

# Advanced Parallel School 2022

## Quantum Computing – Day 5

### Quantum Computing @ CINECA

Mengoni Riccardo, PhD

*18 Feb 2022*

CINECA



# CINECA Overview

## CINECA: Italian HPC center

Rank	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
1	<b>Supercomputer Fugaku</b> - Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D, Fujitsu RIKEN Center for Computational Science Japan	7,630,848	442,010.0	537,212.0	29,899
14	<b>Marconi-100</b> - IBM Power System AC922, IBM POWER9 16C 3GHz, Nvidia Volta V100, Dual-rail Mellanox EDR Infiniband, IBM CINECA Italy	347,776	21,640.0	29,354.0	1,476



List of the 500  
most powerful  
supercomputers  
in the world

# CINECA Overview

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CINECA: Italian HPC center

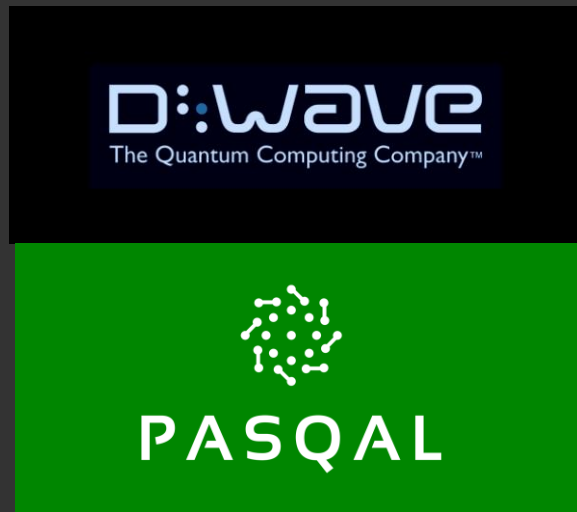


**Leonardo:** Cineca pre-exascale supercomputer

Coming soon. Will be in the **top five most powerful supercomputers in the world**

# CINECA Overview

- **Today Access to:**
  - D-Wave Quantum Annealer
  - Pasqal Neutral Atoms
- **Future:**
  - Soon others..
  - On-site?



# Old School Quantum Algorithms: Overview

## Cryptography

Shor's Algorithm

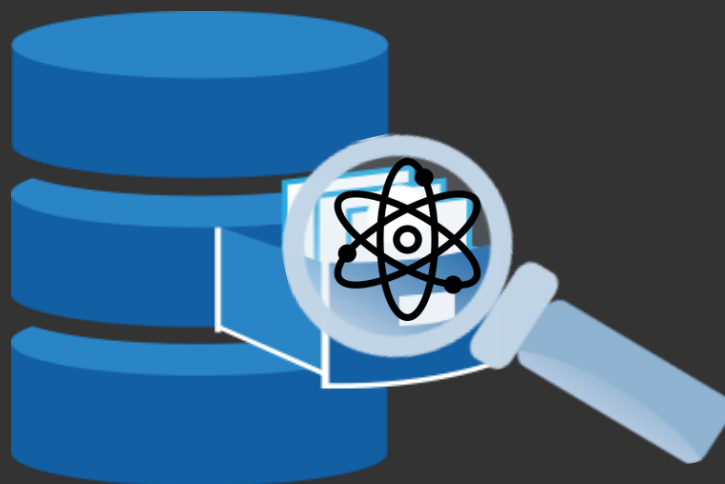
Exponential Speedup



## Optimization

Grover's Algorithm

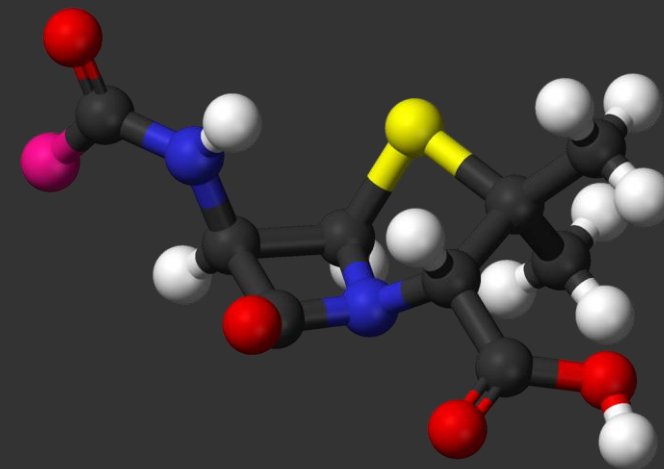
Quadratic Speedup



## Chemistry

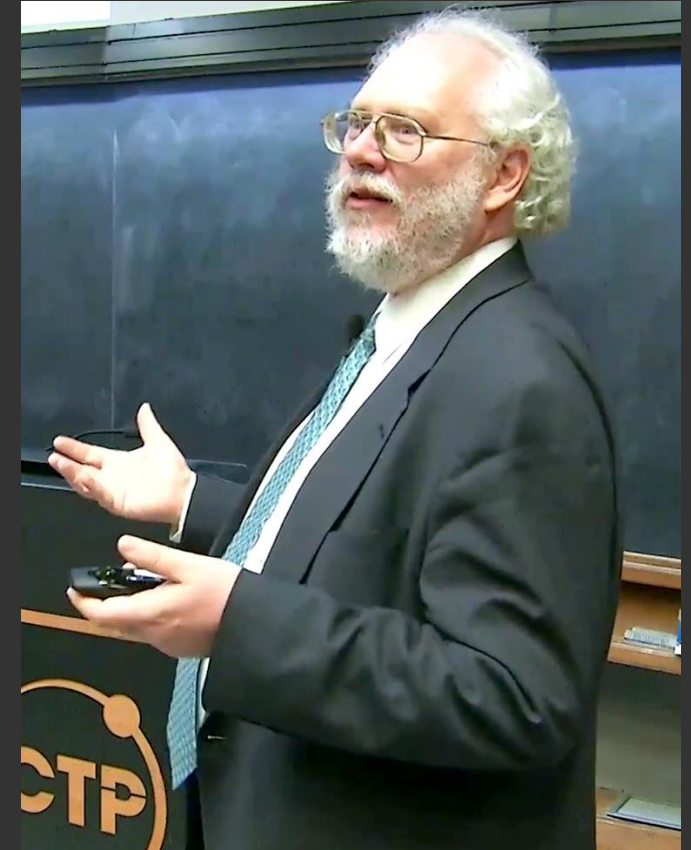
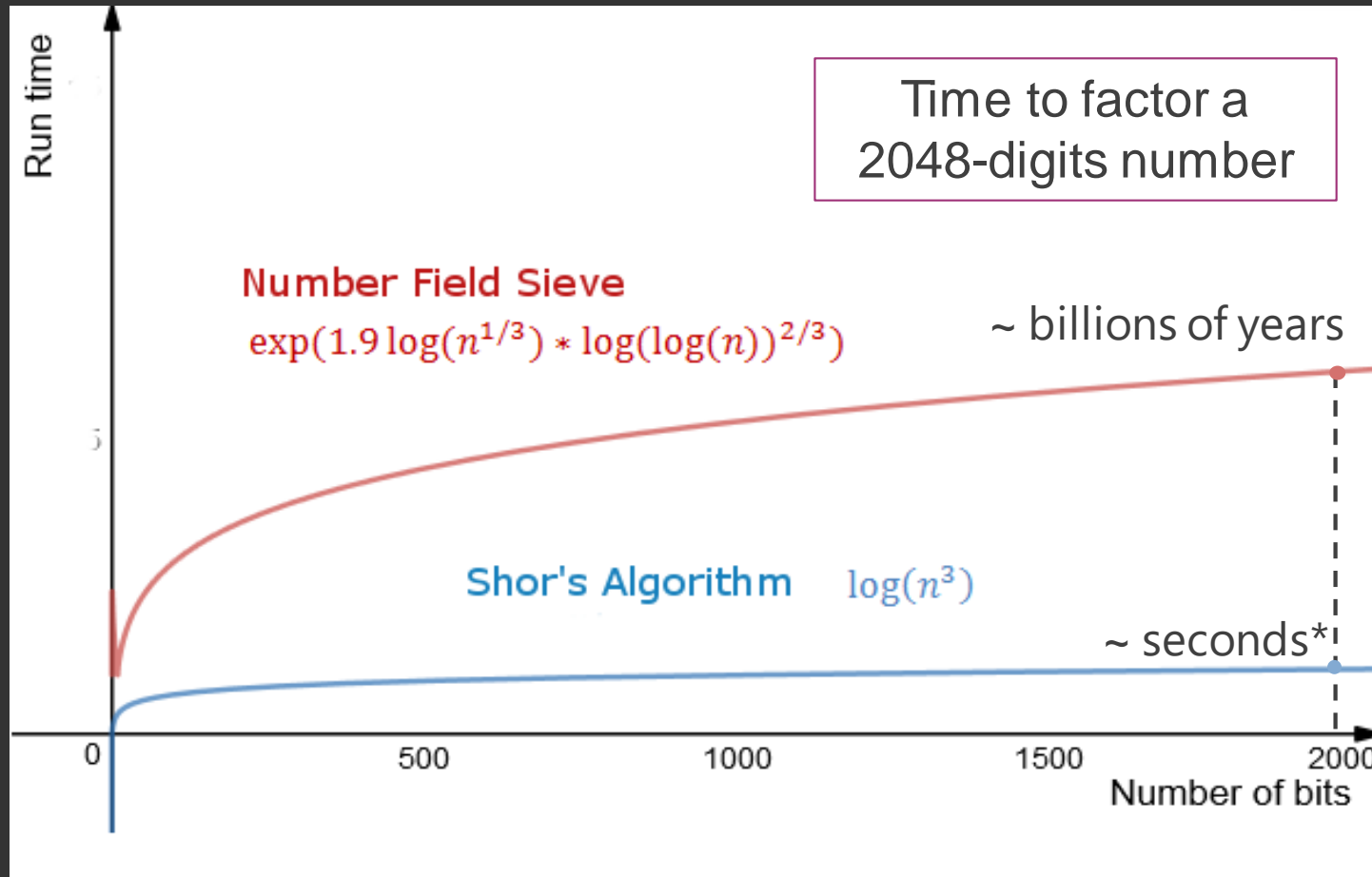
Hamiltonian Simulation

Exponential Speedup





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



\* 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

# Old School Quantum Algorithms: Error Correction

## Cryptography

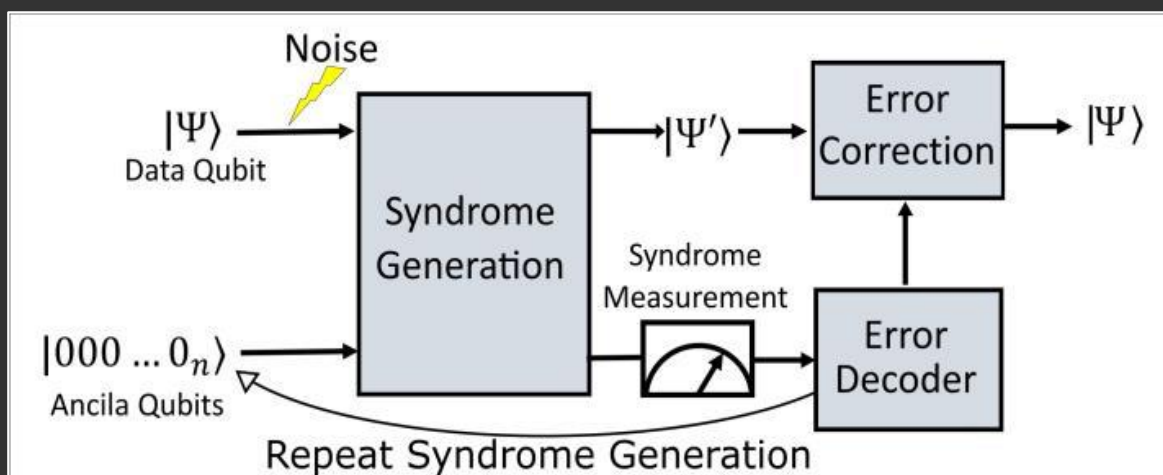
Shor's Algorithm  
Exponential Speedup

## Optimization

Grover's Algorithm  
Quadratic Speedup

## Chemistry

Hamiltonian Simulation  
Exponential Speedup



- Require **error corrected** quantum computers with about **1 million or 100 thousands of qubits**
- Will be **available in 10-20 years**

**NISQ = Noisy Intermediate-Scale Quantum**

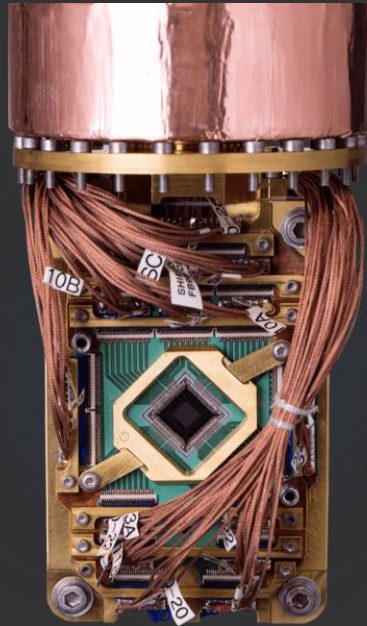
**Intermediate-Scale Quantum computers with no error correction**



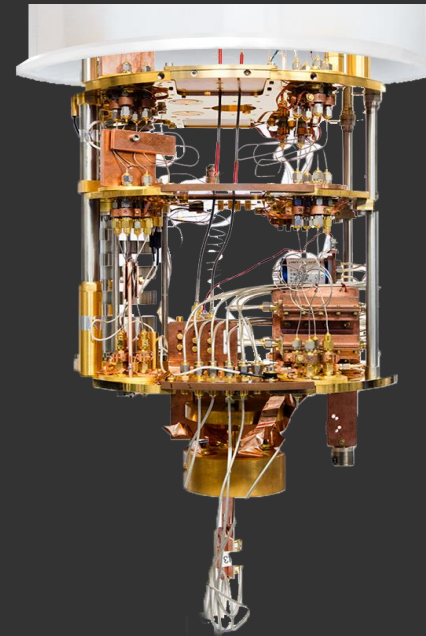
**NISQ = Noisy Intermediate-Scale Quantum**

**Intermediate-Scale Quantum computers with no error correction**

## 1. Quantum Annealers



## 2. Circuit Quantum Computers



**NISQ = Noisy Intermediate-Scale Quantum**

**Intermediate-Scale Quantum computers with no error correction**

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



- Speed up
- Better quality solutions
- Lower energy consumption

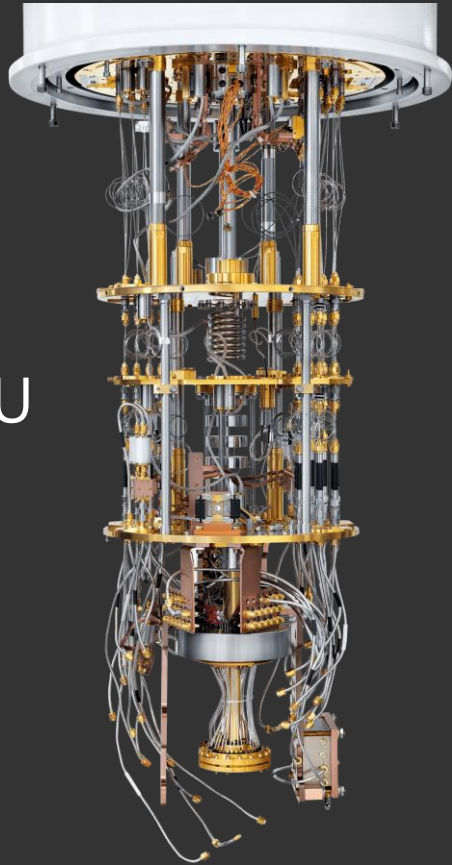


- Quantum Chemistry
- Quantum Optimization
- Quantum AI/Machine Learning

# Cineca Quantum Computing Lab: Vision

Quantum Computing will always be **Hybrid**

QPU

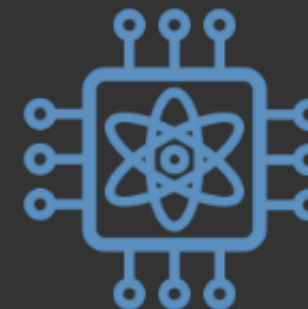


HPC

# Cineca Quantum Computing Lab: Vision

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**Emulators:** develop/test HPC ready software for simulating quantum systems and quantum computers



**Hybrid workflows:** development of problem oriented hybrid QPU-HPC algorithms

**Scheduling hybrid resources:** ensure a task is run with the resources it needs and decide when and how to allocate QPU-HPC resources



**Real-world applications:** chemistry, optimization, machine learning, simulations, etc.

# Cineca Quantum Computing Lab: Emulators

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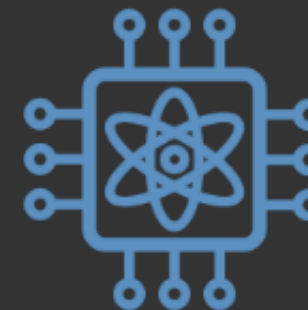
**Emulators:** develop/test HPC ready software for simulating quantum systems and quantum computers



# Cineca Quantum Computing Lab: Emulators

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**Emulators:** develop/test HPC ready software for simulating quantum systems and quantum computers



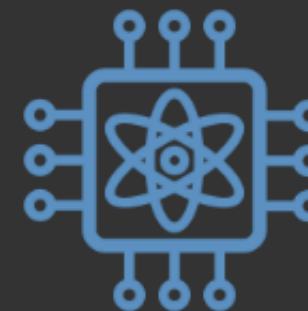
## Usage:

- Development and verification of Quantum Algorithms
- Benchmarking
- Study Noise
- Assess hardware constraint
- Co-design of quantum hardware
- ...



# Cineca Quantum Computing Lab: Emulators

**Emulators:** develop/test HPC ready software for simulating quantum systems and quantum computers



## State-vector emulators

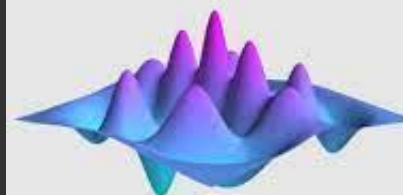
- Single node Multi-threading using OpenMP to achieve state of the art emulation of quantum circuits.
- Working on a multithread/multi-node implementation



Qiskit



Cirq

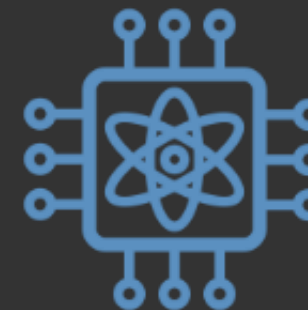


QuTiP

Quantum Toolbox in Python

# Cineca Quantum Computing Lab: Emulators

**Emulators:** develop/test HPC ready software for simulating quantum systems and quantum computers



## State-vector emulators

- Single node Multi-threading using OpenMP to achieve state of the art emulation of quantum circuits.
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NVIDIA  
CuQuantum  
Testing ...

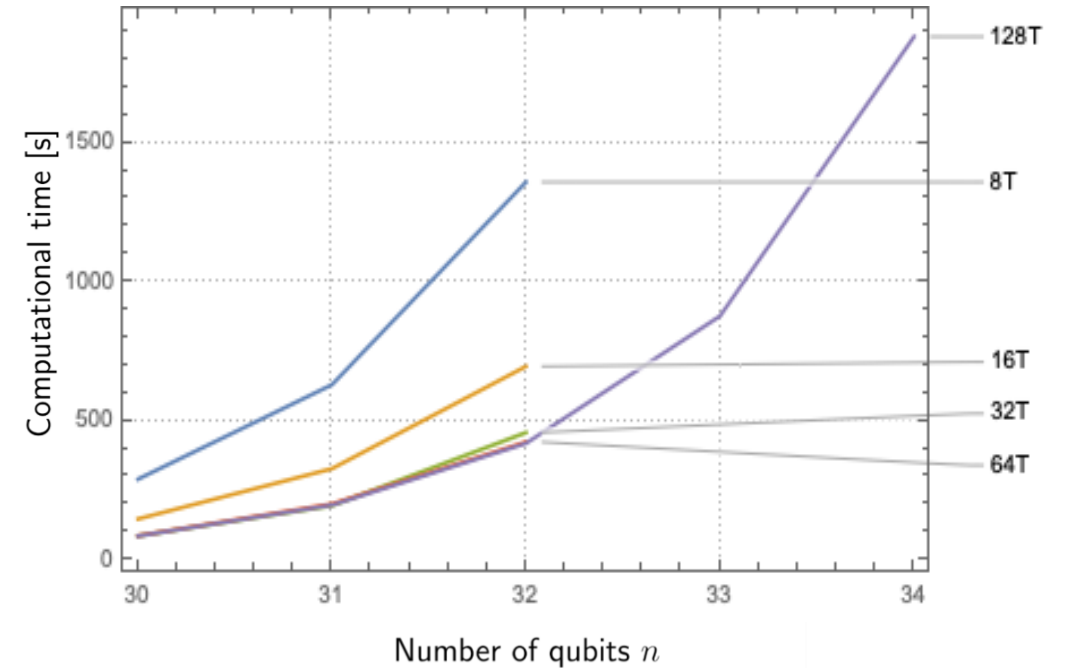
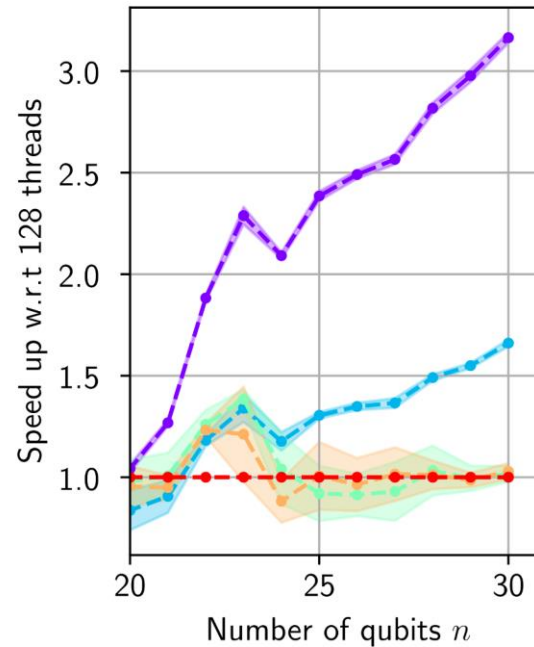
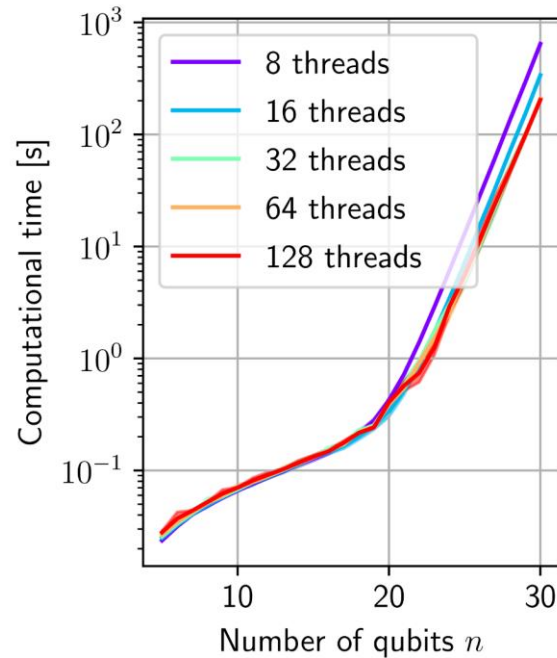


# Cineca Quantum Computing Lab: Emulators

**Emulators:** develop/test HPC ready software for simulating quantum systems and quantum computers

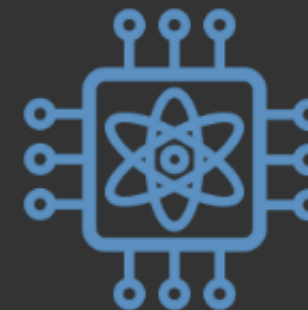


## State-vector emulators



# Cineca Quantum Computing Lab: Emulators

**Emulators:** develop/test HPC ready software for simulating quantum systems and quantum computers



## Tensor Network emulator

- Single node MPS simulator developed in fortran QCOMPS.
- Python interface: qiskit and strawberry fields
- Working on a parallelized implementation



**QCOMPS**



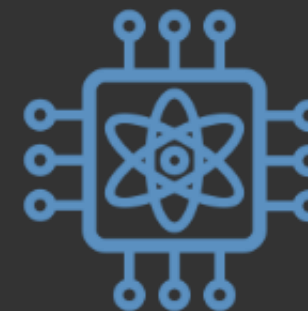
**Qiskit**



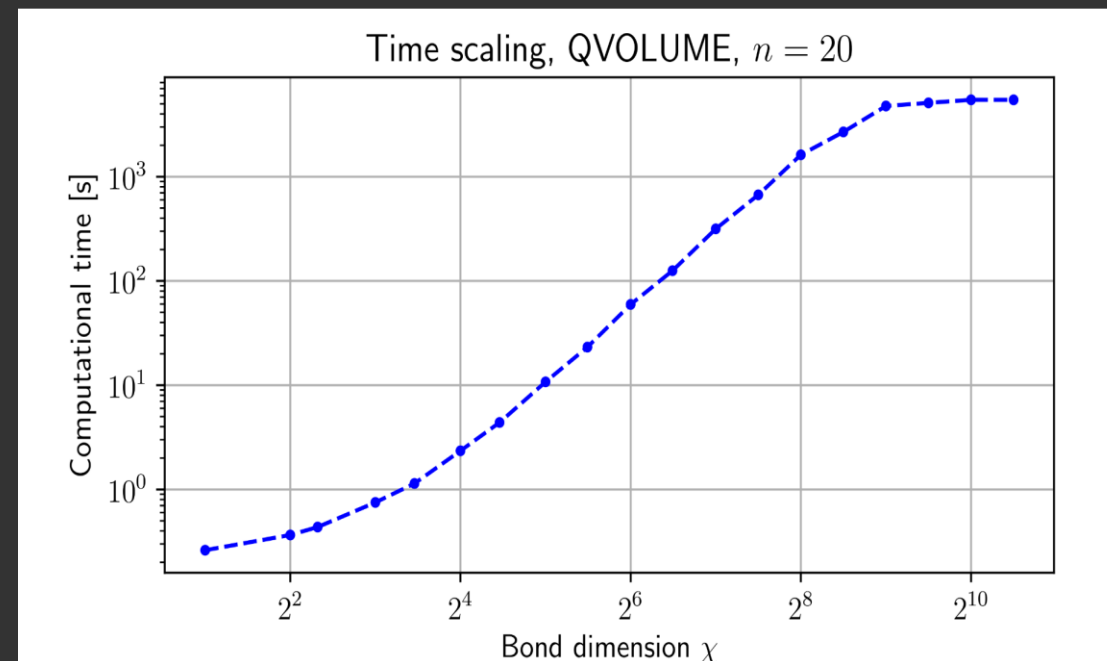
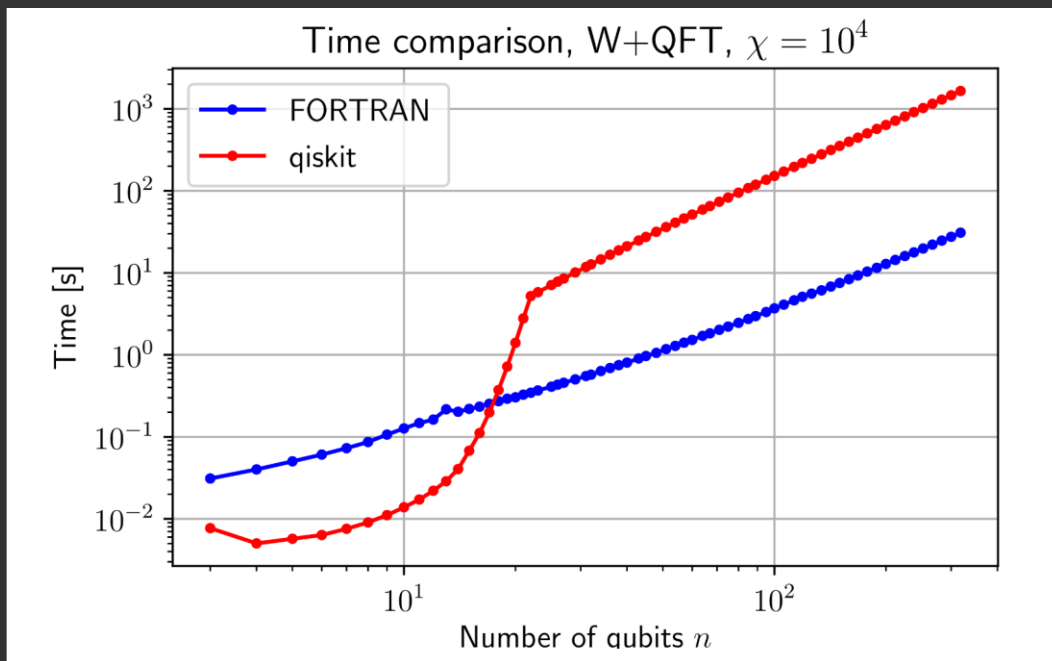
STRAWBERRY FIELDS

# Cineca Quantum Computing Lab: Emulators

**Emulators:** develop/test HPC ready software for simulating quantum systems and quantum computers



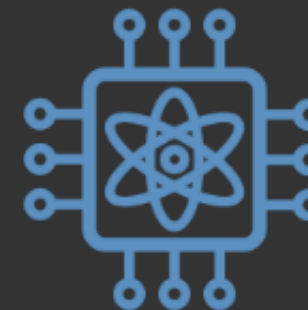
## Tensor Network MPS emulator



# Cineca Quantum Computing Lab: Emulators

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**Emulators:** develop/test HPC ready software for simulating quantum systems and quantum computers



## Simulated Quantum Annealing

- D-Wave neal library for simulated annealing
- SQAOD Collections of solvers/annealers for simulated quantum annealing on CPU and CUDA(NVIDIA GPU).





# Cineca Quantum Computing Lab: Hybrid workflows

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**Hybrid workflows:** development of problem oriented hybrid QPU-HPC algorithms

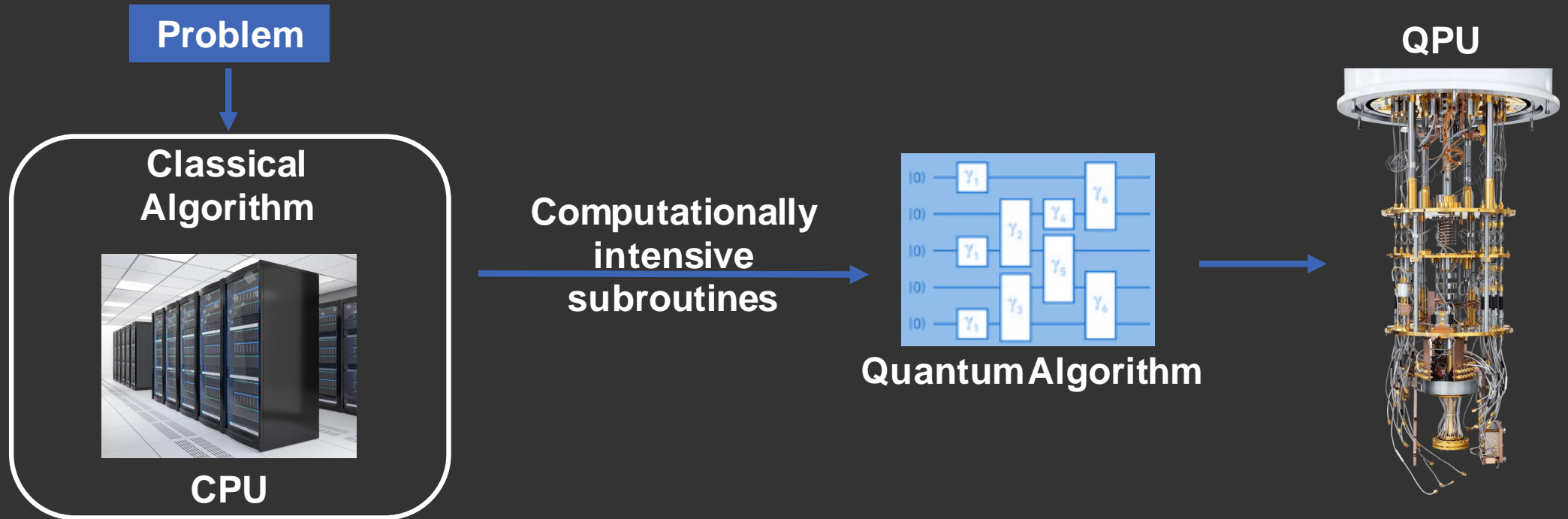


# Cineca Quantum Computing Lab: Hybrid workflows

**Hybrid workflows:** development of problem oriented hybrid QPU-HPC algorithms



## 1. QPU - enhanced computation

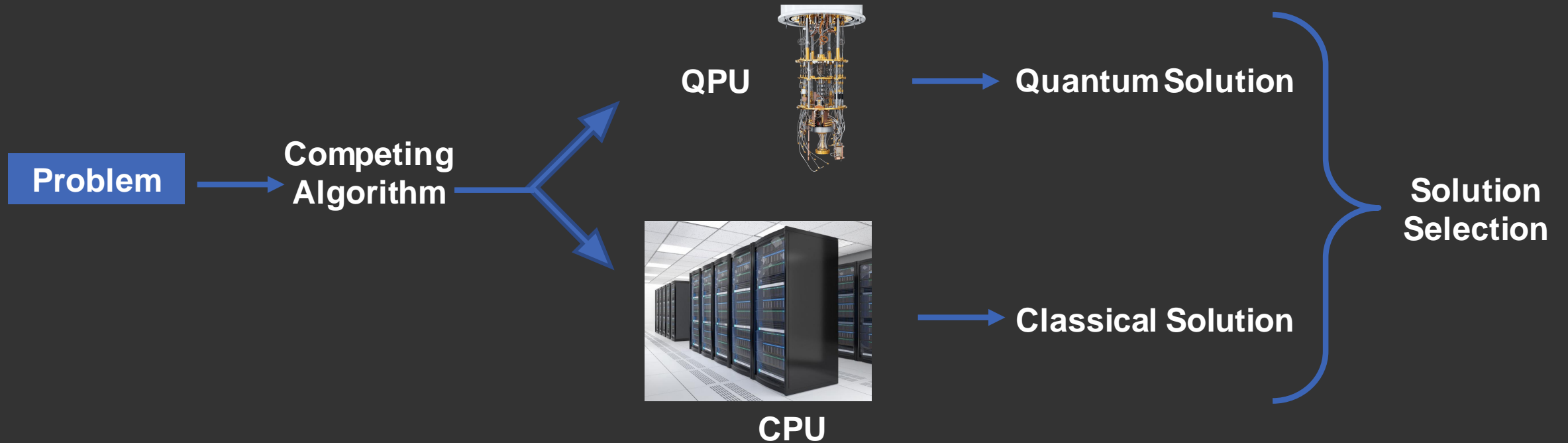


# Cineca Quantum Computing Lab: Hybrid workflows

**Hybrid workflows:** development of problem oriented hybrid QPU-HPC algorithms



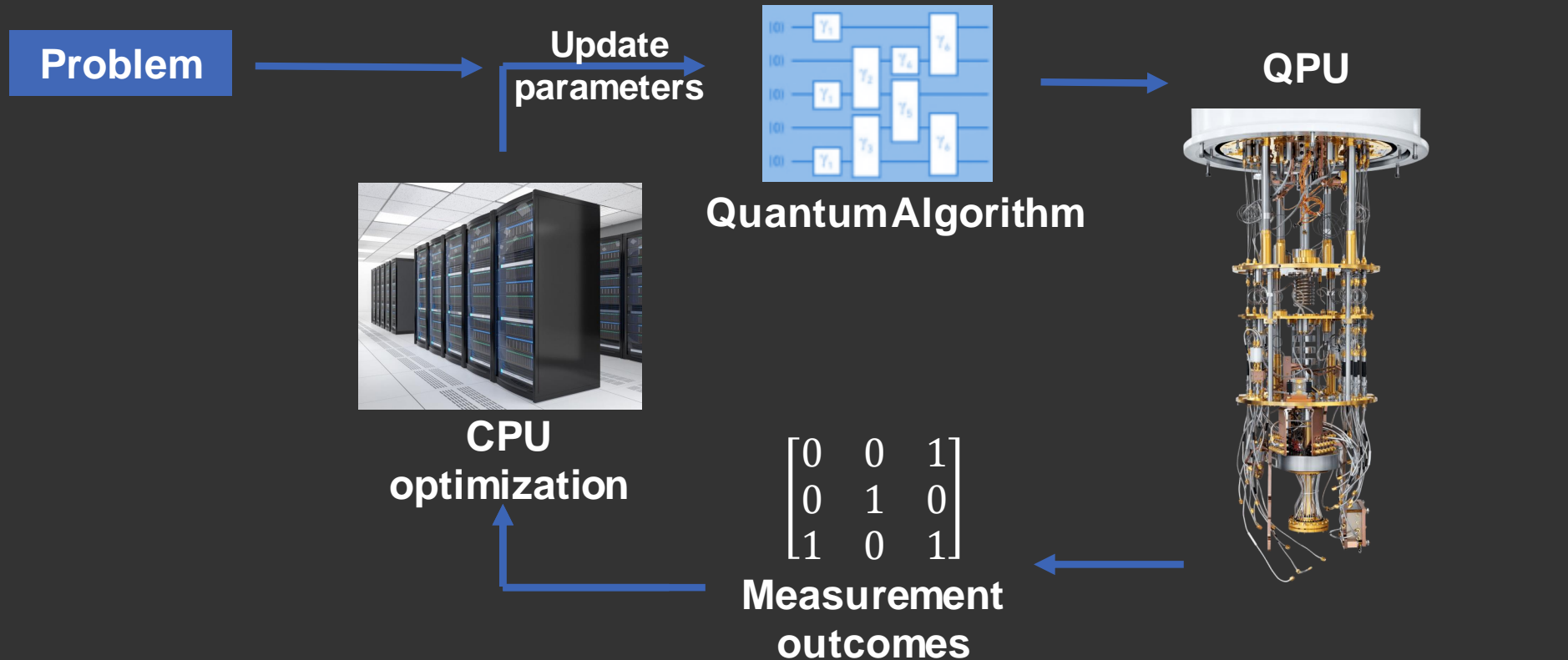
## 2. Competing CPU-QPU



# Cineca Quantum Computing Lab: Hybrid workflows

**Hybrid workflows:** development of problem oriented hybrid QPU-HPC algorithms

## 3. Iterative Hybrid algorithm



# Cineca Quantum Computing Lab: Scheduling

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**Scheduling hybrid resources:** ensure a task is run with the resources it needs and decide when and how to allocate QPU-HPC resources

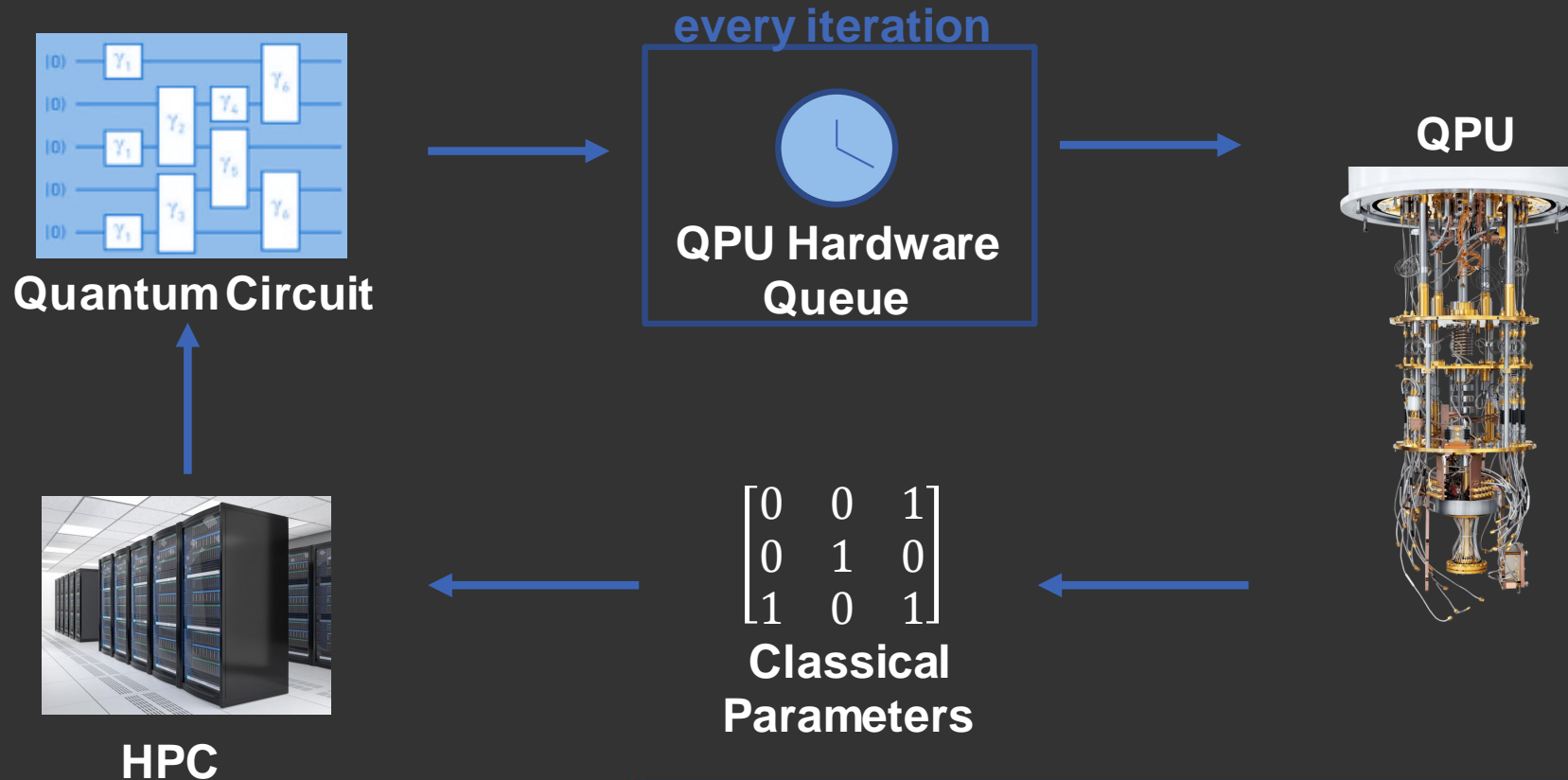


# Cineca Quantum Computing Lab: Scheduling

**Scheduling hybrid resources:** ensure a task is run with the resources it needs and decide when and how to allocate QPU-HPC resources



**Today**





# Cineca Quantum Computing Lab: Scheduling

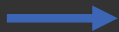
**Scheduling hybrid resources:** ensure a task is run with the resources it needs and decide when and how to allocate QPU-HPC resources



## Future



Hybrid  
Program



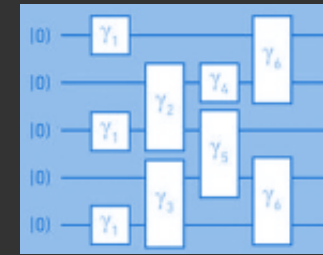
only once



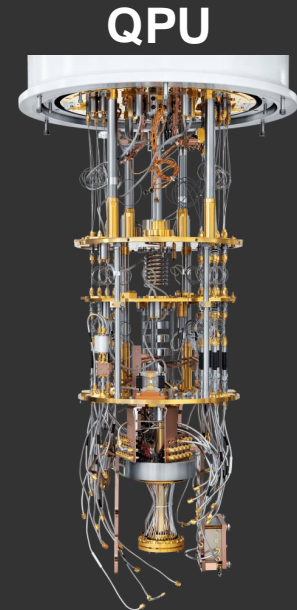
HPC-QPU  
Queue



HPC



Quantum Circuit



QPU

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

Classical  
Parameters



# Cineca Quantum Computing Lab: Applications

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**Real-world applications:** chemistry, optimization, machine learning, simulations, etc.



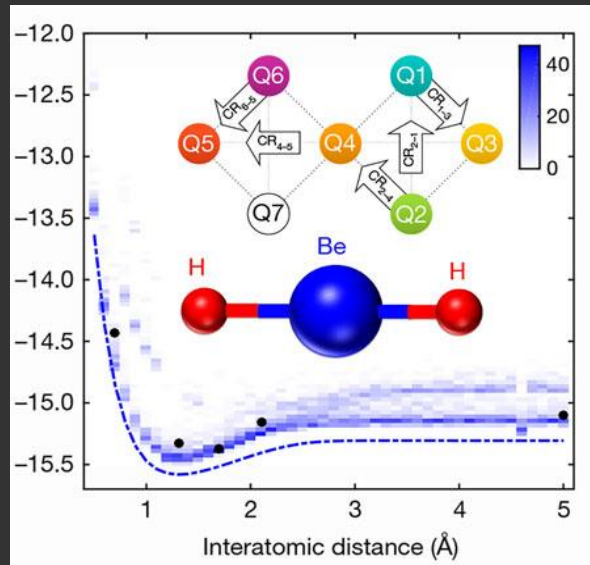
# Cineca Quantum Computing Lab: Applications

**Real-world applications:** chemistry, optimization, machine learning, simulations, etc.

## Gate model QC

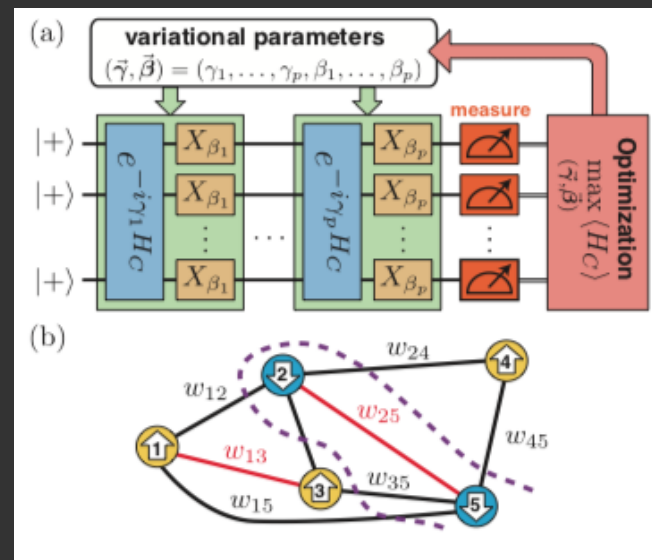


### VQE



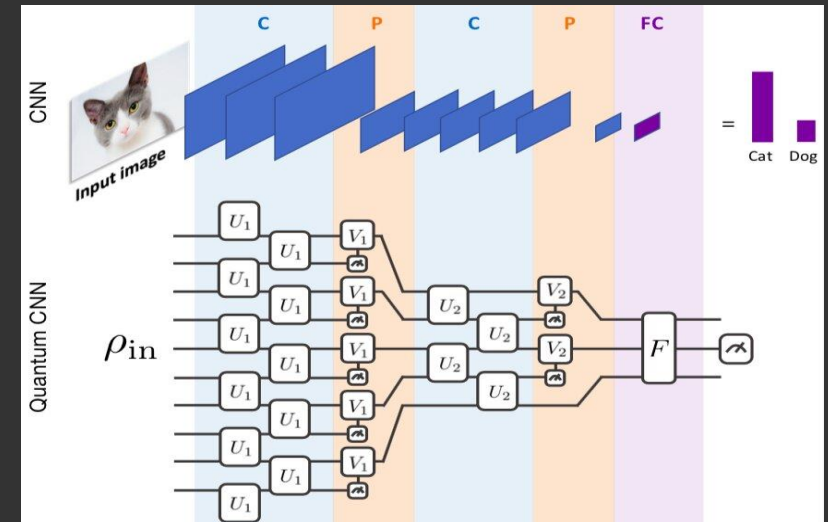
Quantum Chemistry

### QAOA



Quantum Optimization

### QNN



Quantum Machine Learning

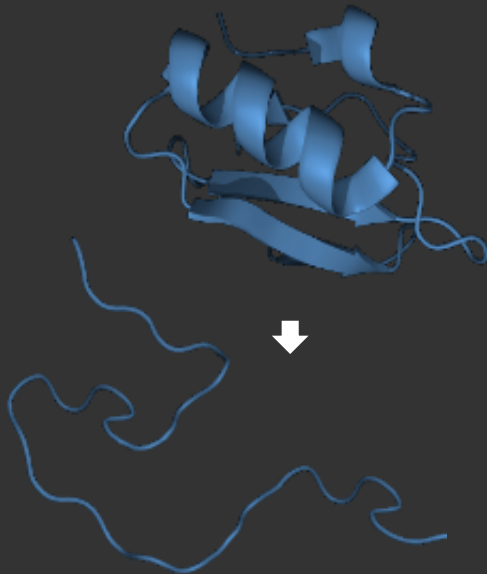
# Cineca Quantum Computing Lab: Applications

**Real-world applications:** chemistry, optimization, machine learning, simulations, etc.

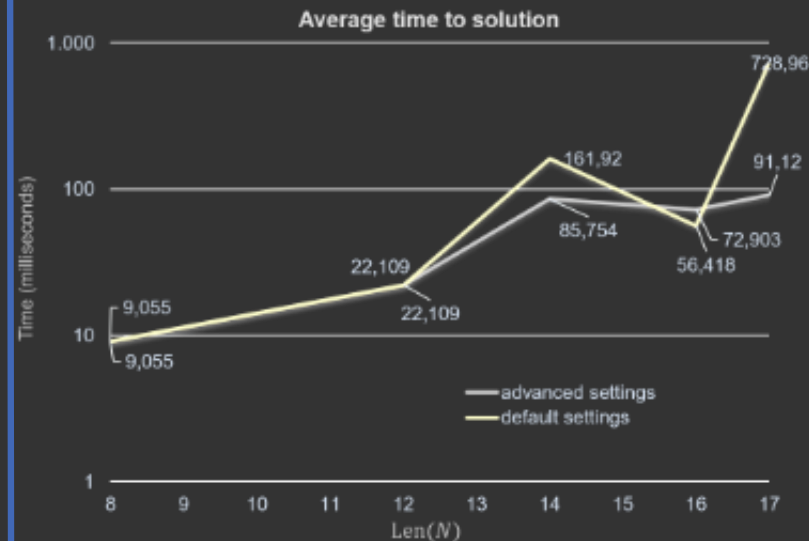


## Quantum Annealing

### Molecular Unfolding



### Factorization



### System of Eqn.s solver

$$AX = \begin{bmatrix} D_1 & B_1^T & & & \\ B_1 & D_2 & B_2^T & & \\ & \ddots & \ddots & \ddots & \\ & & B_{N-2} & D_{N-1} & B_{N-1}^T \\ & & & B_{N-1} & D_N \end{bmatrix} \begin{bmatrix} X_1 \\ X_2 \\ \vdots \\ X_{N-1} \\ X_N \end{bmatrix} = \begin{bmatrix} F_1 \\ F_2 \\ \vdots \\ F_{N-1} \\ F_N \end{bmatrix}$$

# Cineca Quantum Computing Lab: Applications

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**Real-world applications:** chemistry, optimization, machine learning, simulations, etc.



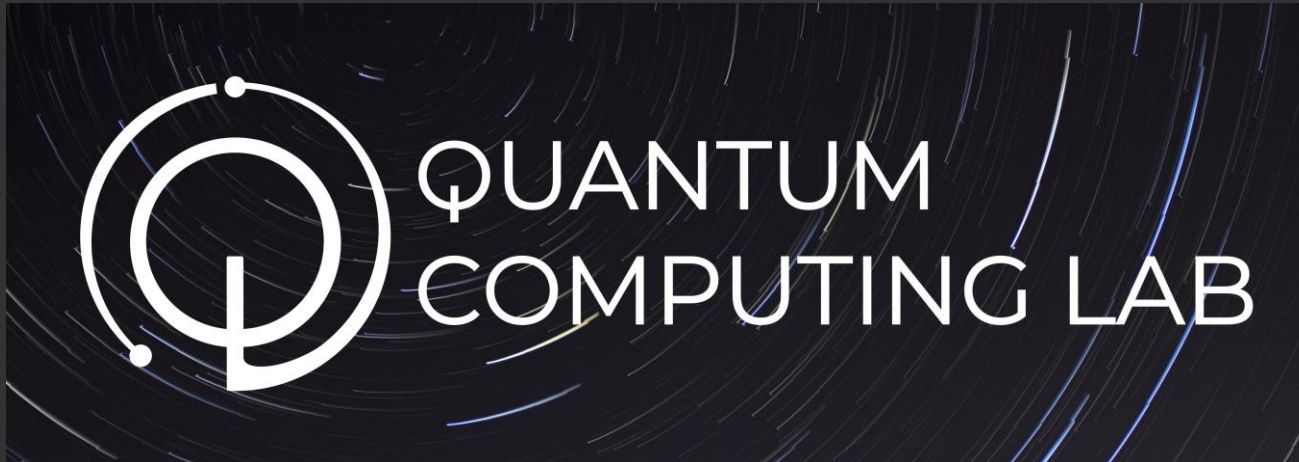
## QUANTUM ADVANTAGE IN THE NISQ ERA?

# Quantum Computing @ CINECA

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## CINECA Quantum Computing Lab:

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



<https://www.quantumcomputinglab.cineca.it>



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