Chapitre 2: Calcul quantique à l’ère NISQ

Les ordinateurs quantiques sont bruités

- Les qubits sont très sensibles à leur environnement
- La profondeur des circuits (nombre de couches de circuits) allonge la durée d'exécution et, par conséquent, ajoute et propage des erreurs.
- Les circuits doivent être aussi courts que possible
- Le circuit doit être exécutable sur une machine donnée

https://www.vecteezy.com/vector-art/23929483-noise-pollution-harmful-sounds-causing-disturbances-affecting-health-and-environment

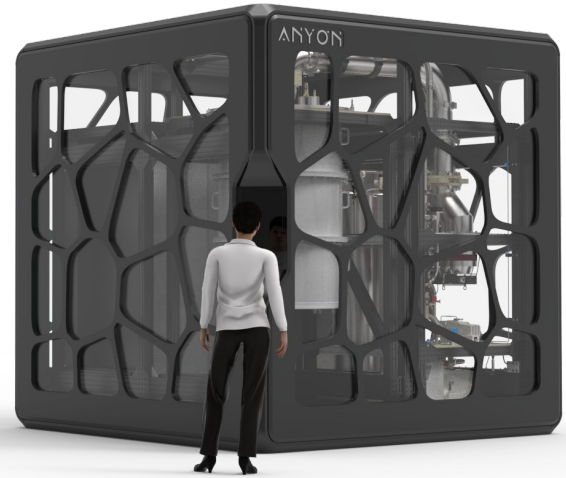
NISQ

Noisy
Intermediate
Scale
Quantum
Computers

Processeurs quantiques disponibles aujourd'hui

Haut niveau de bruit

➔ Nombre limité de qubits
➔ Nombre d'opérations unitaires (portes) limité



MonarQ

Nombre de qubits	24 qubits
Profondeur de circuit	~350 portes à un qubit

Vers l’ère FTQC

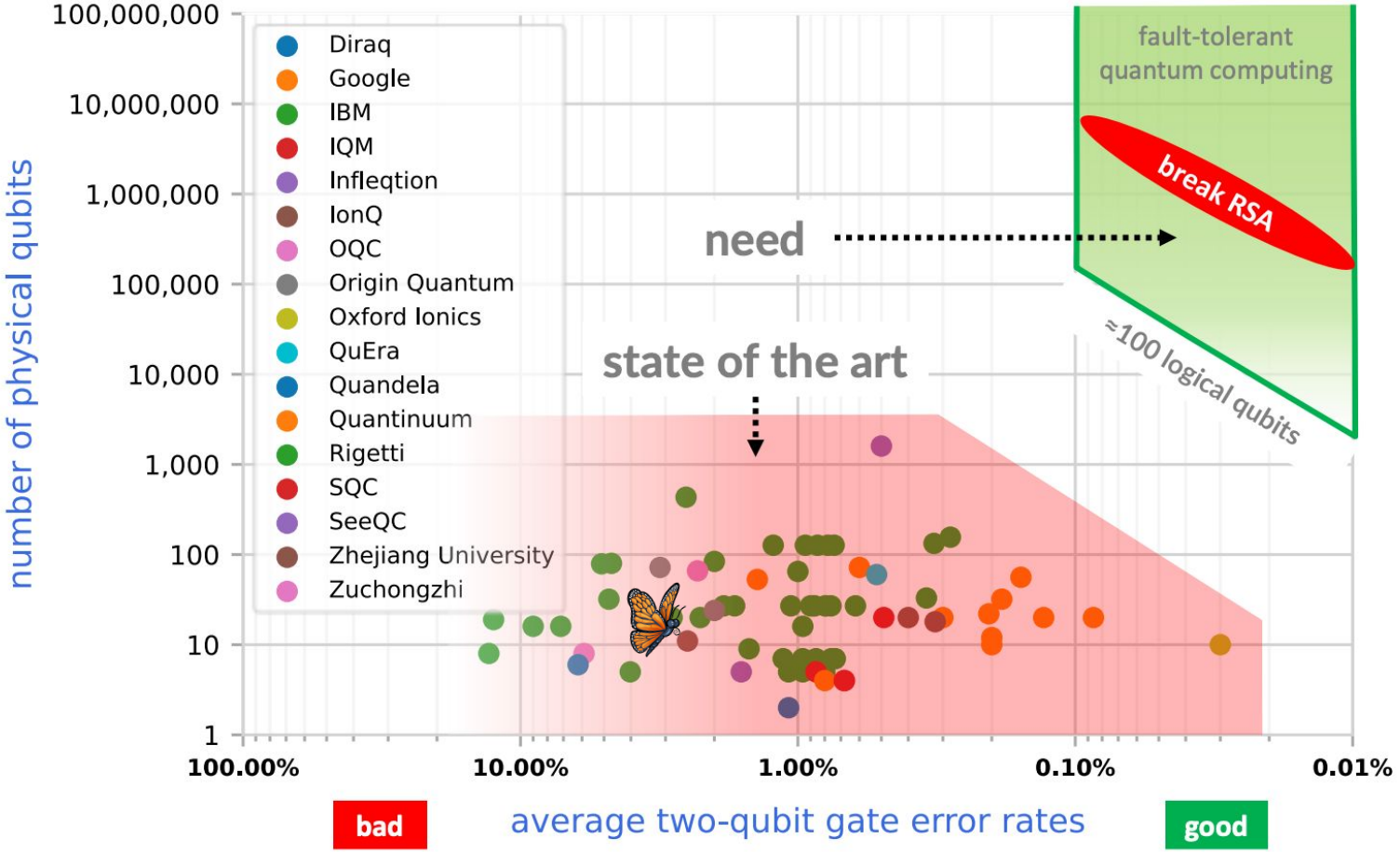
Fault
Tolerant
Quantum
Computers

Objectif à long terme de l'informatique quantique

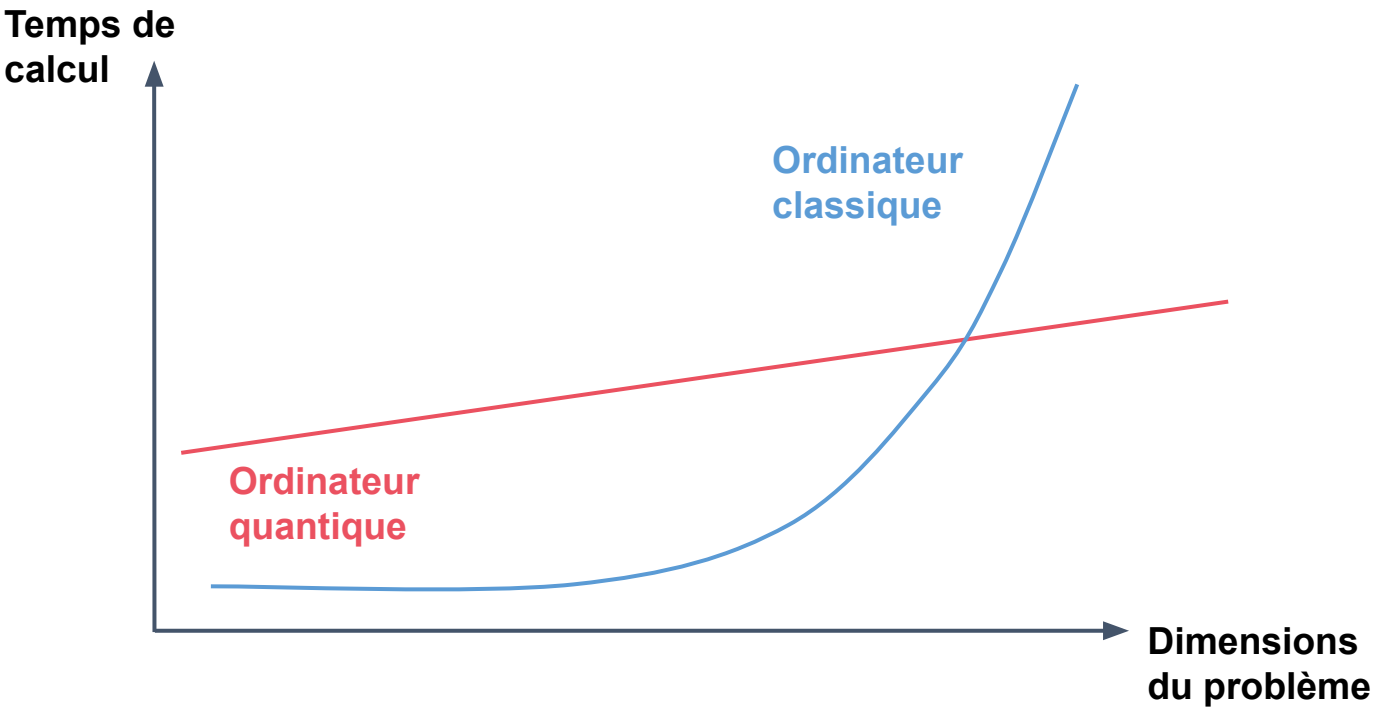
Ordinateurs quantiques avec correction d’erreurs

- ➔ Plus grand nombre de qubits nécessaires pour faire des qubits **logiques** (1000:1)
- ➔ Qubit logique: robuste aux erreurs
- ➔ Sinon on parle de **qubits physiques**
- ➔ Augmentation de la profondeur des circuits

Source : Eur. Phys. J. A (2023) 59:94 https://doi.org/10.1140/epja/s10050-023-01006-7



Quand utiliser un ordinateur quantique?



Quand utiliser un ordinateur quantique?

Un PC suffit

Problèmes compatibles avec NISQ

FTQC requis

- Arithmétique
- Regarder ses courriels

- Chimie
- Apprentissage machine
- Optimisation

… et d’autres domaines de recherche

- Algorithme de Shor
- Transformé de Fourier quantique
- Algorithme de Grover

Adapté de https://learning.quantum.ibm.com/course/quantum-computing-in-practice/what-problems-are-quantum-computers-good-for

SHORTER TERM → LONGER TERM

	Molecular simulation	Quantum optimization	Quantum Monte Carlo	Machine learning	HHL	Decryption[1]
Life sciences	Calculating a drug's binding affinity	Optimizing the location of clinical trial sites	Predicting the spread of disease in epidemics	Improving image classification in diagnostics	Modelling forces for protein-folding simulations	Protecting patient data privacy
Chemicals	Simulating the reaction pathway in synthesis	Optimizing the production process of chemicals	Simulating meso-scale reactor processes	Predicting the properties of new chemicals	Solving fluid dynamics in reaction vessels	Protecting data related to IP and trade secrets
Energy	Designing new materials for carbon capture	Optimizing power dispatching in an electric grid	Forecasting energy prices in the market	Predicting energy production from weather patterns	Solving DC power flow calculations in electrical grids	Protecting access to data on grid infrastructure
Telecom	Designing new semiconductor materials	Optimizing antenna placement	Stress-testing network resilience	Improving customer segmentation	Solving EM-field calculations in antenna design	Protecting the data exchanged over a network
Advanced manufacturing industries	Designing new batteries for electric vehicles	Optimizing the step sequence in car production	Improving the resilience of the supply chain	Improving fault detection in chip manufacturing	Solving aerodynamics simulations	Protecting communication connections
Logistics	N/A	Optimizing the route of a delivery service	Stress-testing logistic schedules for disruptions	Predicting maintenance needs in a fleet	Improving inventory management	Protecting personalized customer data
Finance	N/A	Optimizing the value of an asset portfolio	Modelling credit value at risk in capital allocation	Improving the detection of fraud in transactions	Estimating risk for the future value of an asset	Protecting customer transaction data

Source : Alice & Bob, 2024

NISQ Étude de cas

Chimie

Greene-Diniz et al. *EPJ Quantum Technology* (2022) 9:37
https://doi.org/10.1140/epjqt/s40507-022-00155-w
EPJ.org
EPJ Quantum Technology
a SpringerOpen Journal
COMMENT Open Access

Modelling carbon capture on metal-organic frameworks with quantum computing

Gabriel Greene-Diniz[1], David Zsolt Manrique[1], Wassil Sennane[2], Yann Magnin[3], Elvira Shishenina[4,2], Philippe Cordier[2], Philip Llewellyn[3], Michal Krompiec[1], Marko J. Rančić[2*] and David Muñoz Ramo[1]

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Abstract

Despite the recent progress in quantum computational algorithms for chemistry, there is a dearth of quantum computational simulations focused on material science applications, especially for the energy sector, where next generation sorbing materials are urgently needed to battle climate change. To drive their development, quantum computing is applied to the problem of CO_2 adsorption in Al-fumarate Metal-Organic Frameworks. Fragmentation strategies based on Density Matrix Embedding Theory are applied, using a variational quantum algorithm as a fragment solver, along with active space selection to minimise qubit number. By investigating different fragmentation strategies and solvers, we propose a methodology to apply quantum computing to Al-fumarate interacting with a CO_2 molecule, demonstrating the feasibility of treating a complex porous system as a concrete application of quantum computing. We also present emulated hardware calculations and report the impact of device noise on calculations of chemical dissociation, and how the choice of error mitigation scheme can impact this type of calculation in different ways. Our work paves the way for the use of quantum computing techniques in the quest of sorbents optimisation for more efficient carbon capture and conversion applications.

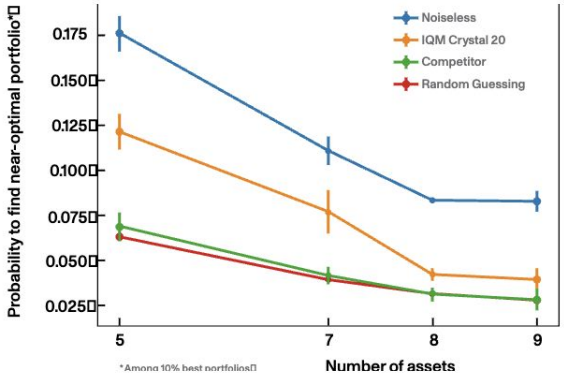
Keywords: Quantum computing; NISQ; Carbon capture; Climate change; Quantum algorithms

Source : https://epjquantumtechnology.springeropen.com/articles/10.1140/epjqt/s40507-022-00155-w

Optimisation

IQM and DATEV advance quantum solutions for portfolio optimization

In our collaboration with DATEV, we developed a specific quantum algorithm tailored to the company's product portfolio optimization challenge. By using the data of DATEV and applying advanced transpilation techniques, we were able to execute the algorithm on our quantum hardware leveraging a quantum processing unit (QPU) with 20 qubits.



Source : https://www.meetiqm.com/lp/the-future-of-portfolio-optimization-is-in-quantum

Apprentissage machine (QML)

Applying Quantum Autoencoders for Time Series Anomaly Detection

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Abstract

Anomaly detection is an important problem with applications in various domains such as fraud detection, pattern recognition or medical diagnosis. Several algorithms have been introduced using classical computing approaches. However, using quantum computing for solving anomaly detection problems in time series data is a widely unexplored research field.
This paper explores the application of quantum autoencoders to time series anomaly detection.

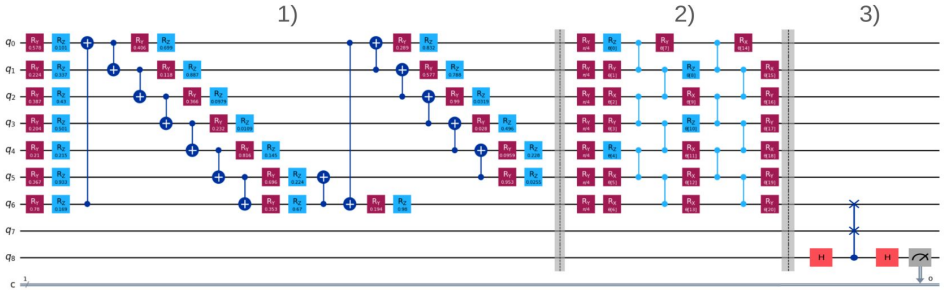

Fig. 8: Illustration of a circuit optimized for execution on real quantum hardware before transpilation.

Source : https://arxiv.org/abs/2410.04154

et d'autres domaines actifs de recherche

Science des matériaux

Quantum Algorithm for Vibronic Dynamics: Case Study on Singlet Fission Solar Cell Design

Danial Motlagh,[1] Robert A. Lang,[1] Jorge A. Campos-Gonzalez-Angulo,[2,3] Tao Zeng,[4] Alan Aspuru-Guzik,[2,3,5,6] and Juan Miguel Arrazola[1]

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[6] *Acceleration Consortium, Toronto, ON, M*

Vibronic interactions between nuclear motion and electronic
modeling of photochemistry. However, accurate simulations of f
ics are often prohibitively expensive for classical methods beyo
present a quantum algorithm based on product formulas for sim
eral vibronic Hamiltonian in real space, capable of handling an a
and vibrational modes. We develop the first trotterization schen

Biologie

A biological sequence comparison algorithm using quantum computers

Büsra Kösoglu-Kind[1], Robert Loredo[2,3], Michele Grossi[4], Christian Bernecker[5], Jody M. Burks[2] & Rüdiger Buchkremer[1]✉

Genetic information is encoded as linear sequences of nucleotides, represented by letters ranging from thousands to billions. Differences between sequences are identified through comparative approaches like sequence analysis, where variations can occur at the individual nucleotide level or collectively due to various phenomena such as recombination or deletion. Detecting these sequence differences is vital for understanding biology and medicine, but the complexity and size of genomic