

Introduction to quantum computing

Quantum Computing Minicourse ICTP-SAIFR

Stefano Carrazza[‡] and Matteo Robbiati[†]

8 April 2024

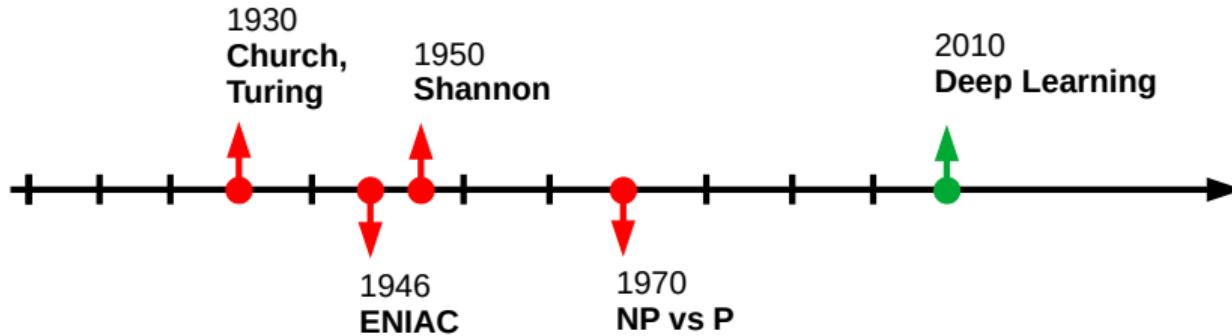
[‡] Associate Professor & Researcher, University of Milan and INFN Milan, Italy.

[†] PhD candidate, University of Milan, Italy and CERN, Switzerland.

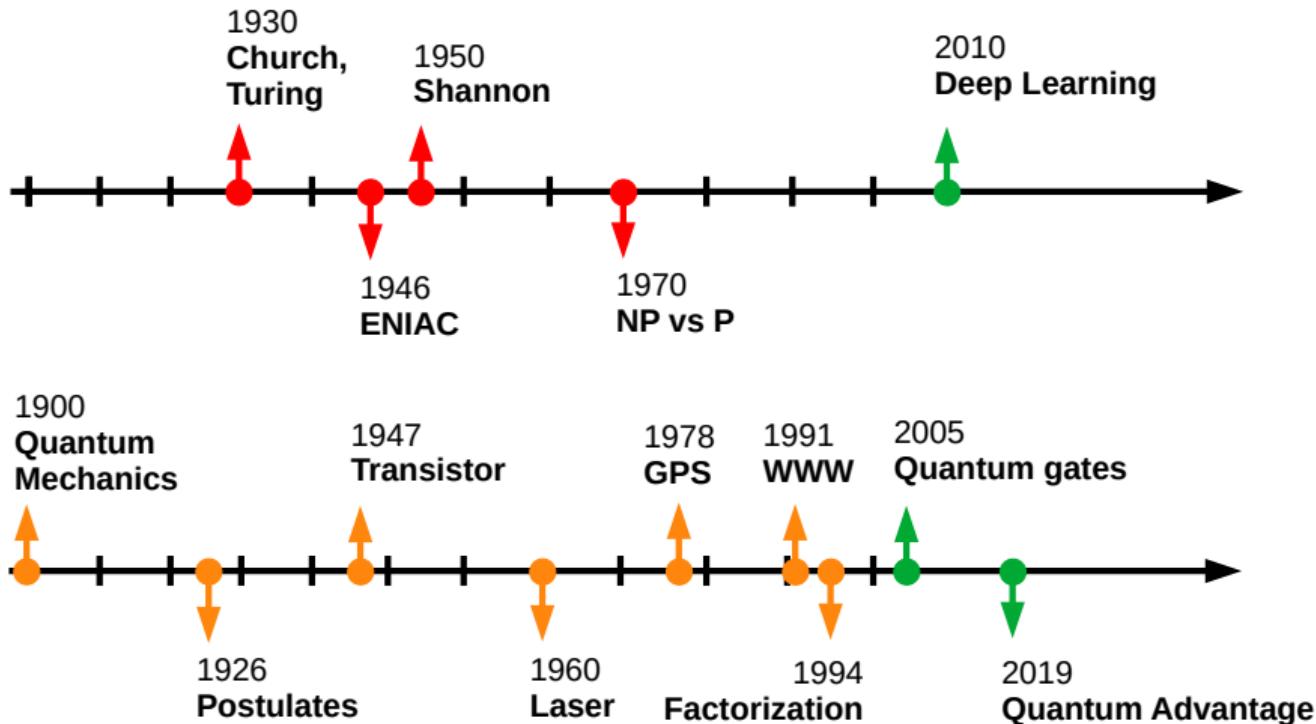


Introduction

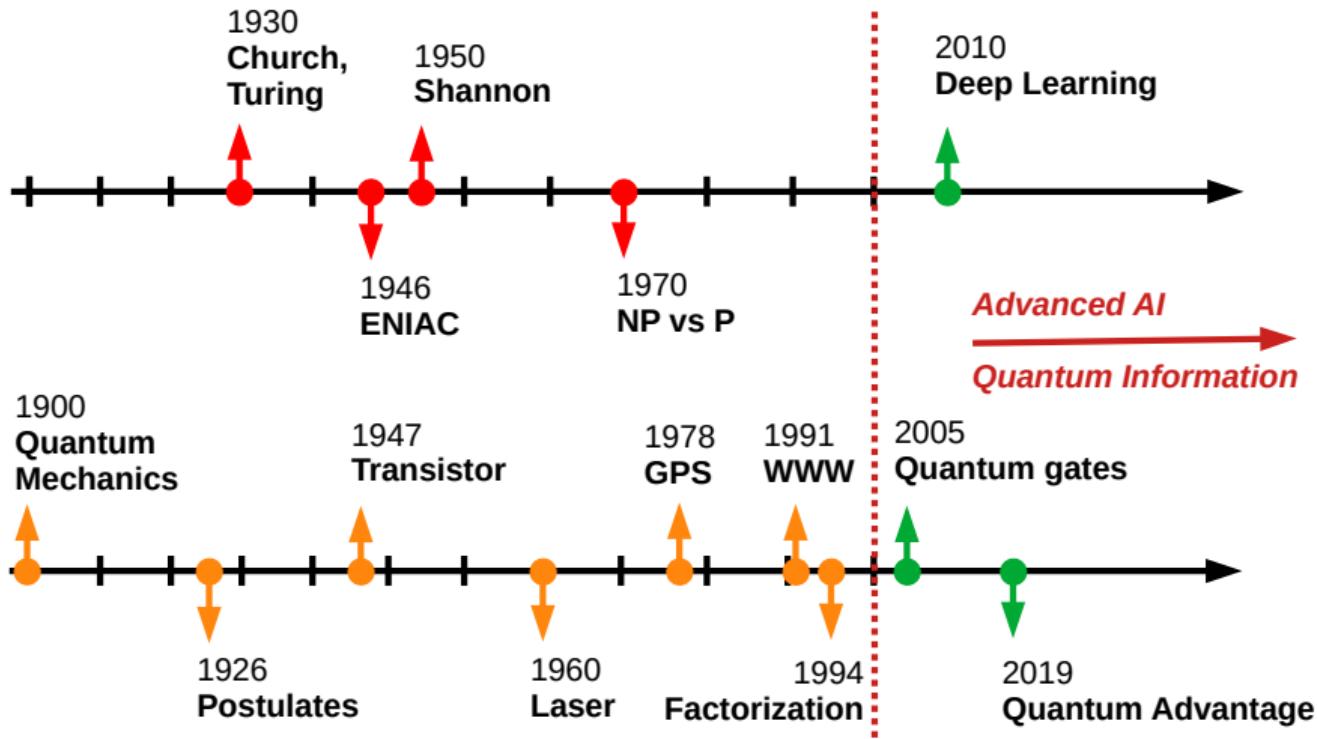
The Quantum Disruption



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R&D and adoption of new technologies

Scientific community is moving towards new technologies, in particular **hardware accelerators**:

CPU



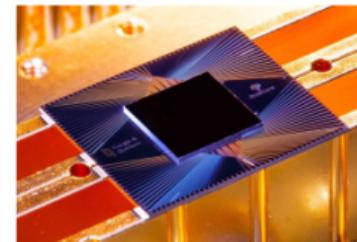
GPU



FPGA/ASIC

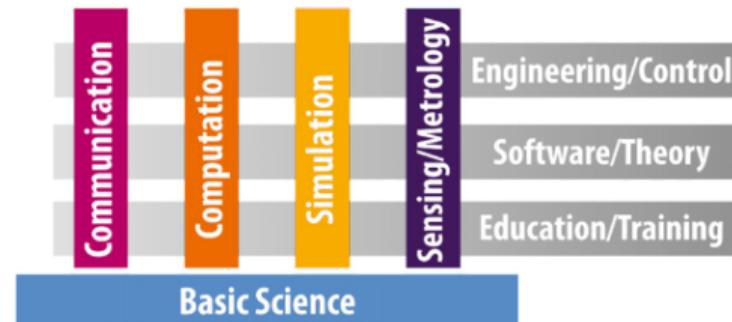


Quantum chip



Moving from **general purpose devices** ⇒ **application specific**

Structure of research field in quantum technologies:

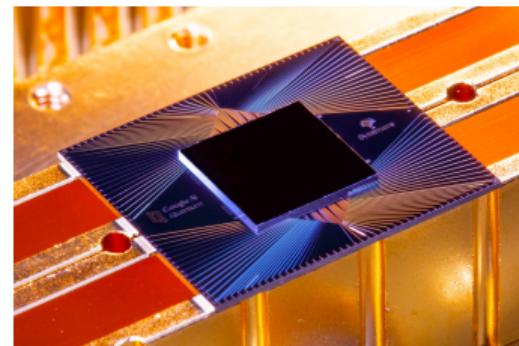
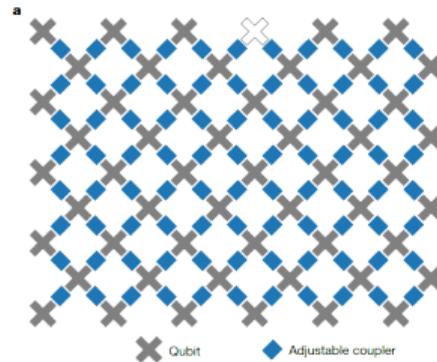


Quantum computing is a paradigm that exploits quantum mechanical properties of matter in order to perform calculations.

⇒ Unitary operators, entanglement, superposition, interference, etc.

Quantum advantage

First quantum computation that can not be reproduced on a classical supercomputer from Google, [Nature 574, 505-510\(2019\)](#):



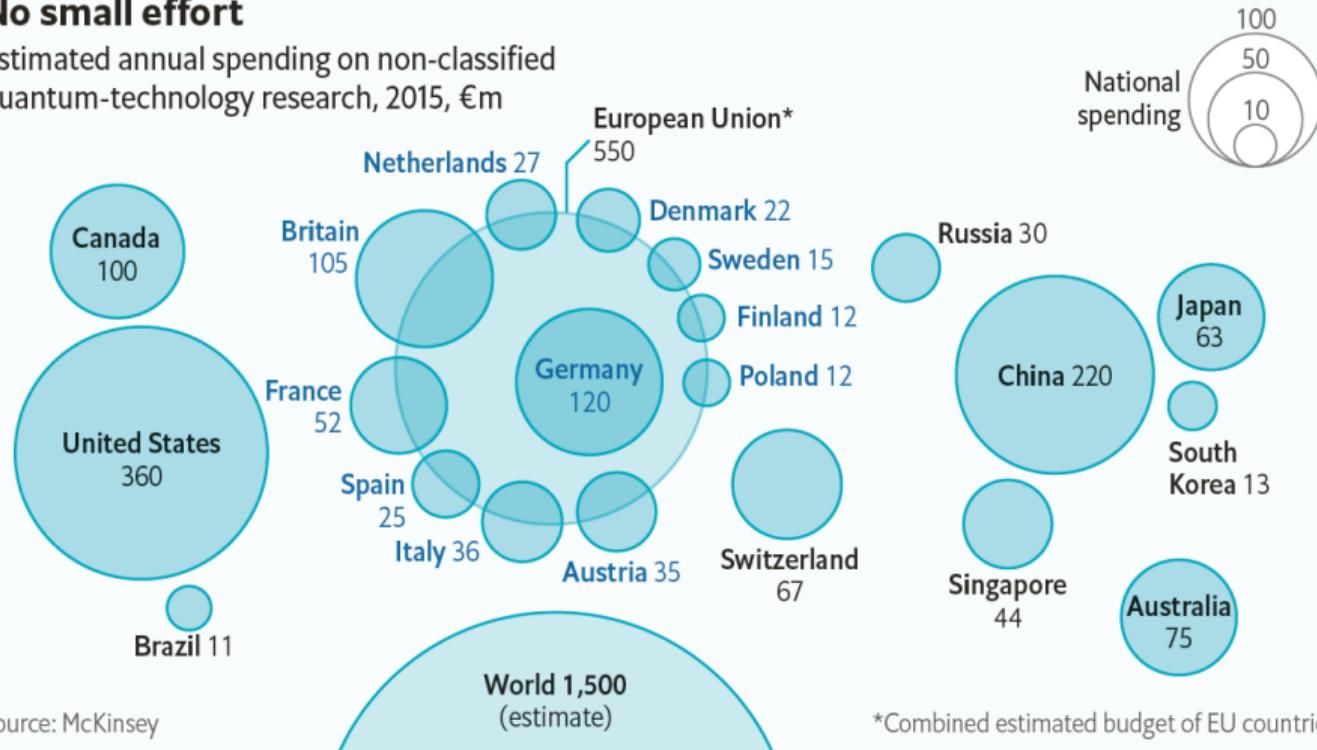
53 qubits (86 qubit-couplers) → Task of sampling the output of a pseudo-random quantum circuit (extract probability distribution).

Classically the probability distribution is exponentially more difficult.

Annual spending on quantum technology

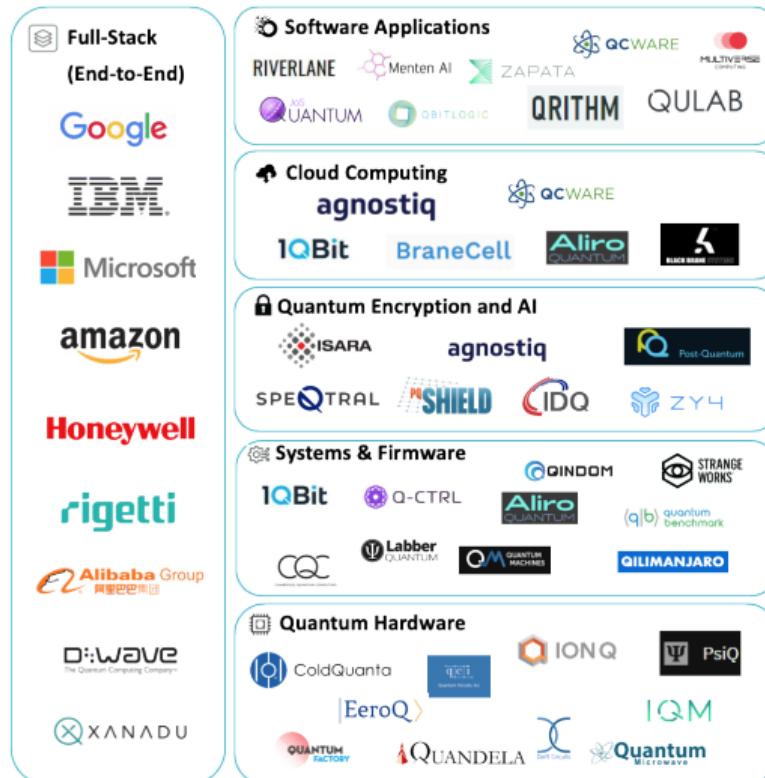
No small effort

Estimated annual spending on non-classified quantum-technology research, 2015, €m

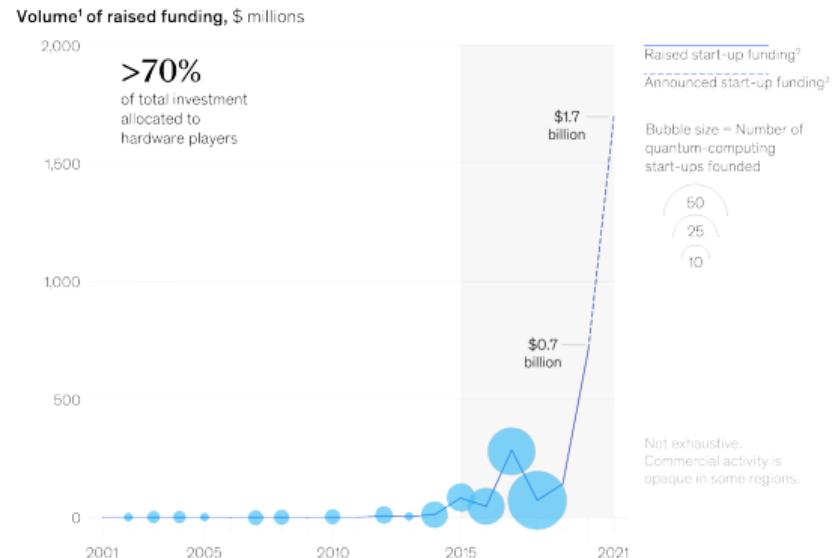


Source: McKinsey

Strong synergy between industry and academics worlds



Start-up activity and investments in quantum computing have skyrocketed since 2015.



¹Based on public investment data recorded in PitchBook; actual investment is likely higher.

²Public announcements of major deals; actual investment is likely higher.

³Start-ups from 2019 and later are likely still in stealth mode or are not yet recognized as quantum-computing companies by relevant platforms and experts.

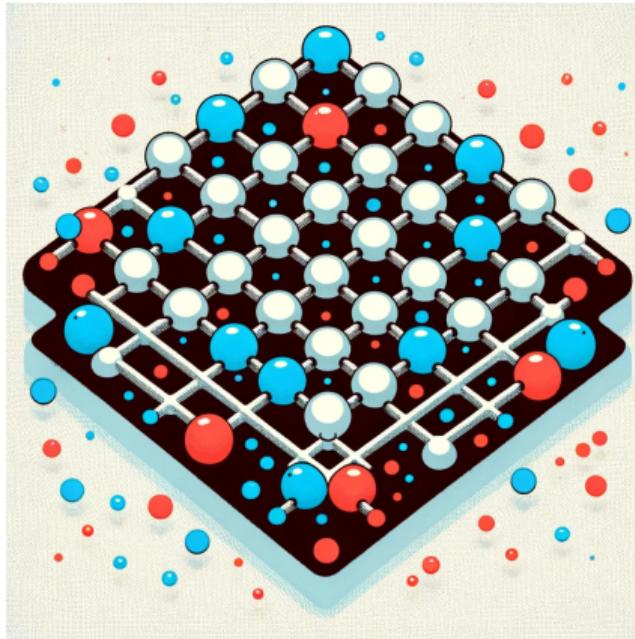
Source: PitchBook, McKinsey analysis

Quantum Systems

Compute quantum mechanics

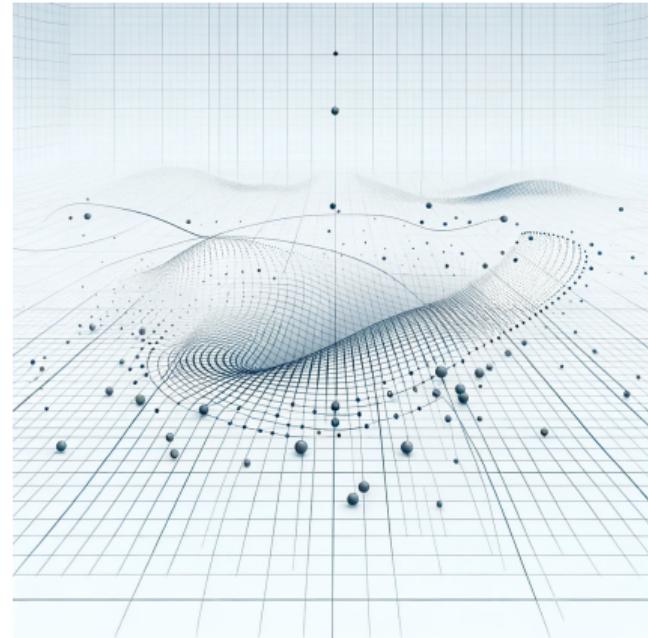
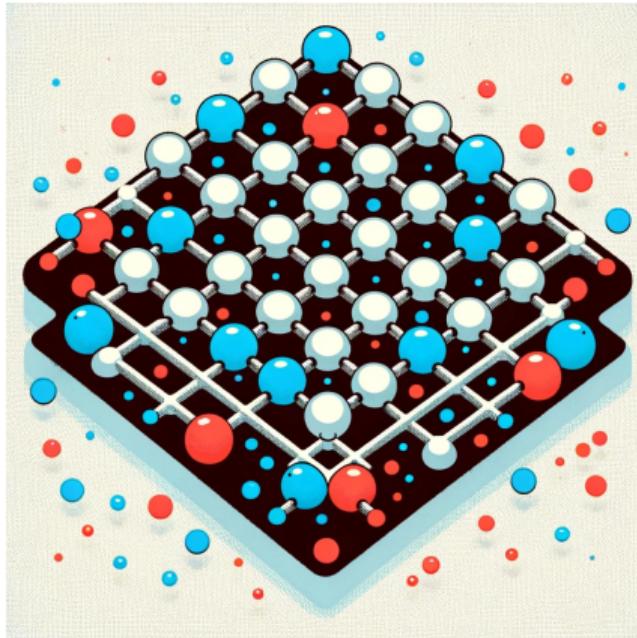
Compute quantum mechanics

- ⚙️ Representing N particles is difficult;



Compute quantum mechanics

- ⚙️ Representing N particles is difficult;
- ⚙️ considering N spins (\uparrow, \downarrow), we deal with a 2^N dimensional Hilbert space!



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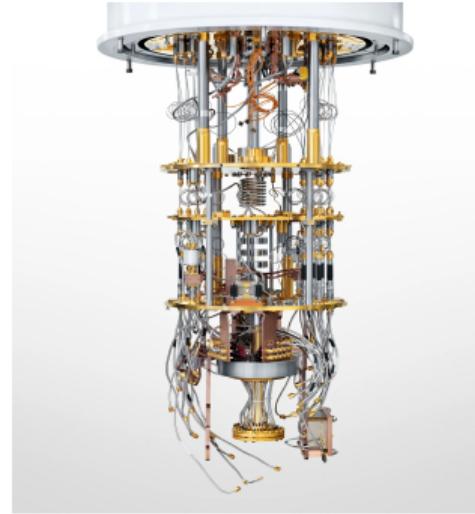


Nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy.

— Richard Feynman, 1982, Simulating Physics with Computers

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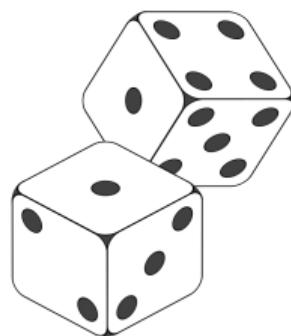


Some smart classical strategies

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1. Variational Monte Carlo (VMC): given a wave function $\Psi(x|\theta)$ and a target H , MC methods are used to minimize:

$$\frac{\int dx \Psi^*(x|\theta) H \Psi(x|\theta)}{\int dx |\Psi(x|\theta)|^2} \geq E_0;$$



arXiv:1508.02989

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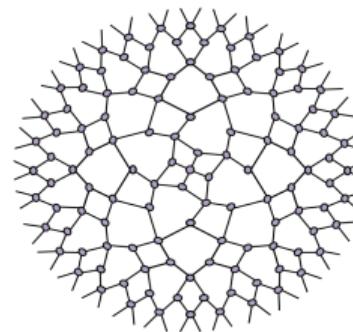
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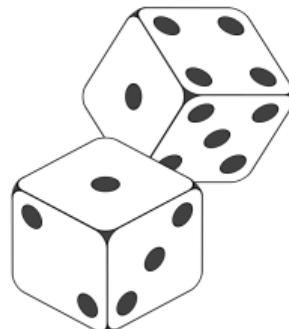
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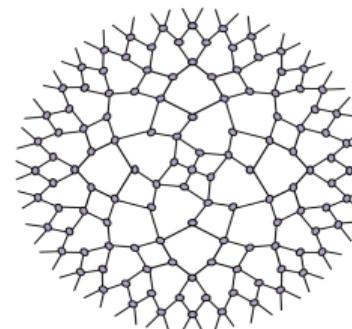
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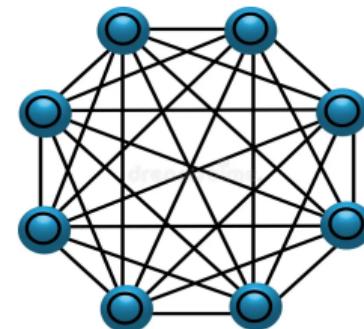
2. Tensor Networks (TNs): contraction of complex systems into simpler structures;
3. Neural Network Quantum States: use complex ANNs to represent the state.



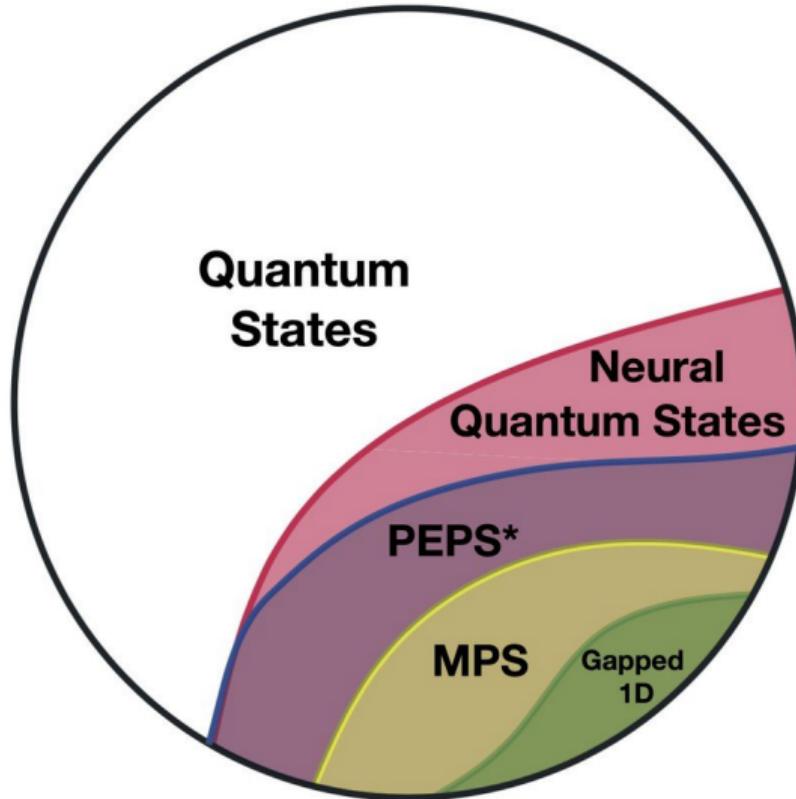
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arXiv:1606.02318

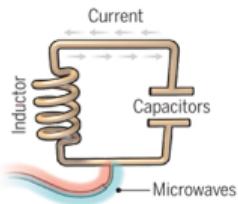


Quantum computing

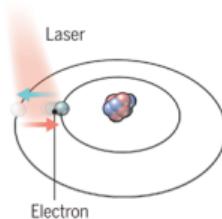
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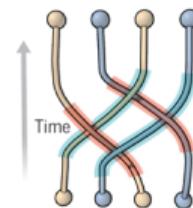
Superconducting loops
A resistance-free current oscillates back and forth around a circuit loop. An injected microwave signal excites the current into superposition states.



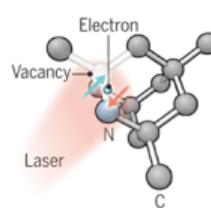
Trapped ions
Electrically charged atoms, or ions, have quantum energies that depend on the location of electrons. Tuned lasers cool and trap the ions, and put them in superposition states.



Silicon quantum dots
These "artificial atoms" are made by adding an electron to a small piece of pure silicon. Microwaves control the electron's quantum state.



Topological qubits
Quasiparticles can be seen in the behavior of electrons channeled through semiconductor structures. Their braided paths can encode quantum information.

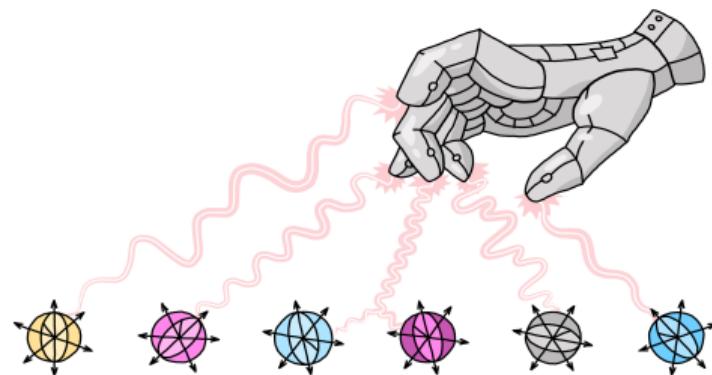


Diamond vacancies
A nitrogen atom and a vacancy add an electron to a diamond lattice. Its quantum spin state, along with those of nearby carbon nuclei, can be controlled with light.

Qubits

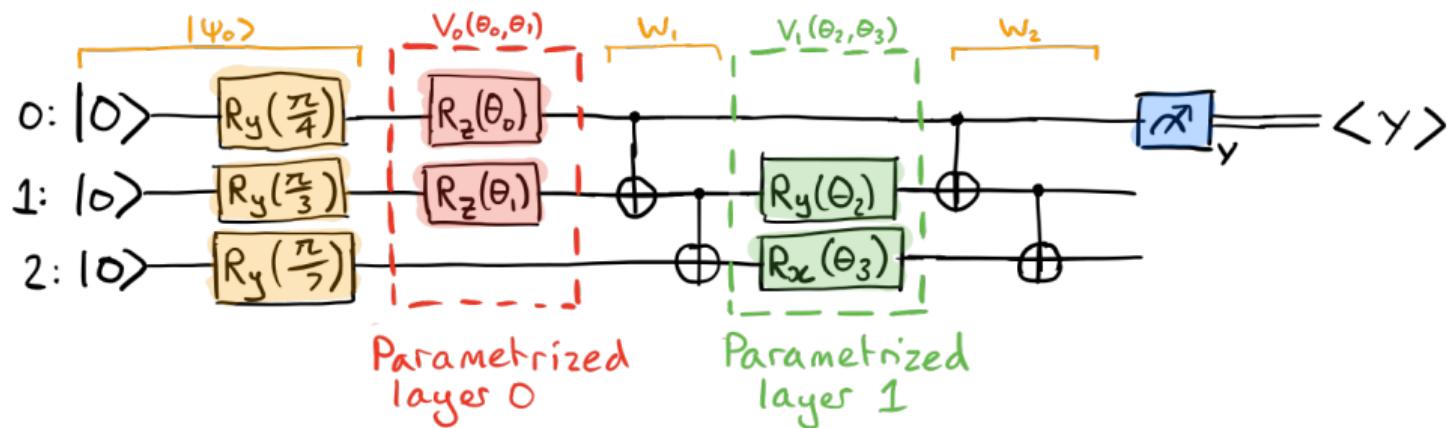
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Typically we use 1-qubit and 2-qubits gates!



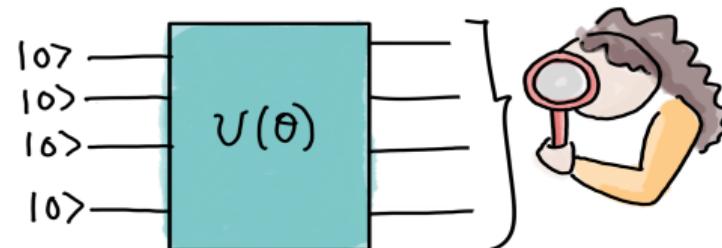
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3. combine together gates to build **quantum circuits**;
4. to access the information we need to measure the system.



What is a qubit?

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Let us consider a two-dimensional **Hilbert space**, we define the computational basis:

$$|0\rangle \rightarrow \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad |1\rangle \rightarrow \begin{bmatrix} 0 \\ 1 \end{bmatrix}.$$

A **quantum bit (qubit)** is the basic unit of quantum information and it is written as:

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle,$$

where α, β are **complex numbers** and the **state is normalized**, i.e. $|\alpha|^2 + |\beta|^2 = 1$.

Multiple qubits states

A system with n qubits lives in 2^n -dimensional Hilbert space, defining the basis:

$$|0\rangle_n = |00\dots00\rangle, |1\rangle_n = |00\dots01\rangle, |2\rangle_n = |00\dots10\rangle, \dots, |2^n - 1\rangle_n = |11\dots1\rangle$$

therefore a generic n qubits state is defined as

$$|\psi_n\rangle = \sum_{i=0}^{2^n-1} \alpha_i |i\rangle_n \quad \text{with} \quad \sum_{i=0}^{2^n-1} |\alpha_i|^2 = 1$$

i.e. a superposition state vector with 2^n complex numbers.

Quantum circuits

The **quantum circuit** model considers a sequence of unitary quantum gates:

$$|\psi'\rangle = U_2 U_1 |\psi\rangle \rightarrow |\psi\rangle \xrightarrow{\boxed{U_1}} \boxed{U_2} |\psi'\rangle$$

The final state $|\psi'\rangle$ is given by:

$$\psi'(\sigma) = \sum_{\sigma'} \textcolor{blue}{U_1 U_2(\sigma, \sigma')} \textcolor{red}{\psi(\sigma_1, \dots, \sigma'_{i_1}, \dots, \sigma'_{i_{N_{\text{targets}}}}, \dots, \sigma_N)},$$

where the sum runs over qubits targeted by the gate.

$\textcolor{blue}{U}_2$ and $\textcolor{blue}{U}_1$ are gate matrices which act on the state vector.

$\textcolor{red}{\psi}$ is a state and it is bounded by memory.

Quantum gates

Single-qubit gates

Pauli gates

Hadamard gate

Phase shift gate

Rotation gates

Two-qubit gates

Controlled gates

Swap gate

fSim gate

Three-qubit gates

Toffoli

Operator	Gate(s)	Matrix
Pauli-X (X)		$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
Pauli-Y (Y)		$\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$
Pauli-Z (Z)		$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
Hadamard (H)		$\frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$
Phase (S, P)		$\begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}$
$\pi/8$ (T)		$\begin{bmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{bmatrix}$
Controlled Not (CNOT, CX)	 	$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$
Controlled Z (CZ)	 	$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$
SWAP	 	$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$
Toffoli (CCNOT, CCX, TOFF)	 	$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \end{bmatrix}$

Pauli gates

X gate

The X gate acts like the classical NOT gate, it is represented by the σ_x matrix,

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

therefore



Z gate

The Z gate flips the sign of $|1\rangle$, it is represented by the σ_z matrix,

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

therefore



Hadamard gate

The Hadamard gate (H gate) is defined as

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

Therefore it creates a superposition of states

$$|0\rangle \xrightarrow{H} \frac{|0\rangle + |1\rangle}{\sqrt{2}} \equiv |+\rangle$$

$$|1\rangle \xrightarrow{H} \frac{|0\rangle - |1\rangle}{\sqrt{2}} \equiv |-\rangle$$

Measurements

In real experiments we perform measurements with a preselected number of shots.

Shots contribute to the reconstruction of the underlying wave-function distribution.

Measurement (M) gate:

Lets consider the following circuit:



The analytic final state is:

$$\frac{|0\rangle + |1\rangle}{\sqrt{2}}$$

When measuring the final state we obtain 0 or 1 each with 50% probability.

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- let's apply a controlled-NOT (CNOT) gate on a second qubit prepared in $|0\rangle$:

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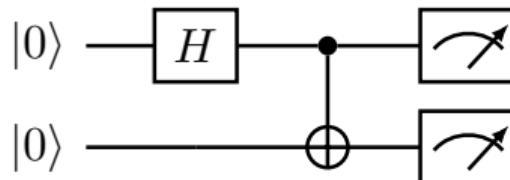
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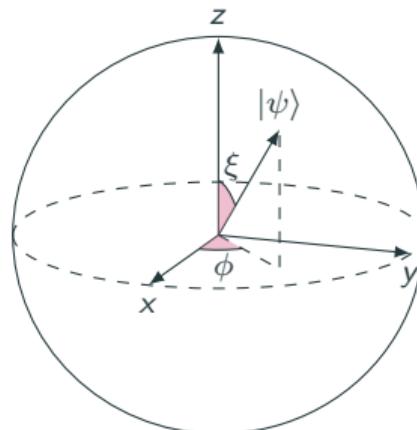
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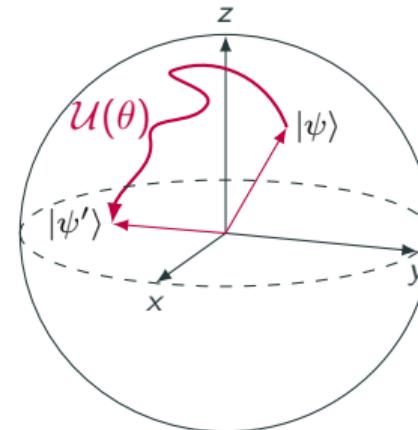
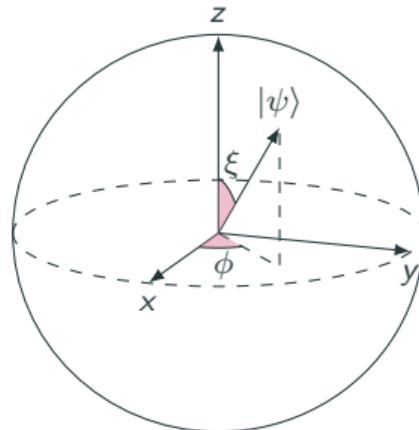


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$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle \quad \text{with} \quad \alpha = \cos\frac{\theta}{2}, \quad \beta = e^{i\phi}\sin\frac{\theta}{2}.$$



We can use as parametric gates the rotation around the axis of the block sphere:

$$R_k(\theta) = \exp[-i\theta\sigma_k], \quad \text{with} \quad \sigma_k \in \{I, \sigma_x, \sigma_y, \sigma_z\}.$$

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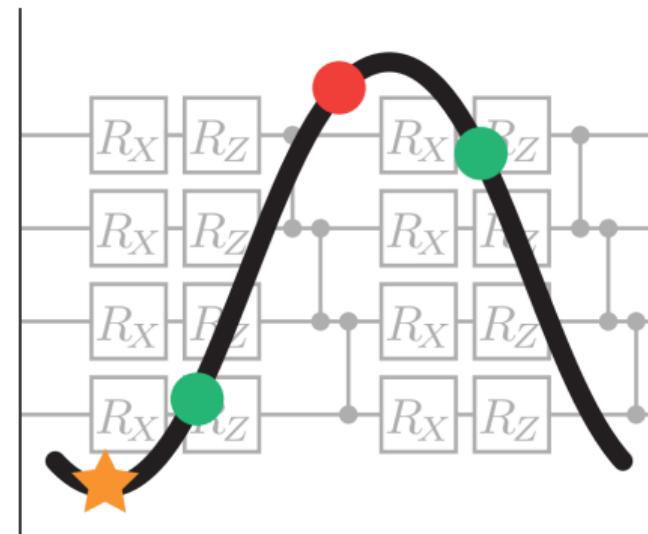
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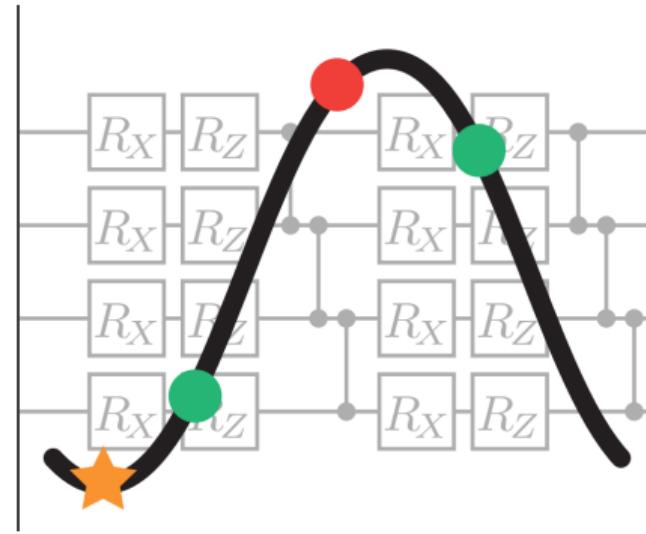


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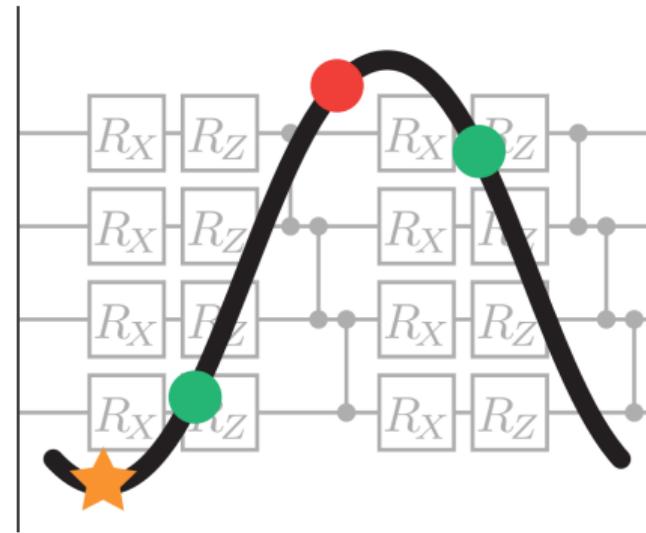


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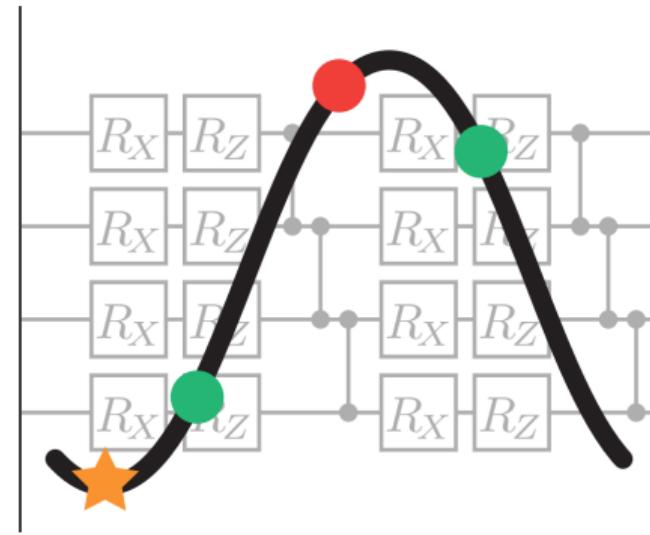


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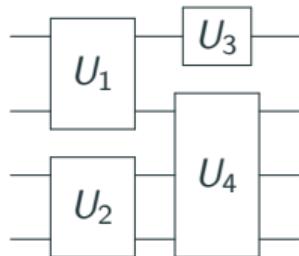
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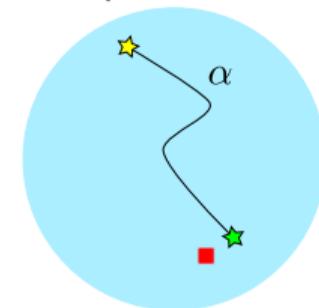
Rational for Variational Quantum Circuits

Rational: Deliver variational quantum states → explore a large Hilbert space.

$$U(\vec{\alpha}) = U_n \dots U_2 U_1$$



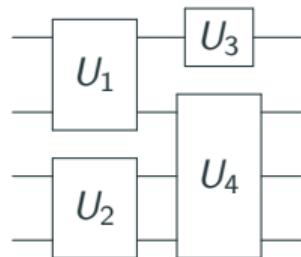
Near optimal solution



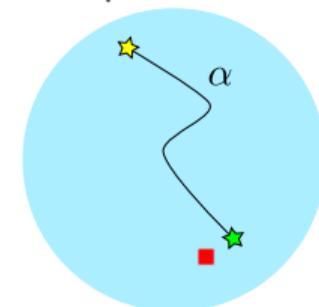
Rational for Variational Quantum Circuits

Rational: Deliver variational quantum states → explore a large Hilbert space.

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Near optimal solution



Idea: Quantum Computer is a machine that generates variational states.

⇒ **Variational Quantum Computer**

Solovay-Kitaev Theorem

Let $\{U_i\}$ be a dense set of unitaries.

Define a circuit approximation to V :

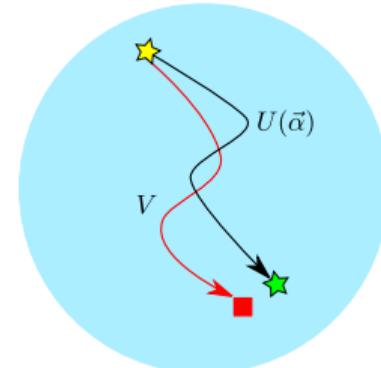
$$|U_k \dots U_2 U_1 - V| < \delta$$

Scaling to best approximation

$$k \sim \mathcal{O} \left(\log^c \frac{1}{\delta} \right)$$

where $c < 4$.

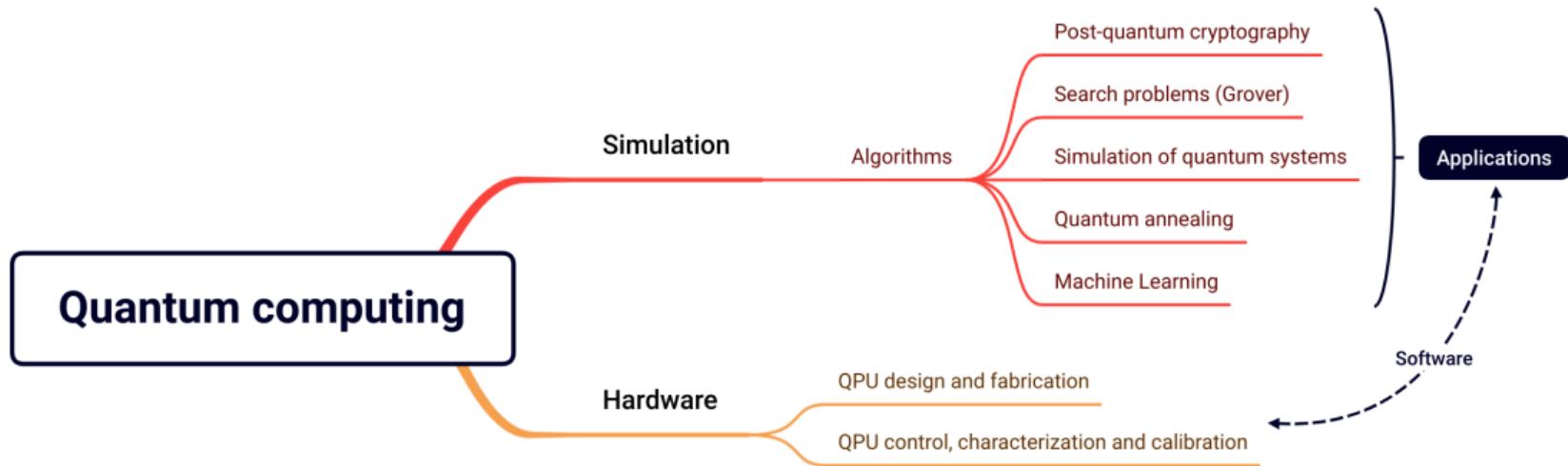
Optimal solution



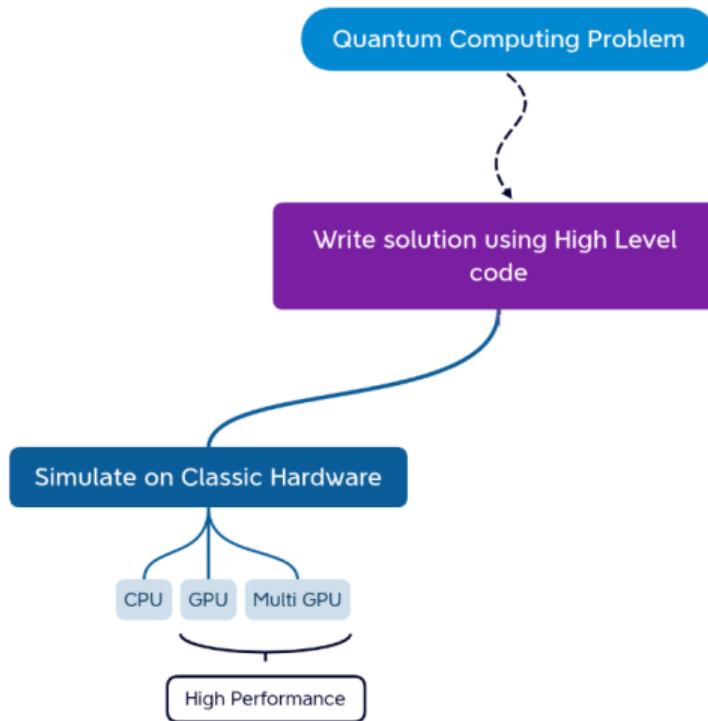
⇒ The approximation is **efficient** and requires a **finite number of gates**.

Quantum software challenges

Software and Quantum Computing



Full-stack deployment process



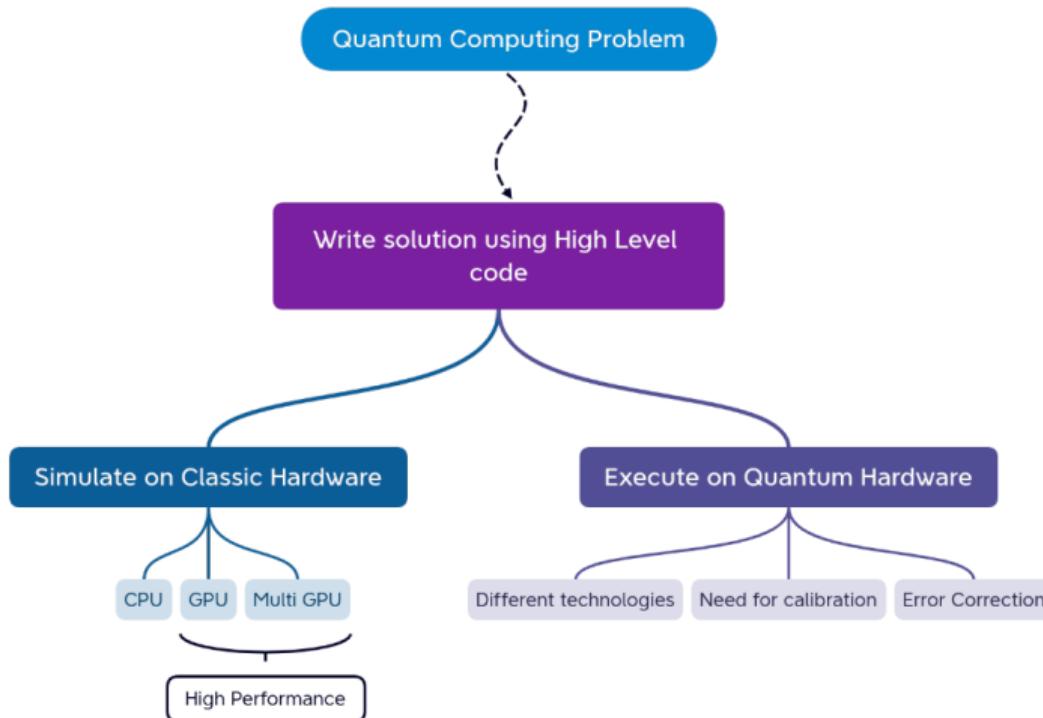
1. Prototyping

High-level programming language

2. Simulation

Fast classical quantum simulation

Full-stack deployment process



1. Prototyping

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Fast classical quantum simulation

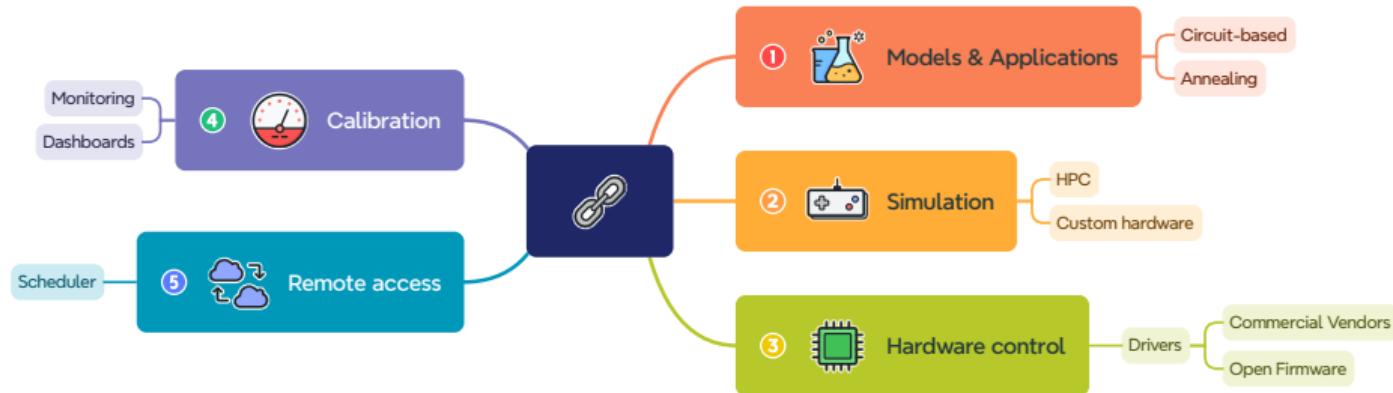
3. Deployment on hardware

Hardware optimization

Software challenges

Requirements for self-hosted quantum hardware:

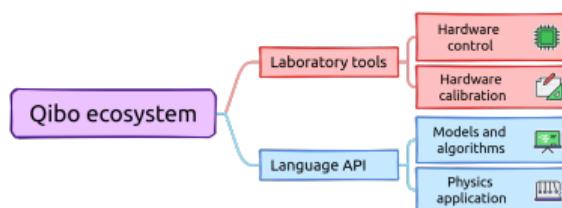
1. Access to **interdisciplinary set of software tools** for:



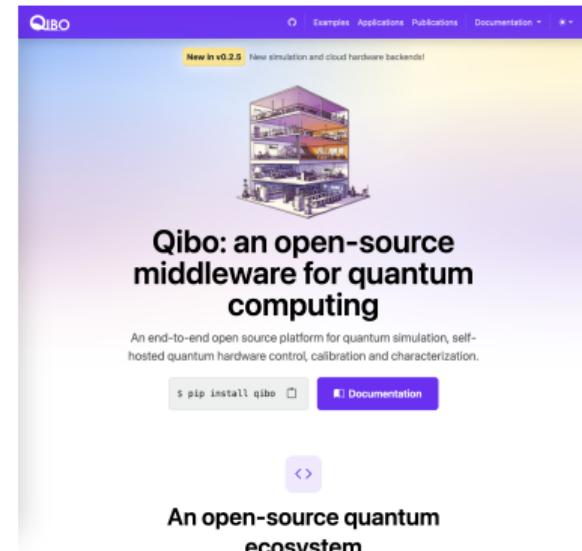
2. **Open-source software** tools supported by benchmarks and publications.

Introducing Qibo

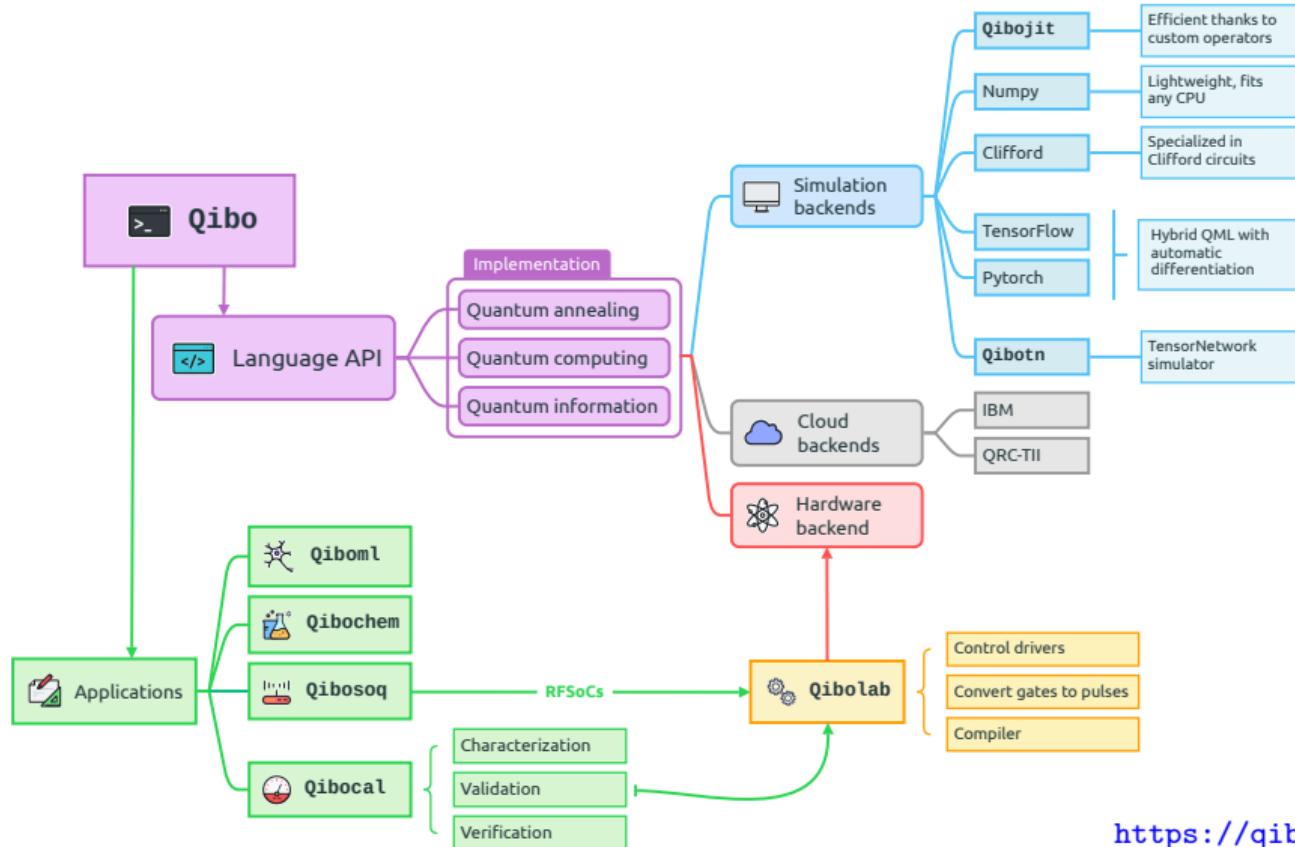
Qibo is an **open-source** hybrid quantum operating system for self-hosted quantum computers.



1. Fully open-source and community driven.
2. Modular layout design with possibility of adding:
 - new backends for simulation,
 - new platforms for hardware control,
 - new drivers for control electronics.
3. Supported by documentation and tests/CI on quantum hardware.



<https://qibo.science>



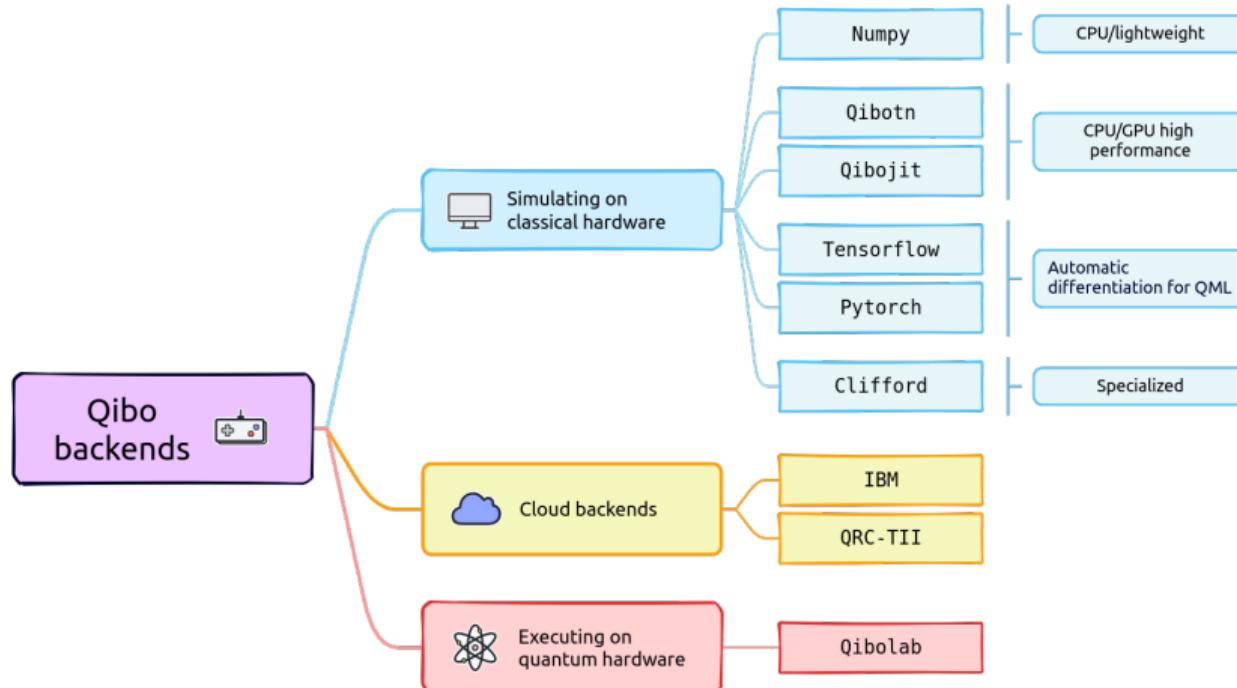
Qibo Contributors (March 2024)



Quantum Simulation

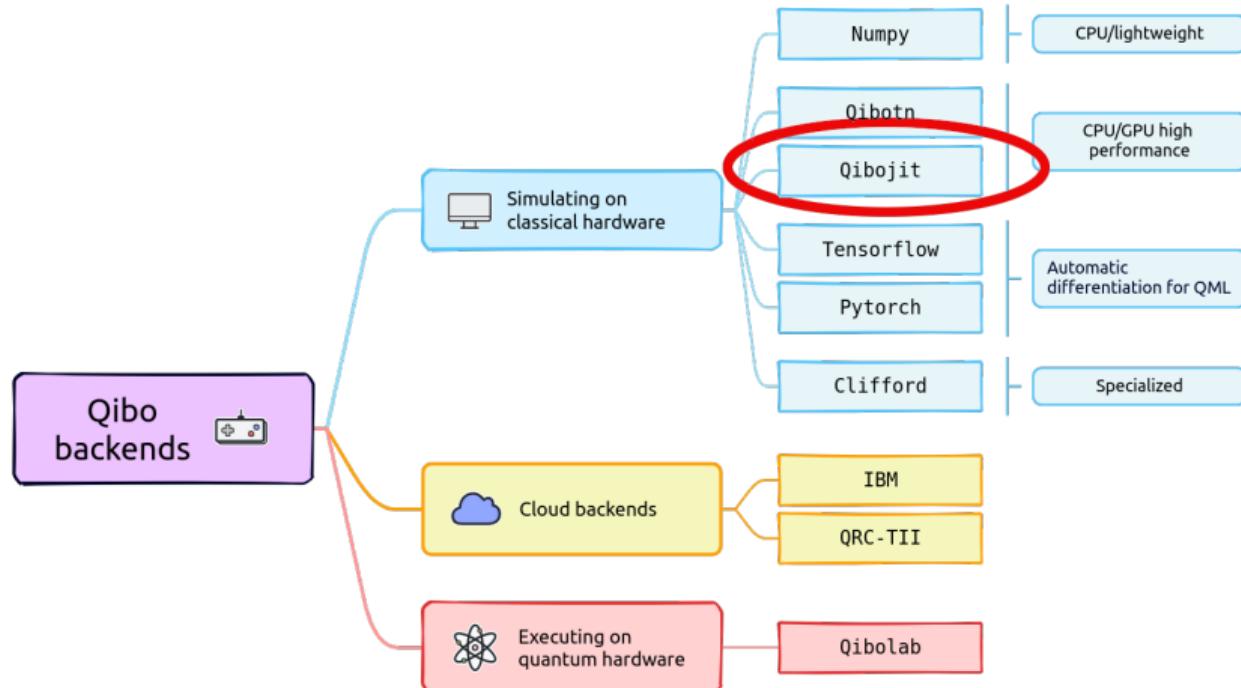
Qibo backends

We provide a modular and extensible framework for quantum computing based on **backends**:



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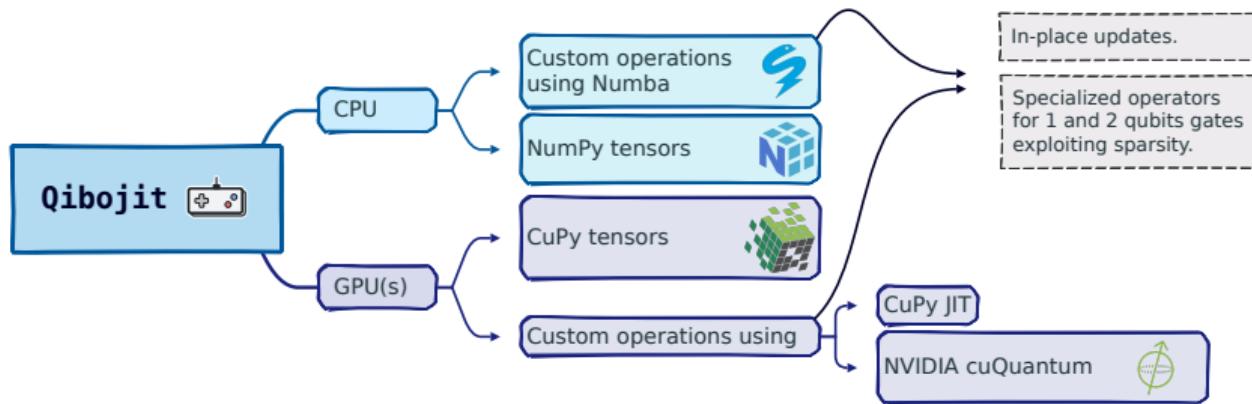


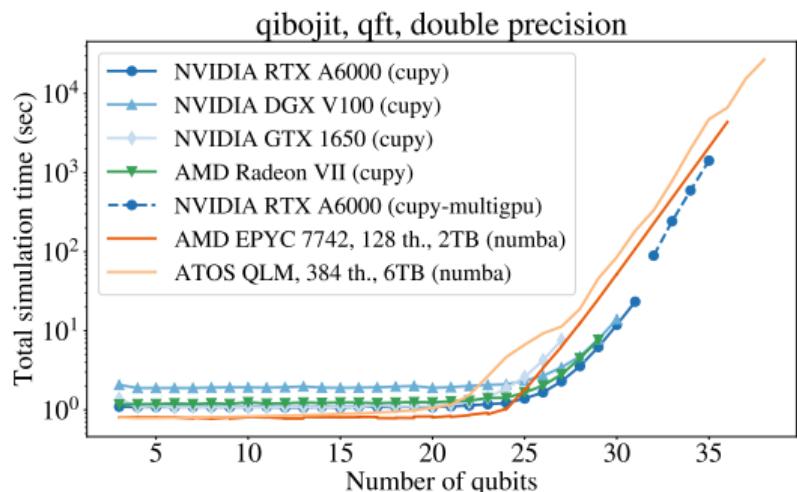
State vector simulation solves:

$$\psi'(\sigma_1, \dots, \sigma_n) = \sum_{\tau'} G(\tau, \tau') \psi(\sigma_1, \dots, \tau', \dots, \sigma_n)$$

The number of operations scales **exponentially** with the number of qubits.

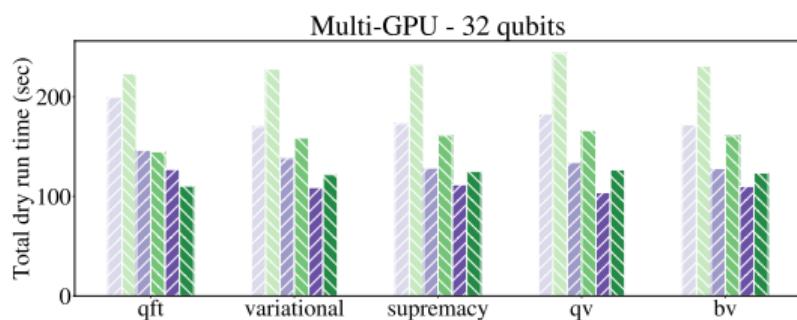
Qibo uses just-in-time technology and hardware acceleration:





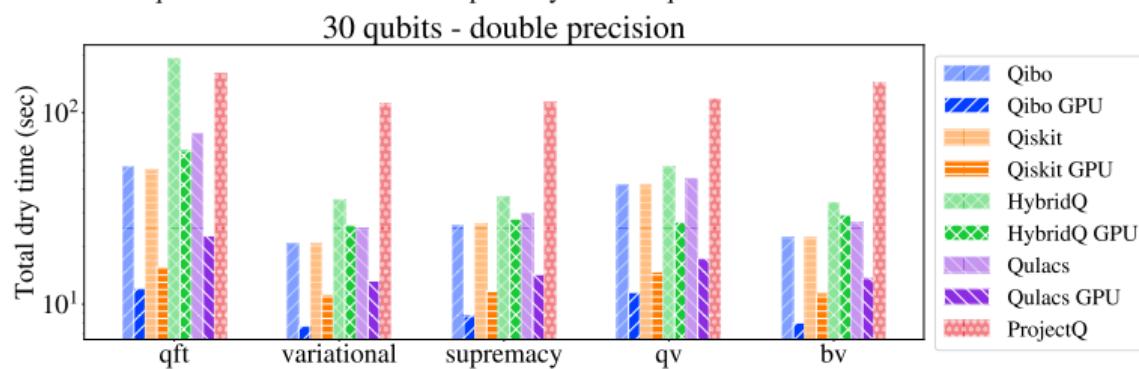
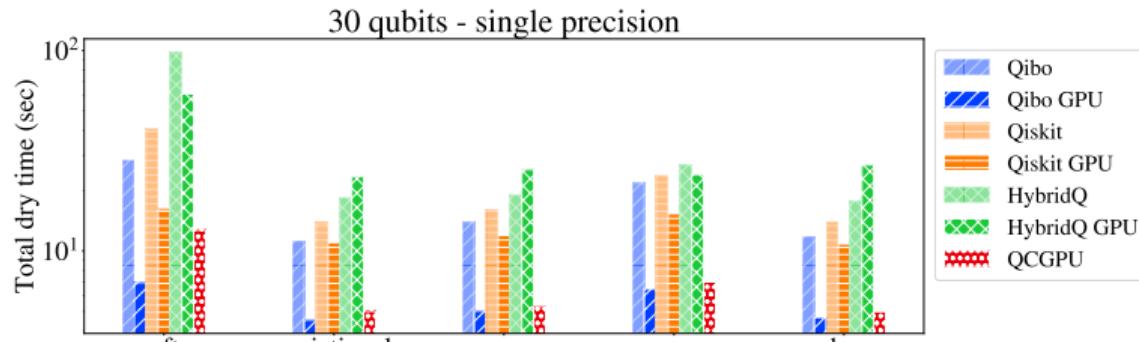
Major features:

- Supports CPU, GPU and multi-GPU.
- NVIDIA and AMD GPUs support.
- Reduced memory footprint.

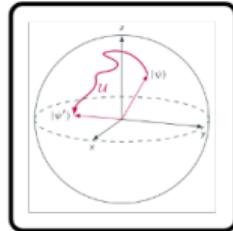
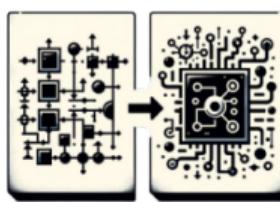
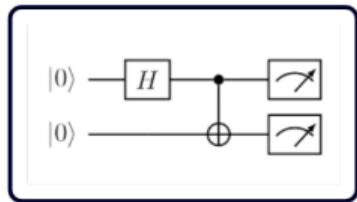


Benchmark library: <https://github.com/qiboteam/qibojit-benchmarks>

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Laboratory modules



Major features:

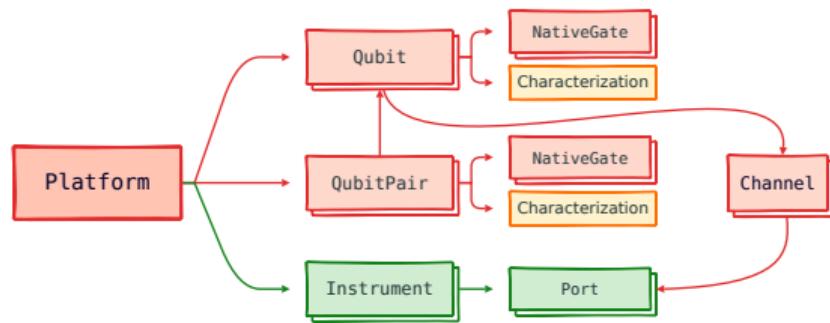
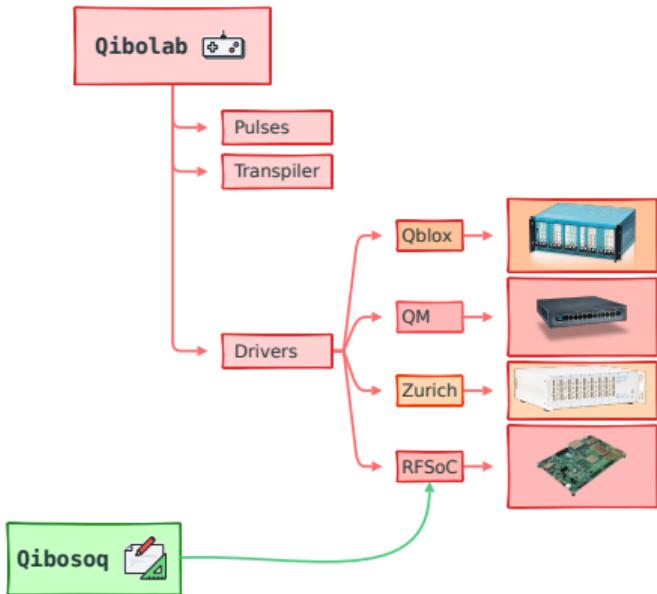
Pulse and pulse sequence API.

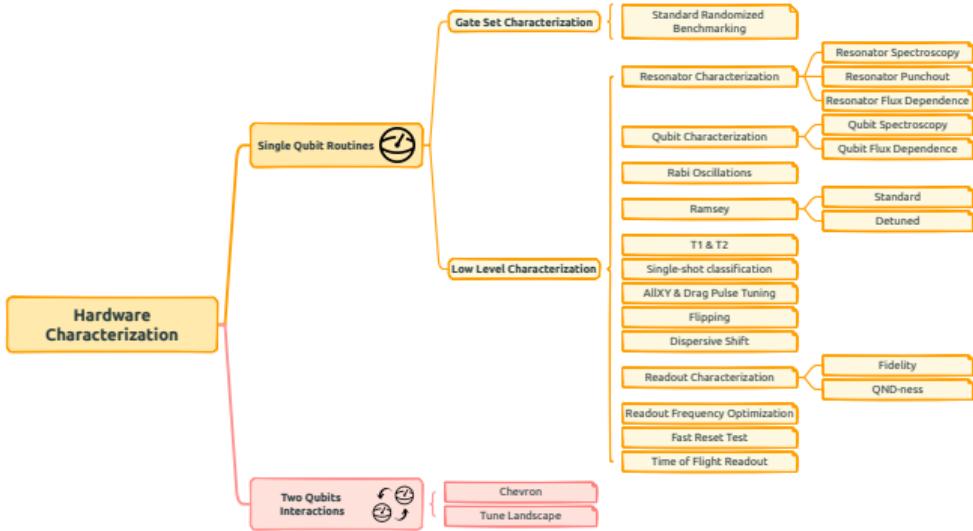
Extensible API to drivers of control instruments.

Hardware sweeps for faster execution of calibration routines.

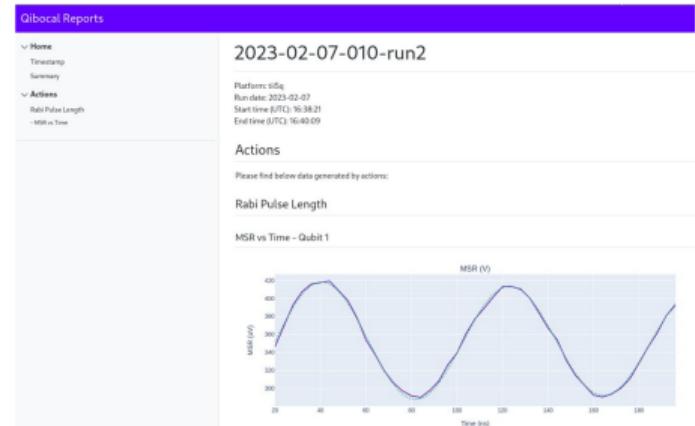
Transpilers from arbitrary circuits to pulses.

C/C++ and Rust APIs

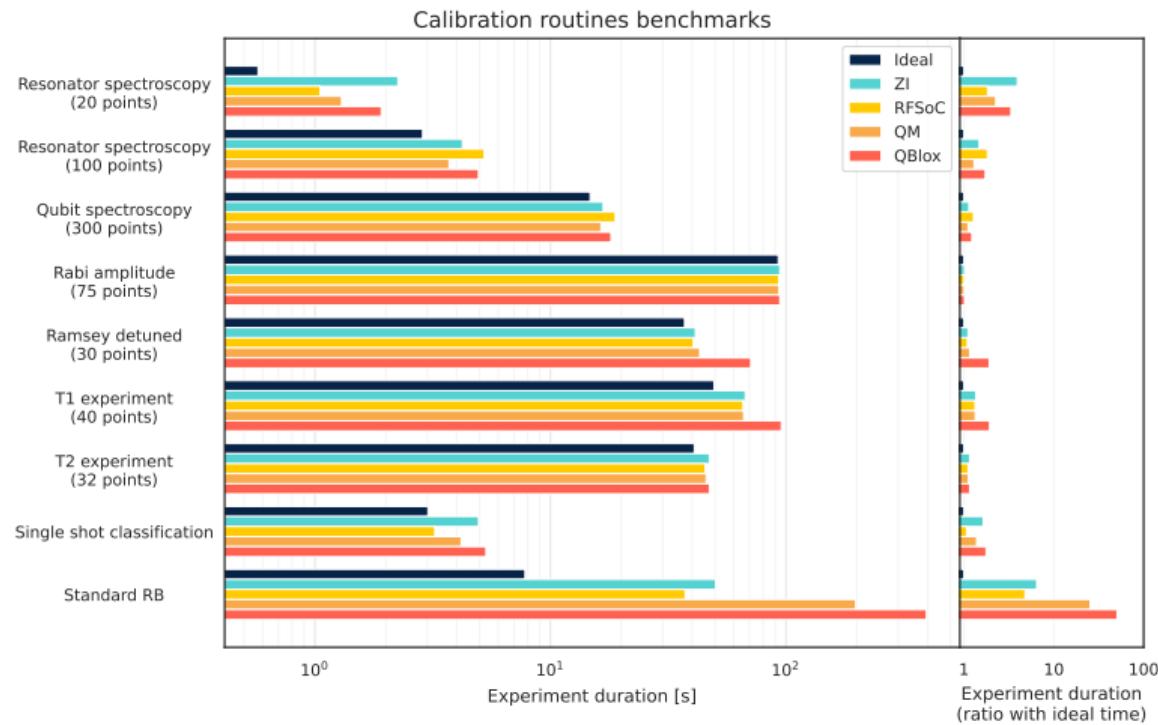




Major features:
Calibration of single and multi-qubit platforms are possible using **Qibo**.

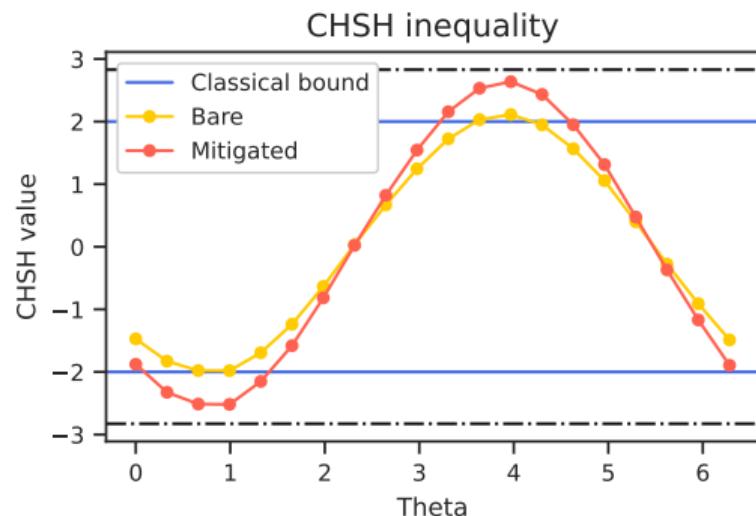
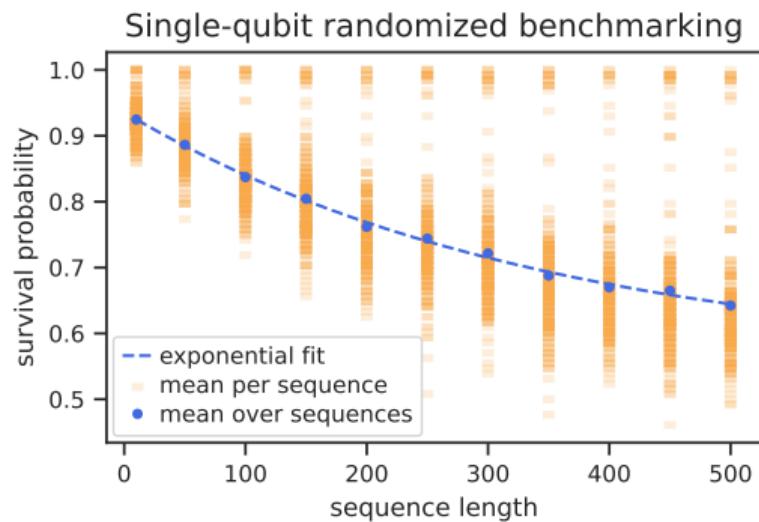


We compare the ideal pulse sequence execution performance to instruments execution duration.



Full-stack applications

Examples of results executed on quantum hardware (single-qubit) after calibration with Qibo:



1. High-Level API (Qibo)

Define model prototype.

Implement training loop.

Perform training using simulation.

2. Calibration (Qibocal)

Calibrate qubit.

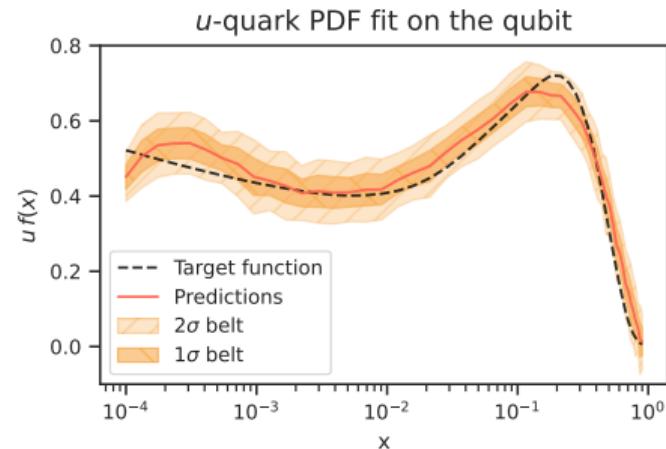
Generate platform configuration.

3. Execution (Qibolab)

Allocate calibrated platform.

Compile and transpile circuit.

Execute model and return results.



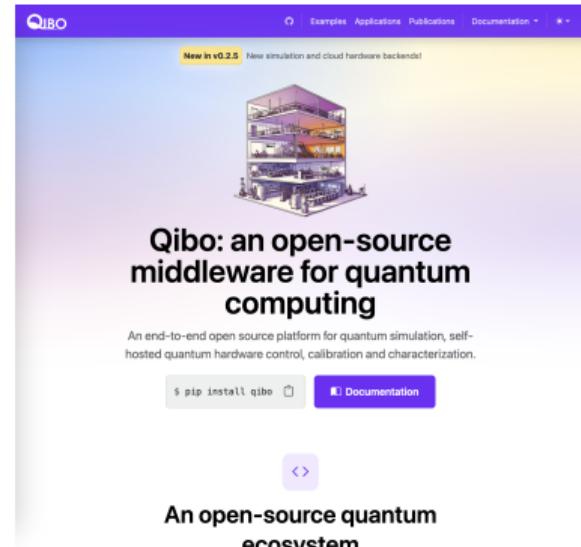
Parameter	Value
N_{data}	50 points
N_{shots}	500
MSE	10^{-3}
Electronics	Xilinx ZCU216
Training time	< 1h

Outlook

What next?

Hands-on tutorials:

1. Setting up Qibo's quantum middleware software environment, building quantum circuits.
2. Quantum circuits, gates and shots. Bell states and ancillary qubits.
3. Grover search algorithm.
4. Introducing quantum noise and quantum hardware limitations
5. Mitigating quantum noise via Quantum Error Mitigation



<https://qibo.science>

Let's code!

