Quantum SPAIN

Agustina infrastructure: Fostering scientific research with High Performance Computing

Sergio Martínez-Losa Del Rincón, Quantum & HPC Support Technician @ BIFI

Gobierno de España · Vicepresidencia Primera del Gobierno · Ministerio de Asuntos Económicos y Transformación Digital · Secretaría de Estado de Digitalización e Inteligencia Artificial
Plan de Recuperación, Transformación y Resiliencia
Financiado por la Unión Europea NextGenerationEU
RES Red Española de Supercomputación
Instituto Universitario de Investigación Biocomputación y Física de Sistemas Complejos Universidad Zaragoza
España | digital 2026

Computation History

Quantum SPAIN

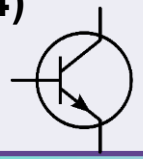
Grace Hopper and COBOL (1958)

IBM360 (1964)

GNU/Linux (1991)

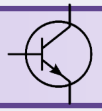
Mechanical Calculator (1837)

Colossus Bletchey Park (1944)



WWII (1939 - 1945)

1950s Business computers



Moore Paradigm

Boole Algebra (1847)

Turing Bomb (1940)

Digital Logic

ENIAC (1946)

Penn
University of Pennsylvania

Von Neumann Architecture (1945)

UNIX (Mid. 60s)

Ken Thompson & Denis Ritchie

BIFI history

- Founded in 2002 as part of an effort towards basic research and applications of complexity concepts as: Biochemistry, Physics, Biology, Computing, Mathematics and Citizen Science. It is financially supported by the Government of Aragon and the University of Zaragoza

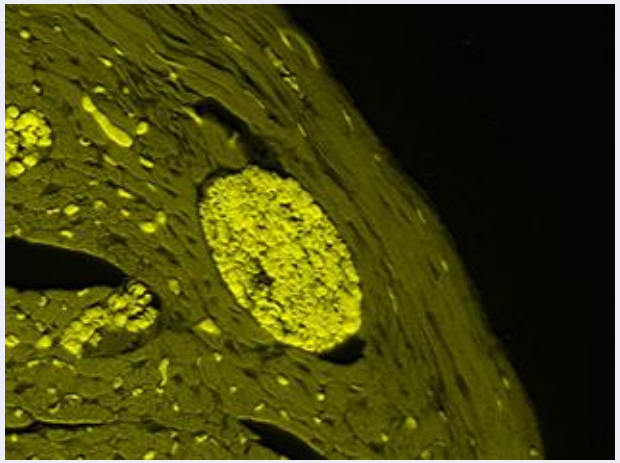
- Member of RES

- CESAR is a powerful computing infrastructure with a computer cluster that is among the most powerful in Spain. The infrastructure covers a wide set of technologies: High Performance Computing (HPC), Cloud Computing, Volunteer Computing and Dedicated Computers.

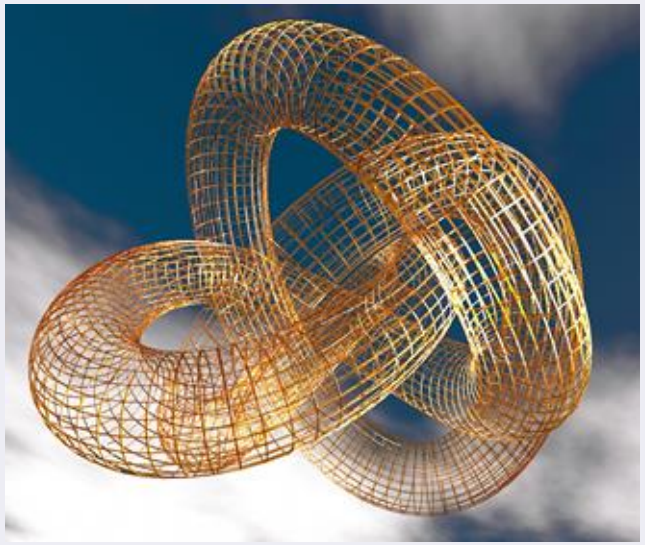
BIFI research lines

Quantum SPAIN

Biochemistry

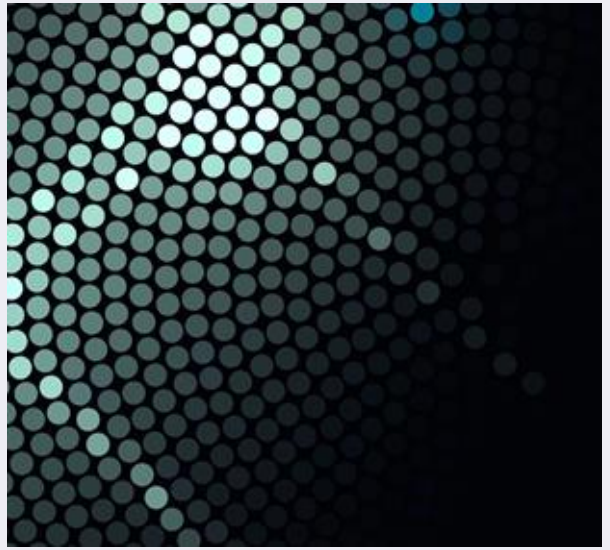


Biophysics

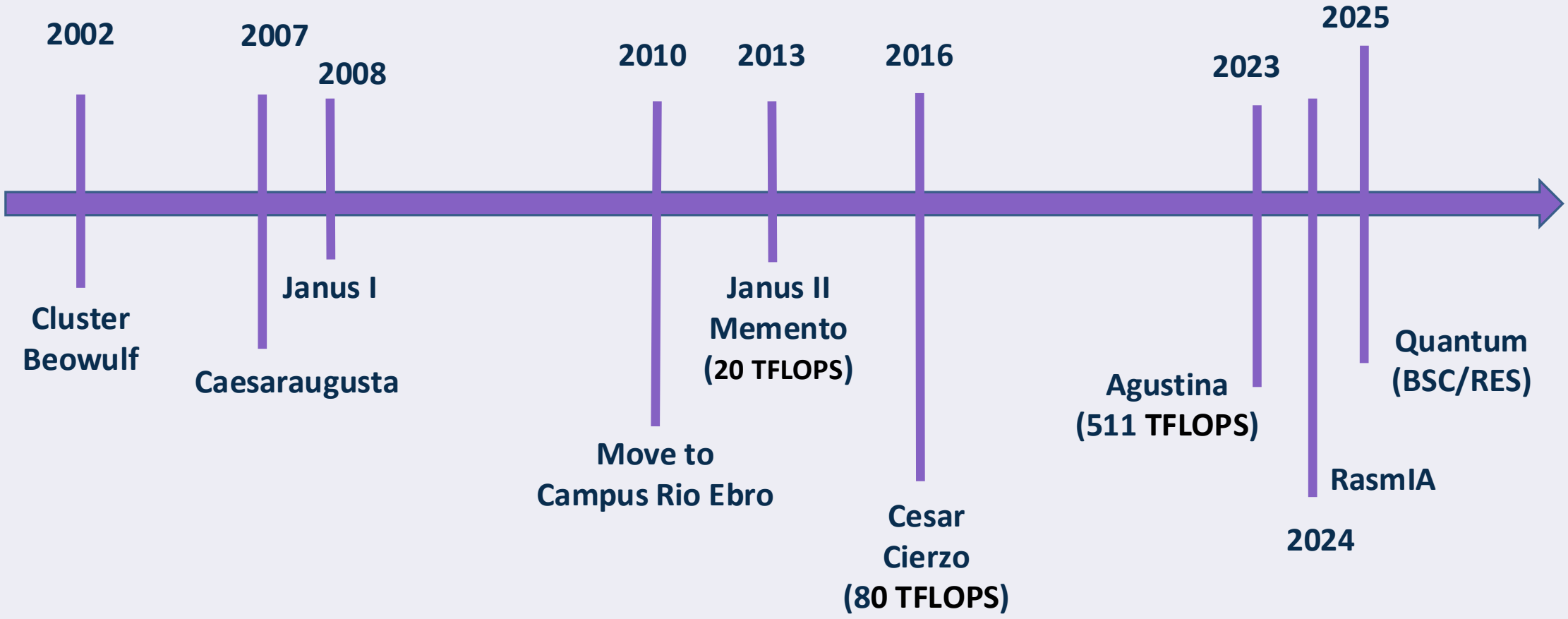


Computing & Data Science

Physics



BIFI computing history (CESAR)



HPC – Cierzo

- **2080 cores** Intel x86_64 architecture
  - 170 CPUs Intel Xeon E5-2680v3 2.5GHz in85 compute nodes
  - 4 CPUs E5-4627v3 2.6GHz in 1 compute node
- 8 GPUs Nvidia Kepler Tesla K40 (12GB RAM x 8)
- 2 Coprocessors Intel Xeon Phi 5110P
- **7,31 TB RAM memory** total DDR4 2133 ECC REG
  - 64 GB x standard compute node
  - 2 TB with 1 FAT node
- **Real computation power ~80TFLOPS (Rmax)**
- Internal InfiniBand connectivity FDR 56Gbps
- External connectivity 10GE
- 288 TB Lustre storage
- Power efficiency of 2,24 GFLOPs/W

https://cesar.unizar.es/hpc/

HPC – Agustina

- **6144 cores** x86_64 architecture with 192 CPUs AMD Epyc7513 2.6GHz placed in 96 compute nodes
  - 93 THIN nodes with 256 GB RAM per node
  - 3 FAT nodes with 512 GB RAM per node
- **25,4 TB RAM memory** DDR4 3200MHz
- Internal connectivity InfiniBand HDR 100Gbps
- External connectivity 10GbE
- 500TB Lustre storage
- **Power peak (Rpeak) of 511 TFLOPS**
- Maximum consumption 57 KW
- InRow water cooling

https://cesar.unizar.es/hpc/

HPC/AI – RasmIA

- **3 nodes:**
  - **3x4 = 12 GPUs Nvidia H100 with 80GB VRAM**
  - RAM: 2TB/node (6TB total)
- **9 nodes:**
  - **9x4 = 36 GPUs Nvidia L40S with 48 GB VRAM**
  - RAM: 1.5TB/node (13.5TB total)

https://cesar.unizar.es/hpc/

Cloud service – Colossus

- **OpenStack-based** Cloud Services Platform
- **1800 cores** Intel Xeon E5-2670-V3
- **20TB RAM** (DDR4 in performance mode)
- **10G Base-T** Internal Connectivity
- **10G Base-T** External Connectivity
- **KVM-based** Virtualization
- **Ceph-based** distributed storage solution with approximately **600TB** of capacity, consisting of SAS and SSD disks

https://cesar.unizar.es/cloud/

HPC and Cloud account

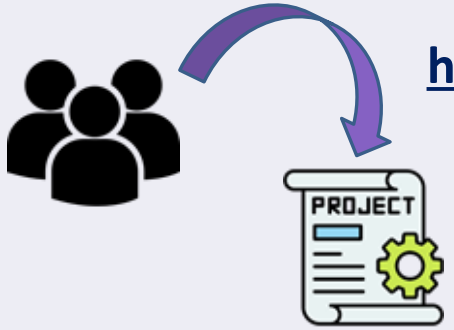
1 .- Register your Project as Project leader in the following link:

https://soporte.bifi.unizar.es/forms/form.php?idForm=1

2 .- Create user accounts for your Project with this form:

https://soporte.bifi.unizar.es/forms/form.php?idForm=2

3 .- Link user accounts to your Project with this form:



https://soporte.bifi.unizar.es/forms/form.php?idForm=4

Some available applications

Quantum SPAIN

QIBO

NVIDIA CUDA

R

ORCA

TensorFlow

STABLE DIFFUSION

Golang

python

Gaussian, Inc.

Ollama

PENNYLANE

miniCONDA

mumax3

GPU-accelerated micromagnetism

Documentation and support

```
$ ssh USER@agustina.bifi.unizar.es
```

https://soporte.bifi.unizar.es

https://doc-publica.bifi.es/agustina/manual_agustina.html

agustina@bifi.es
sergio.martinez@bifi.es

BIFI jump on quantum computation with QuantumSpain project

European Quantum Manifesto 2016

- European answer to **Second Quantum Revolution**
- €1 billion Flagship-scale Initiative in Quantum Technology
- This initiative aims to place Europe at the forefront of the second quantum revolution now unfolding worldwide, bringing transformative advances to science, industry and society

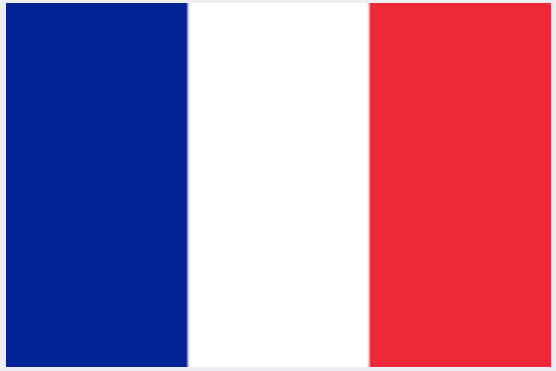
Other public quantum initiatives

Lumi-Q (20 Qbits)

Exa-Q (100 Qbits)

+

Quantum Simulator 100 qubits in Jülich Supercomputing Centre



EuroQCS-France (10 Qbits)

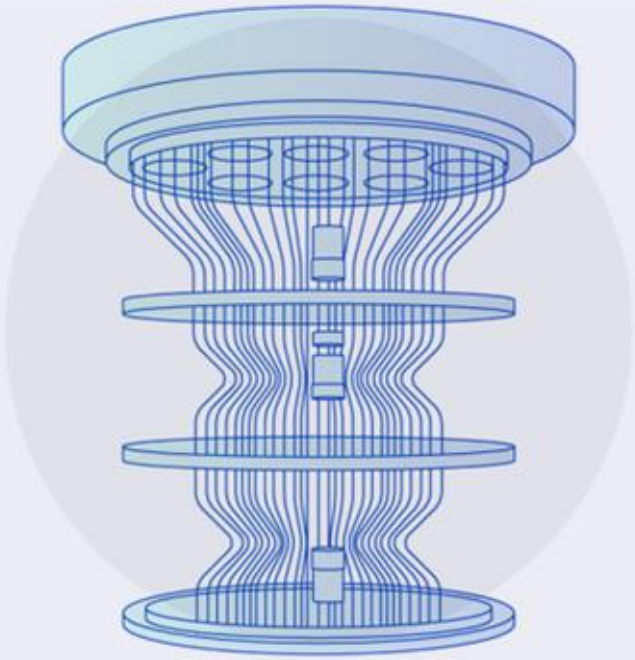
+

Quantum Simulator 100 Qubits Joliot Curie of GENCI

EuroQCS-Italy (Ion trap)

What is QuantumSpain?

https://quantumspain-project.es/



- A collaborative Quantum Infrastructure to **promote and finance** a competitive and complete **quantum computing infrastructure in Spain**
- **Funded with €22 Million (01/01/22 – 31/03/26)**
- First Public European Quantum Infrastructure as a Service
- Based in Superconducting technology brings from 5 to 20 Qubits at the end of 2025
- Member of RES (Red Española de Supercomputacion)

Who takes part?

- Nodos de la RES
- Investigación
- Simuladores HPC
- Computador Cuántico

QuantumSpain roadmap

Quantum SPAIN

2022

1 JAN · 2 FEB · 3 MAR · 4 APR · 5 MAY · 6 JUN · 7 JUL · 8 AUG · 9 SEP · 10 OCT · 11 NOV · 12 DEC

2023

1 JAN · 2 FEB · 3 MAR · 4 APR · 5 MAY · 6 JUN

Achieved:
- Purchase Quantum hardware
- Formative Plan in Quantum Information for Tecnicians

Achieved:
- QC 5-Qbits in Lab and Test
- Creation of learning materials for TalentQ
- First internal research groups

2024

7 JUL · 8 AUG · 9 SEP · 10 OCT · 11 NOV · 12 DEC · 1 JAN · 2 FEB · 3 MAR · 4 APR · 5 MAY · 6 JUN · 7 JUL · 8 AUG · 9 SEP · 10 OCT · 11 NOV · 12 DEC

Achieved:
- Creation of learning materials for TalentQ
- Start user support for QC
- **Installation of QC in BSC**

Achieved:
- Release of material for TalentQ
- Second internal research groups

2025

1 JAN · 2 FEB · 3 MAR · 4 APR · 5 MAY · 6 JUN · 7 JUL · 8 AUG · 9 SEP · 10 OCT · 11 NOV · 12 DEC

2026

1 JAN · 2 FEB · 3 MAR

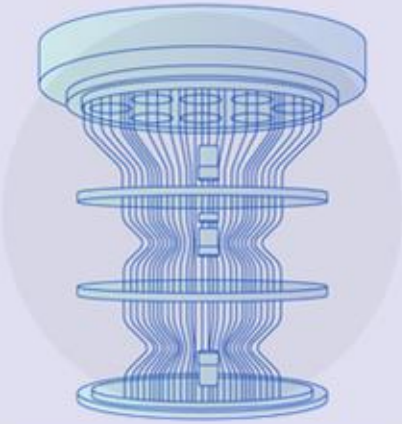
Achieved:
- Deployment of QC >=20-Qbits

Finish

QuantumSpain main activities

Quantum SPAIN

Quantum computer

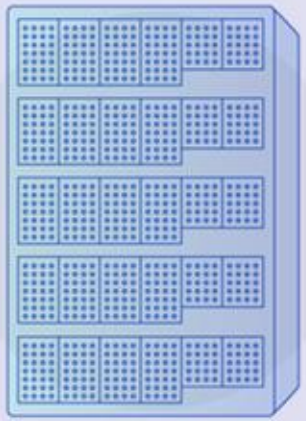


Barcelona Supercomputing Center

Adquisition and installation of a quantum computer based on superconducting qubits technology.

Quantum as a Service

Access



Spanish Supercomputing Network

Provide the access to the quantum computer and High Performance Computing devices for quantum technologies.

Research

Universities and Research centers

Development and research of novel quantum algorithms and their applications in AI.

Training

TalentQ program

Training programs, workshops, schools, seminars and other initiatives to bring quantum computation to all backgrounds.

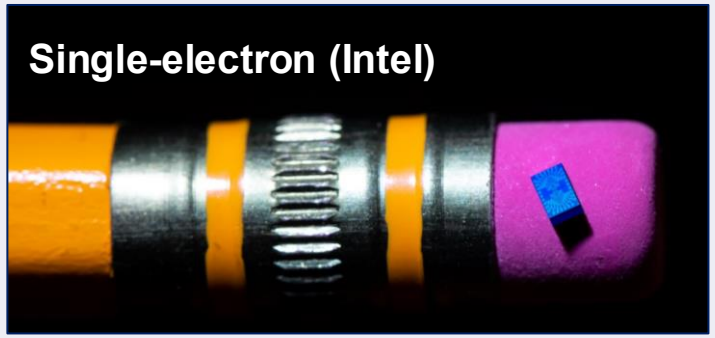
TalentQ program

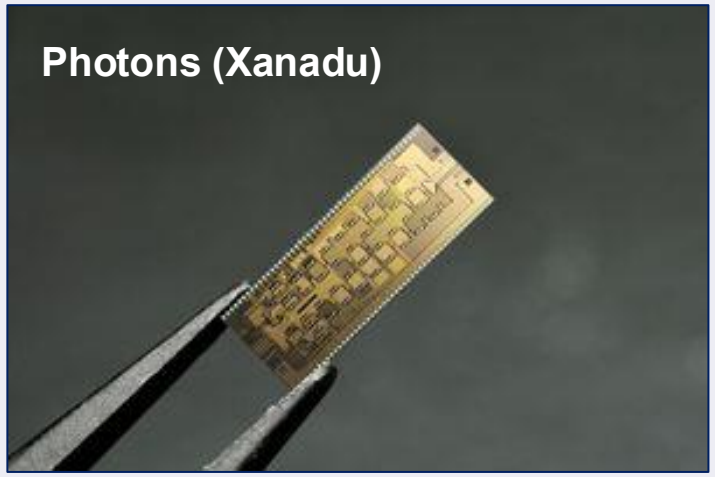
- Learning material created by QuantumSpain Tecnicians
- Starts from basic math level used in Quantum Physics to advanced topics
- Coordinated by Universidad de Santiago de Compostela, CESGA, BSC and PYSQT
- More courses to come…

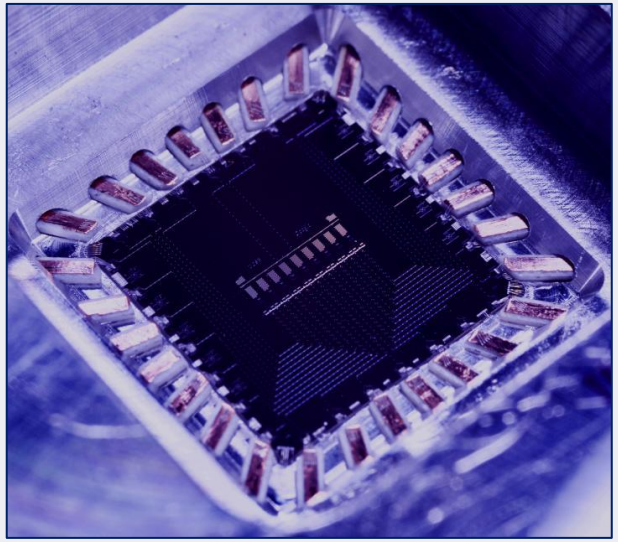
NOW AVAILABLE: Basic Course of Quantum Computing and more…

https://www.talentq.es

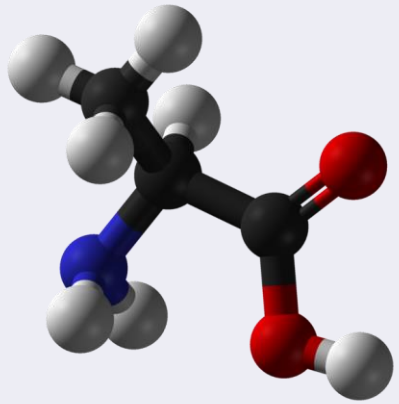
Technology used to create Qubits







Superconductive Rings (Google, IBM…)



Magnetic molecules in superconductive circuits (Zaragoza, Spain)

Superconductive technology

- Superconducting Qubits at very low temperatures (-270ºC)
- Use of magnetic fields
- Electromagnetic pulses to measure
- Vaccumm conditions
- Interconnected Qubits
- Decoherence
- Quantum Errors

Hardware for a Quantum Computer

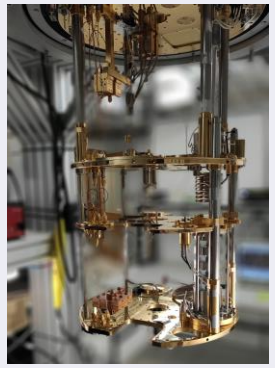
Quantum SPAIN

Power source

Vectorial Analizer | Oscilloscope | Spectrum ananlyzer

Spectra generator | RF generator

Dilution Refrigerator

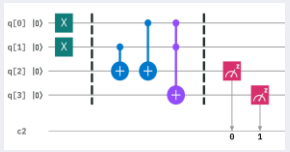


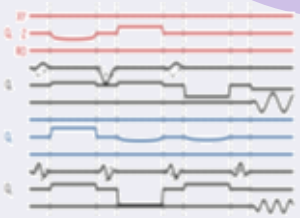
Wiring & Connections

Coax | Amplifiers

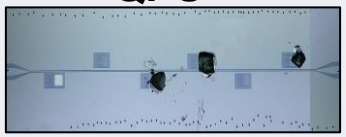
Circulators | Bias-

Pulse Software





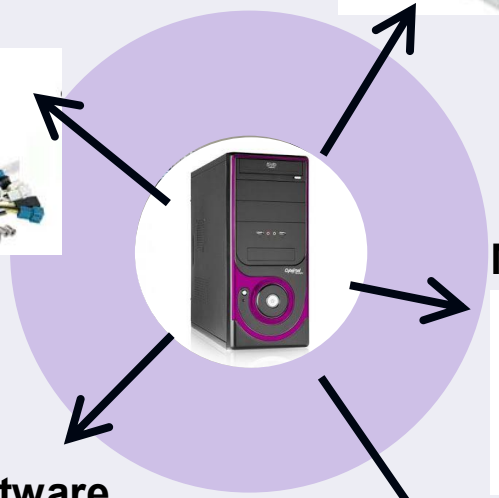
QPU



Building a Quantum Computer

Power source

Fan



Motherboard

Software

```
#include <iostream>

int main()
{
    std::cout << "Hello, world!\n";
    return 0;
}
```

```
b8    21 0a 00 00
a3    0c 10 00 06
b8    6f 72 6c 64
a3    08 10 00 06
b8    6f 2c 20 57
a3    04 10 00 06
b8    48 65 6c 6c
```

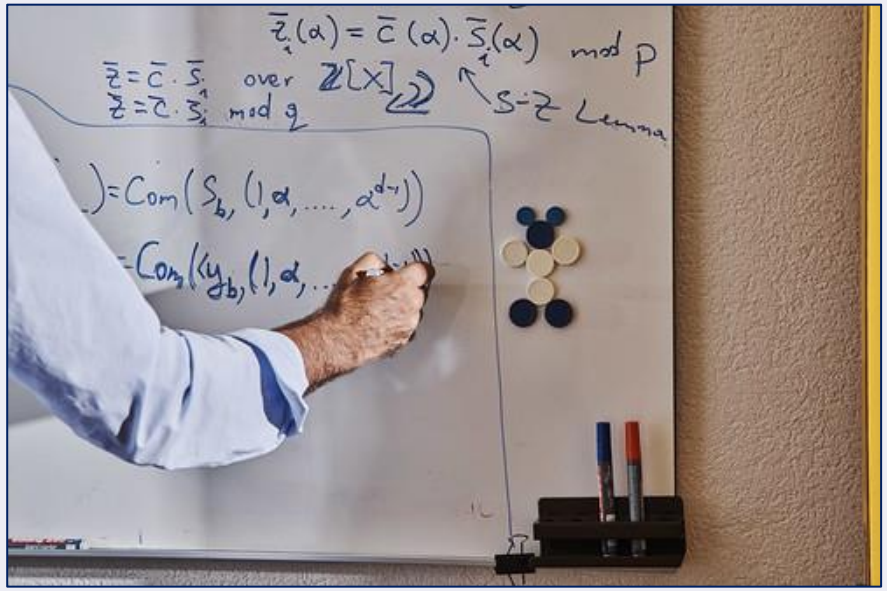
CPU

Post-Quantum Algorithms

Quantum SPAIN

NIST Asks Public to Help Future-Proof Electronic Information

December 20, 2016



1. CRYSTALS-Kyber
2. CRYSTALS-Dilithium
3. FALCON
4. SPHINCS+

6 years later

NIST Announces First Four Quantum-Resistant Cryptographic Algorithms

Federal agency reveals the first group of winners from its six-year competition.

July 05, 2022

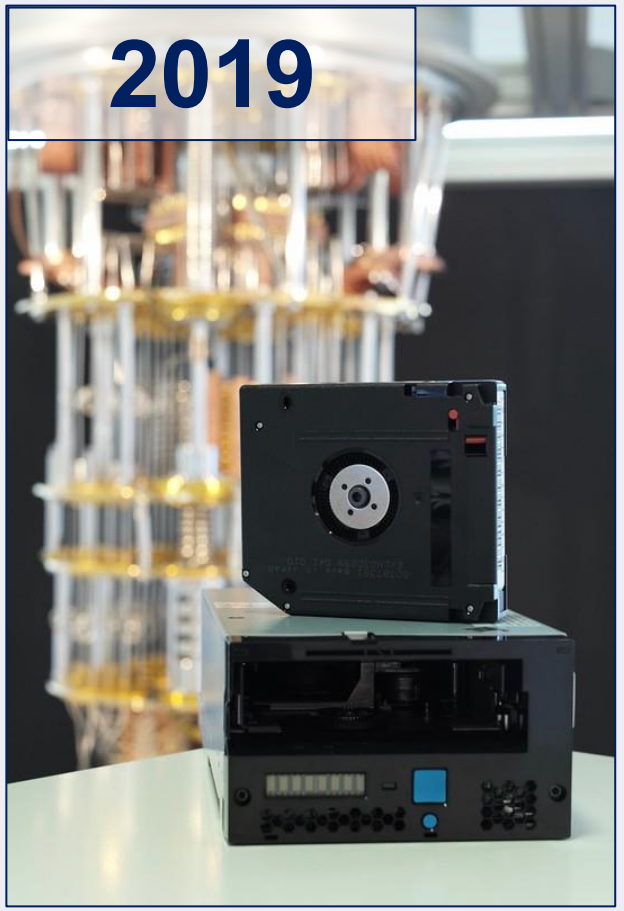
Post-Quantum Algorithms

Quantum SPAIN

IBM — 2019

aws — 2020

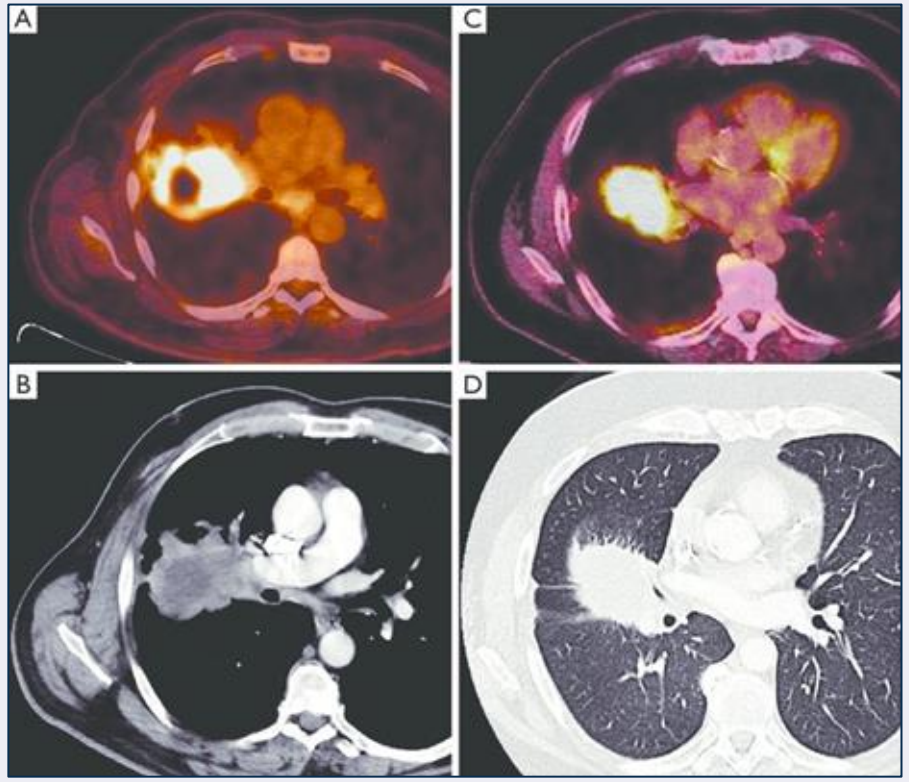
CLOUDFLARE® — 2022



Application of Quantum World

Quantum SPAIN

Molecules simulation



Positron Emission Tomography

Quantum Dots for HQ Imaging

Application of Quantum World

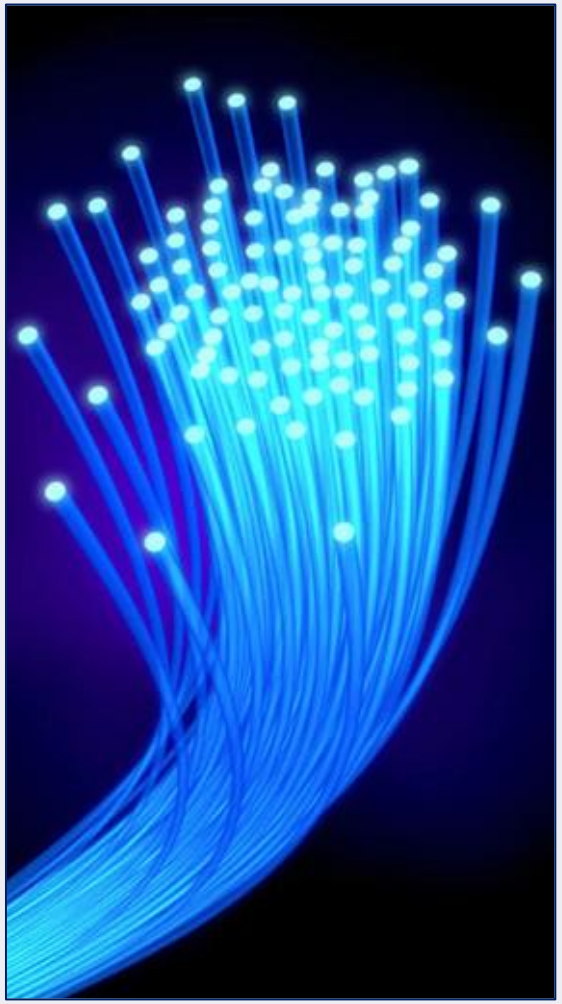
Quantum SPAIN

UNIVERSITY OF KWAZULU-NATAL

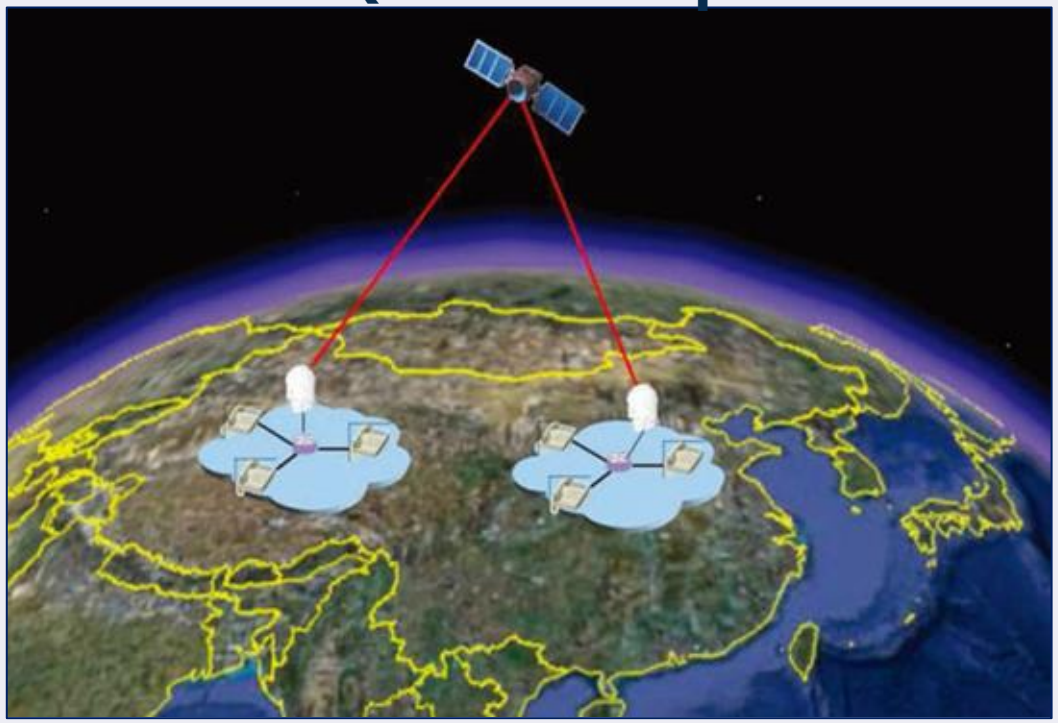
SOUTH AFRICA 2010 FIFA WORLD CUP

Quantum Security

Quantum Internet



Satellite Quantum Teleportation



Where are the Qubits? (BIFI)

Quantum SPAIN

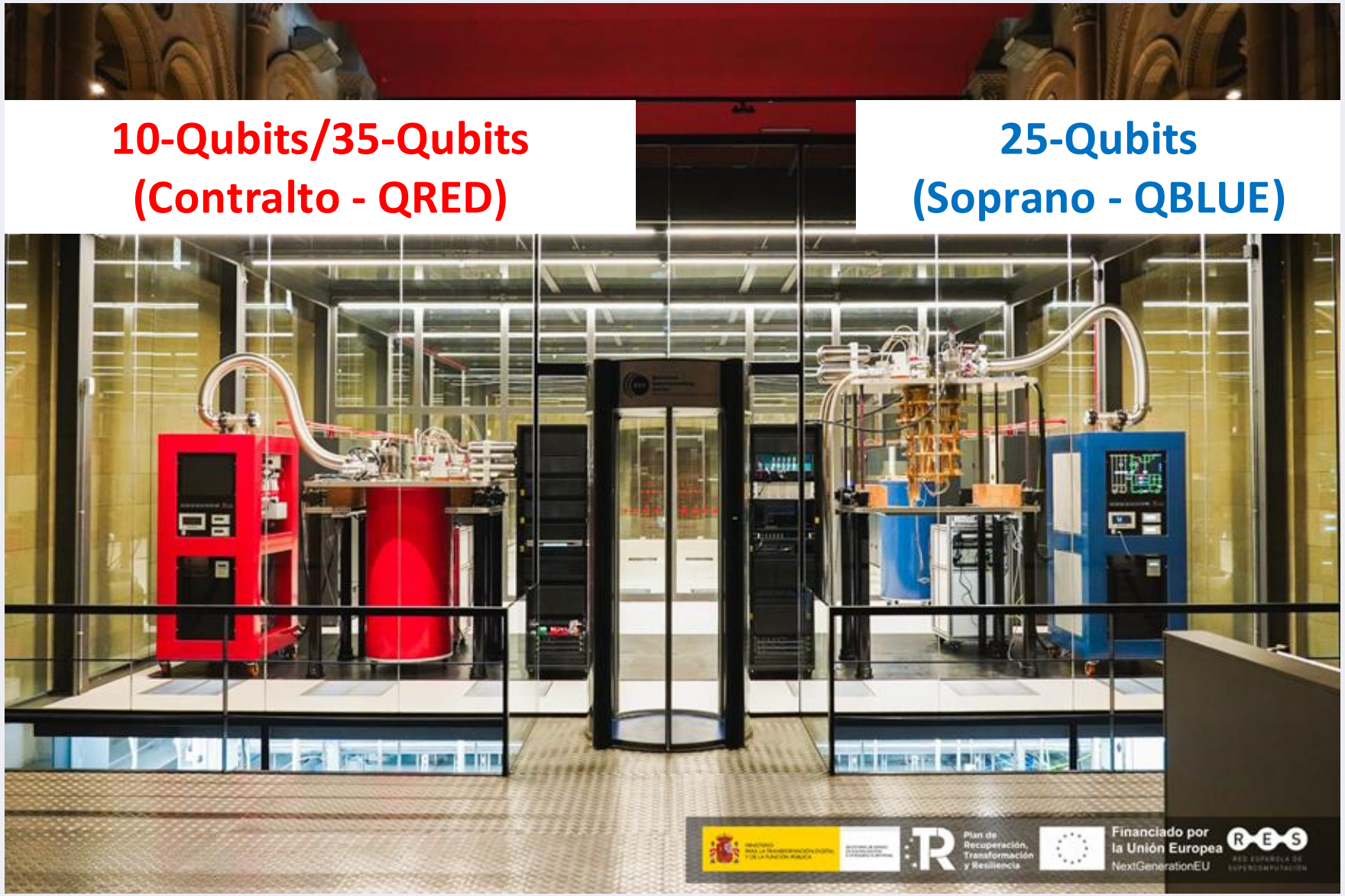
Instituto Universitario de Investigación
Biocomputación y Física
de Sistemas Complejos
Universidad Zaragoza

PENNYLANE

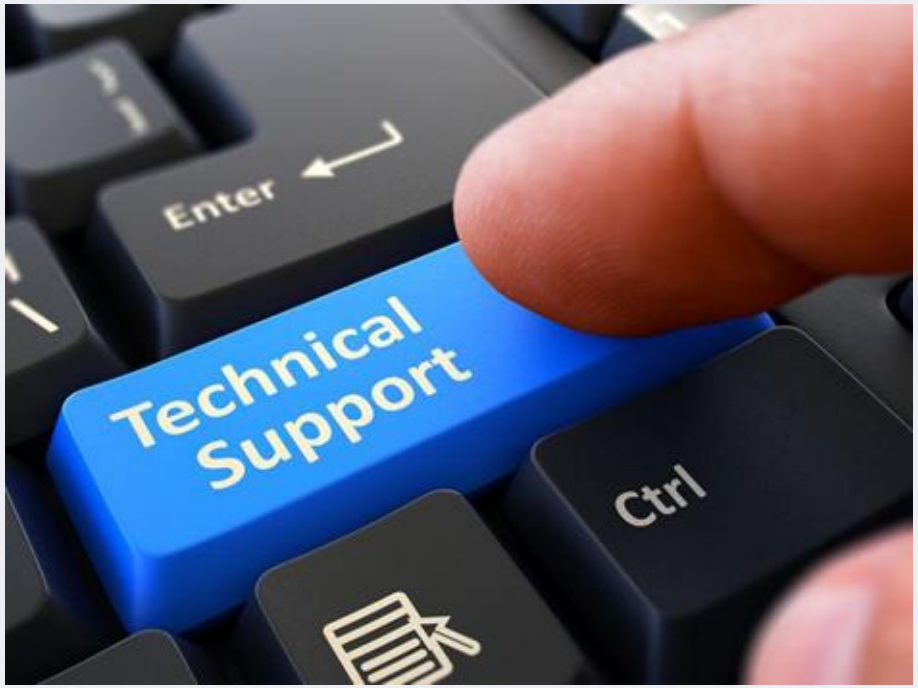
Qiskit

QIBO

Where are the Qubits? (BSC)

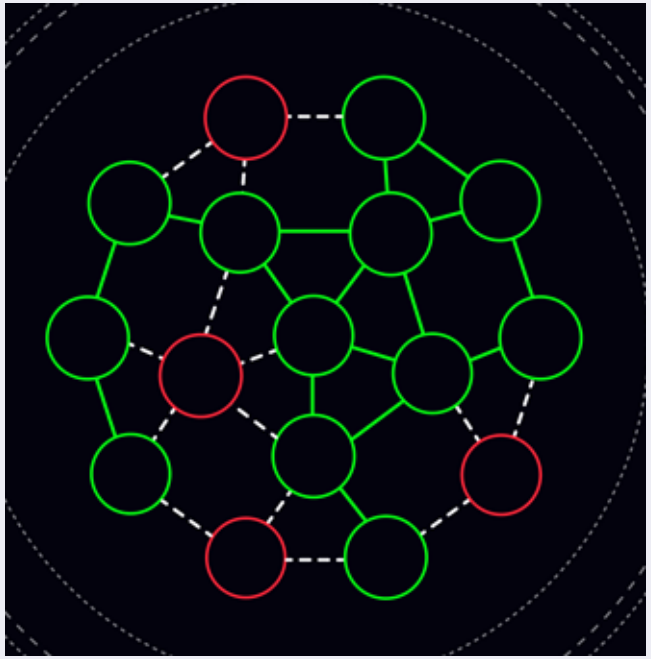


Quantum technical support

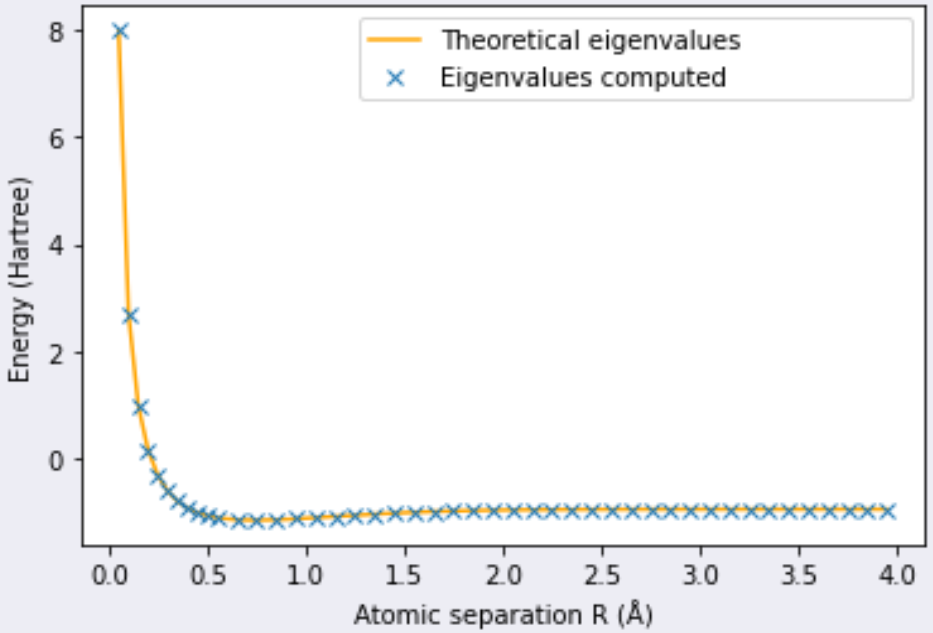


- QuantumSpain is part of RES network, follow the same procedure as a request for HPC
- Give clear indications about the project and how it can take advantage of the Quantum Computer
- Fill the form with detailed information
- Read Qibo documentation and QiboConnection Documentation
- Username and Acces Token grant acces to Quantum Computer in BSC
- Any question concerning the Quantum Technologies can be address to technicians
- Any question about QuantumSpain should be addressed to technicians

Research topics (PT-3)



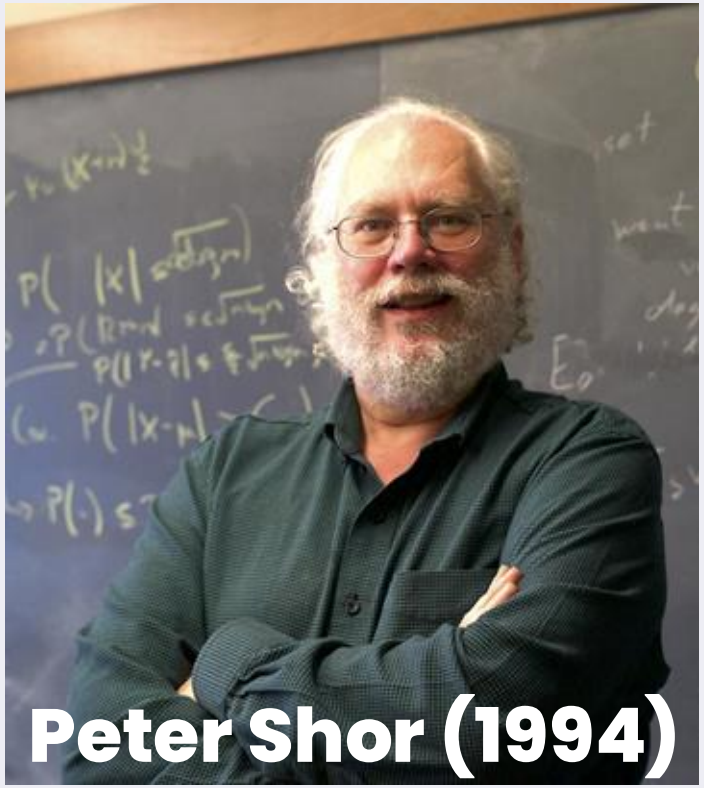
Fault Tolerant Algorithms
(Grover, Shor,
Iterative Phase Estimation)



Variational Quantum Eigensolver
(Ansätze, Optimizers)

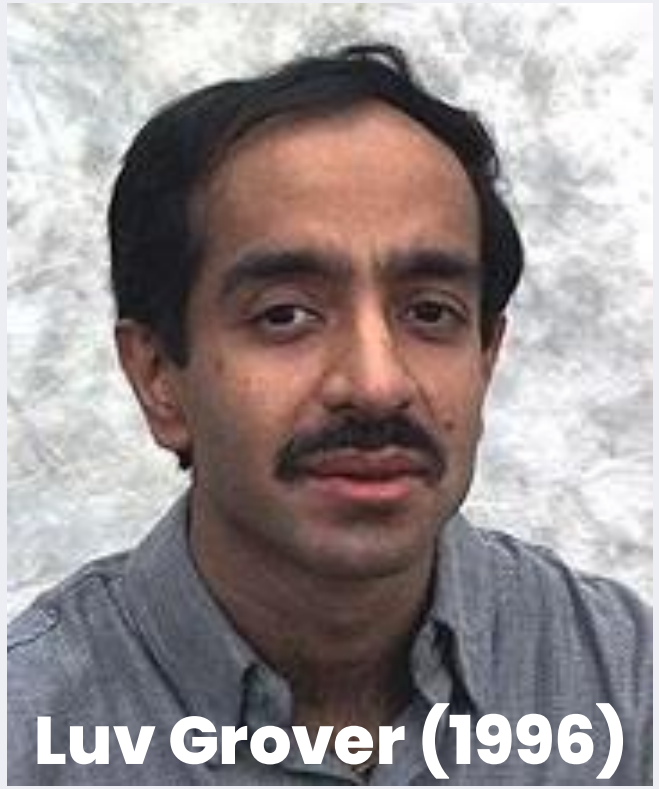
Quantum Machine Learning (Feature
Encoding, QSVM, QKernels)

Fault tolerant algorithms


Peter Shor (1994)

Shor's algorithm is a quantum algorithm for integer factorization that finds the prime factors integer exponentially faster than the best-known classical algorithms

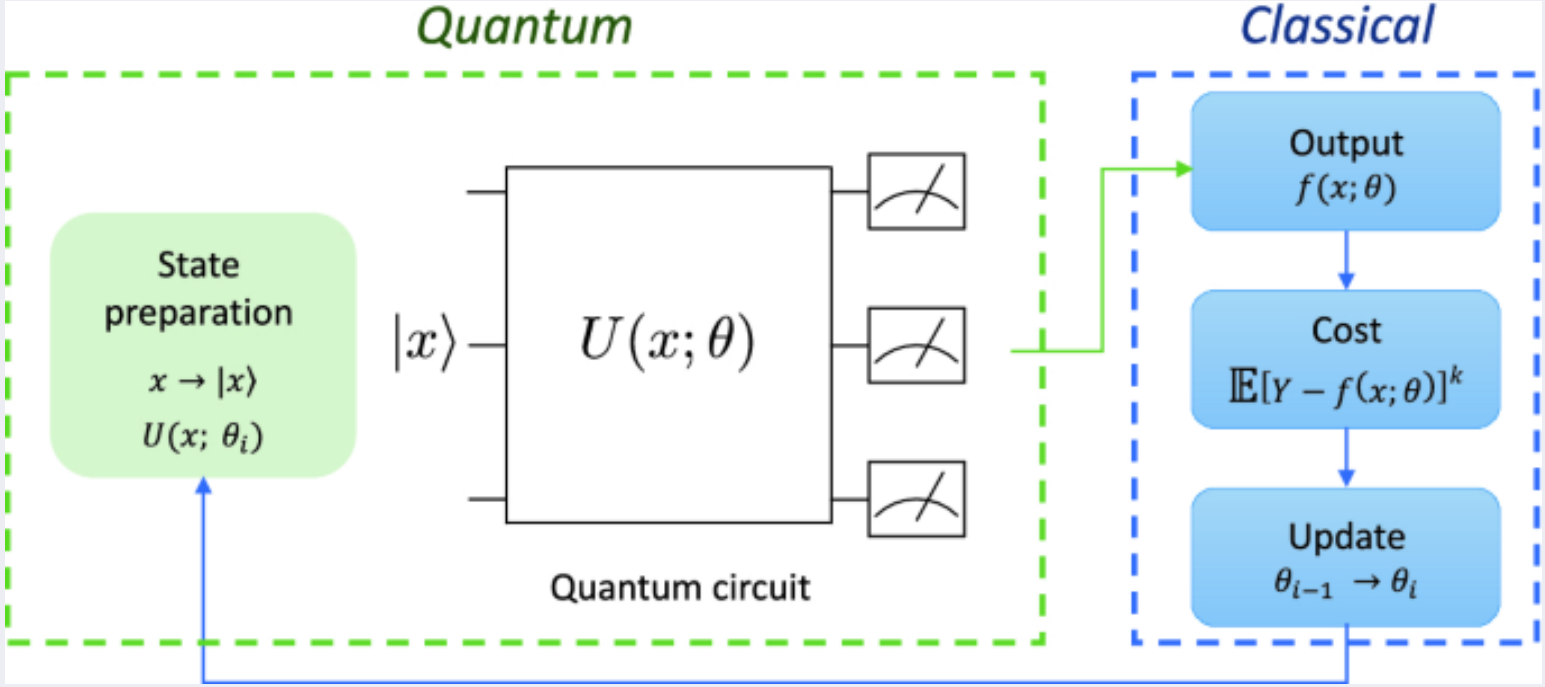
Grover's algorithm is a quantum search algorithm that finds a marked item in an unstructured database of size N, the queries using amplitude amplification


Luv Grover (1996)

Quantum Machine Learning

- Data preprocessing in classical Hardware
- **Data encoding for Quantum Circuit**
- Postprocessing of Quantum Output in a Classical Hardware with a Cost function
- Update input data with new values

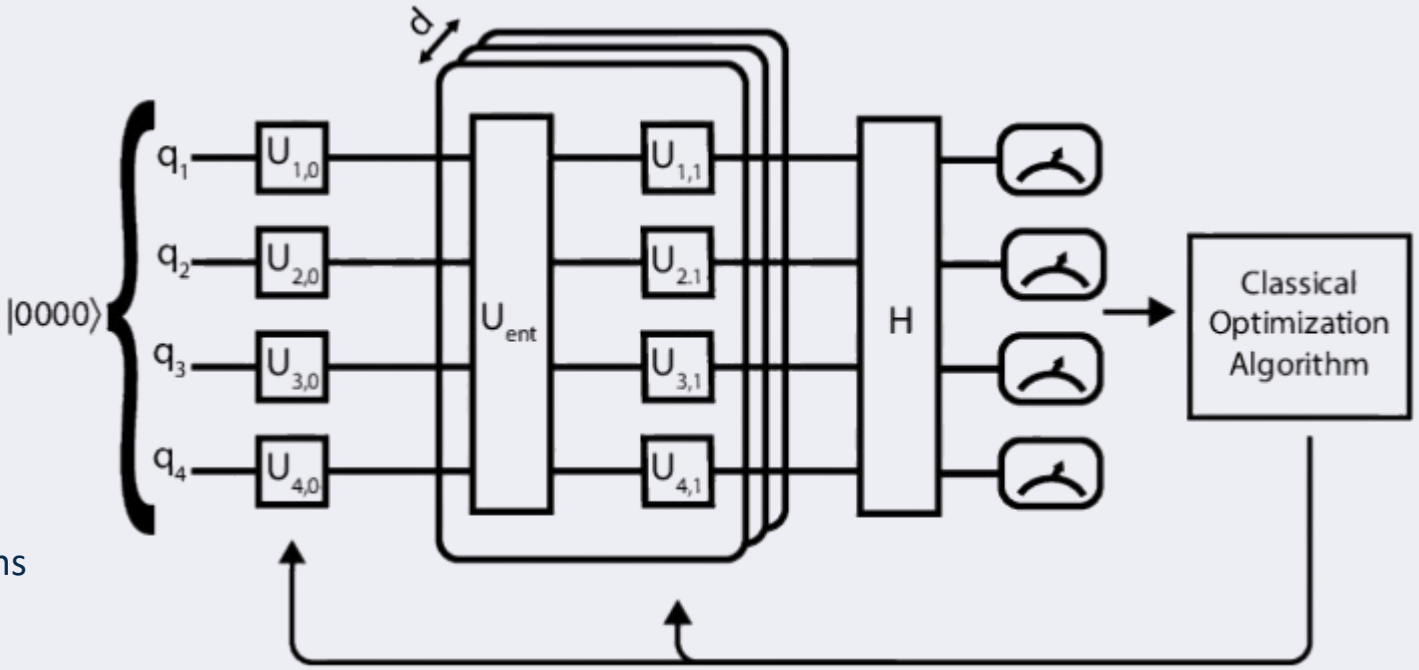
Processing loop of Quantum/Classical Circuit



Quantum Machine Learning uses hybrid approach by using Classical and Quantum Computing

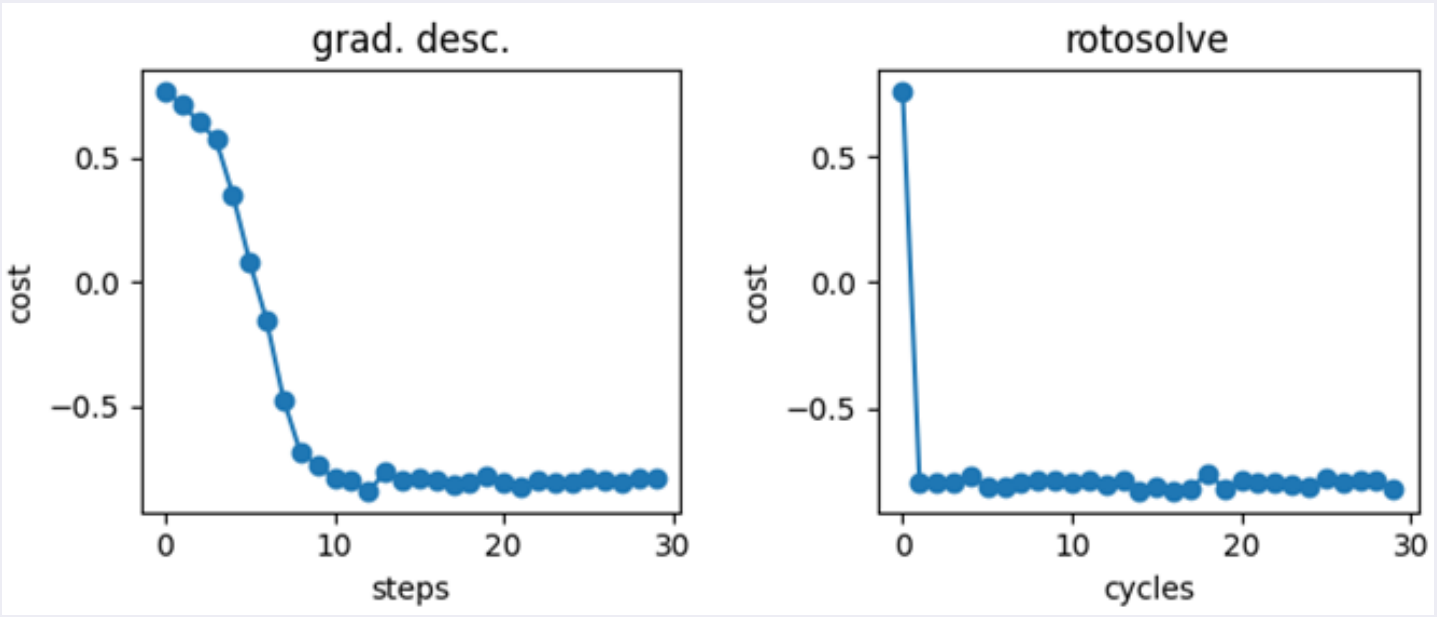
Variational Quantum Eigensolver

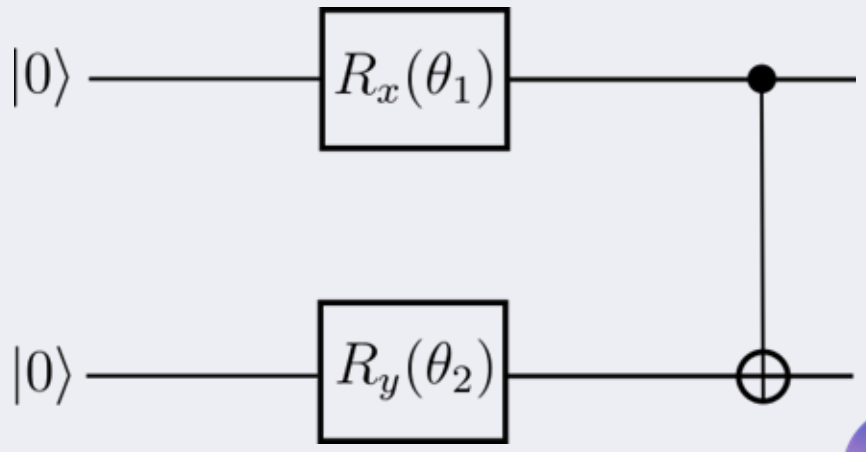
- A Variational Quantum Eigensolver (VQE) is a hybrid quantum–classical algorithm that estimates the ground-state energy of a Hamiltonian by minimizing the expectation value (energy)
- Widely used for solving problems in quantum chemistry and condensed matter physics
- The ansatz is central to VQE, it is the parametrized “search space” for the ground state, and the algorithm’s accuracy and efficiency depend critically on choosing an ansatz that is expressive enough yet compatible with available hardware and optimizers.
- Deeper circuits generally providing better approximations but at the cost of increased computational
- Examples of VQE are the Ising Hamiltonian (models interacting two-level spins) or the H2-molecule energy solving



VQE Optimizers – Rotosolve

- Rotosolve assumes each variational parameter that enters the circuit as a single-parameter rotation so the measured energy depends on that parameter
- The ansatz must be built from rotation gates whose are fixed (typically Pauli-like) and each parameter appears in that rotation
- It determines the parameters with few energy evaluations (commonly 3) and compute the parameter value that minimizes the energy

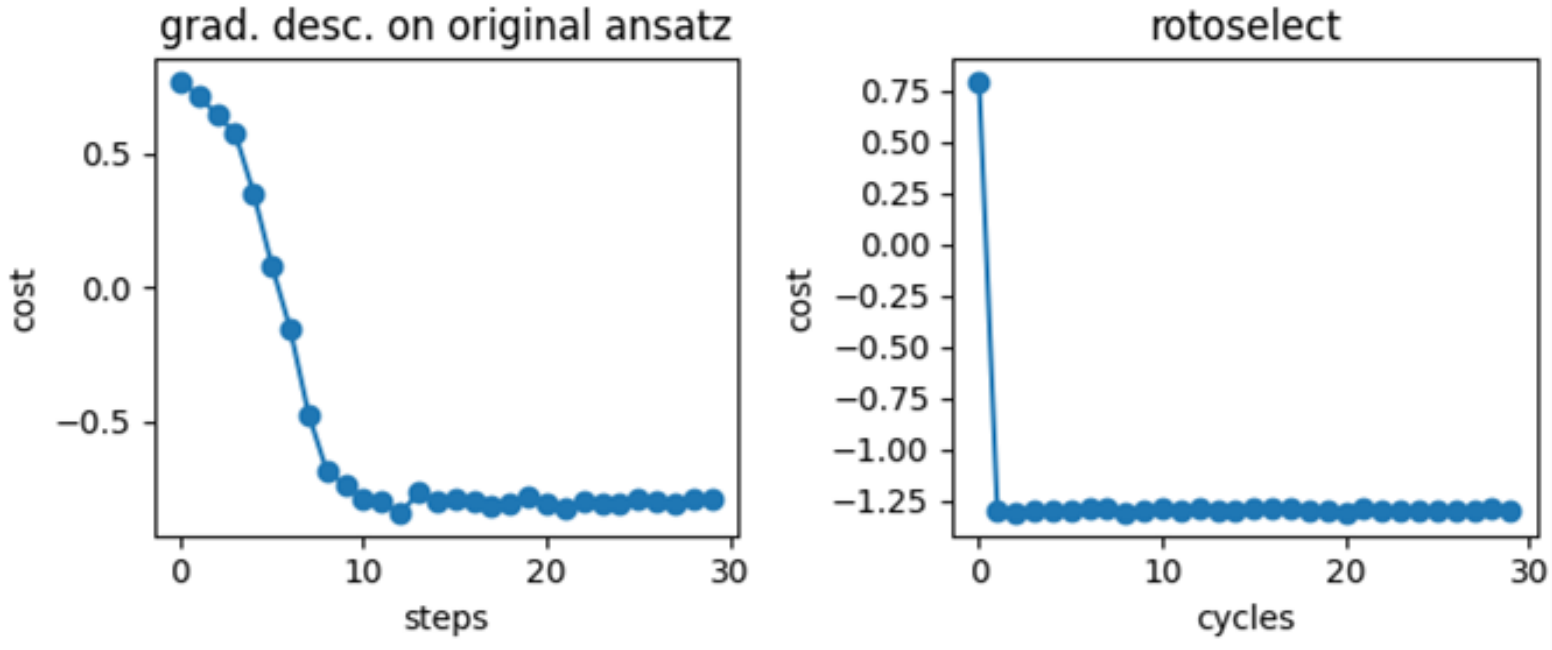


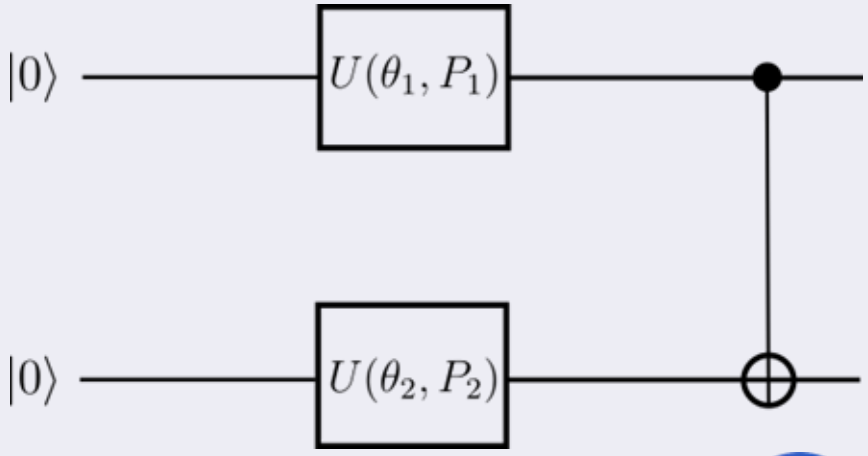


VQE Optimizers – Rotoselect

- Rotoselect assumes the same ansatz form as Rotosolve: each variational parameter appears as a single-parameter rotation, so the energy dependence on that parameter.

- It differs by selecting which parameters to update (or evaluate) at each step rather than updating all parameters every iteration.





RES access to Quantum computer

https://www.res.es/es

Next deadline September 2026 (twice a year)

Final thoughts

- QuantumSpain is the first QaaS in Europe
- Provides Quantum Computer to Universities and Companies
- Foster Quantum Computing/Physics knowledge with TalentQ
- A 35-Qubits Quantum Computer with more than 30 projects calls
- Finally, the second Quantum revolution is taking place in Europe

Quantum SPAIN

Thank you!

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