

High Performance and Disruptive Computing in Remote Sensing Summer School

29 May - 1 June 2023, Iceland

HDCRS Summer School Introduction to Quantum Computing and its Ecosystem*

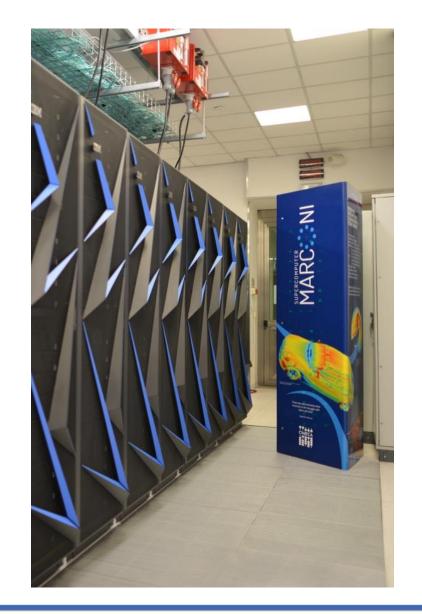
Mengoni Riccardo, PhD

1 June 2023



CINECA Overview

- CINECA is a Consortium composed by 98 Italian universities and public institutions.
- Since its origins in 1969, Cineca offers support to scientific research, public and industrial, through supercomputing and the use of the most innovative computing systems based on state-ofthe-art architectures and technologies.
- HPC Italian National Center, owner of one of the most powerful supercomputer in Europe and the World





CINECA Overview





Leonardo: Cineca preexascale supercomputer

Fourth most powerful supercomputers in the world

Rank	System	Cores	Rmax (PFlop/s)	Rpeak (PFlop/s)	Power (kW)
4	Leonardo - BullSequana XH2000, Xeon Platinum 8358 32C 2.6GHz, NVIDIA A100 SXM4 64 GB, Quad-rail NVIDIA HDR100 Infiniband, Atos EuroHPC/CINECA	1,824,768	238.70	304.47	7,404



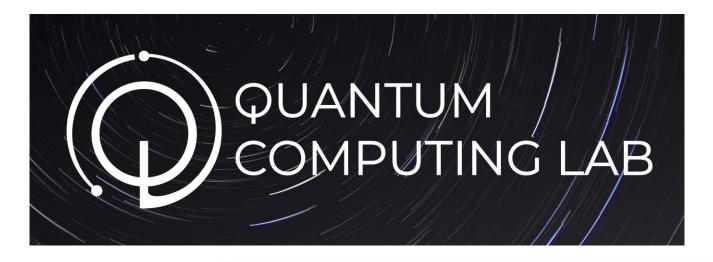
CINECA: Italian HPC center CINECA Quantum Computing Lab:

- Support research Universities, Industries and QC startups
- Internship programs, Courses and Conference (HPCQC)

https://www.quantumcomputinglab.cineca.it

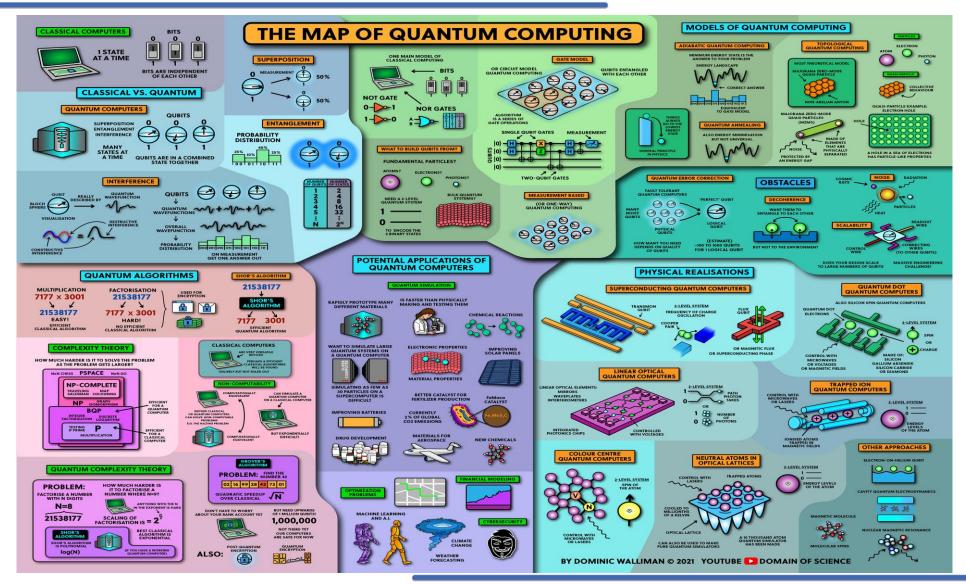


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A Quantum Computer is NOT simply a smaller or faster version of traditional computers or HPC systems





A fundamentally new paradigm for information processing and computation

Based on the principles of Quantum Physics



Quantum Algorithms ≠ Classical Algorithms

 A completely different approach is required to solve problems (because involves quantum mechanics)





Let's take a step back.. What is Quantum Mechanics?



What is Quantum Mechanics?

"If you remove all the physics QM= probability theory + minus sign"

Cit. Scott Aaronson

https://www.youtube.com/watch?v=SczraSQE3MY



What is Quantum Mechanics?

"If you remove all the physics QM= probability theory + minus sign"

Cit. Scott Aaronson

...also Linear algebra Involved

 $| \Psi \rangle = \begin{pmatrix} \Psi_{1} \\ \Psi_{2} \\ \vdots \\ \Psi_{n} \end{pmatrix} \qquad \begin{array}{c} \Psi_{1} \in \mathbb{C} \\ \Psi_{n} \end{pmatrix} \qquad \begin{array}{c} | \phi \rangle \otimes [\Psi \rangle = \\ \text{Complex} \\ \text{Number} \end{array} \qquad \begin{array}{c} | \phi \rangle \otimes [\Psi \rangle = \begin{pmatrix} \psi_{1} \\ \Psi_{2} \\ \Psi_{n} \\ \Psi_{n} \end{pmatrix} \qquad \begin{array}{c} U \cup^{\dagger} = \cup^{\dagger} \cup = \mathbb{I} \\ \Psi_{1} \oplus \psi_{1} \\ \Psi_{2} \\ \Psi_{n} \end{pmatrix} \qquad \begin{array}{c} \Psi_{1} \oplus \Psi_{2} \\ \Psi_{2} \\ \Psi_{n} \end{pmatrix} \qquad \begin{array}{c} \Psi_{1} \oplus \Psi_{2} \\ \Psi_{2} \\ \Psi_{n} \end{pmatrix} \qquad \begin{array}{c} \Psi_{1} \oplus \Psi_{2} \\ \Psi_{2} \\ \Psi_{n} \end{pmatrix} \qquad \begin{array}{c} \Psi_{1} \oplus \Psi_{2} \\ \Psi_{2} \\ \Psi_{n} \end{pmatrix} \qquad \begin{array}{c} \Psi_{1} \oplus \Psi_{2} \\ \Psi_{2} \\ \Psi_{2} \\ \Psi_{2} \\ \Psi_{2} \end{pmatrix} \qquad \begin{array}{c} \Psi_{1} \oplus \Psi_{2} \\ \Psi_{2} \\ \Psi_{2} \\ \Psi_{2} \\ \Psi_{2} \end{pmatrix} \qquad \begin{array}{c} \Psi_{1} \oplus \Psi_{2} \\ \Psi_{2} \\ \Psi_{2} \\ \Psi_{2} \\ \Psi_{2} \\ \Psi_{2} \end{pmatrix} \qquad \begin{array}{c} \Psi_{1} \oplus \Psi_{2} \\ \Psi_{2} \\ \Psi_{2} \\ \Psi_{2} \\ \Psi_{2} \\ \Psi_{2} \\ \Psi_{2} \end{pmatrix} \qquad \begin{array}{c} \Psi_{1} \oplus \Psi_{2} \\ \Psi_{2} \\ \Psi_{2} \\ \Psi_{2} \\ \Psi_{2} \\ \Psi_{2} \\ \Psi_{2} \end{pmatrix} \qquad \begin{array}{c} \Psi_{1} \oplus \Psi_{2} \\ \Psi_{2} \end{pmatrix} \qquad \begin{array}{c} \Psi_{1} \oplus \Psi_{2} \\ \Psi_{2} \\$

CINEC

Nielsen, M. A., & Chuang, I. L. (2011). Quantum Computation and Quantum Information

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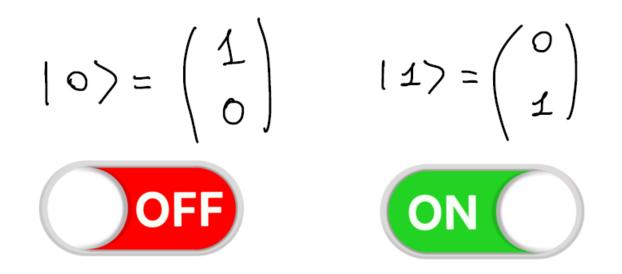
1. Unit of Information



Classically

Unit of classical information is the bit

State of a bit:





Quantumly

To a closed quantum system is associated a space of states *H* which is a Hilbert space. The pure state of the system is then represented by a unit norm vector on such Hilbert space.

The unit of quantum information is the quantum bit a.k.a. Qubit

State of a qubit:

$$|\Psi\rangle = \lambda |0\rangle + \beta |1\rangle = \begin{pmatrix} \lambda \\ \beta \end{pmatrix}$$



Space of states:
$$\mathcal{H} \simeq \mathcal{C}^2$$

State of a qubit:

$$|\Psi\rangle = \langle 0\rangle + \beta |1\rangle = \begin{pmatrix} \lambda \\ \beta \end{pmatrix}$$

 $\langle \beta \in \mathbb{C} \quad |\alpha|^2 + |\beta|^2 = 1$



Space of states:
$$\mathcal{H} \simeq \mathbb{C}^2$$

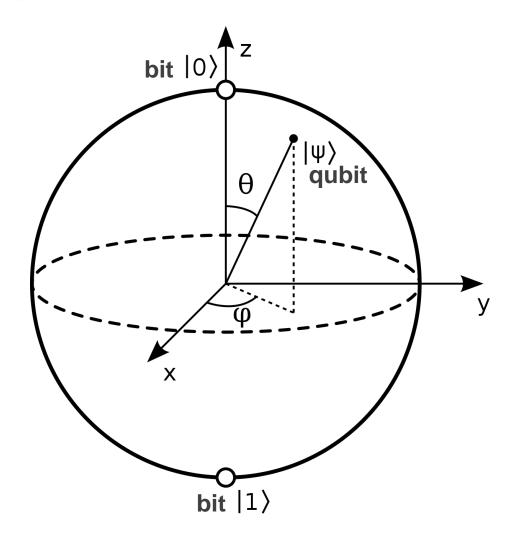
State of a qubit:

$$|\Psi\rangle = d|0\rangle + \beta|1\rangle = \begin{pmatrix} d\\ \beta \end{pmatrix}$$

 $d, \beta \in \mathbb{C}$ $|d|^{2} + |\beta|^{2} = 1$

Can be parametrized as:

$$|\Psi\rangle = \cos\left(\frac{\theta}{2}\right)|0\rangle + e^{i\phi}\sin\left(\frac{\theta}{2}\right)|1\rangle$$
$$\theta \in [0,\pi] \qquad \phi \in [0,2\pi]$$





2. Composite systems



Classically

State of N bits:



Quantumly

The space of states of a composite system is the tensor product of the spaces of the subsystems $(c^2 \otimes (c^2 \otimes ... \otimes (c^2))^2$

State of N qubits:

$$\chi_{1}|000..0\rangle + \chi_{2}|100..0\rangle + \chi_{3}|010..0\rangle + ... \chi_{n}|111..1\rangle$$

 $\chi_{1} \in \mathbb{C} \qquad \sum_{i} |\chi_{i}|^{2} = 1$



Quantum Entanglement

States that can be written as tensor product

$$|\Psi\rangle = |\Psi_1\rangle \otimes |\Psi_2\rangle \otimes \dots \otimes |\Psi_N\rangle$$

are called factorable or product states



Quantum Entanglement

States that **can NOT** be written as tensor product

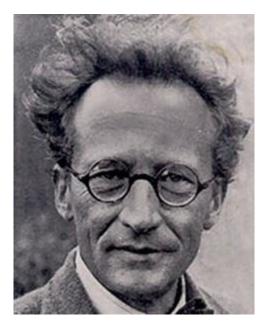
$$|\Psi\rangle \neq |\Psi_1\rangle \otimes |\Psi_2\rangle \otimes ... \otimes |\Psi_N\rangle$$

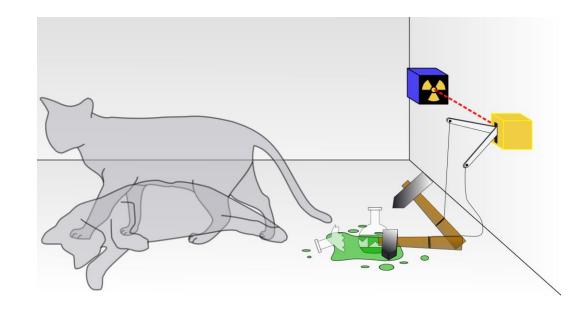
are called entangled states



Quantum Entangled

Example: Schrödinger's Cat







Quantum Entangled Example: Bell's states

$$\frac{1}{N_{2}}\left(100\right) + 1112\right) \qquad \frac{1}{N_{2}}\left(101\right) + 110\right)$$
$$\frac{1}{N_{2}}\left(101\right) + 1102\right)$$
$$\frac{1}{N_{2}}\left(100\right) - 1112\right) \qquad \frac{1}{N_{2}}\left(101\right) - 1102$$





3. State Change



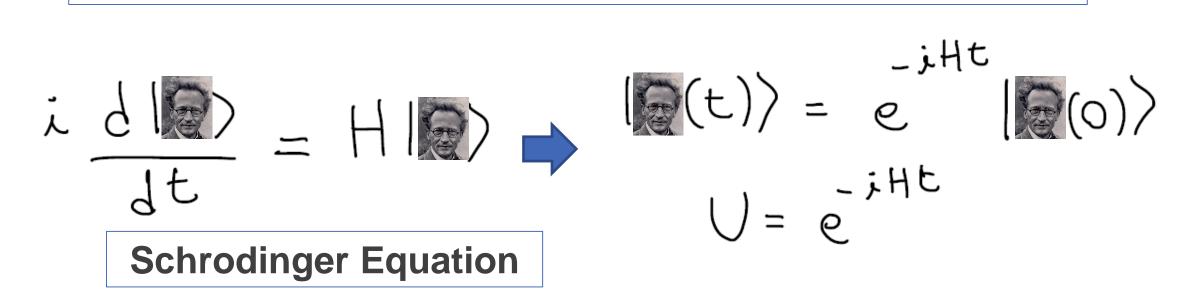
Classically: logic gates

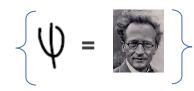
Logic Gate	Symbol	Description	Boolean
AND		Output is at logic 1 when, and only when all its inputs are at logic 1,otherwise the output is at logic 0.	X = A•B
OR		Output is at logic 1 when one or more are at logic 1.If all inputs are at logic 0,output is at logic 0.	X = A+B
NAND		Output is at logic 0 when,and only when all its inputs are at logic 1,otherwise the output is at logic 1	X = •B
NOR		Output is at logic 0 when one or more of its inputs are at logic 1.If all the inputs are at logic 0,the output is at logic 1.	X = A+B
XOR		Output is at logic 1 when one and Only one of its inputs is at logic 1. Otherwise is it logic 0.	Х=А⊕В
XNOR		Output is at logic 0 when one and only one of its inputs is at logic1.Otherwise it is logic 1. Similar to XOR but inverted.	X = A⊕ B
ΝΟΤ		Output is at logic 0 when its only input is at logic 1, and at logic 1 when its only input is at logic 0.That's why it is called and INVERTER	$X = \overline{A}$



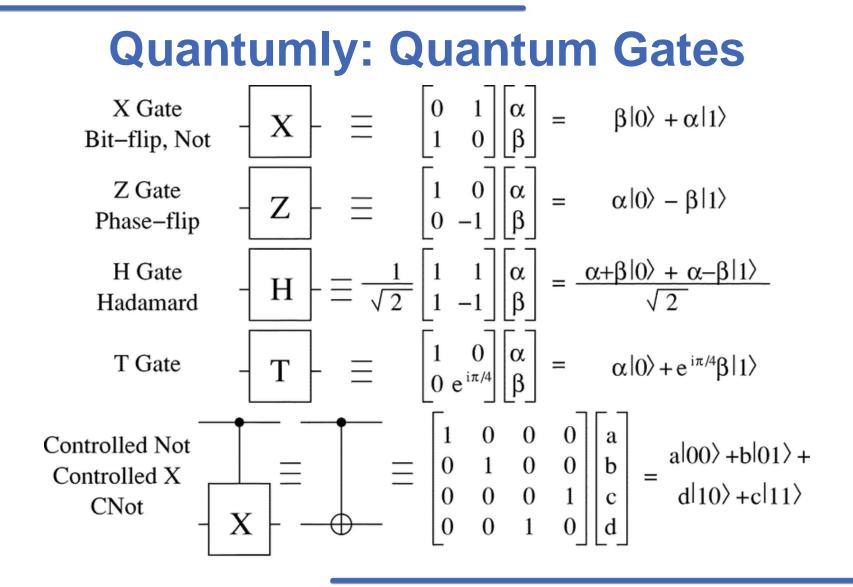
Quantumly

The state change of a closed quantum system is described by a unitary operator











4. Measurement



Classically

Measuring returns the state of a bit with certainty

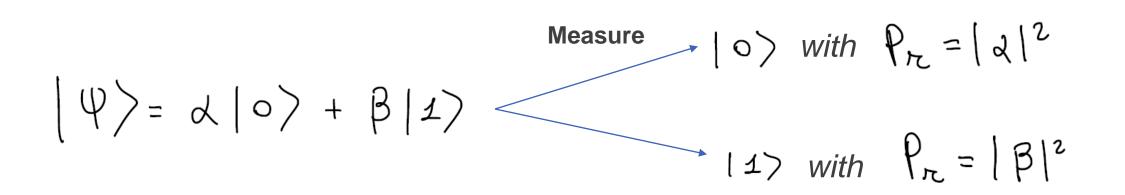


Measurements do not affect the state of a bit



Quantumly

Measuring returns the bit state with some probability



Measurement affects the state of a qubit



Outcome

Quantumly

 To any observable physical quantity is associated an hermitian operator O

$$(| \sigma_i \rangle = \sigma_i | \sigma_i \rangle$$

• A measurement outcomes are the possibile eigenvalues $\{o_i\}$.

 The probability of obtaining o_i as a result of the measurement is

$$P_{r}(\sigma_{i}) = |\langle \Psi | \sigma_{i} \rangle|^{2}$$

• The effect of the measure is to change the state $|\psi\rangle$ into the eigenvector of *O*

$$|\psi\rangle \rightarrow |\sigma_i\rangle$$

When you're a quantum particle in a state of superposition but you're about to pass through a detector

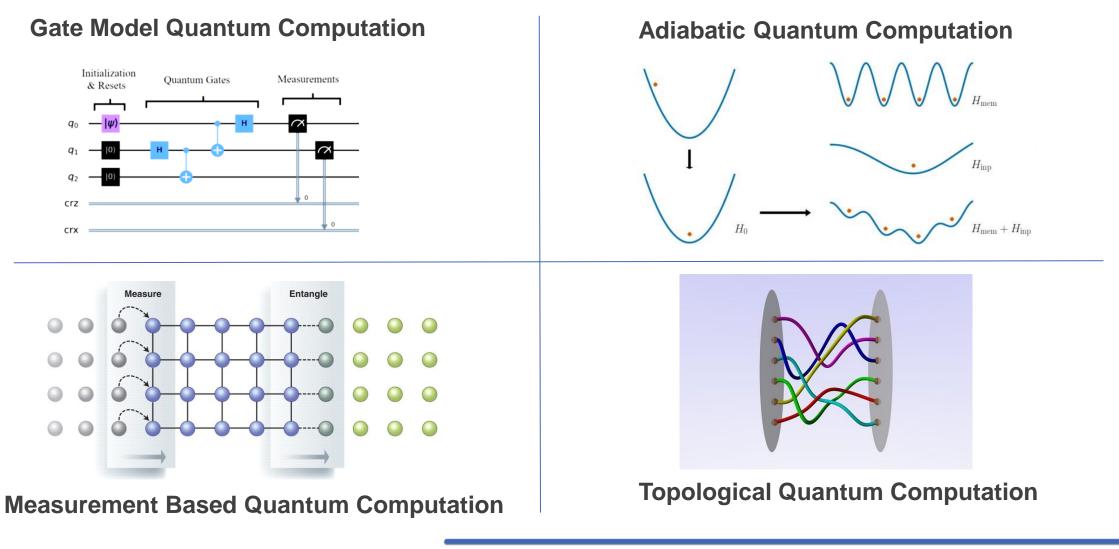




Quantum Computing Models

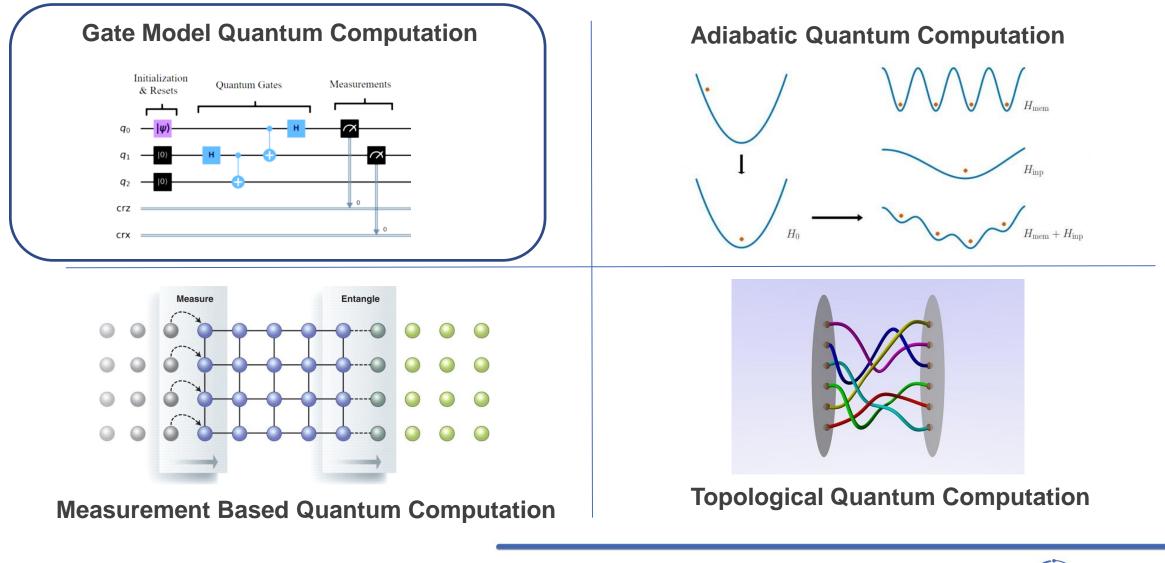


Quantum Computing Models





Quantum Computing Models





Quantum Circuits



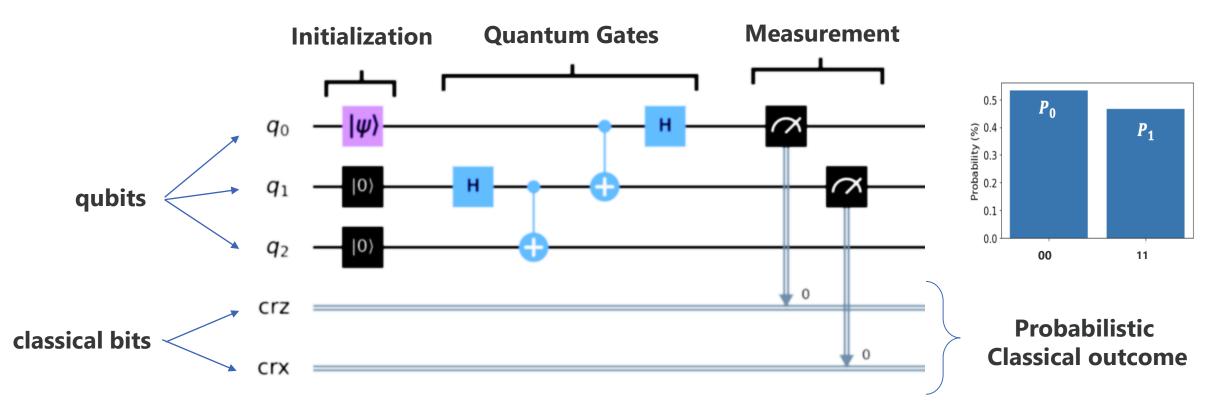
Quantum Algorithm = Quantum Circuit

A quantum circuit with *n* input qubits and *n* output qubits is defined by a unitary transformation

$$\mathcal{J} \in \mathcal{U}(2^{n})$$
 $\begin{pmatrix} U^{\dagger}U = UU^{\dagger} = I \\ U^{-1} = U^{\dagger} \end{pmatrix}$



Quantum Circuits



It is necessary to run the circuit and measure multiple times to reconstruct the probability distribution

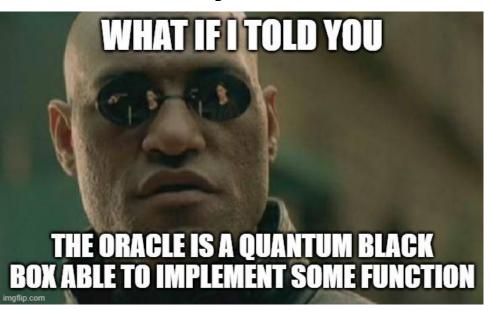






Given a function $f: \{0,1\}^{n} \rightarrow \{0,1\}^{n}$, an algorithm to evaluate such function is given by the unitary \bigcup_{f}

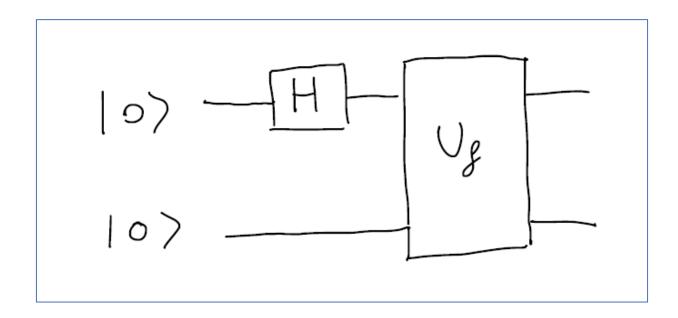
$$\begin{array}{c} (x) | y \rightarrow (x) \\ (x) | y \rightarrow f(x) \\ \text{where} \quad X \in \{0, 1\}^{N} \quad y \in \{0, 1\}^{M} \end{array}$$



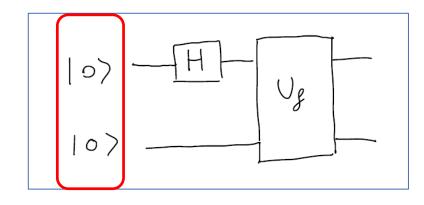


Quantum Parallelism

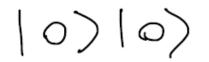
Consider the following quantum circuit



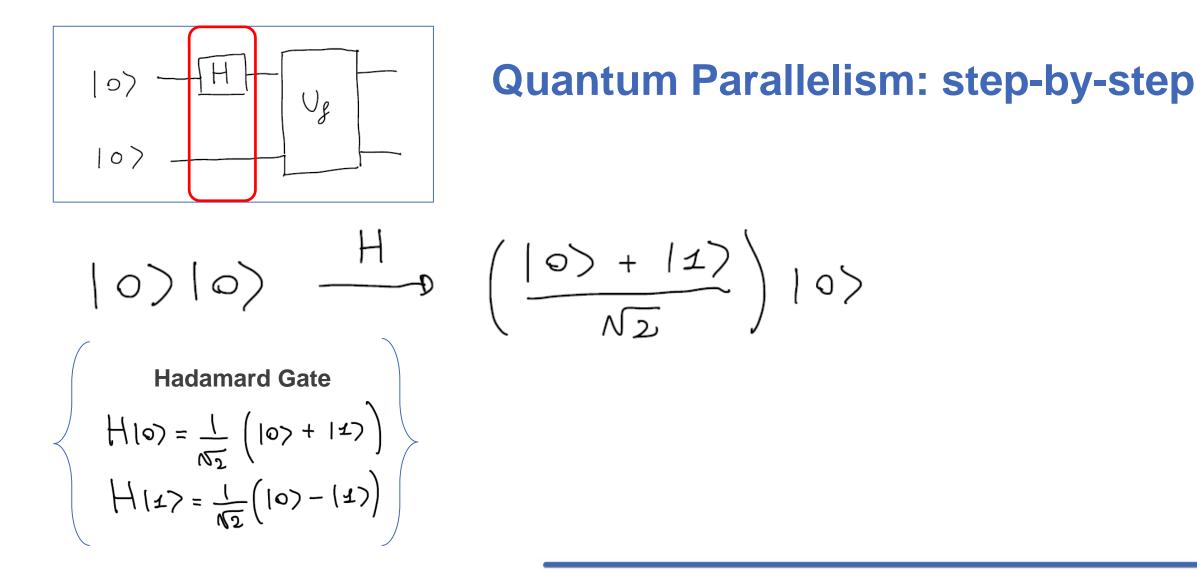




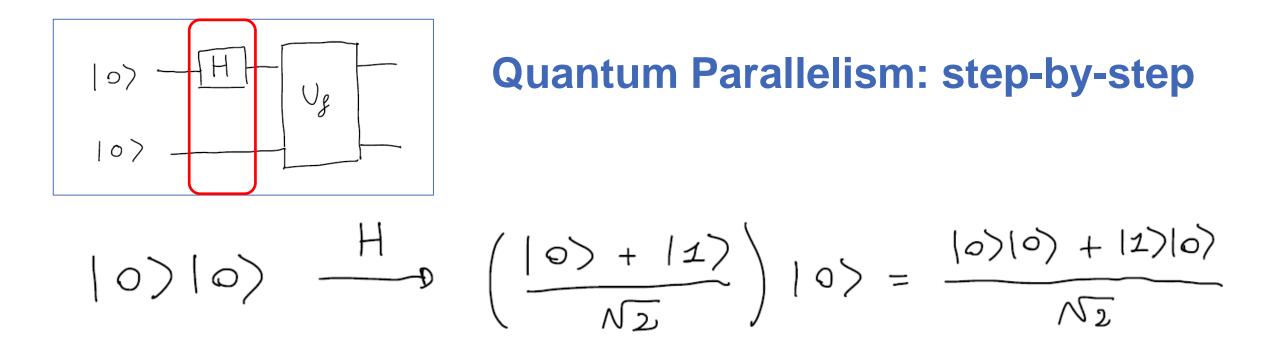
Quantum Parallelism: step-by-step



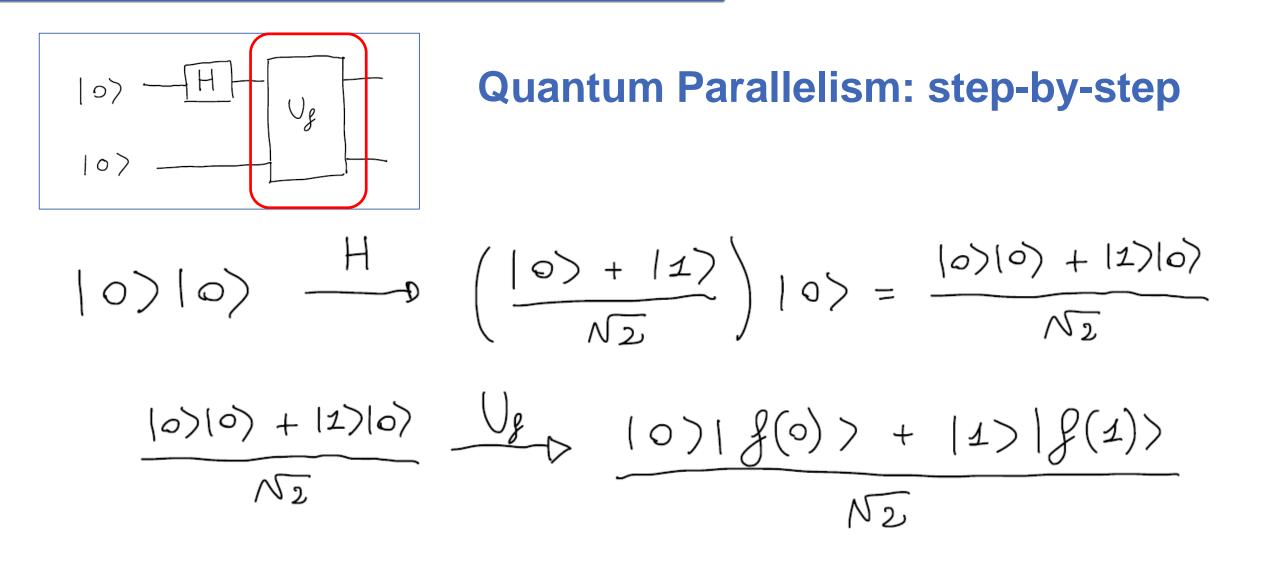




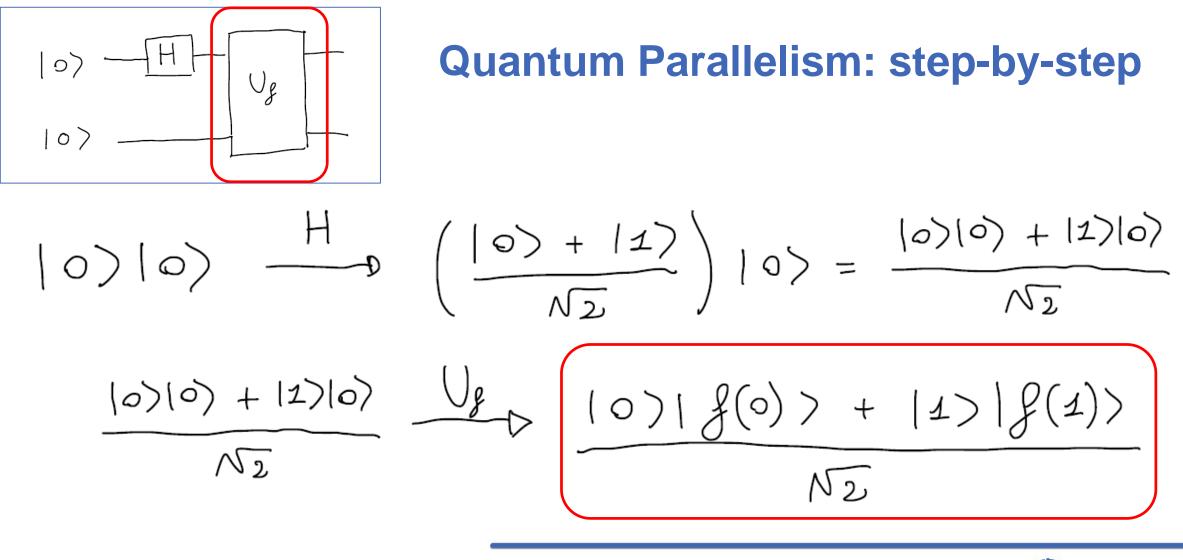














 $|0\rangle|f(0)\rangle + |1\rangle|f(1)\rangle$ N2

This is a remarkable state!

With a single use of the Oracle, we created a quantum superposition containing information about both f(0) and f(1)



$$\frac{10)|f(0)>+|1>|f(1)>}{N_2}$$

This is a remarkable state!

With a **single use of the Oracle**, we created a quantum superposition containing information about both f(0) and f(1)

However, parallelism alone is not **immediately useful!** Measuring would return a random output (either f(0) or f(1)).



Quantum algorithms exploit quantum parallelism to solve some problems faster than classical algorithms



QUANTUM COMPUTERS:

Quantum Algorithms



Facorization Problem

Given \mathbb{N} , find the two prime numbers such that

$$N = p \times q$$

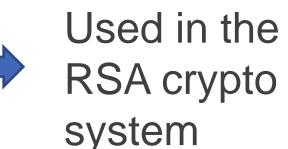


Facorization Problem

Given \mathbb{N} , find the two prime numbers such that

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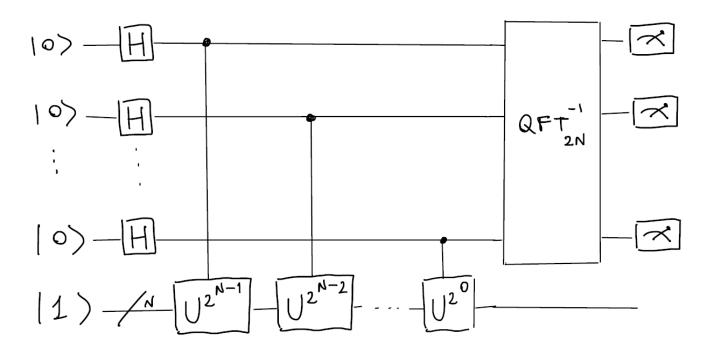
Classically: Finding solution requires exponential time







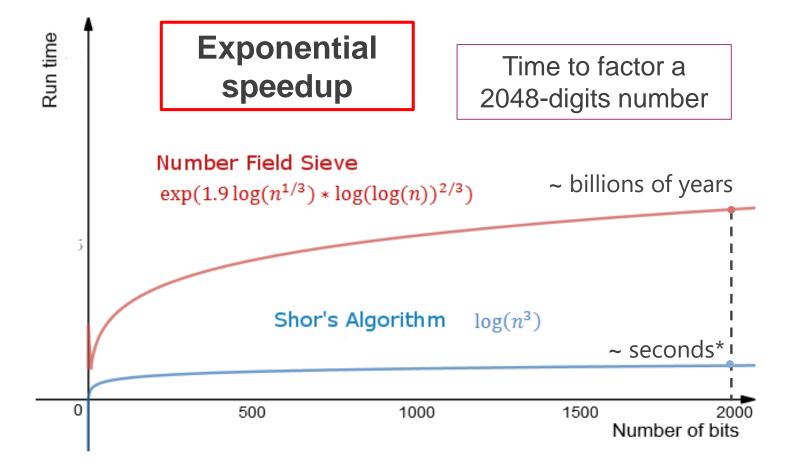
Quantum Algorithm to solve factorization in polynomial time





https://www.youtube.com/watch?v=6qD9XEITpCE



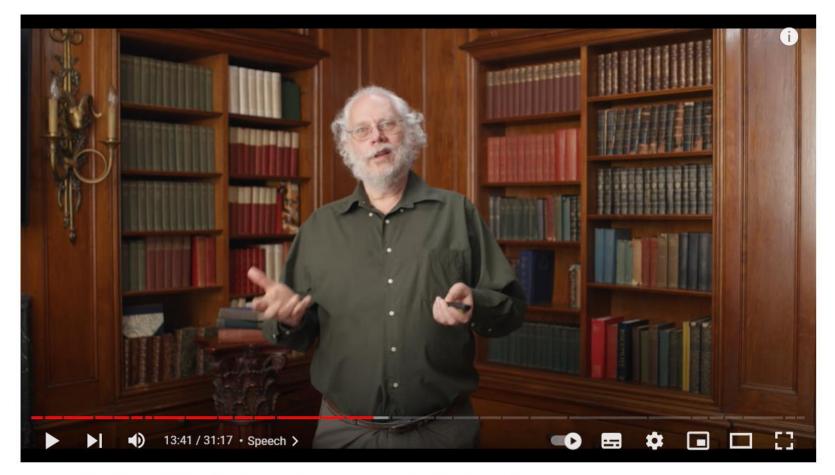




* Assuming we have a fault-tolerant quantum computer capable of executing Shor's algorithm by applying gates at the speed of current quantum computers based on superconducting circuits



https://www.youtube.com/watch?v=6qD9XEITpCE

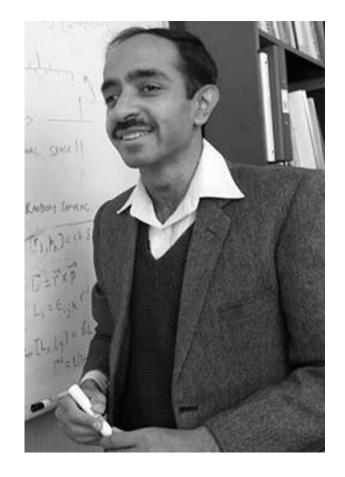


The Story of Shor's Algorithm, Straight From the Source | Peter Shor

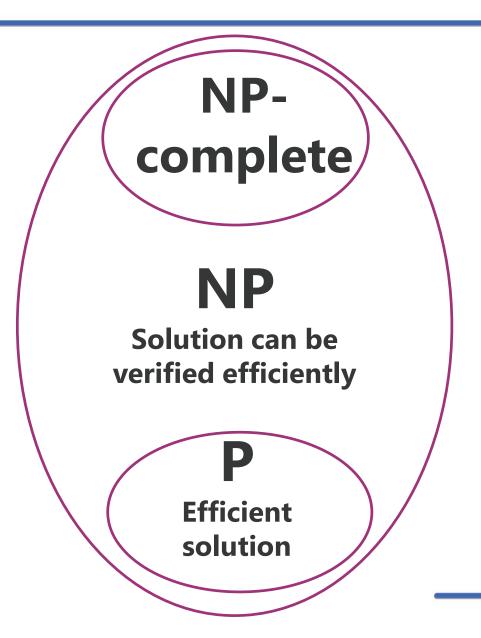


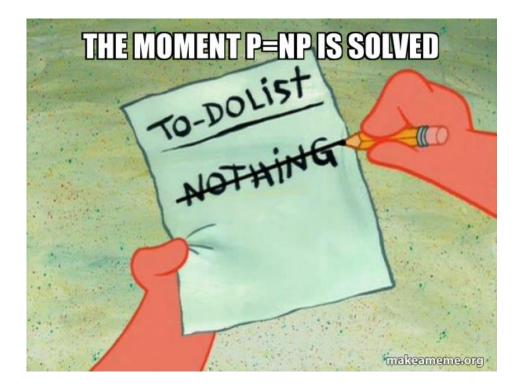
Run-time brute-force algorithm: d^N

Run-time Grover search: $\sqrt{d^N}$

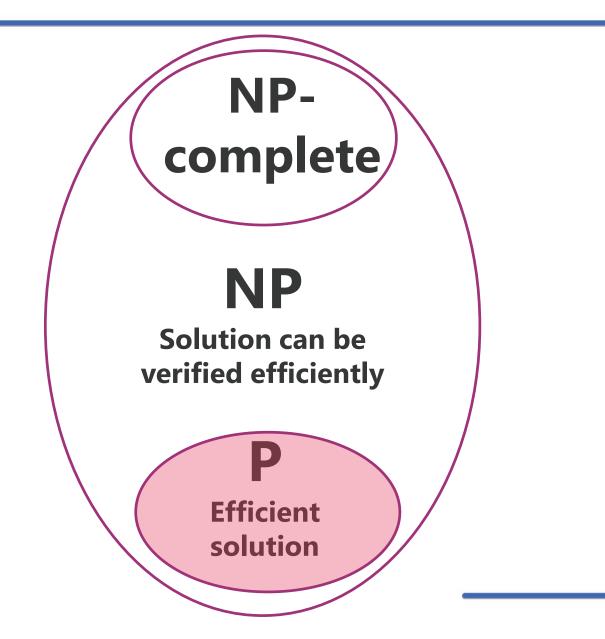




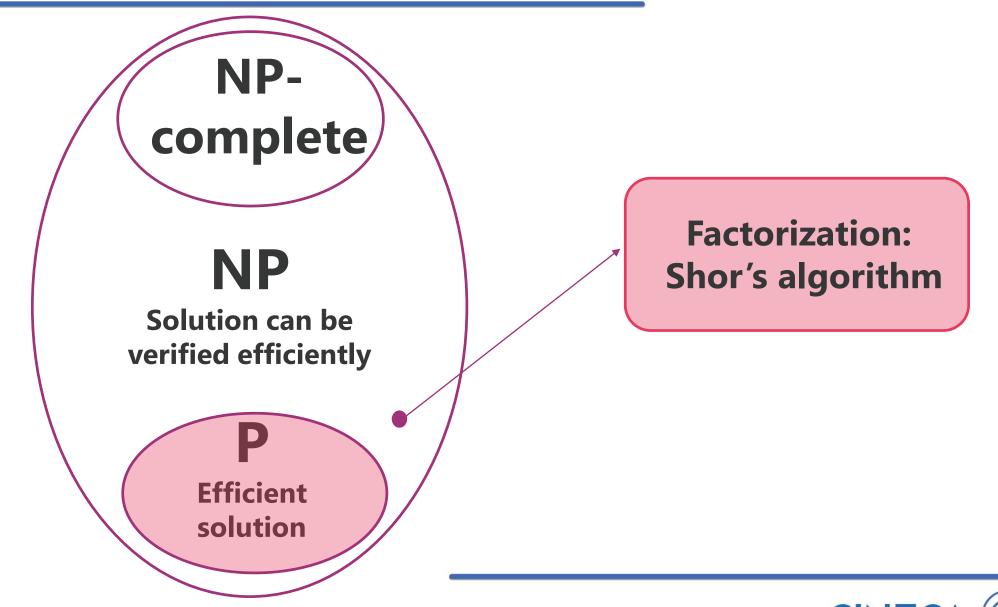




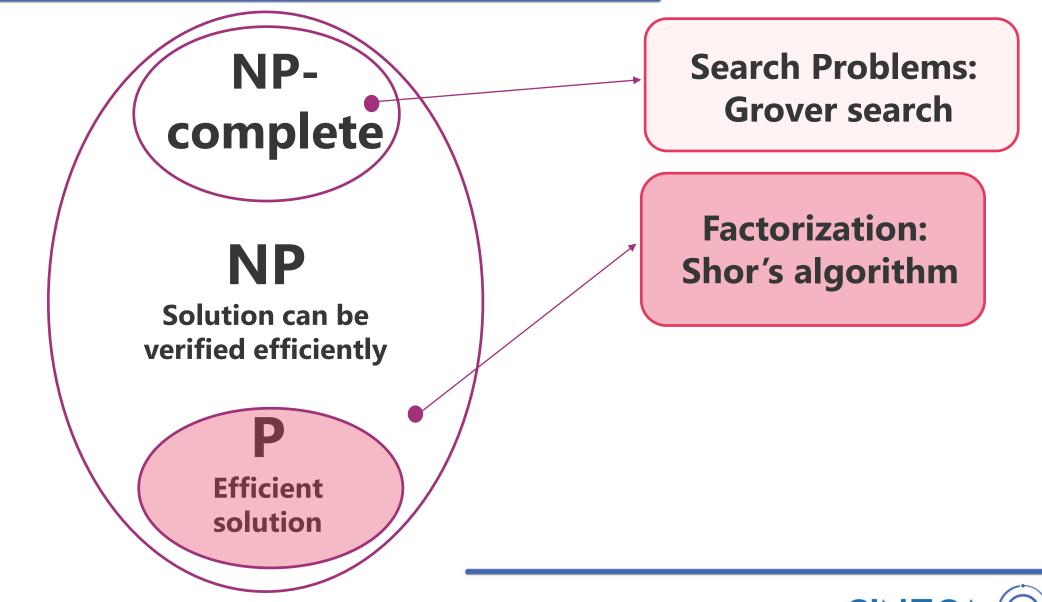




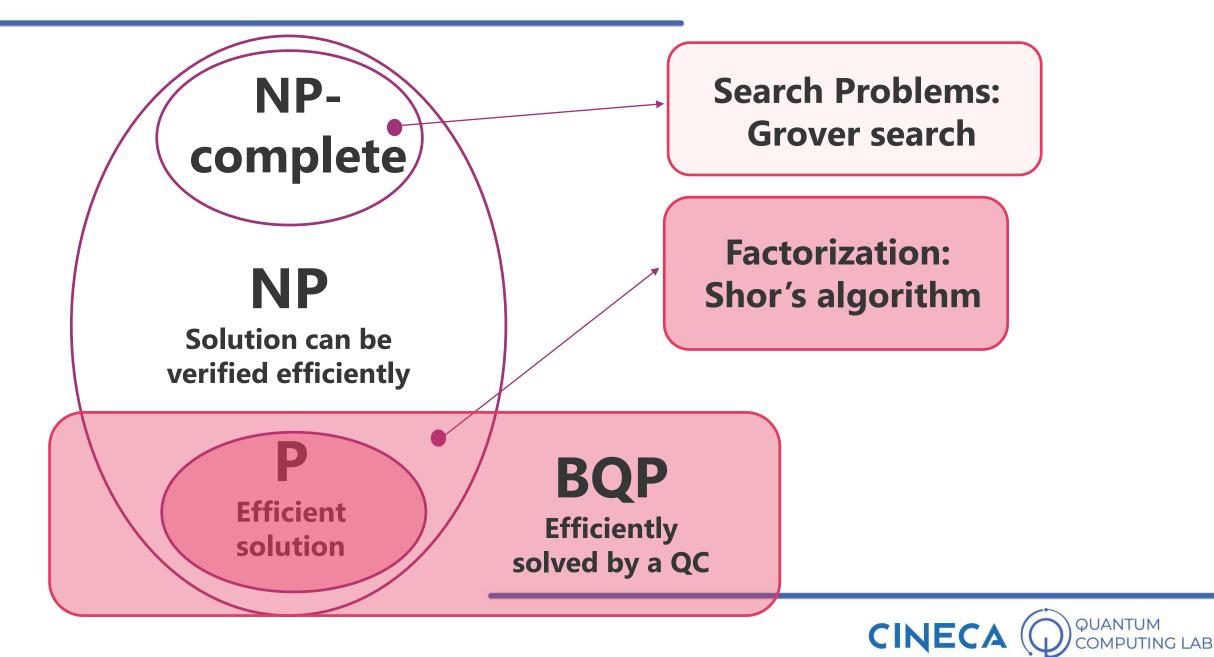


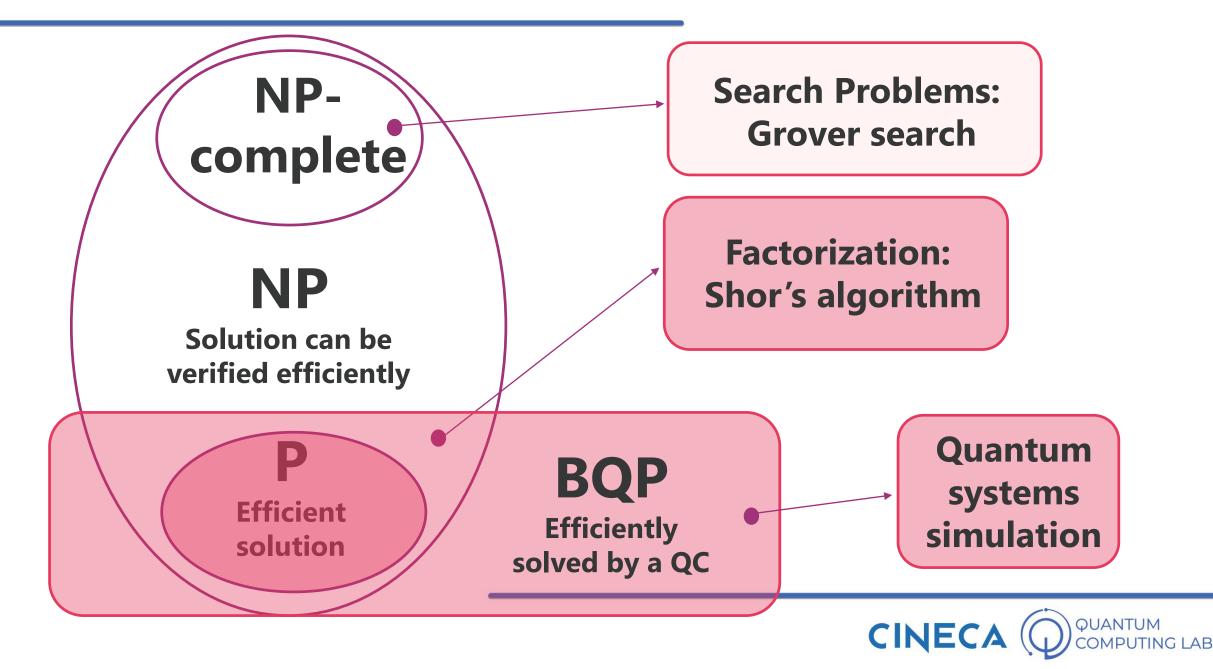


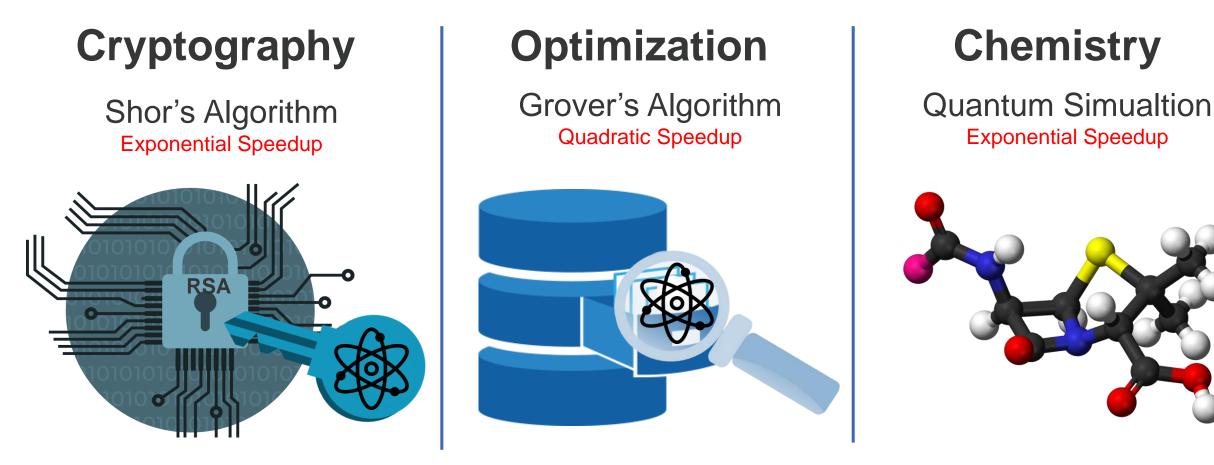












Quantum Algorithm Zoo: https://quantumalgorithmzoo.org/



Cryptography

Shor's Algorithm Exponential Speedup

Optimization

Grover's Algorithm Quadratic Speedup

Chemistry

Quantum Simualtion Exponential Speedup

These algorithms assume to have **ideal qubits** that are **not subjected to noise and errors**

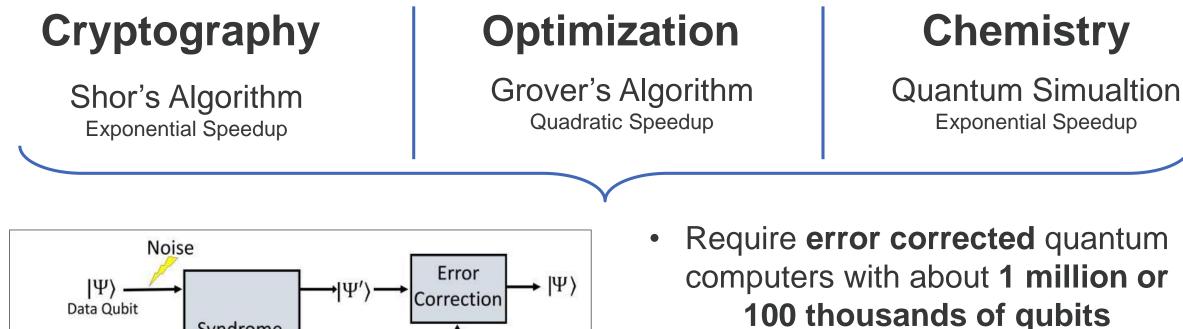
Common sources of errors in QC

- Coherent quantum errors: Gates
 which are incorrectly applied
 - **Decoherence**: errors due to the interaction with the environment
- Initialization errors: failing to prepare the correct initial state
 - Qubit loss



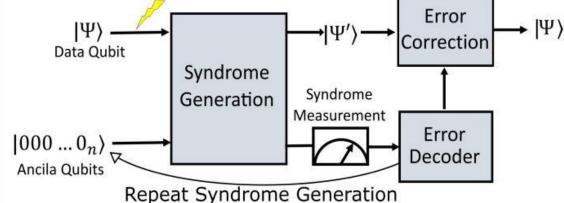
QEC: introductiory guide https://arxiv.org/abs/1907.11157

Old School Quantum Algorithms: Error correction



- Error correction comes with an overhead in the number of physical qubits
 - Will be availabe in 10-20 years





QEC: introductiory guide https://arxiv.org/abs/1907.11157

Old School Quantum Algorithms: Error correction

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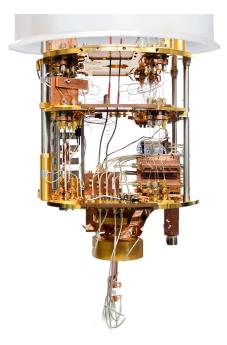
When you see the ratio of physical to logical qubits for fault tolerant quantum computation

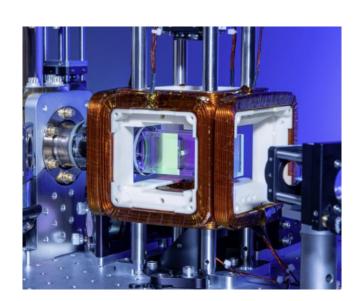


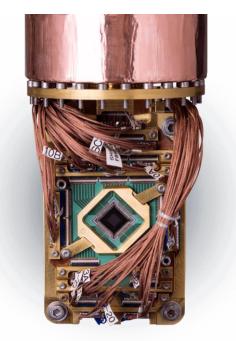
- Require error corrected quantum computers with about 1 million or 100 thousands of qubits
- Error correction comes with an overhead in the number of physical qubits
 - Will be availabe in 10-20 years



How can we use the small and imperfect Quantum Devices (NISQ) we have today?









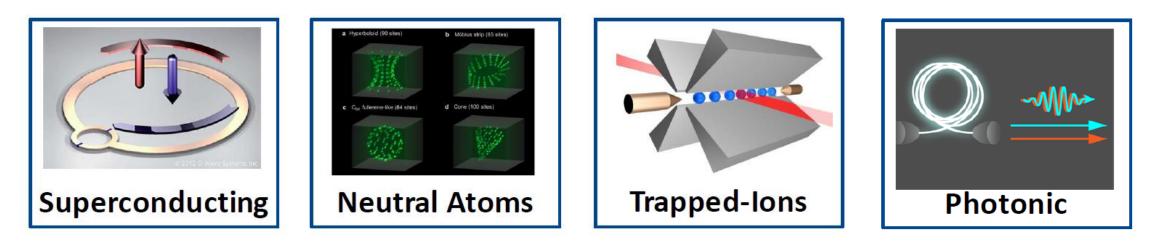
The NISQ Era



NISQ = Noisy Intermediate-Scale Quantum

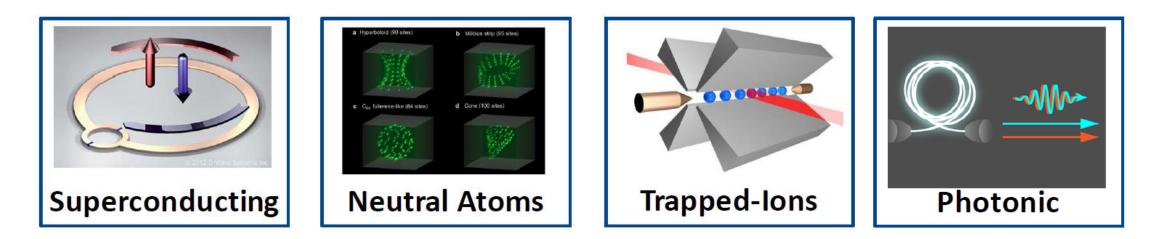
Intermediate-Scale Quantum computers with no error correction

Different Qubit technologies





The NISQ Era



Differences:

Topology: how qubits are connected togerther

Coherence Time (seconds): quantum superposition lifetime

Gate Delay (seconds) : time needed to aplly a gate operation

Gate Fidelity (%) : Fidelity in gate operation



Qubit technologies

	Superconducting	Superconducting	Superconducting	Superconducting
Subtype	Tunable	Fixed Freq.	Parametric	Flux
Coherence Time (seconds)	1.50E-05	1.50E-04	2.00E-05	5.00E-08
Gate Fidelity (%)	99.7%	99.1%	99.2%	
Gate Delay (seconds)	2.0E-08	4.50E-07	1.60E-07	
Environment	20mK	20mK	20mK	20mK
Largest Device	53Q	127Q	80Q	5000Q
Players	Google QuTech Quantum Circuits Inc. IQM SeeQC	IBM OpenSuperQ OQC	Rigetti Bleximo	D-Wave Qilimanjaro

Pros: High gate speeds and fidelities. Can leverage standard lithographic processes. Among first qubit modalities so has a head start.

Cons: Requires cryogenic cooling; short coherence times; microwave interconnect frequencies still not well understood.



https://quantumcomputingreport.com/

Qubit technologies

	Trapped Ions	Trapped Ions
Subtype	Hyperfine	Optical
Coherence Time (seconds)	3	0.2
Gate Fidelity (%)	99.92%	99.6%
Gate Delay (seconds)	2.00E-04	2.0E-04
Environment	Vacuum	Vacuum
Largest Device	32Q	20Q
Notable Players	lonQ Honeywell	AQT AQTION NextGenQ

Pros: Extremely high gate fidelities and long coherence times. Extreme cryogenic cooling not required. lons are perfect and consistent. *Cons*: Slow gate times/ operations and low connectivity between qubits. Lasers hard to

align and scale. Ultra-high

may restrict scalability.

vacuum required. Ion charges



https://quantumcomputingreport.com/

	Photonics	Photonics
Subtype	Si ₃ N ₄	Other
Coherence Time (seconds)		1.50E-04
Gate Fidelity (%)		
Gate Delay (seconds)		1.00E-09
Environment	Ambient, 2K only for Detectors	Ambient, 2K only for Detectors
Largest Device	216 continuos variable Qumode	20 photons
Notable Players	- Xanadu -QuiX	-PsiQ -Orca Computing

Pros: Extremely fast gate speeds and promising fidelities. No cryogenics or vacuums required. Small overall footprint. Can leverage existing CMOS fabs.

Cons: Noise from photon loss; each program requires its own chip. Photons don't naturally interact so 2Q gate challenges.





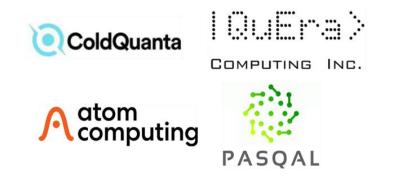


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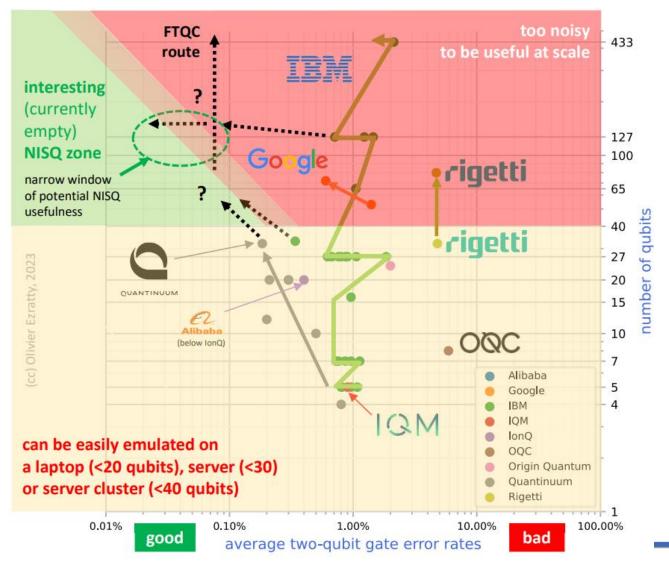
	Neutral Atoms
Coherence Time (seconds)	3.20E-01
Gate Fidelity (%)	Expected to be around 98%
Gate Delay (seconds)	1.00E-06
Environment	Vacuum
Largest Device	200Q
Notable Players	-ColdQuanta -QuEra -Pasqal -Atom Computing

Pros: Long coherence times.
Atoms are perfect and consistent. Strong connectivity, including more than 2Q. External cryogenics not required. *Cons*: Requires ultra-high vacuums. Laser scaling challenging.



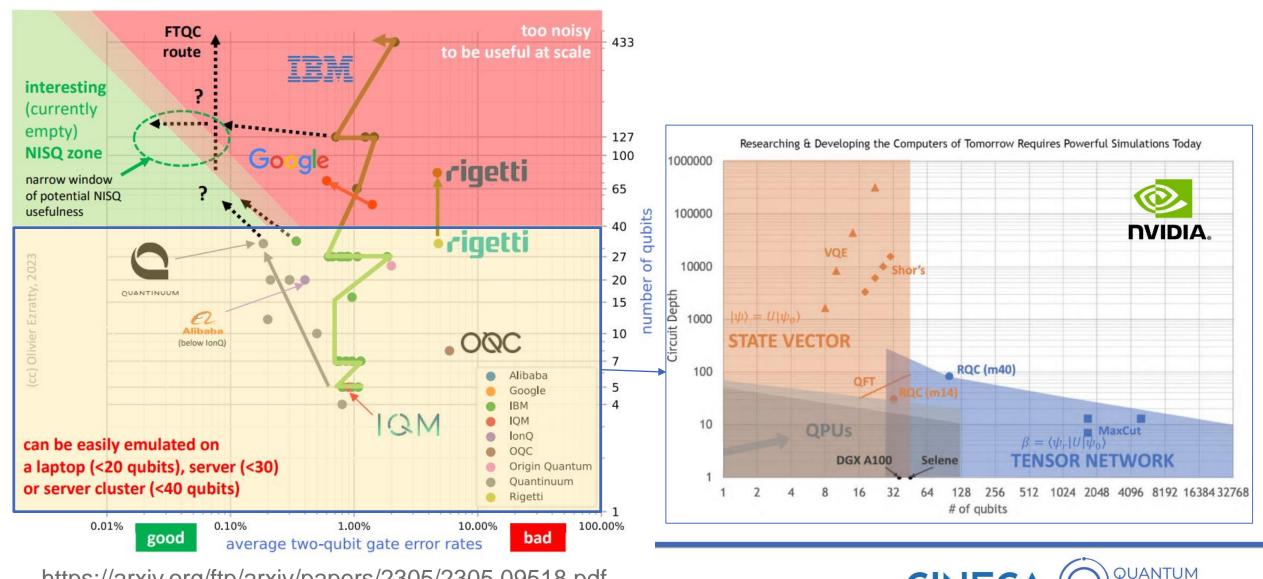


https://quantumcomputingreport.com/



https://arxiv.org/ftp/arxiv/papers/2305/2305.09518.pdf





CINEC

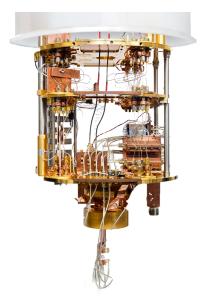
COMPUTING LAB

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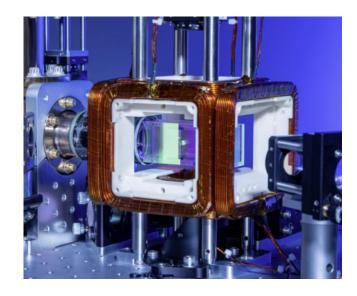
NISQ = Noisy Intermediate-Scale Quantum

Intermediate-Scale Quantum computers with no error correction

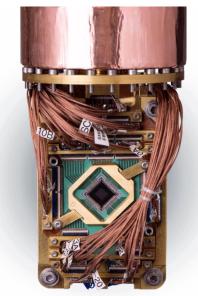
General Purpose QC



Quantum Simulator



Quantum Annealers





Quantum Annealers

Can only run Quantum annealing algorithm

Intermediate-Scale: Up to several thousands of qubits



Noise:

- No need for Quantum Error
 Correction
- Still unclear: noise due to qubit quality could affect scalability (i.e. performance related to large problems)

D-Wave Advantage: 5000 qubits





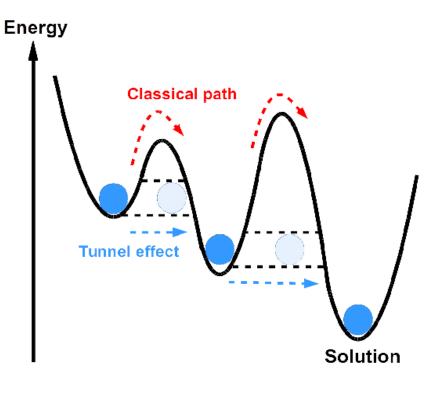
The NISQ Era

Quantum Annealers

Can be used to solve problems
 expressed as QUBO or Ising

$$\sum_{i} h_i \sigma_i^z + \sum_{i < j} J_{ij} \sigma_i^z \sigma_j^z$$

 Use Quantum Tunnelling and Superposition to explore the configuartion space



Quantum Tunnelling

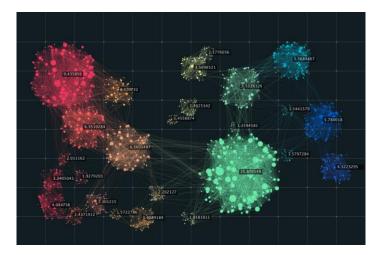


Quantum Annealers

Several real-world hard problems can be formulated as QUBO problems

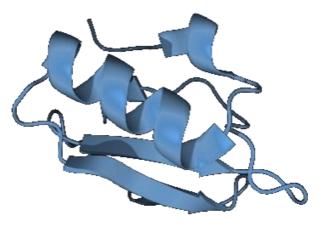
Ising formulation of NP problems: https://arxiv.org/abs/1302.5843

Machine Learning



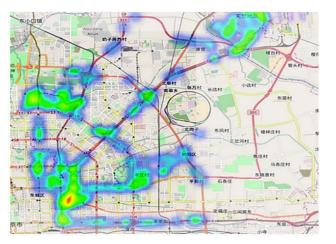
https://arxiv.org/abs/1906.06283

Molecular Dynamics



https://arxiv.org/abs/2107.13607

Scheduling



https://arxiv.org/abs/2006.14162



The NISQ Era

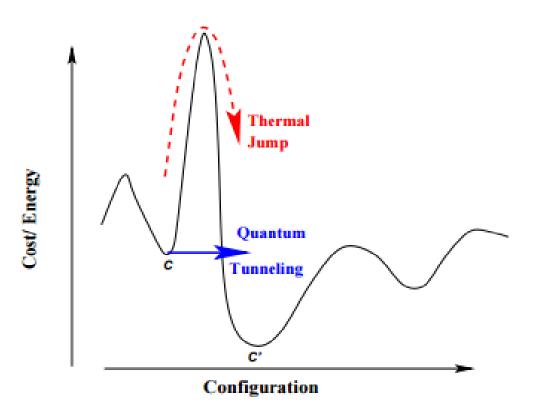
Quantum Annealers

Could have advantage over classical techniques like Simulated Annealing

The transition probability in SA is proportional to
$$e^{-rac{\Delta}{k_BT}}$$

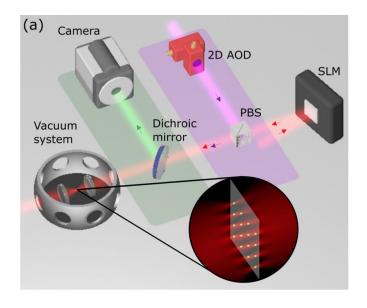
In QA, the strength of transverse field determines the probability of quantum tunneling. The transition probability is proportional to

$$e^{-rac{\sqrt{\Delta}w}{\Gamma}}$$
 with $w\ll\sqrt{\Delta}$

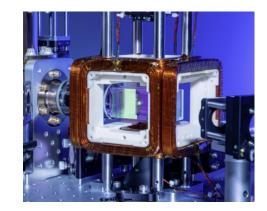




The NISQ Era

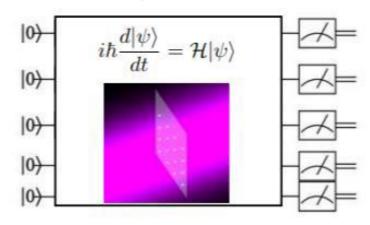


Quantum Simulator



Quantum computing is carried out by directly manipulating the mathematical operator (Hamiltonian) that describes the evolution of the quantum system

Analog processor



https://arxiv.org/abs/2006.12326

$$H = \sum_{i} \frac{\hbar}{2} \left(\Omega(t) \sigma_i^x - \delta(t) \sigma_i^z \right) + \sum_{i < j} U_{ij} \hat{n}_i \hat{n}_j$$

Possible by **varying**:

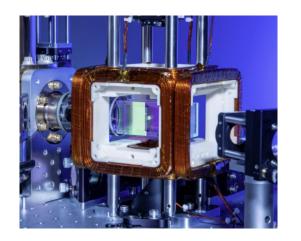
- Intensity and frequency of lasers used to manipulate quantum state
 - Qubit register topology



Quantum Simulator

Can implement a limited set of algorithms

Intermediate-Scale : Up to hundreds of qubits



Noise:

- No Quantum Error Correction: overhead in number of qubit
- Interaction with environment generates errors, this limits the duration of quantum computation

Pasqal: 100 Qubits QuEra: 200 Qubits PASQAL

DUEra>

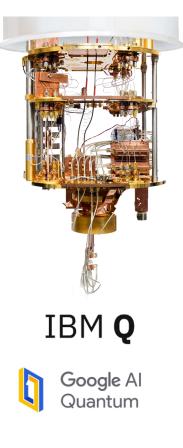


General Purpose QC

Use gates, in theory can run any quantum algorithm

Intermediate-Scale : Up to hundreds of qubits

IBM: 127 Qubits Google: 72 Qubits



Noise:

- No Quantum Error Correction: overhead in number of qubit
- Error rate per single gate affects the depth of the circuit: error rate of 0.1% means that we can run circuits with at most 100 elementary gates (shallow circuits)

CINE



NISQ-ready algorithms

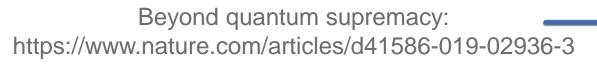
The scientific community believes that NISQ technology could outperform traditional classical computers for specific applications



- Speed up
- Better quality solutions
- Lower energy consumption

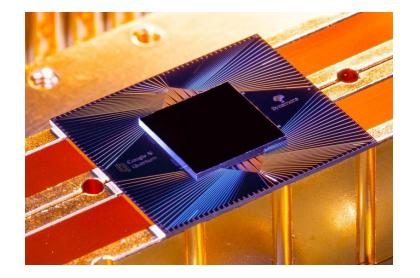


- Quantum Chemistry
- Quantum Optimization
- Quantum AI/Machine Learning





Quantum Supremacy: demonstrating that a programmable quantum device can solve a problem that no classical computer can solve in any feasible amount of time.



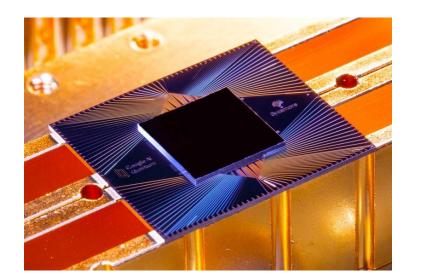
In 2019, researchers at the Google Quantum AI Lab compared the performance of quantum computers to classical supercomputers, using their **Sycamore quantum computer** with **53 qubits.**

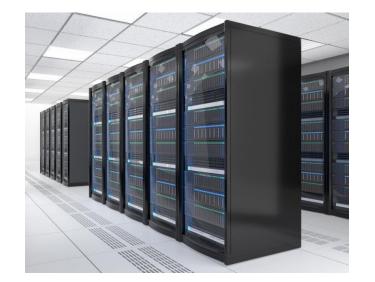
https://www.nature.com/articles/s41586-019-1666-5



Quantum Supremacy: with just 53 qubits, their Sycamore quantum computer was able to run a specific algorithm, called the Random Quantum Circuit (RQC), in 200 seconds. Much less than the 2.5 days estimated to perform the same calculation with most powerful supercomputer.

VS







https://www.nature.com/articles/s41586-019-1666-5

NASA and Google researchers, used a program called qFlex, believed to be the most efficient classic emulator quantum system to implement the RQC algorithm on one of the most powerful supercomputers in the world, Summit.



Lamp for few hours = 0.42KWh

21MWh = 5 families for 1 year

The qFlex implementation required 21 MWh on Summit, while the problem solved by Sycamore device used only 0.42 kWh.

https://arxiv.org/abs/1811.09599



NISQ-ready algorithms

The scientific community believes that NISQ technology could outperform traditional classical computers for specific applications

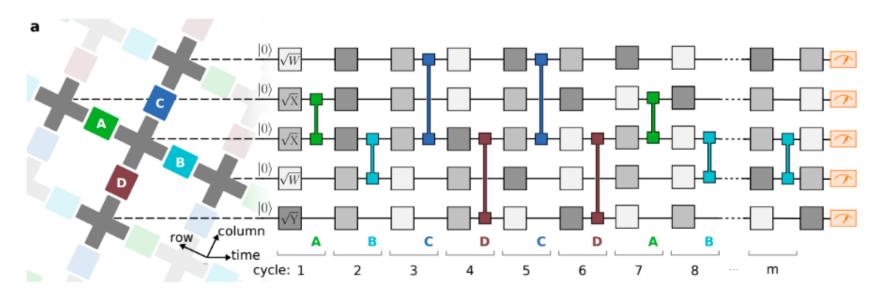
- Speed up
- Better quality solutions
- Lower energy consumption



- Quantum Chemistry
- Quantum Optimization
- Quantum AI/Machine Learning



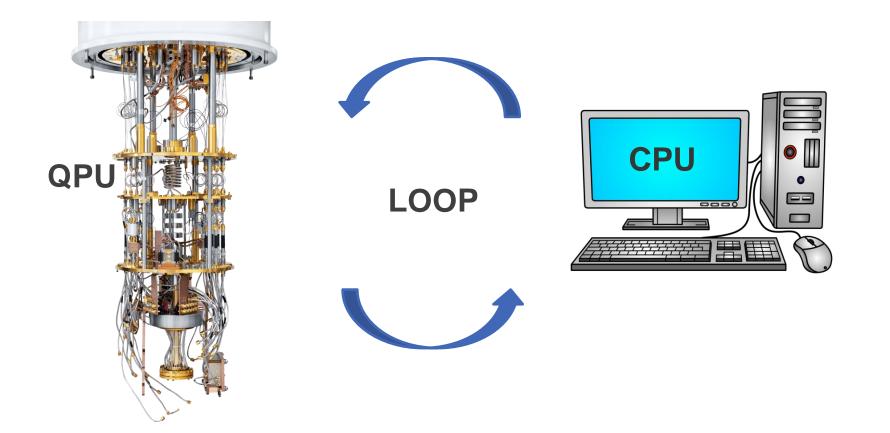
Random Quantum Circuit (RQC) does not solve any useful (real-world) problem. Its purpose is exactly to prove Quantum supremacy



RQC Real World Problems?



Hybrid Quantum-Classical algorithms



Variational Quantum Algorithms: https://arxiv.org/abs/2012.09265



Parametric Quantum Circuits

$\begin{bmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 0$

Quantum Hardware

 Circuits that use gates, or in general, that apply parameterdependent operations to qubits
 (e.g. Arbitrary rotations of angle γ)

 Shallow circuits, i.e. of limited
 depth (1000 gates maximum, due to limited coherence times)

- Circuits in which the error is not corrected

But errors can be mitigated https://arxiv.org/abs/2009.04417



Working principle

Variational Quantum Algorithms: https://arxiv.org/abs/2012.09265



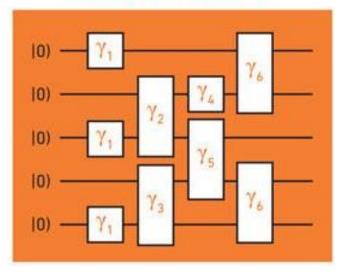
Working principle

1. Choose the parametric circuit you want to use (Variational Ansatz)

2. Implement Variational Ansatz on the QPU

|Ψ**(**θ̃)>

Quantum Hardware



Variational Quantum Algorithms: https://arxiv.org/abs/2012.09265



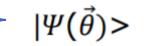
Working principle

1. Choose the parametric circuit you want to use (Variational Ansatz)

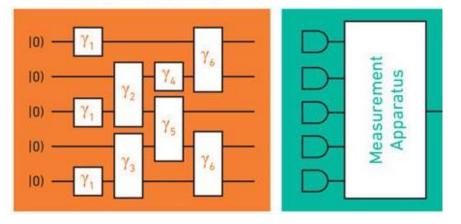
2. Implement Variational Ansatz on the QPU

3. Measure the qubits and calculate the cost function

$$\mathsf{E}_{\vec{\theta}} = < \Psi(\vec{\theta}) |\mathbf{H}| \Psi(\vec{\theta}) >$$



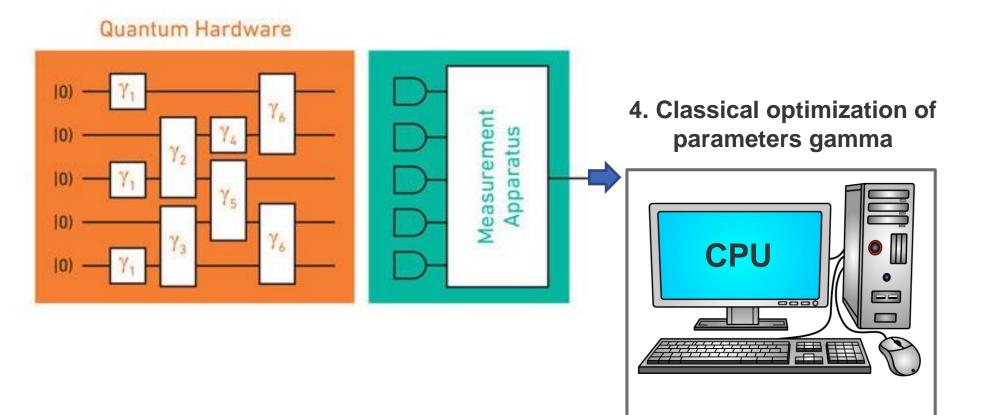
Quantum Hardware



Variational Quantum Algorithms: https://arxiv.org/abs/2012.09265



Working principle



Variational Quantum Algorithms: https://arxiv.org/abs/2012.09265



Working principle

1. Choose the parametric circuit you want to use (Variational Ansatz)

2. Implement Variational Ansatz on the QPU

3. Measure the qubits and calculate the cost function

4. Use a classic computer to optimize the circuit parameters

The **optimization** of the set of parameters could be **gradient-based** or **gradientfree** (BFGS, COBYLA, L-B, SPSA, Bayesian Opt.) Depending on the type of cost function being evaluated

Variational Quantum Algorithms: https://arxiv.org/abs/2012.09265



Working principle

1. Choose the parametric circuit you want to use (Variational Ansatz)

2. Implement Variational Ansatz on the QPU

3. Measure the qubits and calculate the cost function

4. Use a classic computer to optimize the circuit parameters

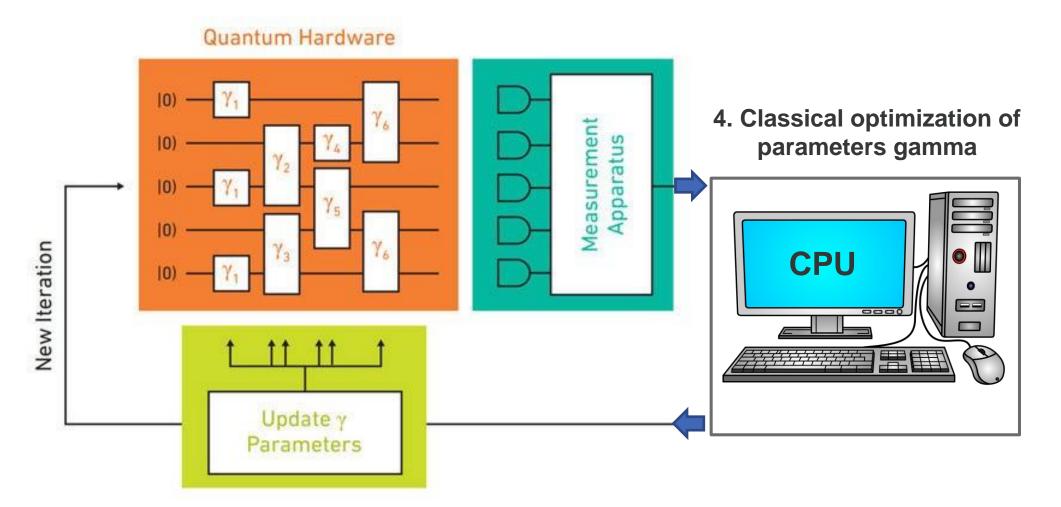
This cycle is repeated until convergence. The final state gives us an approximation of the solution

> Heuristic Algorithm

Variational Quantum Algorithms: https://arxiv.org/abs/2012.09265



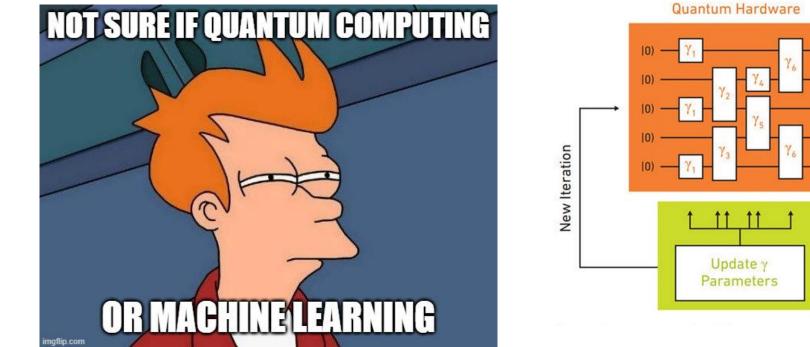
Working principle

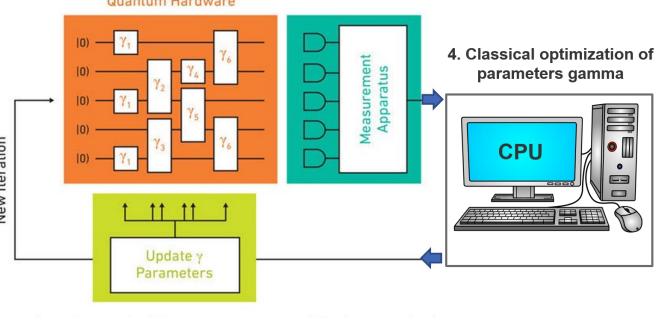


Variational Quantum Algorithms: https://arxiv.org/abs/2012.09265



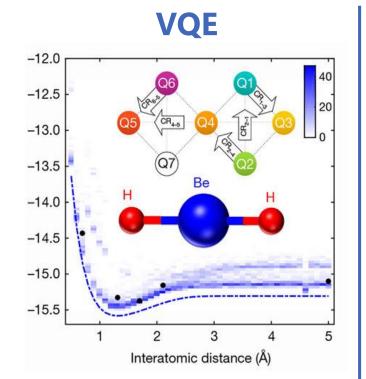
Working principle





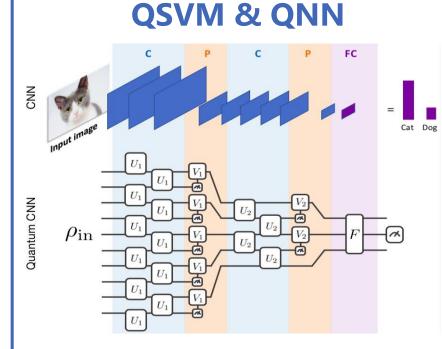
Variational Quantum Algorithms: https://arxiv.org/abs/2012.09265





Quantum Chemistry

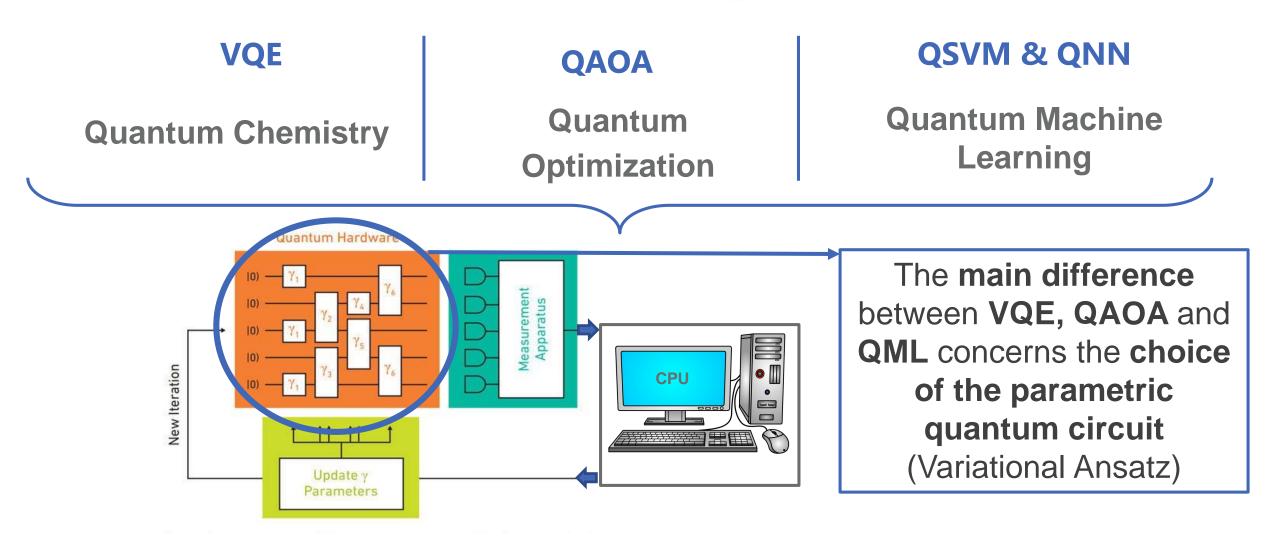
QAOA (a) variational parameters $\vec{\beta}$) = (γ_1 , ..., γ_p , β_1 , ..., β_p) max $\langle H_C \rangle$ |+)+(b) w_{45} w_{13} w_{15} Quantum **Optimization**



Quantum Machine Learning

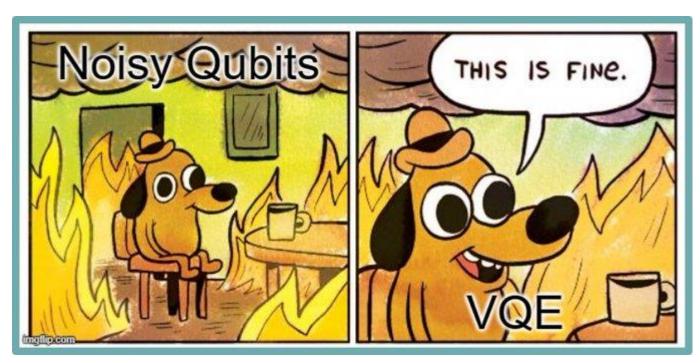


Quantum algorithms for NISQ Devices: General Purpose QC





Variational Quantum Eigensolver (VQE)

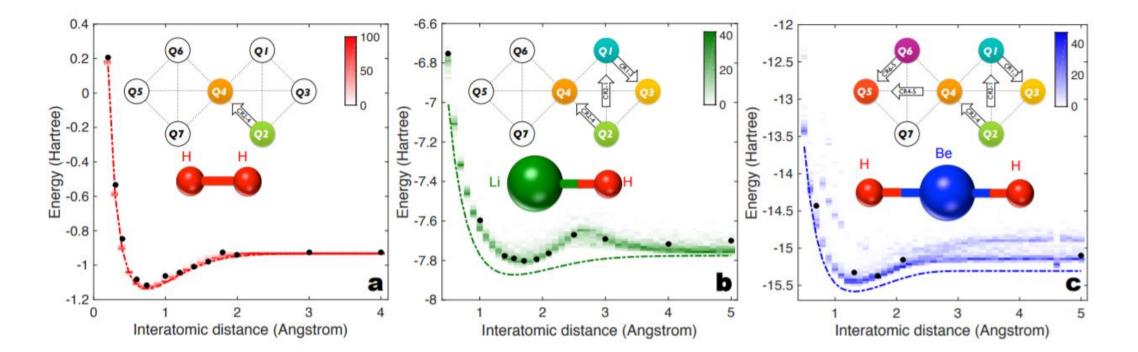


https://arxiv.org/abs/2011.01125



Variational Quantum Eigensolver (VQE) – QUANTUM CHEMISTRY

Objective: finding the ground state energy of molecules





Variational Quantum Eigensolver (VQE) – QUANTUM CHEMISTRY

Objective:

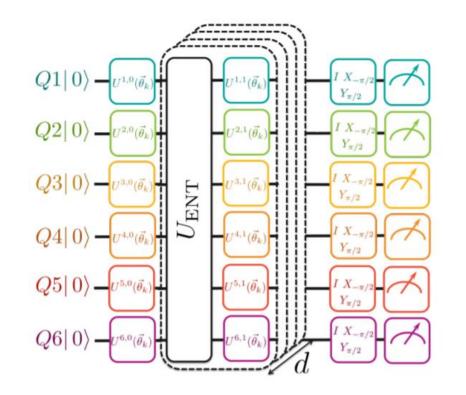
to calculate the ground state of molecules

Method:

Ansatz is a provisional molecular ground state

Possible Advantage:

Simulate complex quantum molecular wavefunctions in polynomial time





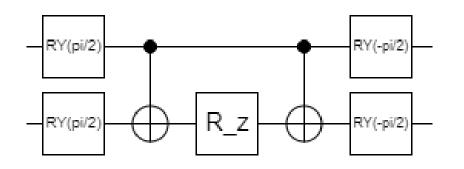
Variational Quantum Eigensolver (VQE) – Ansatz

 $|\psi'\rangle$

VQE uses:

 $|\psi_0\rangle$

 $|\psi_1\rangle$



 $U3(\theta_2, \phi_2, \lambda_2)$

 $U3(\theta_3, \phi_3, \lambda_3)$

Chemical-inspired Ansatz, such as the Unitary Coupled Cluster (UCC) method

(Challenge : may be harder to implement on real hardware)

or a Hardware-efficient Ansatz

(<u>Challenge</u> : easy to implement on hardware but lack of any physical meaning)

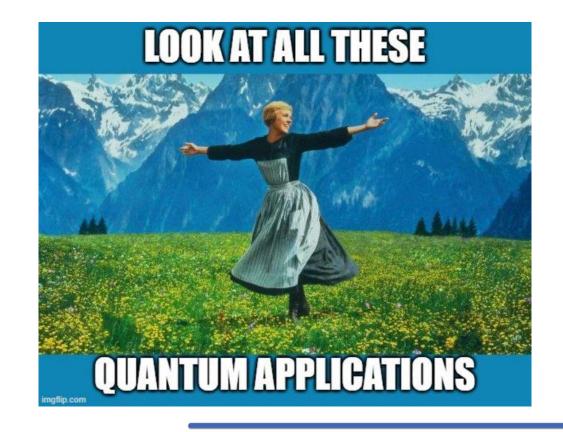
https://arxiv.org/abs/1704.05018

 $U3(\theta_0,\phi_0,\lambda_0)$

 $U3(\theta_1,\phi_1,\lambda_1)$



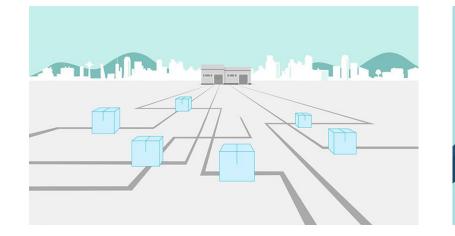
Quantum Approximate Optimization Algorithm (QAOA)





Quantum Approximate Optimization Algorithm (QAOA) – QUANTUM OPTIMIZATION

Optimization Problems



Routing



Scheduling



Portfolio Optimization



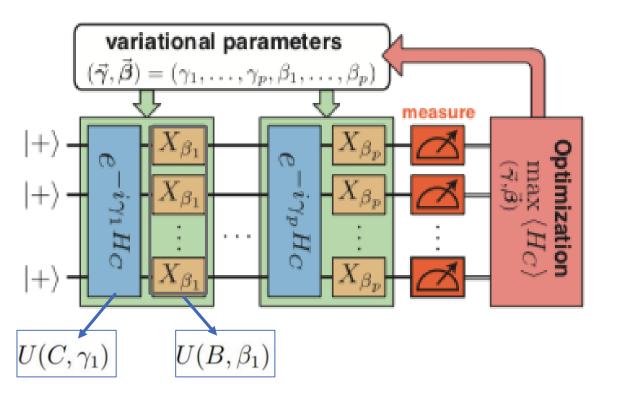
Quantum Approximate Optimization Algorithm (QAOA) – QUANTUM OPTIMIZATION

Objective: to solve a combinatorial optimization problem

<u>Method</u>: Ansatz encodes two alternating circuits, U(C) and U(B), each parameterized by a number, γ and β.

Ideally, the circuit provides the solution
 |γ,β> to a combinatorial problem implicit
 in the definition of U(C).

A Quantum Approximate Optimization Algorithm: https://arxiv.org/abs/1411.4028 $|\boldsymbol{\gamma},\boldsymbol{\beta}\rangle = U(B,\beta_p) U(C,\gamma_p) \cdots U(B,\beta_1) U(C,\gamma_1) |s\rangle$





Quantum Approximate Optimization Algorithm (QAOA) – QUANTUM OPTIMIZATION

$$\begin{array}{c} |\boldsymbol{\gamma},\boldsymbol{\beta}\rangle = U(B,\beta_p) \, U(C,\gamma_p) \cdots U(B,\beta_1) \, U(C,\gamma_1) \, |s\rangle \\ & & & & & & \\ & & & & & \\ & & & & & & & \\ & & & & & & \\ & &$$

$$U(C,\gamma) = e^{-i\gamma C} = \prod_{\alpha=1}^{m} e^{-i\gamma C_{\alpha}}$$

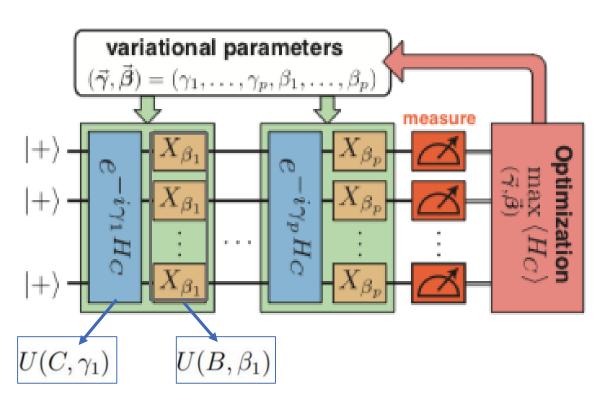
Encodes the optimization problem to solve

(e.g. C could be some Qubo problem)

$$U(B,\beta) = e^{-i\beta B} = \prod_{j=1}^{n} e^{-i\beta\sigma_{j}^{x}}$$

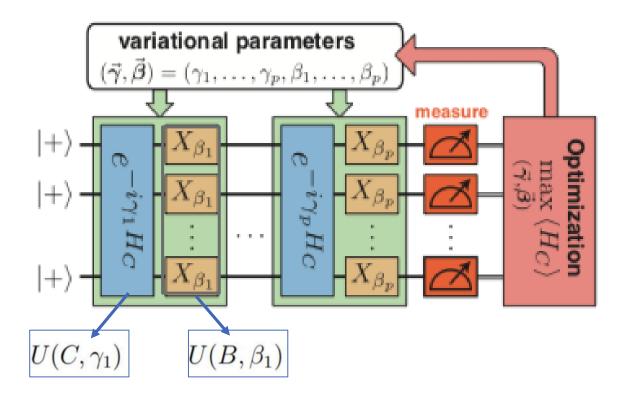
Possible Advantage:

Allow the quantum exploration of the solution space



Quantum Approximate Optimization Algorithm (QAOA) – QUANTUM OPTIMIZATION

<u>Challenge</u>: find a class of problems for which QAOA is strictly better than the best classical algorithms.



A Quantum Approximate Optimization Algorithm: https://arxiv.org/abs/1411.4028



Quantum Machine Learning (QML)



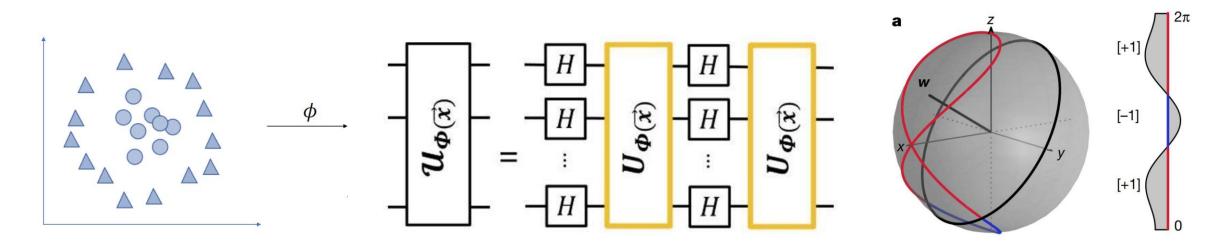


Quantum Machine Learning (QML) – Quantum Feture Map

Quantum Feature map maps classical vector

into a quantum state

$$\vec{x} \mapsto |\Phi(\vec{x})\rangle = \mathcal{U}_{\Phi(\vec{x})}|0\rangle^{\otimes n}$$



Quantum enhanced feature spaces: https://arxiv.org/abs/1804.11326



Quantum Machine Learning (QML) – Quantum SVM

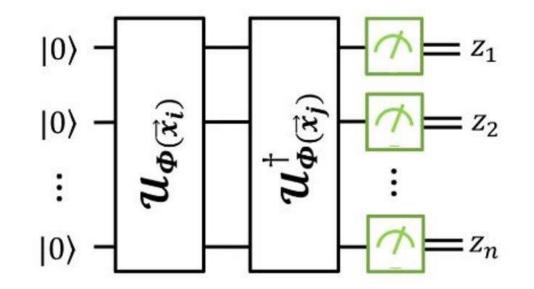
Quantum Kernel 🔿

$$K(\vec{x}_i, \vec{x}_j) = \left| \langle \Phi(\vec{x}_i) | \Phi(\vec{x}_j) \rangle \right|^2 = \left| \langle 0 | \mathcal{U}_{\Phi(\vec{x}_j)}^{\dagger} \mathcal{U}_{\Phi(\vec{x}_i)} | 0 \rangle^{\otimes n} \right|^2$$

<u>Goal</u>: Address a classification problem (like classical SVMs)

Challenge: More complex feature map at low computational cost

Quantum enhanced feature spaces: https://arxiv.org/abs/1804.11326





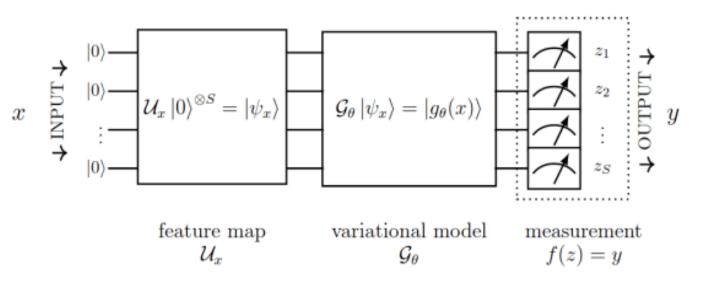
Quantum Machine Learning (QML) – Quantum NN

Goal: Address a supervised machine learning problem

Method: Ansatz consists of a feature map that serves to represent classical data and a variational part for learning

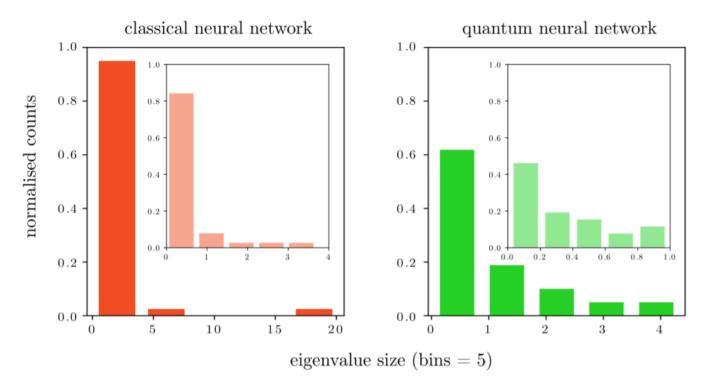
The power of quantum neural networks https://arxiv.org/abs/2011.00027

- **Feature map**: Store the inputs in a quantum state
- Variational circuit: Learnable parameter circuit
- Expectation value: Measurements introduce non-linearity



Quantum Machine Learning (QML) – Quantum NN

The Power of QNNs



More evenly spread eigenvalues of the Fisher information for the QNN wrt classical NN with same number of parameters

Ţ

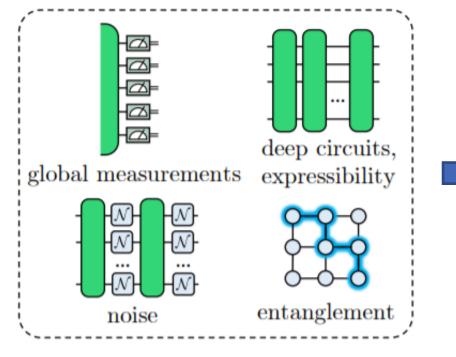
Better Generalization (how accurately the algorithm is able to predict outcome values for previously unseen data.)

The power of quantum neural networks https://arxiv.org/abs/2011.00027

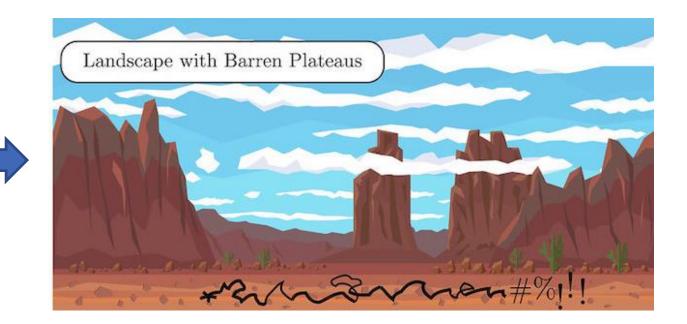


Quantum Machine Learning (QML) – Quantum NN

Barren Plateaus: Vanishing loss function Gradient that make it hard to train the QNN



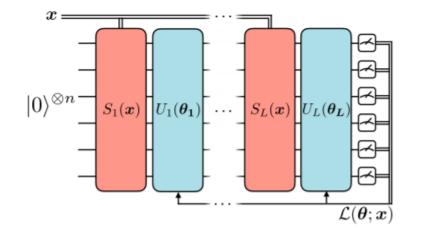
Features that may induce Barren Plateaus

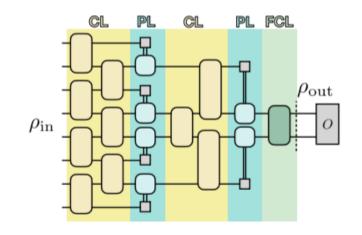


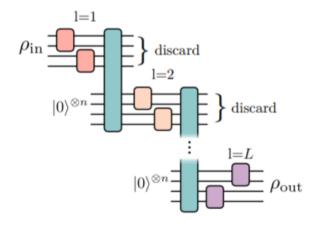
Subtleties in the trainability of QML models: https://arxiv.org/pdf/2110.14753.pdf



Quantum Machine Learning (QML) – Quantum NN







Re-Uploding QNN

Universal function approximator

https://arxiv.org/abs/2009.00298

Convolutional QNN

Absence of Barren Plateaus https://arxiv.org/abs/2011.02966

Dissipative QNN

Backpropagation-like training

https://arxiv.org/abs/1902.10445

Quantum computing models for NN https://arxiv.org/abs/2102.03879



QUANTUM ADVANTAGE IN THE NISQ ERA?



NISQ gate-based hardware resource requirements

resources	initial estimates	realistic estimates and constraints			
qubit number	50 qubits for a computational advantage (Preskill)	100s to 1000s qubits for many practical NISQ algorithms to obtain a speedup advantage (Guerreschi, Albino).			
computing depth	use shallow algorithms with under 10-gate cycles	most NISQ algorithms in the quantum advantage regime have >100s gate cycles			
available fidelities	NISQ is to use currently available qubit fidelities that are in the 99.9% to 99% range	current QPUs either have low fidelities and >30 qubits (transmons) or better fidelities and <30 qubits (trapped ions)			
required fidelities	error rate $\ll \frac{1}{\# \ qubits * algo \ depth}$ for QAOA, but seemingly for other NISQ algorithms as well <u>https://iopscience.iop.org/article/10.1088/2058- 9565/abae7d</u> error rate usually relates to the two-qubit error rate, which should ideally be its minimum error rate and not median/average rate.	the fidelities requirements are not matched by actual hardware even for the shallowest computing depth 1/(1121 q * 8 d) => 99,99% possible? 1/(127 q * 8 d) => 99,9% IBM Heron's 133 qubit QPU in 2024? 1/(65 q * 8 d) => 99,8% not available. 1/(53 q * 8 d) => 99,7% Google Sycamore is at 98,6%. minimum ansatz depth of 8 gate cycles			

https://arxiv.org/ftp/arxiv/papers/2305/2305.09518.pdf









PENNYLANE







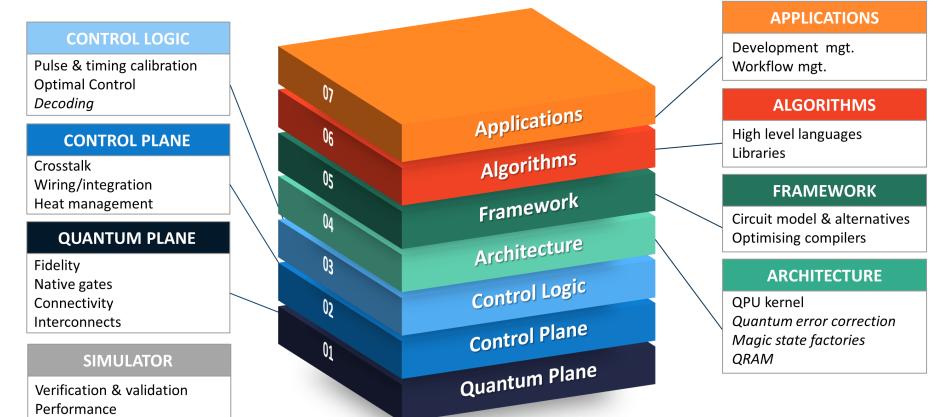
Qiskit



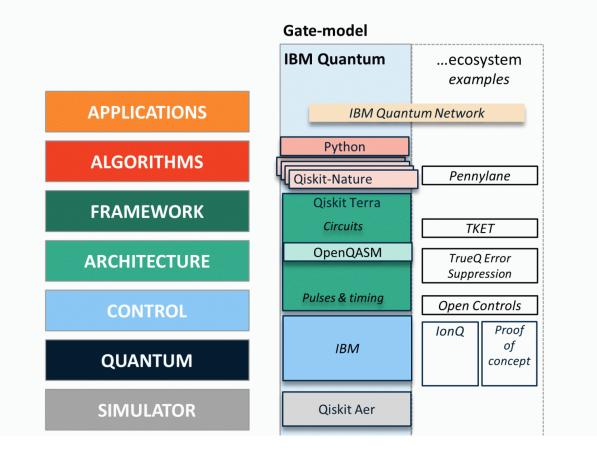


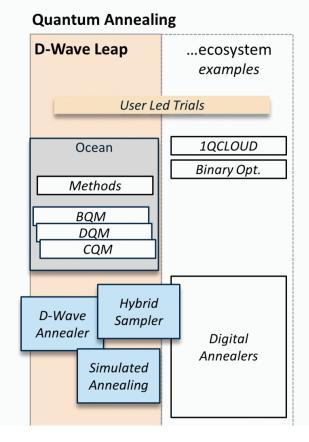


The quantum stack



Quantum pioneers



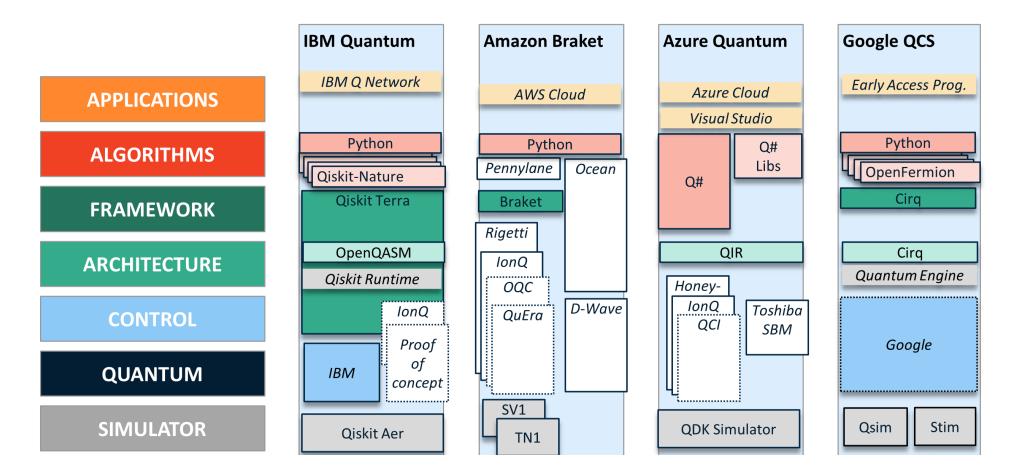


Early gate-model full-stack players

	IBM Quantum	Google QCS	Rigetti QCS	Xanadu	OriginQ Cloud	Pasqal
APPLICATIONS	IBM Q Network	Early Access Prog.		TensorFlow PyTorch NumPy	Industry Alliance	
ALGORITHMS	Python	Python	Python	Python	C++	Python
	Qiskit-Nature	OpenFermion	Grove	Pennylane	ChemiQ	
FRAMEWORK	Qiskit Terra	Cirq	pyQuil	Strawberry Fields	QPanda	
	Circuits					
ARCHITECTURE	OpenQASM	Cirq	Quil	Blackbird	QRunes	Pulser
ARCHITECTORE	Qiskit Runtime	Quantum Engine	Quantum Kernel			
CONTROL	Pulses & timing		Quil-T			
CONTROL		Casala		Xanadu	OriginQ	
QUANTUM	IBM	Google	Rigetti			Pasqal
SIMULATOR	Qiskit Aer	Qsim Stim	QVM	CV Simulators	GPUEmulator	QuTiP based



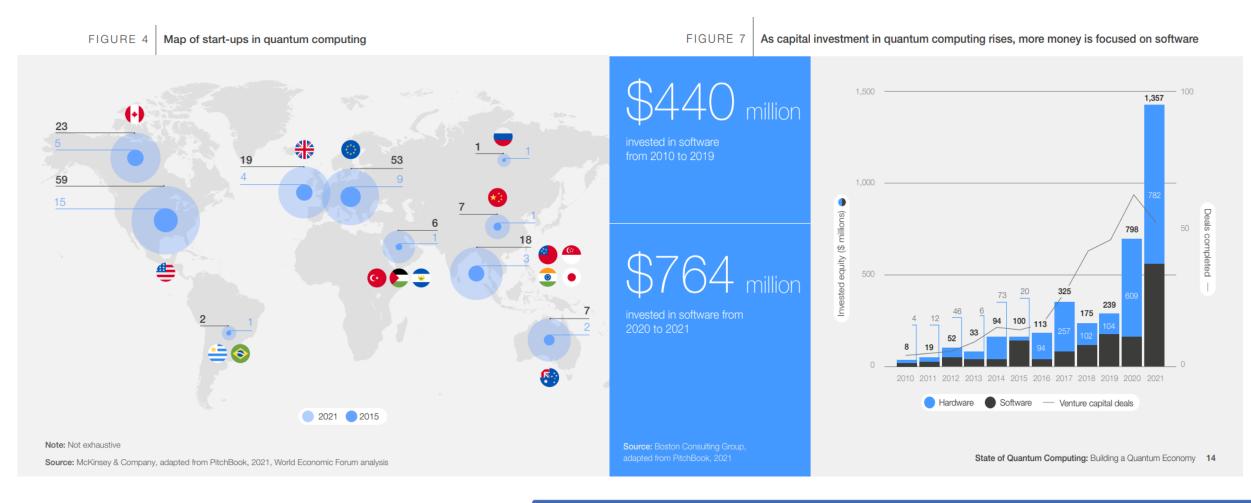
Quantum PaaS (Platform as a Service)







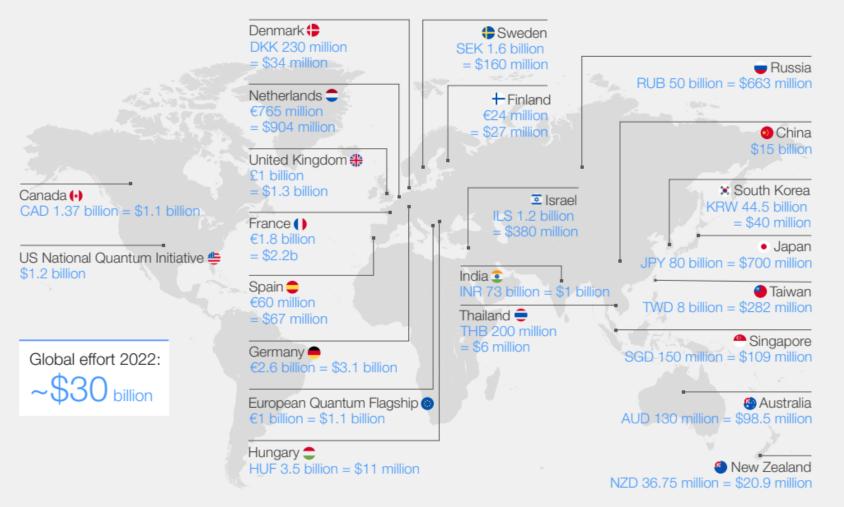
Startup and Private companies



https://www3.weforum.org/docs/WEF_State_of_Quantum_Computing_2022.pdf

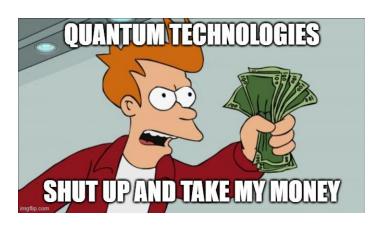






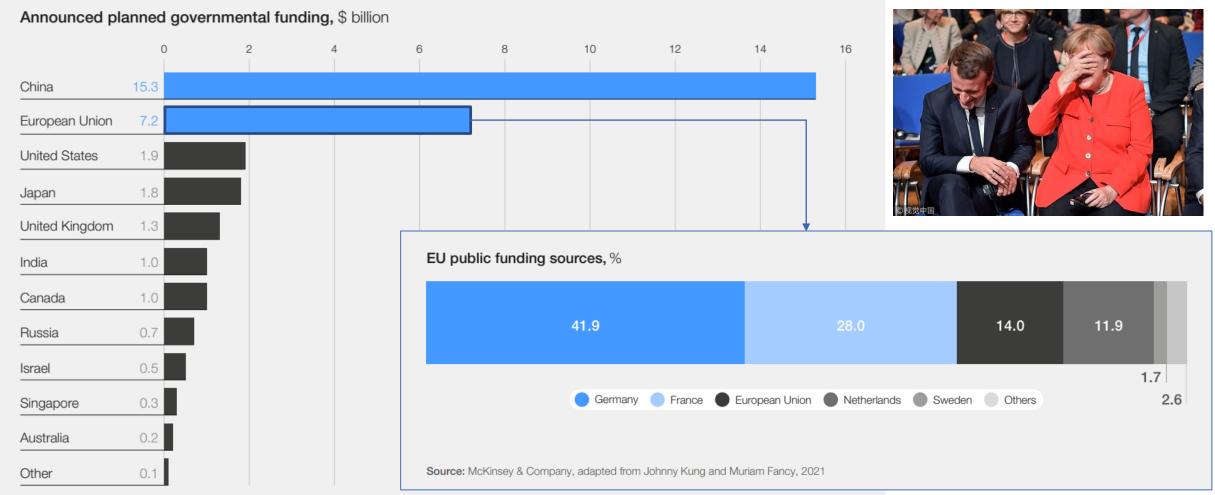
Map of global public investments in quantum technologies

> Global effort: 30 Billion dollars





Public investments



QUANTUM

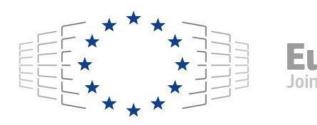
OMPUTING

LAB

CINEC/

https://www3.weforum.org/docs/WEF_State_of_Quantum_Computing_2022.pdf







- May 2016: The Manifesto, addressed to the European Commission, said in essence: we have the opportunity to compete for a new kind of technological independence, let's take it.
- October 2018: The European Commission launched the Quantum Flagship program: 1.3 billions of Euro to support 10 year of quantum technologies research and development.
- The European High Performance Computing Joint Undertaking (EuroHPC JU) is a joint initiative between the EU, European countries and private partners to develop a World Class Supercomputing Ecosystem in Europe.
- The European Processor Initiative (EPI) is a project whose aim is to design and implement a roadmap for a new family of low-power European processors for extreme scale computing, high performance Big-Data and a range of emerging applications.



The **HPCQS** consortium was born with the idea of combining HPC and QC hardware and software.

For the realization of Quantum Computers, the French company PASQAL was chosen, which produces quantum computers based on Neutral Atoms technology

During the 4 years of the project, the most efficient way to connect Pasqal computers to EuroHPC supercomputers will be studied.

The ultimate goal of the project is the creation of an interconnected network of quantum computers throughout Europe, able to communicate with each other and through the support of EUROHPC supercomputers.

(HPC|@S)



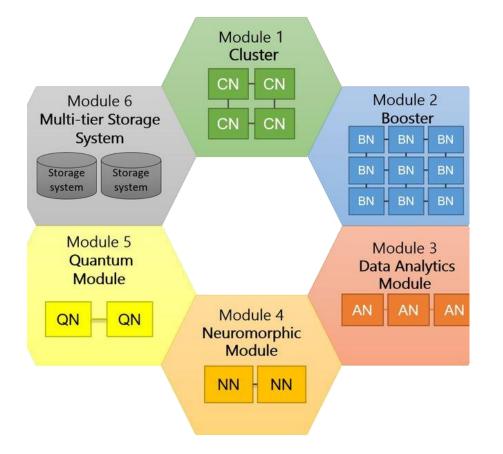
https://www.hpcqs.eu/



Modular Supercomputer Architecture

- Integrate the QPU as a new module into the supercomputer
- Low-latency connection to other modules via federated, high-speed network
- Integration in the scheduling and resource management on the system level

(HPC @S)











Projects and Fundings: ITALY

• ISCRA-C: Quantum Computing as a Service

D-Wave Quantum Annealer

- Since 01/03/2021 possibility to request calculation hours to be used on D-Wave quantum machines
- More than 15 projects already approved (almost fully allocated monthly calculation hours budget)

Scientific collaboration with Pasqal

- On 03/15/2021 start of scientific collaboration with Pasqal's Neutral Atoms simulation systems
- Preliminary preparation phase for future collaboration

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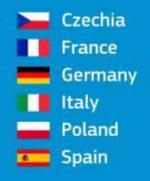
ISC

https://www.hpc.cineca.it/services/iscra





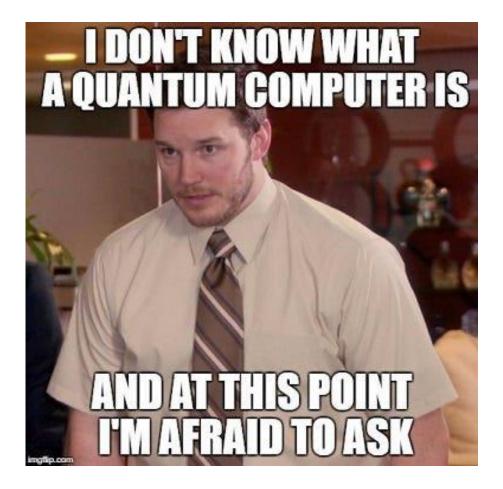
The EuroHPC JU has selected six sites across the European Union to host and operate the first EuroHPC quantum computers in:





https://eurohpc-ju.europa.eu/selection-six-sites-host-first-european-quantum-computers-2022-10-04_en

I hope you don't feel like this..





CINECA: Italian HPC center CINECA Quantum Computing Lab:

- Support research Universities, Industries and QC startups
- Internship programs, Courses and Conference (HPCQC)

https://www.quantumcomputinglab.cineca.it



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