm{REM}} = \begin{bmatrix} 2.25 & -0.75 & -0.75 & 0.25 \\ -0.75 & 2.25 & 0.25 & -0.75 \\ -0.75 & 0.25 & 2.25 & -0.75 \\ 0.25 & -0.75 & -0.75 & 2.25 \end{bmatrix} \times \begin{bmatrix} m|00\rangle \\ m|01\rangle \\ m|10\rangle \\ m|11\rangle \end{bmatrix}$$

- Note that applied in this simple manner, we can end up having negative probabilities/counts for some states
  - A bit more sophisticated methods needed to keep the probabilities positive, but the idea is essentially the same
- There will be a demo on REM later today!

Summary and musings

We need to create valuable classical support-software for quantum

- Bridges the gap between end-users and quantum-accelerated HPC
- Plenty of **classical** software development needed
- Need to actively make HPC (seen as) useful!

Making existing modelling workflows quantum-ready: dynamic shift towards increasing quantum-acceleration

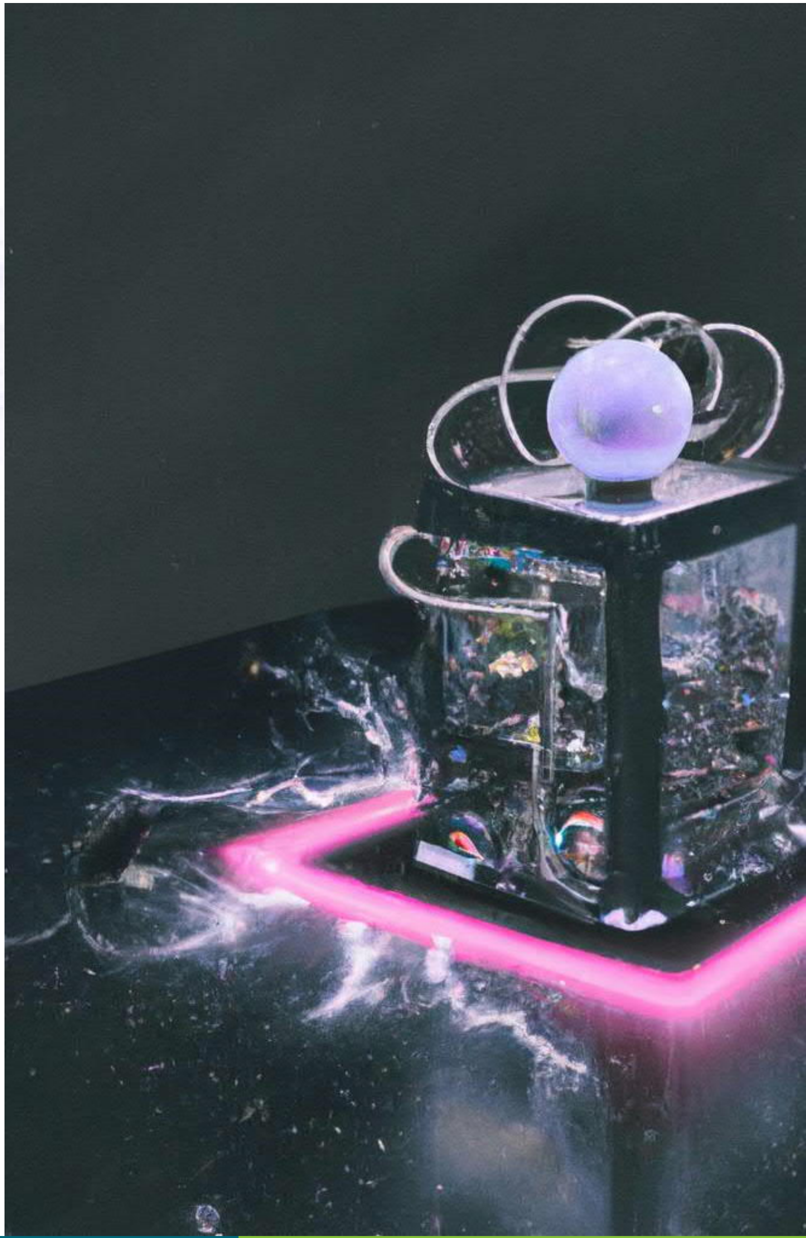
- Closely coupled with HPC-ification in general

Quantum advantage is already here!

- On-board those users that can utilise this already now, to build momentum in the end-user base

Quantum computing is a high-risk/*very*-high gain type of project

- Will need public support to truly get flying
- The role of HPC centres is to provide the best modelling tools available to our customers: **also the tools of the future!**
- Early support can bring us closer to all forms of quantum advantage: **every year counts**



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Dr. Mikael Johansson

Manager, Quantum Technologies
mikael.johansson@csc.fi

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