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Quantum Computing

Introduction & State of the art

Orléans – 09.12.2022

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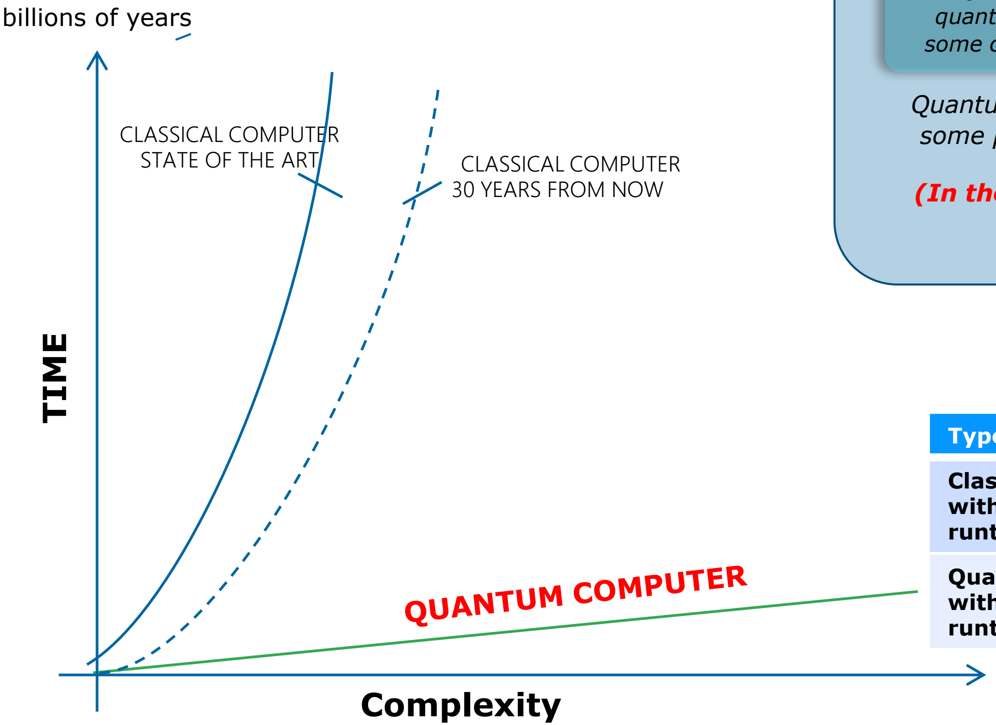
Classical computing “limitations”



Quantum computing relies on one promise:

Quantum computing is based on the promise that, when quantum computers are available, it will be possible to solve some complex problems faster than the current most powerful HPC systems.

Quantum computing will massively reduce the complexity of some problems currently intractable to classical computers

(In theory) Taking advantage of exponential growth : 2^n

Theoritical view ☺

Type of scaling	Time to solve the problem*:			
Classical algorithm with exponential runtime	2 mins	330 years	3300 years	**Age of the universe**
Quantum algorithm with polynomial runtime	2 mins	10 mins	11 mins	**~24 mins**

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Quantum Computing : Where we are ☺

1981: **First basic model** of a quantum computer
R. Feynman

1994: **Quantum algorithm development** to factorize large numbers. *P. Shor*

2016: IBM Q Network *(5 qubits)*

2017: Atos introduced **Quantum Learning Machine**

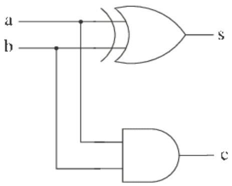
mid-term 2023/2026
- up to 5000 qubits
- NISQ devices : « Quantum Advantage »

2035+: **Logical qubits**
- *FTQC (Fault Tolerant Quantum Computers)*

Discovery phase | **NISQ Era** *(Noisy Intermediate-Scale Quantum)* | FTQC era

Today
- **NISQ HW (10-500 qubits)** (IBM, Google, Intel, DWave, Rigetti, Honeywell… Pasqal Quandela, IQM, AQT …
- **Emulators / Learning Systems** (Atos QLM, NVIDIA …)

Classical Information …. ☺



Boolean gates
Boolean circuit

Serial logic

bit 1	bit 2	bit 3	bit 4
0	1	1	0

- Each bit is in a definite state : 0 or 1
- Reading a bit does not change the state
- You can copy a bit
- All of the information of a bit is stored in that bit
- bits do not interact

0 0

0 1

1 0

1 1

0 0 0

0 0 1

…

1 1 1

0 0 0 0

…

1 1 1 1

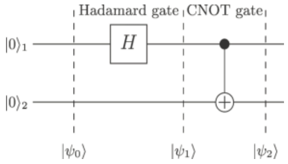
…

011100110

….

Quantum Computing

A few fundamental notions



Quantum gates
Quantum circuit

Parallel logic

QUANTUM BIT "QUBIT"

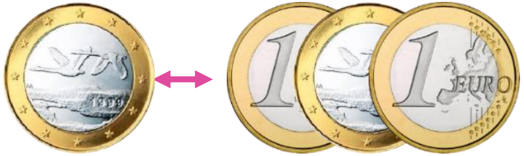
- ✓ **Basic unit** of quantum information
- ✓ **Two-state** quantum-mechanical system

- ✓ In QC, the **computational power** of a system is expressed in # of qubits
- ✓ **N qubits ➔** 2^N information

STATE SUPERPOSITION and MEASUREMENT

Qubits can be in **superposed |0> and |1> states**

When measured, they **collapse** to one of the states: |0> or |1>



N-qubit system ➔ 2^N states

QUANTUM ENTANGLEMENT

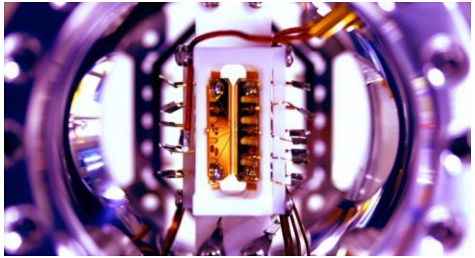
Entangled qubits have their states in **interaction** with each other. They cannot be described independently of the state of the others

q_0

Measurement of a single qubit will influence the entangled system as a whole!

Quantum Computing Challenges (1/3) : making Qubits

Ions



Credit: S. Debnath and E. Edwards/JQI
Monroe Group, University of Maryland/JQI

Photons

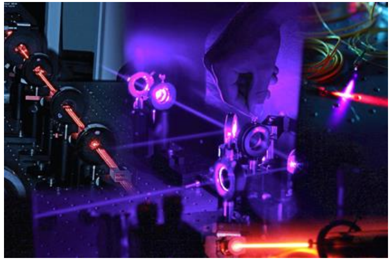


Image from the Centre for Quantum Computation & Communication Technology, credit Matthew Broome

Neutral Atoms

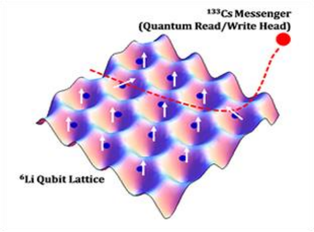


Image from Cheng Group, University of Chicago

Solid-state defects

NV Centers, Phosphorous in Si, SiC defects, etc.

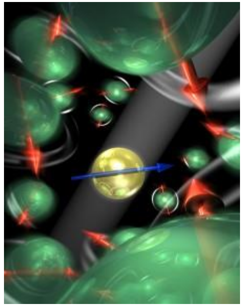
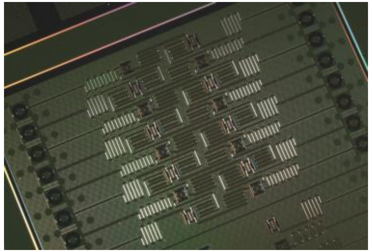
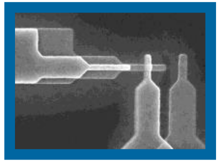
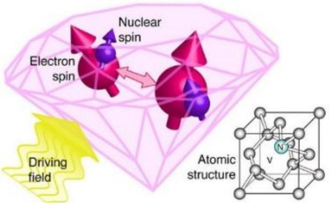


Image from Hanson Group, Delft

Superconducting Circuits



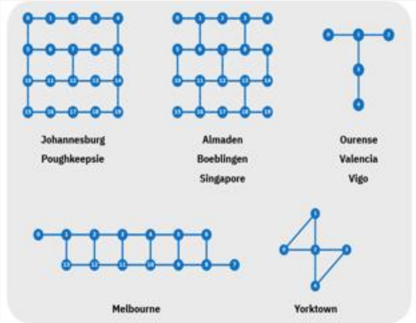




Quantum Computing Challenges (2/3): Connecting qubits

Connecting 2 or 3 qubits is easy ☺ ☺

Adding more qubits is complicated

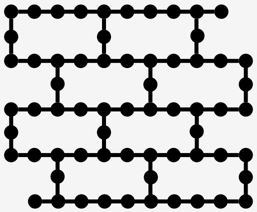


- Several possibilities for noisy qubits exists :

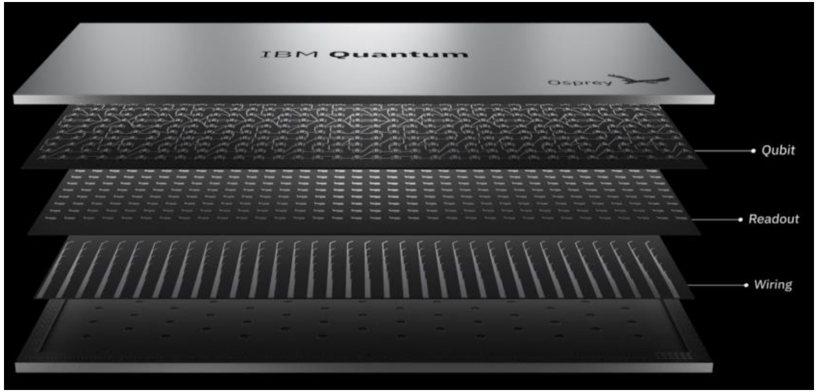
But

- A major engineering problem is : scaling !
- Difficulty is exponential
- State of the art (Nov. 2022 : 433 qubits IBM), no error correction
- 500-4000 uncorrected qubits expected in the coming 3 years
- But the goal is to reach …… one million of qubits !!

IBM 65 Q
Hummingbird



IBM Osprey 433 qubits



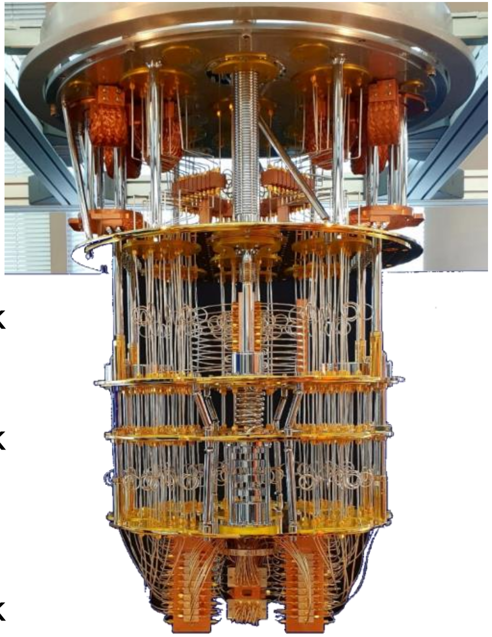
Quantum Computing Challenges (3/3):

2.7 K

0.8 K

0.1 K

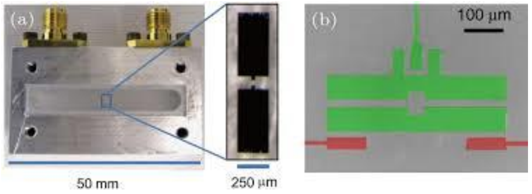
0.02K



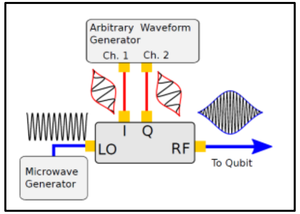
Temperature
near abs.zero (-273.15°C)

- **Cryostat**
- **Cabling and multiplexing**
- **Amplifiers**

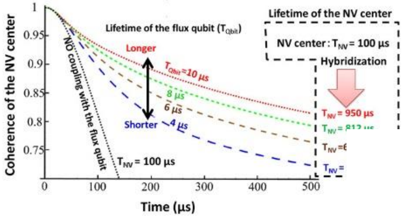
(Some) Factors contributing to the overall system
Where do the « errors » come from **(noisy qubits & NISQ Era)**



- Qubit size
- Gate Fidelity / Errors (single qubit, multiple qubits)

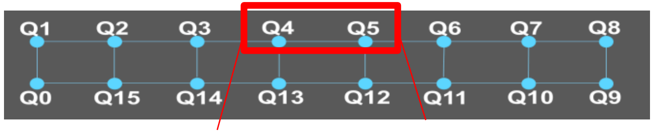


- Coherence time : How long a quantum state live (#100us to ms)
- Measurement Fidelity
- Connectivity between qubits
- « Crosstalk» / Spectator errors



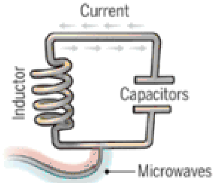
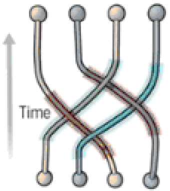
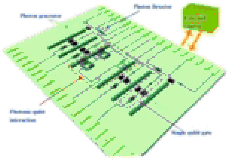
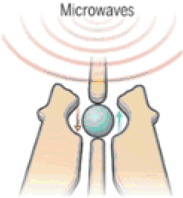
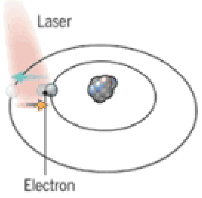
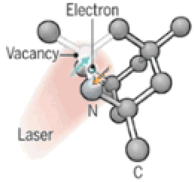
Maud Vinet, Grenoble

	Superconductor	Si spin	Trapped ions	Photons	NV centers	Neutral atoms
Size	(100µm)²	(100nm)²	(1mm)²	~(100µm)²	~(100µm)²	(1µm)²
Fidelity	~99.3%	~99.6%	~99.9%	50% (mesure) 98% (portes)	98% (probabilistic)	95%
Speed	100 ns	~1 µs	100 µs	1 ms	100ms	1 ms
Manufacturing						
Qubit Variability	3%	0.1%-0.5%	0.0001%	0.5%	0.001%	0.0001%
Operation T°	50mK	10mK-1K	300K	4K	4K	300K
Connectivity	4	4	10	2	5	10
Entangled qubits	53	6	20	18	20	192



Two-qubit exchange interaction is mediated by the bus resonator.

Quantum eco-system

					
boucles supra-conductrices	**qubits topologiques**	**optique linéaire**	**quantum dots silicium**	**ions piégés**	**impuretés diamants**
IBM	Microsoft	XANADU	intel	IONQ	QDTI
intel	NOKIA	hp	cea	MIT	cea
Google	TU Delft	PSIQUANTUM	Yale University	University of Maryland	MIT
QuTech	QuTech	TUNDRA SYSTEMS GLOBAL LTD.	NTT	Sandia National Laboratories	University of Maryland
rigetti		University of Oxford	NOKIA	Harvard University	TU Delft
qci		University of Bristol		JGU	Universität Stuttgart
UCSB		universität wien		universität innsbruck	
cea		Università degli Studi di Milano		IQOQI	
OXFORD QUANTUM		Sapienza Università di Roma		IQST	
Raytheon					

Alice&Bob

PASQAL

QUANDELA

C12

cea

cnrs

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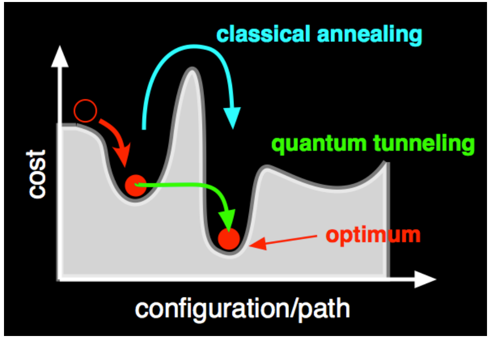
Types of Quantum Computers (1/2)

Quantum Annealers

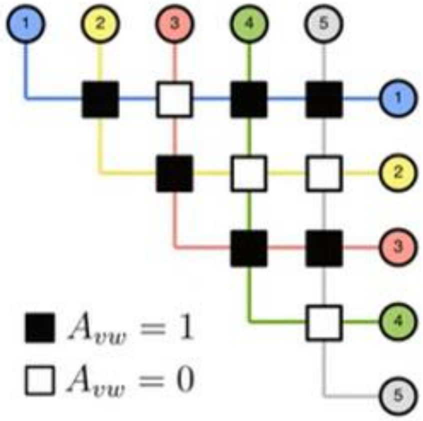
Optimization Problems

- Machine learning
- Fault analysis
- Optimization, logistics, time scheduling
- etc…



- Ground state of an Ising model
- Many ‘noisy’ qubits can be built (# 4000) today
- Quantum speedup unclear (not demonstrated)

Quantum Simulators



- Finding the ground state of an Ising model
- # 100/1000 qubits today

Quantum Gate based Computers

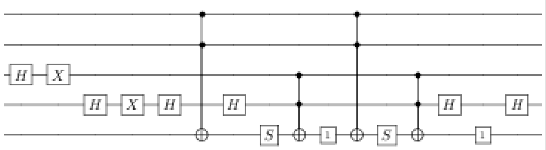
Larger Class of problems; Execution of arbitrary Quantum Algorithms

- Material discovery
- Quantum chemistry
- Optimization
- Machine Learning

Algebraic algorithms
(machine learning, cryptography,…)

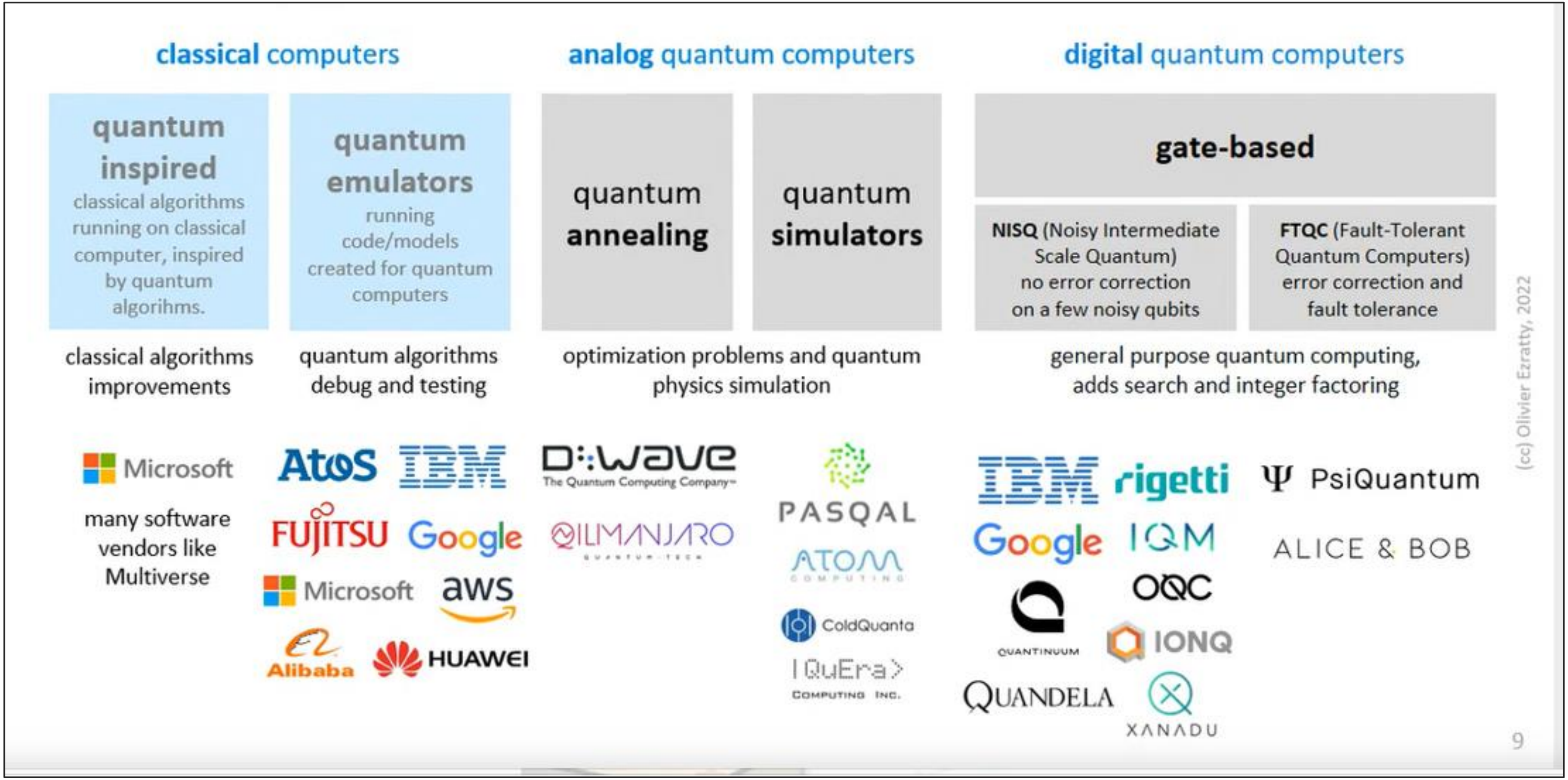
- Combinatorial optimization
- Digital simulation of quantum systems

Quantum Programs



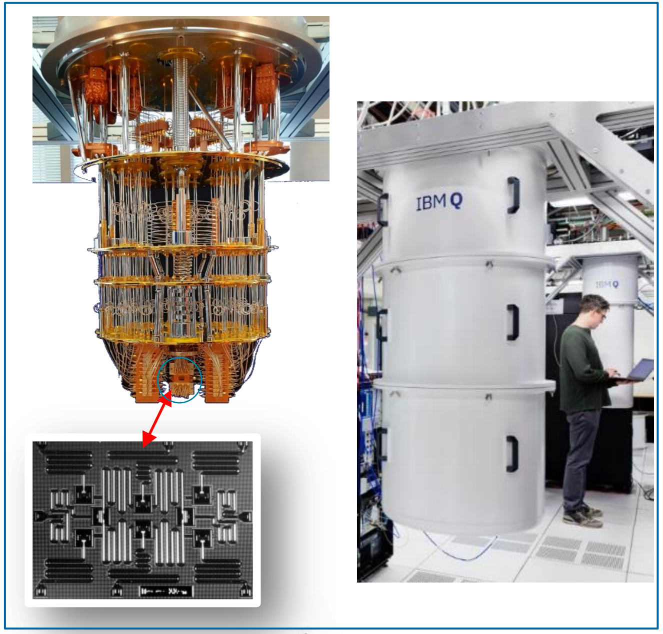
- Limited ‘noisy’ qubits can be built (# 10-500) today

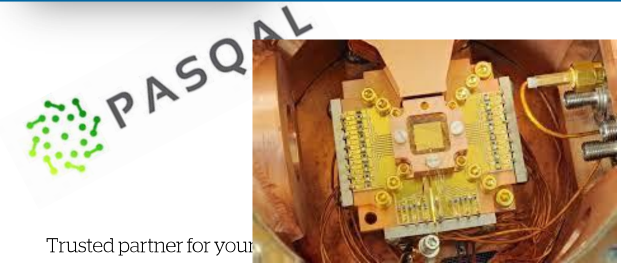
Types of Quantum Computers (2/2)



(*) Slide from Olivier Ezratty, 2022

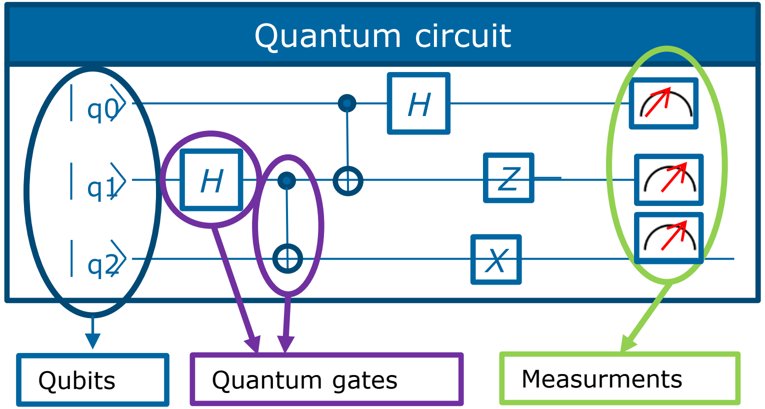
Existing (NISQ) solutions …





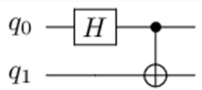
Quantum Computing – Programming in a nutshell

(Quantum gate based model)



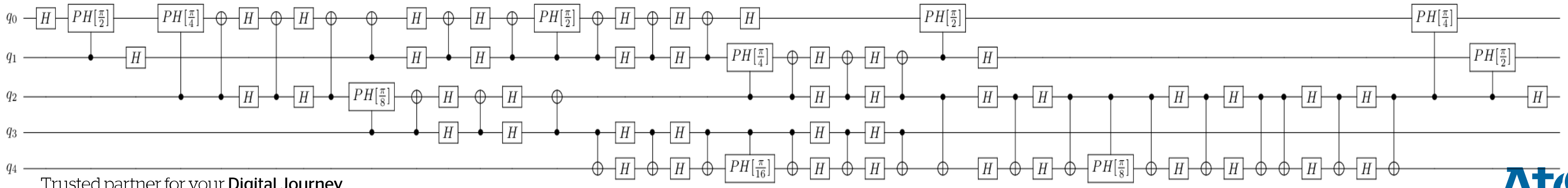
- Create a program
- Allocate some qubits
- Apply some quantum gates
- Export the program to a circuit
- Display the circuit

```
from qat.lang.AQASM import Program, H, CNOT
from qat.qpus import LinAlg
qprog = Program()
qbits = qprog.qalloc(2)
qprog.apply(H, qbits[0])
qprog.apply(CNOT, qbits)
circuit = qprog.to_circ()
%qatdisplay circuit
```



Quantum Gates are "manipulated" through Python

Example : a QFT on 5 qubits …



Writing your first circuit

A few notions: standard gates

Operator	Gate(s)	Matrix
Pauli-X (X)	X, ⊕	$\begin{bmatrix}0 & 1\\1 & 0\end{bmatrix}$
Pauli-Y (Y)	Y	$\begin{bmatrix}0 & -i\\i & 0\end{bmatrix}$
Pauli-Z (Z)	Z	$\begin{bmatrix}1 & 0\\0 & -1\end{bmatrix}$
Hadamard (H) ☆	H	$\frac{1}{\sqrt{2}}\begin{bmatrix}1 & 1\\1 & -1\end{bmatrix}$
Phase (S, P)	S	$\begin{bmatrix}1 & 0\\0 & i\end{bmatrix}$
$\pi/8$ (T)	T	$\begin{bmatrix}1 & 0\\0 & e^{i\pi/4}\end{bmatrix}$

Operator	Gate(s)	Matrix
Controlled Not (CNOT, CX)		$\begin{bmatrix}1&0&0&0\\0&1&0&0\\0&0&0&1\\0&0&1&0\end{bmatrix}$
☆ Controlled Z (CZ)	Z	$\begin{bmatrix}1&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&-1\end{bmatrix}$
SWAP		$\begin{bmatrix}1&0&0&0\\0&0&1&0\\0&1&0&0\\0&0&0&1\end{bmatrix}$
Toffoli (CCNOT, CCX, TOFF)		$\begin{bmatrix}1&0&0&0&0&0&0&0\\0&1&0&0&0&0&0&0\\0&0&1&0&0&0&0&0\\0&0&0&1&0&0&0&0\\0&0&0&0&1&0&0&0\\0&0&0&0&0&1&0&0\\0&0&0&0&0&0&0&1\\0&0&0&0&0&0&1&0\end{bmatrix}$

For non-standard gates, **abstract gates** could be defined by a matrix or a routine

$$XX[\theta] = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 0 & 0 & -ie^{i\theta}\\0 & 1 & -i & 0\\0 & -i & 1 & 0\\-ie^{-i\theta} & 0 & 0 & 1\end{pmatrix}$$

03. Application domains and use cases

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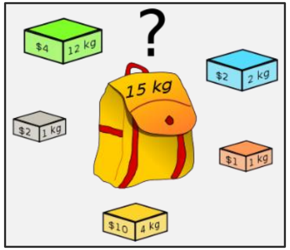
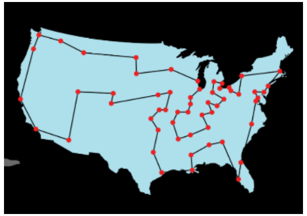
Why quantum computing?

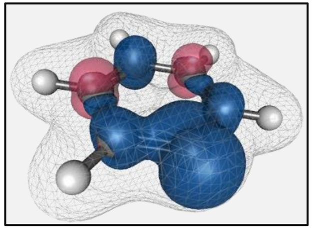
Classically solved problems

Classically intractable problems

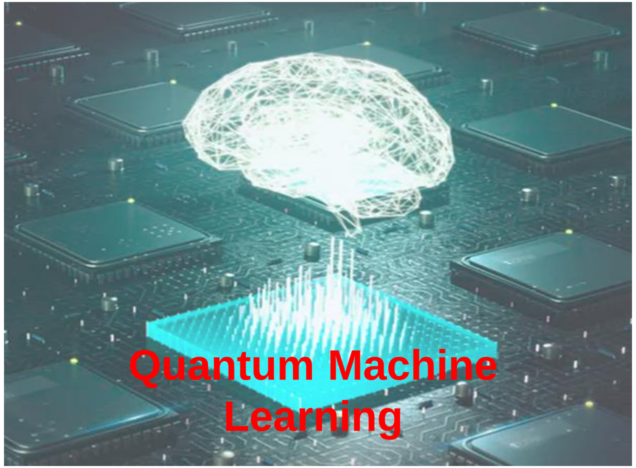
Quantum Computing addressable problems



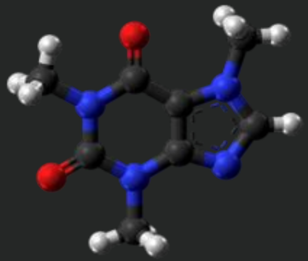




Quantum Circuits for Applications



Quantum Simulations

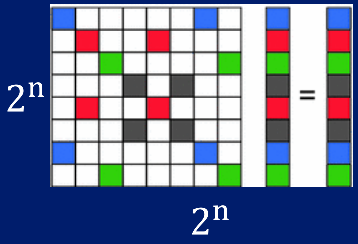


Physics

Chemistry

Materials discovery

Linear Systems ($Ax = b$)



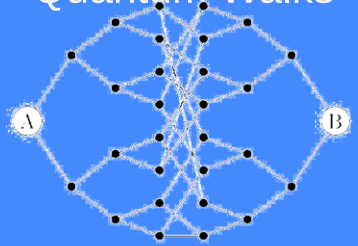
Network analysis

Differential equations

Option pricing, heat transfer

Classification (Machine Learning)

Quantum Walks



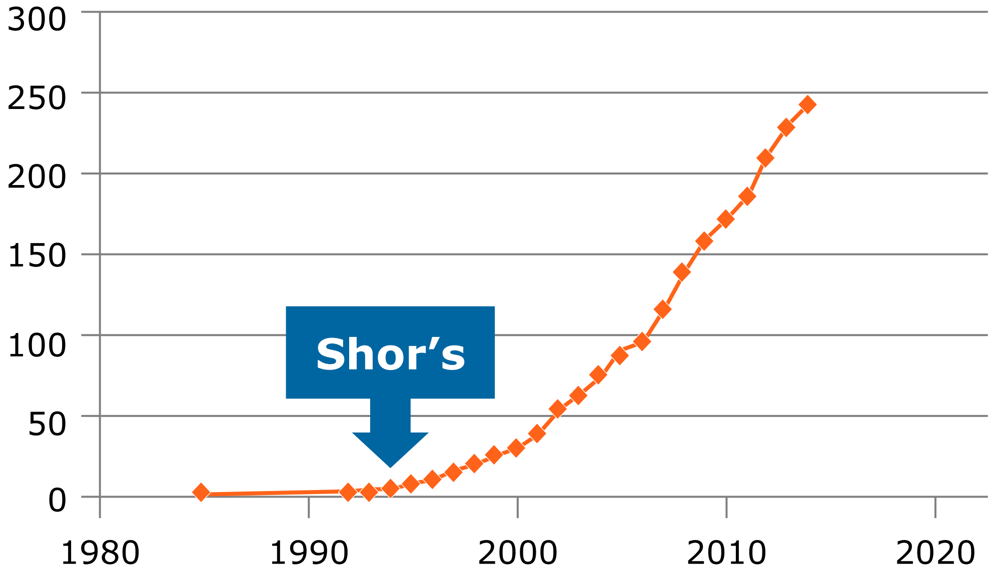
Graph properties (network flows, electrical resistance)

Search

Collision finding

Known Quantum Algorithms with a Speedup

Progress in QC Algorithms



math.nist.gov/quantum/zoo

Quantum Computing applications

Numerous cross-industry impacts

Manufacturing

- Autonomous vehicle
- Logistics
- Supply chain
- Software validation
- Batteries
- Polymers

Public Sector & Defense

- Neural networks
- Process optimization
- Cryptanalysis
- Material science
- Nanotechnologies

Chemistry & material Science

- Materials science
- NanoTech.
- Batteries
- Polymers
- Catalysts, enzyme design
- Molecular modeling
- Protein folding
- Drug discovery

Financial Services & Insurance

- Fraud detection
- Trading strategies
- Market simulation
- Portfolio optimization
- Risk assessment
- Cryptocurrency

Telecom, Media & Technology

- Personalized content
- 5G antenna location
- Chip layout optimization
- Post-quantum cryptography

Resources & Services

- Smart grids
- Flight scheduling
- Oil well optimization
- Yield management
- Cybersecurity
- Carbon dioxide capture

Health & Life Sciences

- Genomics
- Virtual screening
- Protein folding
- Drug discovery
- Personalized medicine

Chemistry

One of today's most active application areas!

Goal

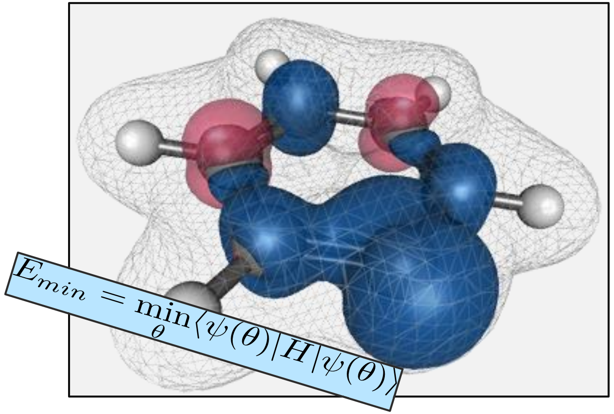
- Compute the exact energy of large molecules
  - This is intractable today
  - Cost: 2 qubits per orbital even without error correction!

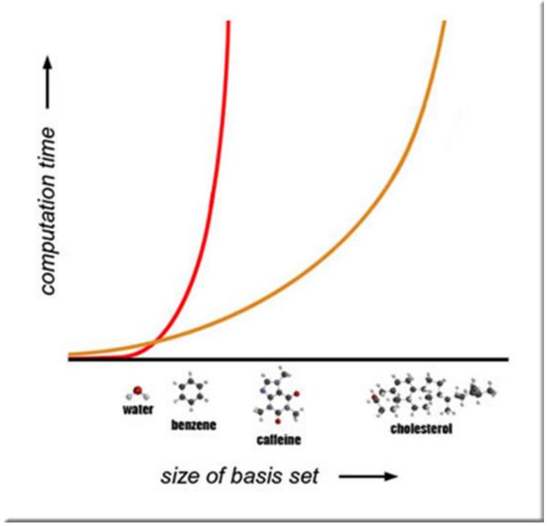
Star algorithms

- Variational Quantum Algorithms (VQE and derivatives)

Impact

- New discovery and energy savings in synthesis for fertilizers, lubricants, …





Atos in the Quantum Landscape

- HPC Manufacturer. #3 in the world
- Invested in Quantum Research since 2016

- **Atos Platform**
  - Built an HPC fat node (up to 48 TB memory)
  - Complete quantum framework
  - Embeds high performance emulators (perfect, simulation of quantum physics noise)
  - **Hardware agnostic hybridization**
- Used in 30+ HPC Centers

- We already integrate quantum processors into supercompuetrs
  - IQM at LRZ
  - Pasqal Analog simulator at GENCI
  - ..

Our solutions:

- Identify use cases in your production
- Design and test their quantum version
- Educate your teams
- Provide a hardware-agnostic high performance quantum simulator

Atos Quantum Learning Machine

Programming environment and a quantum processor emulator

PROGRAMMING

AQASM
Assembly language to build quantum circuits

pyAQASM
Python extension to AQASM

CIRC
Binary format of quantum circuits

QLIB
AQASM & pyAQASM libraries

CO problems class
Describe any Combinatorial Optimization problem

INTEROP.
Connectors with other frameworks

ProjectQ

OPTIMIZATION

PBO
Pattern based optimizer

NNIZER
Topology constraint solver

Circuit Optimizer
Generic circuit optimizer

SIMULATION

SIMULATORS

Digital QC Simulators
Quantum-Inspired Simulators

PHYSICS

Physical Noise models

Atos Quantum - A universal gateway to quantum technologies

Atos

1 Atos Quantum Learning Machine

On-Premise solution

- Advanced simulation
  - Noise modelling
  - Optimization
  - Quantum annealing
- Multi-tenancy
- Performance
  - Optional GPU acceleration

2 myQLM

Universal programming environment

Desktop solution

- Freeware
- Entry-level simulation
- Open-source plugins

Interoperability

Proprietary programming frameworks

Universal front-end for quantum technologies

Any Quantum Computing hardware

- Superconducting
- Trapped ions
- Rydberg atoms
- ...

myQLM documentation : https://myqlm.github.io/

Quantum Learning Machine: jupyter notebooks tutorial

myQLM-1.5.1

The Quantum Learning Machine provides a software environment to program, compile and execute quantum pro
simulators or on an actual chip whose interface has been implemented.

It comes with a python software stack named "*Quantum Application Toolset*" (QAT), available under the general r

Getting started

The getting started notebook provides the basic steps to write and simulate your first quantum circuit.

Tutorial notebooks: overview per theme

- Basics
- AQASM: the quantum programming language of the QLM
- Ideal (noise-less) circuit simulation
- Customizing computational stack with Plugins
- Interoperability

Full table of contents

Atos Worldwide Quantum Community

From research to productive applications

Hartree Centre
Science & Technology Facilities Council

ICHEC
Irish Centre for High-End Computing

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Argonne NATIONAL LABORATORY

Stanford University

OAK RIDGE National Laboratory

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CaSciModOT
Calcul Scientifique et Modélisation Orléans Tours

Merci et au plaisir de poursuivre ces échanges ☺

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