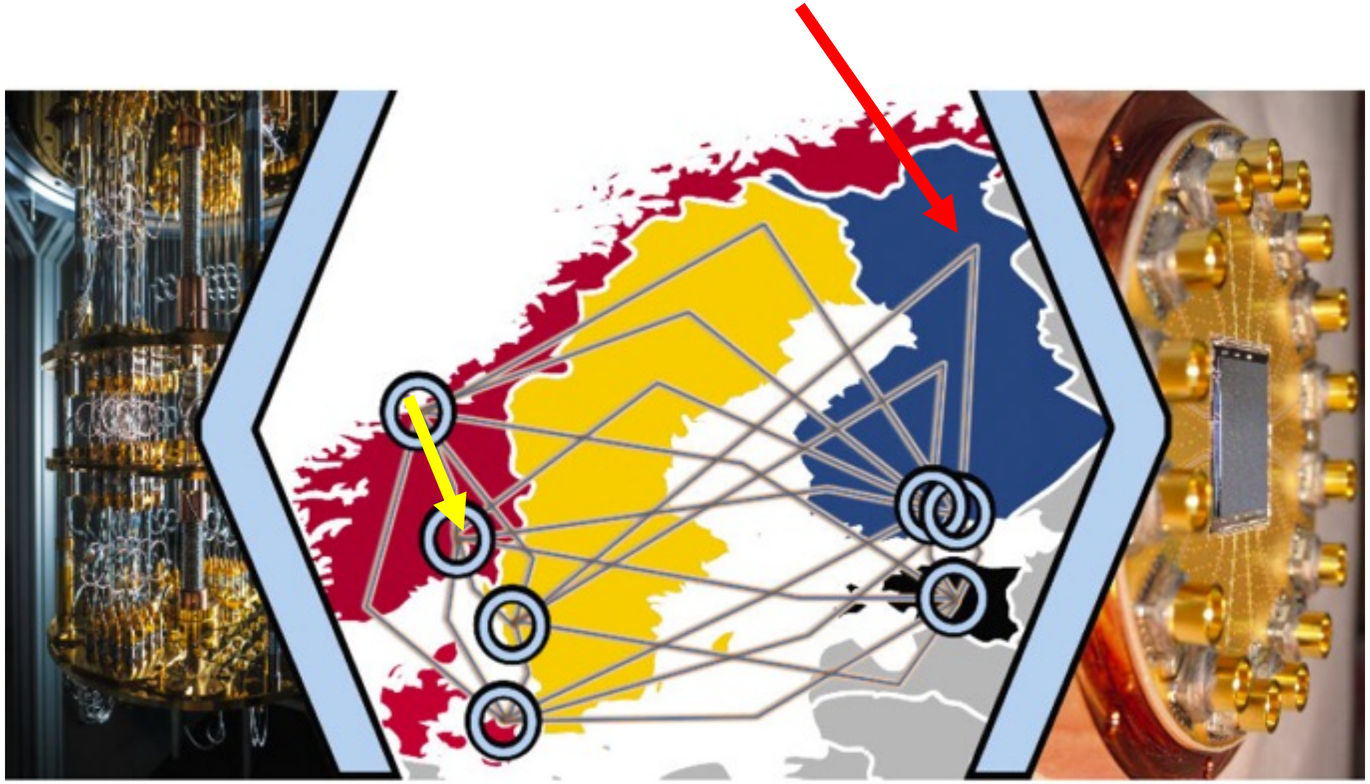
NordiQuEst HPC-QC ecosystem

2022-2025

LUMI pre-exascale HPC in Kajaani



EuroHPC JU

LUMI-Q ….. ?

(CSC, VTT, Chalmers, NeIC, IQM …)

Horizon Europe

OpenSuperQ Plus !

(FPA Roadmap 2022-2029:
Chalmers, VTT, CSC, IQM, ….)

SGA1 2023-2025 !

SGA2 2026-2029 ….

NordIQuEst

Nordic-Estonian Quantum Computing e-Infrastructure Quest

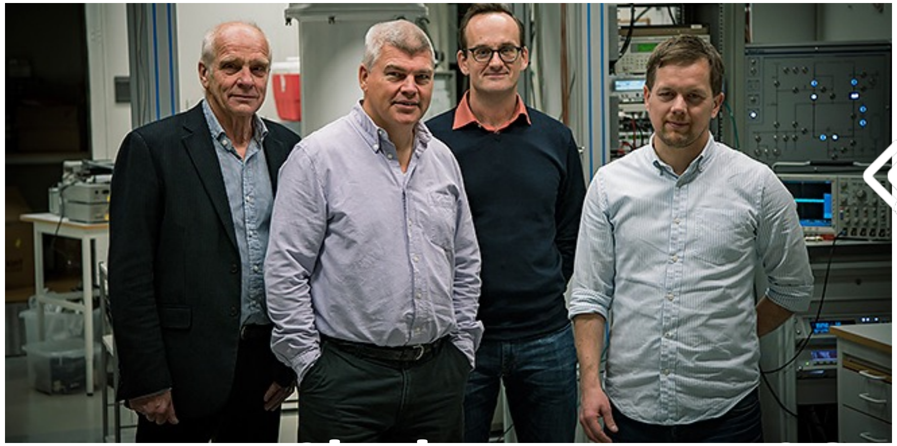
Institution	Country	Contact person	Position
CHALMERS	Sweden	Miroslav Dobsicek	Research Scientist
CSC	Finland	Mikael Johansson	Technology Strategist
DTU	Denmark	Sven Karlsson	Assoc. prof.
SINTEF	Norway	Franz Fuchs	Research Scientist
SRL	Norway	Shaukat Ali	Professor
UTartu	Estonia	Dirk Oliver Theis	Assoc.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

Sweden’s quantum technology programme

Wallenberg Centre for Quantum Technologies

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

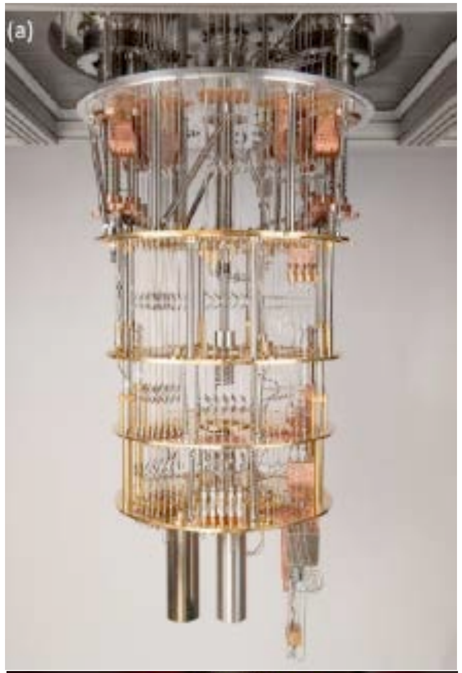
12 years, 150 M€

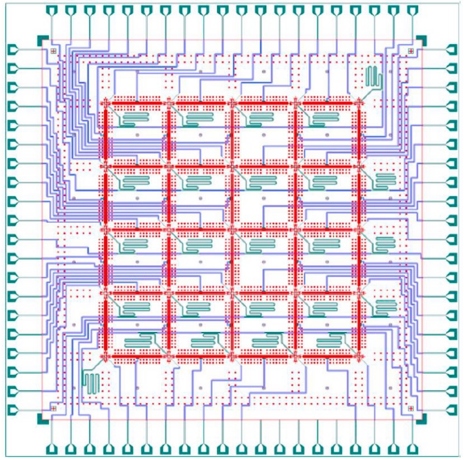


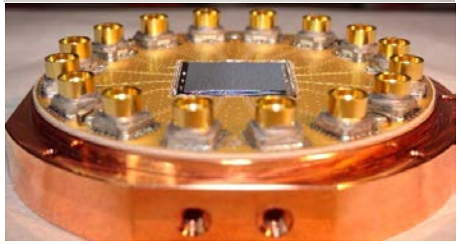
Mission: to build a quantum processor with 100+ superconducting qubits by 2025

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

Cryostat
≈ 10 mK

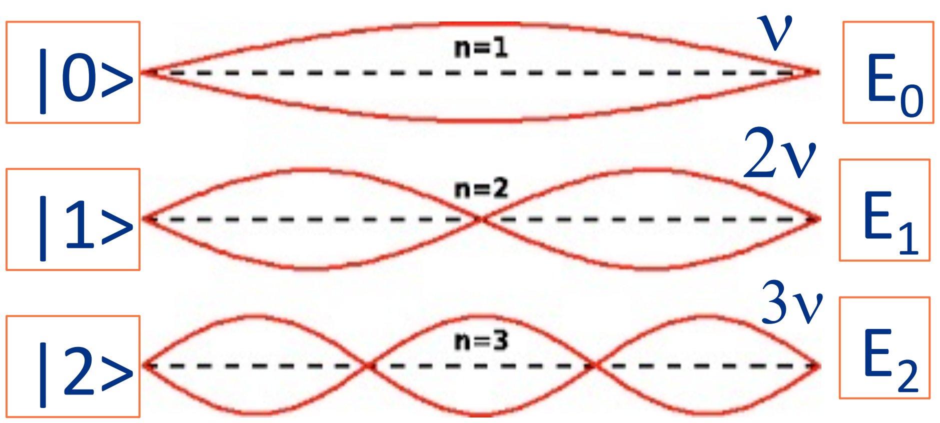




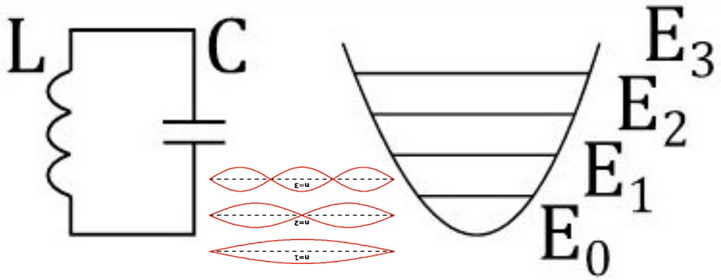


25q Transmon chip under testing

QC/QPU: Superconducting Transmon qubit

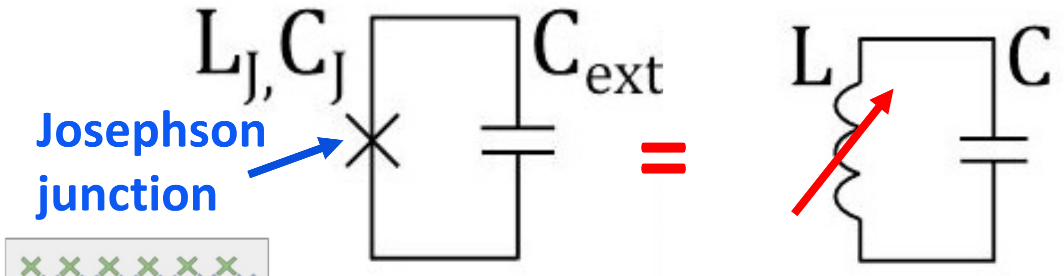


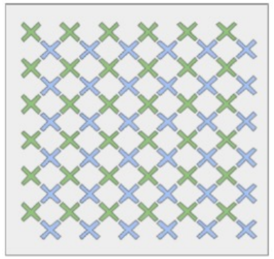
$$E = (n+1/2)\ \hbar\omega$$



Harmonic oscillator

$$|\psi> = a|0> + b|1> + c\ |2> + ...$$

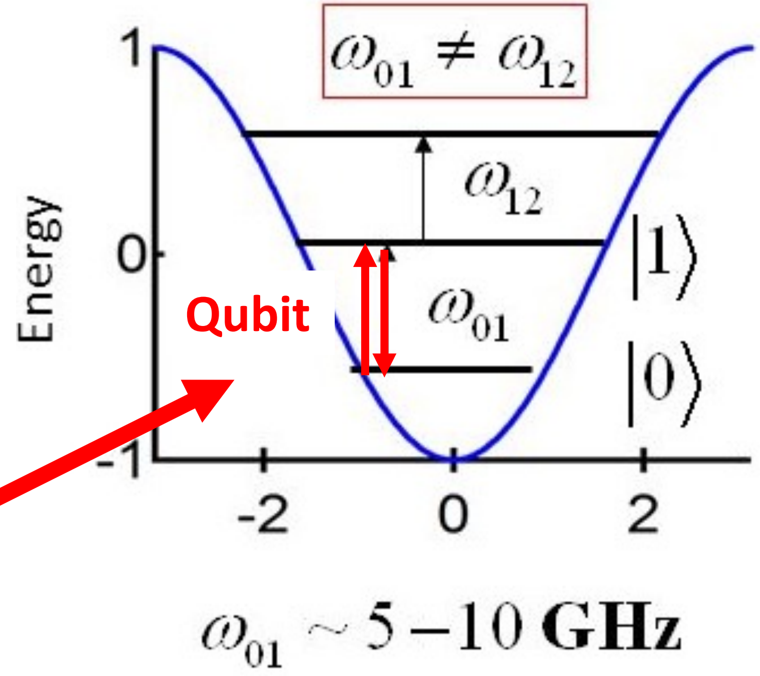




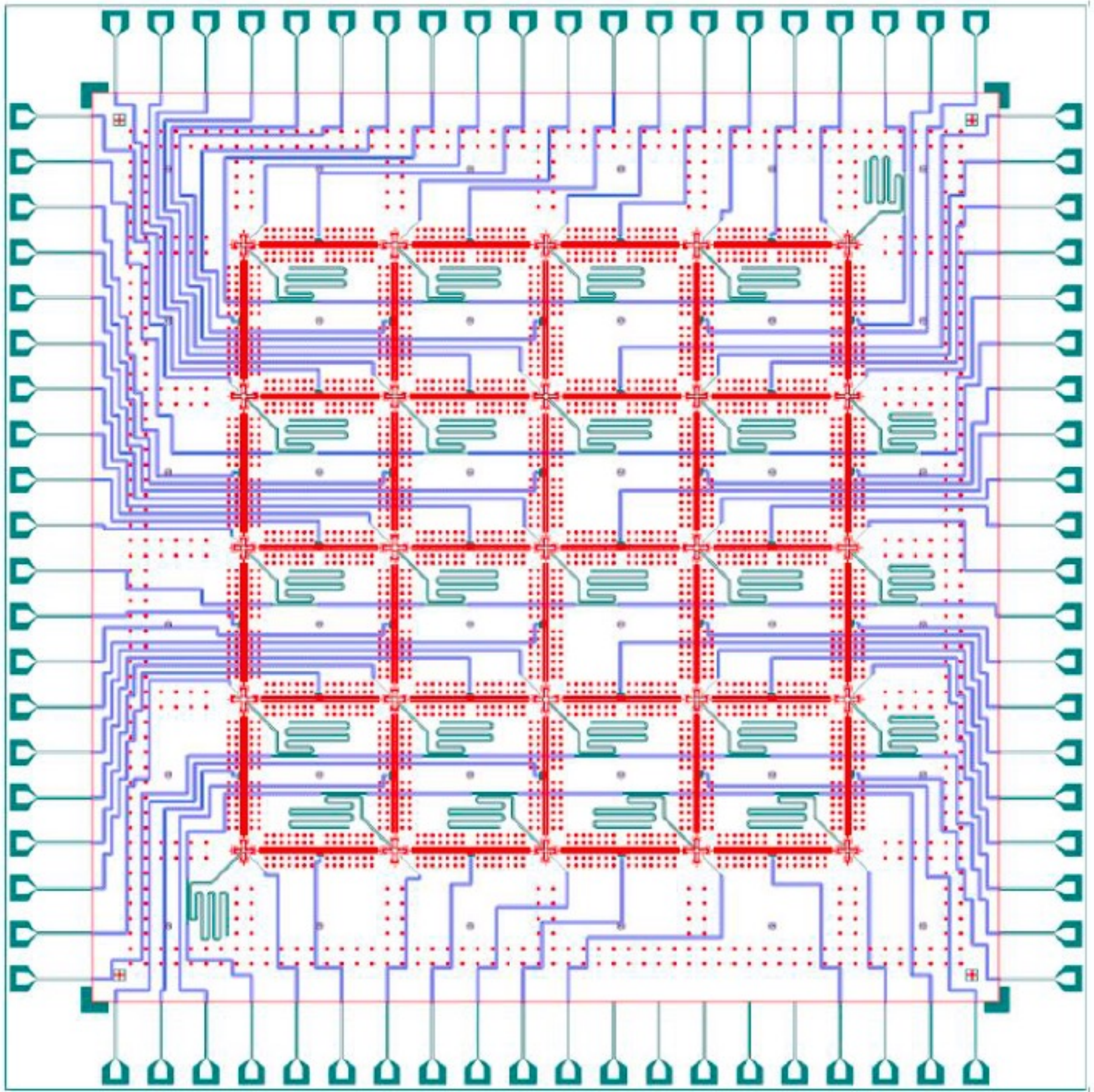
Qubit

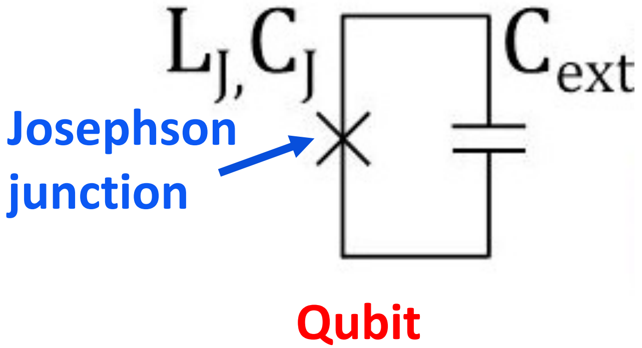
Non-linear quantum resonator

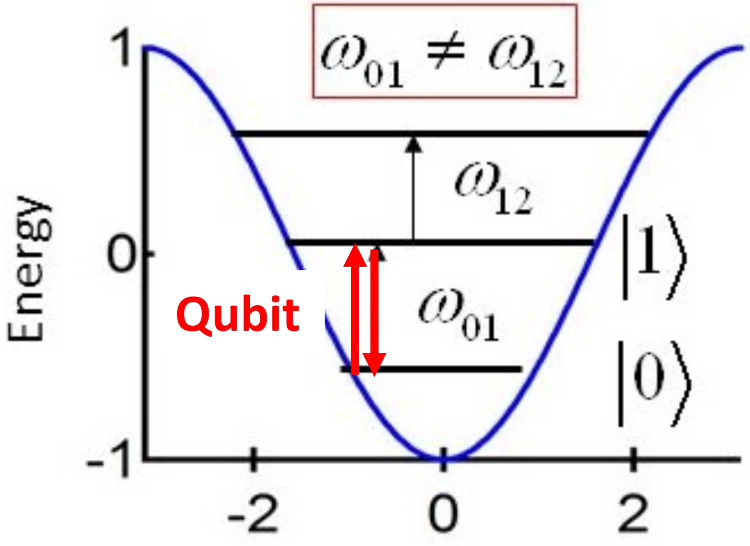
Anharmonic oscillator



QC/QPU: Superconducting Transmon qubit







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

Why do we need quantum computers ?

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

The original "killer application": Shor's algorithm for factorisation (1995)

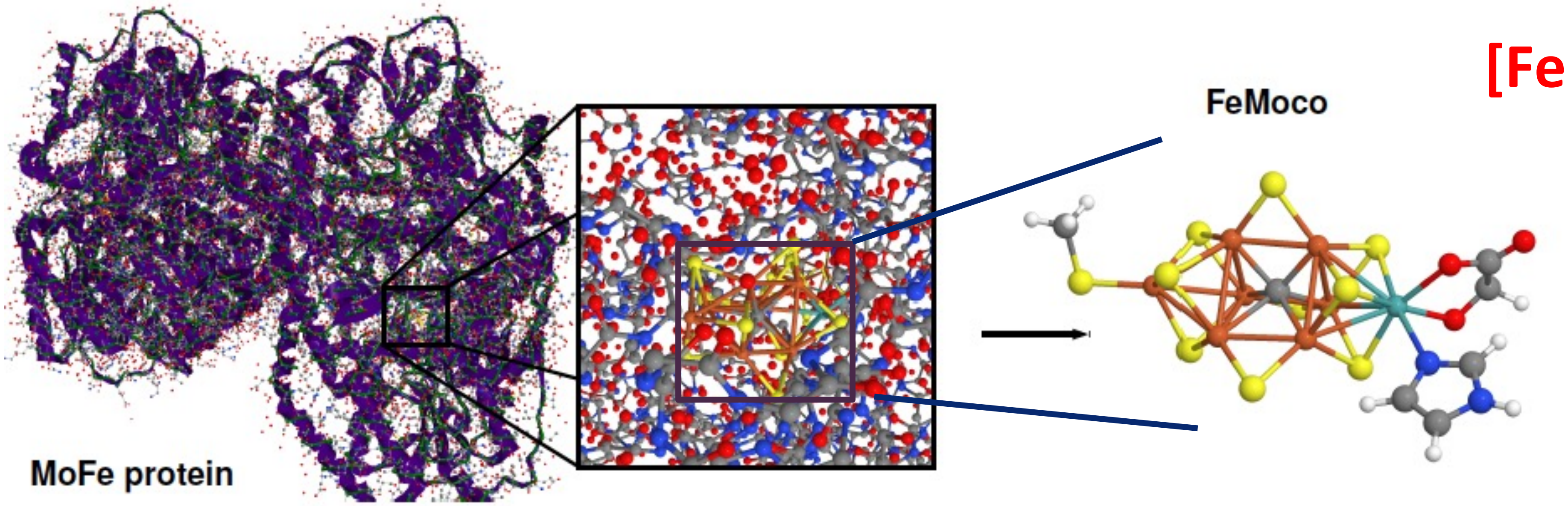
Today, the typical killer applications are "use cases":

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

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

The killer application

Nitrogenase protein: iron molybdenum cofactor FeMoco



[FeS]$_n$

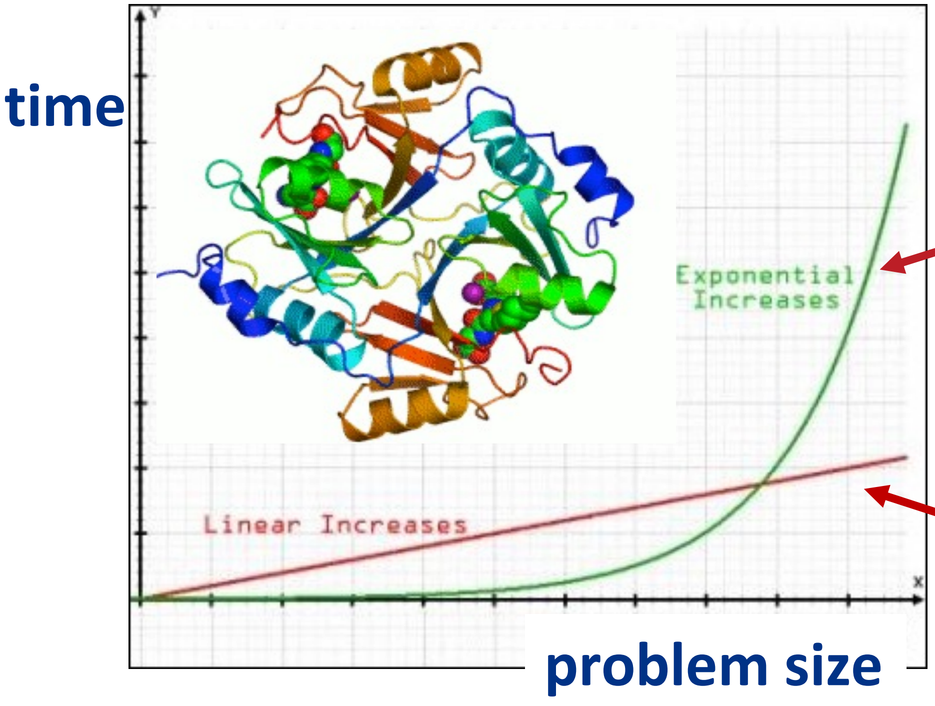
Elucidating reaction mechanisms on quantum computers

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

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

Quantum Advantage

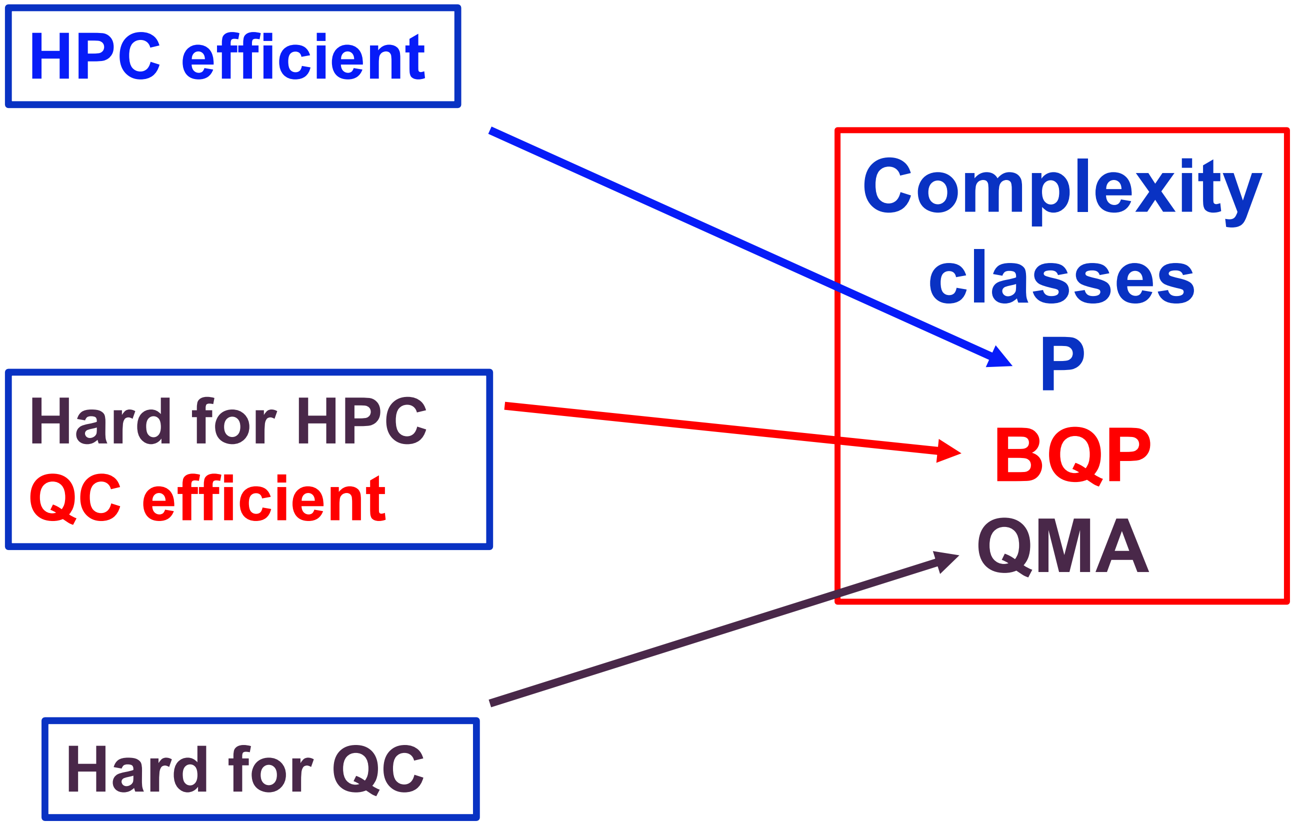
Quantum computers offer, in principle,
exponential speed-up for certain classes of hard problems



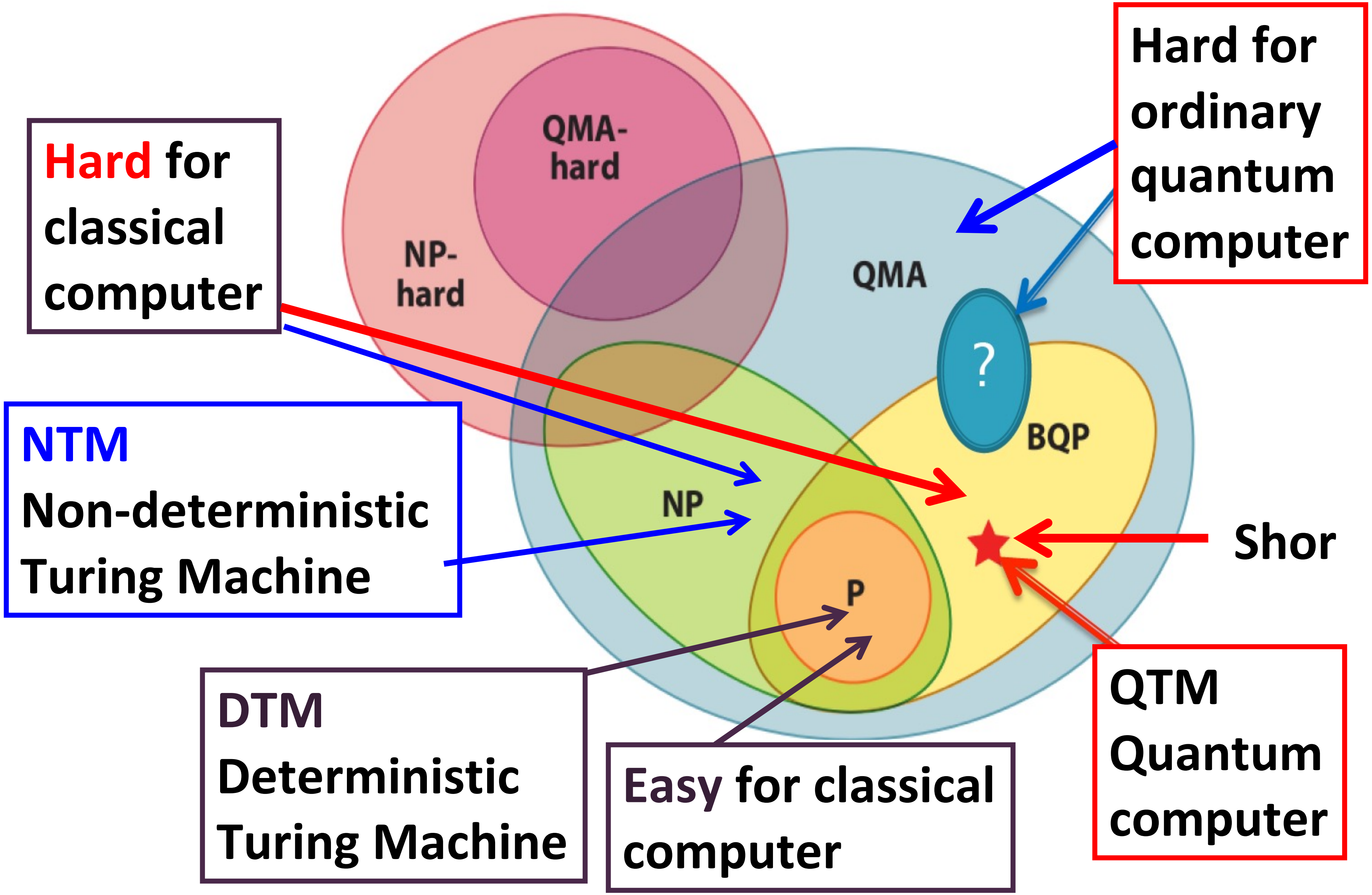
TTS for a HPC:
Grows exponentially

TTS for a quantum computer:
Grows linearly/polynomially

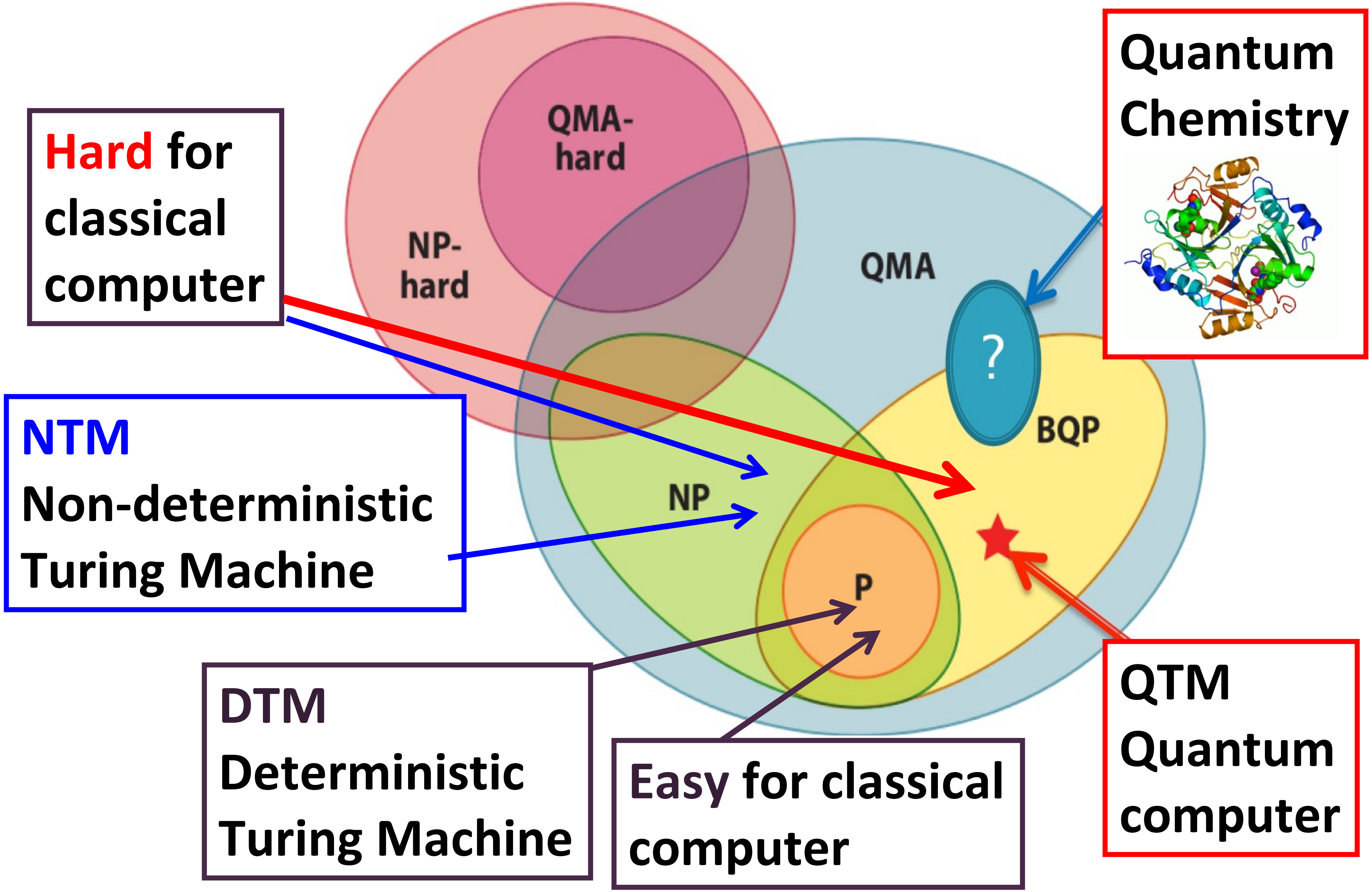
No Quantum Advantage


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

Complexity classes



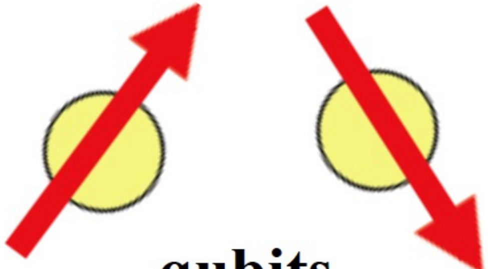
Complexity classes – Quantum Chemistry



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

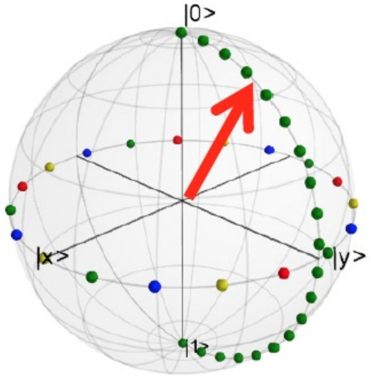
-Quantum physics

- -Coherence
- -Superposition
- -Parallelism
- -Entanglement

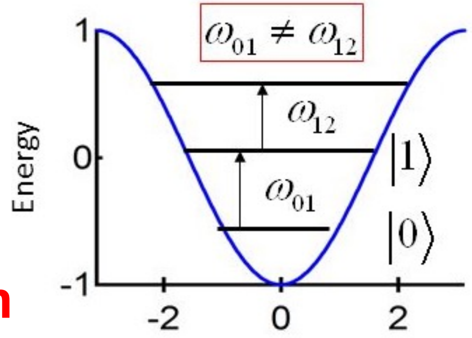


qubits

Bloch sphere



qubit = 2-level system



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

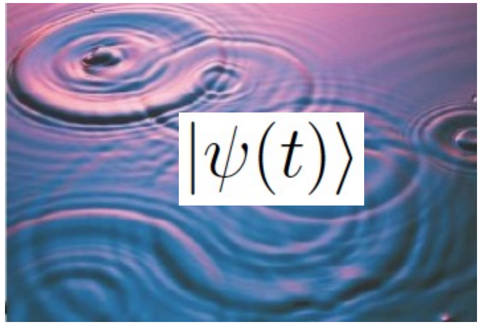
|0> , |1>

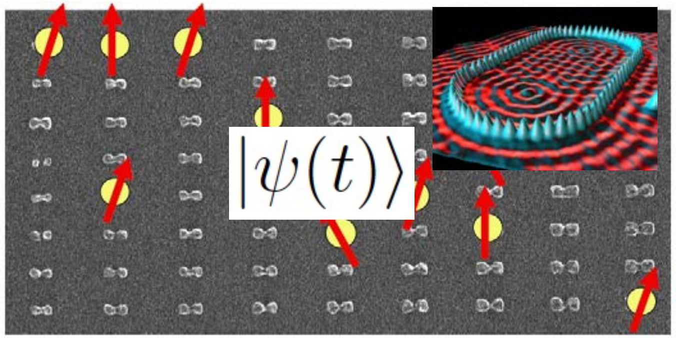
a|0> + b|1>

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>

$|\psi(t)\rangle$

$n=2^N$

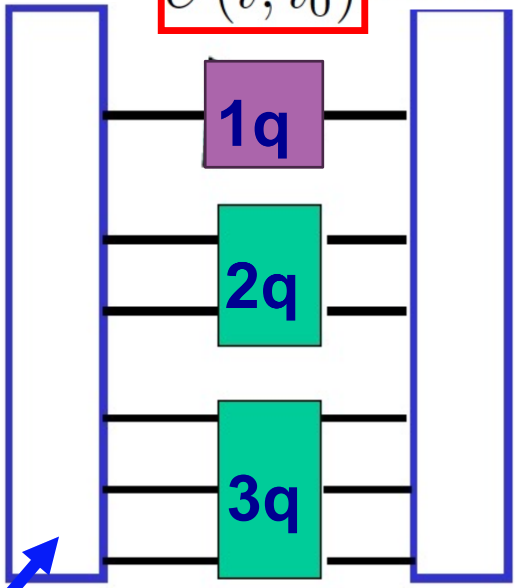
Quantum gates and states: superposition and entanglement

N qubits, n = 2^N states

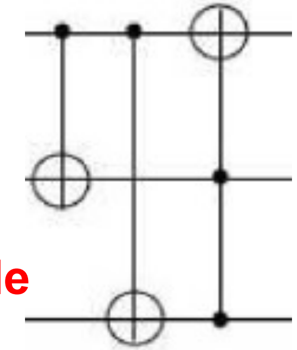
$|00..000\rangle$ +
$|00..001\rangle$ +
$|00..010\rangle$ +
$|00..011\rangle$ +
.... +
$|11..110\rangle$ +
$|11..111\rangle$ =
$|0\rangle 0\rangle..|0\rangle|0\rangle|0\rangle$

Product state
Not entangled

$|\psi(t_0)\rangle$ > $\hat{U}(t, t_0)$ $|\psi(t)\rangle$



Qubit (memory) register



Reversible gates

U

Rotation

NOT, Hadamard

CNOT
CPHASE

C-Rotation

c-c-NOT
c-swop

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

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

Superposition of 2^N state configurations - entanglement

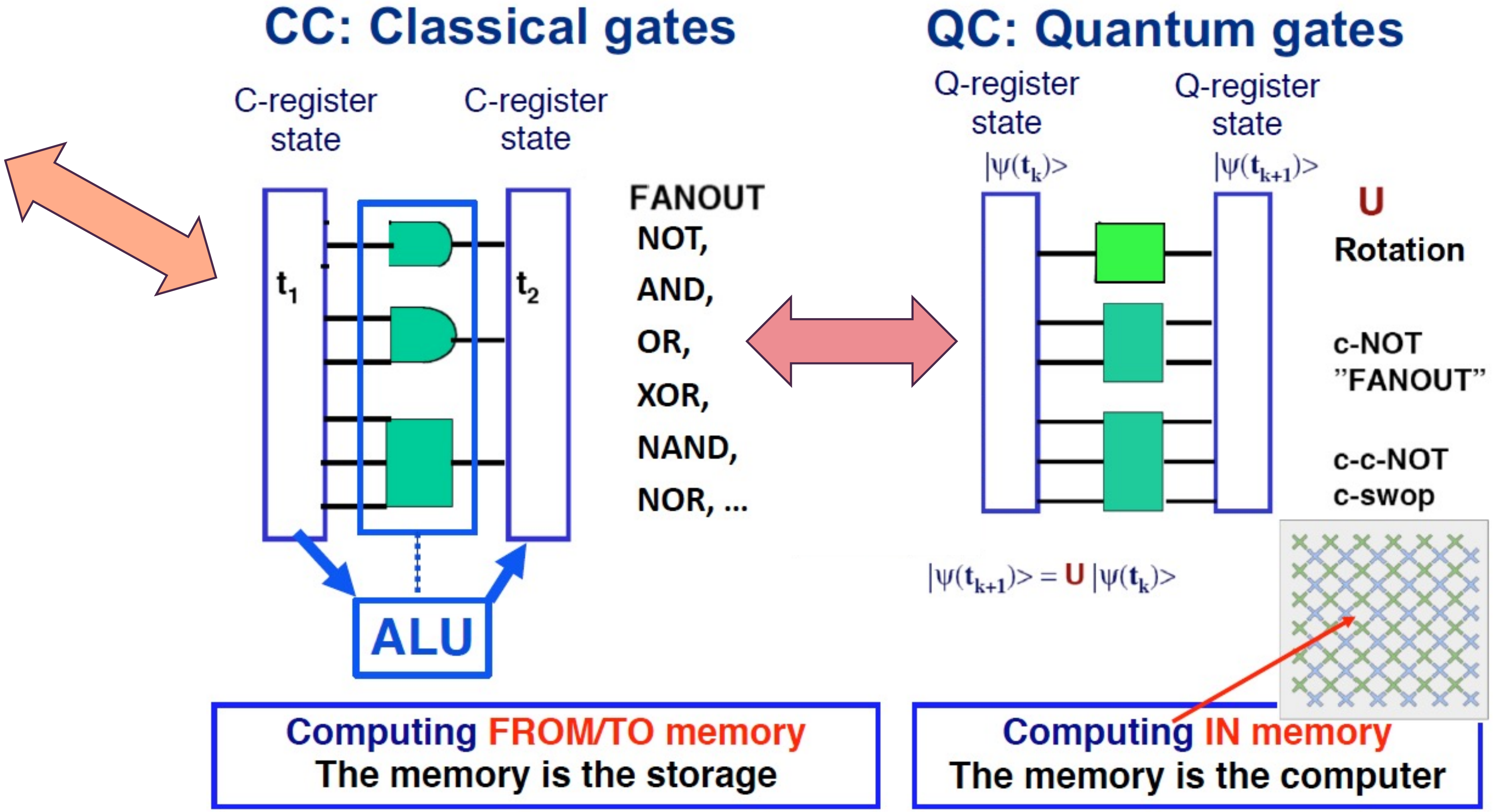
$$|\psi(t)\rangle = U(t, t_0)|\psi(t_0)\rangle$$

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

Generic quantum gate

Series expansion →
Quantum gate circuit

HPC-Q = Classical computer + q-accelerator



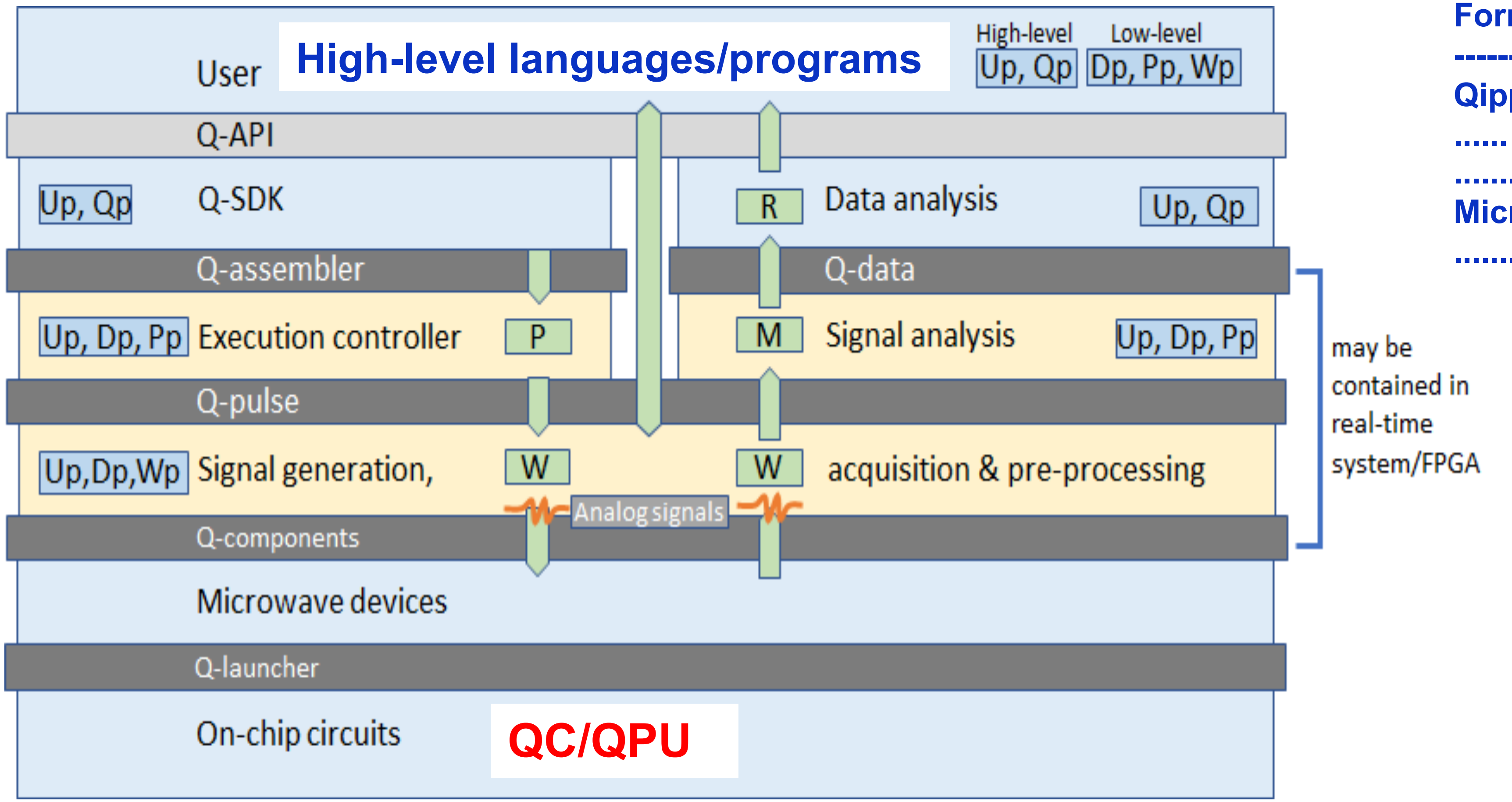
HPC-Q hybrid computer

HPC (mainframe/control) + QC (accelerator/subroutines)

Qiskit (IBM)
Cirq (Google)
Forrest (Rigetti)

Qipper
......
....
Microsoft
....

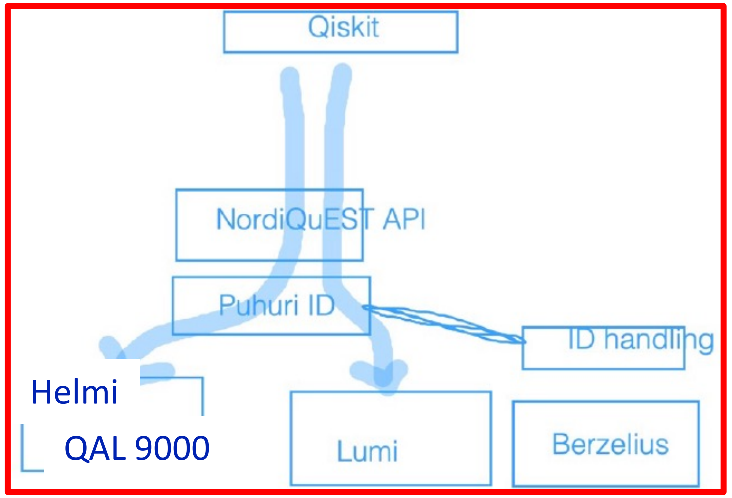
HPC
& cl.
control

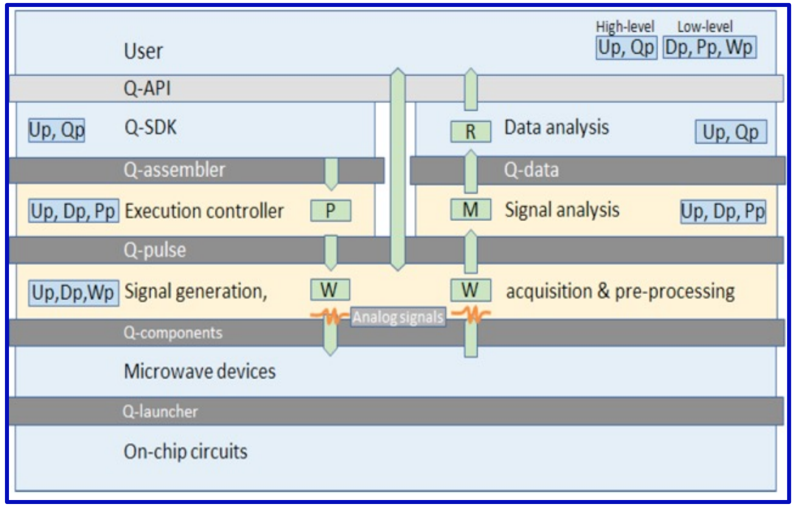


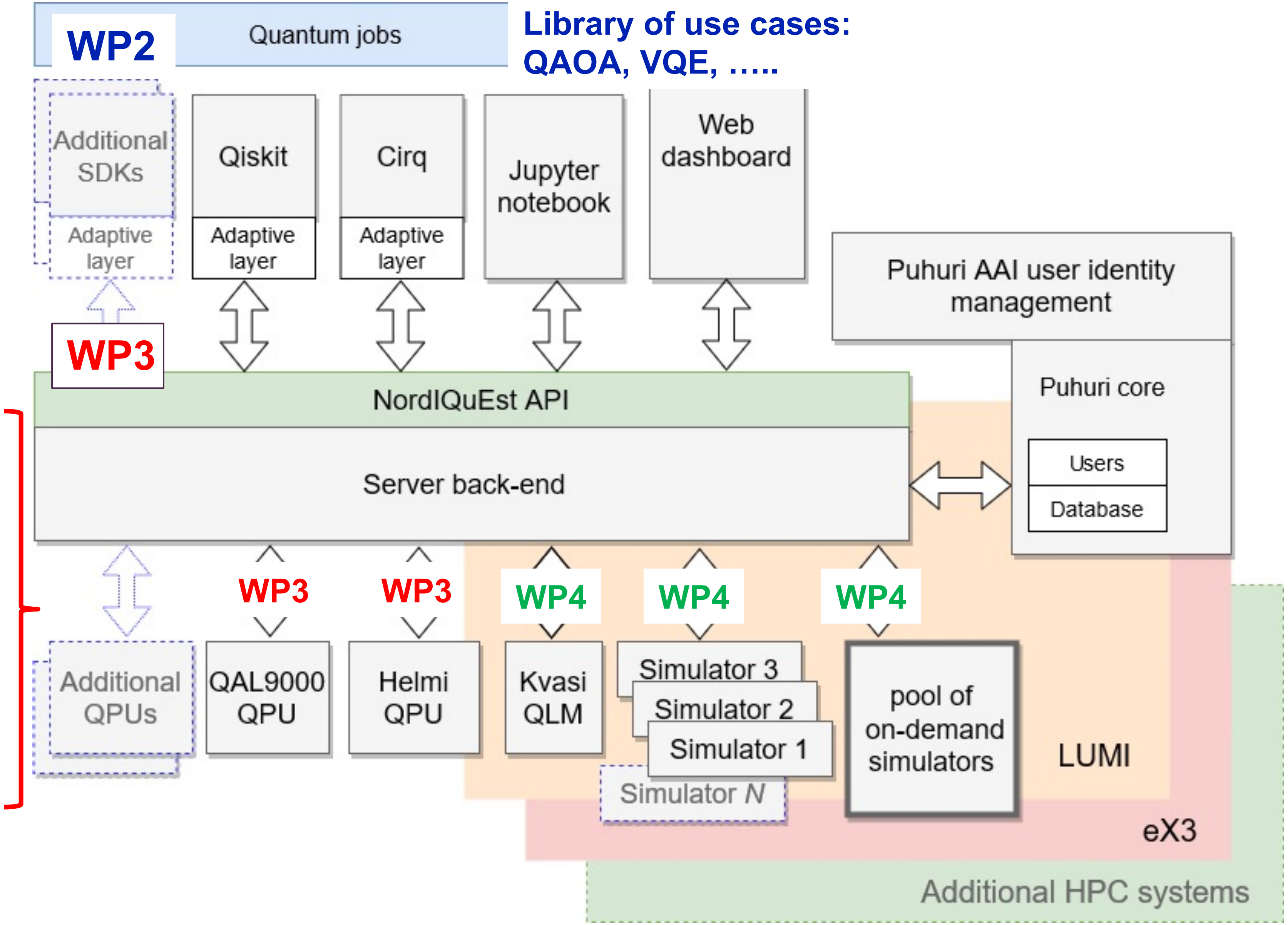
IBM
Google
Rigetti
Alibaba
Baidu
ETH

Innsbruck
IonQ
Sandia
Honeywell

NordiQuEst in a nutshell







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

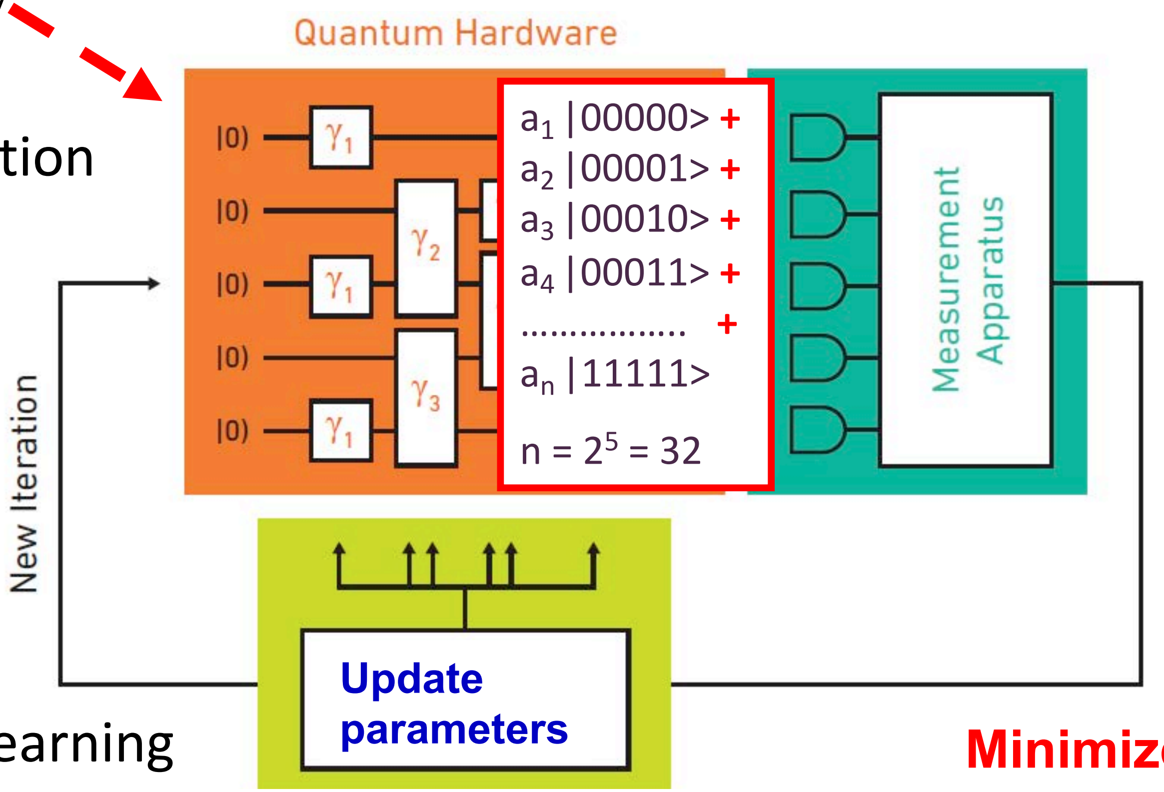
QC **HPC**

Quantum circuit trial function $|\psi(\theta)\rangle$

Optimisation

Quantum Approximate Optimization Algorithm (QAOA)

Quantum Variational Eigensolver (VQE)



Machine learning

Evaluate cost function

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

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

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

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

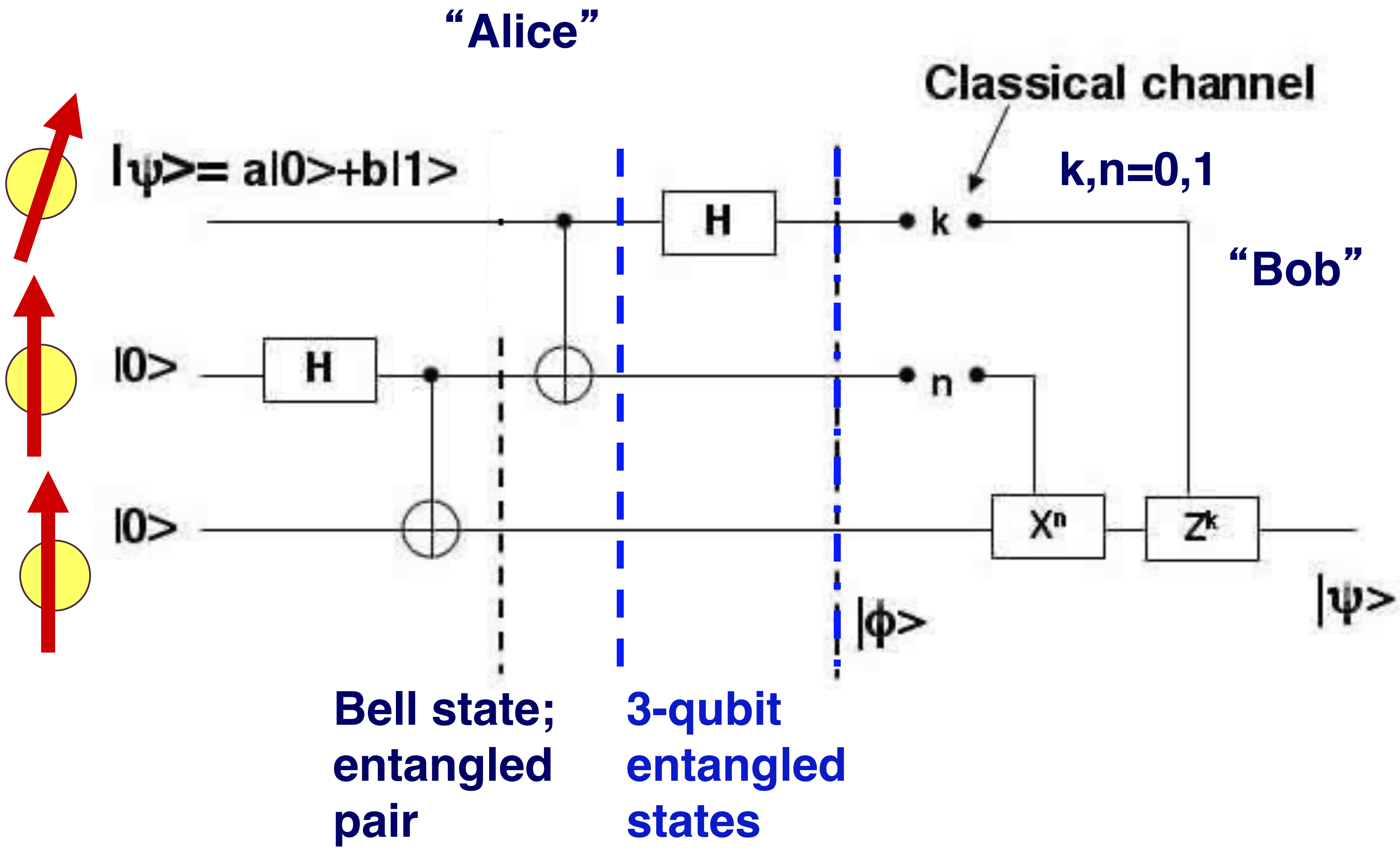
Cost function $\hat{H} = \sum_{i\alpha} h_{i\alpha}\,\sigma_{i\alpha} + \sum_{i\alpha,j\beta} h_{i\alpha,j\beta}\,\sigma_{i\alpha}\sigma_{j\beta} + \sum_{i\alpha,j\beta,k\gamma} h_{i\alpha,j\beta,k\gamma}\,\sigma_{i\alpha}\sigma_{j\beta}\sigma_{k\gamma} + \ldots\ldots$

Background for hands-on exercises: Teleportation

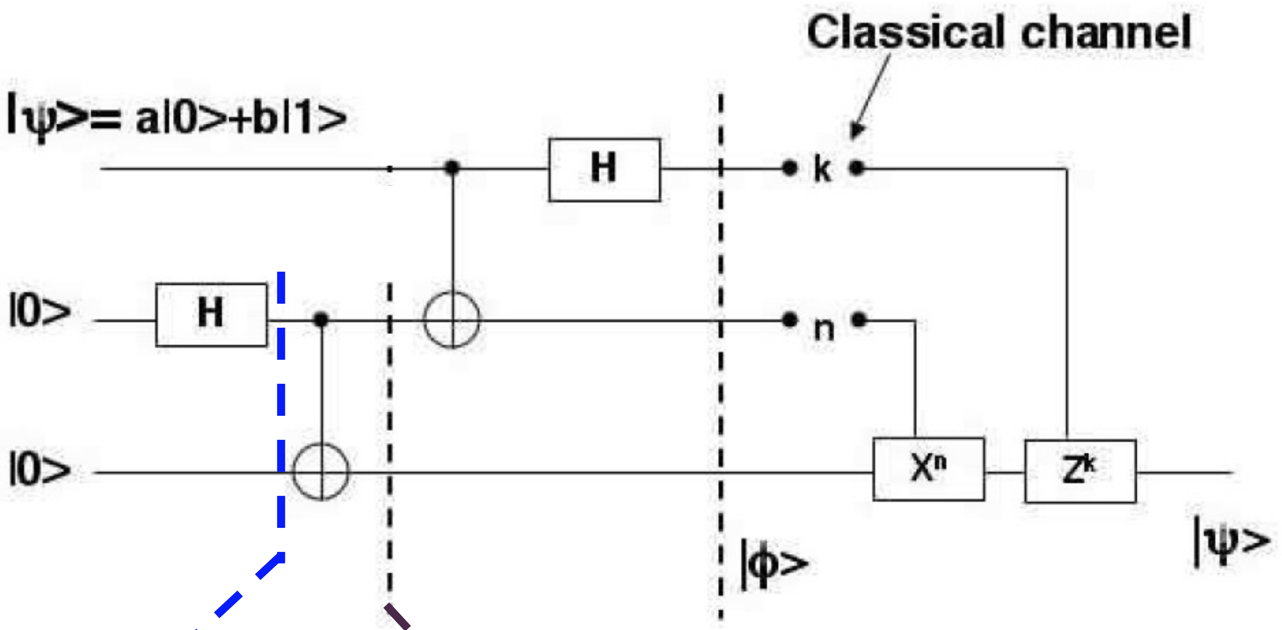
Exemplifies:

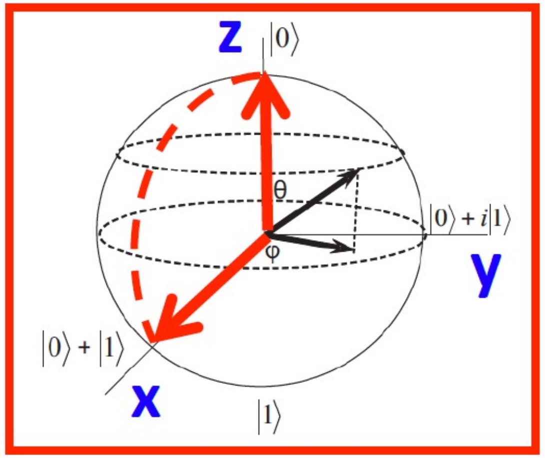
- Quantum circuits
- 1q Hadamard gate
- Superposition
- 2q CNOT (XOR)
- Entanglement
- Coding– decoding
- Intro to quantum error correction (QEC)

Teleportation



Teleportation - Bell state generation





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

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

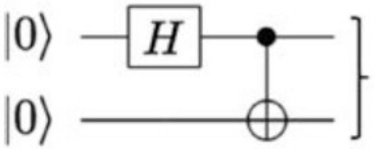
00 -> 00
01 -> 01
10 -> 11
11--> 10

Hadamard

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

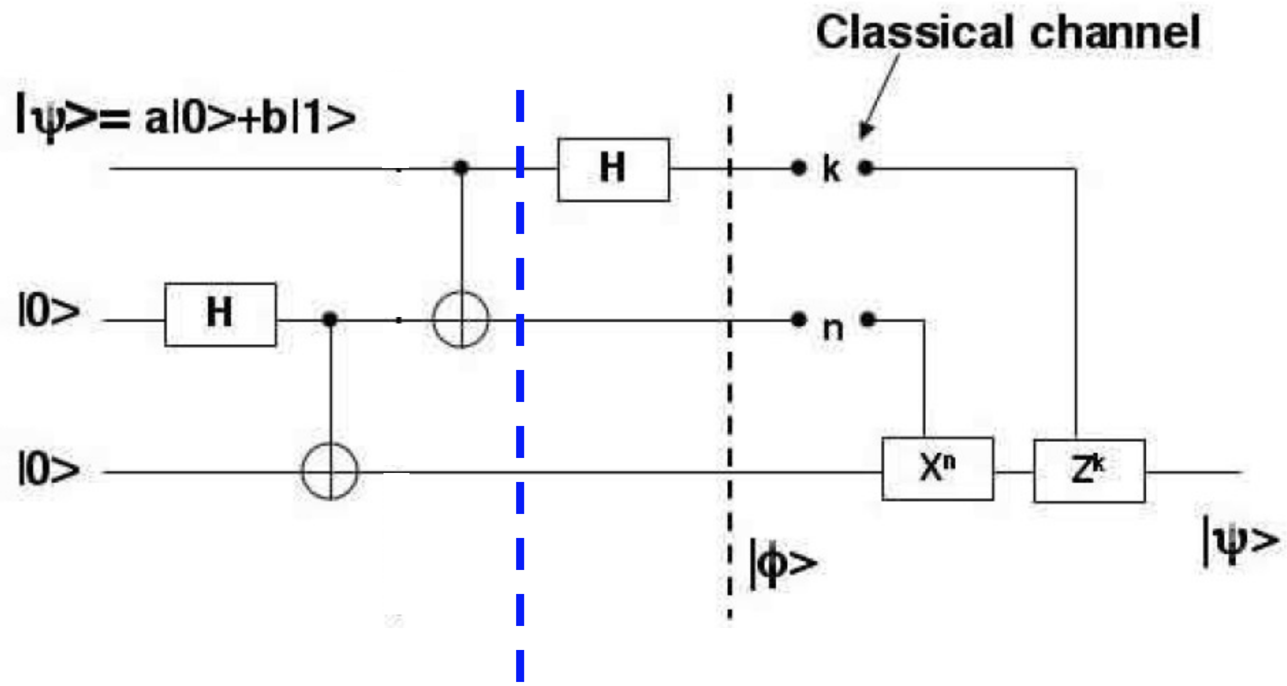
√NOT

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



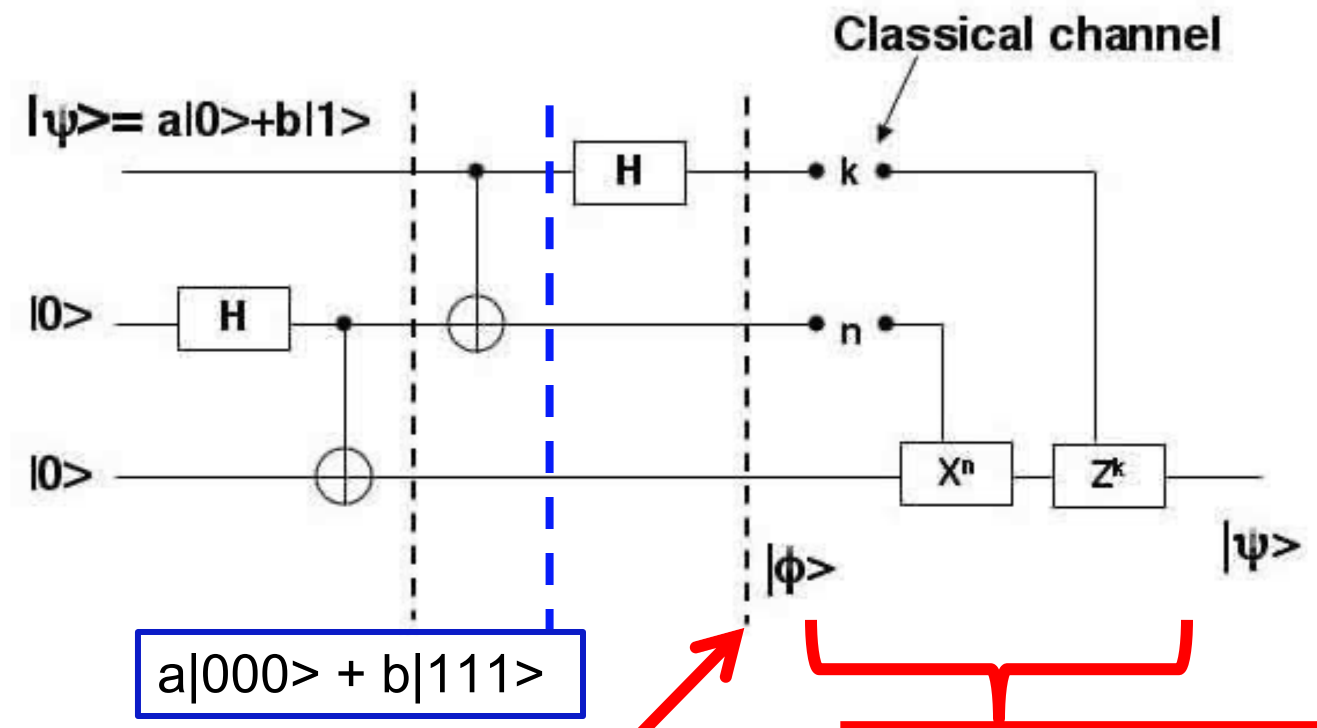
$$\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$

Teleportation – entangling input state with Bell state



a|000> + b|111>

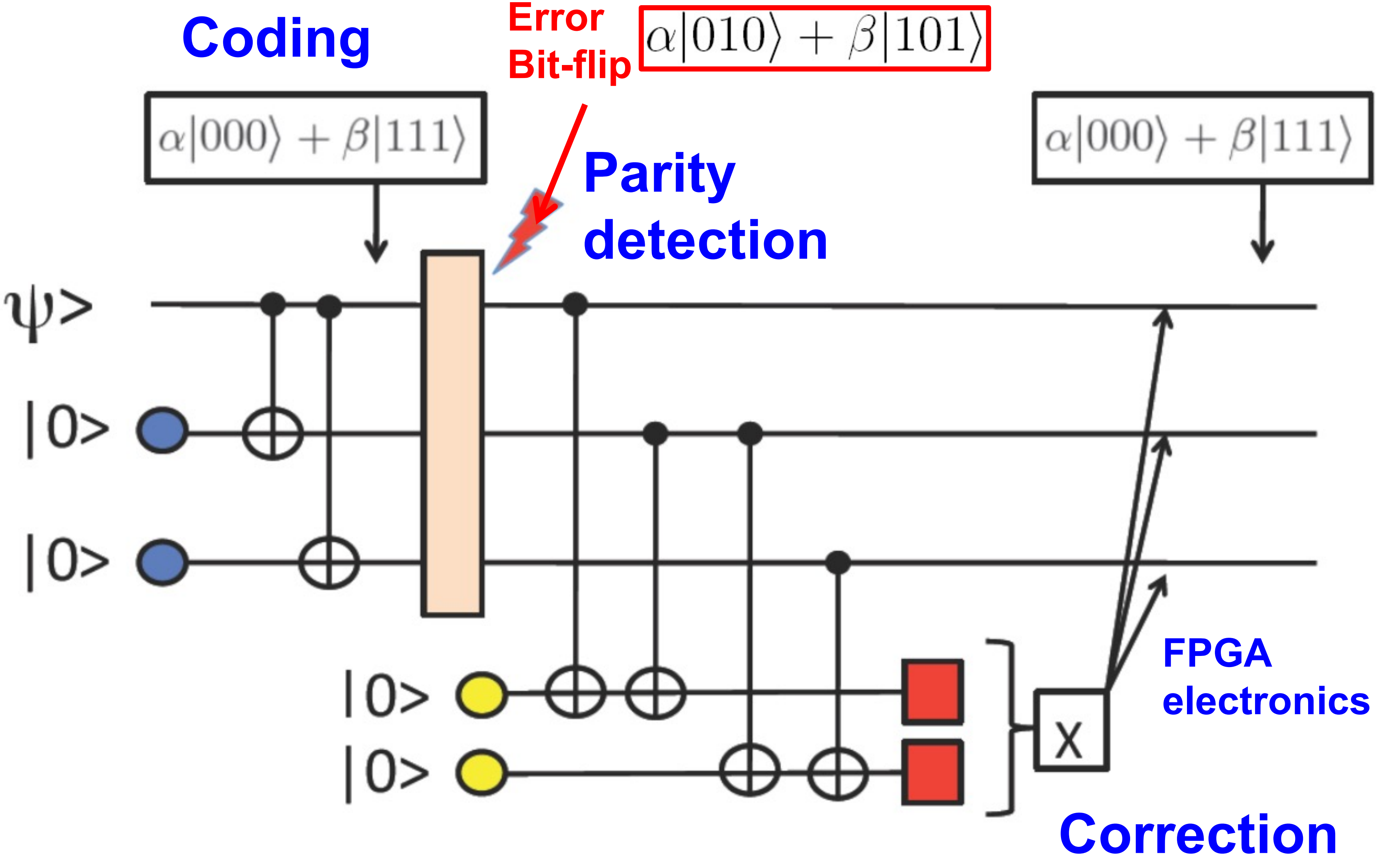
Teleportation – decoding entangled state + meas't + restoring (Bob)



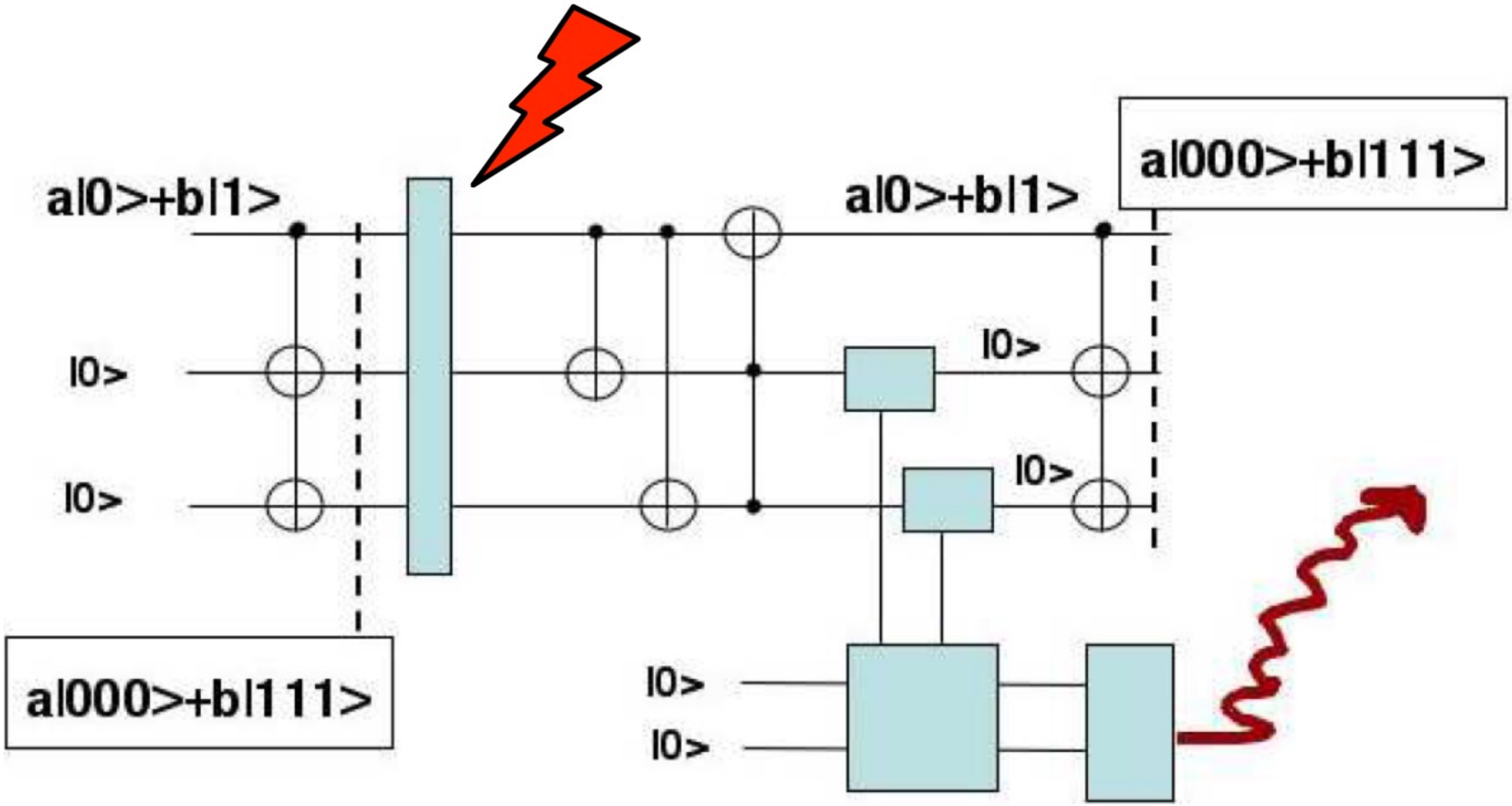
$$
\begin{aligned}
&|00\rangle(a|0\rangle + b|1\rangle)\\
&+ |01\rangle(b|0\rangle + a|1\rangle)\\
&+ |10\rangle(a|0\rangle - b|1\rangle)\\
&+ |11\rangle(-b|0\rangle + a|1\rangle)
\end{aligned}
$$

$$
\begin{aligned}
I(a|0\rangle + b|1\rangle) &= |\psi\rangle\\
\sigma_x(b|0\rangle + a|1\rangle) &= |\psi\rangle\\
\sigma_z(a|0\rangle - b|1\rangle) &= |\psi\rangle\\
\sigma_z\sigma_x(-b|0\rangle + a|1\rangle) &= |\psi\rangle
\end{aligned}
$$

Quantum Error Correction - QEC



Quantum Error Correction - QEC



That’s All Folks!