Introduction to Quantum Computing Day 4 – QC with Neutral Atoms and NISQ devices

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24 June 2021



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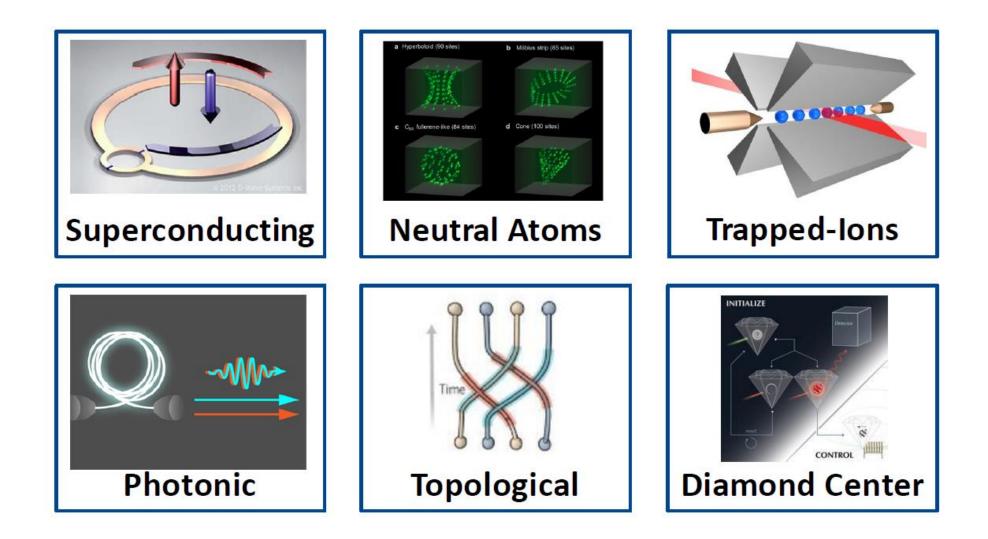
- Intro and Recap
- Pasqal Quantum Hardware: QC with Neutral Atoms
- Pulser: Control Software for Pasqal QC
- Quantum algorithms for NISQ Devices
- Application: QAOA & MIS problem



Intro and Recap

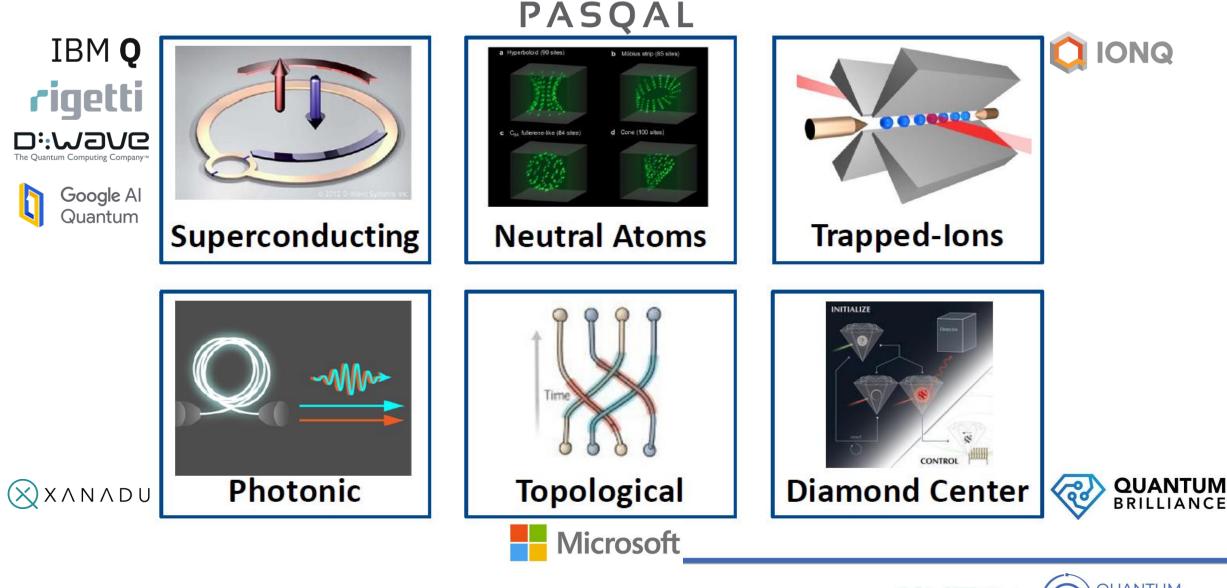


Hardware state of the art – qubit physical realization

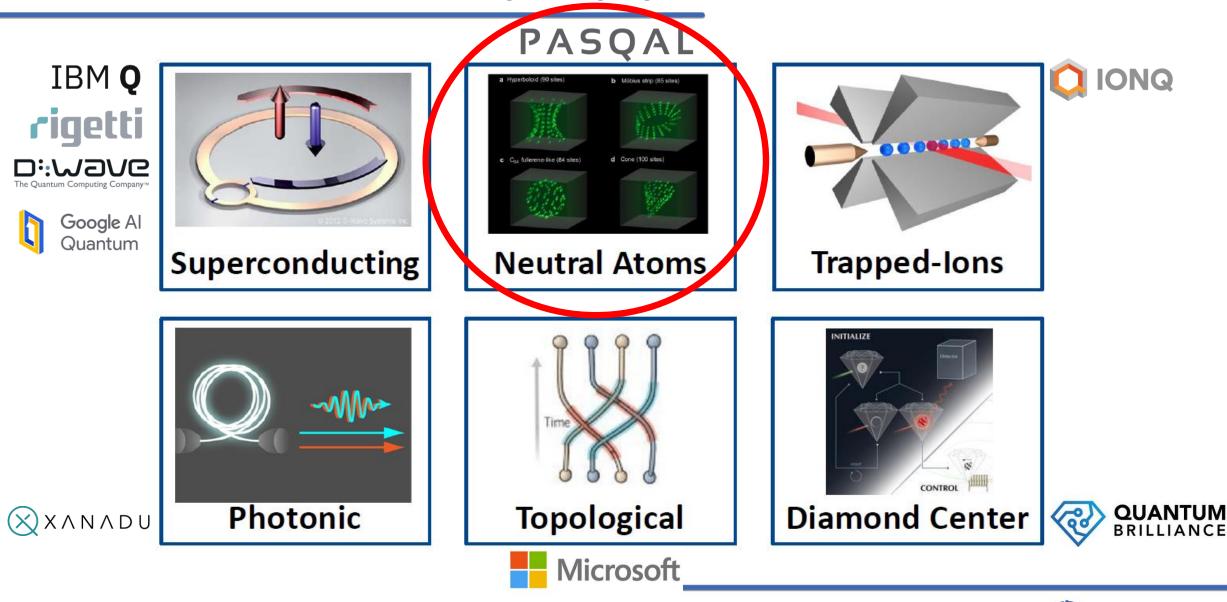




Hardware state of the art – qubit physical realization



Hardware state of the art – qubit physical realization



QUANTUM

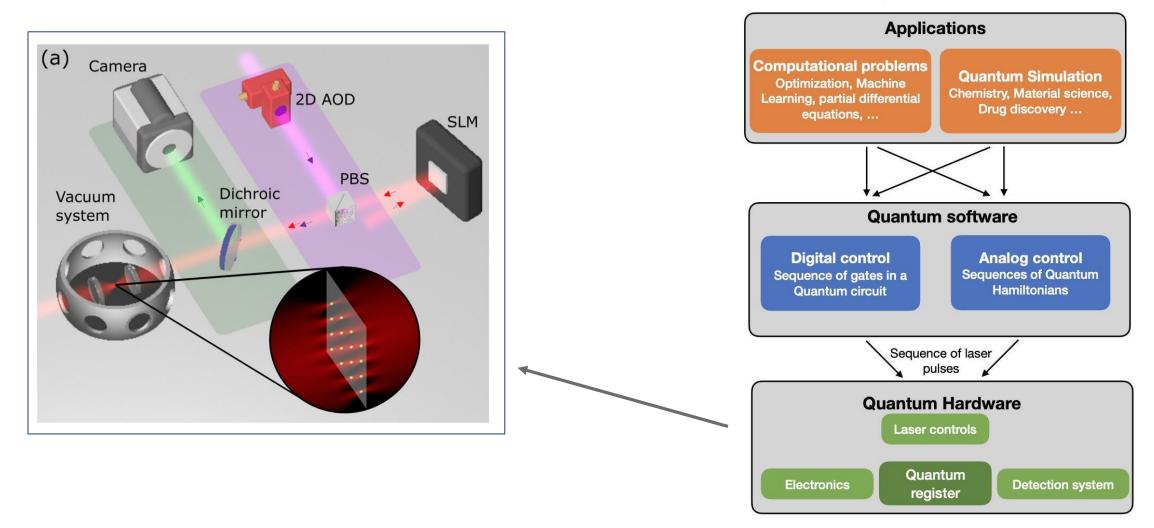
IPUTING LAB

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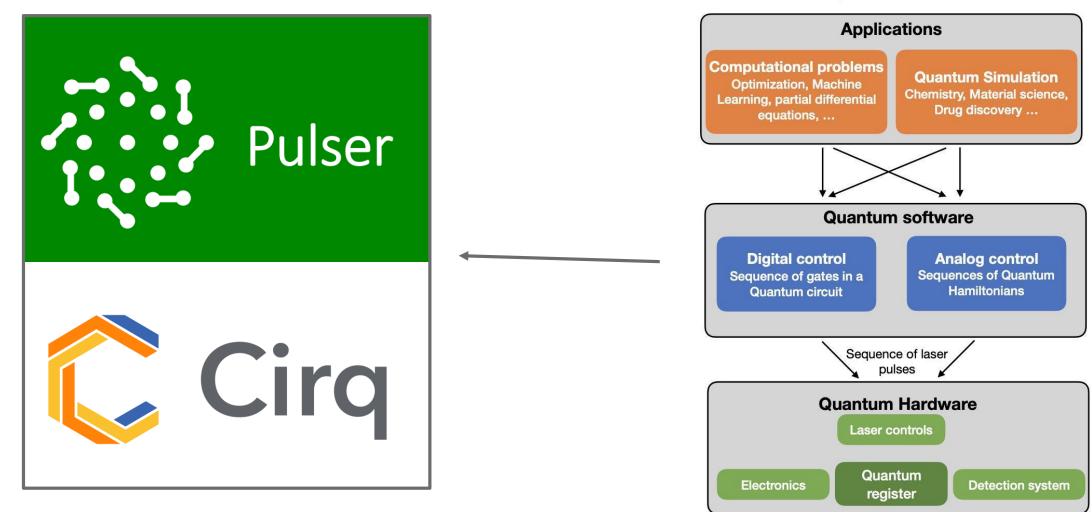
- The **project** will last 4 years, during which it will be created the **conditions** to **integrate quantum simulators with the European HPC network**.
- The **aim** is to create an **integrated ecosystem**.
- PASQAL announced that it already has a quantum simulator prototype with 100 qubits (scalable up to 1000).





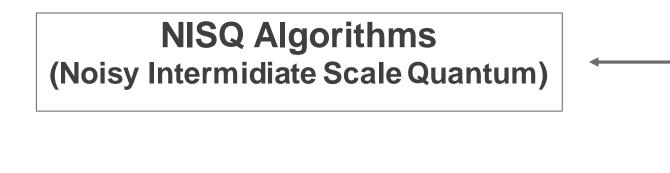


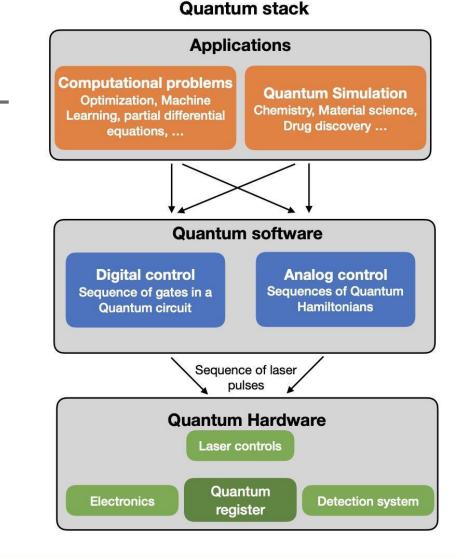


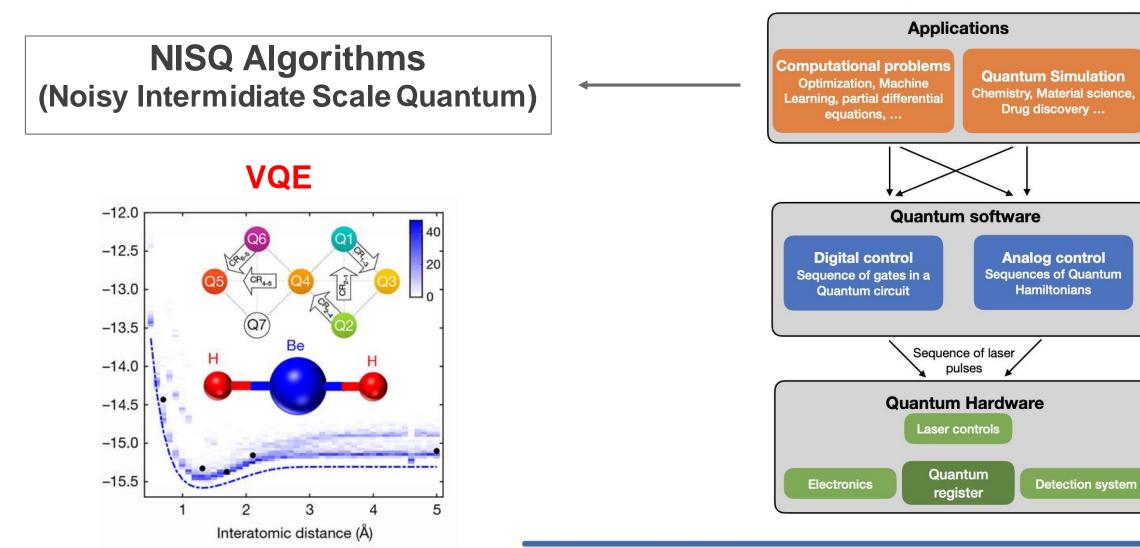




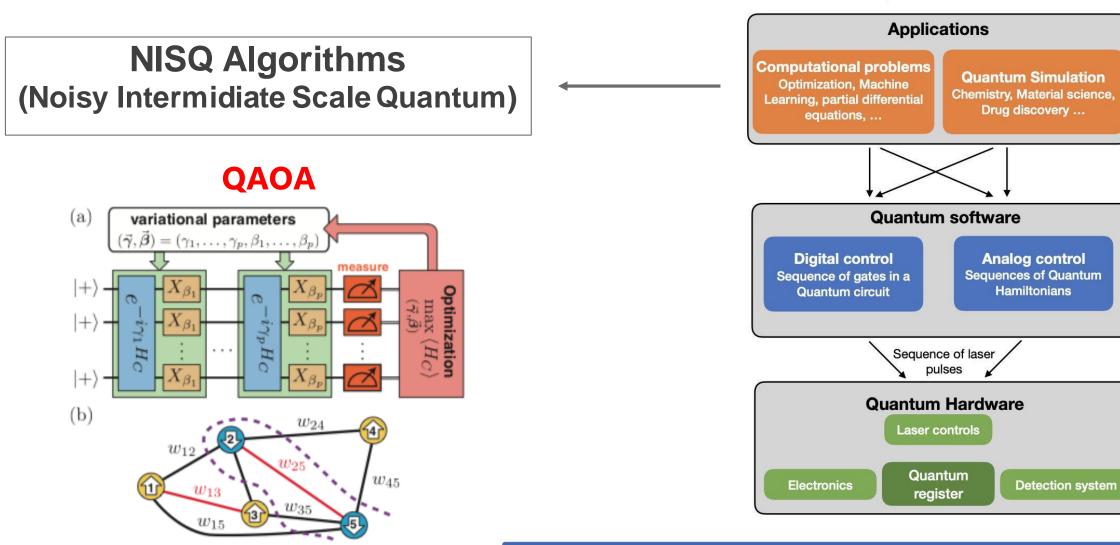




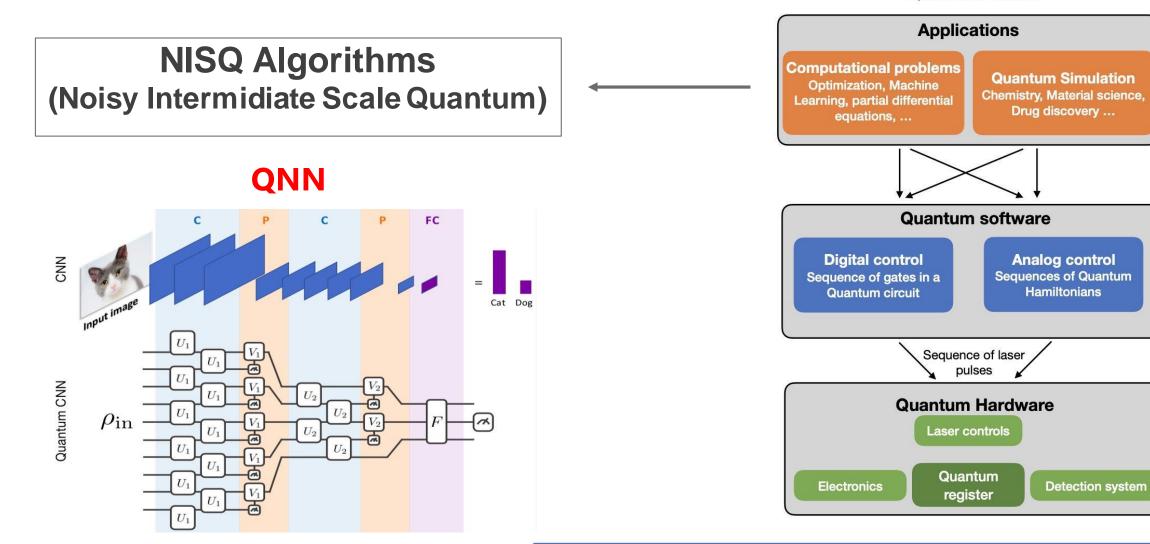




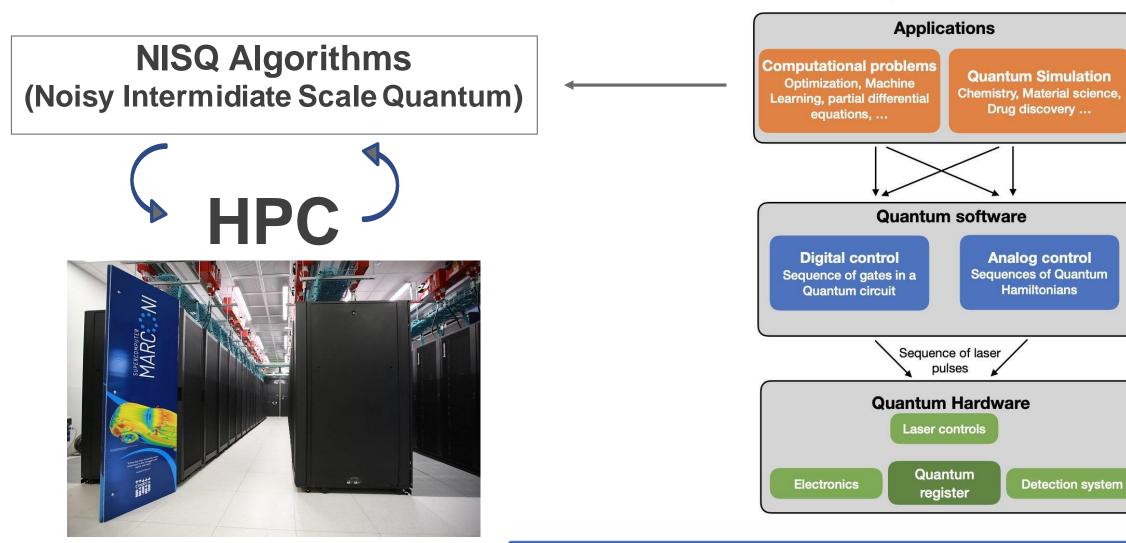




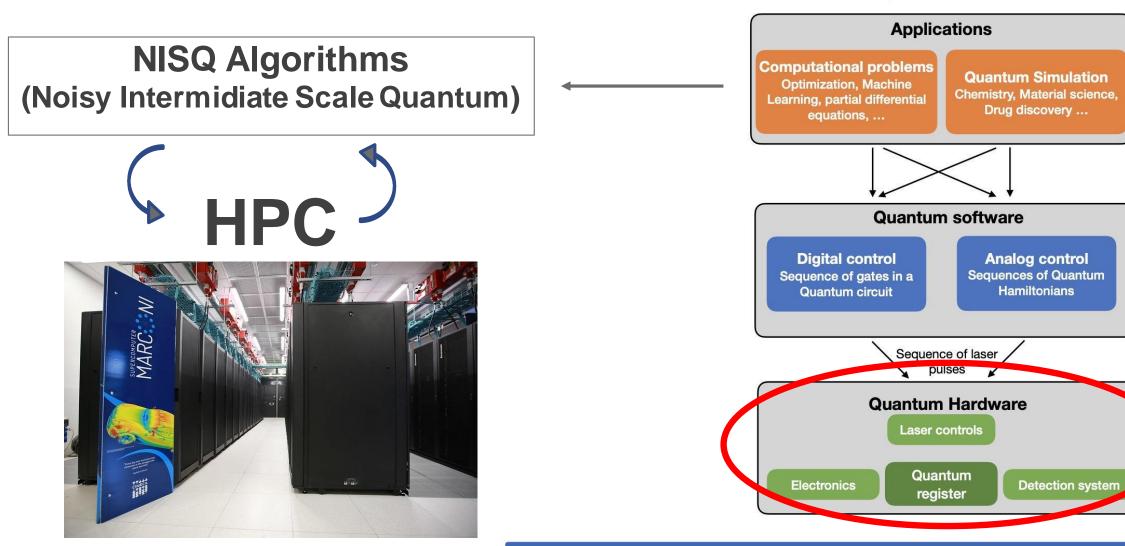








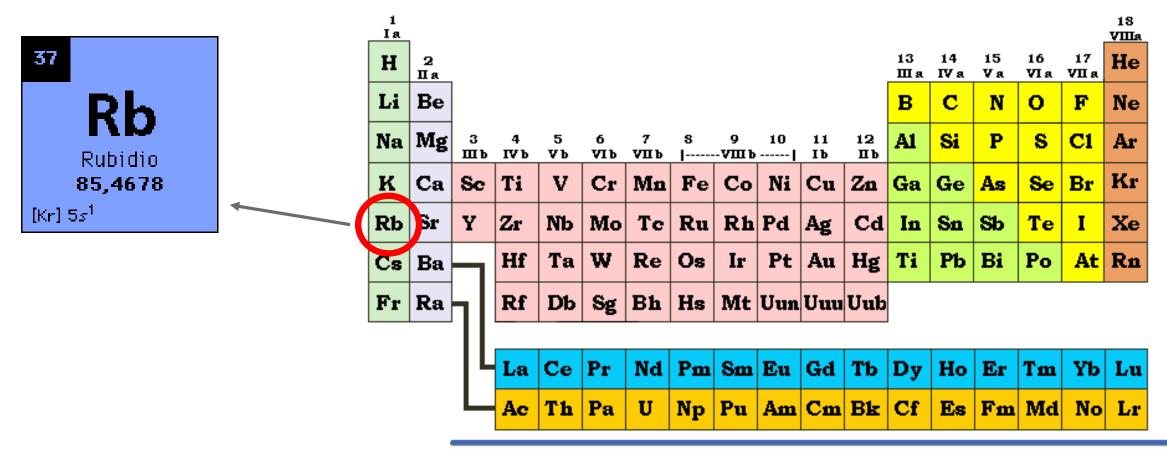






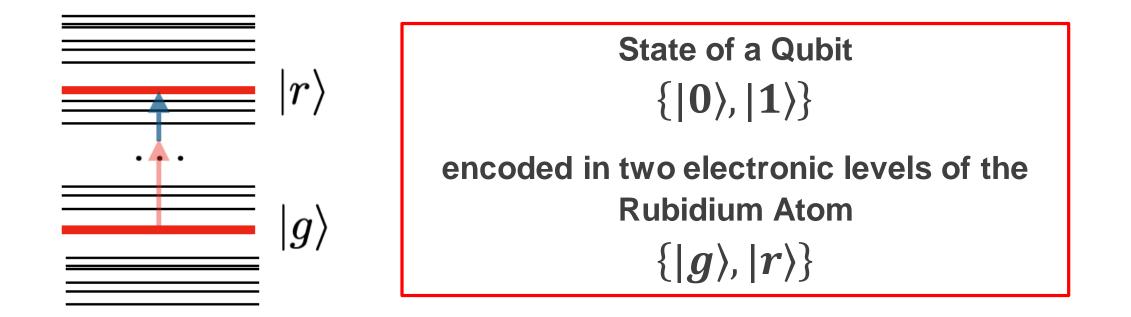


Pasqal employs Rubidium Atoms for its Neutral Atoms Quantum Computer





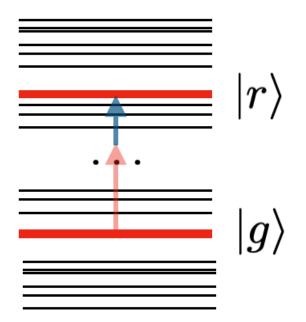
Pasqal employs Rubidium Atoms in the construction of the QPU



Since the **atoms** are **indistinguishable**, even the **qubits are strictly identical**. This is a **great advantage** for obtaining **low error levels** when calculating.



Pasqal employs Rubidium Atoms in the construction of the QPU

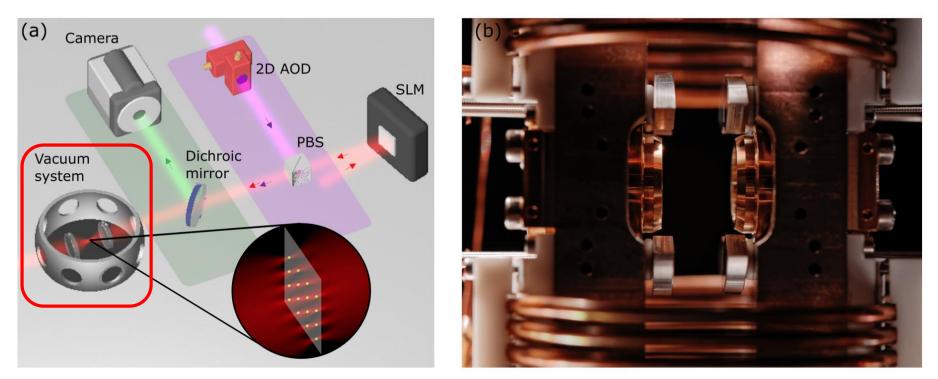


 $\{|g\rangle, |r\rangle\}$ are ground and «Rydberg» states characterized by:

- Long decay time: if excited to the state |r>,
 the atom tends to stay in that state and does not decays immediately in ground state |g>
- Strong interaction between atoms

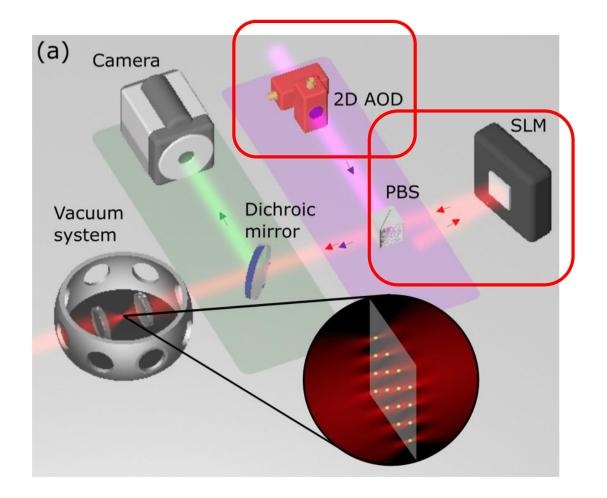


Pasqal employs Rubidium Atoms in the construction of the QPU



The atomic vapor is introduced into an ultra-high vacuum system operating at room temperature



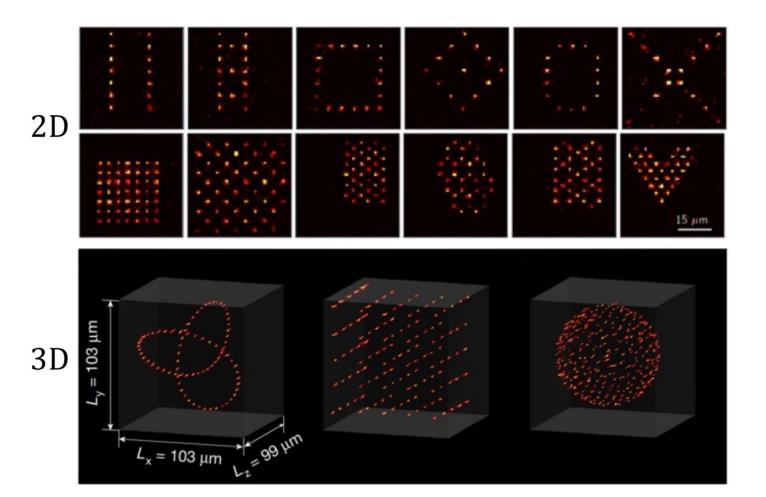


Rubidium atoms are trapped and held by laser beams, in particular:

- Optical Tweezers (purple beam) controlled by 2D acousto-optic laser deflector (AOD)
- Laser (red beam) reflected by spatial light modulator (SLM) which gives the correct phase

Every Tweezers traps a single atom



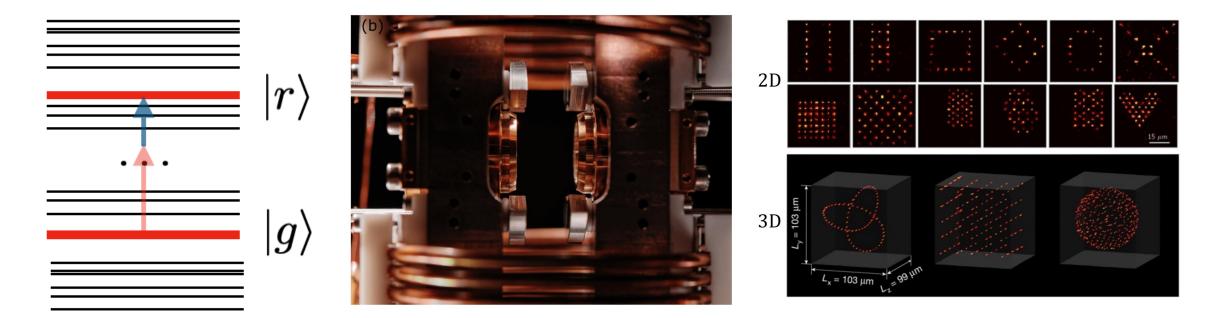


By moving the optical tweezers it is possible to arrange the topology of the Rubidium atoms and therefore of the qubits

Depending on the application, it is useful to vary the Topology which can be 1D, 2D or even 3D

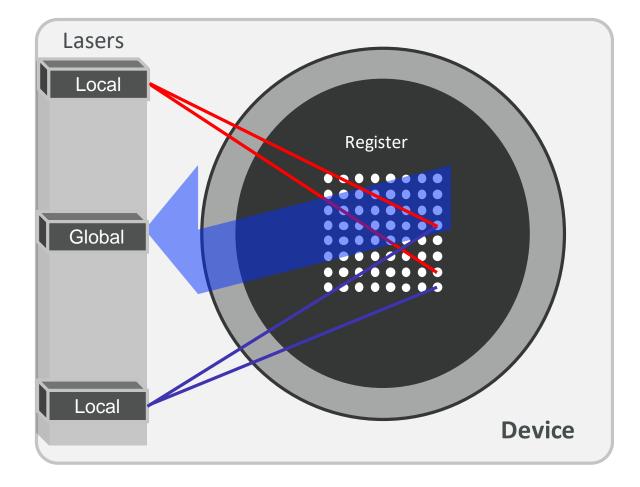


Pasqal employs Rubidium Atoms in the construction of the QPU



How does quantum computation happen?





Local and global laser beams control the state of qubit registers and allow to:

Act on single qubit

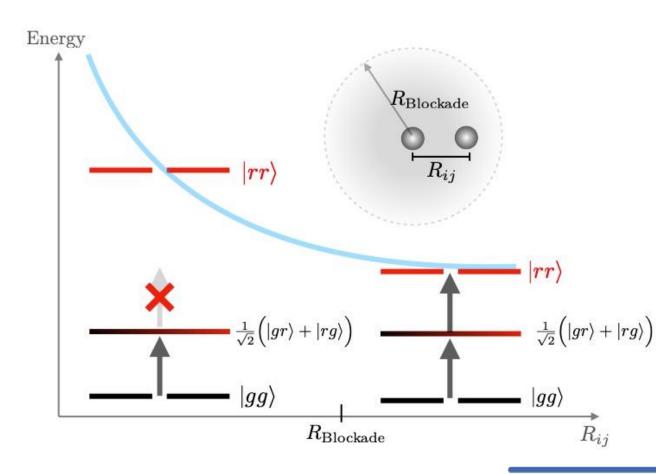
e.g. |g
angle
ightarrow |r
angle

Make qubit interact

e.g. $|gg\rangle \rightarrow \frac{1}{\sqrt{2}} (|gr\rangle + |rg\rangle)$



Rydberg Blockade: principle used to create entangled states

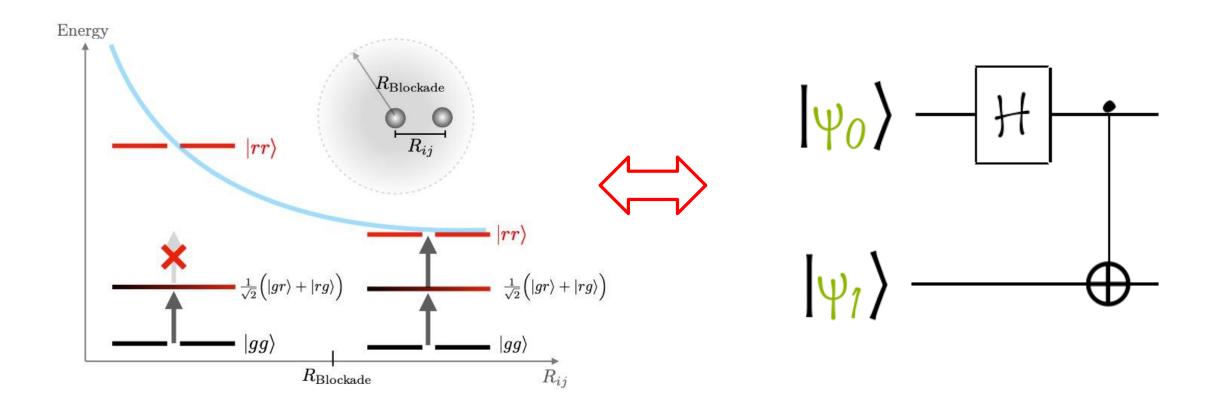


Qubits that are within range of the Rydberg blockade interact with each other.

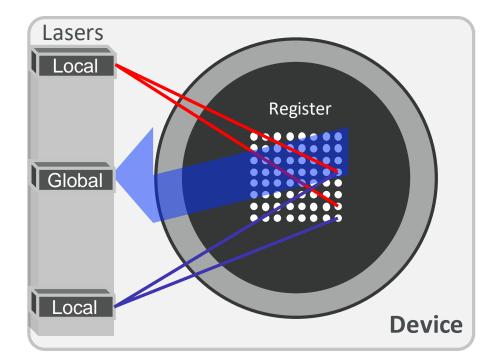
The interaction within this radius is strong enough to make the state |rr> inaccessible

The resulting state is an **entangled state**, the same as obtained after a Hadamard gate followed by a CNOT

Rydberg Blockade: principle used to create entangled states



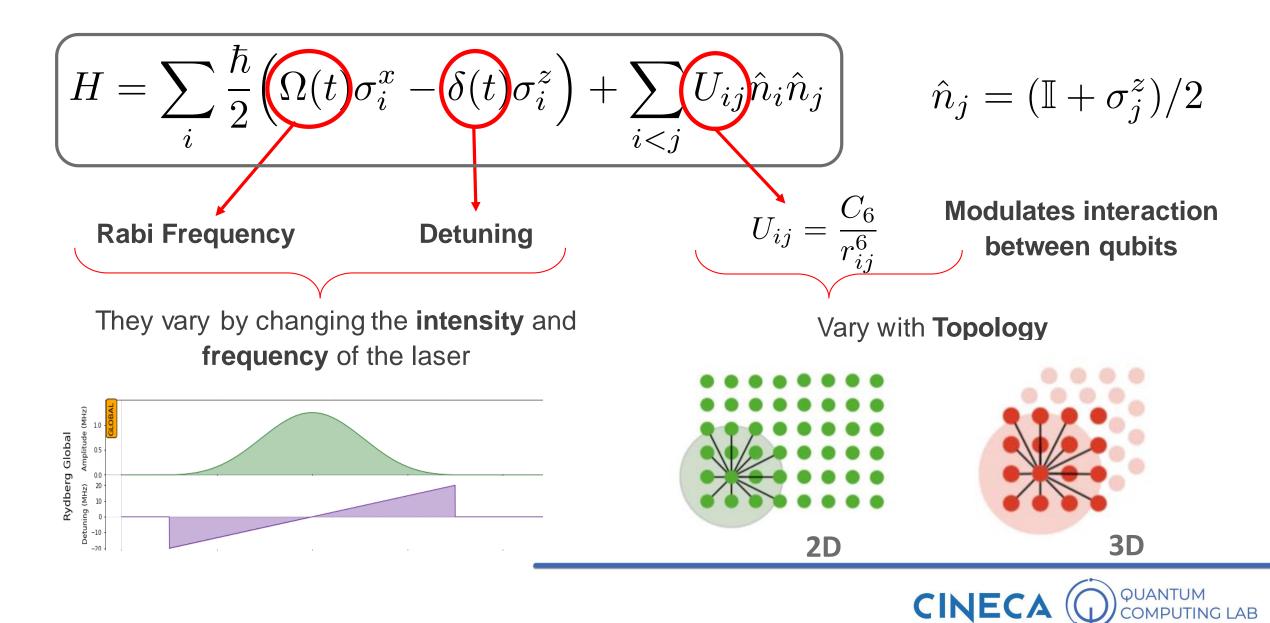


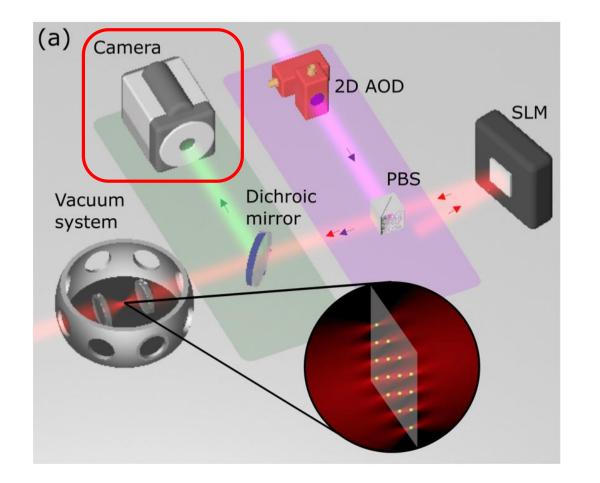


Mathematically, lasers interact with qubits, modifying the Hamiltonian, which is a function that describes the energy of the entire qubit system

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



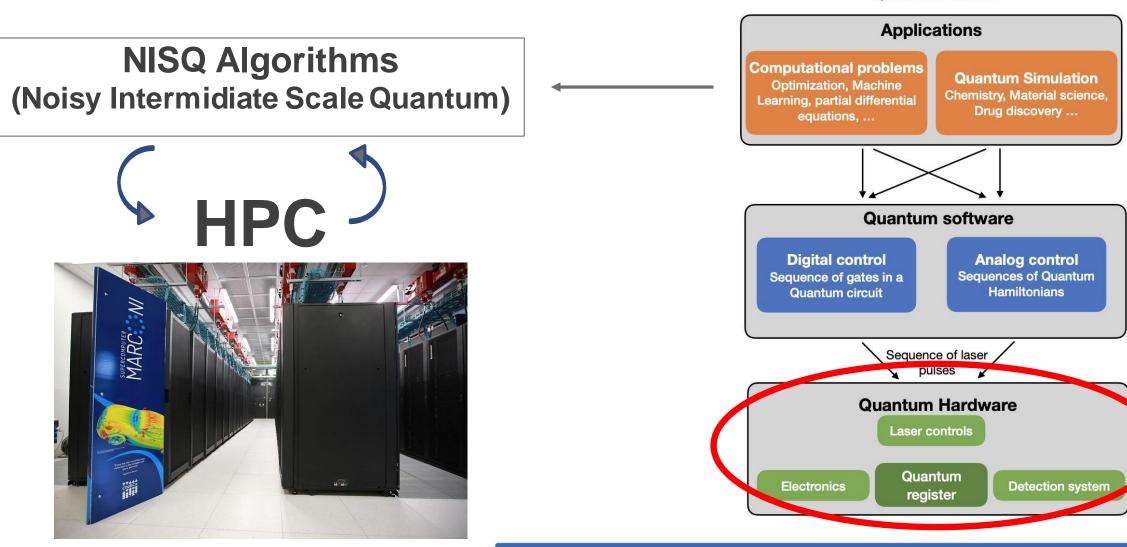




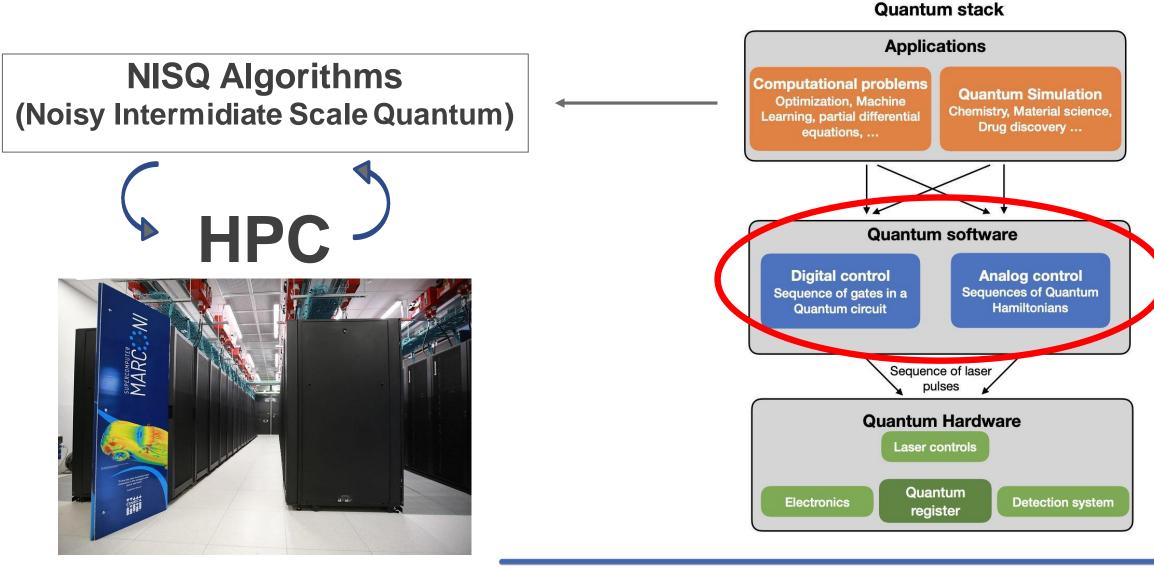
At the end of the computation, the qubit register is measured by observing the final fluorescence image (green beam).

The measurement process is performed in such a way that each atom in the qubit state | 0> appears bright, while the atoms in the qubit state | 1> remain dark.





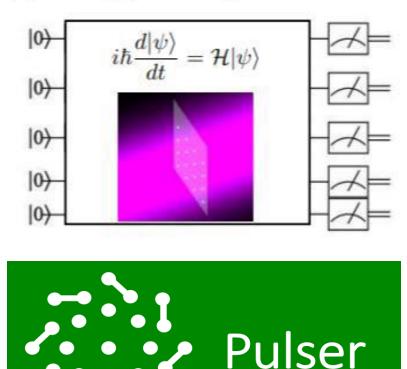






Lower level programming

(b) Analog processing



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

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

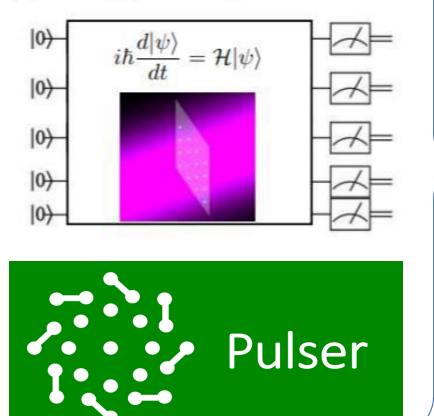
Possible by **varying**:

- Intensity and frequency of lasers
 - Qubit register topology



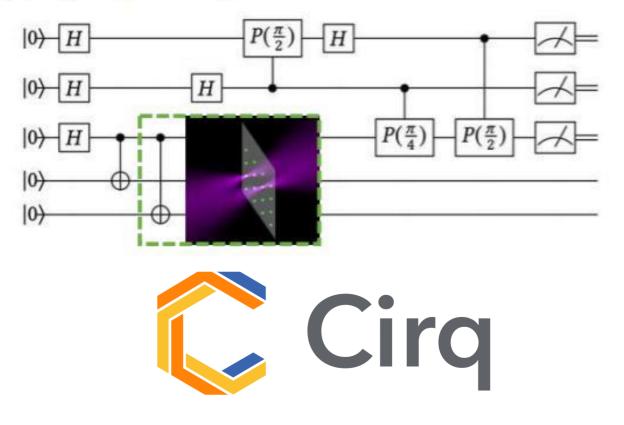
Lower level programming

(b) Analog processing

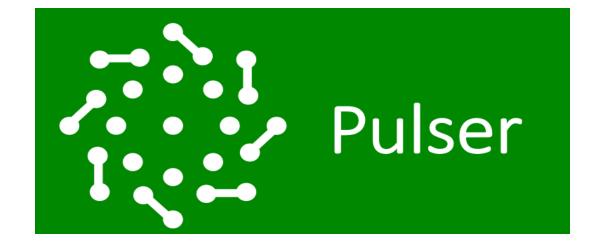


Higher level programming

(a) Digital processing







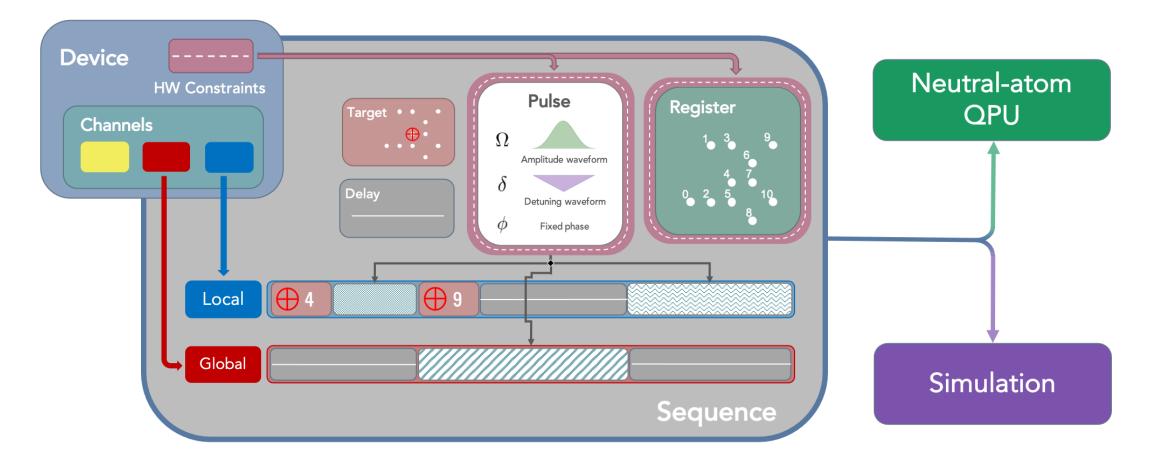
Python software library for programming Pasqal devices at the laser pulse level.

It allows to **design pulse sequences** that represent the physical parameters relevant to the computation.

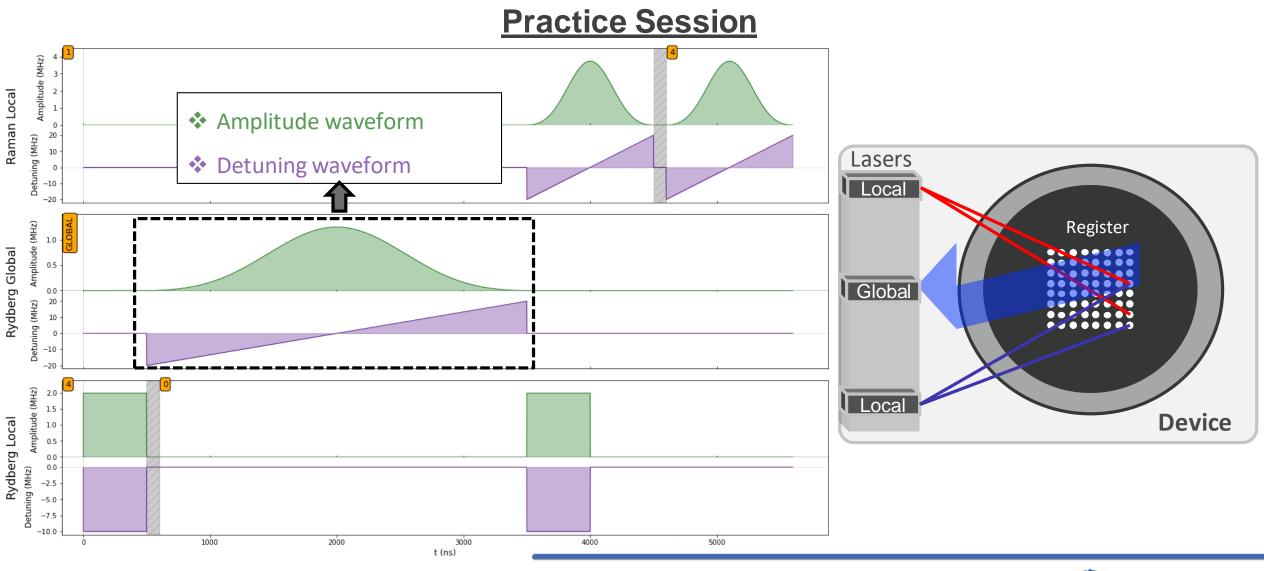
The sequences can be read and executed by the QPU or by an emulator



In Pulser, local and global pulse sequences can be defined







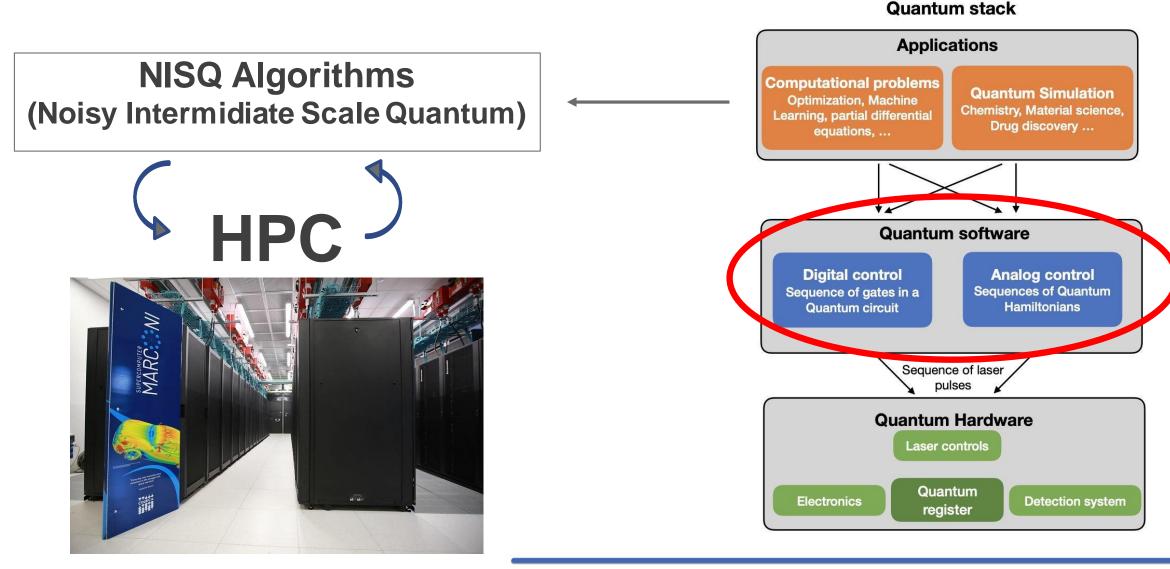


Practice Session

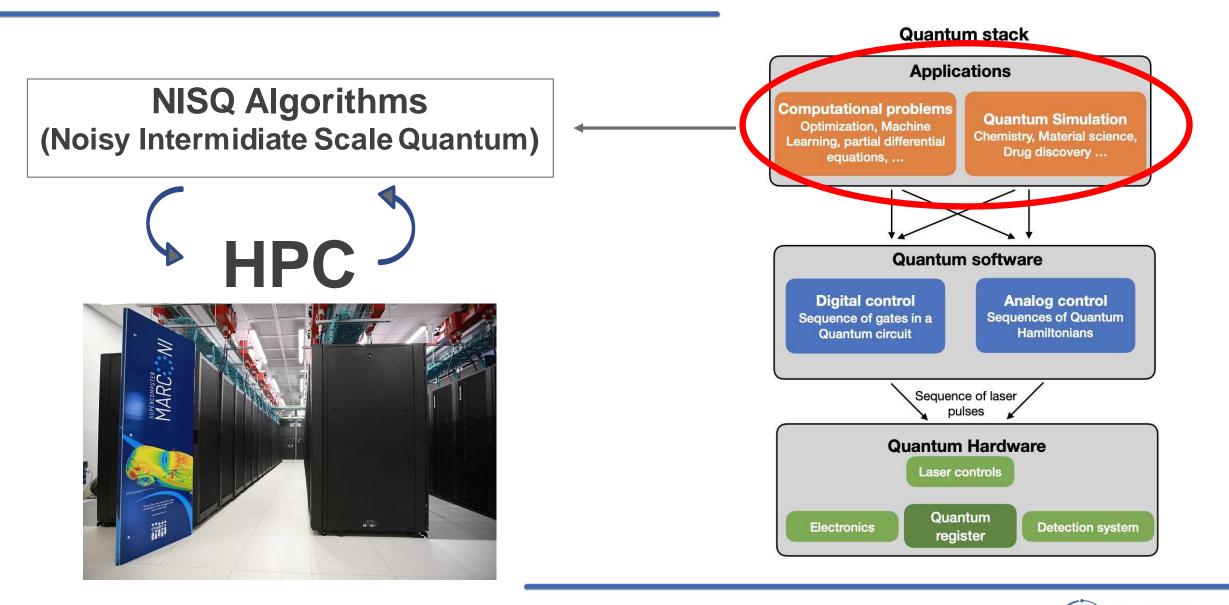
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https://github.com/pasqal-io/Pulser









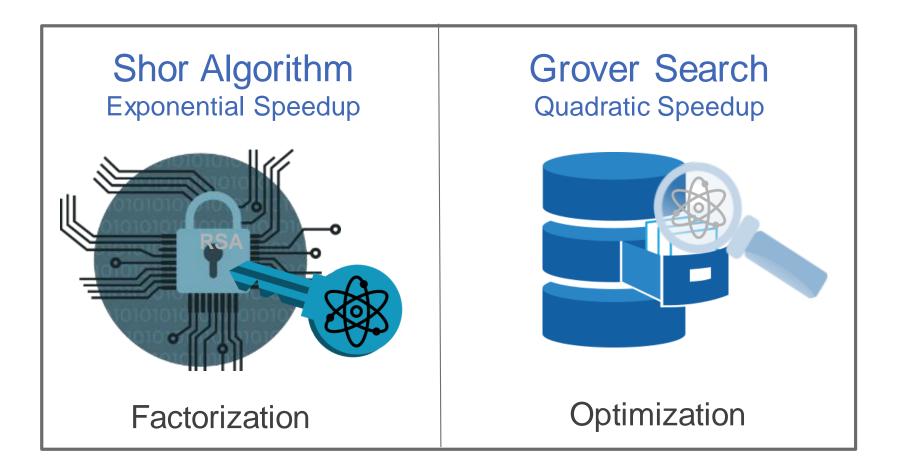
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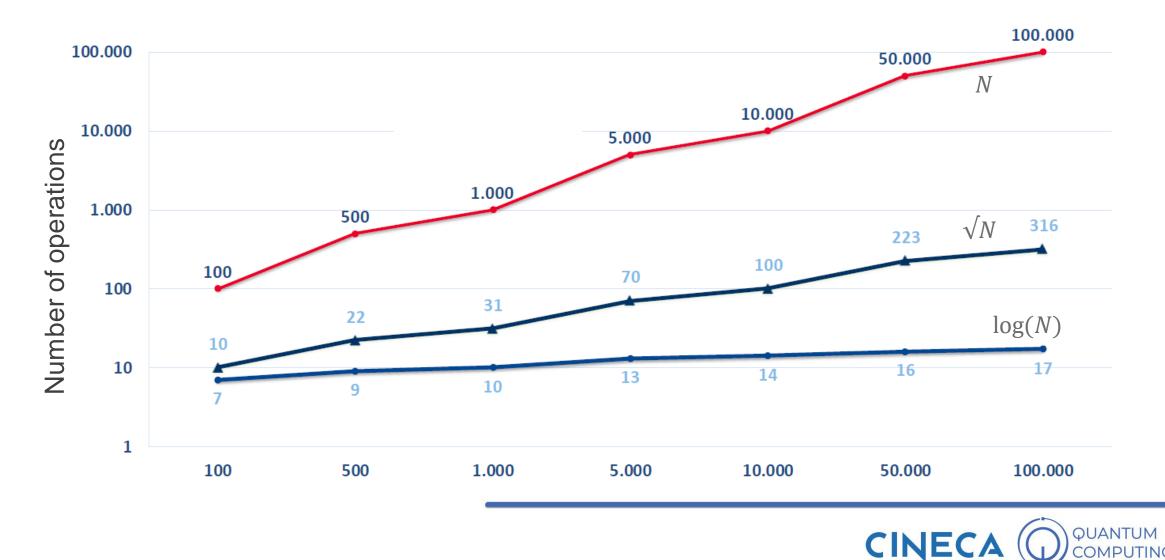


Before NISQ – Old School Quantum Algorithms



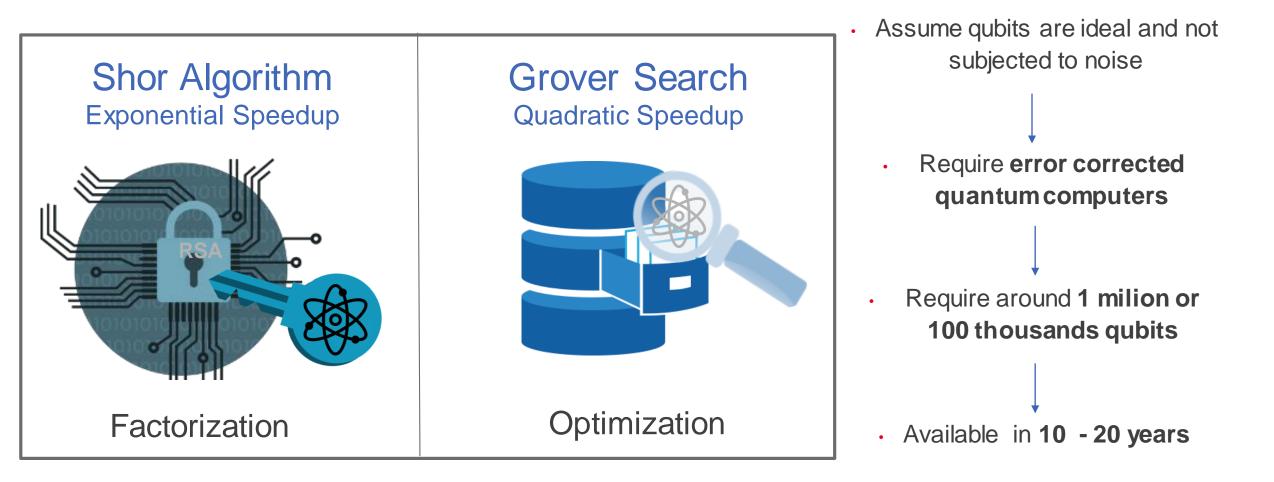


Before NISQ – Old School Quantum Algorithms



LAB

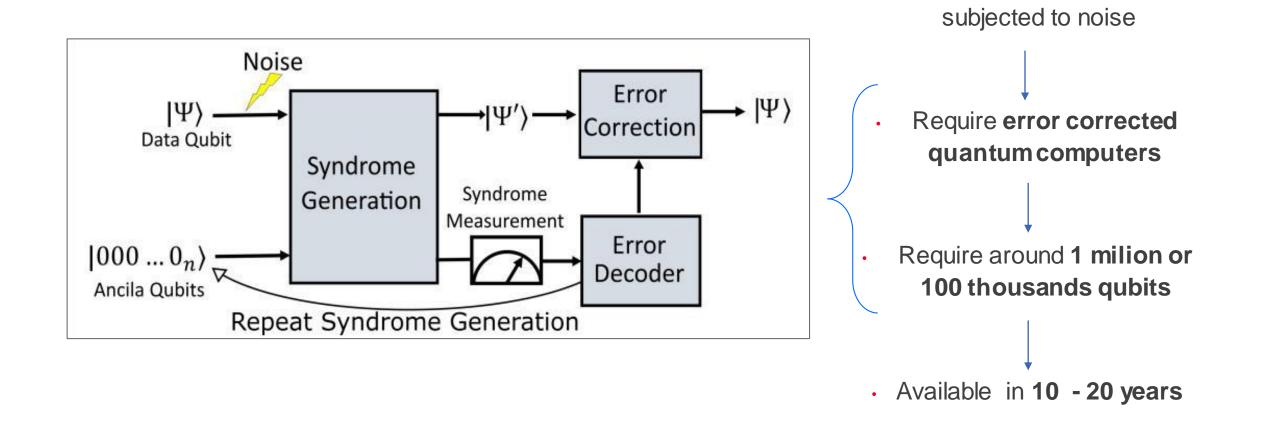
Before NISQ – Old School Quantum Algorithms



CINE

Before NISQ – Old School Quantum Algorithms

Assume qubits are ideal and not



We entered the NISQ era

NISQ = Noisy Intermediate-Scale Quantum

Intermediate-Scale

General Purpose QC

50 up to hundreds of qubits

IBM: 65 Qubits Google: 53 Qubits

Quantum Annealers

Thousands of qubits

D-Wave Advantage: 5000Q



We entered the NISQ era

NISQ = Noisy Intermediate-Scale Quantum

Noisy - noise due to interaction with environment

General Purpose QC

- 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 1000 elementary gates (shallow circuits)

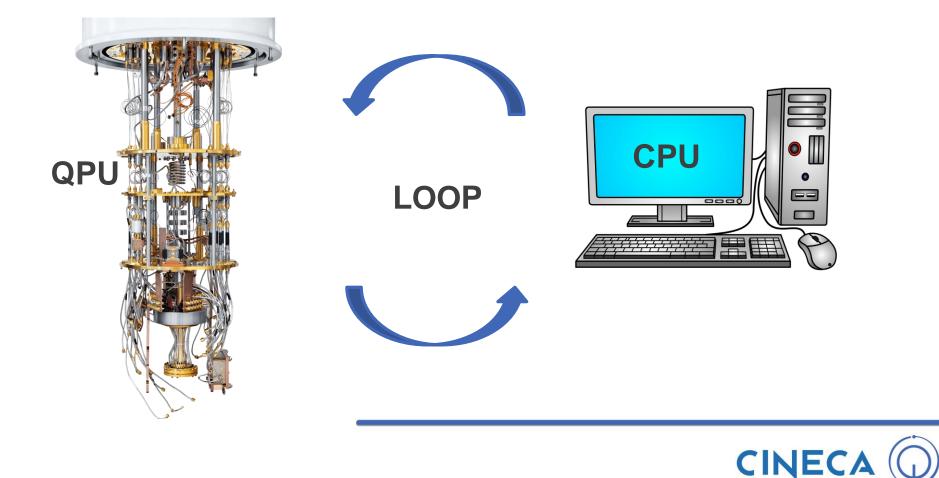
Quantum Annealers

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



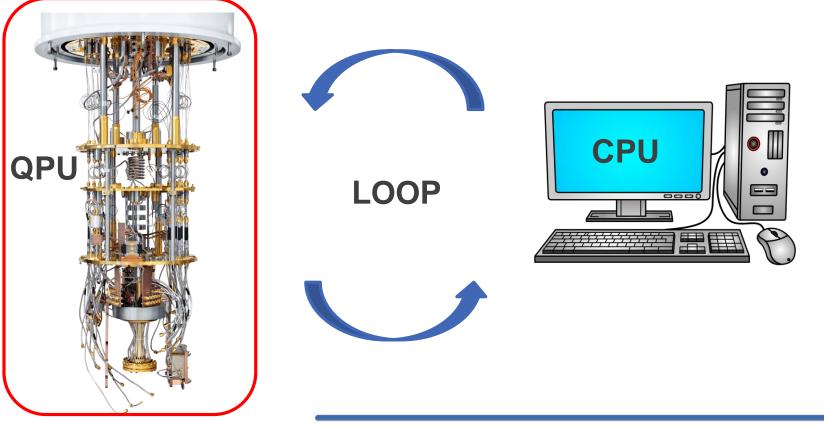
NISQ-ready algorithms for general purpose QPU

Hybrid Quantum-Classical algorithms



NISQ-ready algorithms for general purpose QPU

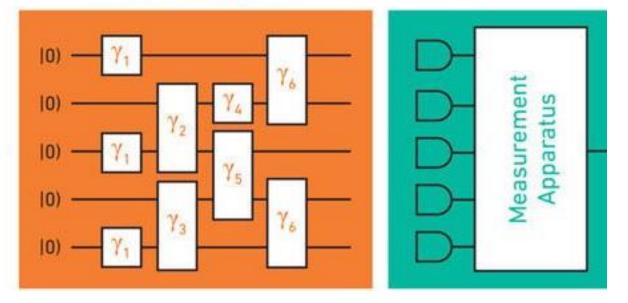
Hybrid Quantum-Classical algorithms





NISQ-ready algorithms for general purpose QPU

Parametric Quantum Circuits



Quantum Hardware

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

- Circuits in which the error is not corrected

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



NISQ-ready algorithms for general purpose QPU

Working principle

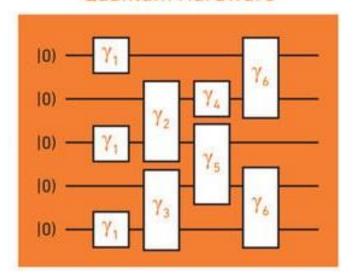


NISQ-ready algorithms for general purpose QPU

Working principle

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

2. Implement Variational Ansatz on the QPU



 $|\Psi(\vec{\theta})\rangle$



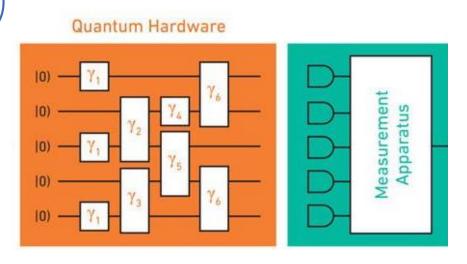
NISQ-ready algorithms for general purpose QPU

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

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

 $|\Psi(\vec{\theta})>$





NISQ-ready algorithms for general purpose QPU 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

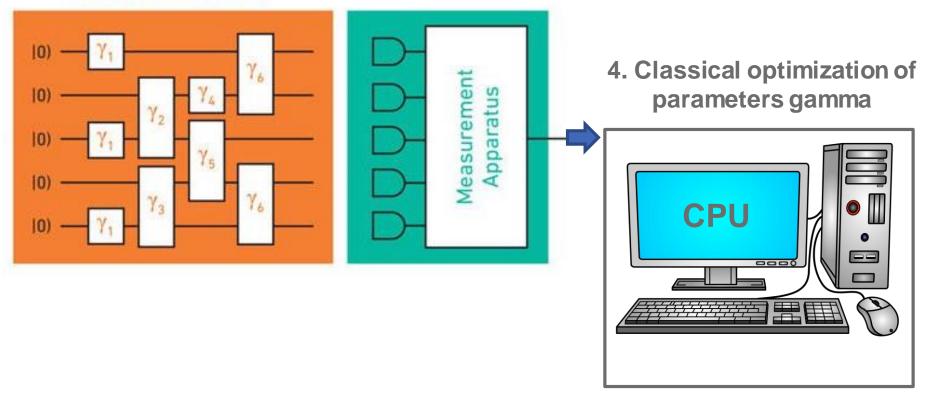
4. Use a classic computer to optimize the circuit parameters

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



NISQ-ready algorithms for general purpose QPU

Quantum Hardware





NISQ-ready algorithms for general purpose QPU

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

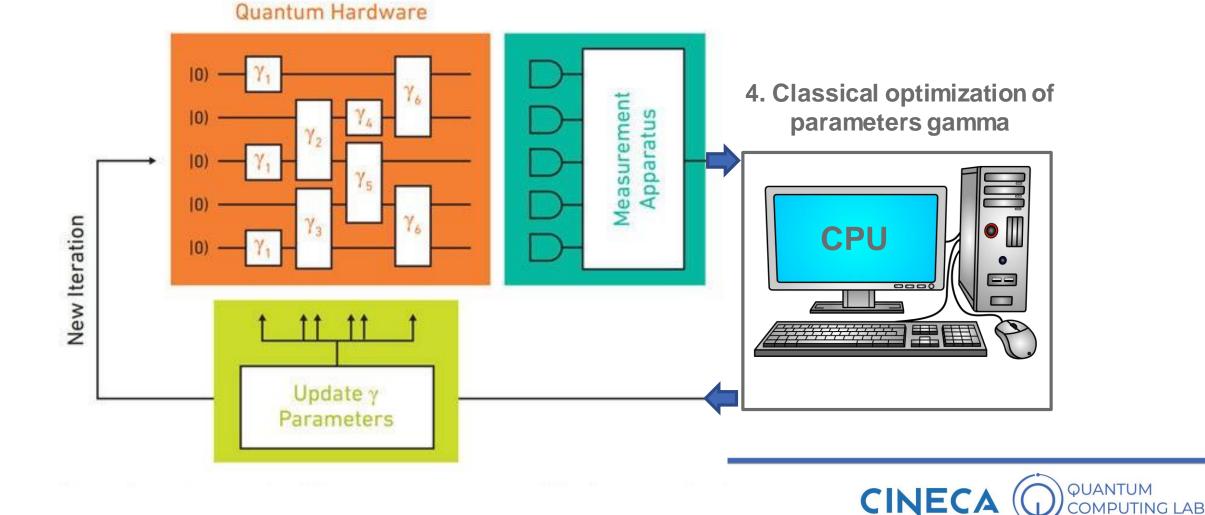
4. Use a classic computer to optimize the circuit parameters

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

> Heuristic Algorithm



NISQ-ready algorithms for general purpose QPU



NISQ-ready algorithms for general purpose QPU

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

It means both getting the **same classic solutions faster**, and/or finding **new, better solutions**

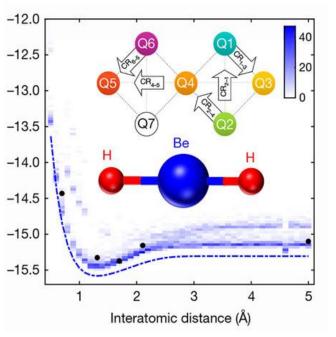


- Quantum Chemistry
- Quantum Optimization
- Quantum Al/Machine Learning



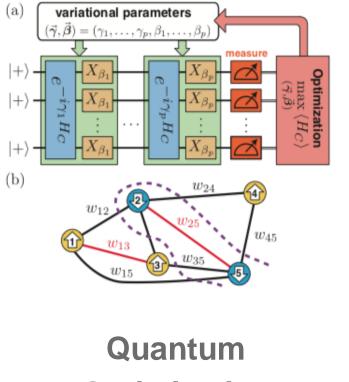
NISQ-ready algorithms for general purpose QPU

VQE

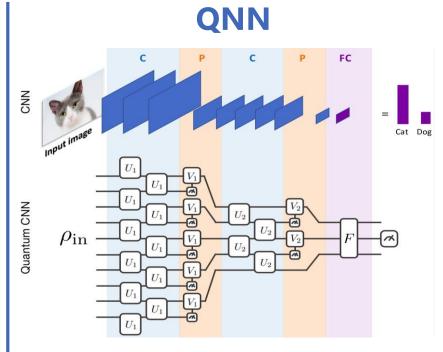


Quantum Chemistry

QAOA



Optimization

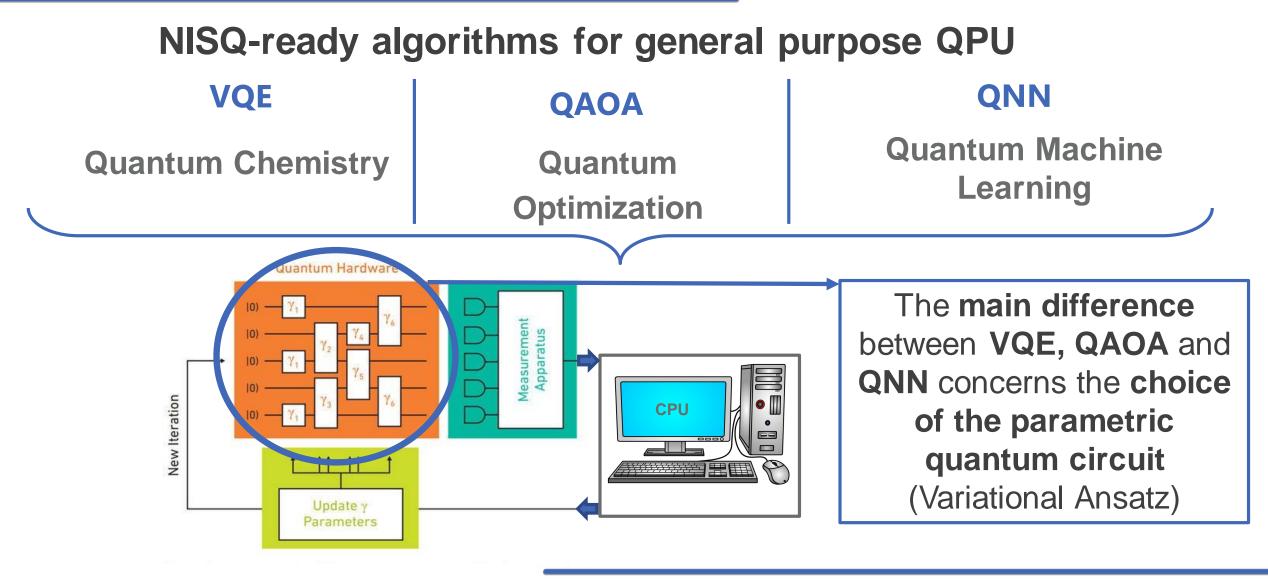


Quantum Machine Learning

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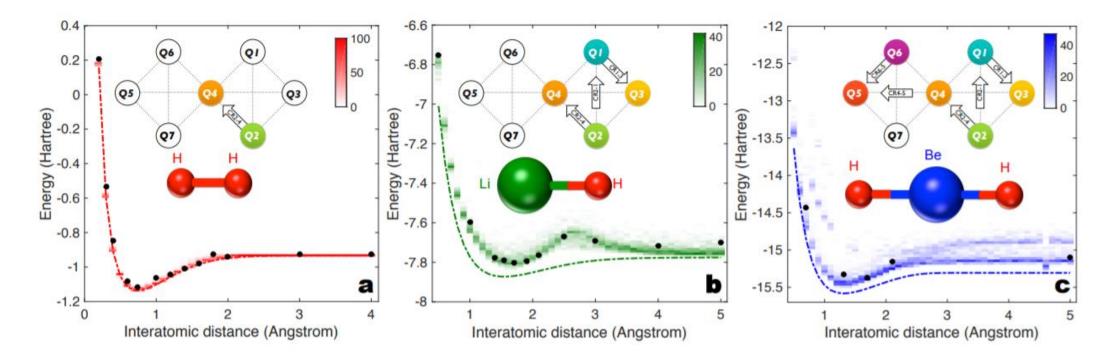
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NISQ-ready algorithms for general purpose QPU Variational Quantum Eigensolver (VQE) – QUANTUM CHEMISTRY



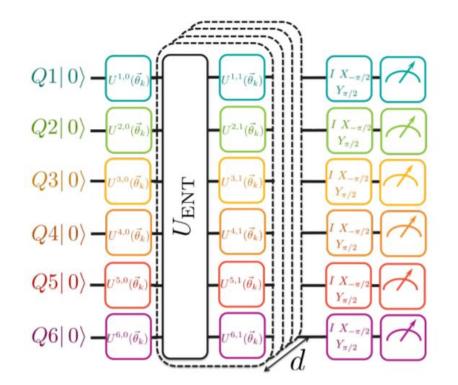
https://arxiv.org/abs/1704.05018



NISQ-ready algorithms for general purpose QPU Variational Quantum Eigensolver (VQE) – QUANTUM CHEMISTRY

<u>Objective</u>: to calculate the ground state of molecules (we want to go beyond the approximation of the mean field, which is classically very expensive in terms of resources)

<u>Method</u>: the VQE uses chemical-inspired Ansatz, such as the Unitary Coupled Cluster (UCC) method or a "hardware-efficient" ansatz



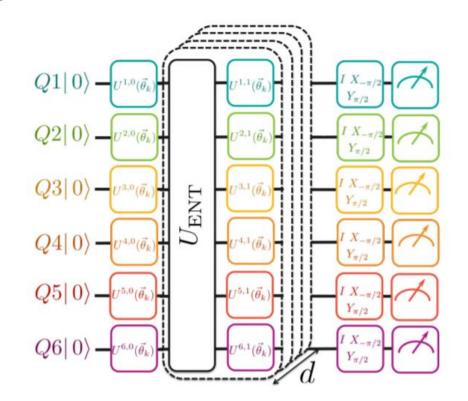
https://arxiv.org/abs/1704.05018



NISQ-ready algorithms for general purpose QPU Variational Quantum Eigensolver (VQE) – QUANTUM CHEMISTRY

- Ansatz is a provisional molecular ground state
- The classic optimizer evaluates the suitability of candidate solution based on its energy.

This holds the promise to study large molecules with unprecedented accuracy



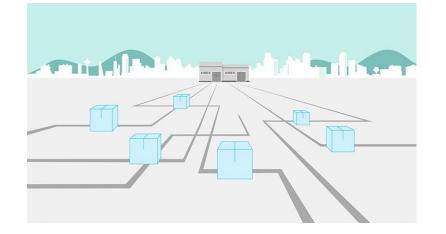
https://arxiv.org/abs/1704.05018



NISQ-ready algorithms for general purpose QPU

Quantum Approximate Optimization Algorithm (QAOA) – QUANTUM OPTIMIZATION

Optimization Problems



Routing



Scheduling



Portfolio Optimization



NISQ-ready algorithms for general purpose QPU

Quantum Approximate Optimization Algorithm (QAOA) – QUANTUM OPTIMIZATION

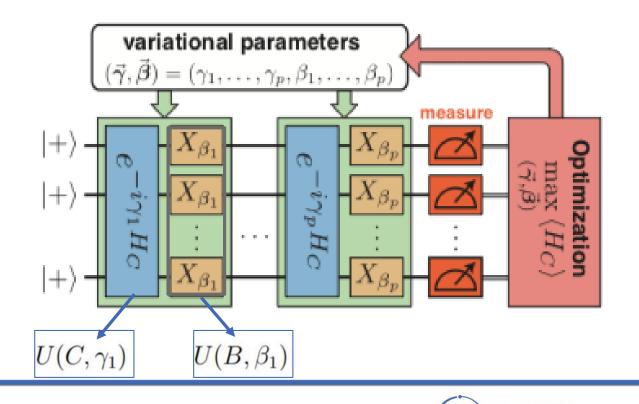
Objective: to solve a combinatorial optimization problem

<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).

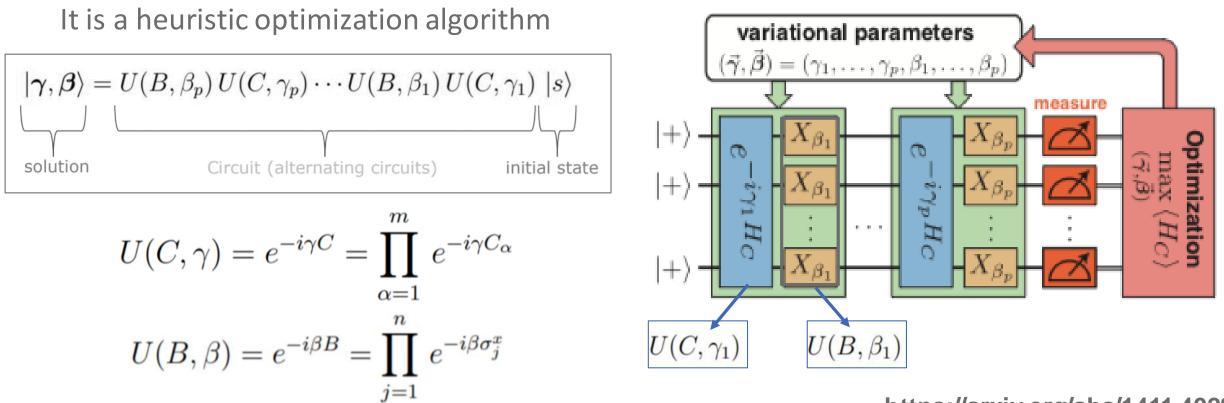
https://arxiv.org/abs/1411.4028

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



NISQ-ready algorithms for general purpose QPU

Quantum Approximate Optimization Algorithm (QAOA) – QUANTUM OPTIMIZATION



https://arxiv.org/abs/1411.4028



NISQ-ready algorithms for general purpose QPU

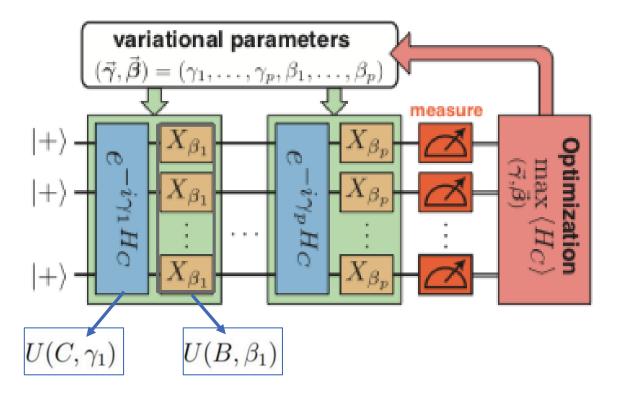
Quantum Approximate Optimization Algorithm (QAOA) – QUANTUM OPTIMIZATION

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

Encodes the optimization problem to solve (e.g. C could be some Qubo problem)

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

Allow the exploration of the solution space



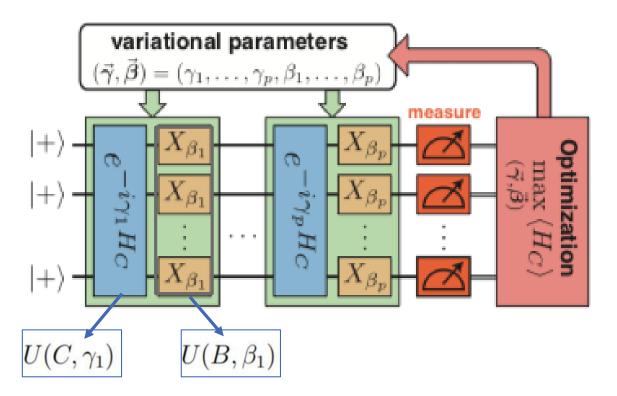
https://arxiv.org/abs/1411.4028



NISQ-ready algorithms for general purpose QPU

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.



https://arxiv.org/abs/1411.4028

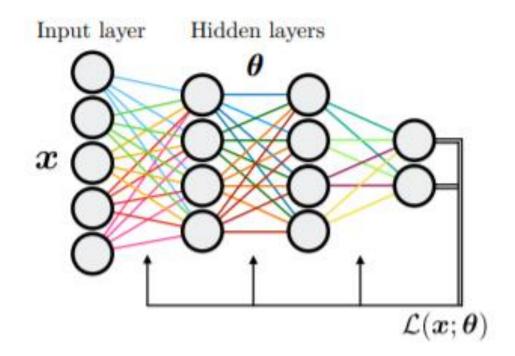


NISQ-ready algorithms for general purpose QPU

Quantum Neural Networks (QNN) – QUANTUM MACHINE LEARNING

Supervised learning: the algorithm is asked to **reproduce the relations** between some inputs and outputs.

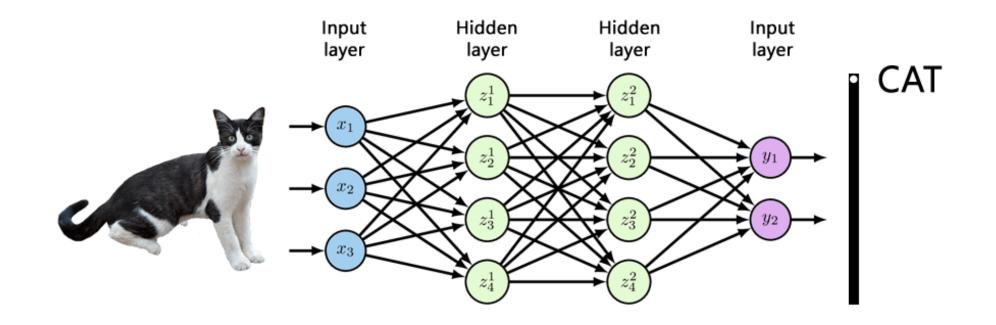
If properly trained, the NN is able to classify new data, i.e. data that was not used during training





NISQ-ready algorithms for general purpose QPU

Quantum Neural Networks (QNN) – QUANTUM MACHINE LEARNING



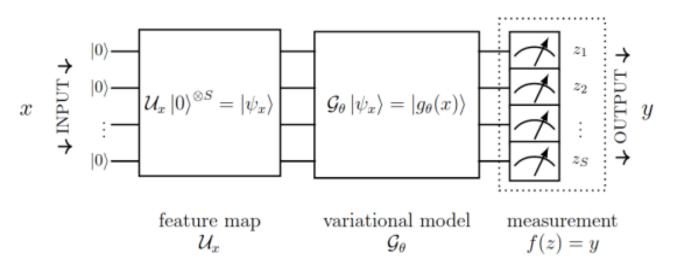


NISQ-ready algorithms for general purpose QPU

Quantum Neural Networks (QNN) – QUANTUM MACHINE LEARNING

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 circuit learns to classify new inputs based on the examples seen in the training phase

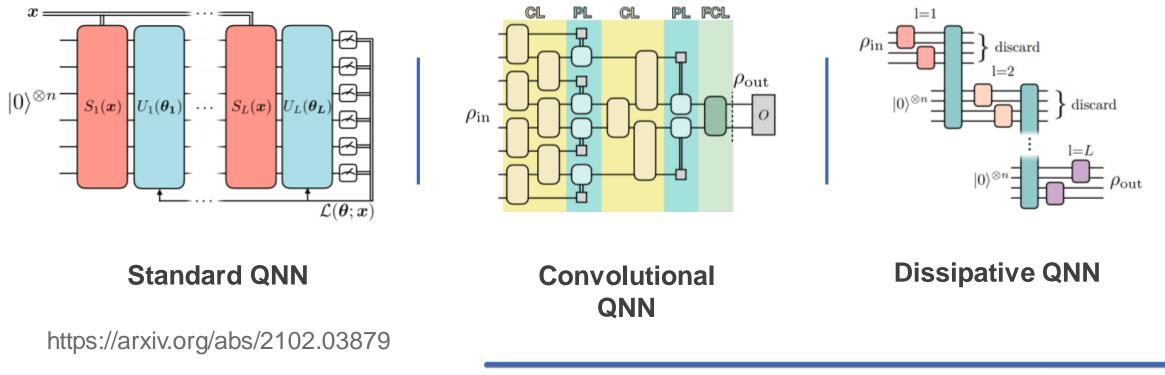
https://arxiv.org/abs/2011.00027



NISQ-ready algorithms for general purpose QPU

Quantum Neural Networks (QNN) – QUANTUM MACHINE LEARNING

We can also have several Ansatz for QNNs

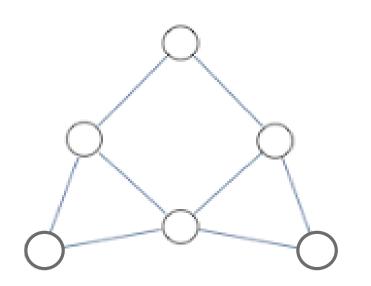






Maximal Independent Set (MIS) Problem

<u>Definition</u>: Given a graph, color the largest number of nodes avoiding that nodes of the same color are connected together



It is a hard **combinatorial optimization**

problem (complexity class NP-hard)

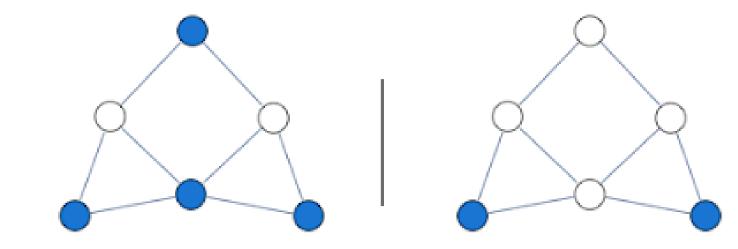
Applications:

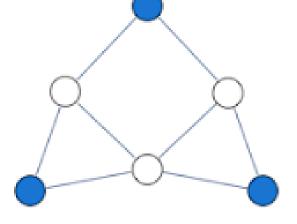
- Modeling and Optimization in Massive Datasets
 - Modeling Wireless Networks
 - Matching Molecular Structures



Maximal Independent Set (MIS) Problem

Definition: Given a graph, **color** the **largest number of nodes avoiding** that **nodes of the same color** are **connected** together





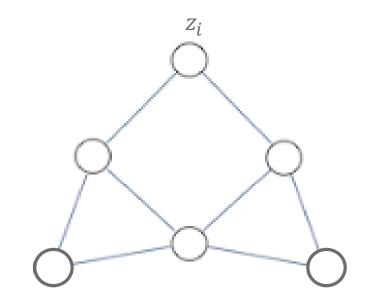
Not an independent set

Independent set but on maximal Maximal Independent Set



Maximal Independent Set (MIS) Problem

Definition: Given a graph, **color** the **largest number of nodes avoiding** that **nodes of the same color** are **connected** together



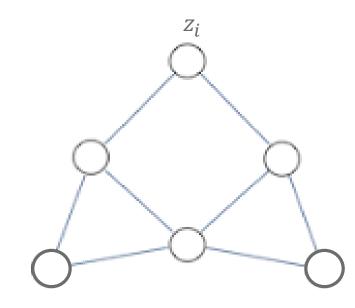
Combinatorial formulation

We can attribute a binary variable z_i to each node, where $z_i = 1$ if node *i* is colored (therefore it belongs to the independent set) and $z_i = 0$ otherwise.



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The Maximum Independent Set corresponds to the minimum of the following cost function:

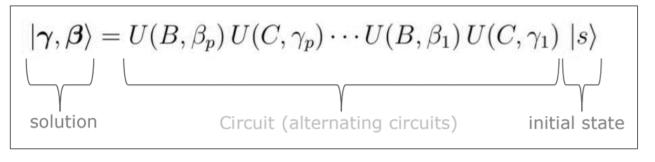
$$C(z_1,\ldots,z_N) = -\sum_{i=1}^N z_i + U \sum_{\langle i,j
angle} z_i z_j$$

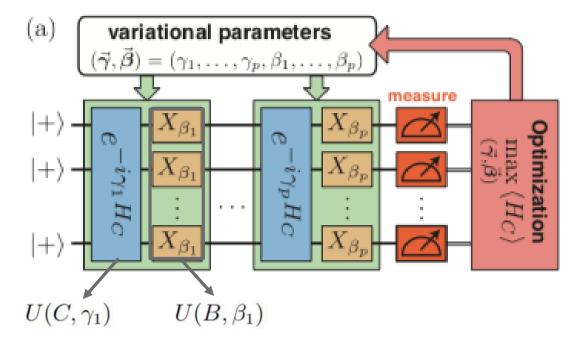
 $U \gg 1$



Maximal Independent Set (MIS) Problem

QAOA Ansatz

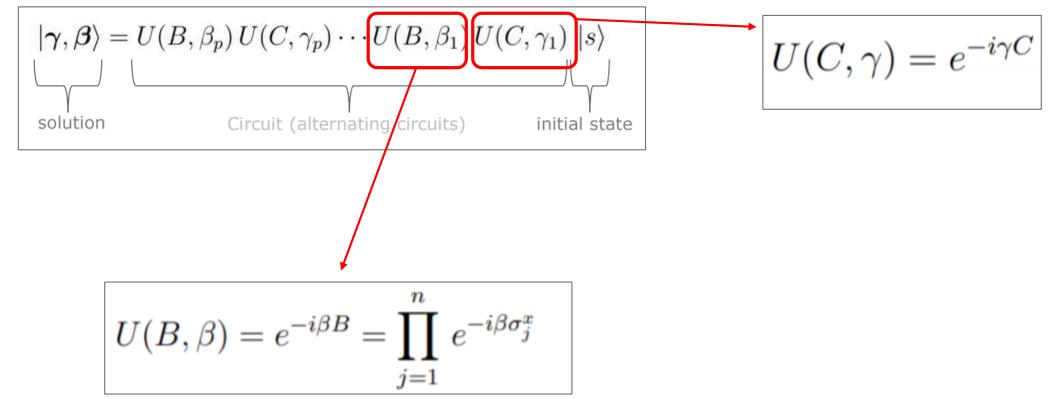






Maximal Independent Set (MIS) Problem

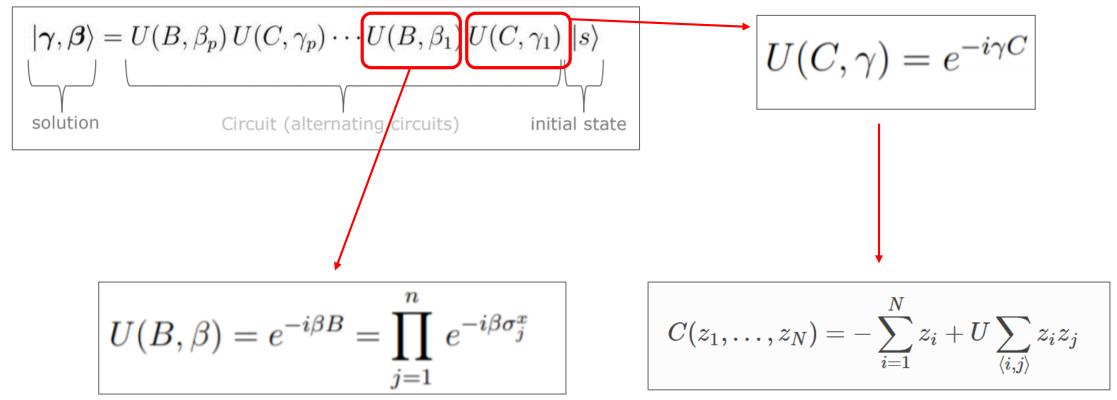
QAOA Ansatz





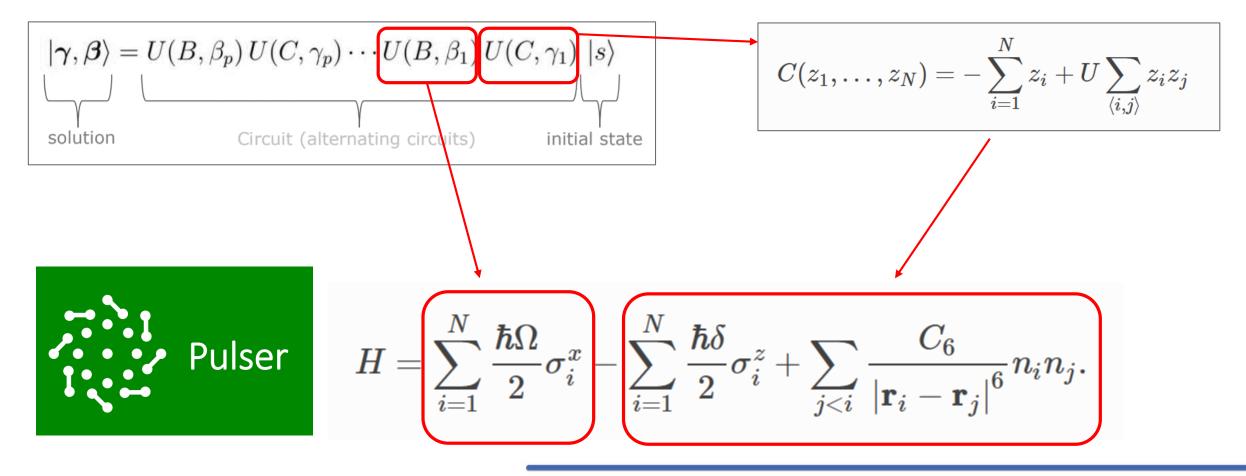
Maximal Independent Set (MIS) Problem

QAOA Ansatz



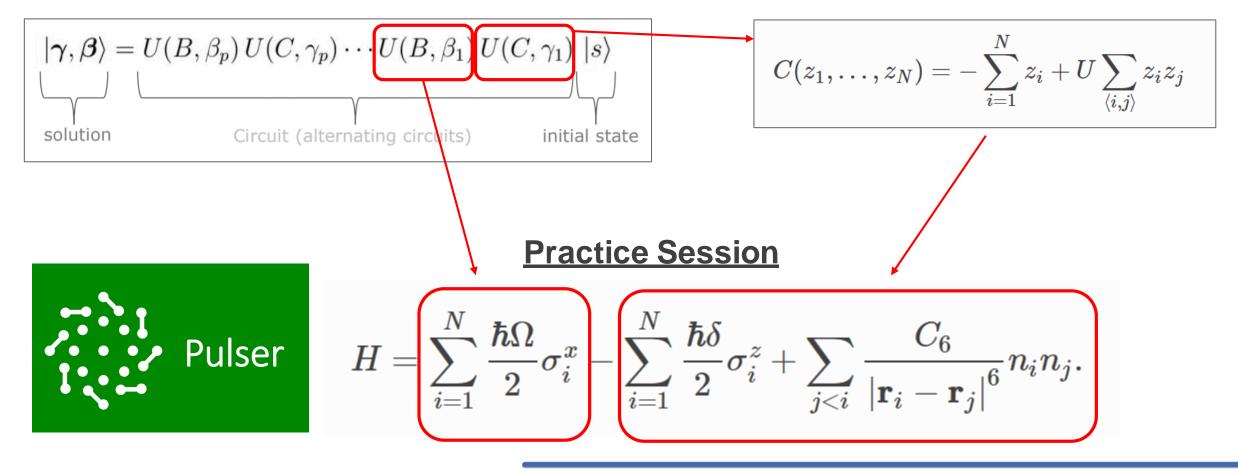


Maximal Independent Set (MIS) Problem





Maximal Independent Set (MIS) Problem





Appendix

Useful Software





Quantum Computing @ CINECA

CINECA: Italian HPC center CINECA Quantum Computing Lab:

- Research with Universities, Industries and QC startups
- Internship programs, Courses and Conference (HPCQC)

https://www.quantumcomputinglab.cineca.it



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