DA VINCI DIALOGUES

SÉMINAIRE DEEP TECH

9-10 AVRIL 2024

CHÂTEAU LOUISE DE LA VALLIÈRE
REUGNY, INDRE-ET-LOIRE

LES TECHNOLOGIES QUANTIQUES AU SERVICE DE LA SANTÉ

Olivier Ezratty

DA VINCI LABS

les technologies quantiques au service de la santé

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Tours, 10 avril 2024
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quantum sensors

- less invasive imaging (MRI, MEG) and better precision biological sensors (NV centers).

drugs discovery

- DNA sequence alignment.
- de novo DNA sequence.
- protein folding and interactions with ligands.
- force field and electronic structure computation.
- screening and generation of molecular entities as drug candidates.
- drug retargeting.

diagnostics

- medical images classification and reconstruction.
- disease assessement based on genomic samples.
- clinical data classification and analysis.
- disease risk prediction.
- clustering of similar individuals.

treatments

- persistence and health-related behavior prediction.
- treatment and intervention effectiveness forecasting.
- disease outbreak prediction and spread modeling.
- precision oncology.
- tailored radiotherapy.
- hospital capacities optimization.

simulating nature

- chemical simulations.

data processing

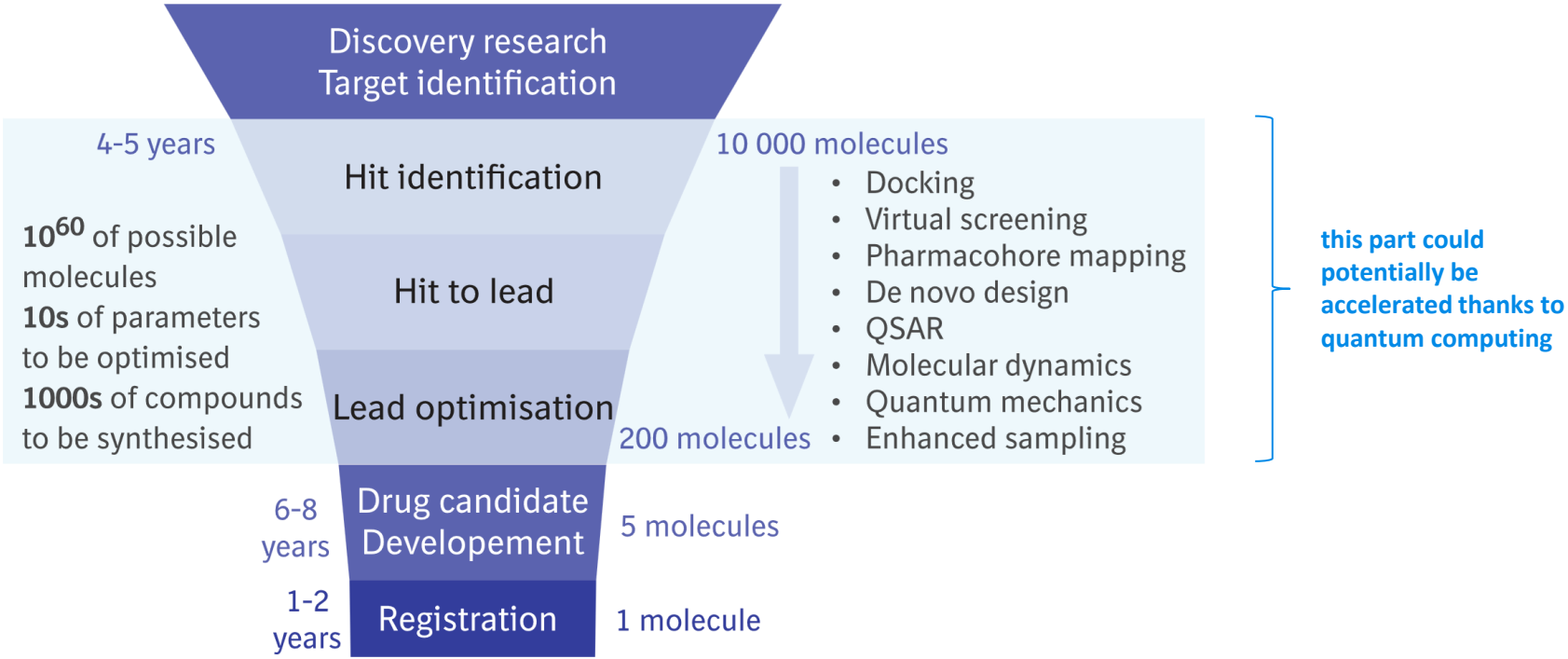
- images and structured data.
- quantum machine learning.

search and optimizations

- various datasets.

inspired from "The state of quantum computing applications in health and medicine" by Frederik F. Flöther, IBM Quantum, January 2023.

fasten drug discovery

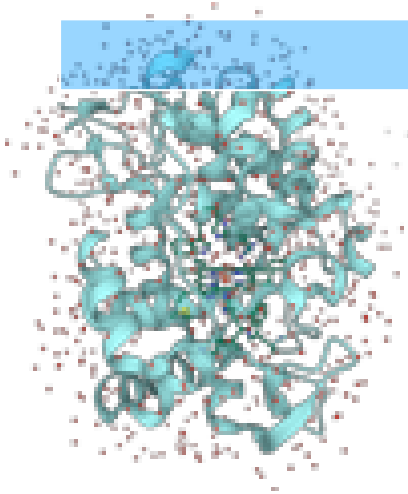


Source: Drug design on quantum computers by Raffaele Santagati, Alan Aspuru-Guzik, Nathan Wiebe et al, January 2023 (9 pages)

common electronic structure methods employed on classical computers

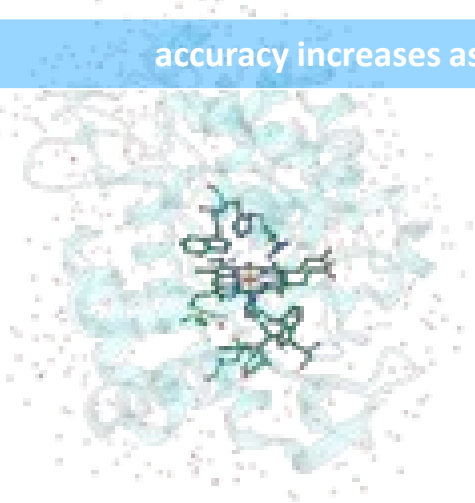
commonly used quantum chemistry methods to solve the electronic structure problem. In the left column, we zoom in on the Compound I intermediate of Cytochrome c Peroxidase (PDB ID: 1ZBZ [71{73]).

accuracy increases as molecule are smaller



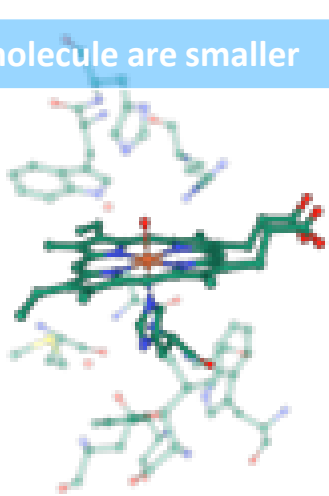
Cytochrome in solution

Force Fields/ Semi-empirical Methods
Methods that cannot fully describe quantum mechanical effects but can be tuned with information from quantum methods.



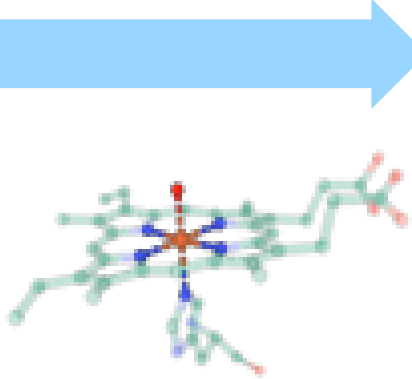
Cytochrome binding site

Hartree-Fock/Density Functional Theory (DFT)
Mean-field methods treat electrons in the presence of the average potential of the other electrons. DFT includes electronic correlation, while Hartree-Fock does not.



Cytochrome heme site

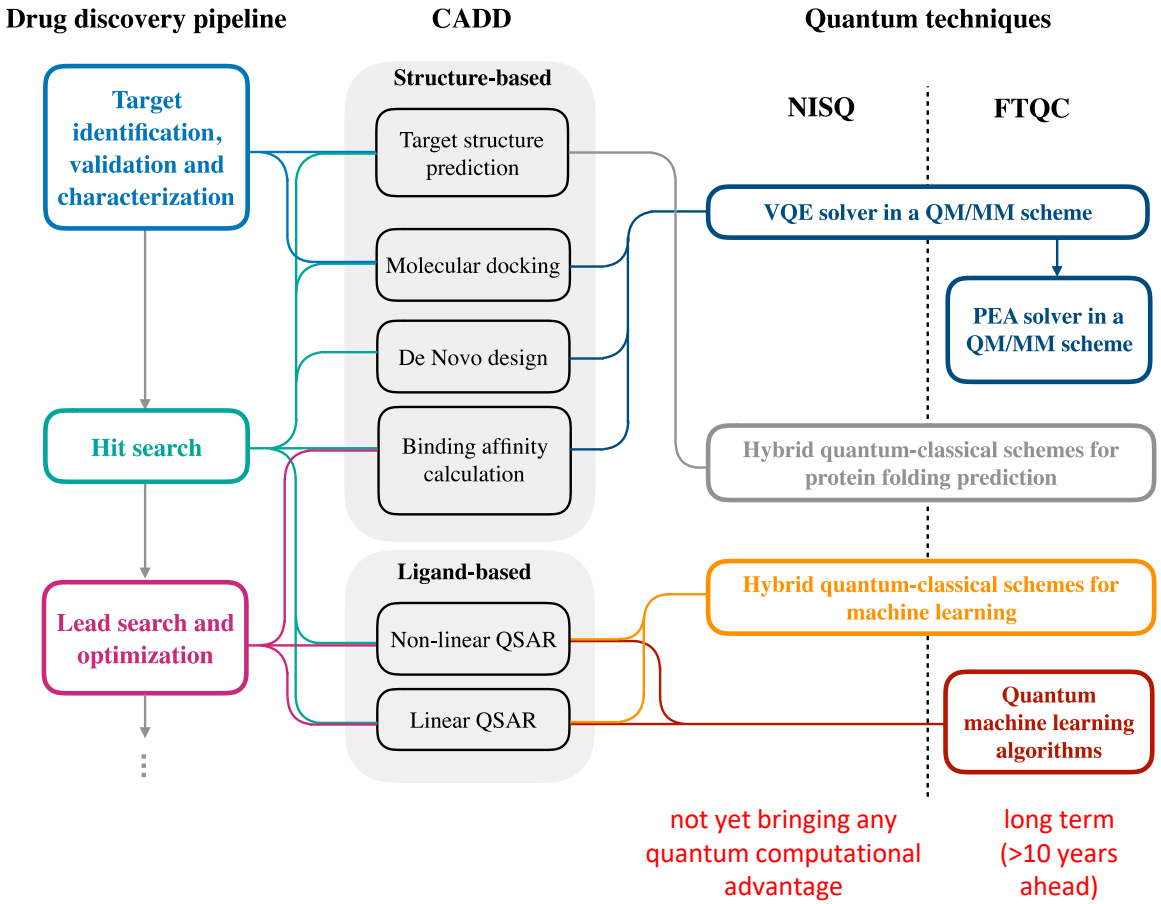
Coupled-Cluster (CC)
Cluster wavefunction methods that expand around a single mean-field reference.



Cytochrome iron cluster

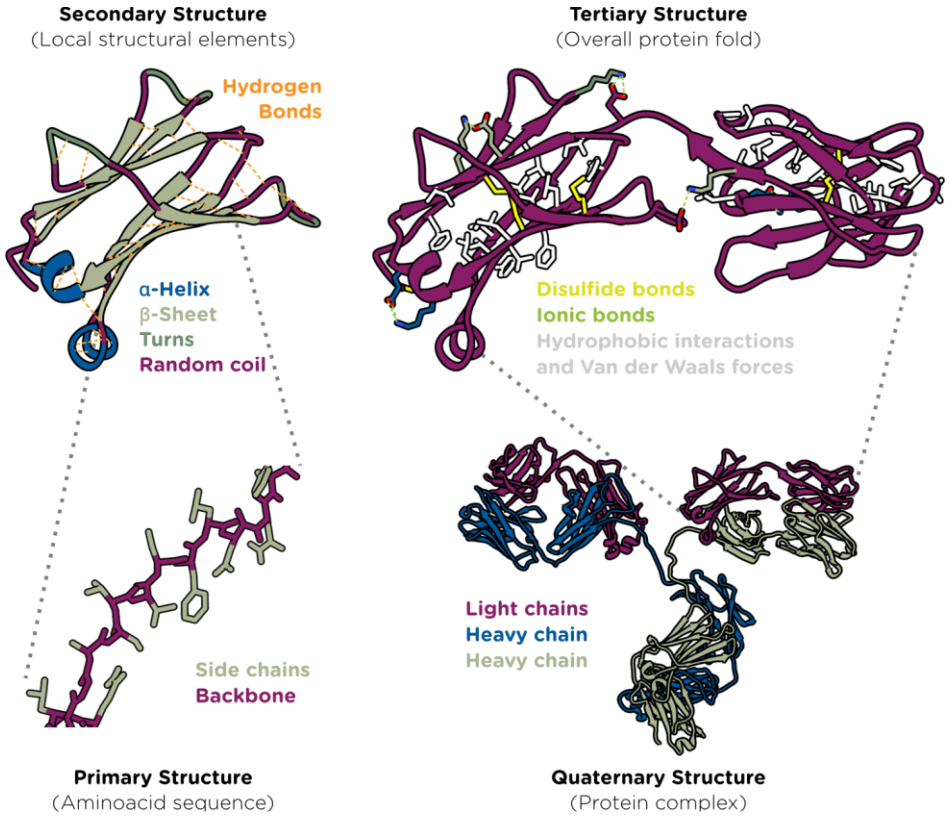
Full Configuration Interaction (FCI)
Method that delivers the exact energy of the electronic structure problem within a finite basis set.

Source: Drug design on quantum computers by Raffaele Santagati, Alan Aspuru-Guzik, Nathan Wiebe et al, January 2023 (9 pages)



Source: Potential of quantum computing for drug discovery by Alán Aspuru-Guzik et al, 2018 (18 pages).

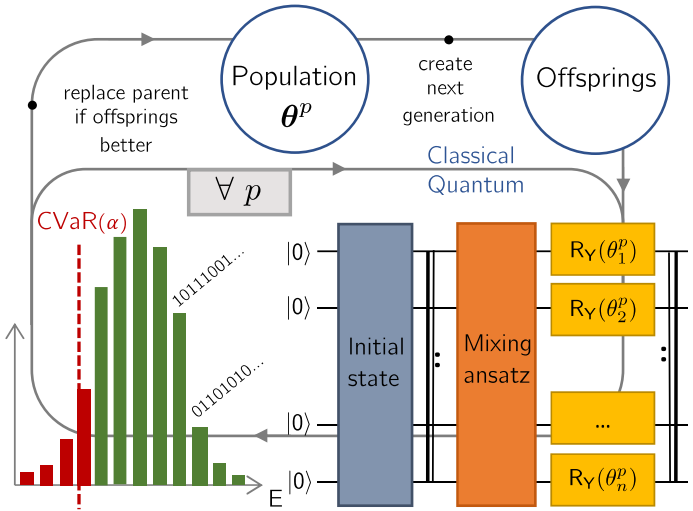
protein folding requirements



Source: FAQS Higher Order Structure and HOS Comparisons Explained.

quantum-based protein folding simulation

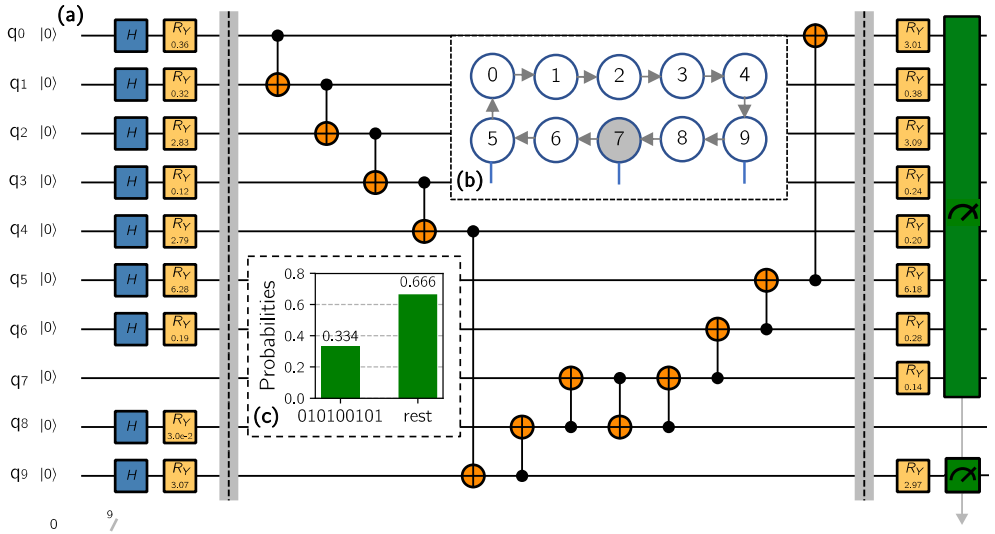
quantum variational algorithm
+ genetic algorithm optimize



$\Rightarrow O(N^4)$

N=number of amino acids

10 amino acid Angiotensin on 22 qubits

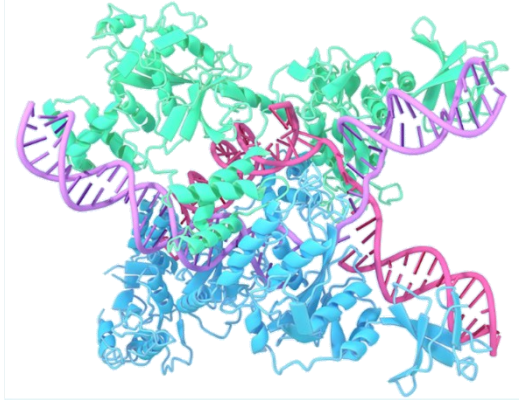


current AlphaFold record is with 450 amino acids.

source: Resource-efficient quantum algorithm for protein folding, Anton Robert et al, 2020.

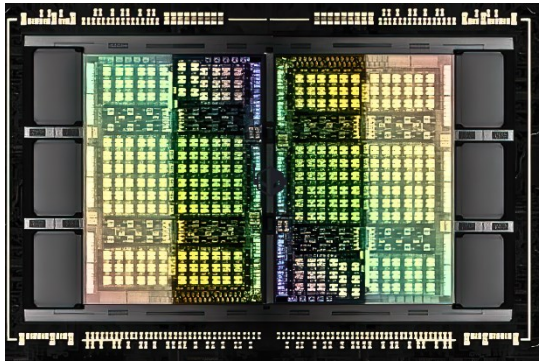
challenges

Google DeepMind



AlphaFold 3 can now generate predictions for nearly all molecules in the Protein Data Bank (PDB), frequently reaching atomic accuracy

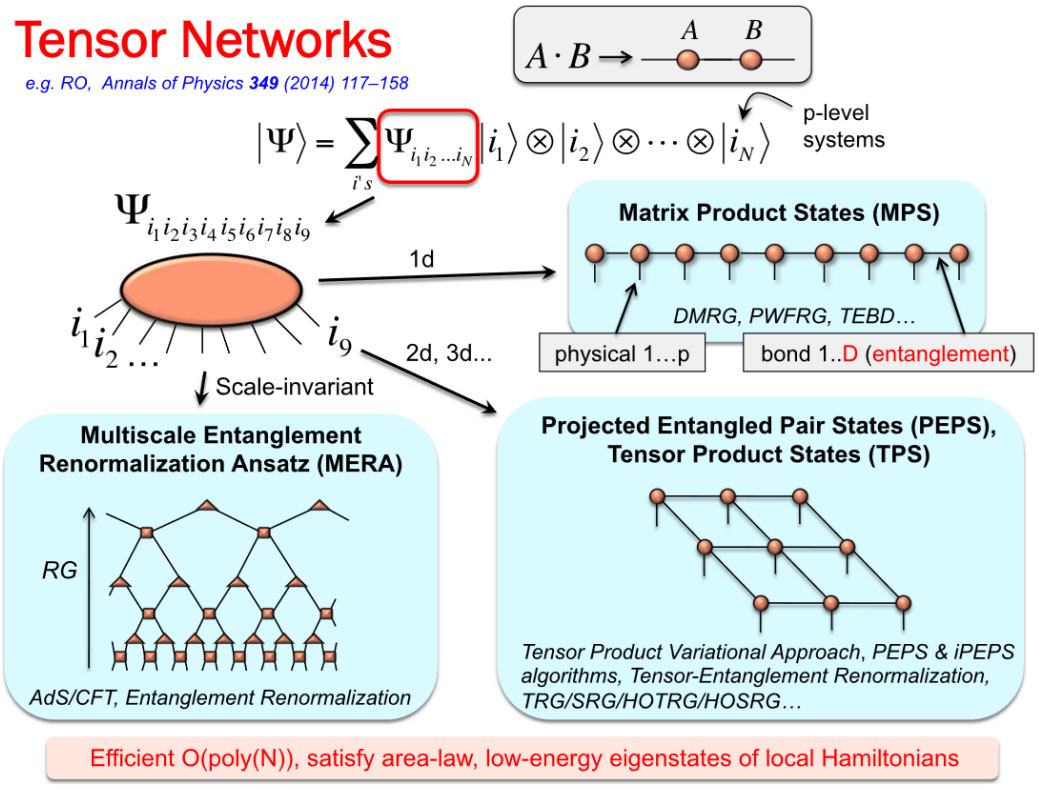
NVIDIA®

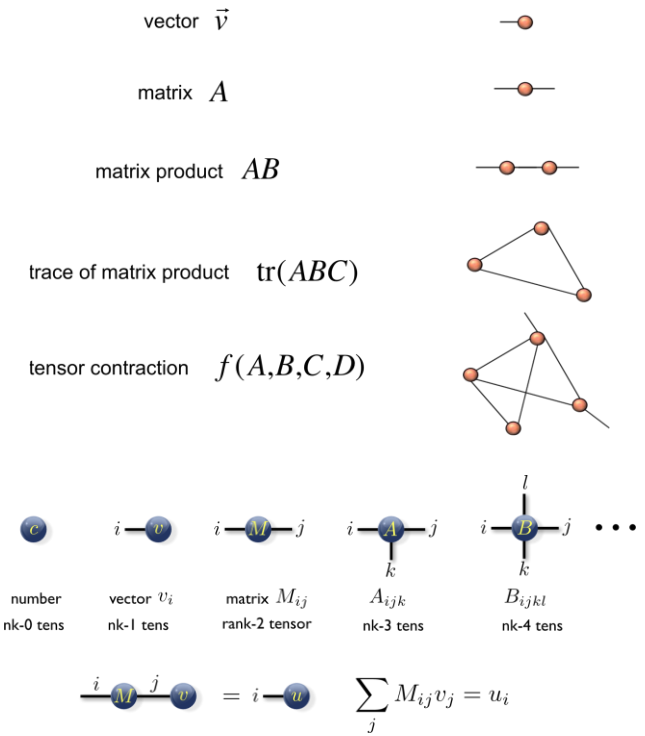


Blackwell GPU with 200 billion transistors and DGX B200 with 8 B200, 144 petaFLOPS inference workloads.

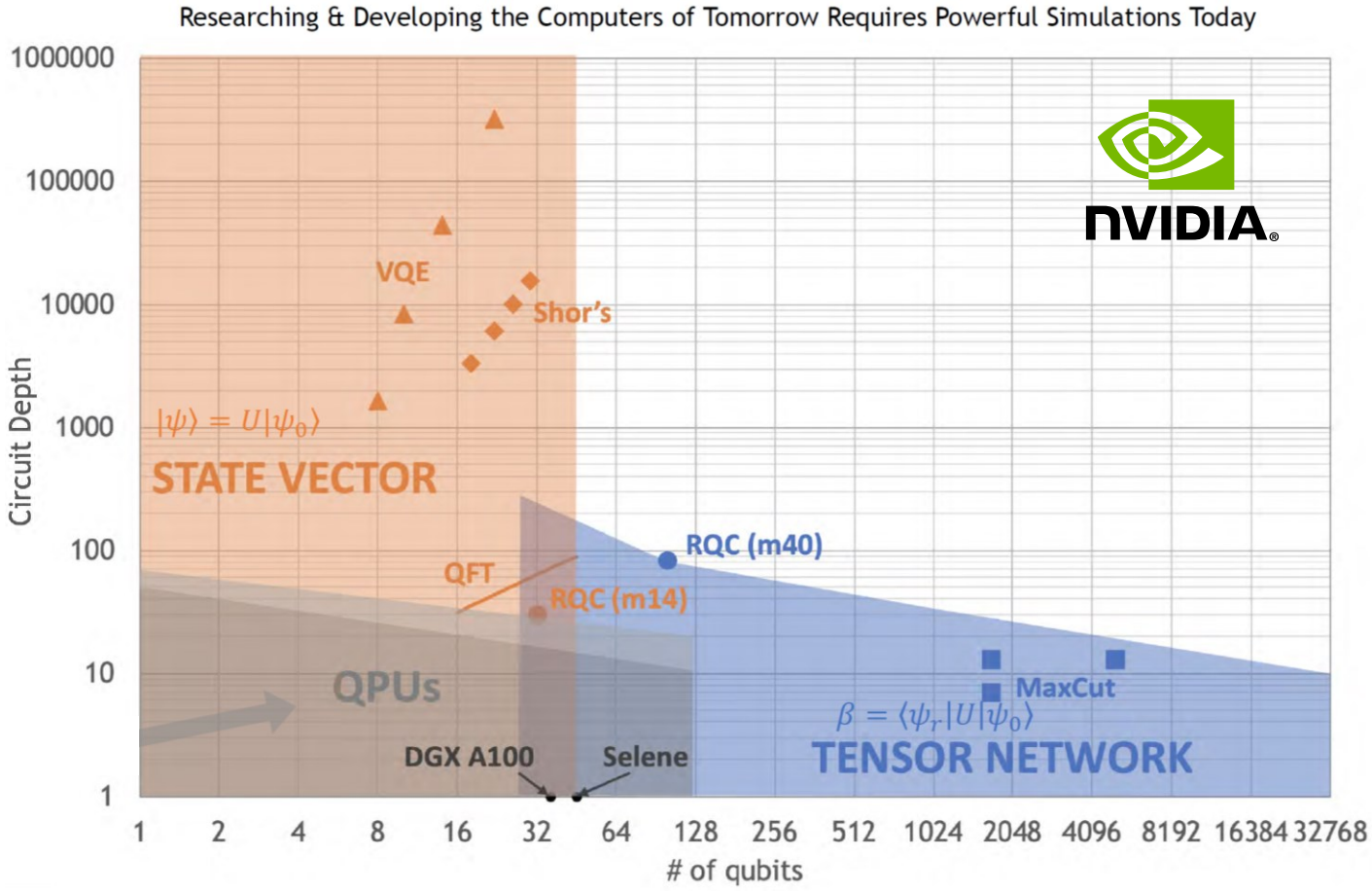
Source: A glimpse of the next generation of AlphaFold, Google DeepMind AlphaFold team and Isomorphic Labs team, October 2023.

tensor network techniques





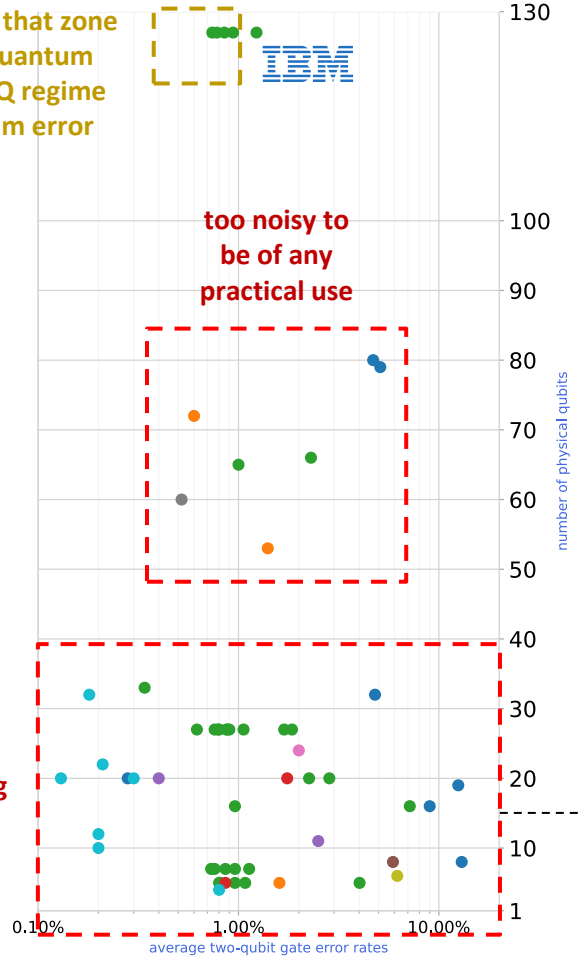
sources: Introduction to Tensor Network States and Methods by Román Orús, DIPC & Multiverse Computing, 2020 (229 slides) and Lecture 1: tensor network states by Philippe Corboz, Institute for Theoretical Physics, University of Amsterdam (56 slides).

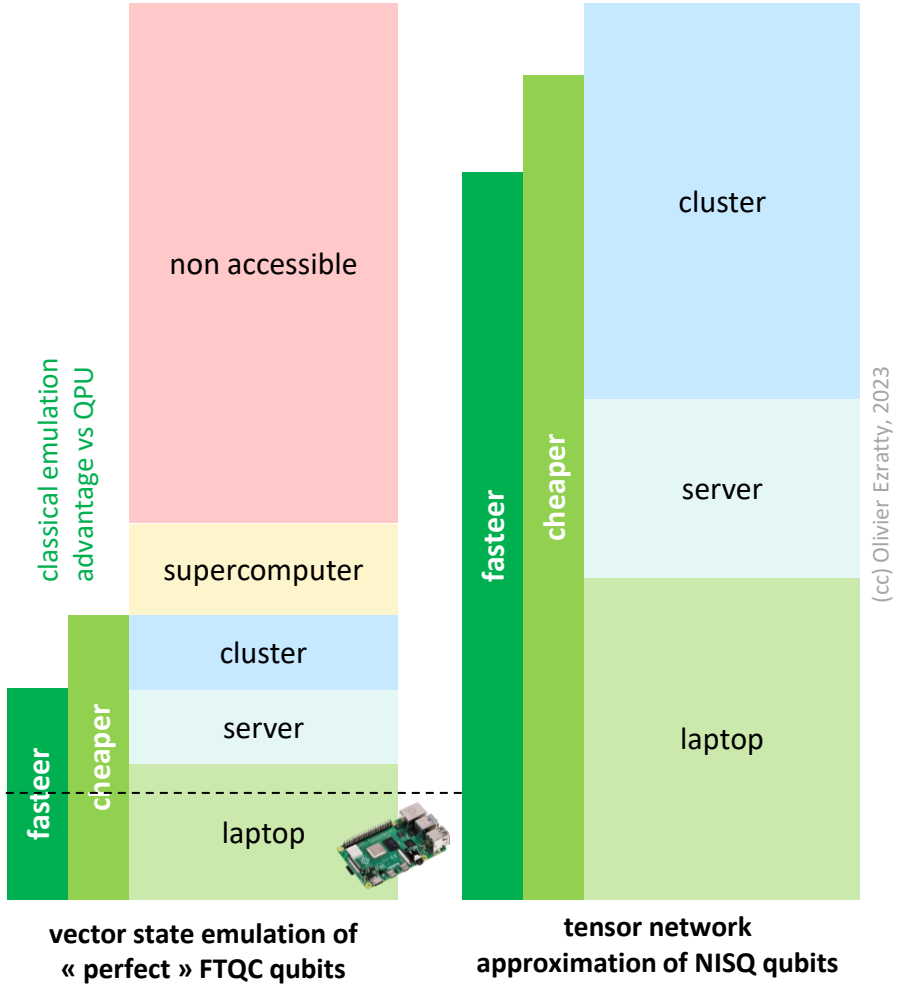

Researching & Developing the Computers of Tomorrow Requires Powerful Simulations Today
1000000
100000
10000
1000
100
10
1
Circuit Depth
VQE
Shor's
$|\psi\rangle = U|\psi_0\rangle$
STATE VECTOR
QFT
RQC (m40)
RQC (m14)
QPUs
MaxCut
$\beta = \langle\psi_r|U|\psi_0\rangle$
TENSOR NETWORK
DGX A100
Selene
1 2 4 8 16 32 64 128 256 512 1024 2048 4096 8192 16384 32768
# of qubits

a QPU case study in that zone may bring some quantum advantage in a NISQ regime with using quantum error mitigation

too noisy to be of any practical use

any QPU case study in that zone cannot bring any business value

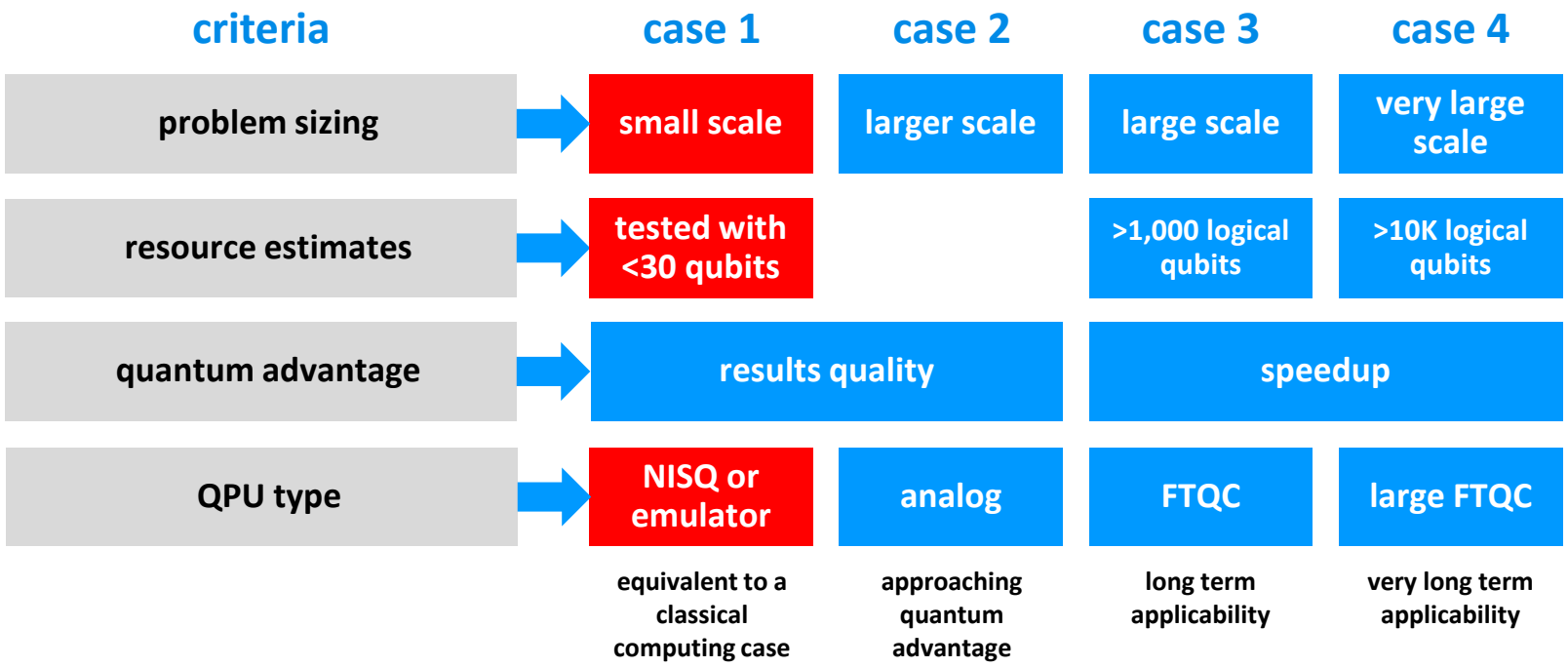




vector state emulation of « perfect » FTQC qubits

tensor network approximation of NISQ qubits

assessing QC case studies



understanding « case studies »

Quantum algorithm for bioinformatics to compute the similarity between proteins

February 2024

Anthony Chagneau[1], Yousra Massaoudi[2], Imene Derbali[2], and Linda Yahiaoui[2]

[1]Expleo Group, Agence Méditerranée, 2 Impasse de Chasles, Z.A Cap Horizon, Vitrolles, 13127, France
[2]Expleo Group, 21 Rue André Lwoff, Saint-Priest, 69800, France

- **QAOA algorithm on a 5 noisy IBM QPU qubits.**
- **50 amino acid string generation.**
- *"Quantum Needleman-Wunsch does **not** give good results for a random protein provided with the quantum generator contrary to Quantum Smith-Waterman algorithm. Moreover, the structure of the scoring matrix constructed with the Needleman-Wunsch algorithm is less adapted for QAOA. **QAOA has difficulty finding the fundamental state of the quantum system** due the spectrum of the scoring matrix is globally symmetrical, resulting in a **very slow resolution time**, which is not the case for the Smith-Waterman or the Conflict graph algorithms".*

Quantum Support Vector Machine for Prostate Cancer Detection: A Performance Analysis

W. El Maouaki*[1], T. SAID[1], and M. BENNAI[1,2]

[1]Quantum Physics and Magnetism Team, LPMC, Faculty of Sciences Ben M'Sik, Hassan II University of Casablanca, Morocco
[2]Lab of High Energy Physics, Modeling and Simulations, Faculty of Sciences, University Mohammed V-Agdal, Rabat, Morocco

March 2024

- **tested on 8 qubits on a Qiskit emulator.**
- **no "quantum" advantage.**

other cases studies

Brain Tumor Diagnosis Using Quantum Convolutional Neural Networks

Muhammad Al-Zafar Khan[¶‖], Nouhaila Innan[‡*], Abdullah Al Omar Galib[§†], Mohamed Bennai[‡**]
[¶]Quantum United Arab Emirates (QUAE), UAE
[‡]Quantum Physics and Magnetism Team, LPMC, Faculty of Sciences Ben M'sick,
Hassan II University of Casablanca, Morocco
[§]Independent Researcher
[‖]m.khan@quae.ae,[*]nouhaila.innan-etu@etu.univh2c.ma,[†]abdullahalomargalib@gmail.com,[**]mohamed.bennai@univh2c.ma

January 2024

- **good results.**
- **tested on a 5-qubit emulator.**
- **no "quantum" speedup advantage.**
- **this is classical computing.**

Peptide Binding Classification on Quantum Computers

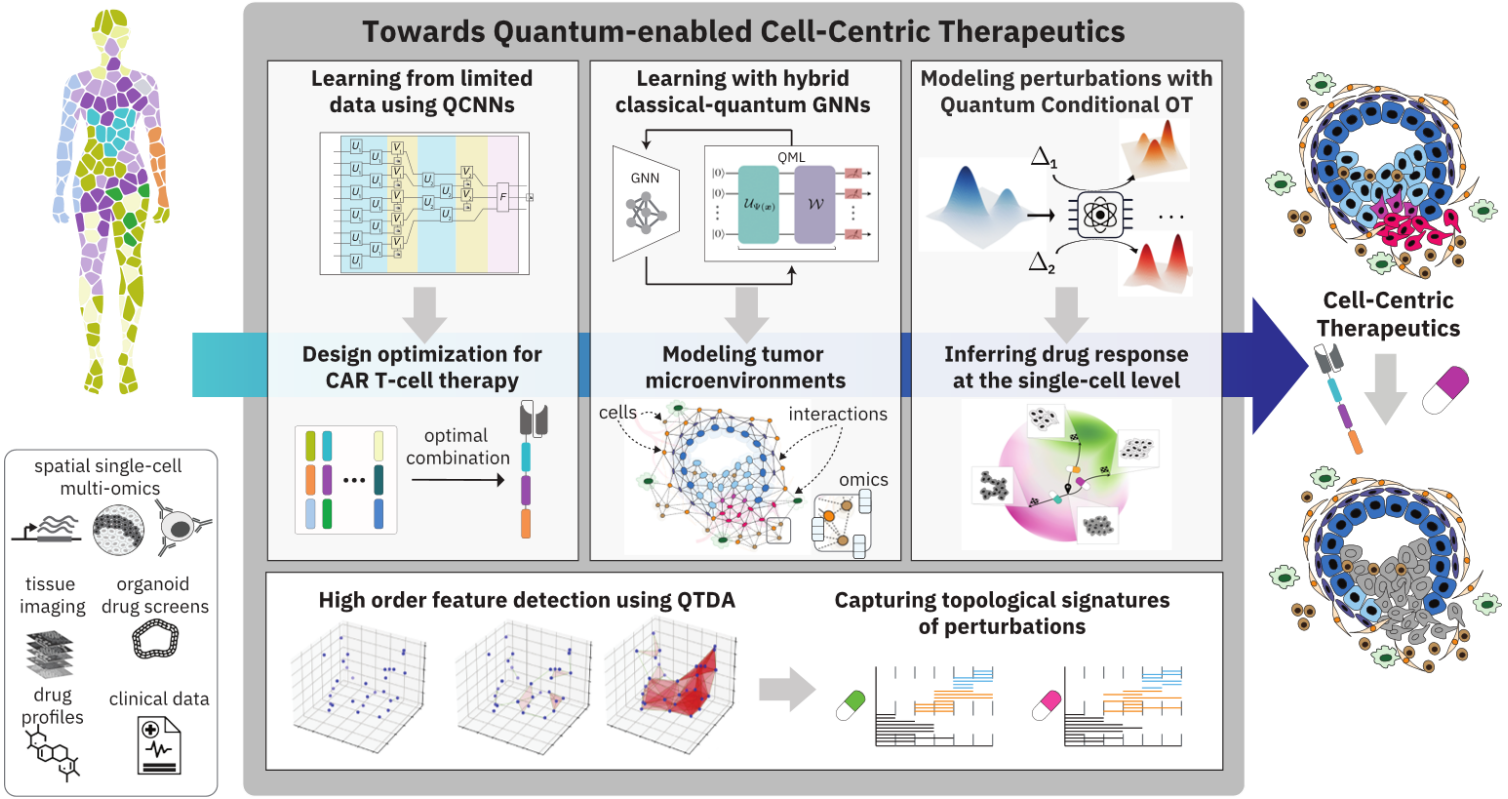
Charles London[1†] Douglas Brown[1†] Wenduan Xu[1] Sezen Vatansever[2]
Christopher James Langmead[2] Dimitri Kartsaklis[1] Stephen Clark[1]
Konstantinos Meichanetzidis[1]
{charles.london; douglas.brown; wenduan.xu; dimitri.kartsaklis; steve.clark; k.mei}@quantinuum.com
{svatanse; clangmea}@amgen.com

[1]Quantinuum, 17 Beaumont St., Oxford, OX1 2NA, UK
[2]Amgen, 1 Amgen Center Dr., Thousand Oaks, 91320, CA, USA

November 2023

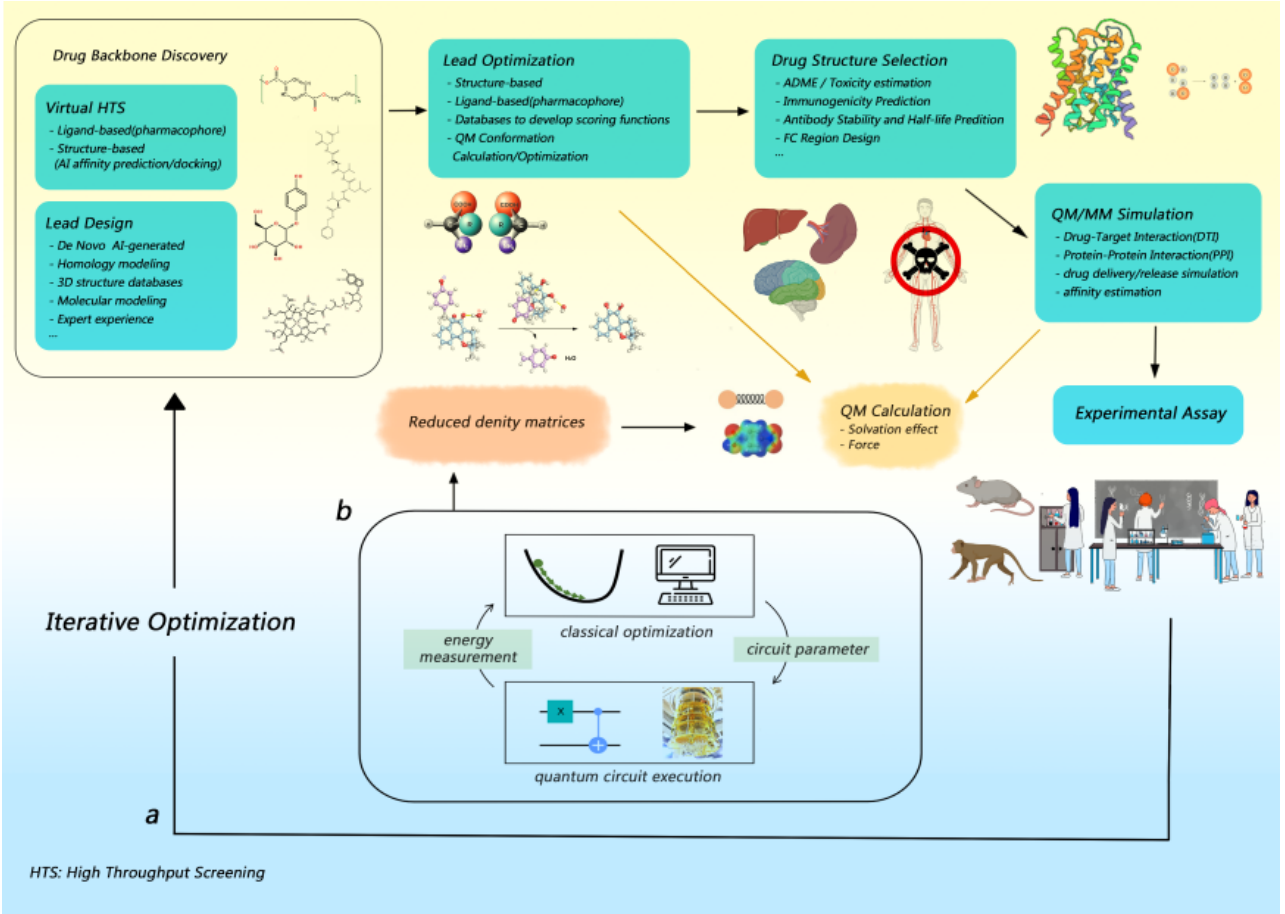
- **good results.**
- **tested on a 8-qubit Quantinuum QPU.**
- **no "quantum" speedup advantage.**

quantum-based multi-omics



source: Towards quantum-enabled cell-centric therapeutics by Saugata Basu et al, IBM Research, July 2023.

drug discovery pipeline



source: Generalizable Quantum Computing Pipeline for Real World Drug Discovery by Weitang Li et al, arXiv, January 2024.

TABLE II. Comparison of computational wall times for classical computing (CASCI) and quantum computing (VQE) on solving the active space of molecule **4**, **5**, **6**, and **TS**.

	Computational Wall Time (s)	
Molecule	CASCI	VQE
4	358	424
5	3	63
6	97	161
TS	360	424

classical method

current VQE NISQ based method

source: Generalizable Quantum Computing Pipeline for Real World Drug Discovery by Weitang Li et al, arXiv, January 2024.

river lane

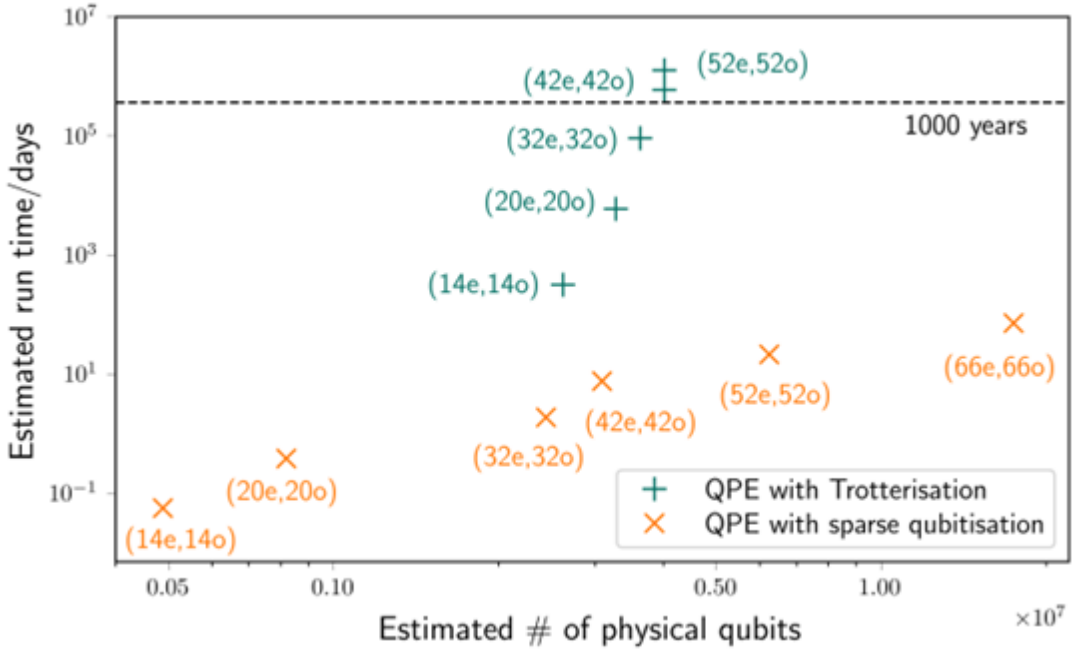


Figure 7: Comparison of resources (runtime and total number of physical qubits) using two QPE algorithms. The first (orange) used qubitisation, and the Hamiltonian was truncated to remove small terms up to an error budget. The second (green) used textbook QPE with Trotterisation and no truncation of the Hamiltonian. The latter algorithm has a much steeper scaling in runtime. Even for a (14e,14o) active space the runtime is multiple orders of magnitude more expensive.

source: A perspective on the current state-of-the-art of quantum computing for drug discovery applications by Nick S. Blunt et al, June 2022-March 2023.


IBM
IBM Quantum
System One
Cleveland Clinic

D-Wave use cases in healthcare

cancers classification

multi-omics: genomics + symptoms in QML

source: D-Wave

de-novo proteins and polypeptides creation

with hybrid computing, tests in research against the covid-19 virus.

source: D-Wave

liver donor optimization

NP-complet complete problem using QUBO

source: Accenture, D-Wave

drug retargeting

with Biogen, 1QBit and Accenture research

source: D-Wave

radiotherapy optimization

to minimized x-ray dose

source: Roswell Park, D-Wave

Pasqal use cases in healthcare

quantum algorithms able to sample equilibrium water solvent molecules configurations within proteins thanks to analog quantum computing

Leveraging Analog Quantum Computing with Neutral Atoms for Solvent Configuration Prediction in Drug Discovery

Mauro D'Arcangelo[1, +], Daniele Loco[2, +], Fresnel team[1], Nicolaï Gouraud[2,3,4], Stanislas Angebault[2], Jules Sueiro[2], Pierre Monmarché[3], Jérôme Forêt[2], Louis-Paul Henry[1], Loïc Henriet[1,*], and Jean-Philip Piquemal[2,4,*]

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[2]Qubit Pharmaceuticals, Advanced Research Department, 24 rue du Faubourg Saint-Jacques, 75014 Paris, France
[3]Sorbonne Université, Laboratoire Jacques-Louis Lions, UMR 7589 CNRS, 75005, Paris, France
[4]Sorbonne Université, Laboratoire de Chimie Théorique, UMR 7616 CNRS, 75005, Paris, France
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[+]these authors contributed equally to this work

PASQAL

Qubit PHARMACEUTICALS

Quantum Feature Maps for Graph Machine Learning on a Neutral Atom Quantum Processor

Boris Albrecht,[1,*] Constantin Dalyac,[1,2,*] Lucas Leclerc,[1,3,*] Luis Ortiz-Gutiérrez,[1,*] Slimane Thabet,[1,2,*] Mauro D'Arcangelo,[1] Vincent E. Elfving,[1] Lucas Lassablière,[1] Henrique Silvério,[1] Bruno Ximenez,[1] Louis-Paul Henry,[1] Adrien Signoles,[1] and Loïc Henriet[1,†]

[1]*PASQAL, 7 rue Léonard de Vinci, 91300 Massy, France*
[2]*LIP6, CNRS, Sorbonne Université, 4 Place Jussieu, 75005 Paris, France*
[3]*Université Paris-Saclay, Institut d'Optique Graduate School, CNRS, Laboratoire Charles Fabry, 91127 Palaiseau, France*
(Dated: November 30, 2022)

toxicity screening experiment, consisting of a binary classification protocol on a biochemistry dataset comprising 286 molecules of sizes ranging from 2 to 32 nodes, and obtain results which are comparable to those using the best classical kernels

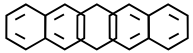
A blueprint for a Digital-Analog Variational Quantum Eigensolver using Rydberg atom arrays

Antoine Michel,[1,2,*] Sebastian Grijalva,[3] Loïc Henriet,[3] Christophe Domain,[1] and Antoine Browaeys[2]

[1]*Electricité de France, EDF Recherche et Développement, Département Matériaux et Mécanique des Composants, Les Renardières, F-77250 Moret sur Loing, France*
[2]*Université Paris-Saclay, Institut d'Optique Graduate School, CNRS, Laboratoire Charles Fabry, F-91127 Palaiseau Cedex, France*
[3]*PASQAL, 7 rue Léonard de Vinci, F-91300 Massy, France*
(Dated: April 25, 2023)

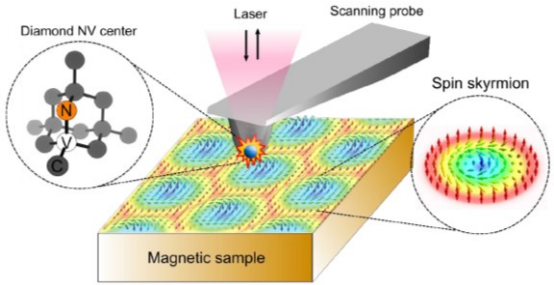
estimating the ground-state energy of Hamiltonians coming from chemistry. Study numerically the behavior of a digital-analog variational quantum eigensolver for the H2, LiH and BeH2 molecules.

chemistry and healthcare QC startups



quantum sensors in healthcare

Qnami

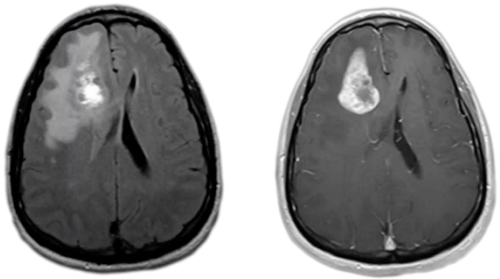


magnétomètres ultrasensibles

$210\ \mathrm{fT}/\sqrt{\mathrm{Hz}}$

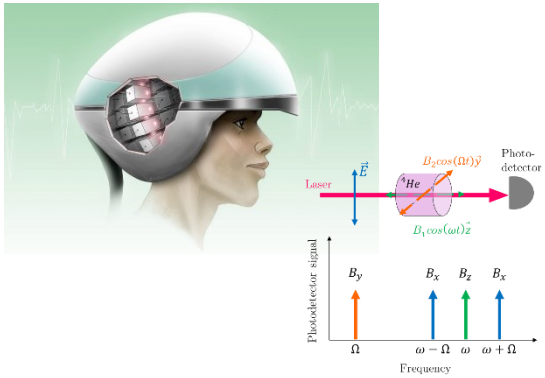
medical imaging
biological analysis

chipiron



SQUID based
ultra-low field MRI

MAG 4He alth

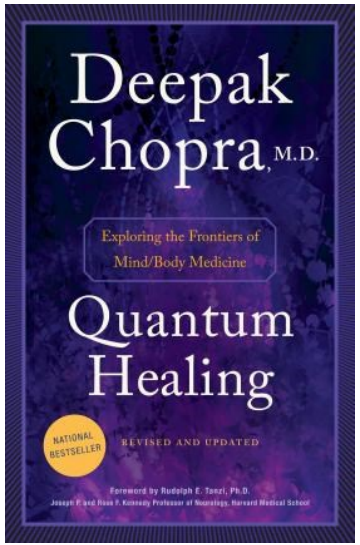


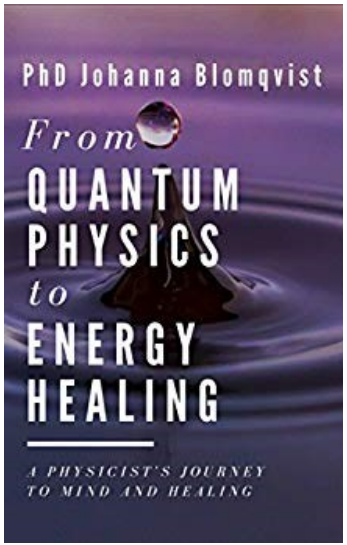
helium 4 nucleus spin
MEG brain imaging

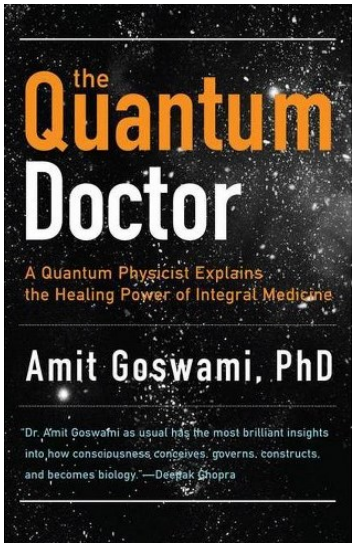
key takeaways

1. quantum computing can bring significant advantage like with **quantum simulations** for drug discovery but only in a FTQC regime.
2. it will require a **large number of logical and physical qubits** and require some patience.
3. quantum algorithms can be tested at **small scales** with existing QPUs or emulators.
4. there are some interesting **analog quantum computing** use cases, particularly for optimizations.
5. **quantum sensors** already work.

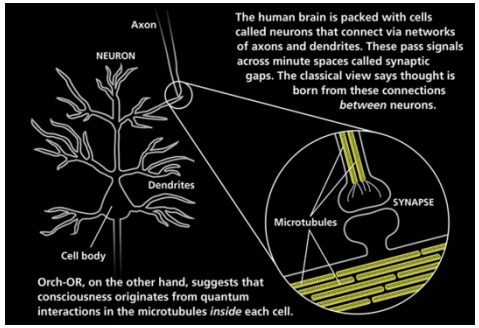
exponential b . . . . . t



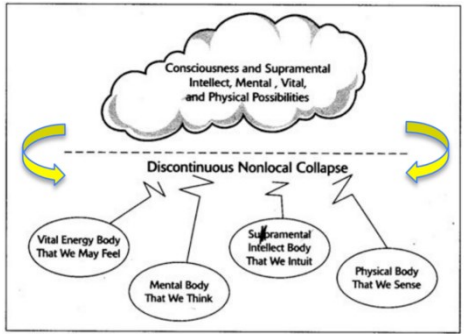




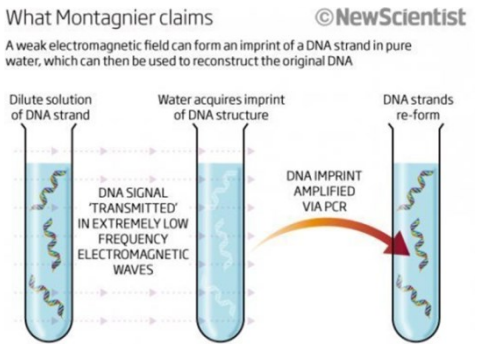
fake quantum medicines



Roger Penrose's Orch-OR theory

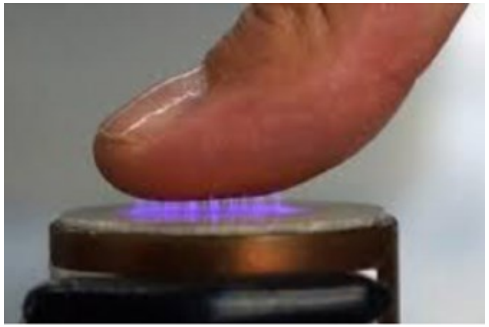


Quantum consciousness



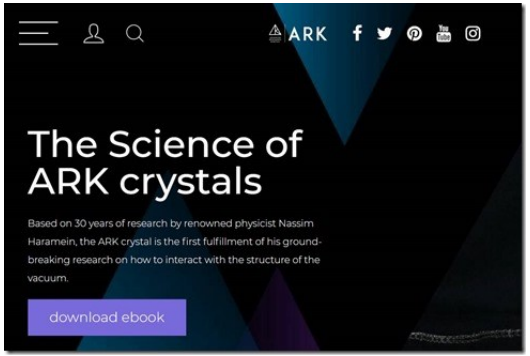
Water memory

Structured water



Biophotons detectors

Scalar waves generators



Magic quantum crystals

Quantum Shield medallions

5G BioShield
"quantum holographic catalyst"

Roll over image to zoom in

i9Bottle Chakra - Healing Crystals, Reusable Glass Water Bottle, Yoga Bottle, Relieve Stress, Super Hydration, Increases Physical Fitness, Body Detox, Chakra Balancing, Sustainable Gifts, Zero Waste, Meditation

Brand: i9

4.5 out of 5 stars 102 ratings

Amazon's Choice for "i9 bottle"

$59.90

No Import Fees Deposit & $13.89 Shipping to France Details

Material	Glass, Silicone
Brand	I9
Capacity	1.4 Pounds
Age Range (Description)	Women aged 30 to 70 years
Special Feature	The bottle improves water quality

$59.90

No Import Fees Deposit & $13.89 Shipping to France Details

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