# Advanced Parallel School 2022 Quantum Computing – Day 4 QC with Neutral Atoms and NISQ devices

Mengoni Riccardo, PhD

17 Feb 2022



#### **Content**

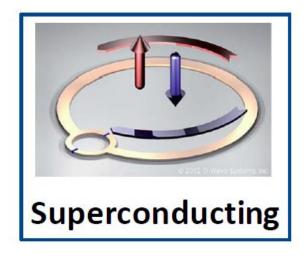
- Intro and Recap
- Pasqal Quantum Hardware: QC with Neutral Atoms
- Pulser: Control Software for Pasqal QC
- Quantum algorithms for NISQ Devices
- Application: QAOA & MIS problem

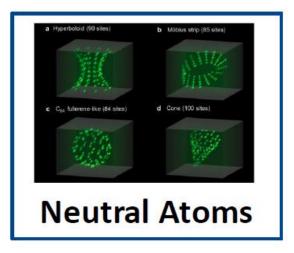


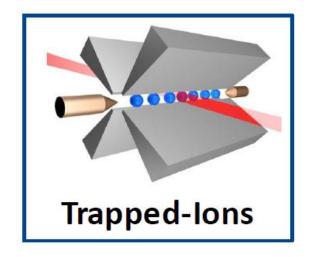
# **Intro and Recap**

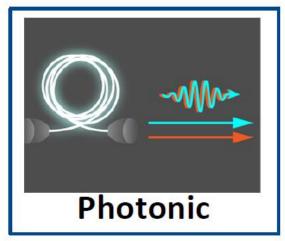


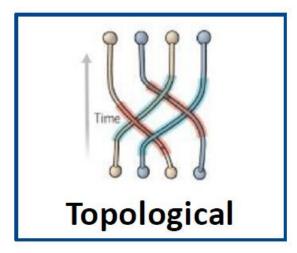
#### Hardware state of the art – qubit physical realization











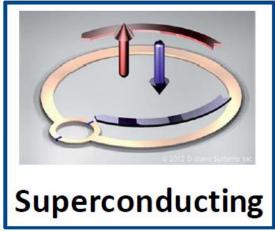




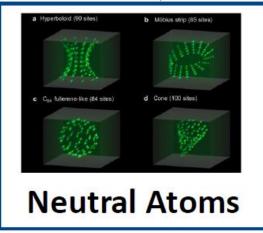
#### Hardware state of the art – qubit physical realization

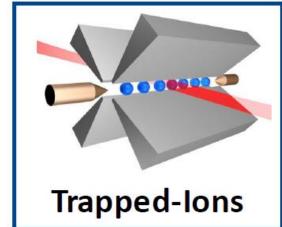




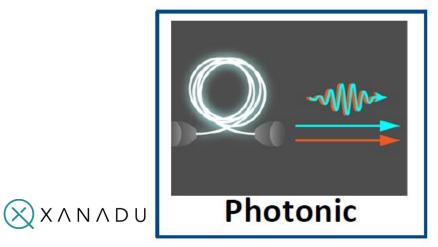


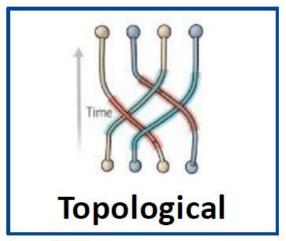
#### PASQAL















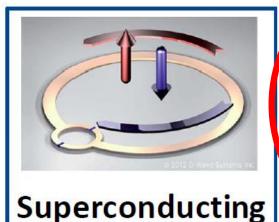


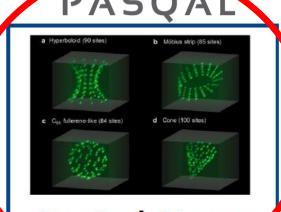


#### Hardware state of the art – qubit physical realization

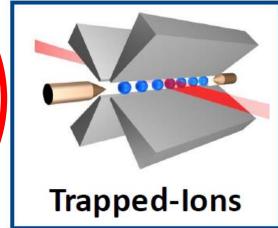




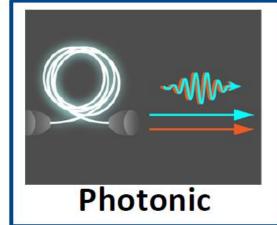


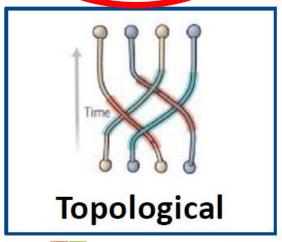


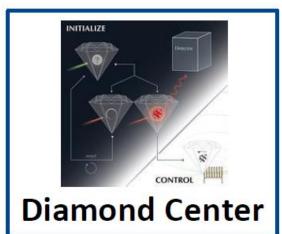












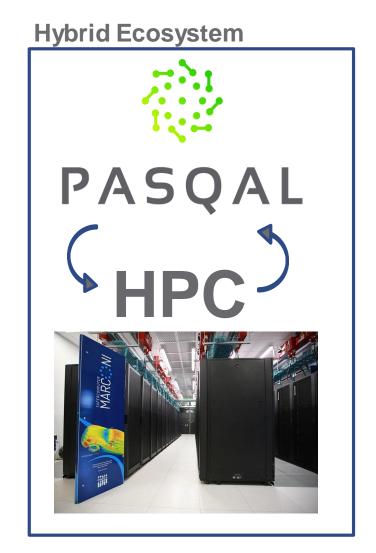




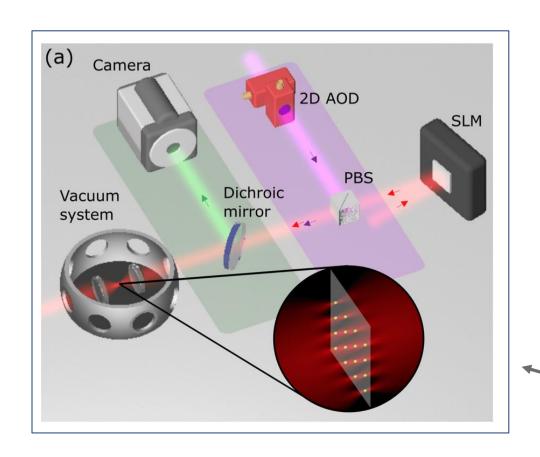


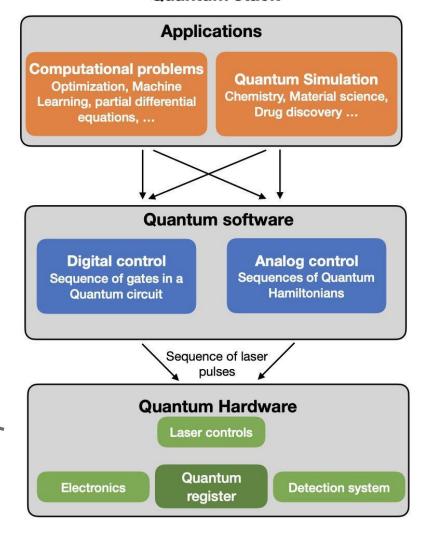


- The project will last 4 years, during which it will be created the conditions to integrate quantum simulators with the European HPC network.
- The aim is to create an integrated ecosystem.
- PASQAL announced that it already has a quantum simulator prototype with 100 qubits (scalable up to 1000).



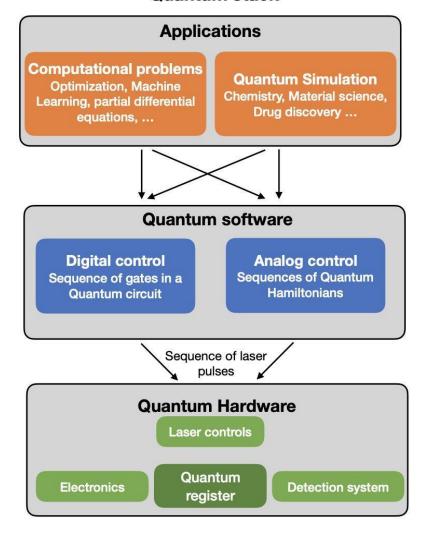






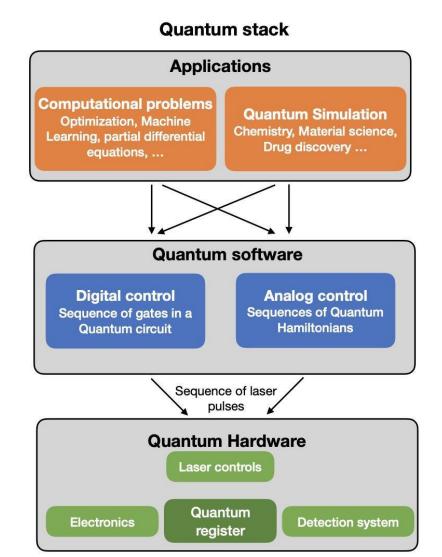






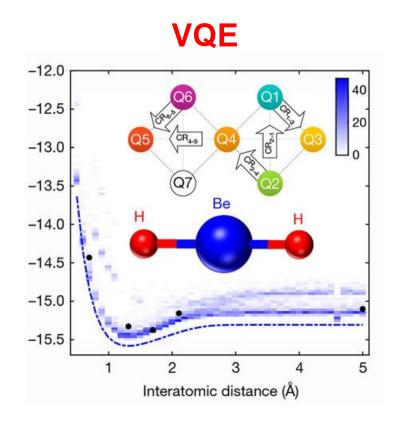


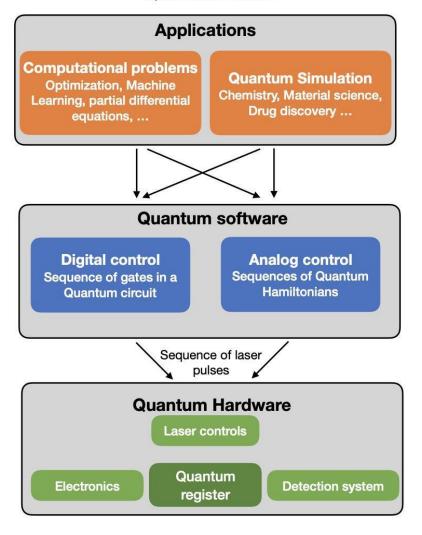
NISQ Algorithms
(Noisy Intermidiate Scale Quantum)





NISQ Algorithms
(Noisy Intermidiate Scale Quantum)

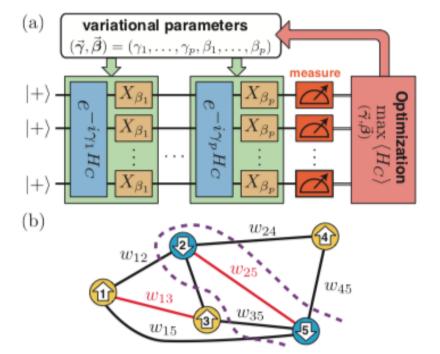


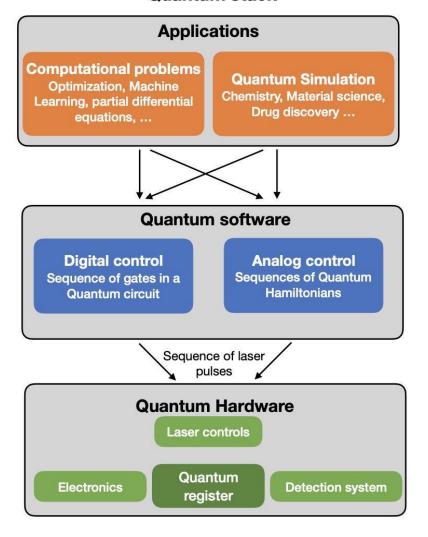




NISQ Algorithms
(Noisy Intermidiate Scale Quantum)

#### **QAOA**

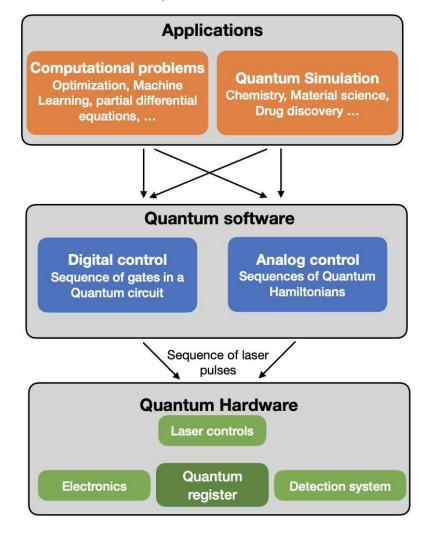






NISQ Algorithms
(Noisy Intermidiate Scale Quantum)

# QNN $\begin{array}{c} C & P & C \\ \hline U_1 & U_1 & U_2 & U_2$

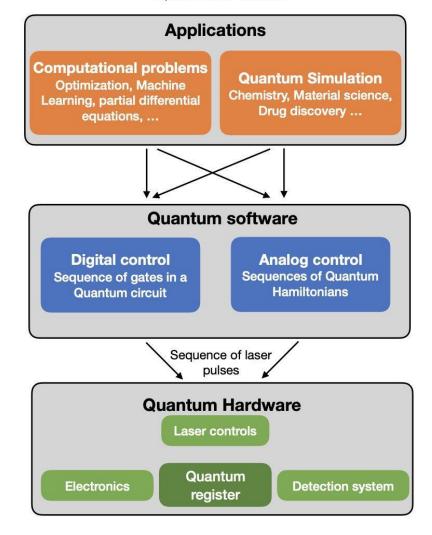




NISQ Algorithms
(Noisy Intermidiate Scale Quantum)





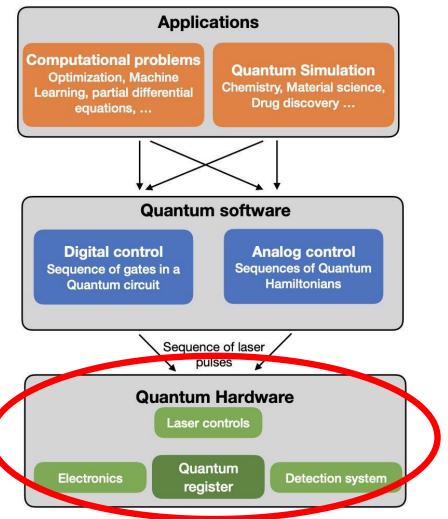




NISQ Algorithms
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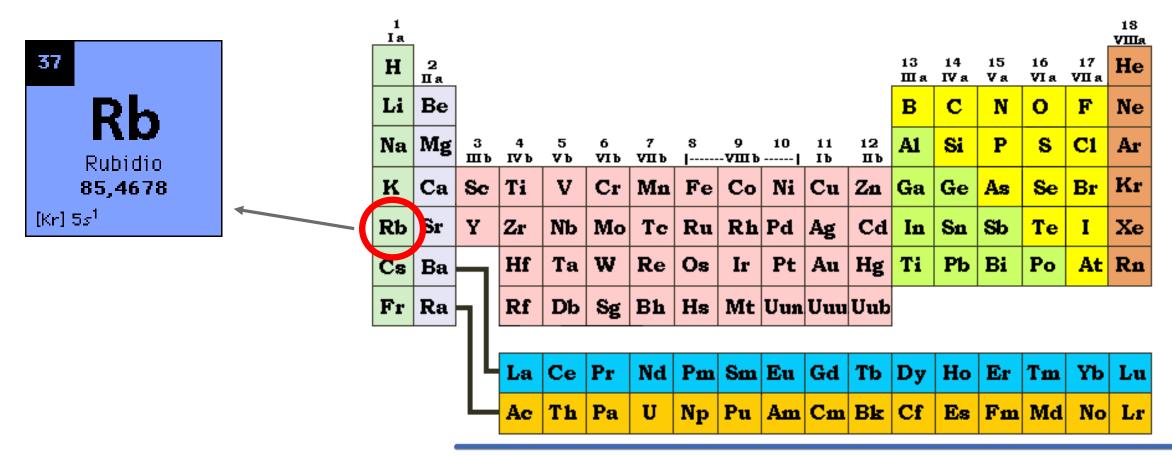






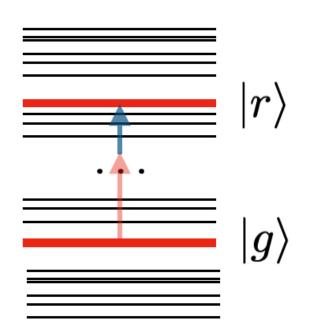


Pasqal employs Rubidium Atoms for its Neutral Atoms Quantum Computer





Pasqal employs Rubidium Atoms in the construction of the QPU

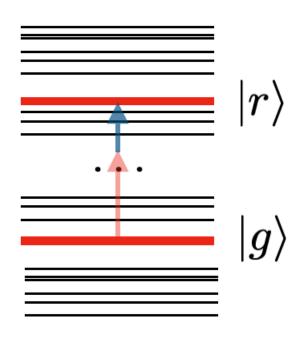


State of a Qubit 
$$\{|0
angle, |1
angle\}$$
 encoded in two electronic levels of the Rubidium Atom  $\{|g
angle, |r
angle\}$ 

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

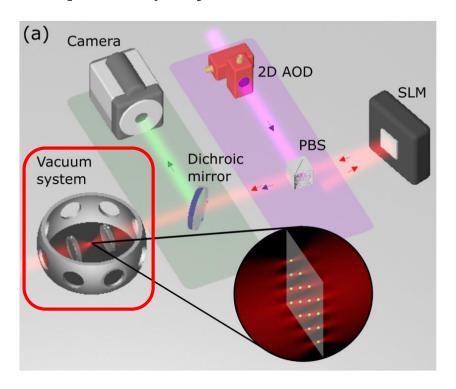


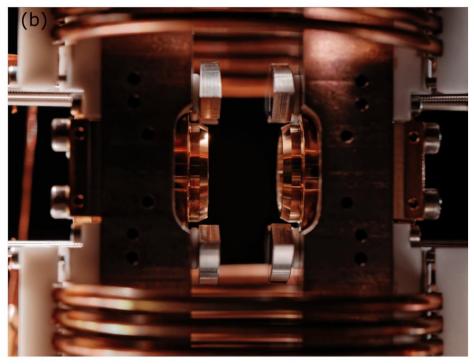
 $\{|g\rangle,|r\rangle\}$  are ground and «Rydberg» states characterized by:

- 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



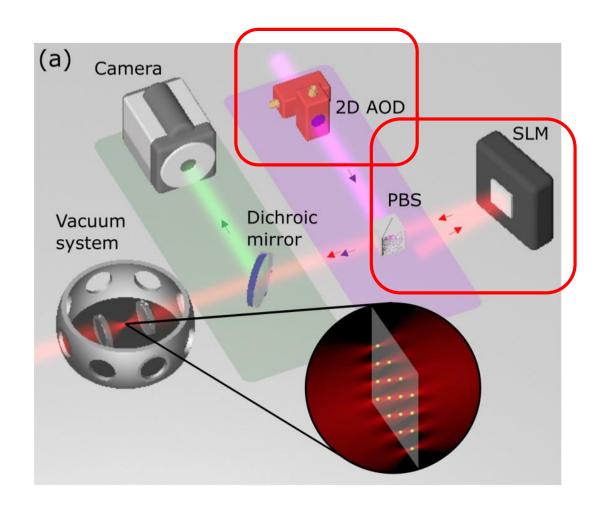
Pasqal employs Rubidium Atoms in the construction of the QPU





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



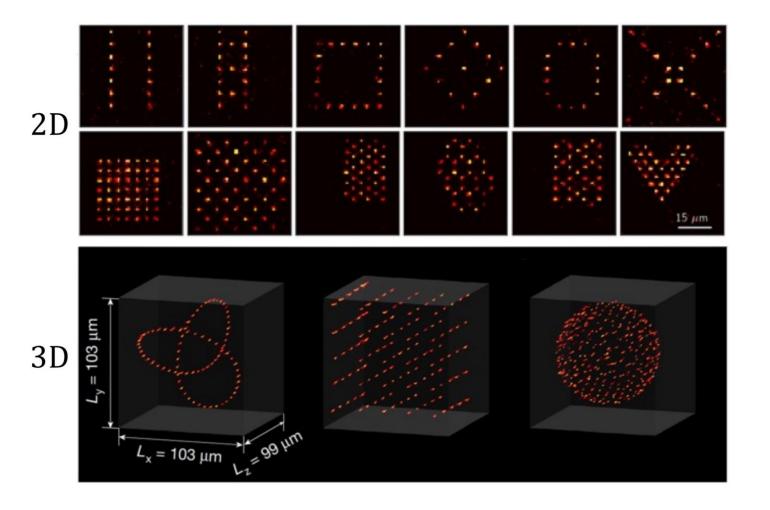


Rubidium atoms are trapped and held by laser beams, in particular:

- 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** 

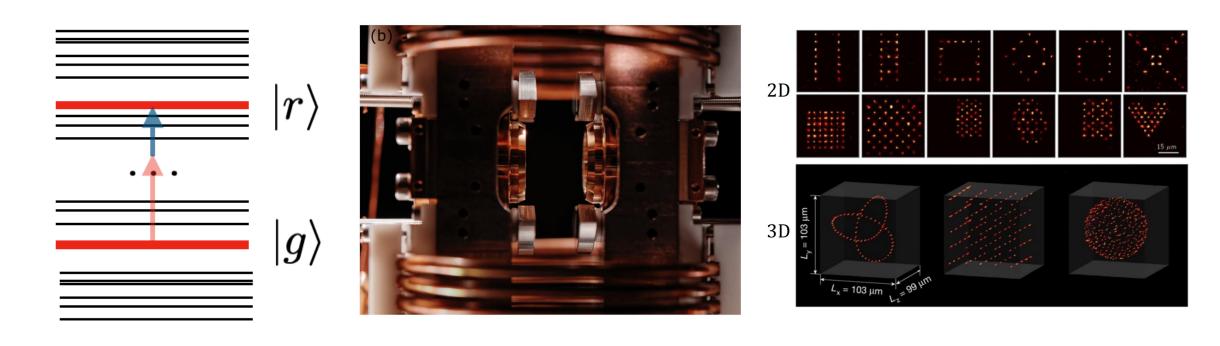




By moving the optical tweezers it is possible to arrange the topology of the Rubidium atoms and therefore of the qubits

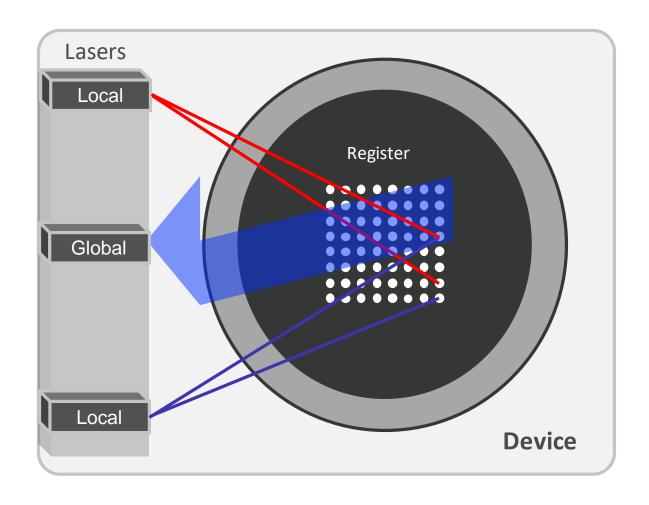
Depending on the application, it is useful to vary the Topology which can be 1D, 2D or even 3D

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

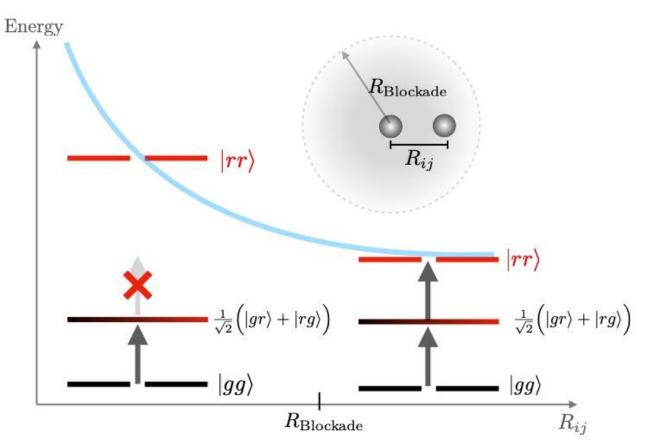
e.g. 
$$|g
angle 
ightarrow |r
angle$$

Make qubit interact

e.g. 
$$|gg
angle 
ightarrow rac{1}{\sqrt{2}} \Big( |gr
angle + |rg
angle \Big)$$



#### Rydberg Blockade: principle used to create entangled states



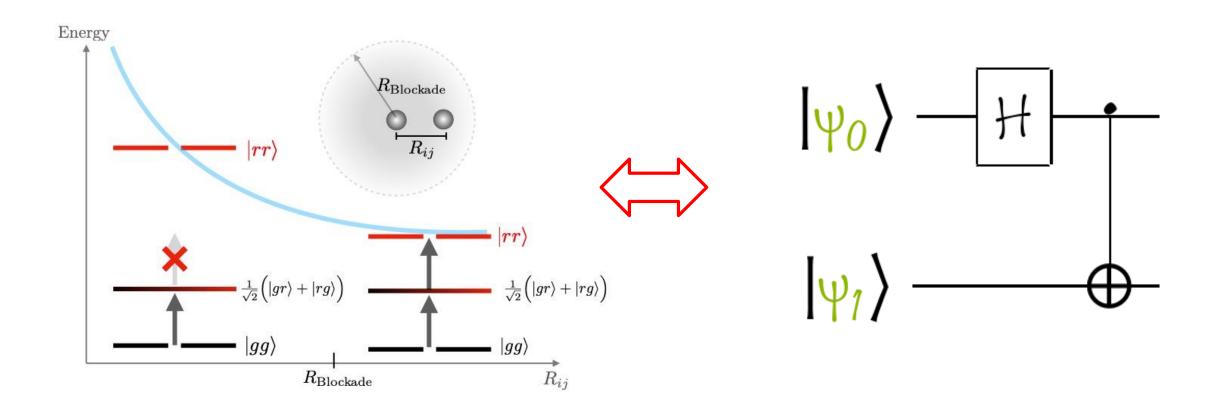
**Qubits** that are **within range** of the Rydberg blockade **interact** with each other.

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

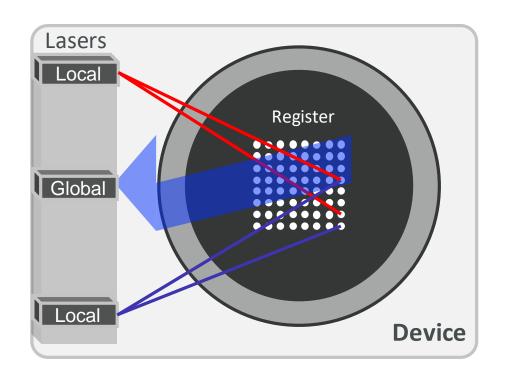
The resulting state is an **entangled state**, the same as obtained after a Hadamard gate followed by a CNOT



#### Rydberg Blockade: principle used to create entangled states



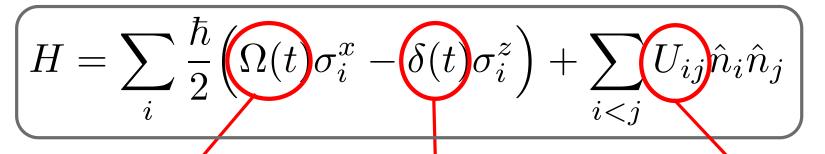




Mathematically, lasers interact with qubits, modifying the Hamiltonian, which is a function that describes the energy of the entire qubit system

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





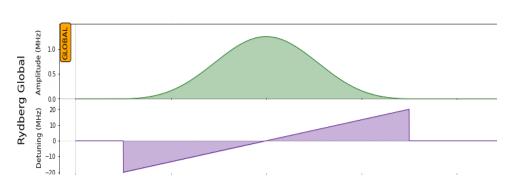
 $\hat{n}_j = (\mathbb{I} + \sigma_j^z)/2$ 

Rabi Frequency

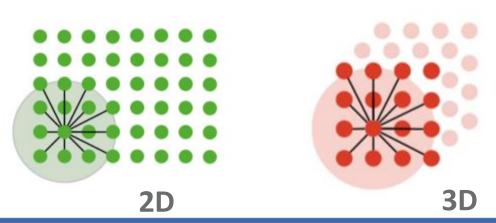
**Detuning** 

 $r_{ij} = rac{C_6}{r_{ij}^6}$  Modulates interaction between qubits

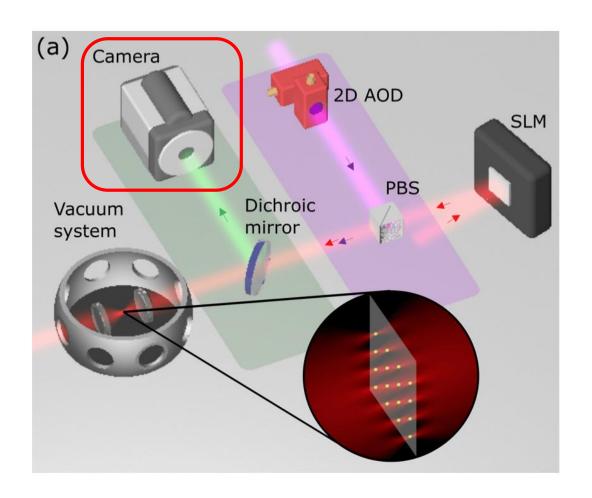
They vary by changing the **intensity** and **frequency** of the laser



Vary with **Topology** 







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

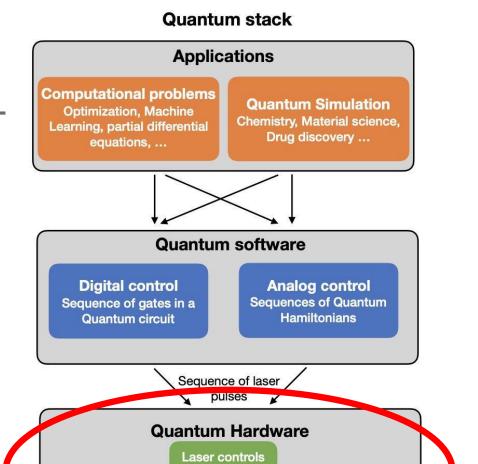
The measurement process is performed in such a way that each atom in the qubit state | 0 
appears bright, while the atoms in the qubit state | 1 
remain dark.



NISQ Algorithms
(Noisy Intermidiate Scale Quantum)







Quantum

register

**Electronics** 

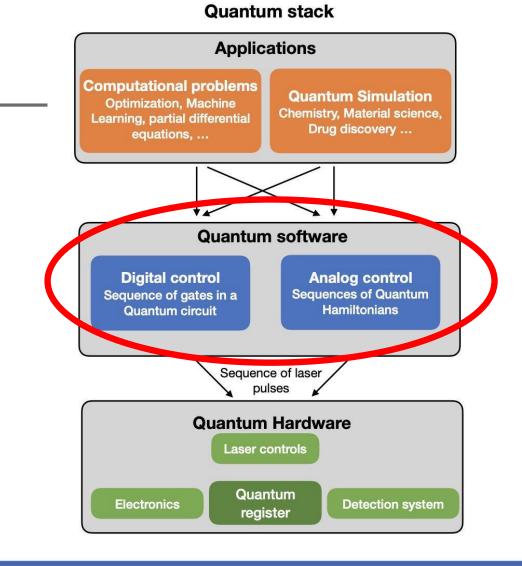


**Detection system** 

NISQ Algorithms
(Noisy Intermidiate Scale Quantum)



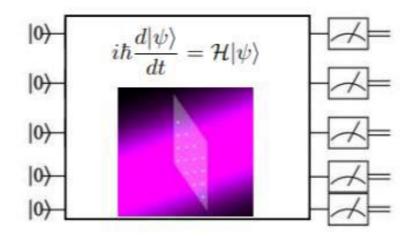


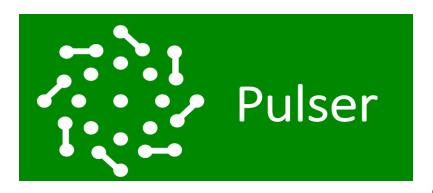




#### Lower level programming

#### (b) Analog processing





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

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

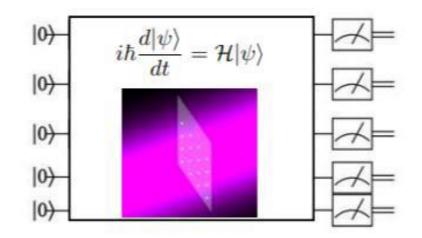
Possible by varying:

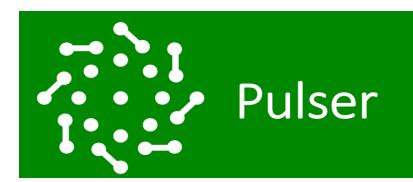
- Intensity and frequency of lasers
  - Qubit register topology



#### Lower level programming

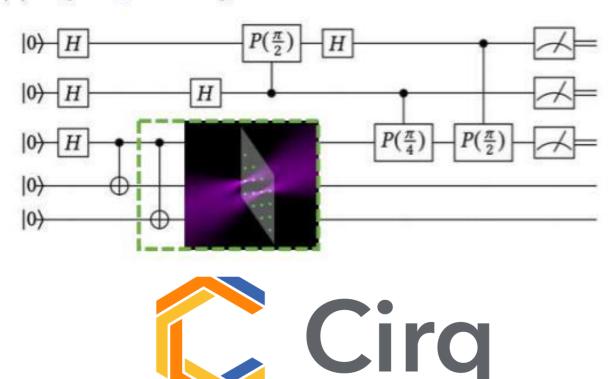
(b) Analog processing



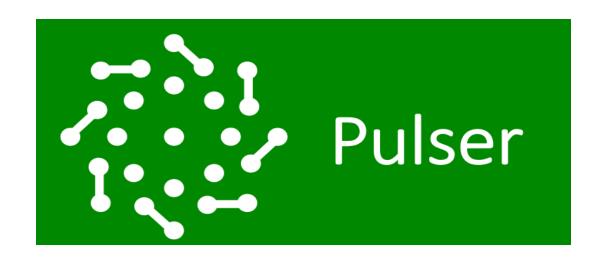


#### Higher level programming

(a) Digital processing







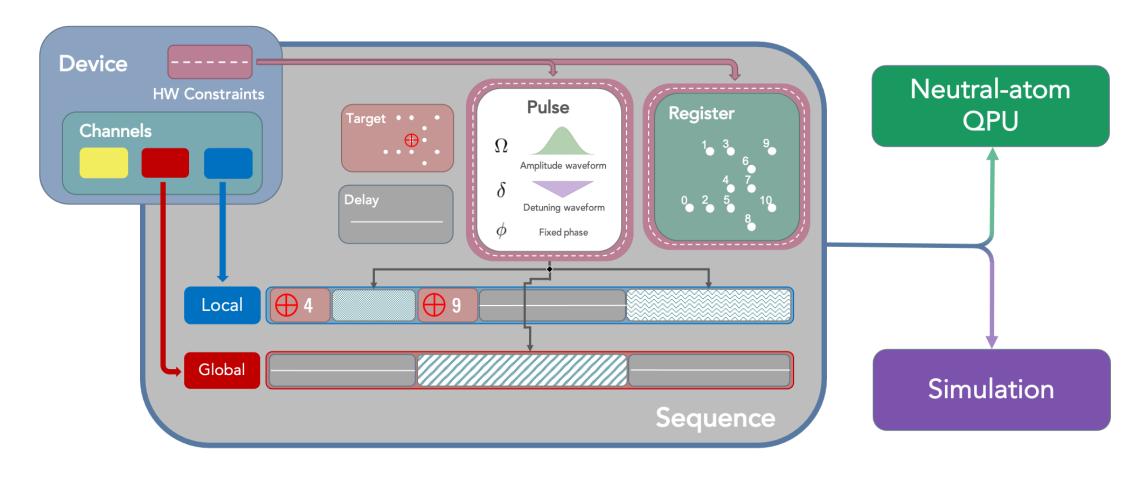
Python software library for programming Pasqal devices at the laser pulse level.

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

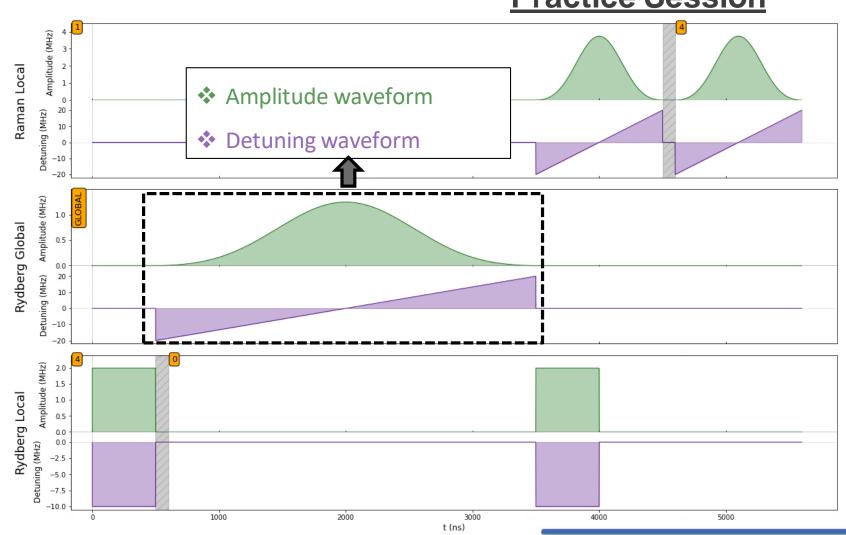


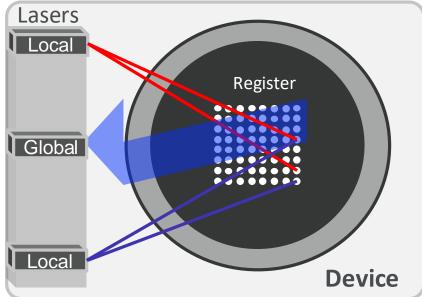
In Pulser, local and global pulse sequences can be defined





#### **Practice Session**

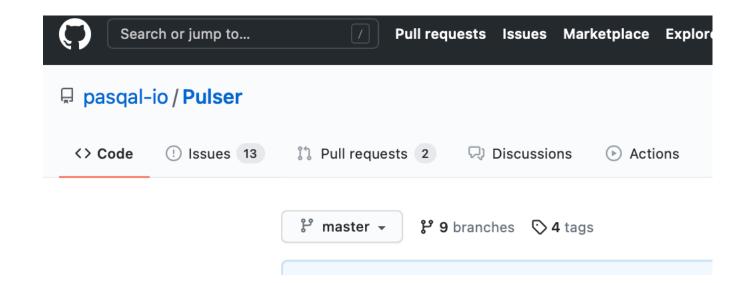






#### **Practice Session**





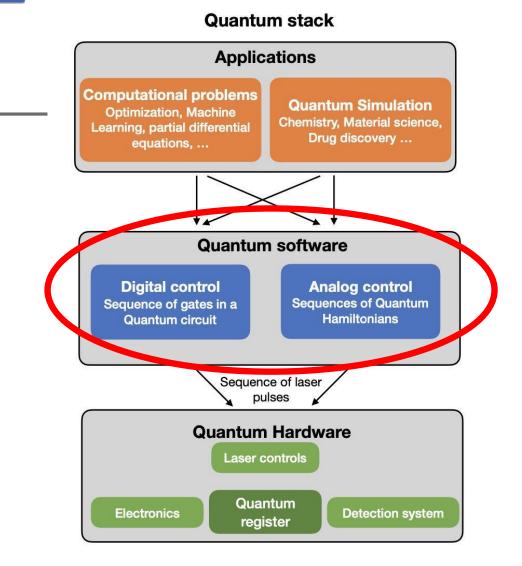
https://github.com/pasqal-io/Pulser



NISQ Algorithms
(Noisy Intermidiate Scale Quantum)





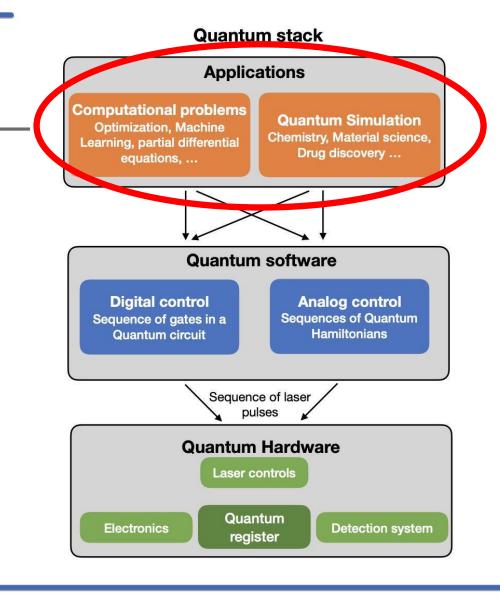




NISQ Algorithms
(Noisy Intermidiate Scale Quantum)











#### Quantum Algorithms: Shor's algorithm (1994)

# **Exampe: Facorization**

Given N, find  $p \times q = N$ 

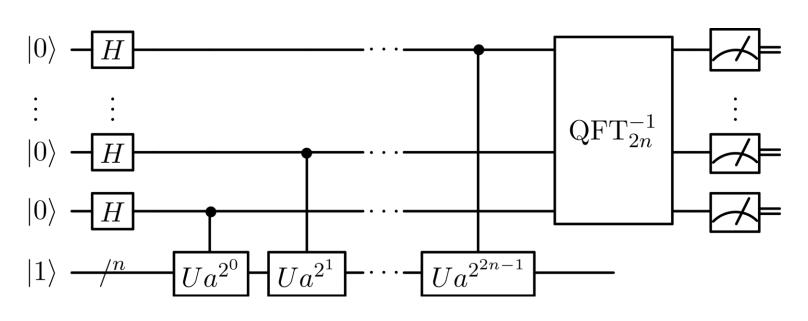
Hard for classical computer

Finding solution requires exponential time





#### Quantum Algorithms: Shor's algorithm (1994)





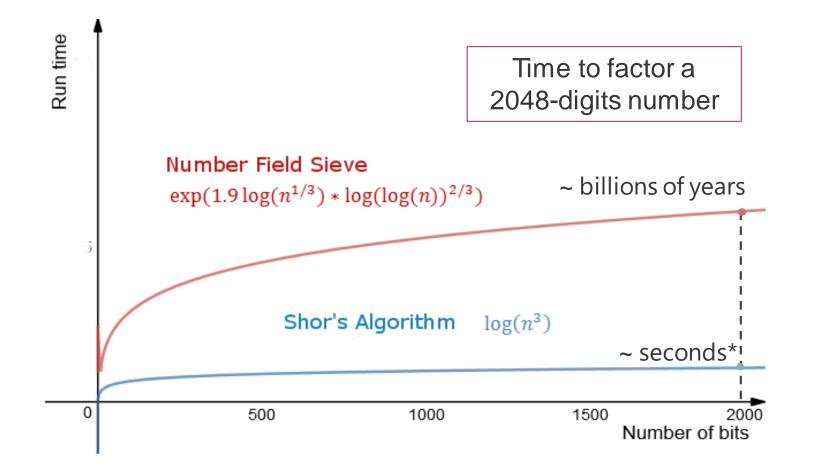
**Efficiently solve Factorization** 



**Exponential Speedup** 



#### Quantum Algorithms: Shor's algorithm (1994)





<sup>\*</sup> 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

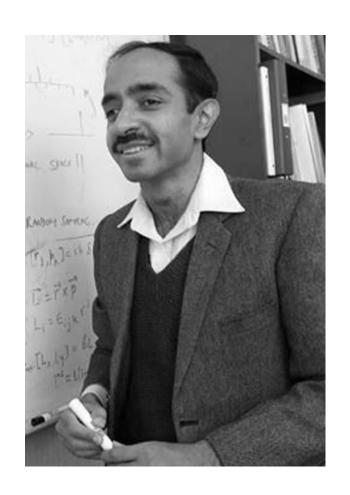


#### **Quantum Algorithms: Grover search algorithm (1996)**

# Run-time brute-force algorithm: $d^N$

**Run-time Grover search:** 

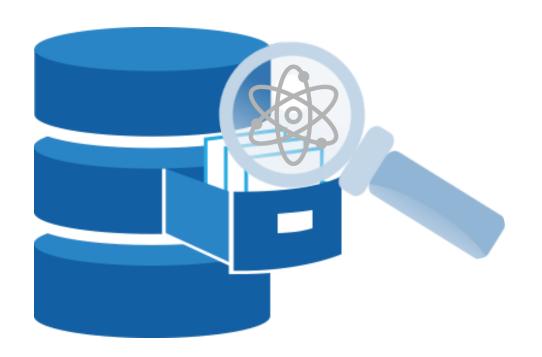
$$\sqrt{d^N}$$

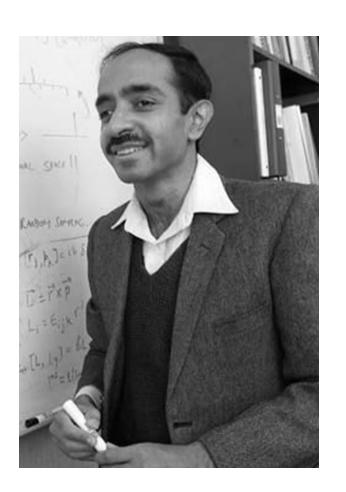




#### **Quantum Algorithms: Grover search algorithm (1996)**

# Original application: Database Search









# NP

Solution can be verified efficiently

P Efficient solution





# NP

Solution can be verified efficiently

Efficient solution



NPcomplete

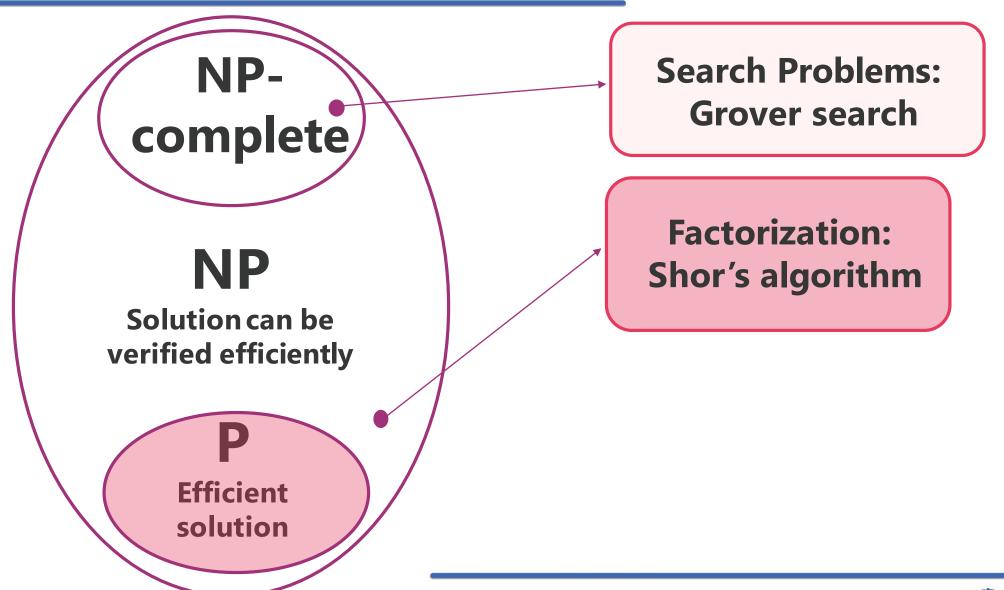
NP

Solution can be verified efficiently

Efficient solution

**Factorization: Shor's algorithm** 

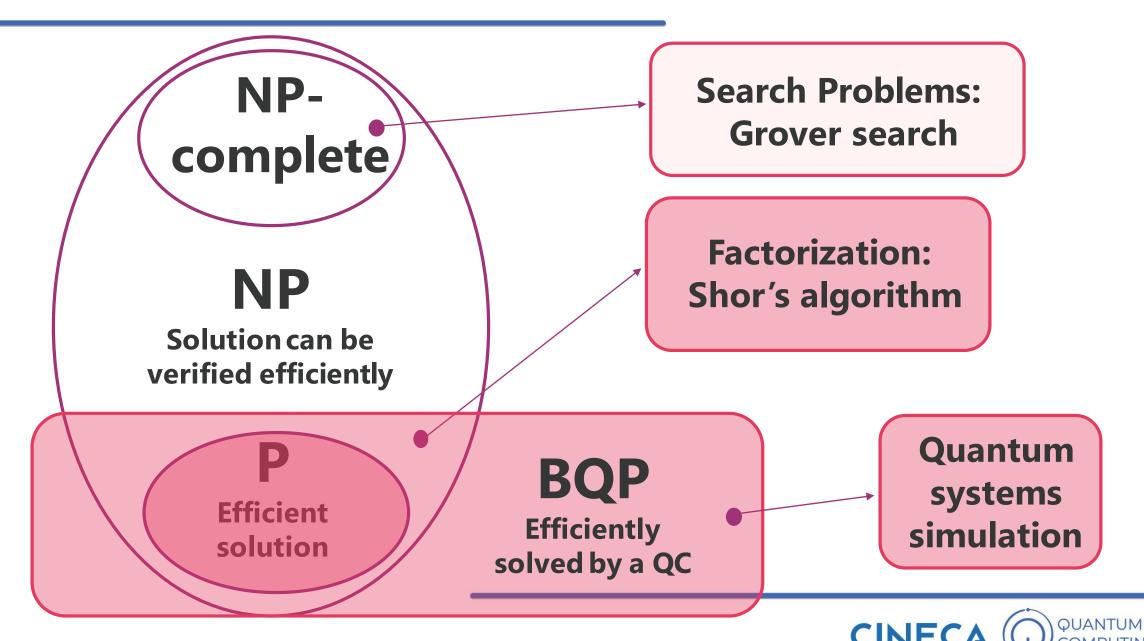






NP-complete **Search Problems: Grover search Factorization:** NP Shor's algorithm Solution can be verified efficiently **BQP Efficient Efficiently** solution solved by a QC



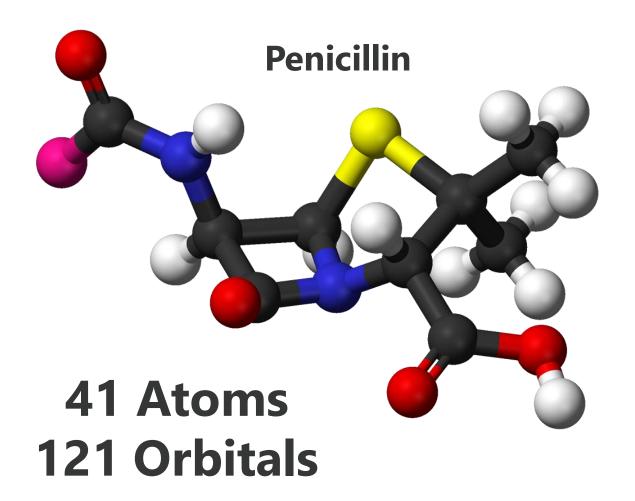


Use a quantum system (the quantum computer)

to

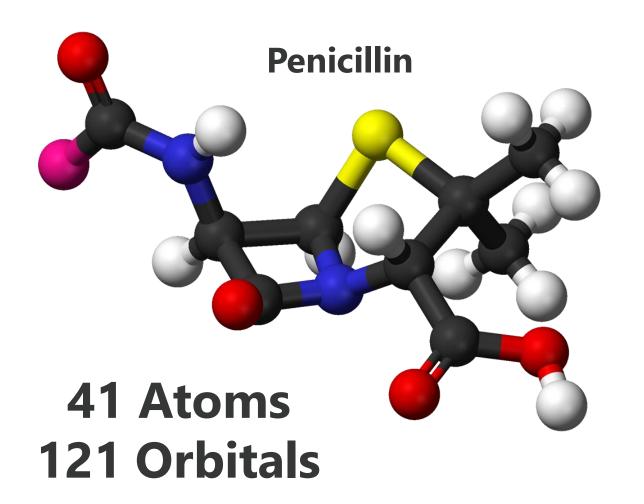
simulate a quantum system (nature)





~10<sup>86</sup> bits to exactly decribe such molecule on a classical computer





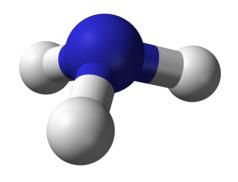
# 286 quantum bits with an ideal QC

# Quantum Simulation (exponential speedup)

It is believed that for any physically realistic Hamiltonian H on n degrees of freedom, the corresponding time evolution operator can be implemented using poly(n,t) gates. This problem is not solvable in general on a classical computer in polynomial time.



#### **Ammonia NH**₃



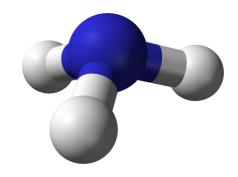
#### **Used for fertilizers:**

- Produced at High preassure and high temperatures
- Every year, 2% of the panet energy goes into the productuon of **NH3**





#### Ammonia NH₃



- Efficient Production
- Save energy and money

#### **Used for fertilizers:**

- Produced at High preassure and high temperatures
- Every year, 2% of the panet energy goes into the productuon of **NH3**

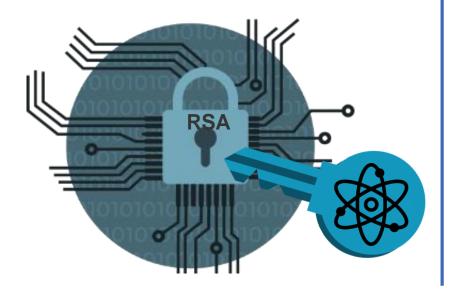


Simulate NH3 with a Quantum Computer could give us information about chemical properties and reactions



# Cryptography

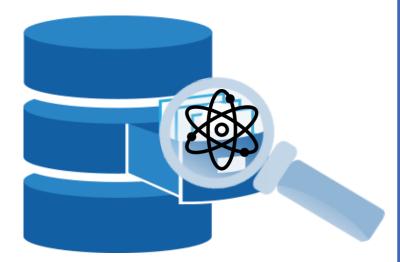
Shor's Algorithm
Exponential Speedup



### **Optimization**

Grover's Algorithm

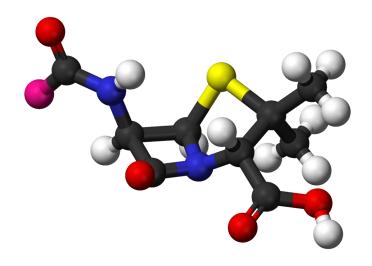
Quadratic Speedup



#### Chemistry

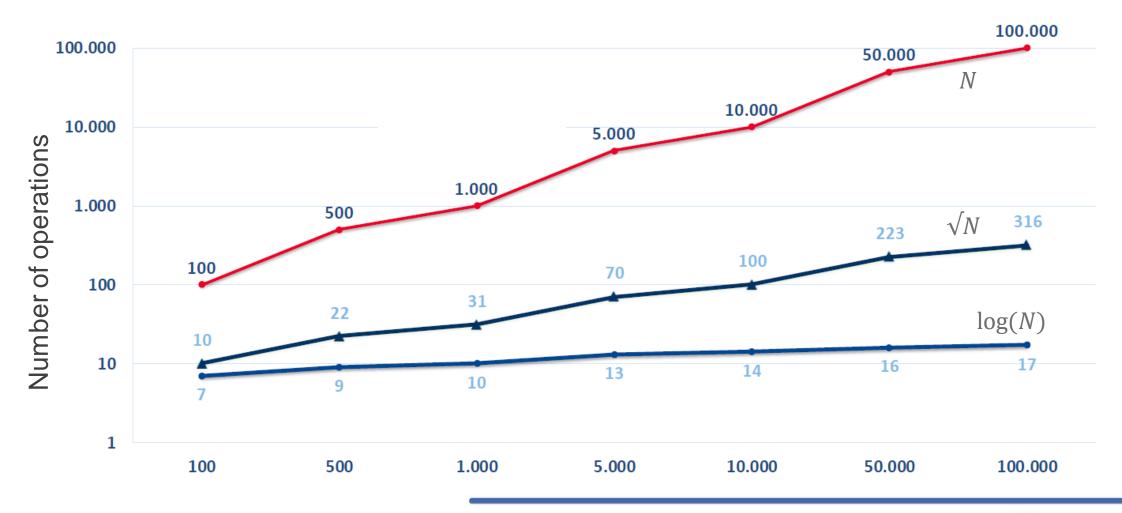
**Quantum Simualtion** 

**Exponential Speedup** 





#### Before NISQ – Old School Quantum Algorithms





### 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



# 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

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



#### **Old School Quantum Algorithms: Error correction**

# Cryptography

Shor's Algorithm
Exponential Speedup

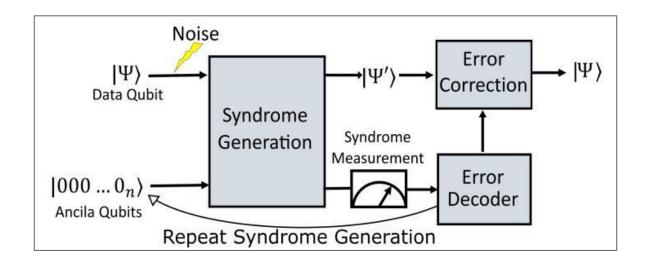
# **Optimization**

Grover's Algorithm

Quadratic Speedup

# Chemistry

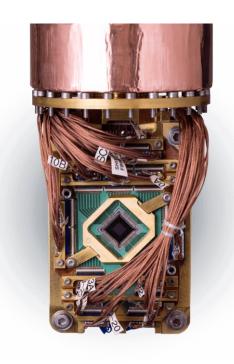
Quantum Simualtion
Exponential Speedup



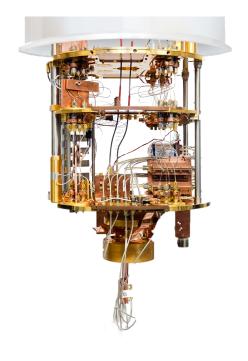
- Require error corrected quantum computers with about 1 million or 100 thousands of qubits
- Error correction comes with an overhead in the number of physical qubits
- Will be availabe in 10-20 years



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





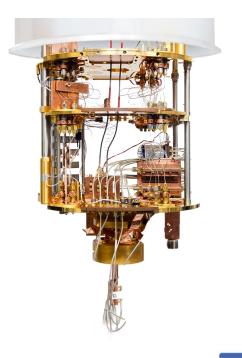


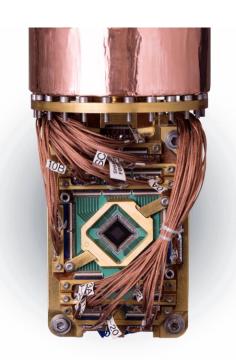


#### We entered the NISQ era

NISQ = Noisy Intermediate-Scale Quantum

1. General Purpose QC





2. Quantum Annealers



#### We entered the NISQ era

NISQ = Noisy Intermediate-Scale Quantum

#### Intermediate-Scale

#### **General Purpose QC**

50 up to hundreds of qubits

IBM: 127 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)

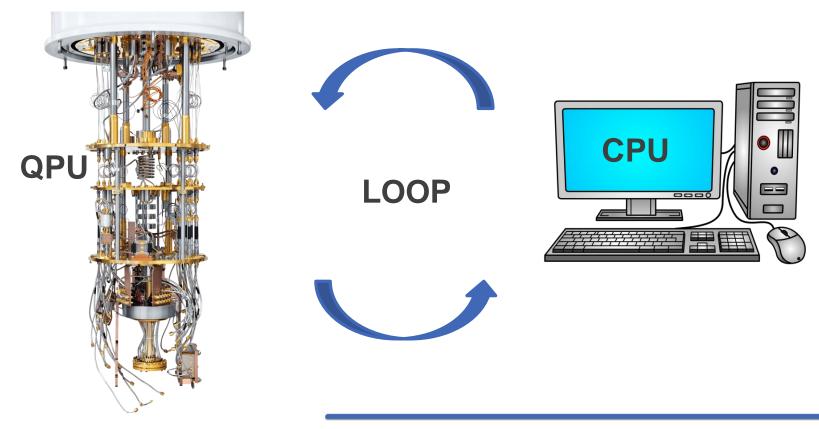
#### **Quantum Annealers**

- 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

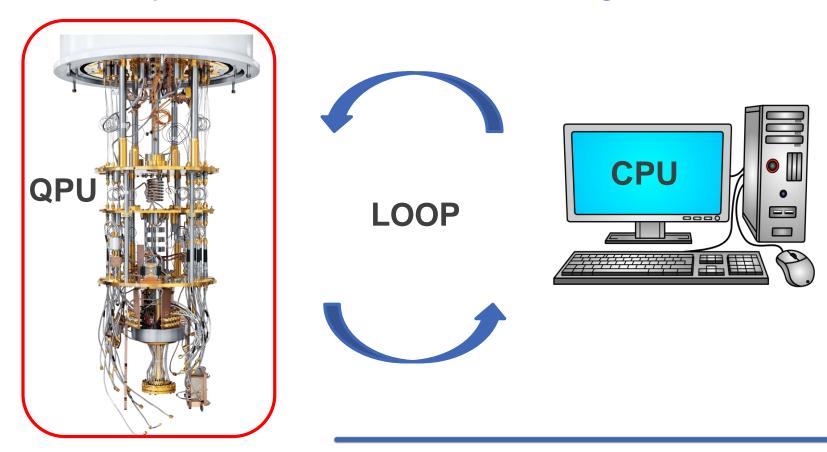
Hybrid Quantum-Classical algorithms





#### NISQ-ready algorithms for general purpose QPU

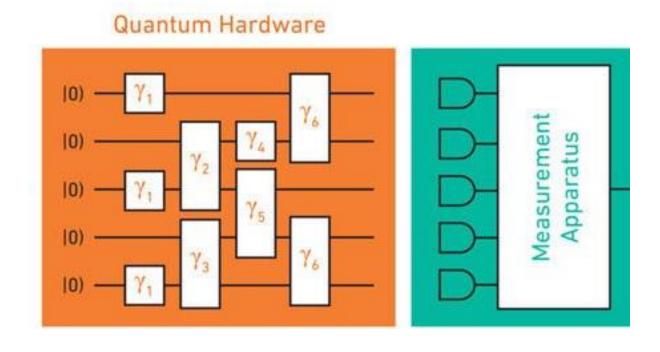
Hybrid Quantum-Classical algorithms





#### NISQ-ready algorithms for general purpose QPU

#### Parametric Quantum Circuits



- Circuits that use gates, or in general, that apply parameter-dependent 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

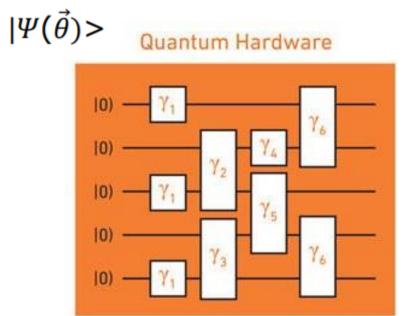


#### NISQ-ready algorithms for general purpose QPU

#### Working principle

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

2. Implement Variational Ansatz on the QPU



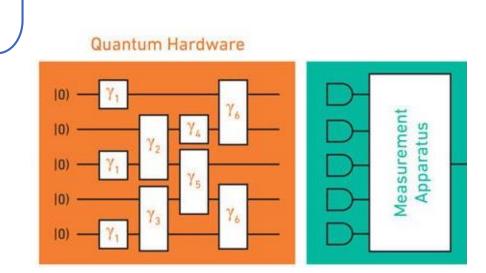


#### NISQ-ready algorithms for general purpose QPU

#### 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

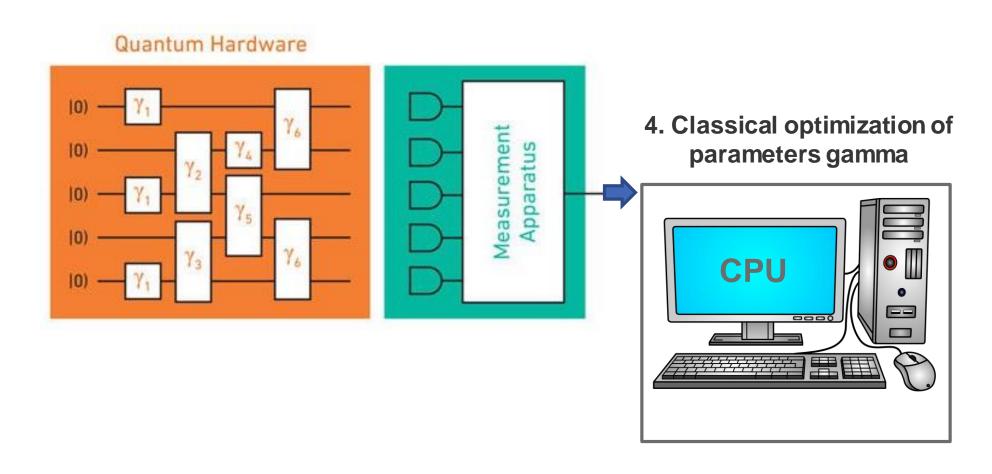
#### Working principle

- 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 gradient-free (BFGS, COBYLA, L-B, SPSA, Bayesian Opt.)
Depending on the type of cost function being evaluated



#### NISQ-ready algorithms for general purpose QPU





# NISQ-ready algorithms for general purpose QPU

#### Working principle

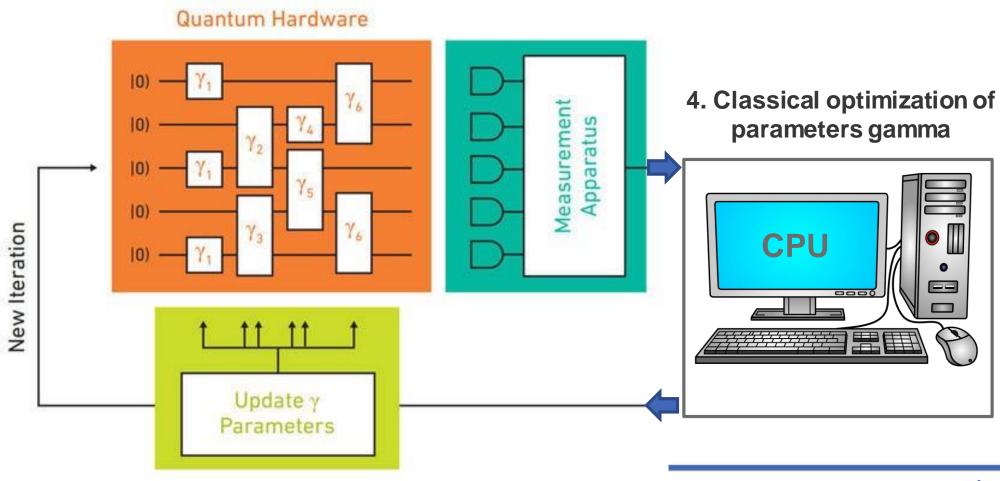
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This cycle is repeated until convergence. The final state gives us an approximation of the solution

**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



- Speed up
- Better quality solutions
- Lower energy consumption

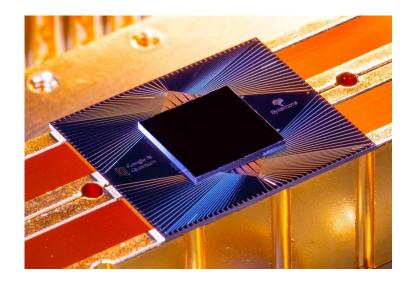


- Quantum Chemistry
- Quantum Optimization
- Quantum Al/Machine Learning



#### NISQ-ready algorithms for general purpose QPU

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

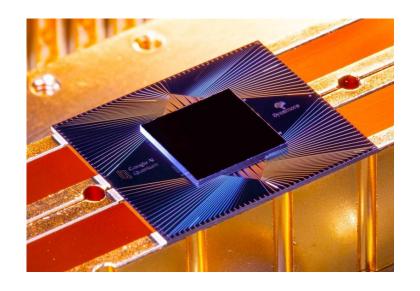


In 2019, researchers at the Google Quantum AI Lab compared the performance of quantum computers to classical supercomputers, using their **Sycamore quantum computer** with **53 qubits.** 

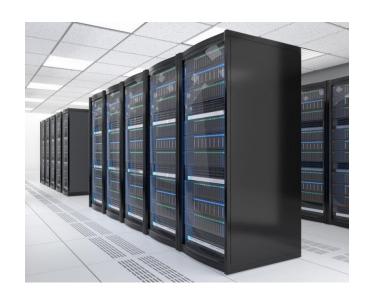


#### NISQ-ready algorithms for general purpose QPU

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





## NISQ-ready algorithms for general purpose QPU

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.



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



## NISQ-ready algorithms for general purpose QPU

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



- Speed up
- Better quality solutions
- Lower energy consumption



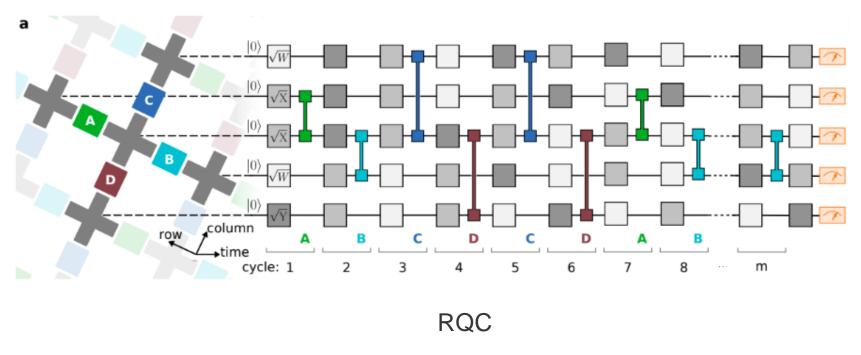
- Quantum Chemistry
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## NISQ-ready algorithms for general purpose QPU

Random Quantum Circuit (RQC) does not solve any useful (real-world) problem.

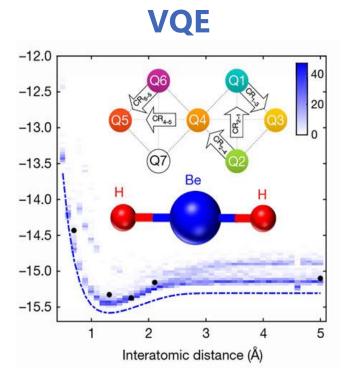
Its purpose is exactly to prove Quantum supremacy



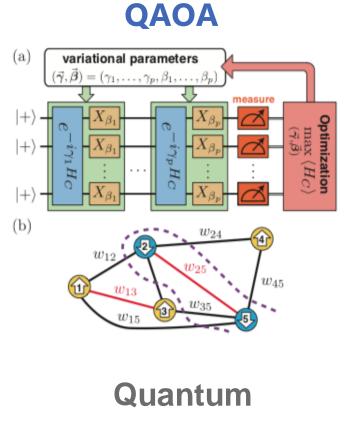
**Real World Problems?** 



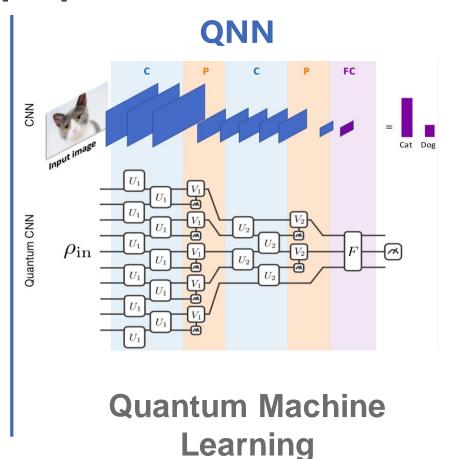
#### NISQ-ready algorithms for general purpose QPU



**Quantum Chemistry** 



**Optimization** 





#### NISQ-ready algorithms for general purpose QPU

**VQE** 

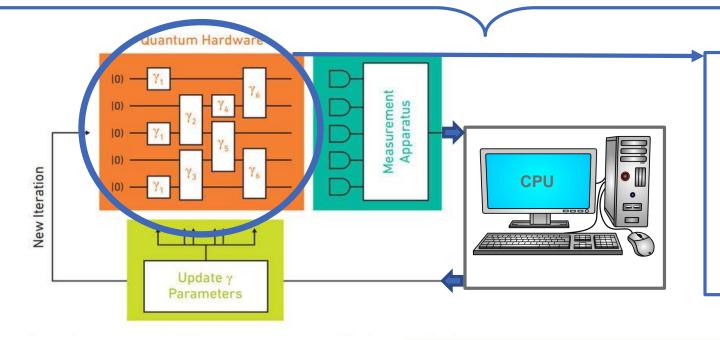
**Quantum Chemistry** 

**QAOA** 

**Quantum Optimization** 

QNN

Quantum Machine Learning

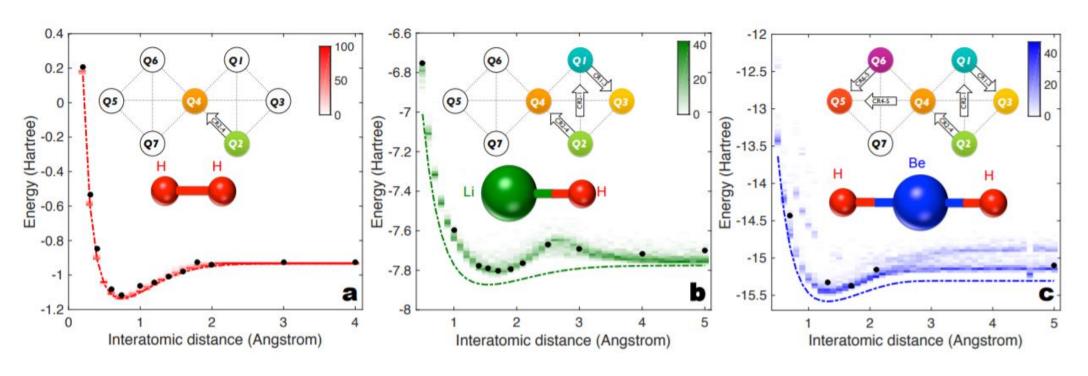


The main difference
between VQE, QAOA and
QNN concerns the choice
of the parametric
quantum circuit
(Variational Ansatz)



#### NISQ-ready algorithms for general purpose QPU

#### Variational Quantum Eigensolver (VQE) – QUANTUM CHEMISTRY



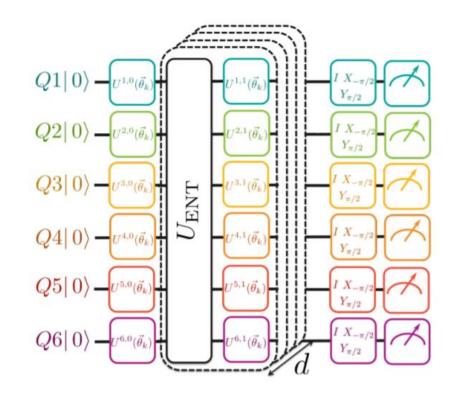


# NISQ-ready algorithms for general purpose QPU

Variational Quantum Eigensolver (VQE) – QUANTUM CHEMISTRY

Objective: 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)

Method: the VQE uses chemical-inspiredAnsatz, such as the Unitary Coupled Cluster(UCC) method or a "hardware-efficient" ansatz



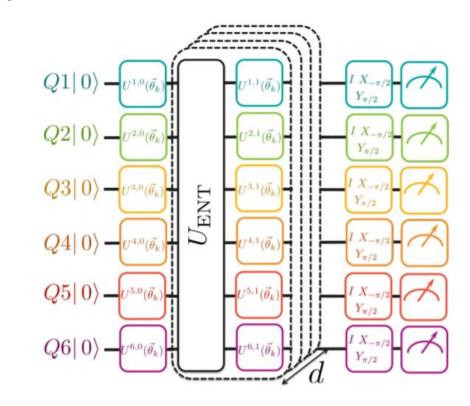


## NISQ-ready algorithms for general purpose QPU

#### 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

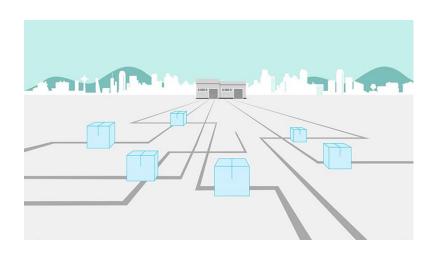




#### NISQ-ready algorithms for general purpose QPU

**Quantum Approximate Optimization Algorithm (QAOA) – QUANTUM OPTIMIZATION** 

#### **Optimization Problems**



Routing



**Scheduling** 



**Portfolio Optimization** 



## NISQ-ready algorithms for general purpose QPU

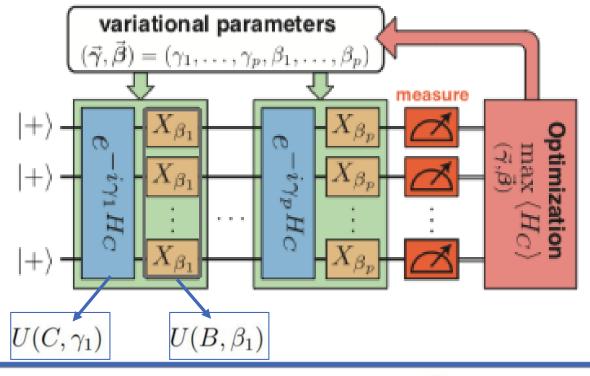
**Quantum Approximate Optimization Algorithm (QAOA) – QUANTUM OPTIMIZATION** 

Objective: to solve a combinatorial optimization problem

Method: 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).

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

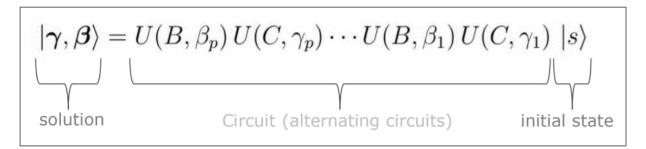




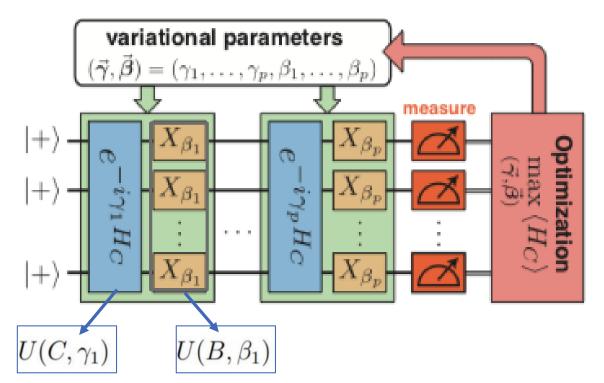
# NISQ-ready algorithms for general purpose QPU

#### **Quantum Approximate Optimization Algorithm (QAOA) – QUANTUM OPTIMIZATION**

It is a heuristic optimization algorithm



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





## NISQ-ready algorithms for general purpose QPU

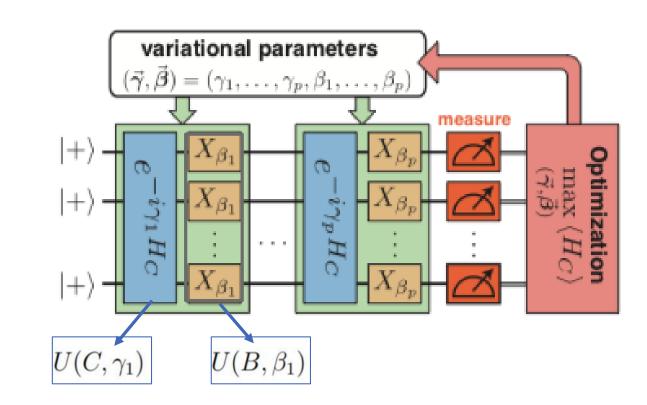
**Quantum Approximate Optimization Algorithm (QAOA) – QUANTUM OPTIMIZATION** 

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

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

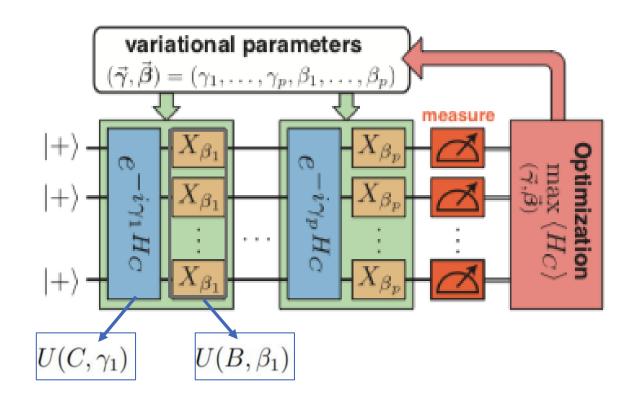




#### NISQ-ready algorithms for general purpose QPU

**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.



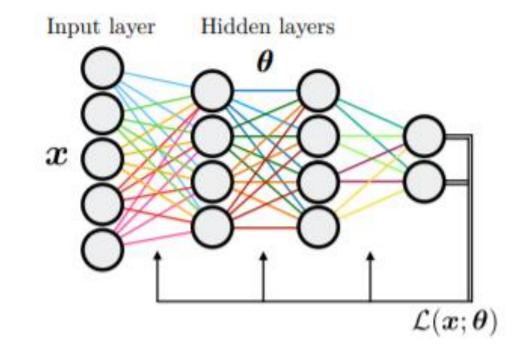


## NISQ-ready algorithms for general purpose QPU

**Quantum Neural Networks (QNN) – QUANTUM MACHINE LEARNING** 

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

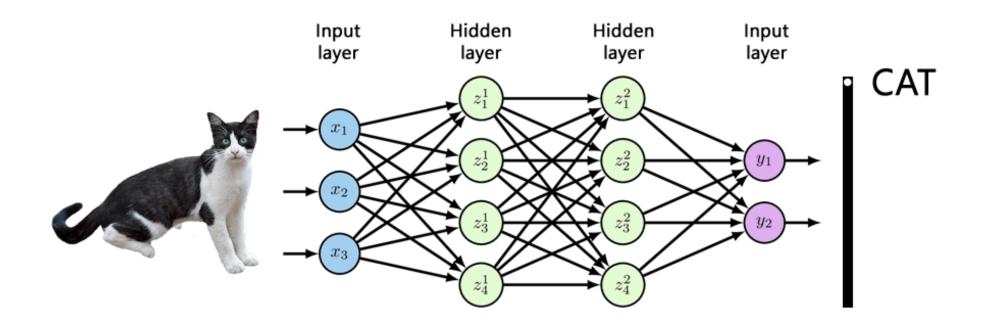
If properly trained, the NN is able to classify new data, i.e. data that was not used during training





#### 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

 $x \xrightarrow{\text{JDdNI}} |0\rangle \longrightarrow \mathcal{U}_{x} |0\rangle \otimes S = |\psi_{x}\rangle \qquad \mathcal{G}_{\theta} |\psi_{x}\rangle = |g_{\theta}(x)\rangle \qquad \mathcal{J}_{z_{2}} \xrightarrow{\text{JDdIDO}} y$   $\text{feature map} \qquad \text{variational model} \qquad \text{measurement}$   $\mathcal{U}_{x} \qquad \mathcal{G}_{\theta} \qquad f(z) = y$ 

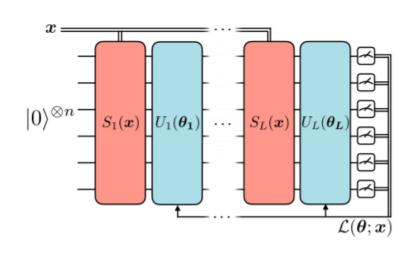
The circuit learns to classify new inputs based on the examples seen in the training phase

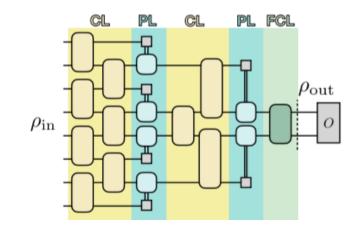


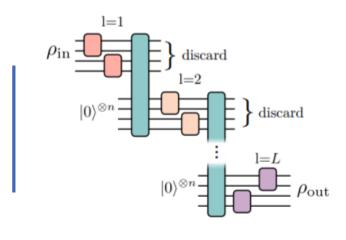
#### NISQ-ready algorithms for general purpose QPU

**Quantum Neural Networks (QNN) – QUANTUM MACHINE LEARNING** 

#### We can also have several Ansatz for QNNs







**Standard QNN** 

Convolutional QNN

**Dissipative QNN** 

https://arxiv.org/abs/2102.03879



#### NISQ-ready algorithms for general purpose QPU

#### **Main Challenges**

- Trainability / optimization of parameters: best optimization scheme or technique
  - Barren plateaus: Vanishing gradients that make it hard to optimize
  - Ansatz and initialization strategies: structure of the parametric circuit
- Efficiency: precision required in the output per the amount of resources consumed
- Accuracy: the degree to which output conforms to the correct value or a standard.
- Hardware noise / Error mitigation: optimal techniques to reduce errors without an overhead in resources



# **NISQ-ready algorithms**

# **QUANTUM ADVANTAGE IN THE NISQ ERA?**



# **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



r.mengoni@cineca.it

