Introduction to
Quantum Computing
& Hybrid HPC-QC Systems

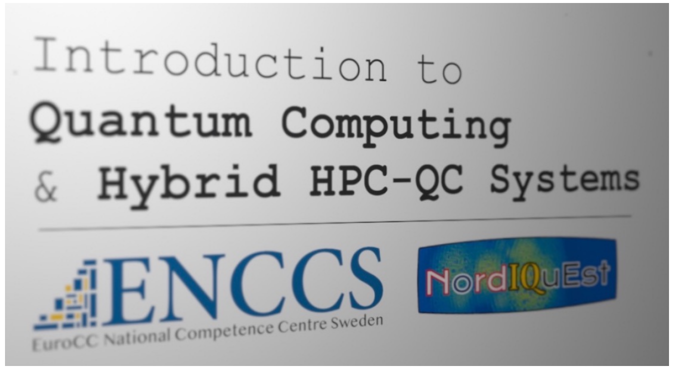
ENCCS
EuroCC National Competence Centre Sweden

L1

The HPC-QC landscape

Göran Wendin
Chalmers

How does QC differ from classical HPC?
What is the relation between HPC and QC for the foreseeable future?



NeIC = Nordic e-Infrastructure Collaboration

ENCCS = European National Competence Centre Sweden

NordIQuEst = Nordic-Estonian Quantum Computing e-Infrastructure Quest

Introduction to Quantum Computing & Hybrid HPC-QC Systems

ENCCS EuroCC National Competence Centre Sweden

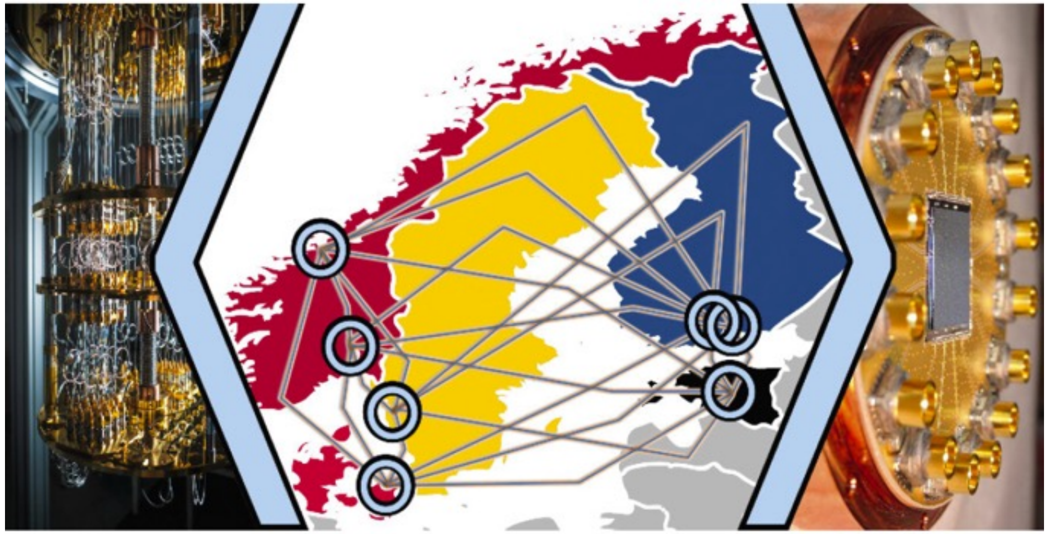
NordIQuEst

NordIQuEst

neic

	Wed 8 June 2022
9-9:45 L1	The HPC-QC landscape: how does QC differ from classical HPC? What is the relation between HPC and QC for the foreseeable future?
10-10:45 L2	Introduction to digital QC: quantum states, qubits, logic gates, quantum algorithms.
11-11:45 L3	Overview of different QC hardware approaches (superconducting, trapped ions, semiconductors) and QC types (digital, analogue, adiabatic, annealing). Hybrid HPC+QC systems, how the non-expert end-user will benefit.
12-13	Lunch
13-16 L4 E1	Introduction to high-level languages for QC (Qiskit, Cirq, Q#) How to download program packages: Qiskit: Hands-on experience with quantum gates and quantum circuits: - Downloading quantum programming environments: Qiskit - Execution of simple examples controlling 1q and 2q gates: 1q rotations, teleportation.

	Thu 9 June 2022
9-9:45 L5	The hybrid HPC-QC approach Systems: HPC-QC integration, facts and fiction. Co-located and distributed systems. Software control of quantum error mitigation and correction.
10-10:45 L6	Overview of the software stack, ranging from ready-made Q-libraries for common tasks to circuit level assembly and hardware-level coding.
11-11:45 L7	Hybrid classical/quantum algorithms Methods: Optimisation and variational methods: QAOA/QUBO, VQE, and more Applications: Introduction to use cases for quantum chemistry, optimisation and finance.
12-13	Lunch
13-16 E2	Hands-on experience with 13-14 - quantum software testing on simulator including downloading the tool and using it to test quantum circuits in Qiskit. 14-15 - Qiskit applied to use cases for optimisation 15-16 - Qiskit applied to use cases for quantum chemistry



NordIQuEst

Nordic-Estonian Quantum Computing e-Infrastructure Quest

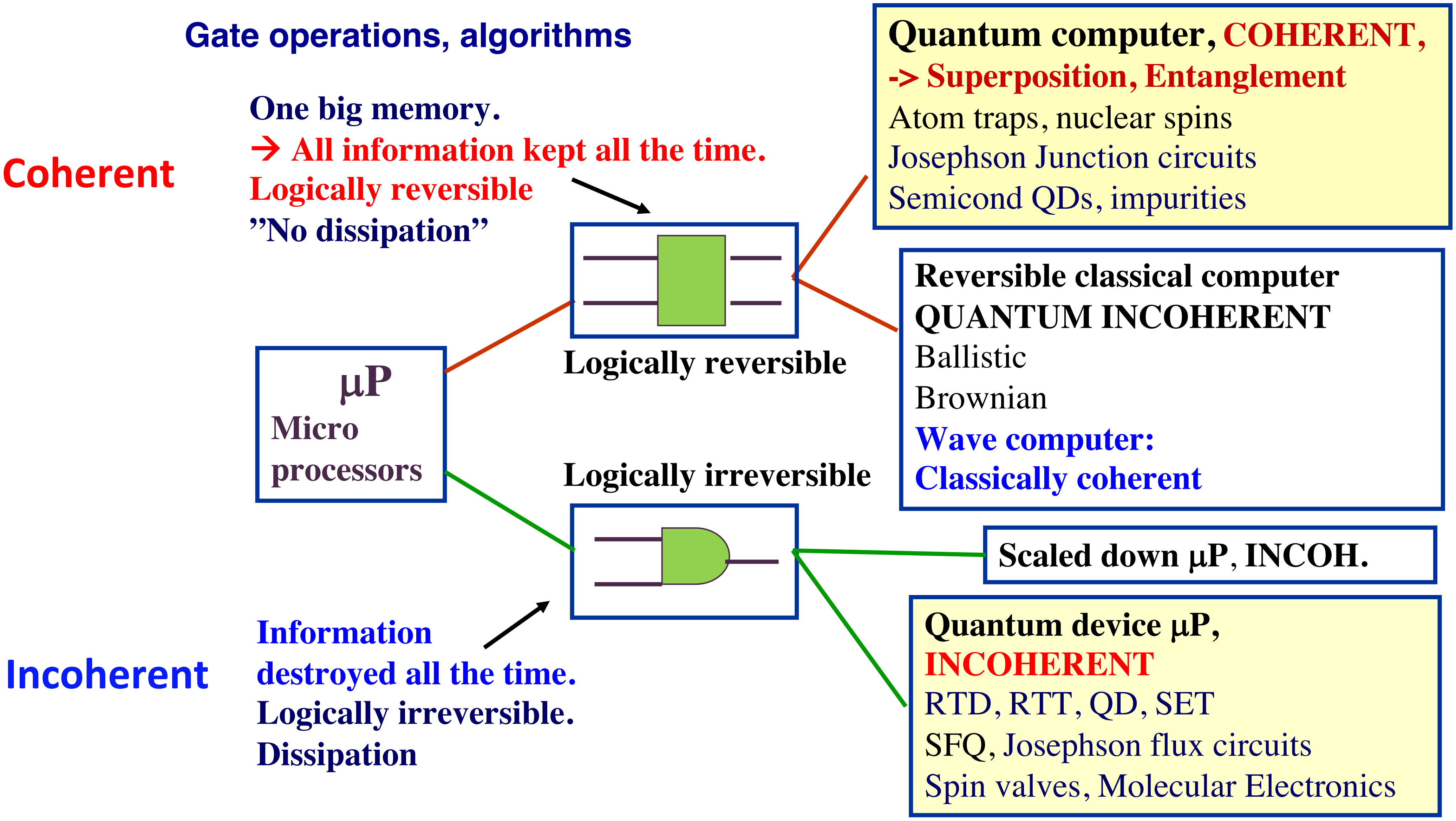
Institution	Country	Contact person	Position
CHALMERS	Sweden	Miroslav Dobsicek	Research Scientist
CSC	Finland	Mikael Johansson	Quantum Strategist
DTU	Denmark	Sven Karlsson	Assoc. prof.
SINTEF	Norway	Franz Fuchs	Research Scientist
SRL	Norway	Shaukat Ali	Professor
UTartu	Estonia	Dirk Oliver Theis	Assoc. prof.
VTT	Finland	Ville Kotovirta	Research Team Leader

NordIQuEst group leaders and Lecturers

How does QC differ from classical HPC?

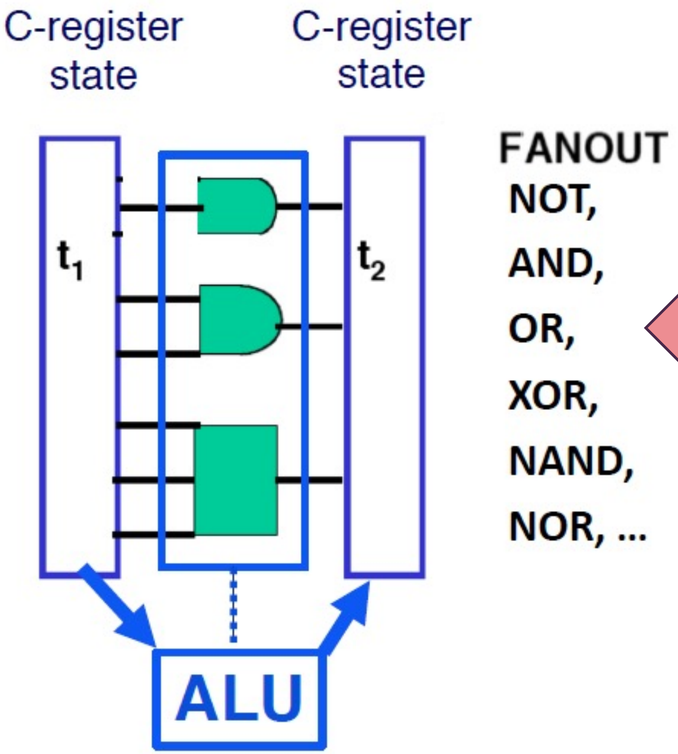
Reversible/coherent – irreversible/incoherent computing !!

Reversible - irreversible computing

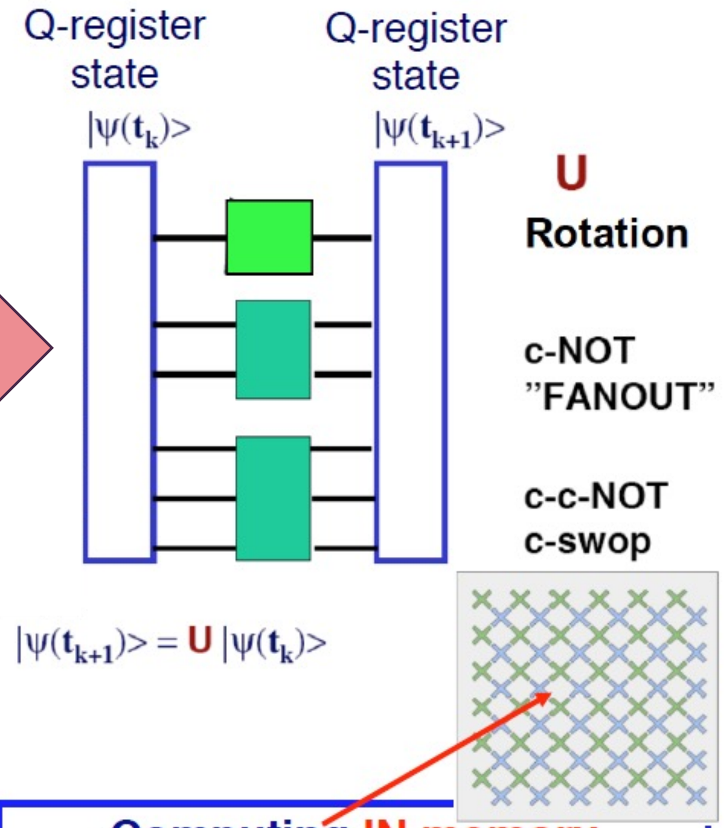


HPC-QC = Classical computer + Q-accelerator

CC: Classical gates



QC: Quantum gates



Computing FROM/TO memory
The memory is the storage

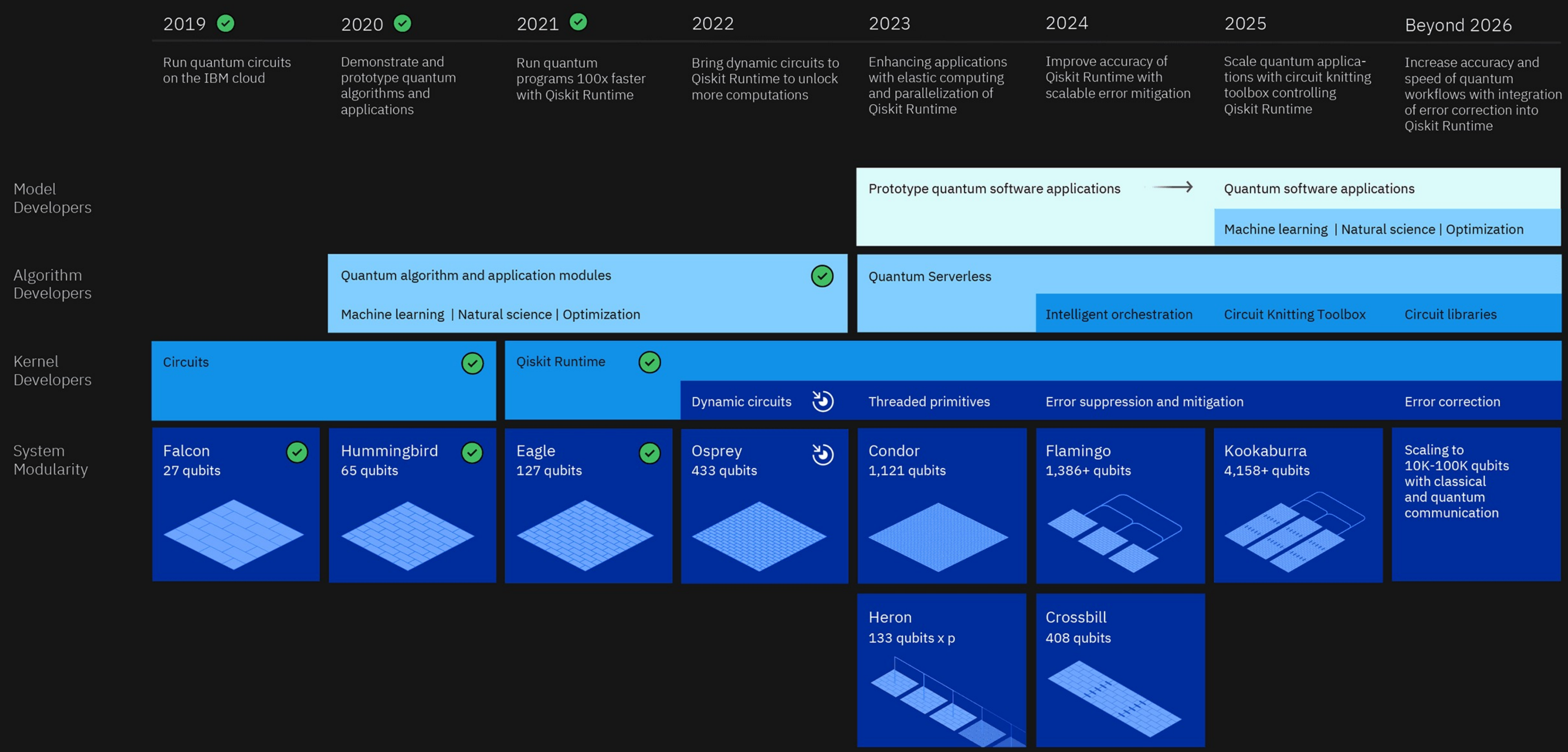
Computing IN memory
The memory is the computer

What is the relation between HPC and QC for the foreseeable future?

Superconducting qubits Cloud service	IBM Google Rigetti Alibaba QuTech (Delft) ……….. -----------	Semiconductor qubits Cloud service	QuTech (Delft) ……….. -----------
Ion trap qubits Cloud service	Innsbruck IonQ Sandia Honeywell Amazon …….	Photonic qubits Cloud service	Not yet ? …….

Development Roadmap | Executed by IBM On target

IBM Quantum

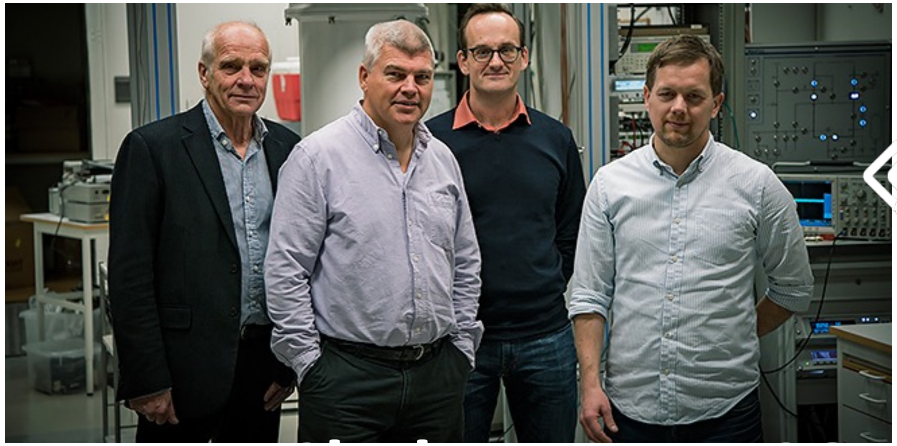


Sweden's quantum technology programme

Wallenberg Centre for Quantum Technologies

WACQT, 2018-2029   MC2, Chalmers U of Tech, Sweden

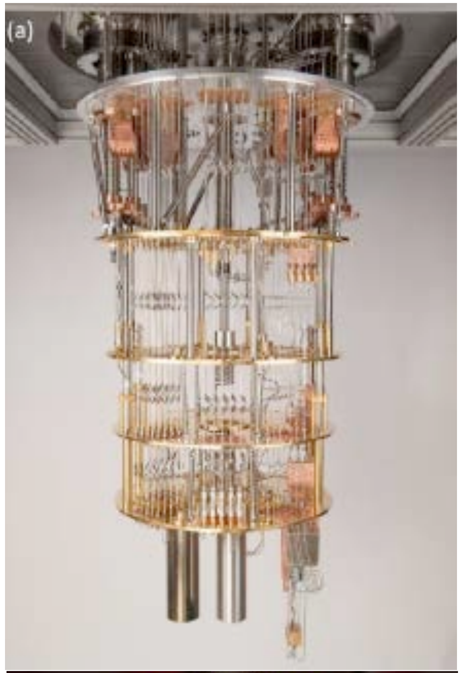
12 years, 150 M€

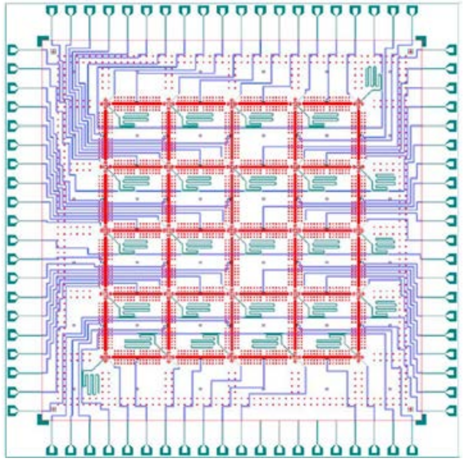


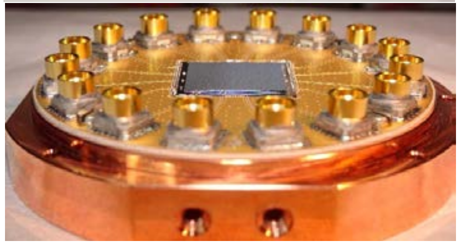
Mission: to build a quantum processor with 100+ superconducting qubits by 2025

https://www.chalmers.se/en/centres/wacqt/Pages/default.aspx

Cryostat
≈ 10 mK





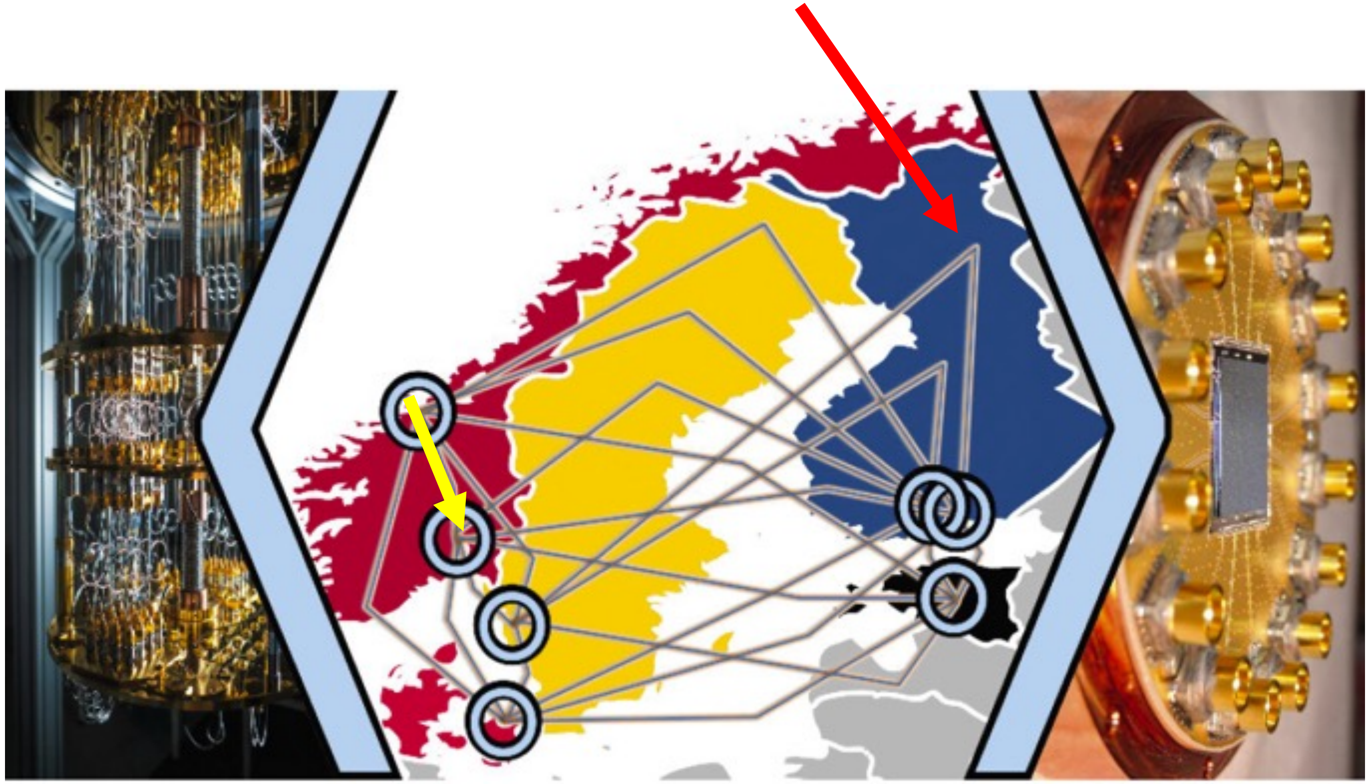


25q Transmon chip under testing

NordiQuEst HPC-QC ecosystem

2022-2025

LUMI pre-exascale HPC in Kajaani



According to plans:
25 qubits by 2023
50 qubits by 2025

Accessible for users via a LUMI portal

EuroHPC JU

LUMI-Q ….. ? (in preparation)

(CSC, VTT, Chalmers, NeIC, IQM …)

Horizon Europe

OpenSuperQ Plus !

FPA Roadmap 2022-2029:

Chalmers, VTT, CSC, IQM, ….

SGA1 2023-2025 (100q)

SGA2 2026-2029 (1000q)

Why is quantum computing interesting?

Because of hard future limits for classical High-Performance Computing (HPC):

- End of Moore's Law for semiconductor component scaling
- Scaling of classical computational power will hit hard limits (ultimately - electrical power)

POWER

Computers:

Big computers and internet servers are built from many **parallel** PC-type processors

1 processor typically consumes about **~ 100 W**
The computation itself (bit flops) consumes about
1V x 3 GHz x 10^10 transistors ≈ **5 W**
The rest is losses dissipated as heat.

20 000 processors x 100 W → 2 10^6 W **= 2 MW**
→ Needs a dedicated power station!

One is planning for 1000 times more powerful – exaflop - computers → **10^9 W = 1000 MW**

→ Requires a dedicated nuclear power station!!

POWER

Internet-of-Things (IoT): a rough estimate

10^{10} people (10 x Kina today)
100 W/person at home (only for IoT)
→ 10^{12} Watt = **1000 nuclear power reactors**

Moreover: every internet server will need a dedicated nuclear power reactor!!
Suppose the world will need 1000 IoT servers

→ **2 000 nuclear power reactors needed for internet/IoT**

→ **Information processing in the near future will need very big electric power!**

→ We need **exponential speed-up** to be able to solve (approximately!) hard problems with finite resources (time, memory).

→ We may need new computational paradigms → **Quantum computing?**

The original quantum “killer application”: Shor’s algorithm for factorisation (1995)

Today, the typical killer applications are “use cases”:

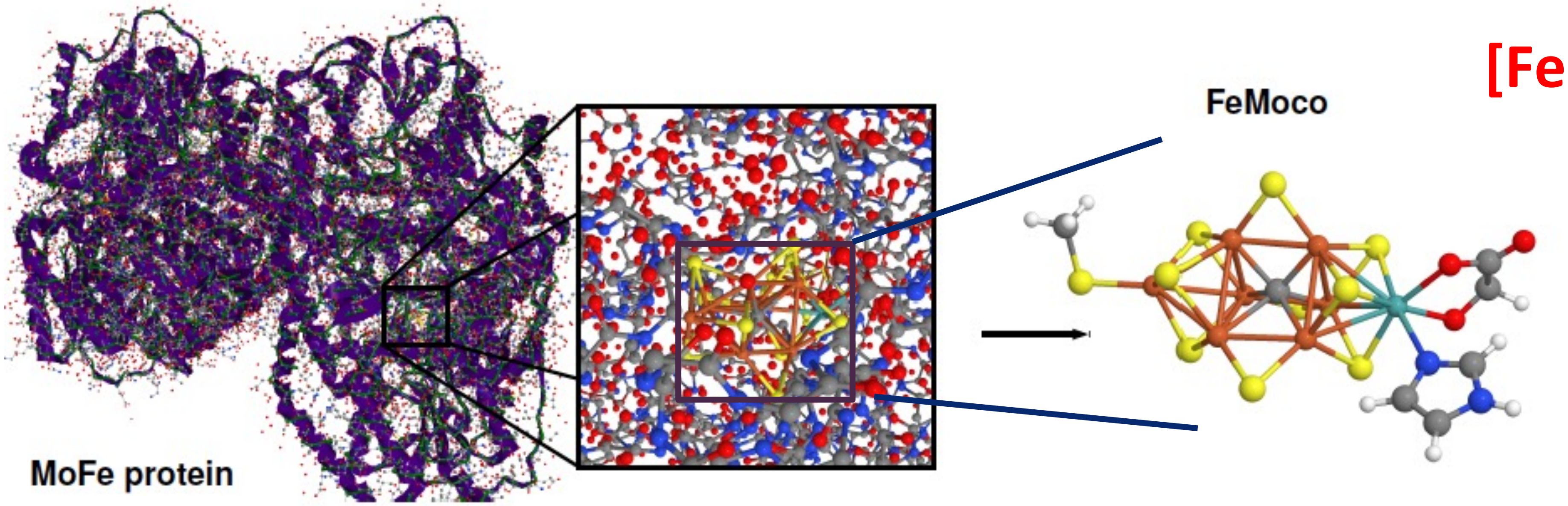
- **Quantum Chemistry** – designing enzymes and catalysers
- **Materials science** – describing strong electron correlations
- **Optimization** - logistics, scheduling, ...

→ **There is no lack of algorithms and applications.**

→ **But there is lack (absence!) of large-scale coherent quantum processors**

The killer application today

Nitrogenase protein: iron molybdenum cofactor FeMoco



$[FeS]_n$

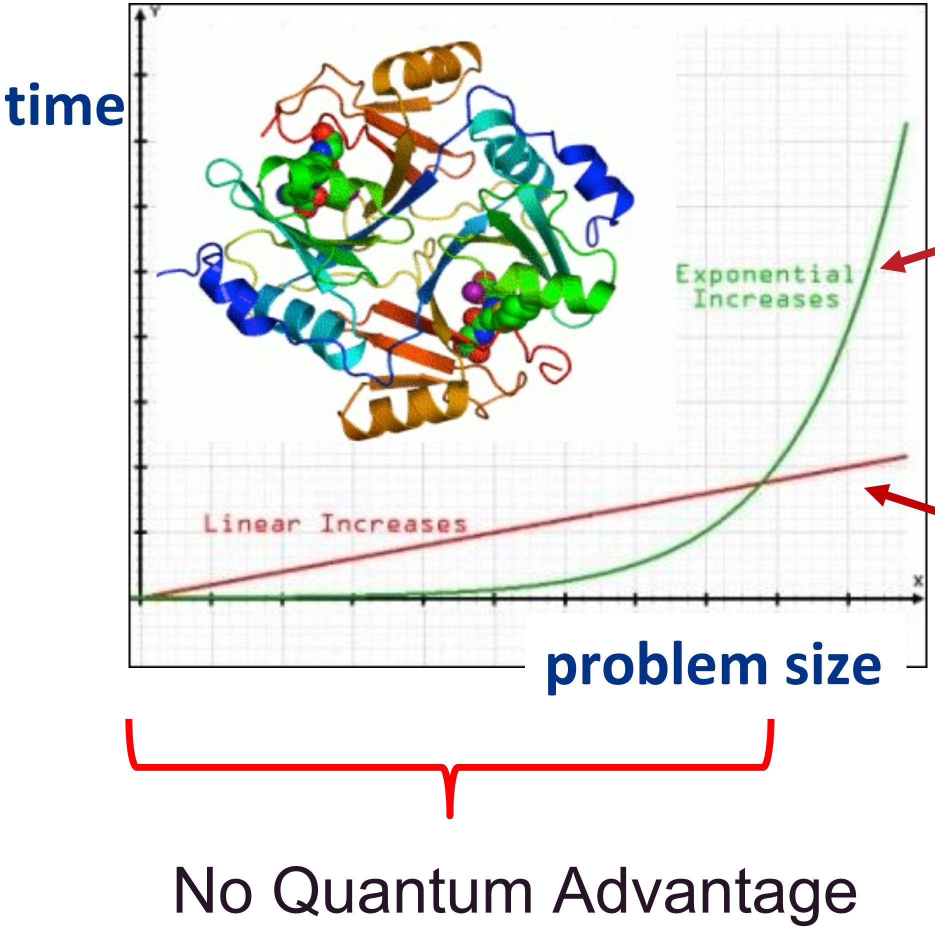
Elucidating reaction mechanisms on quantum computers

M. Reiher, N. Wiebe, K. M. Svore, D. Wecker, and M. Troyer

PNAS **114**, 7555-7560 (2017)

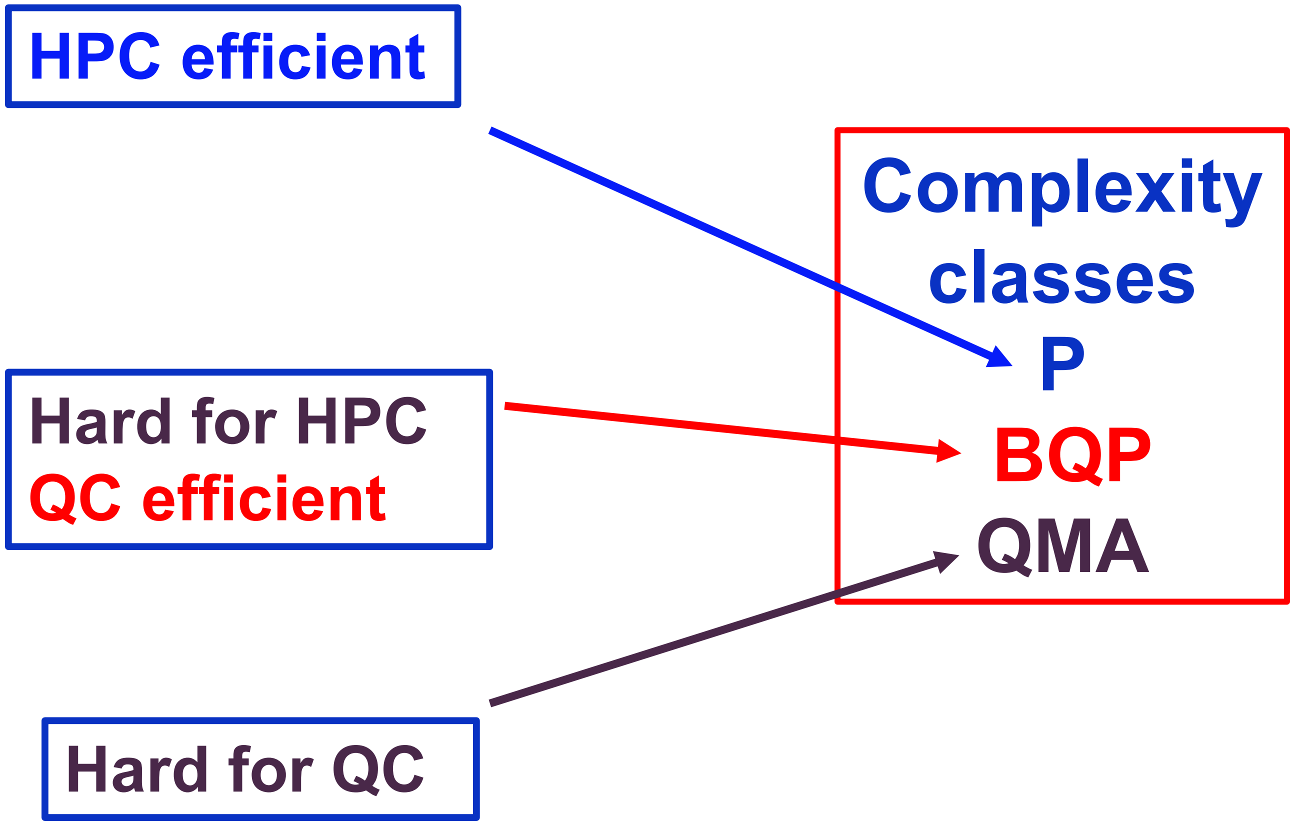
Quantum Advantage

Quantum computers offer, in principle, exponential speed-up for certain classes of hard problems

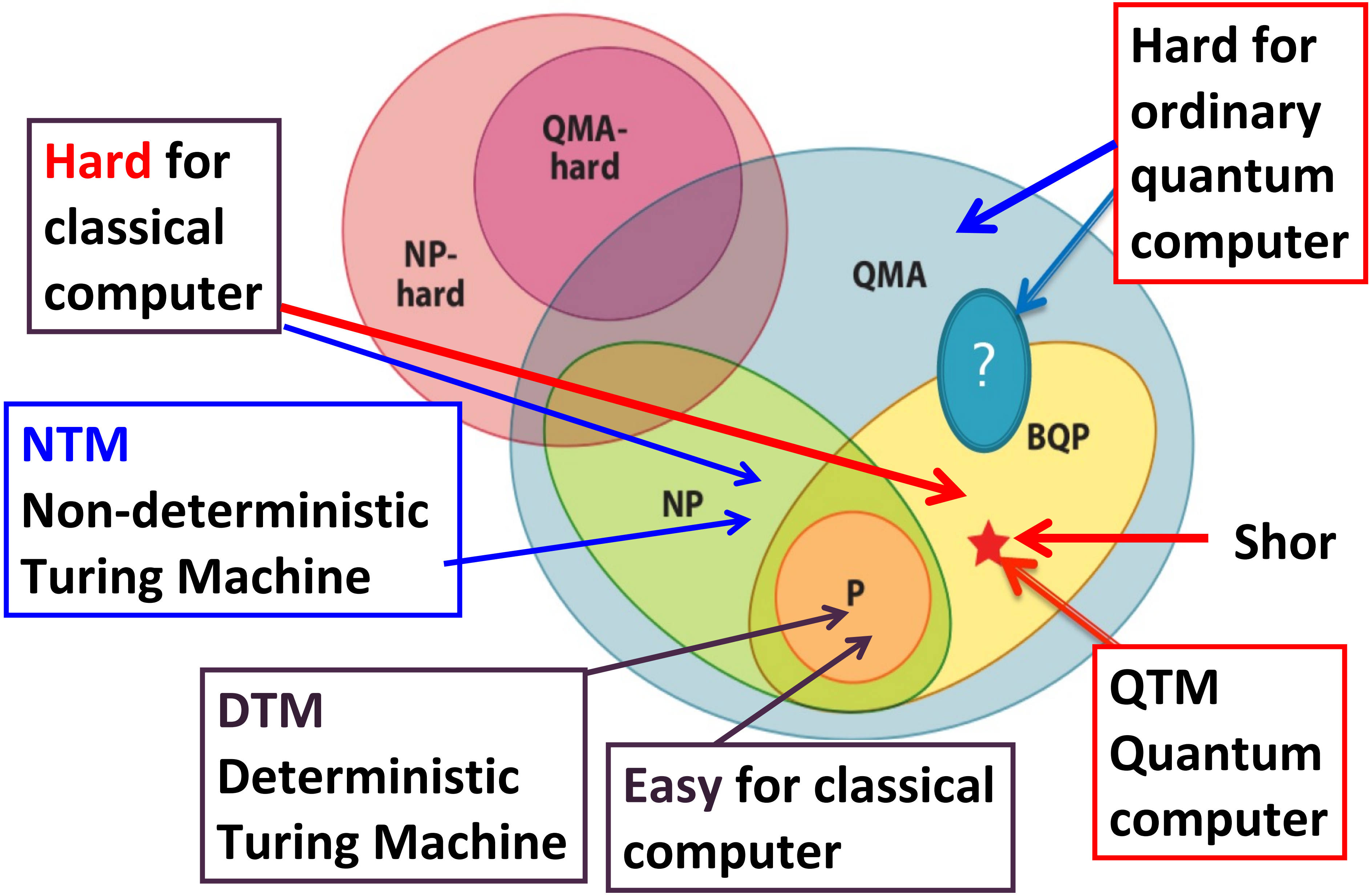


TTS for a HPC:
Grows exponentially

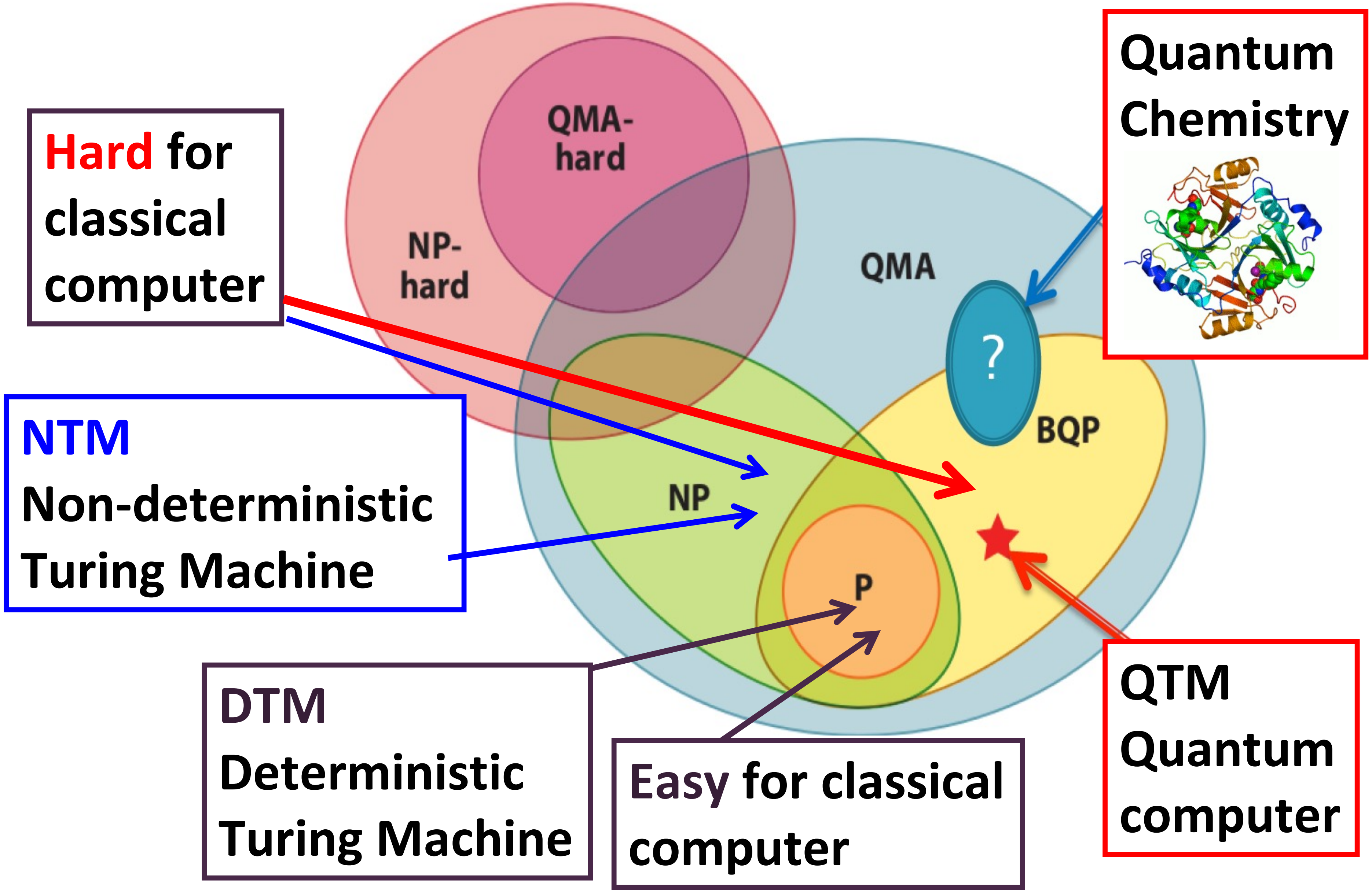
TTS for a quantum computer:
Grows linearly/polynomially


HPC efficient
Hard for HPC
QC efficient
Hard for QC
Complexity classes
P
BQP
QMA

Complexity classes

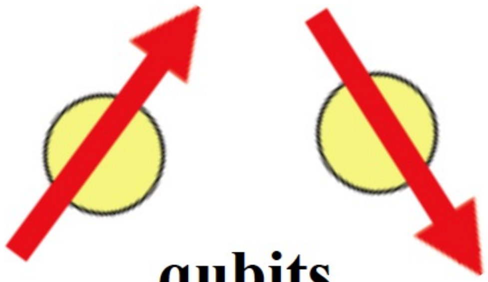


Complexity classes – Quantum Chemistry



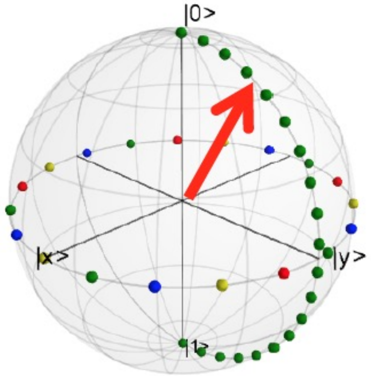
QC makes use of some fundamental properties of matter at "atomic & molecular" levels (like NMR):

- -Quantum physics
- -Coherence
- -Superposition
- -Parallelism
- -Entanglement

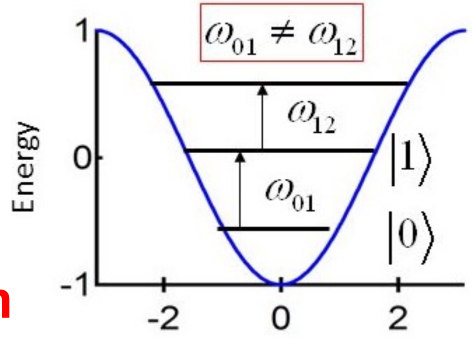


qubits

Bloch sphere



qubit = 2-level system



$\omega_{01} \sim 5-10$ GHz

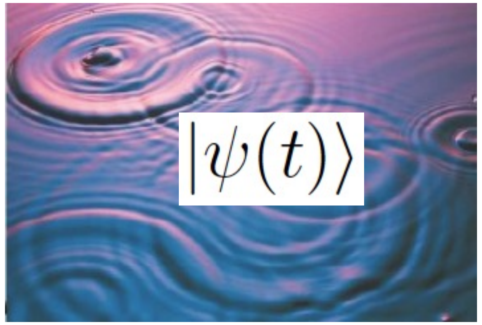
|0> , |1>

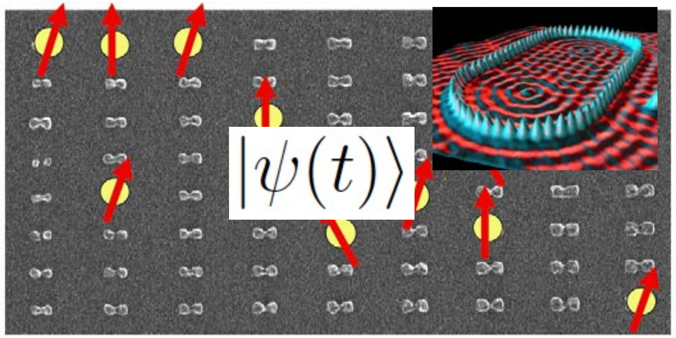
a|0> + b|1>

vector on the unit sphere

QC solves problems by generating and interpreting dynamics of quantum wave patterns in registers of quantum bits (qubits ) – "quantum matter"

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t) = \left[\frac{-\hbar^2}{2\mu}\nabla^2 + V(\mathbf{r},t)\right]\Psi(\mathbf{r},t)$$





Superposition of 2^N registers of N-qubit registers

a_1 I00..000> +
a_2 I00..001> +
a_3 I00..010> +
a_4 I00..011> +
.... +
a_{n-1} I11..110> +
a_n I11..111>

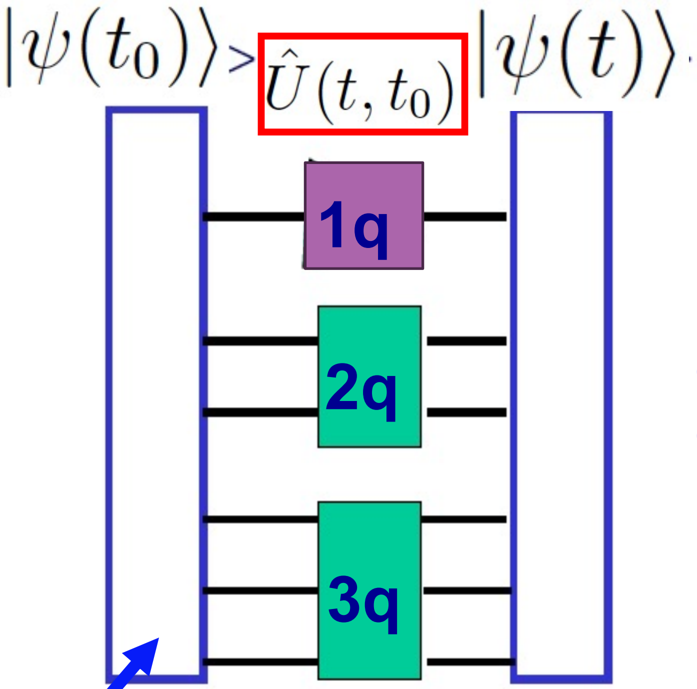
$|\psi(t)\rangle$

$n=2^N$

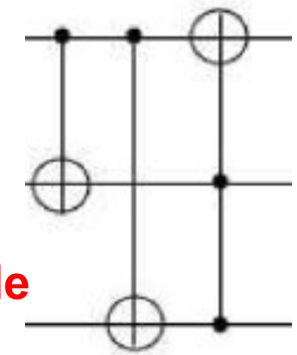
Quantum gates and states: superposition and entanglement

|00..000> +
|00..001> +
|00..010> +
|00..011> +
.... +
|11..110> +
|11..111> =
|>|> ... |>

Product state
Not entangled



Qubit (memory) register



Reversible gates

U

Rotation
NOT, Hadamard

CNOT
CPHASE

C-Rotation
c-c-NOT
c-swop

N qubits, n = 2^N states

$|\psi(t)\rangle = f_1(t)\,|0...00\rangle$
$+ f_2(t)\,|0...01\rangle$
$+ f_3(t)\,|0...10\rangle$
$+ ....$
$+ f_n(t)\,|1...11\rangle$

Super-position of 2^N states; Not possible classically

Superposition of 2^N state configurations - entanglement

$$|\psi(t)\rangle = U(t, t_0)|\psi(t_0)\rangle$$

$$U(t, t_0) = e^{-\frac{i}{\hbar}\hat{H}(t-t_0)}$$

Generic quantum gate

Series expansion → Quantum gate circuit

Quantum variational methods

Rayleigh-Ritz

$$E(\theta) = \langle \psi(\theta)|\hat{H}|\psi(\theta)\rangle \geq E_0; \quad \hat{H} = \sum_i \hat{H}_i$$

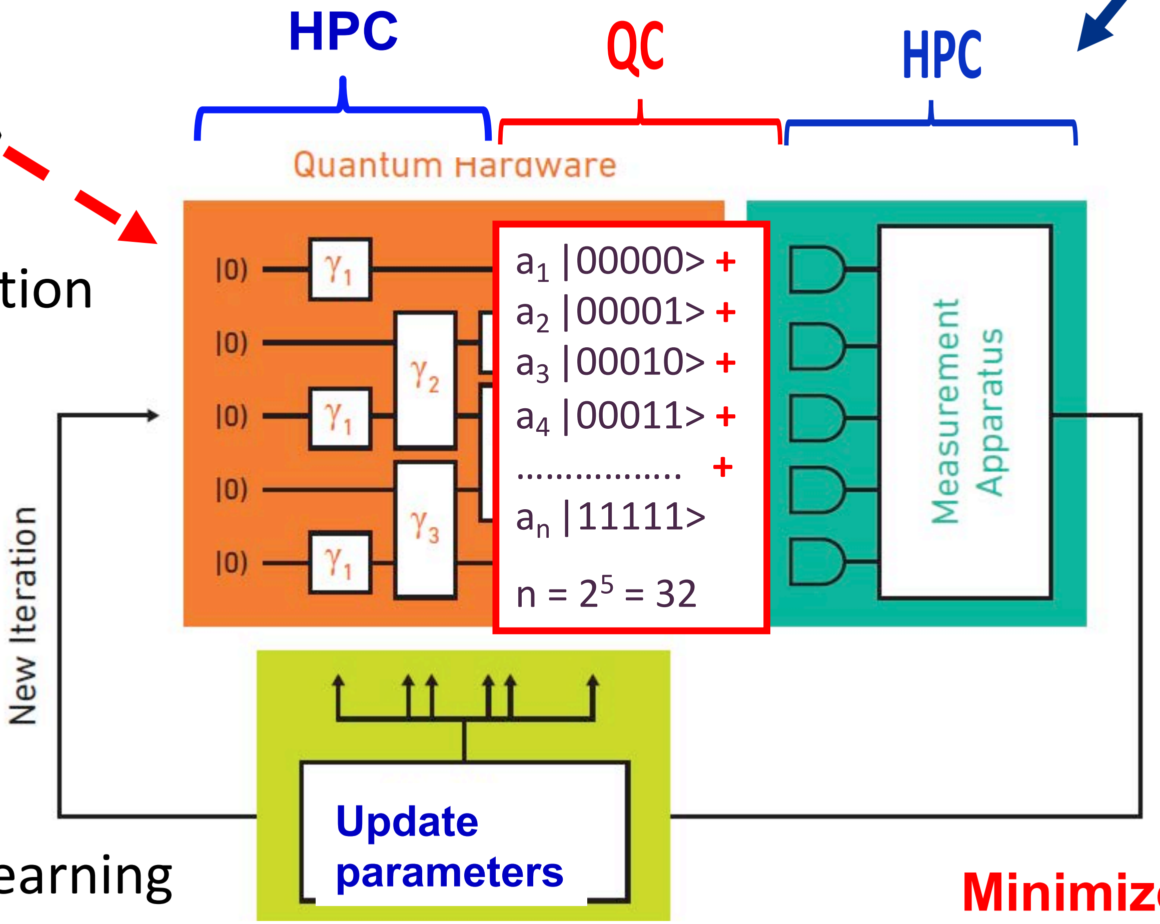
Quantum state tomography

Quantum circuit trial function (HPC-generated) → $|\psi(\theta)\rangle$

Optimisation

Quantum Approximate Optimization Algorithm (QAOA)

Quantum Variational Eigensolver (VQE)



$$\sigma_1 = \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\sigma_2 = \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$\sigma_3 = \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Evaluate cost function

Machine learning

Minimize $\sum_i \langle \psi|\hat{H}_i|\psi\rangle$

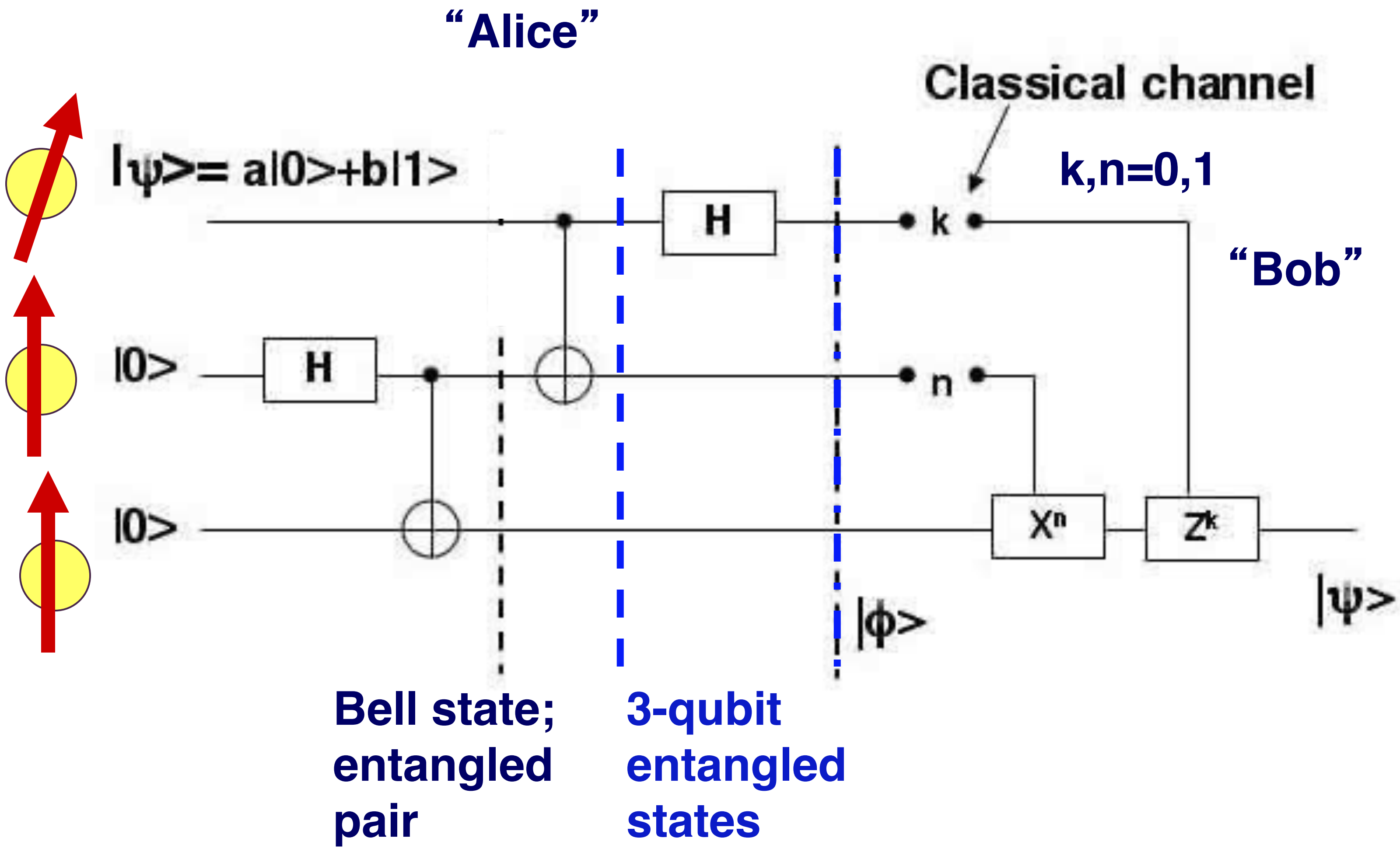
Cost function $\hat{H} = \sum_{i\alpha} h_{i\alpha}\, \sigma_{i\alpha} + \sum_{i\alpha, j\beta} h_{i\alpha,j\beta}\, \sigma_{i\alpha}\sigma_{j\beta} + \sum_{i\alpha,j\beta,k\gamma} h_{i\alpha,j\beta,k\gamma}\, \sigma_{i\alpha}\sigma_{j\beta}\sigma_{k\gamma} + \ldots\ldots$

Background for L2 and exercises: Teleportation

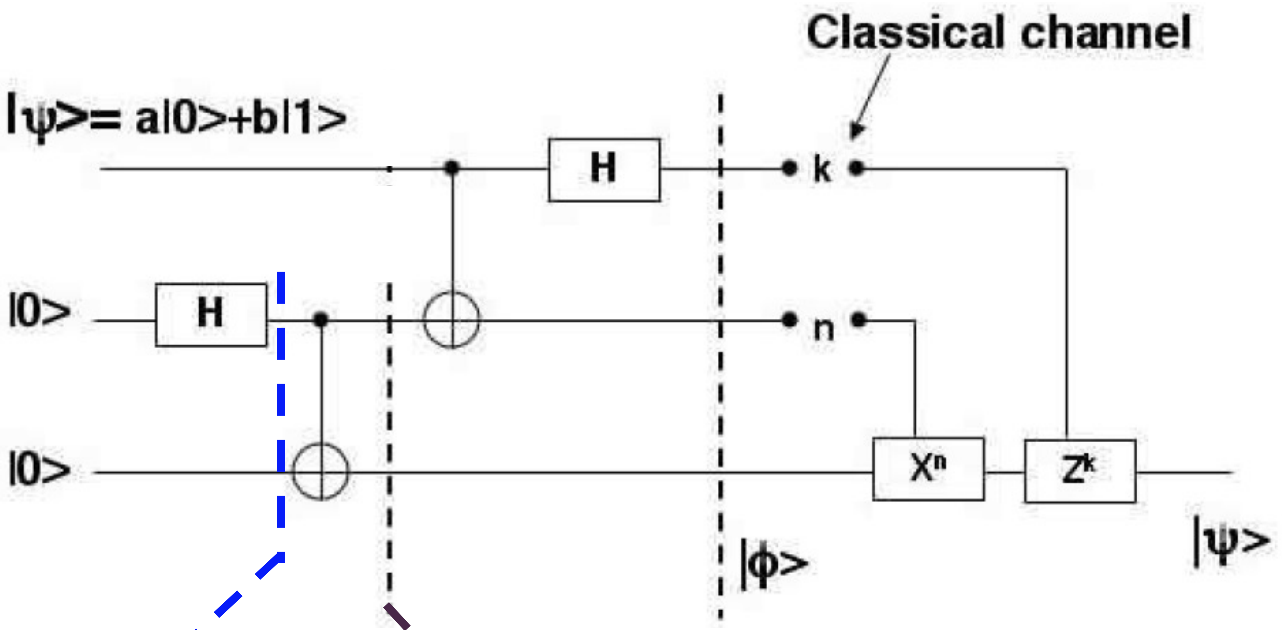
Exemplifies:

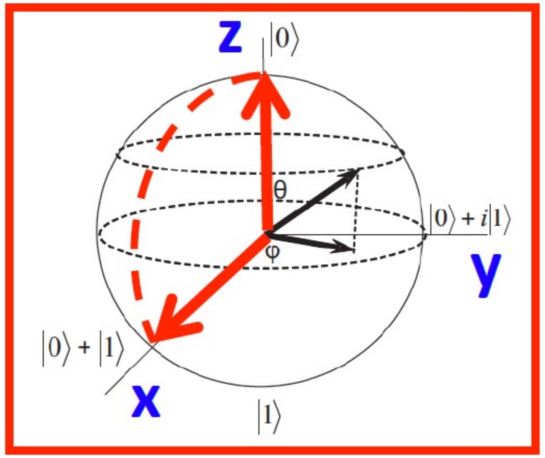
- Quantum circuits
- 1q Hadamard gate
- Superposition
- 2q CNOT (XOR)
- Entanglement
- Coding– decoding
- Intro to quantum error correction (QEC)

Teleportation



Teleportation - Bell state generation





(|0> + |1>) |0> = |00>+|10>

CNOT(|00>+|10>) = (|00>+|11>

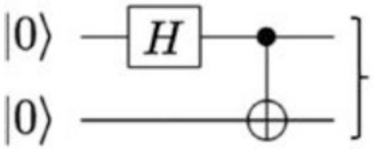
00 -> 00
01 -> 01
10 -> 11
11--> 10

Hadamard

$$H = \frac{1}{\sqrt{2}}\begin{bmatrix}1 & 1\\ 1 & -1\end{bmatrix}$$

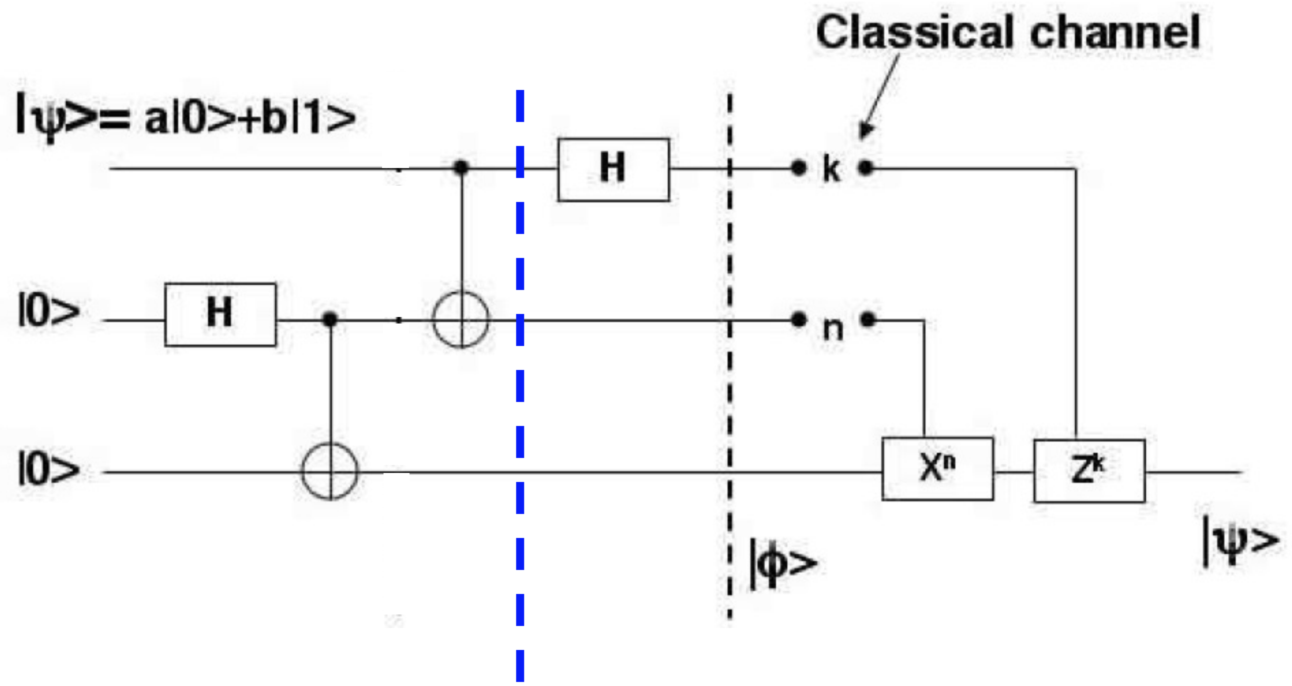
√NOT

$$\text{CNOT} = \text{CX} = \text{Ctrl}\ R_y(\pi) = \begin{pmatrix}1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & 0 & 1\\ 0 & 0 & 1 & 0\end{pmatrix}$$



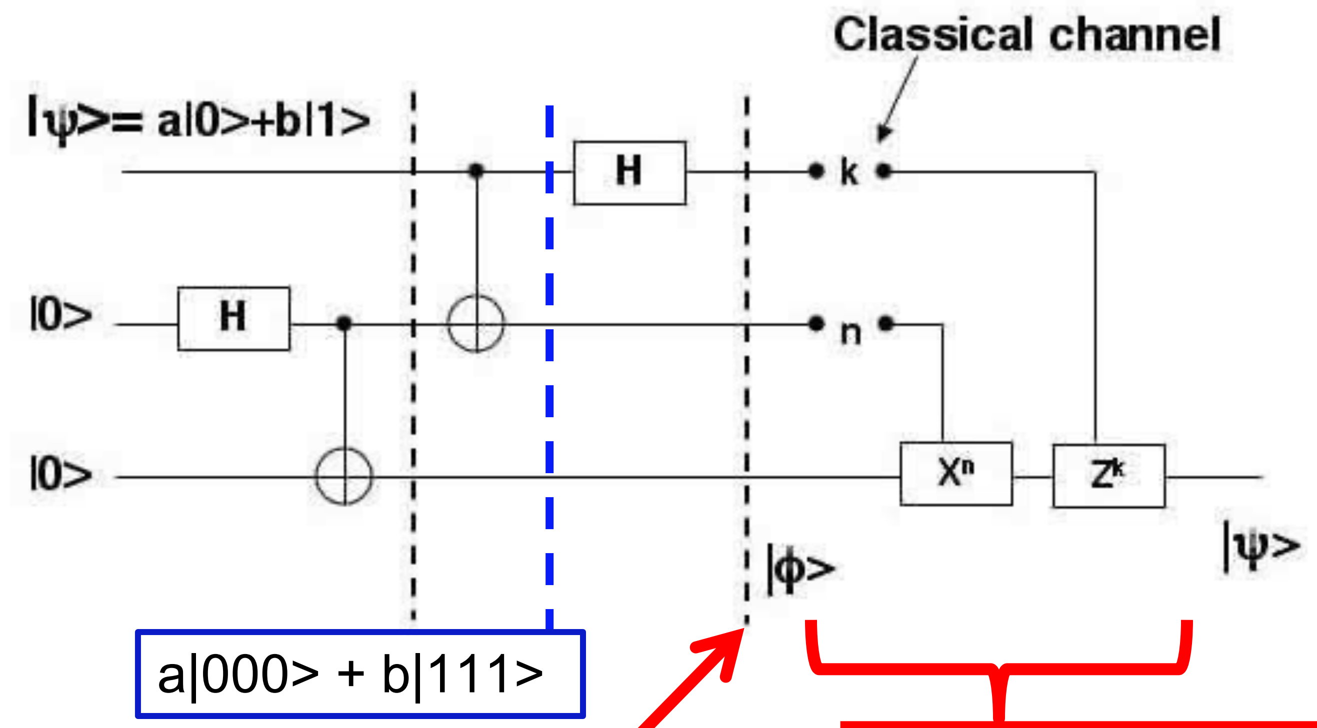
$\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$

Teleportation – entangling input state with Bell state



a|000> + b|111>

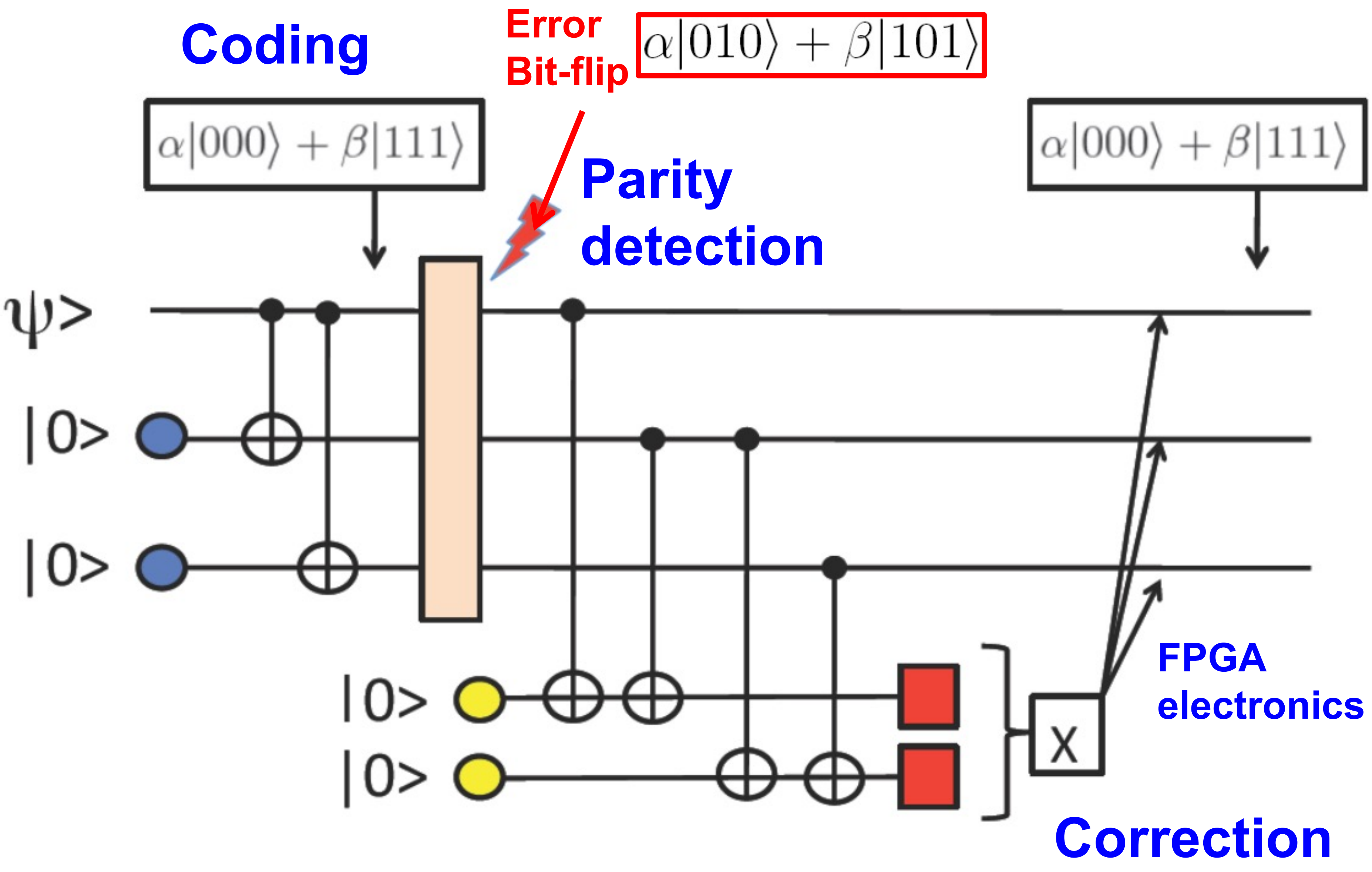
Teleportation – decoding entangled state + meas't + restoring (Bob)



$$|00\rangle(a|0\rangle + b|1\rangle)$$
$$+ |01\rangle(b|0\rangle + a|1\rangle)$$
$$+ |10\rangle(a|0\rangle - b|1\rangle)$$
$$+ |11\rangle(-b|0\rangle + a|1\rangle)$$

$$I(a|0\rangle + b|1\rangle) = |\psi\rangle$$
$$\sigma_x(b|0\rangle + a|1\rangle) = |\psi\rangle$$
$$\sigma_z(a|0\rangle - b|1\rangle) = |\psi\rangle$$
$$\sigma_z\sigma_x(-b|0\rangle + a|1\rangle) = |\psi\rangle$$

Quantum Error Correction - QEC



Quantum Error Correction - QEC