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FMF
Fakulteta za matematiko
in fiziko

Jožef Stefan Institute, Ljubljana, Slovenia

how quantum technologies and other sciences help each other

olivier ezratty

⟨ author | … ⟩

Ljubljana, April 16th, 2024

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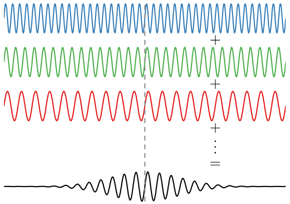
the second quantum revolution

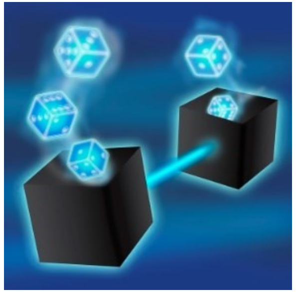
superposition

linked to wave-particle duality and linearity of Schrödinger’s equation



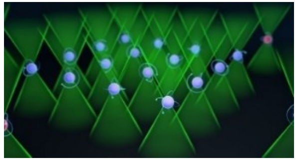
entanglement

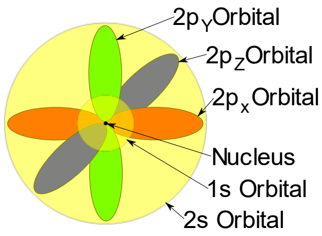
state correlation of distant quantum objects, but random and after measurement

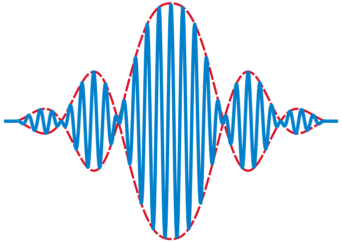


individual control of quantum objects

electrons, photons, atoms







quantum computing

quantum telecommunications

quantum cryptography

quantum sensing

quantum technologies sciences

physics

electromagnetism

quantum physics

quantum matter

thermodynamics

fluids mechanics

photonics

engineering

materials design

electronics engineering

cryogenics

mathematics

linear algebra

groups theory

analysis

complexity theories

computer science

information theory

algorithms design

programming

classical computing

telecommunications

machine learning

human sciences

philosophy

epistemology

sociology

technology ethics

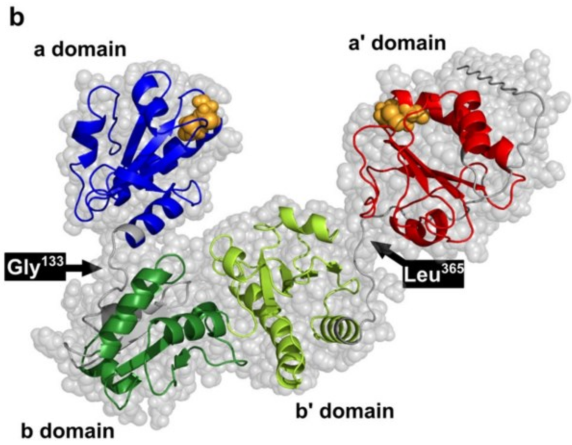
economics of innovation

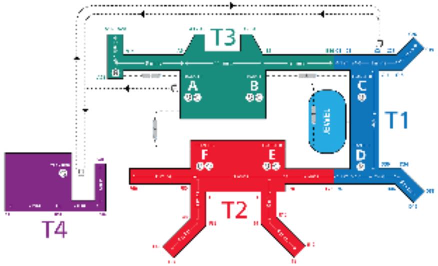
R&D policy making

geopolitics

startups ecosystem

typical difficult problems



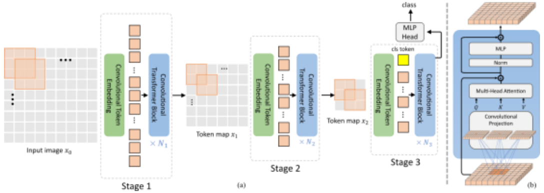


combinatorial optimizations

$$\begin{aligned}
\frac{\partial^2 u_1}{\partial x_1^2}+\frac{\partial^2 u_2}{\partial x_2 \partial x_1}+\frac{\partial^2 u_3}{\partial x_3 \partial x_1}+\frac{\partial^2 u_1}{\partial x_1^2}+\frac{\partial^2 u_1}{\partial x_2^2}+\frac{\partial^2 u_1}{\partial x_3^2}+f_1&=0\\
\frac{\partial^2 u_1}{\partial x_1 \partial x_2}+\frac{\partial^2 u_2}{\partial x_2^2}+\frac{\partial^2 u_3}{\partial x_3 \partial x_2}+\frac{\partial^2 u_2}{\partial x_1^2}+\frac{\partial^2 u_2}{\partial x_2^2}+\frac{\partial^2 u_2}{\partial x_3^2}+f_2&=0\\
\frac{\partial^2 u_1}{\partial x_1 \partial x_3}+\frac{\partial^2 u_2}{\partial x_2 \partial x_3}+\frac{\partial^2 u_3}{\partial x_3^2}+\frac{\partial^2 u_3}{\partial x_1^2}+\frac{\partial^2 u_3}{\partial x_2^2}+\frac{\partial^2 u_3}{\partial x_3^2}+f_3&=0
\end{aligned}$$

solving partial derivative equations

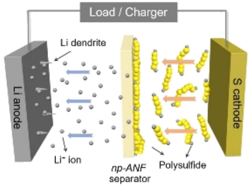
$$i\hbar\frac{\partial \Psi(x,t)}{\partial t}=-\frac{\hbar^2}{2m}\frac{\partial^2 \Psi(x,t)}{\partial x^2}+V(x)\Psi(x,t)$$



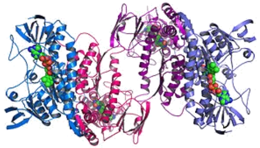
solving Schrodinger's wave equation
to simulate quantum matter

machine learning
and deep learning

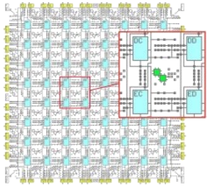
quantum computing science applications



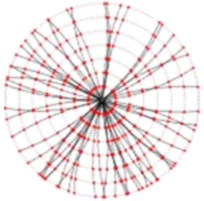
batteries



drugs

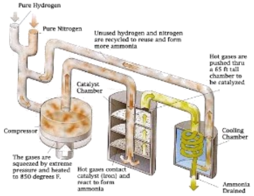


semiconductors

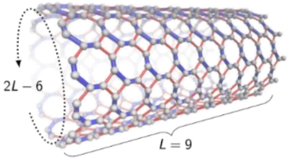


high-energy particle physics

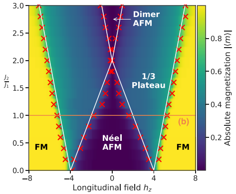
nuclear fusion



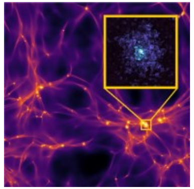
fertilizers production



materials design

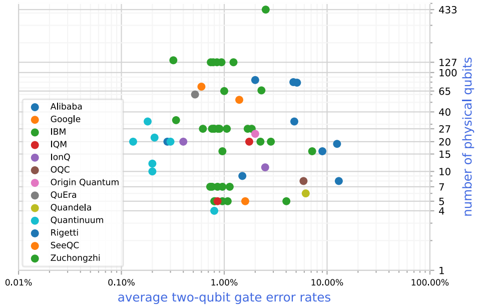


condensed matter physics

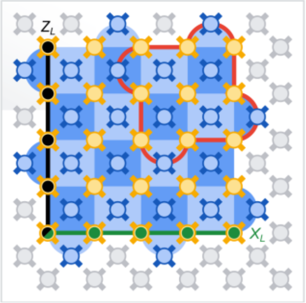


astrophysics

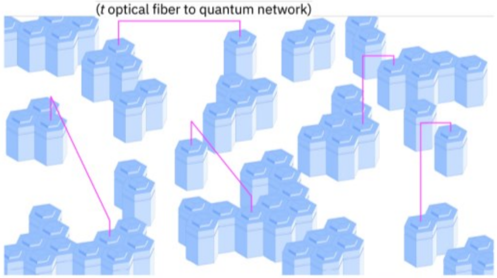
key QPU challenges



qubits fidelities

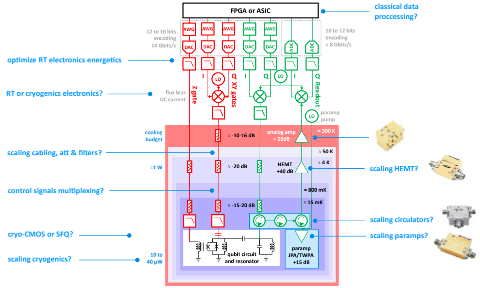


errors mitigation and correction

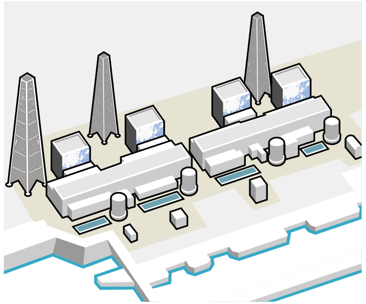


(e) t type modularity involves microwave-to-optical transduction to link QPUs in different dilution refrigerators.

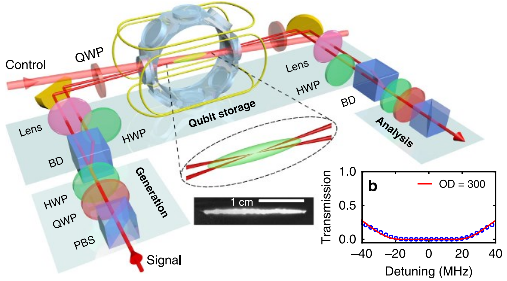
quantum interconnect



enabling technologies scalability

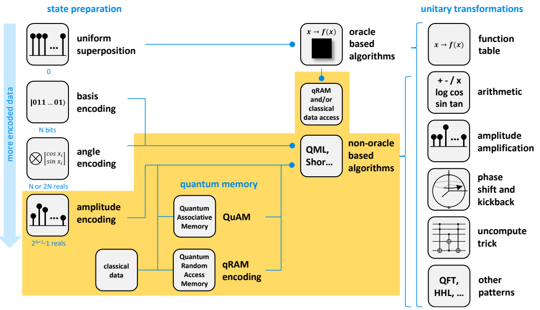


energy consumption

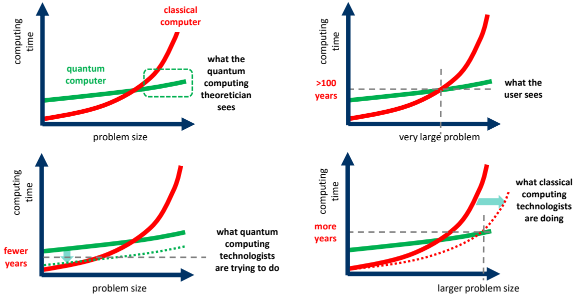


quantum memory

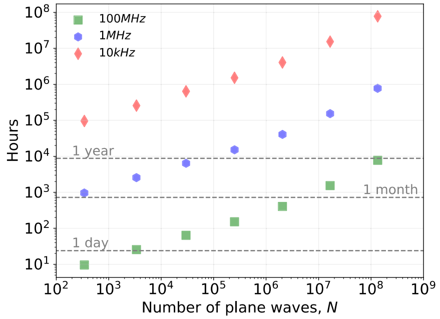
some software challenges



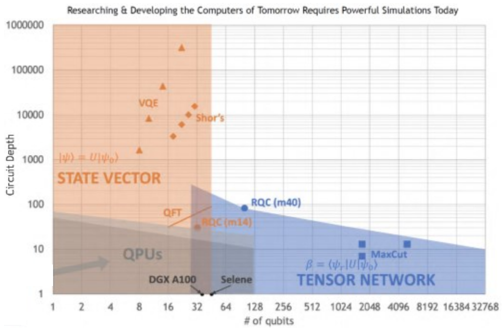
data loading



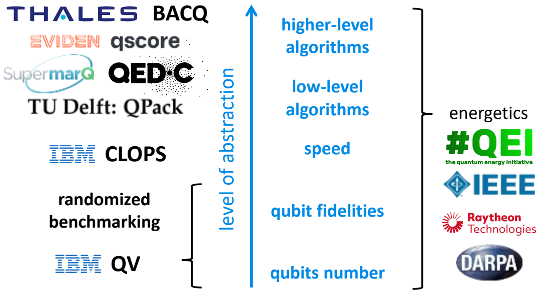
actual speedups



actual computing time



tensor networks competition



THALES BACQ

EVIDEN qscore

SupermarQ QED-C

TU Delft: QPack

IBM CLOPS

randomized benchmarking

IBM QV

level of abstraction

higher-level algorithms

low-level algorithms

speed

qubit fidelities

qubits number

energetics

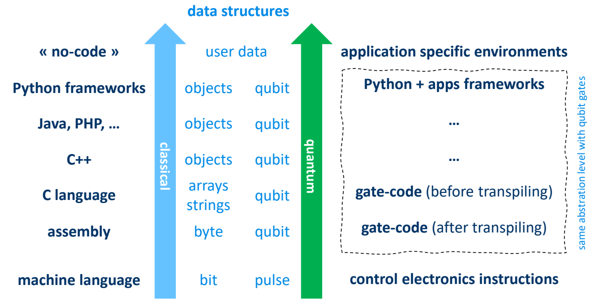
#QEI the quantum energy initiative

IEEE

Raytheon Technologies

DARPA

benchmarking



classical	data structures	quantum	
« no-code »	user data		application specific environments
Python frameworks	objects	qubit	Python + apps frameworks
Java, PHP, …	objects	qubit	…
C++	objects	qubit	…
C language	arrays strings	qubit	gate-code (before transpiling)
assembly	byte	qubit	gate-code (after transpiling)
machine language	bit	pulse	control electronics instructions

same abstraction level with qubit gates

coding abstraction level

what is being practically done

classical computers

quantum inspired

- financial services solutions improvements.
- machine learning improvements.

ALPHARAIL
NatWest

quantum emulators

- code learning.
- code debugging.
- designing new algorithms.
- simulating qubit physics.
- simulating error correction codes.

Qubit PHARMACEUTICALS

analog quantum computers

quantum **annealing computers**

analog **quantum simulators**

- solving optimization problems at mid-sized scale, in transportation (Volkswagen, Denso), retail (Ocado, Pattison), job shop scheduling and financial services (Mastercard, CACIB).
- physics simulations (statistical physics, spin glass, ferromagnetism, topological matter, …).
- potential energetic advantage.

CaixaBank
CRÉDIT AGRICOLE CORPORATE & INVESTMENT BANK
Raiffeisen Bank International Member of RBI Group

digital quantum computers

gate-based

NISQ (Noisy Intermediate Scale Quantum)

- low-level physics simulations ("IBM quantum utility" with 127 qubits and kicked Ising model).
- creating and testing algorithms at small scale (QML, optimizations, chemical simulations).

eDF
AIRBUS
MBDA MISSILE SYSTEMS
TOTAL

FTQC (Fault-Tolerant Quantum Computing)

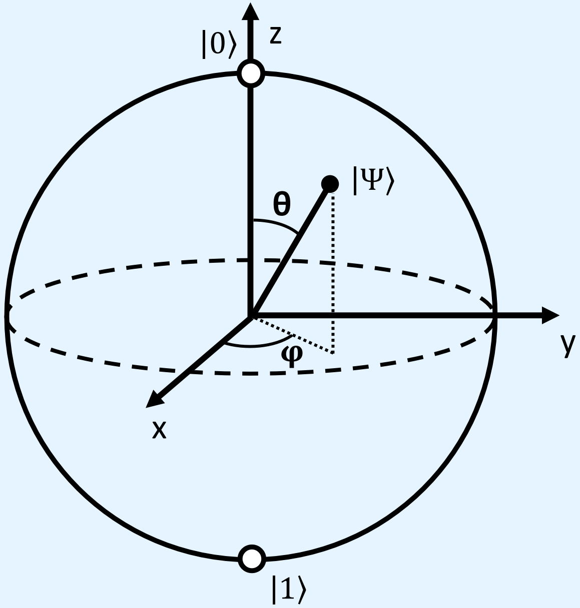
- large algorithms and resource estimations.
- creating and testing error correction codes (Google, Quantinuum, QuEra, PsiQuantum, …).

HYUNDAI
J.P.Morgan
Goldman Sachs

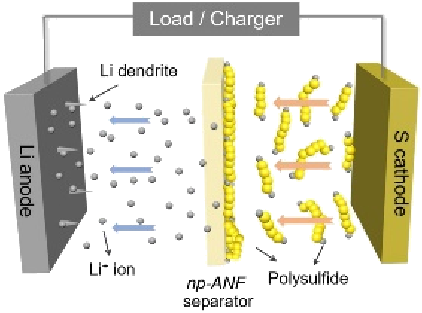
assessing QC case studies

criteria	case 1	case 2	case 3	case 4
problem sizing	small scale	larger scale	large scale	very large scale
resource estimates	tested with <30 qubits		>1,000 logical qubits	>10K logical qubits
quantum advantage	results quality energetic costs		speedup	
QPU type	NISQ or emulator	analog	FTQC	large FTQC
	equivalent to a classical computing case	approaching quantum advantage	long-term applicability	very long-term applicability

quantum technologies and the environment



simulate matter for…



quantum digital twins to create better batteries

MITSUBISHI CHEMICAL

battery simulation

lithium-oxygen

source: IBM

Mercedes-Benz

battery simulation

estimating the cost of electrolyte simulation on PsiQuantum's future QPU.

source: PsiQuantum, Mercedes-Benz

HYUNDAI

battery simulation

model lithium oxide to understand how batteries age over time

source: Hyundai, IonQ

DAIMLER

battery simulation

lithium-sulfur battery design

source: IBM

SAMSUNG

battery simulation

simulating magnetism and spins

source: Samsung, Honeywell

TotalEnergies

battery materials design

simulating Mott insulator transitions in battery electrode materials and ceramic superconductors and discharge curve of Li_xCoO_2.

source: Total, Pasqal

Li-Ion battery chemical simulation

needs…

6,652 logical qubits

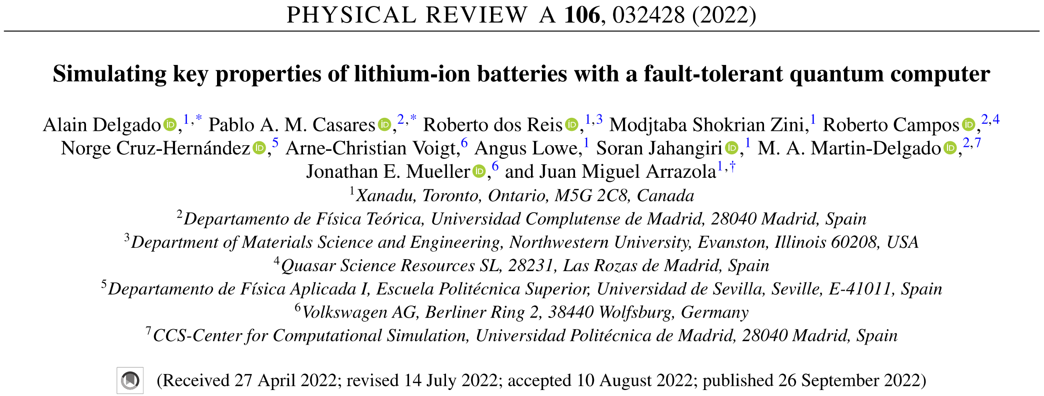
10^{-12} error rate

computing times in months/years

VOLKSWAGEN

XANADU

source: Simulating key properties of lithium-ion batteries with a fault-tolerant quantum computer by Alain Delgado et al, April-September 2022 (31 pages).



PHYSICAL REVIEW A **106**, 032428 (2022)

Simulating key properties of lithium-ion batteries with a fault-tolerant quantum computer

Alain Delgado,[1,*] Pablo A. M. Casares,[2,*] Roberto dos Reis,[1,3] Modjtaba Shokrian Zini,[1] Roberto Campos,[2,4]
Norge Cruz-Hernández,[5] Arne-Christian Voigt,[6] Angus Lowe,[1] Soran Jahangiri,[1] M. A. Martin-Delgado,[2,7]
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[3]*Department of Materials Science and Engineering, Northwestern University, Evanston, Illinois 60208, USA*
[4]*Quasar Science Resources SL, 28231, Las Rozas de Madrid, Spain*
[5]*Departamento de Física Aplicada I, Escuela Politécnica Superior, Universidad de Sevilla, Seville, E-41011, Spain*
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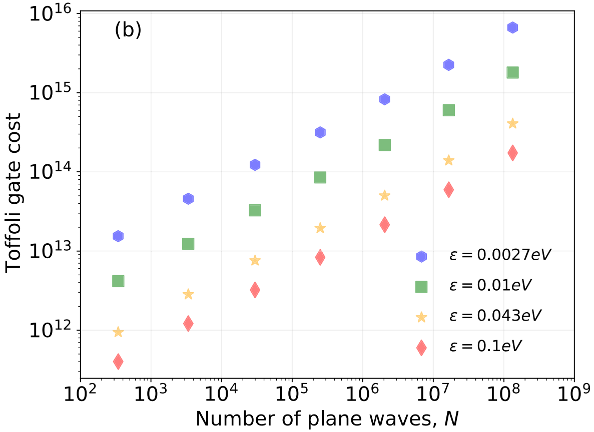
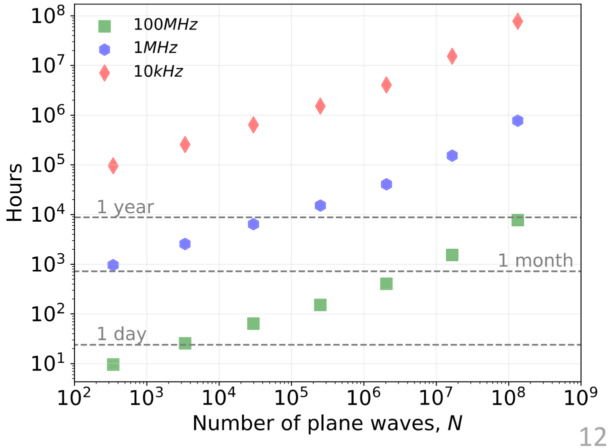
(Received 27 April 2022; revised 14 July 2022; accepted 10 August 2022; published 26 September 2022)





LNO battery simulation

Google

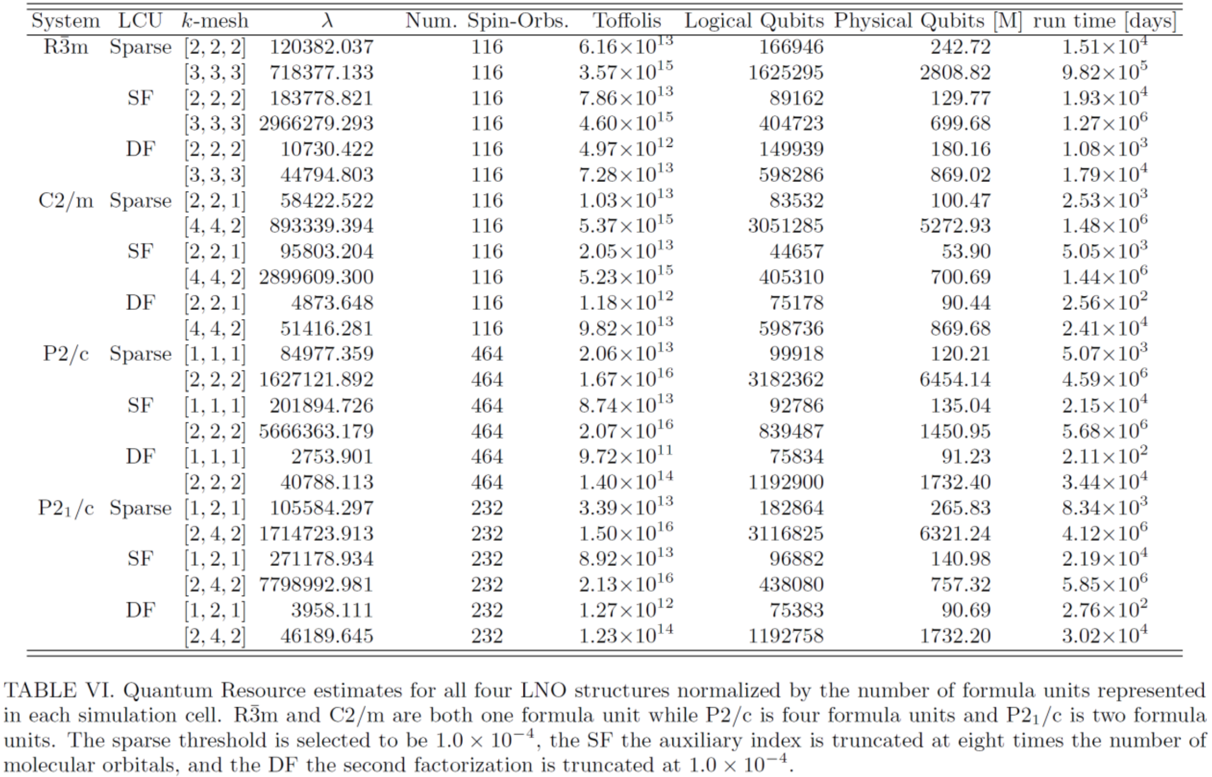
$LiNiO_2$ chemistry simulation

from 75K to 3M logical qubits and 91M to 6G physical qubits

requires physical qubits with 0.01% error rates

computing time from one year to 2,739 years

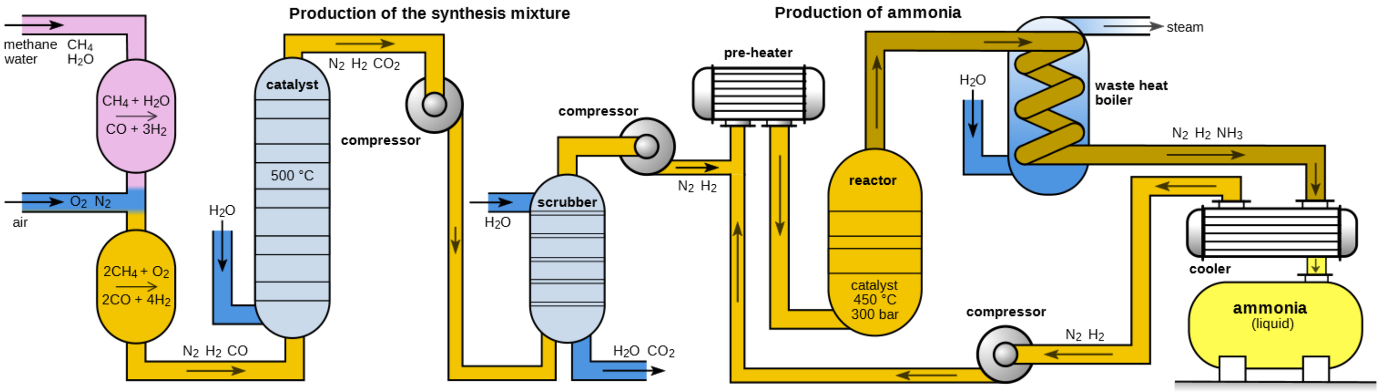
source: Fault-tolerant quantum simulation of materials using Bloch orbitals, Nicholas C. Rubin, Ryan Babbush et al, February 2023 (58 pages).

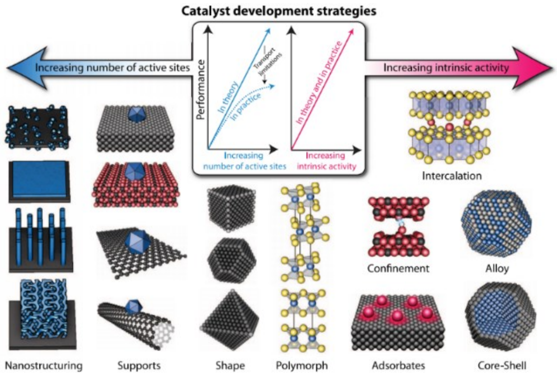


System	LCU	k-mesh	λ	Num. Spin-Orbs.	Toffolis	Logical Qubits	Physical Qubits [M]	run time [days]
$R\bar{3}m$	Sparse	[2, 2, 2]	120382.037	116	6.16×10^{13}	166946	242.72	1.51×10^{4}
		[3, 3, 3]	718377.133	116	3.57×10^{15}	1625295	2808.82	9.82×10^{5}
	SF	[2, 2, 2]	183778.821	116	7.86×10^{13}	89162	129.77	1.93×10^{4}
		[3, 3, 3]	2966279.293	116	4.60×10^{15}	404723	699.68	1.27×10^{6}
	DF	[2, 2, 2]	10730.422	116	4.97×10^{12}	149939	180.16	1.08×10^{3}
		[3, 3, 3]	44794.803	116	7.28×10^{13}	598286	869.02	1.79×10^{4}
$C2/m$	Sparse	[2, 2, 1]	58422.522	116	1.03×10^{13}	83532	100.47	2.53×10^{3}
		[4, 4, 2]	893339.394	116	5.37×10^{15}	3051285	5272.93	1.48×10^{6}
	SF	[2, 2, 1]	95803.204	116	2.05×10^{13}	44657	53.90	5.05×10^{3}
		[4, 4, 2]	2899609.300	116	5.23×10^{15}	405310	700.69	1.44×10^{6}
	DF	[2, 2, 1]	4873.648	116	1.18×10^{12}	75178	90.44	2.56×10^{2}
		[4, 4, 2]	51416.281	116	9.82×10^{13}	598736	869.68	2.41×10^{4}
$P2/c$	Sparse	[1, 1, 1]	84977.359	464	2.06×10^{13}	99918	120.21	5.07×10^{3}
		[2, 2, 2]	1627121.892	464	1.67×10^{16}	3182362	6454.14	4.59×10^{6}
	SF	[1, 1, 1]	201894.726	464	8.74×10^{13}	92786	135.04	2.15×10^{4}
		[2, 2, 2]	5666363.179	464	2.07×10^{16}	839487	1450.95	5.68×10^{6}
	DF	[1, 1, 1]	2753.901	464	9.72×10^{11}	75834	91.23	2.11×10^{2}
		[2, 2, 2]	40788.113	464	1.40×10^{14}	1192900	1732.40	3.44×10^{4}
$P2_1/c$	Sparse	[1, 2, 1]	105584.297	232	3.39×10^{13}	182864	265.83	8.34×10^{3}
		[2, 4, 2]	1714723.913	232	1.50×10^{16}	3116825	6321.24	4.12×10^{6}
	SF	[1, 2, 1]	271178.934	232	8.92×10^{13}	96882	140.98	2.19×10^{4}
		[2, 4, 2]	7798992.981	232	2.13×10^{16}	438080	757.32	5.85×10^{6}
	DF	[1, 2, 1]	3958.111	232	1.27×10^{12}	75383	90.69	2.76×10^{2}
		[2, 4, 2]	46189.645	232	1.23×10^{14}	1192758	1732.20	3.02×10^{4}

TABLE VI. Quantum Resource estimates for all four LNO structures normalized by the number of formula units represented in each simulation cell. $R\bar{3}m$ and $C2/m$ are both one formula unit while $P2/c$ is four formula units and $P2_1/c$ is two formula units. The sparse threshold is selected to be 1.0×10^{-4}, the SF the auxiliary index is truncated at eight times the number of molecular orbitals, and the DF the second factorization is truncated at 1.0×10^{-4}.

simulate matter for…





producing fertilizers with less energy

FeMoCo role in nitrogen fixation

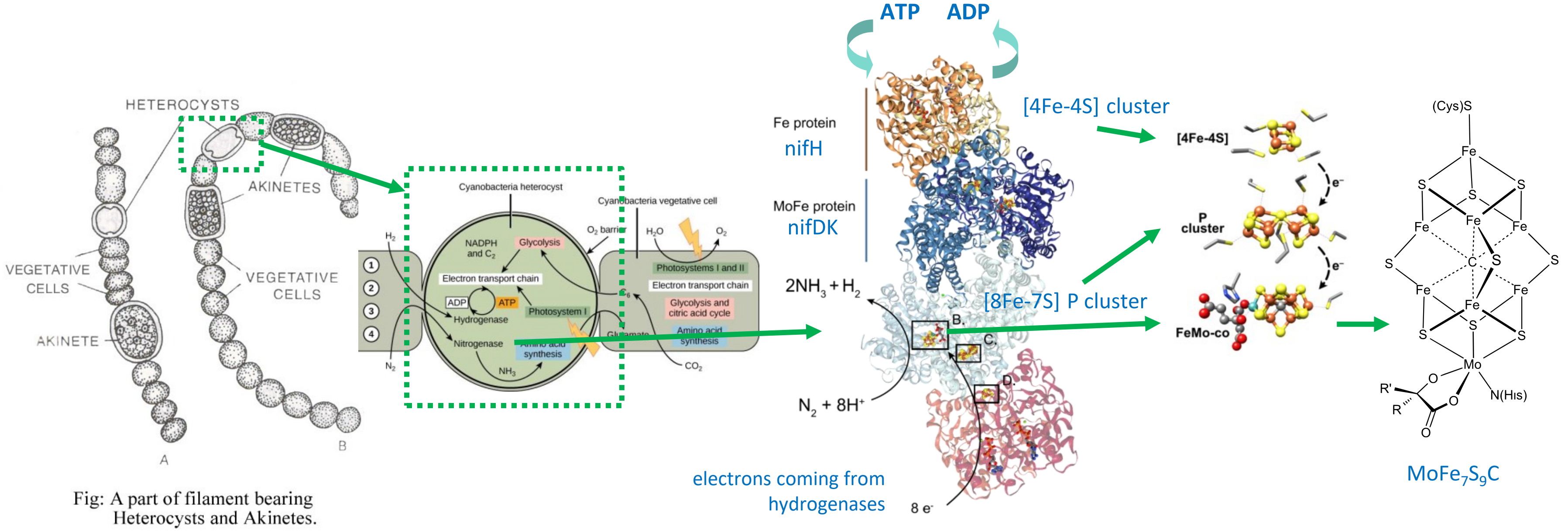


Fig: A part of filament bearing Heterocysts and Akinetes.

cyanobacteria

bacteria producing ammonia in soil and water or legume plants root nodules

heterocyst

cell within cyanobacteria that support the chemical pathways producing ammonia using dinitrogen

nitrogenase

protein complex producing ammonia in heterocyst cells

FeMoCo complex

part of the two nidDK proteins in some nitrogenases that is involved in ammonia production

simulating FeMoCo

need…

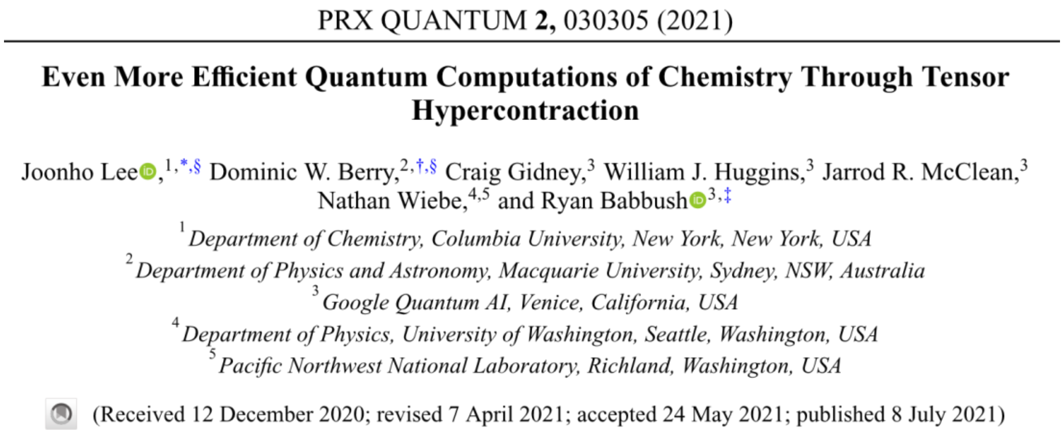
2,142 logical qubits

4M physical qubits

4 days computing time

real need:

- **simulate full NH_3 creation chemical pathway.**
- **design a new industry-grade pathway.**
- **simulate it with a lot of tries.**
- **optimize it with real-life scenario.**



PRX QUANTUM **2,** 030305 (2021)

Even More Efficient Quantum Computations of Chemistry Through Tensor Hypercontraction

Joonho Lee,[1,*,§] Dominic W. Berry,[2,†,§] Craig Gidney,[3] William J. Huggins,[3] Jarrod R. McClean,[3]
Nathan Wiebe,[4,5] and Ryan Babbush[3,‡]

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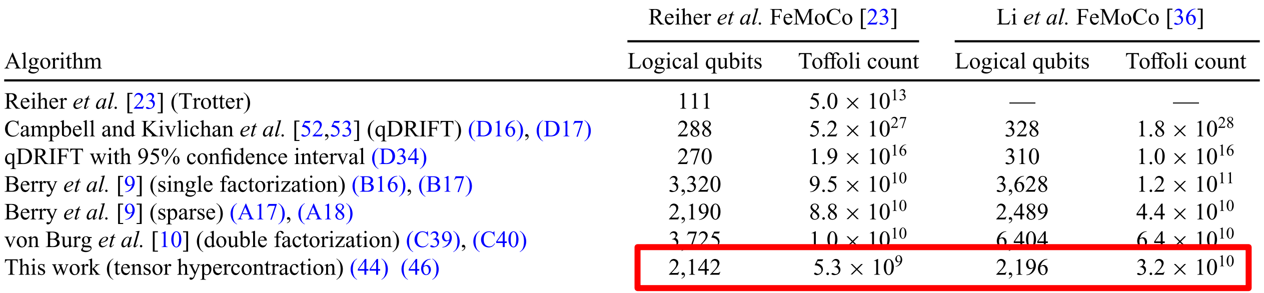
[5] *Pacific Northwest National Laboratory, Richland, Washington, USA*

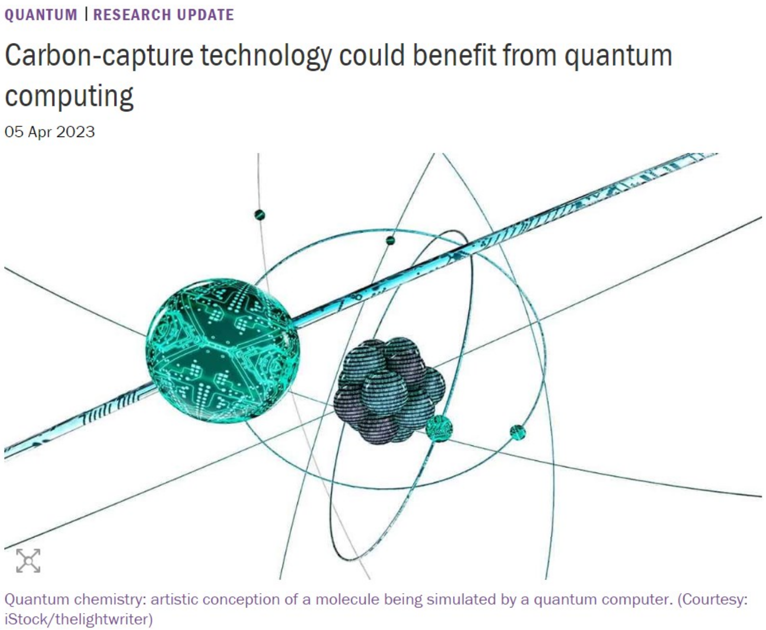
(Received 12 December 2020; revised 7 April 2021; accepted 24 May 2021; published 8 July 2021)



	Reiher *et al.* FeMoCo [23]		Li *et al.* FeMoCo [36]	
Algorithm	Logical qubits	Toffoli count	Logical qubits	Toffoli count
Reiher *et al.* [23] (Trotter)	111	5.0×10^{13}	—	—
Campbell and Kivlichan *et al.* [52,53] (qDRIFT) (D16), (D17)	288	5.2×10^{27}	328	1.8×10^{28}
qDRIFT with 95% confidence interval (D34)	270	1.9×10^{16}	310	1.0×10^{16}
Berry *et al.* [9] (single factorization) (B16), (B17)	3,320	9.5×10^{10}	3,628	1.2×10^{11}
Berry *et al.* [9] (sparse) (A17), (A18)	2,190	8.8×10^{10}	2,489	4.4×10^{10}
von Burg *et al.* [10] (double factorization) (C39), (C40)	3,725	1.0×10^{10}	6,404	6.4×10^{10}
This work (tensor hypercontraction) (44) (46)	2,142	5.3×10^{9}	2,196	3.2×10^{10}

source: Even More Efficient Quantum Computations of Chemistry Through Tensor Hypercontraction by Joonho Lee, Craig Gidney et al, July 2021 (62 pages). https://journals.aps.org/prxquantum/pdf/10.1103/PRXQuantum.2.030305

CO2 capture

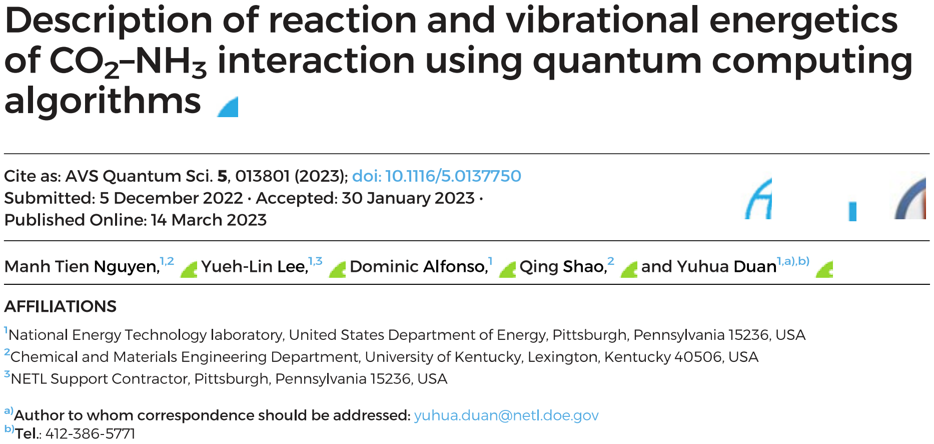


QUANTUM | RESEARCH UPDATE

Carbon-capture technology could benefit from quantum computing

05 Apr 2023

Quantum chemistry: artistic conception of a molecule being simulated by a quantum computer. (Courtesy: iStock/thelightwriter)



Description of reaction and vibrational energetics of CO_2–NH_3 interaction using quantum computing algorithms

Cite as: AVS Quantum Sci. **5**, 013801 (2023); doi: 10.1116/5.0137750
Submitted: 5 December 2022 · Accepted: 30 January 2023 ·
Published Online: 14 March 2023

Manh Tien Nguyen,[1,2] Yueh-Lin Lee,[1,3] Dominic Alfonso,[1] Qing Shao,[2] and Yuhua Duan[1,a),b)]

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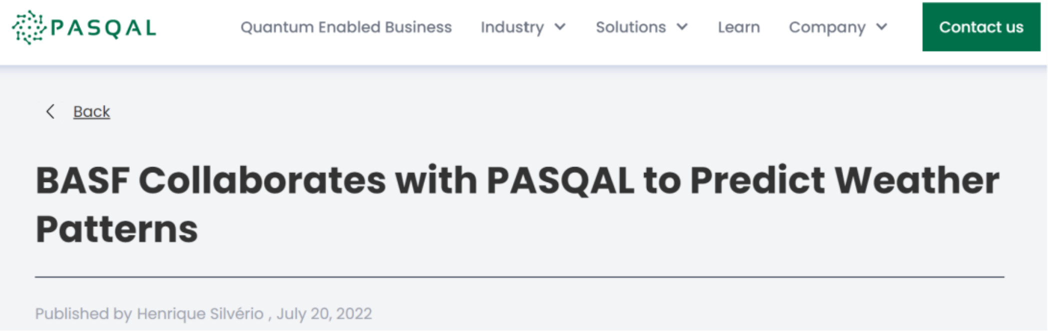
[3] NETL Support Contractor, Pittsburgh, Pennsylvania 15236, USA

[a)] Author to whom correspondence should be addressed: yuhua.duan@netl.doe.gov
[b)] Tel.: 412-386-5771

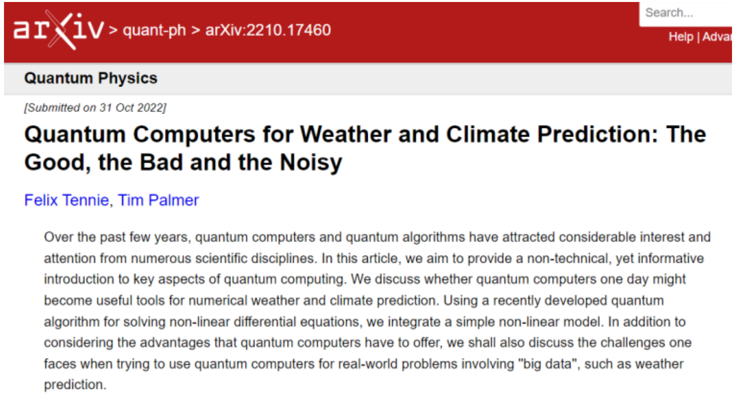
- **VQE algorithm tested on 20 qubits.**
- **not yet in a quantum advantage regime.**
- **not a solution for carbon capture.**

modeling climate and weather



BASF Collaborates with PASQAL to Predict Weather Patterns

Published by Henrique Silvério , July 20, 2022



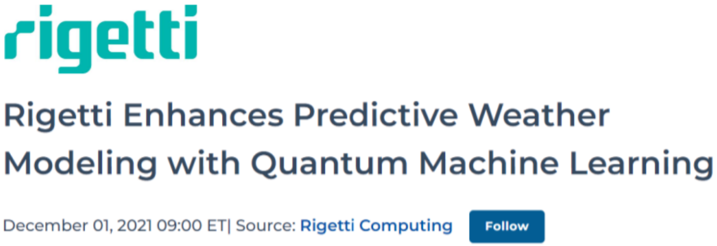
Quantum Physics

[Submitted on 31 Oct 2022]

Quantum Computers for Weather and Climate Prediction: The Good, the Bad and the Noisy

Felix Tennie, Tim Palmer

Over the past few years, quantum computers and quantum algorithms have attracted considerable interest and attention from numerous scientific disciplines. In this article, we aim to provide a non-technical, yet informative introduction to key aspects of quantum computing. We discuss whether quantum computers one day might become useful tools for numerical weather and climate prediction. Using a recently developed quantum algorithm for solving non-linear differential equations, we integrate a simple non-linear model. In addition to considering the advantages that quantum computers have to offer, we shall also discuss the challenges one faces when trying to use quantum computers for real-world problems involving "big data", such as weather prediction.

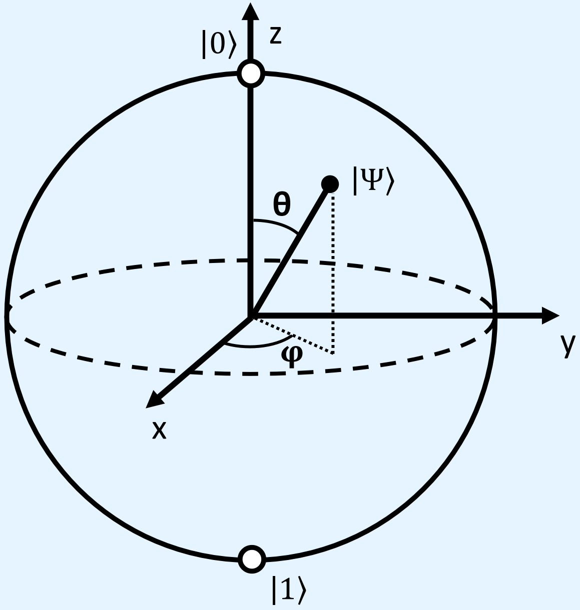


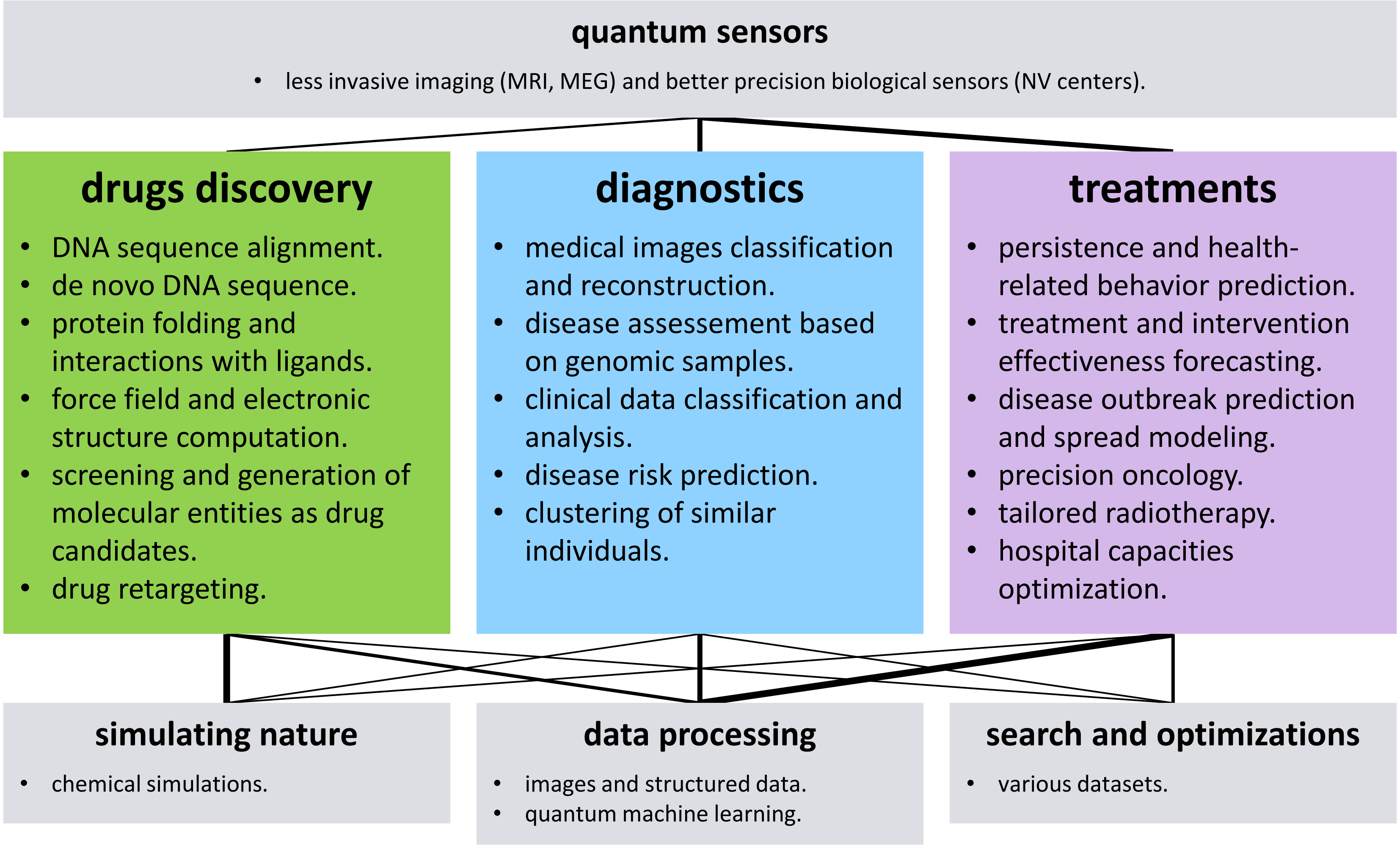
Rigetti Enhances Predictive Weather Modeling with Quantum Machine Learning

December 01, 2021 09:00 ET| Source: Rigetti Computing

with 32 qubits!

quantum technologies in healthcare





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

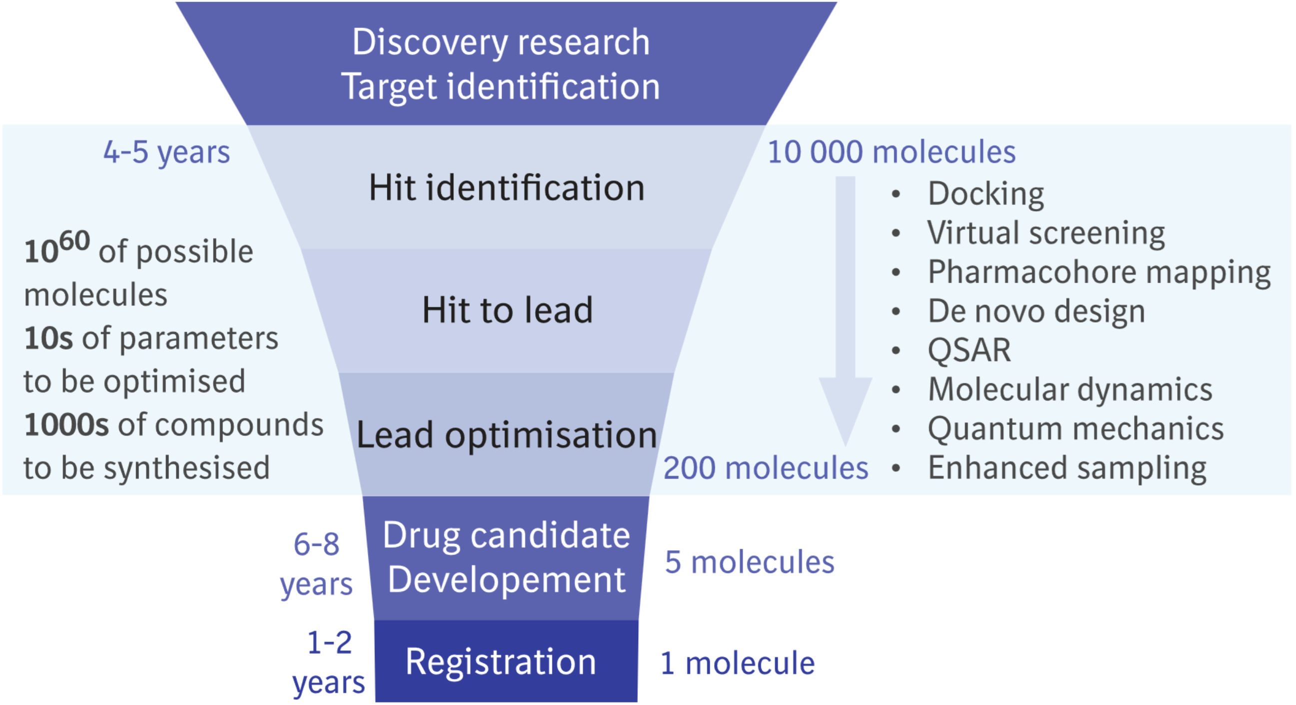
- images and structured data.
- quantum machine learning.

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



Discovery research
Target identification

4-5 years

Hit identification

Hit to lead

Lead optimisation

10^{60} of possible molecules
10s of parameters to be optimised
1000s of compounds to be synthesised

10 000 molecules

- Docking
- Virtual screening
- Pharmacohore mapping
- De novo design
- QSAR
- Molecular dynamics
- Quantum mechanics
- Enhanced sampling

200 molecules

6-8 years

Drug candidate
Developement

5 molecules

1-2 years

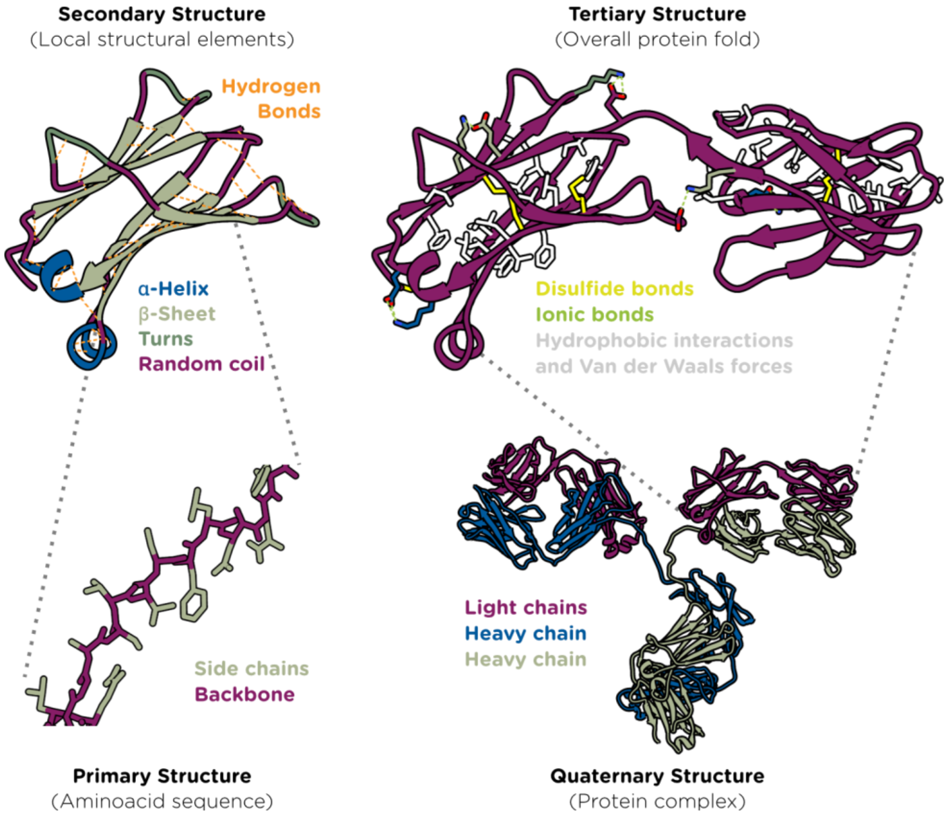
Registration

1 molecule

this part could potentially be accelerated thanks to quantum computing

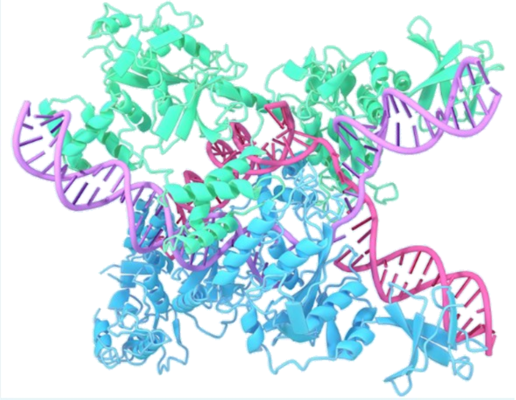
Source: Drug design on quantum computers by Raffaele Santagati, Alan Aspuru-Guzik, Nathan Wiebe et al, January 2023 (9 pages)

protein folding requirements

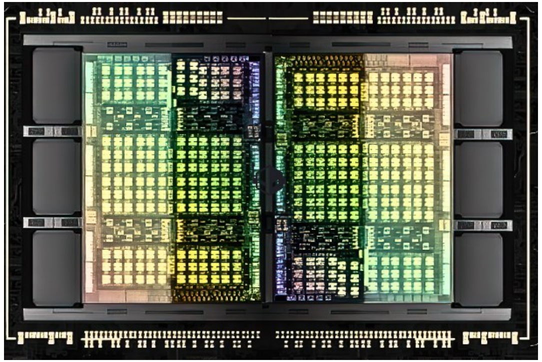


Source: FAQS Higher Order Structure and HOS Comparisons Explained.

challenges



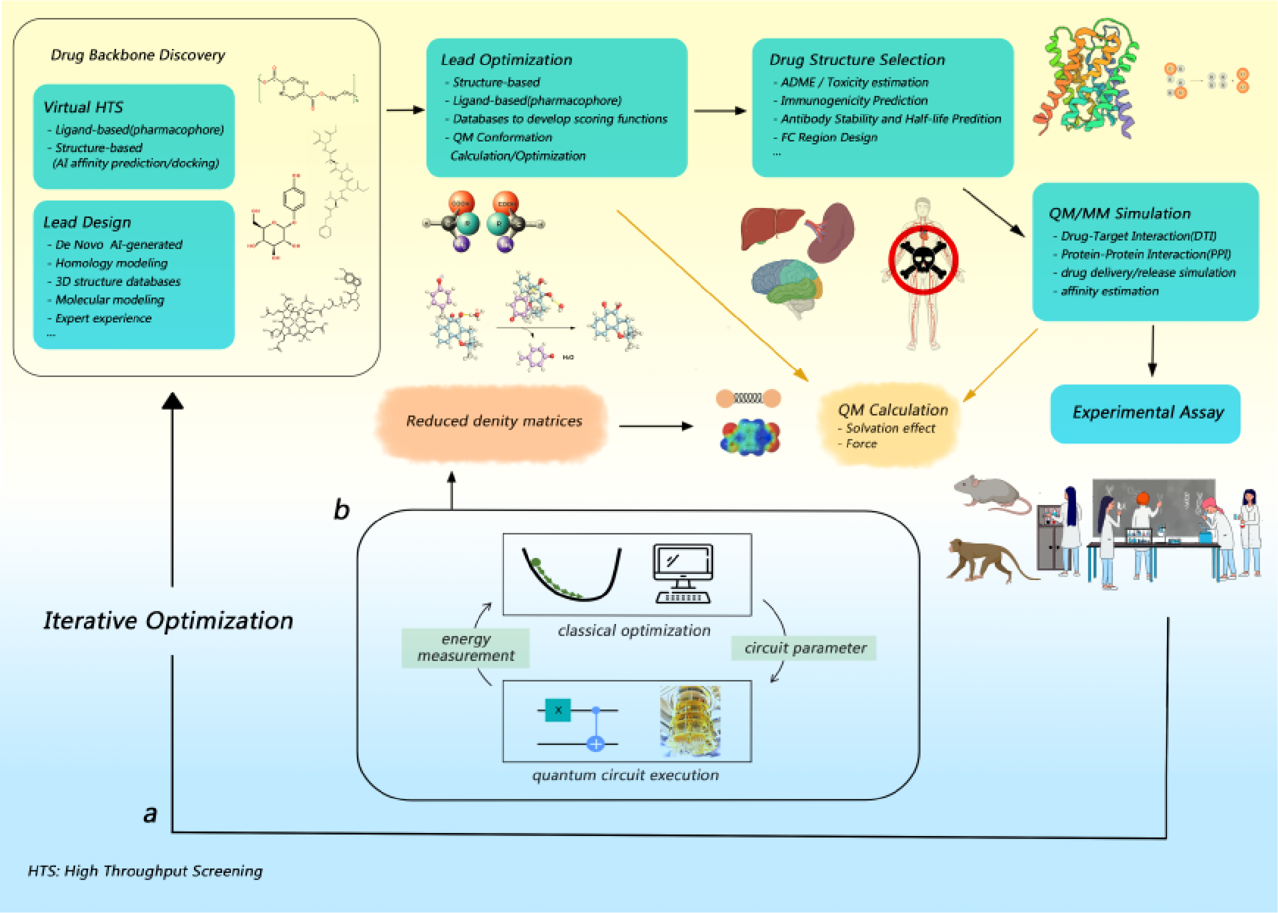
AlphaFold 3 can now generate predictions for nearly all molecules in the Protein Data Bank (PDB), frequently reaching atomic accuracy



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.

drug discovery pipeline



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

D-Wave use cases in healthcare

genuity science

cancers classification

multi-omics: genomics + symptoms in QML

source: D-Wave

menten.AI FLATIRON INSTITUTE

de-novo proteins and polypeptides creation

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

source: D-Wave

accenture

liver donor optimization

NP-complet complete problem using QUBO

source: Accenture, D-Wave

accenture 1QBit Biogen

drug retargeting

with Biogen, 1QBit and Accenture research

source: D-Wave

ROSWELL PARK
COMPREHENSIVE CANCER CENTER

radiotherapy optimization

to minimized x-ray dose

source: Roswell Park, D-Wave

D:wave
The Quantum Computing Company™

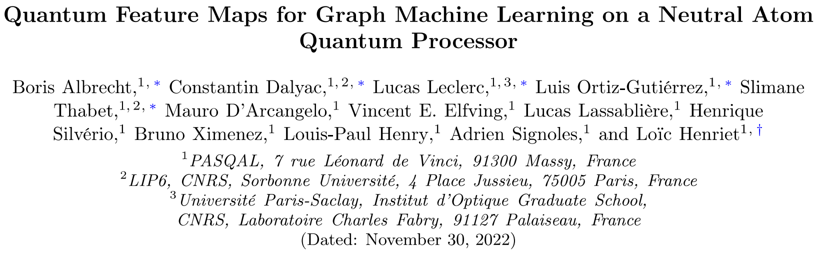
Pasqal use cases in healthcare

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,*]

[1]Pasqal, 7 Rue Léonard de Vinci, 91300 Massy, France
[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
[*]loic.henriet@pasqal.com, jean-philip.piquemal@sorbonne-universite.fr
[+]these authors contributed equally to this work

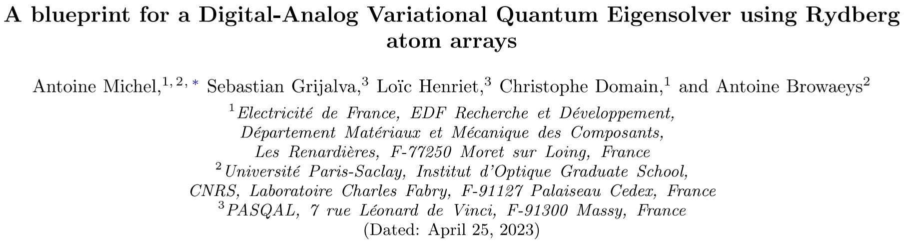


Quantum Feature Maps for Graph Machine Learning on a Neutral Atom Quantum Processor

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

algorithmiq
AQEMIA
apply
ChemAlive
ColibrITD
Creative Quantum
CULGI

Entropica Labs
FACCTs
FOQUS
GOOD CHEMISTRY
HQS QUANTUM SIMULATIONS
ingenii ACCELERATING DATA ENGINEERING

Jij
KUANO
menten.AI
mol|ket⟩
MQS Molecular Quantum Solutions
NETRAMARK

OTI
PHASECRAFT
POLARISQB
ProteinQure
Q1t
QSIMULATE

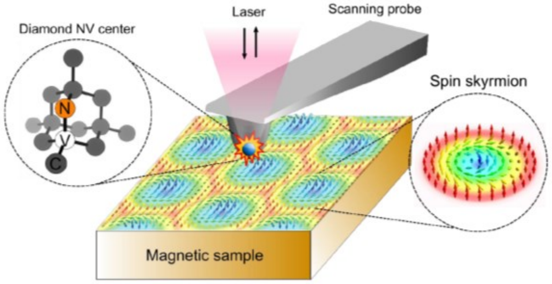
Quantistry
Qubit PHARMACEUTICALS
Quantum Native Systems QunaSys
river lane
SolidStateAI

quantum sensors in healthcare

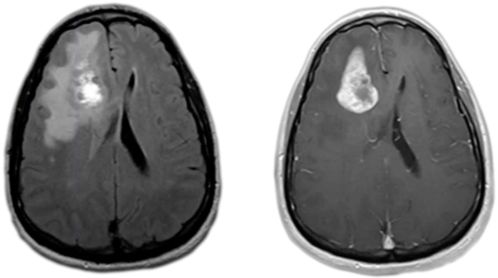
qnami

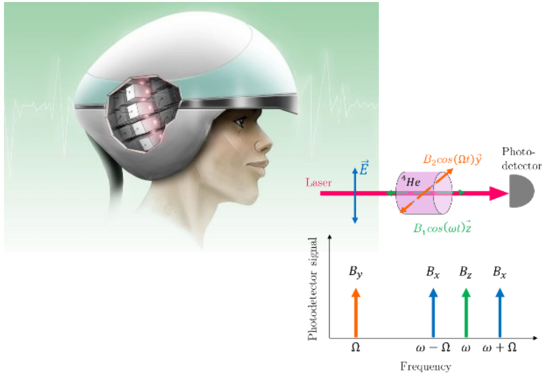
chipiron

MAG^{4}Health



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



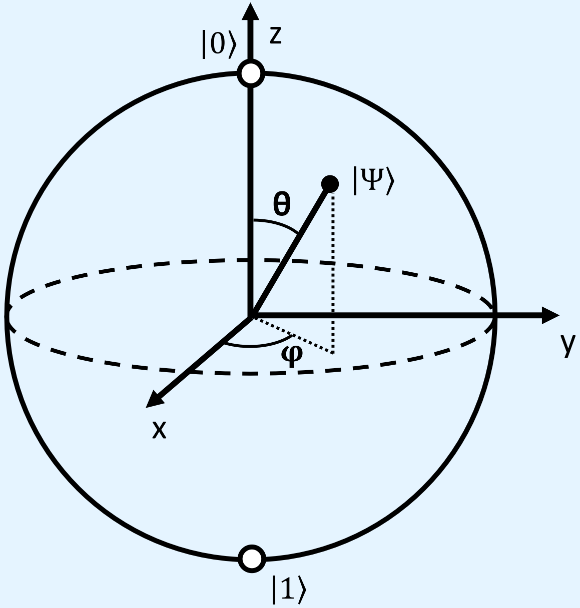


medical imaging
biological analysis

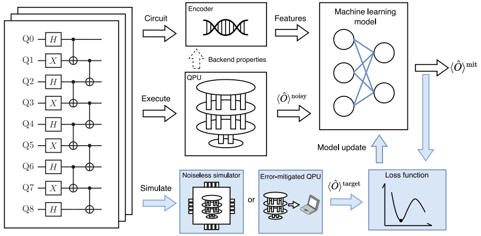
SQUID based
ultra-low field MRI

helium 4 nucleus spin
MEG brain imaging

AI for quantum technologies



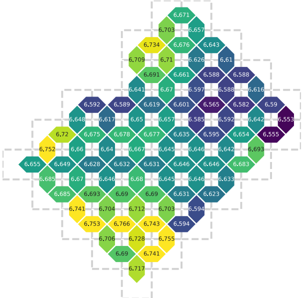
machine learning helps everywhere



quantum error mitigation

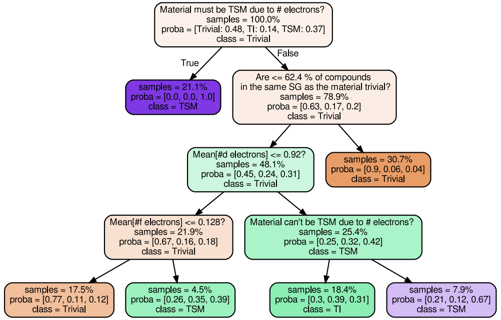
https://arxiv.org/abs/2309.17368

https://arxiv.org/abs/2207.00298



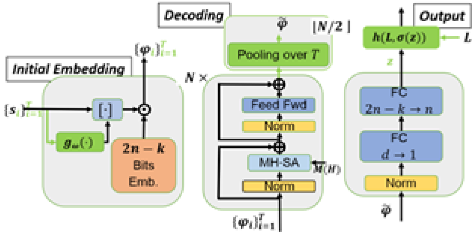
optimizing qubit frequency allocations

https://arxiv.org/abs/1910.11333



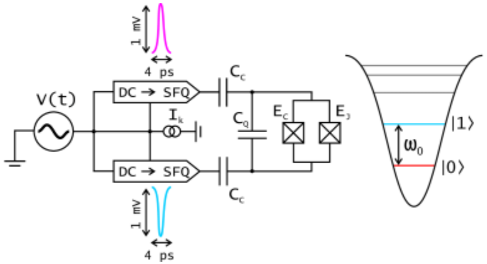
identification of topological materials

https://arxiv.org/abs/1910.10161



QEC error syndrome detection

https://arxiv.org/abs/2301.11930



driving qubit control electronics

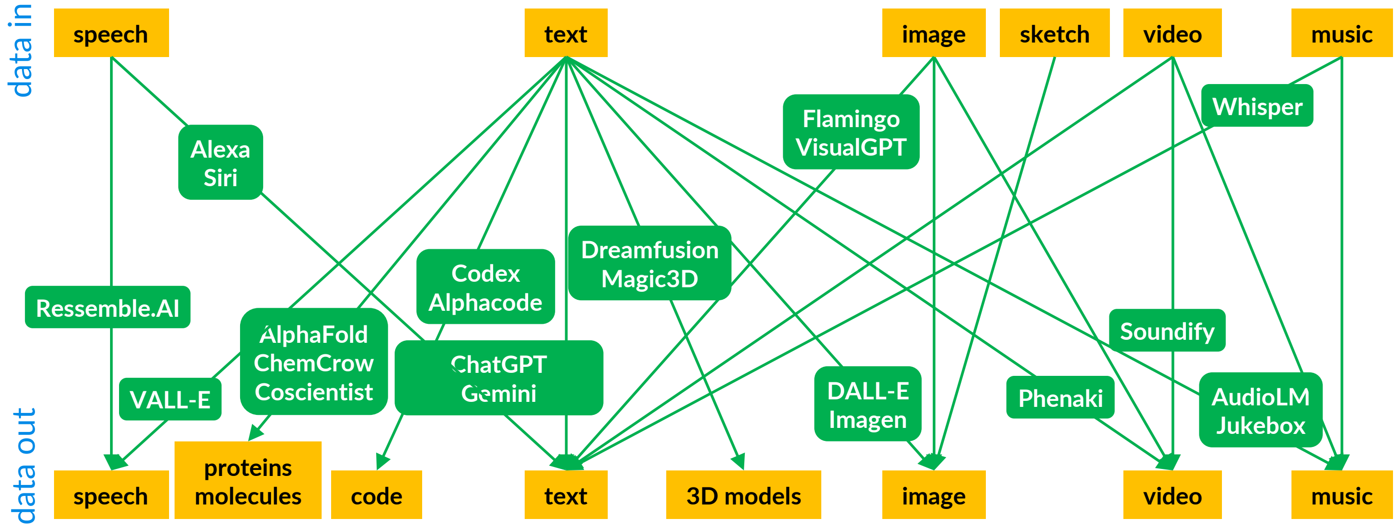
https://arxiv.org/abs/2209.09790

correcting quantum sensor noise

https://arxiv.org/abs/1807.09753

physics lab experiments analysis

generative AI landscape



generative AI data type in/out examples

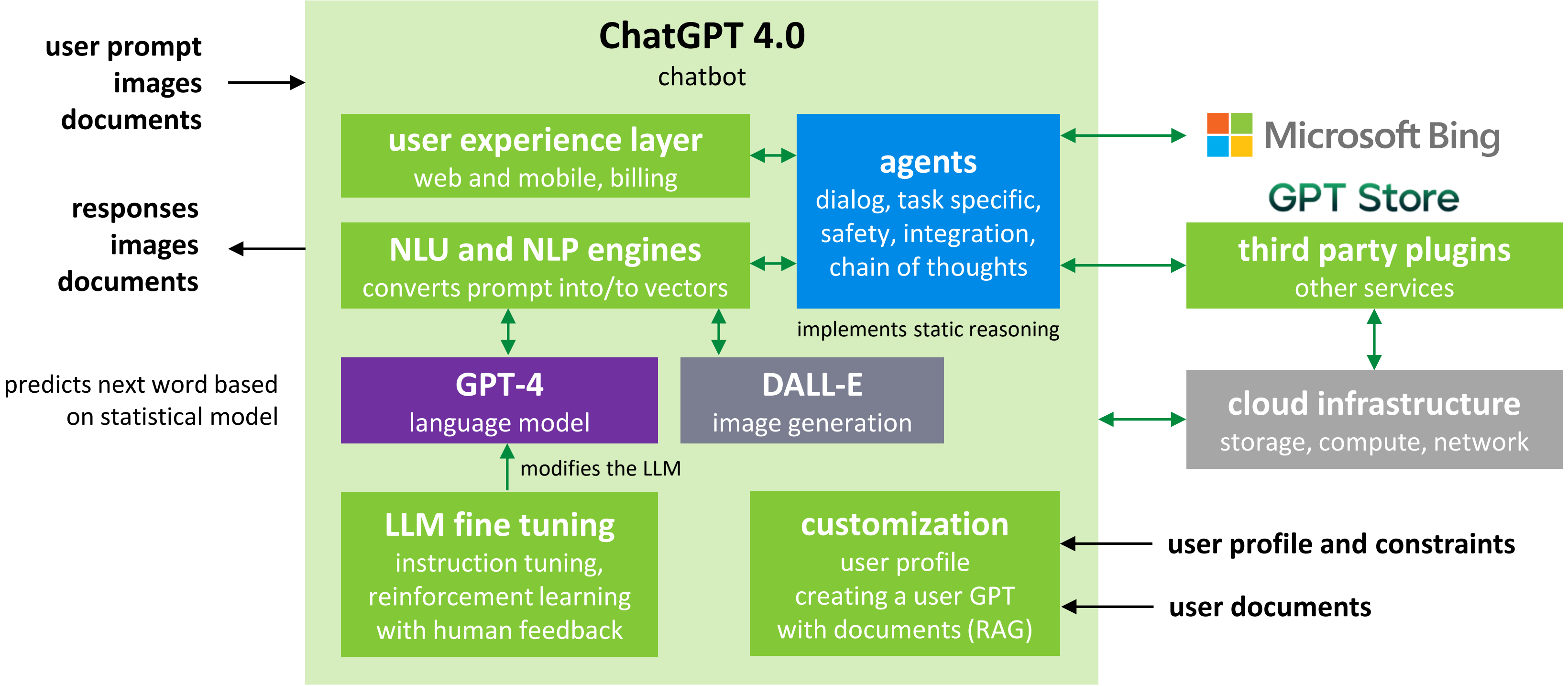
- LLM-based chatbots are one broad category of "generative AI" solutions.
- but they are bound to integrate many other gen AI solutions in their UI.

generic LLM-based chatbot capabilities

answer to questions
summarizing texts
commenting and evaluating texts
producing synopsis and memos
translating texts
creating text “ala” somebody

creating a quiz
identifying images content
creating images based on description
creating data charts
creating software code

ChatGPT 4.0 overall architecture



user prompt
images
documents

responses
images
documents

predicts next word based on statistical model

ChatGPT 4.0
chatbot

user experience layer
web and mobile, billing

NLU and NLP engines
converts prompt into/to vectors

agents
dialog, task specific, safety, integration, chain of thoughts

implements static reasoning

GPT-4
language model

DALL-E
image generation

modifies the LLM

LLM fine tuning
instruction tuning, reinforcement learning with human feedback

customization
user profile
creating a user GPT with documents (RAG)

Microsoft Bing

GPT Store

third party plugins
other services

cloud infrastructure
storage, compute, network

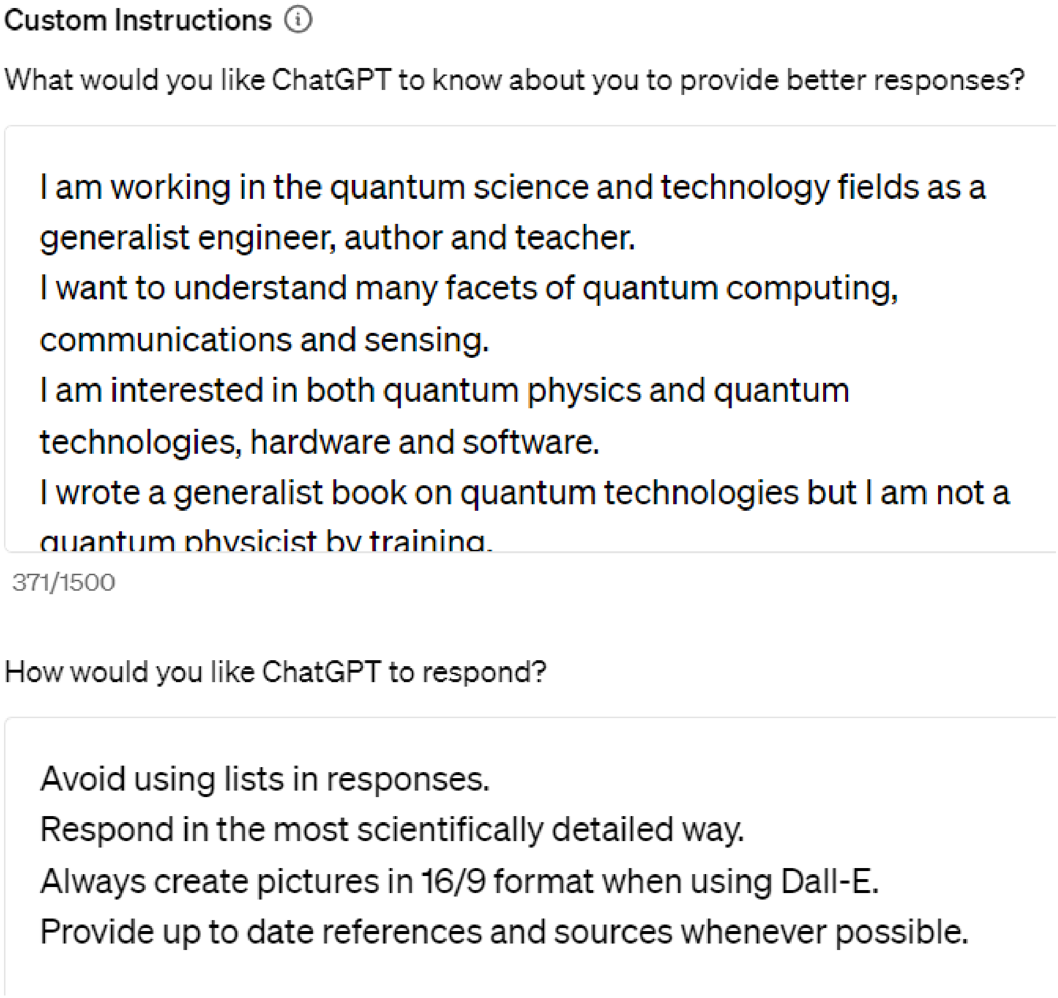
user profile and constraints

user documents

#1
define your user profile

#2
learn prompt engineering

#3
fact check results



Custom Instructions

What would you like ChatGPT to know about you to provide better responses?

I am working in the quantum science and technology fields as a generalist engineer, author and teacher.
I want to understand many facets of quantum computing, communications and sensing.
I am interested in both quantum physics and quantum technologies, hardware and software.
I wrote a generalist book on quantum technologies but I am not a quantum physicist by training.

371/1500

How would you like ChatGPT to respond?

Avoid using lists in responses.
Respond in the most scientifically detailed way.
Always create pictures in 16/9 format when using Dall-E.
Provide up to date references and sources whenever possible.

current *amazing* use cases

basic quantum science knowledge: well done in most fields.

figures of merit: single photon sources, detectors, PNR, circulators, TWPA

inventories: materials used in superconducting qubits, research avenues in some domain,

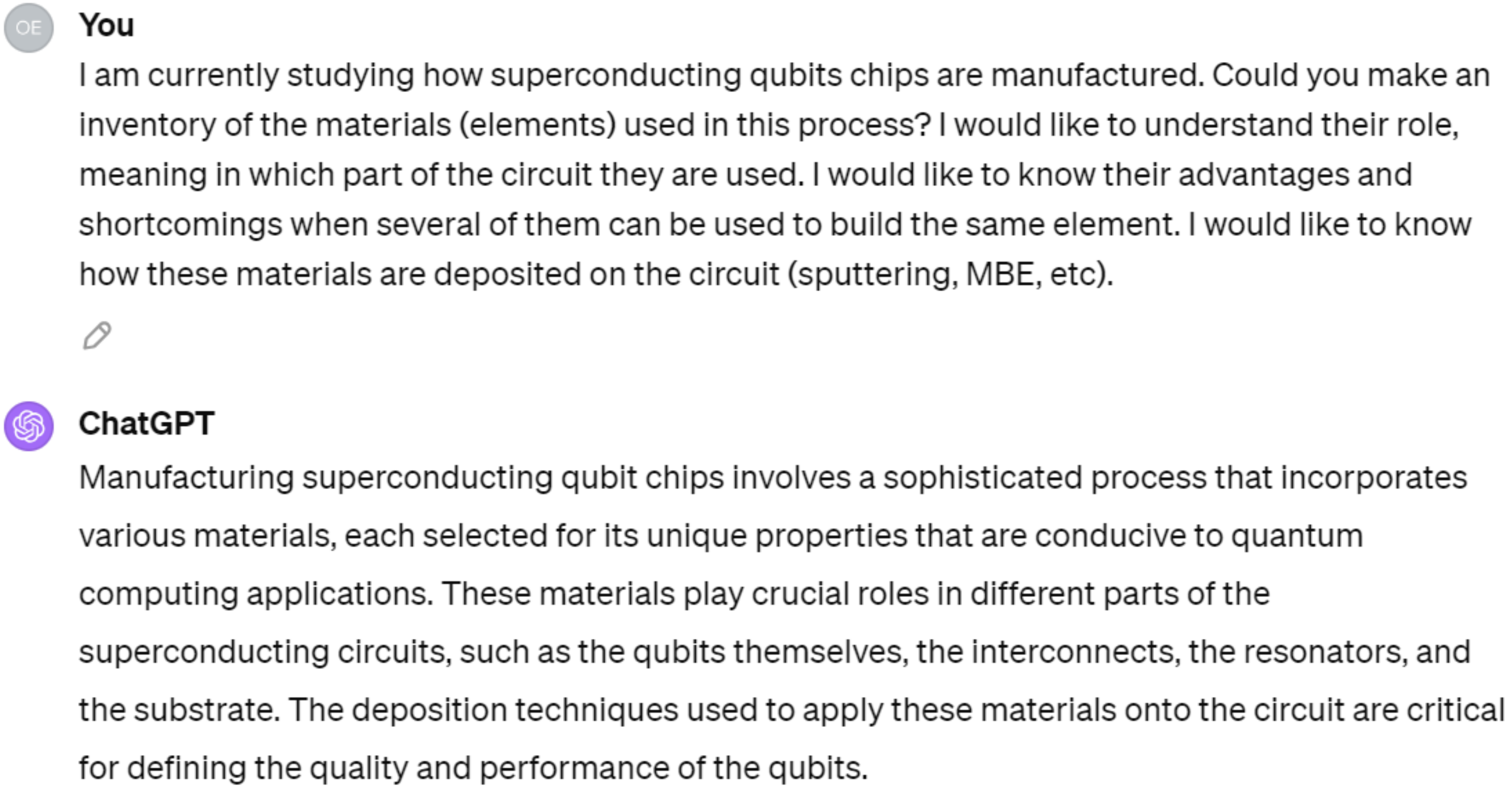
simple maths and logic and continuously improving.

bibliography: getting better with ChatGPT 4.0.

quiz: 48 multiple choice questions on everything quantum.

coding: Python for creating charts, PHP, regex, VBA, …

inventories

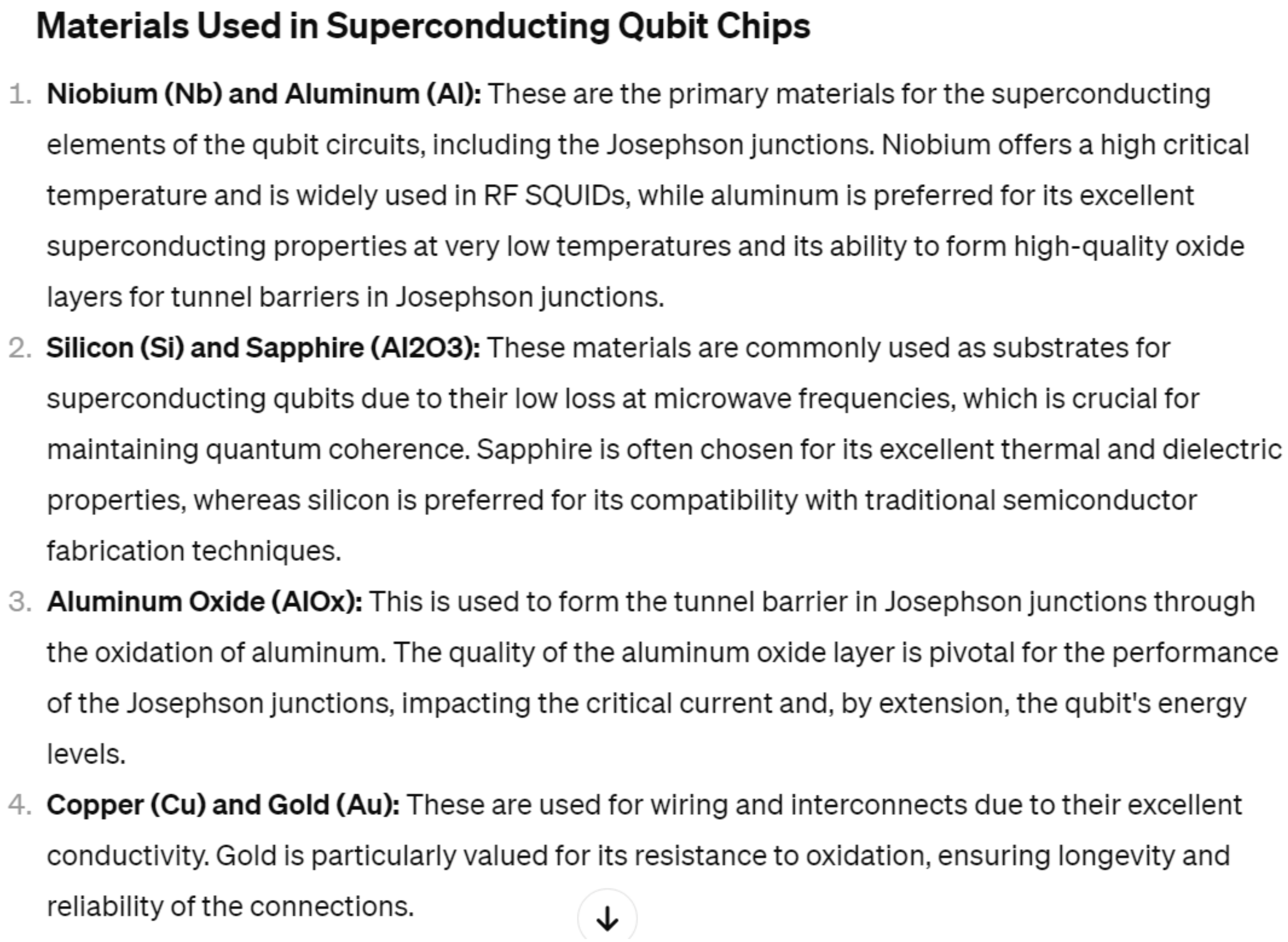


You

I am currently studying how superconducting qubits chips are manufactured. Could you make an inventory of the materials (elements) used in this process? I would like to understand their role, meaning in which part of the circuit they are used. I would like to know their advantages and shortcomings when several of them can be used to build the same element. I would like to know how these materials are deposited on the circuit (sputtering, MBE, etc).

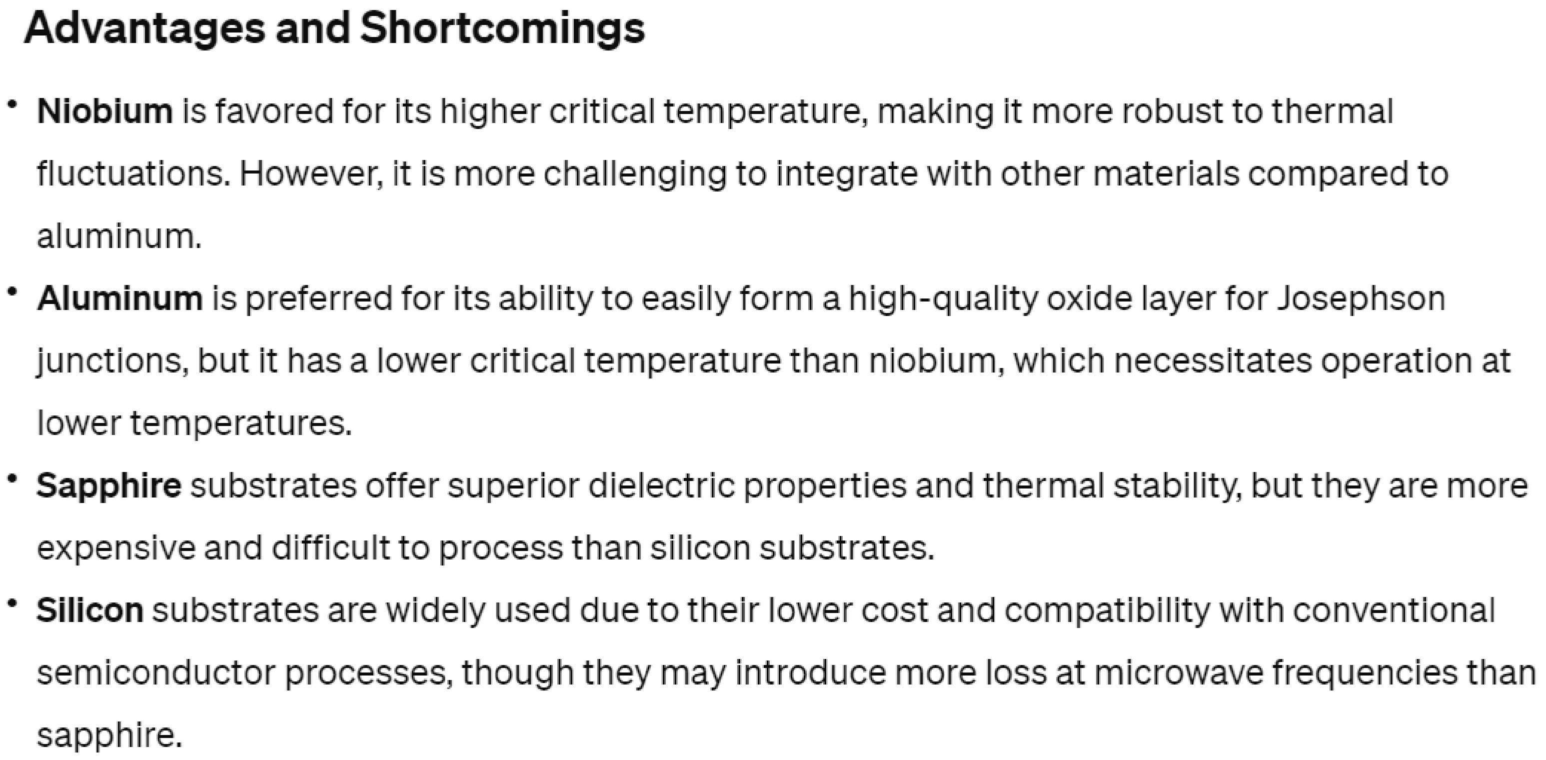
ChatGPT

Manufacturing superconducting qubit chips involves a sophisticated process that incorporates various materials, each selected for its unique properties that are conducive to quantum computing applications. These materials play crucial roles in different parts of the superconducting circuits, such as the qubits themselves, the interconnects, the resonators, and the substrate. The deposition techniques used to apply these materials onto the circuit are critical for defining the quality and performance of the qubits.



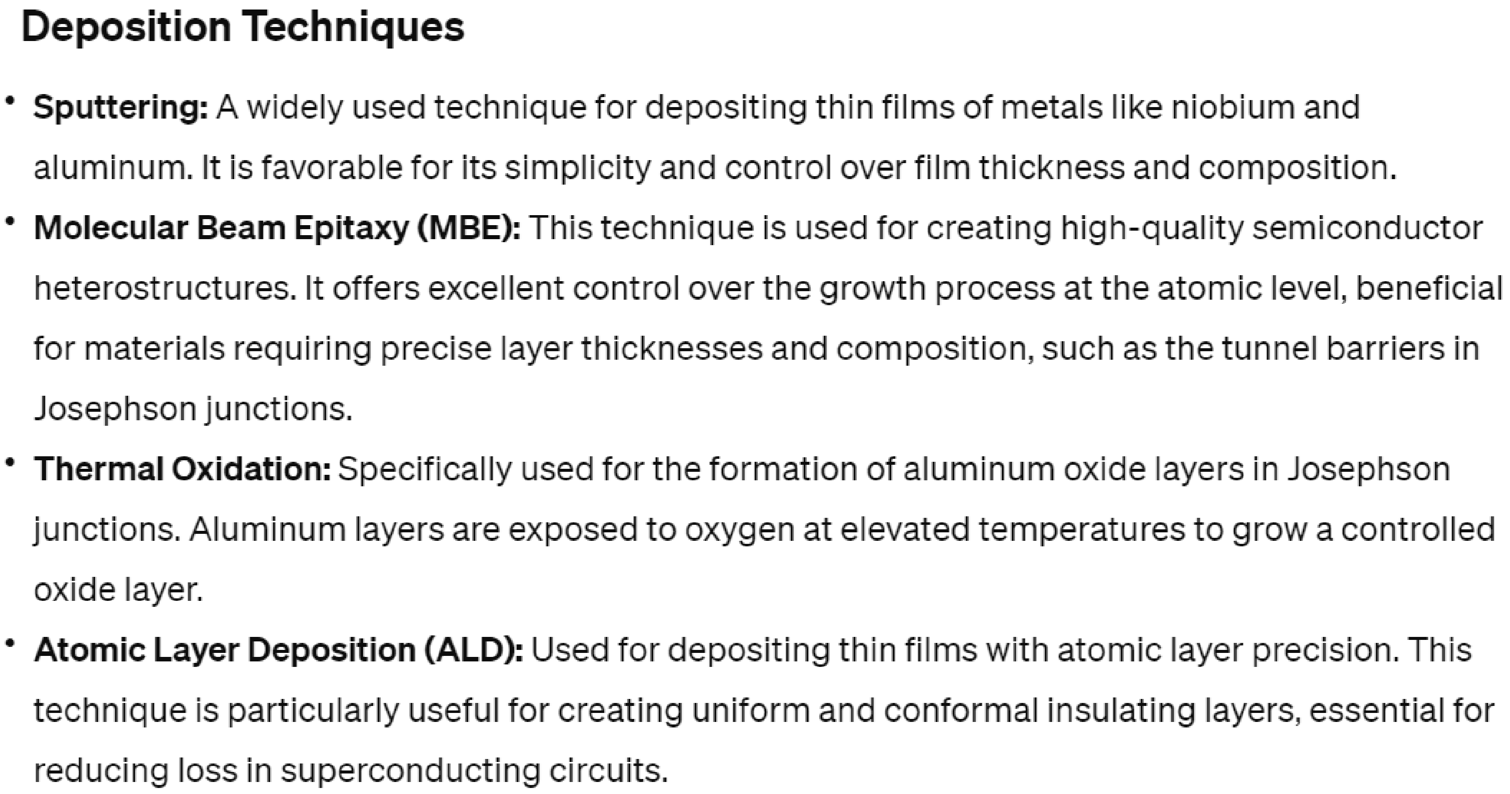
Materials Used in Superconducting Qubit Chips

1. **Niobium (Nb) and Aluminum (Al):** These are the primary materials for the superconducting elements of the qubit circuits, including the Josephson junctions. Niobium offers a high critical temperature and is widely used in RF SQUIDs, while aluminum is preferred for its excellent superconducting properties at very low temperatures and its ability to form high-quality oxide layers for tunnel barriers in Josephson junctions.
2. **Silicon (Si) and Sapphire (Al2O3):** These materials are commonly used as substrates for superconducting qubits due to their low loss at microwave frequencies, which is crucial for maintaining quantum coherence. Sapphire is often chosen for its excellent thermal and dielectric properties, whereas silicon is preferred for its compatibility with traditional semiconductor fabrication techniques.
3. **Aluminum Oxide (AlOx):** This is used to form the tunnel barrier in Josephson junctions through the oxidation of aluminum. The quality of the aluminum oxide layer is pivotal for the performance of the Josephson junctions, impacting the critical current and, by extension, the qubit's energy levels.
4. **Copper (Cu) and Gold (Au):** These are used for wiring and interconnects due to their excellent conductivity. Gold is particularly valued for its resistance to oxidation, ensuring longevity and reliability of the connections.



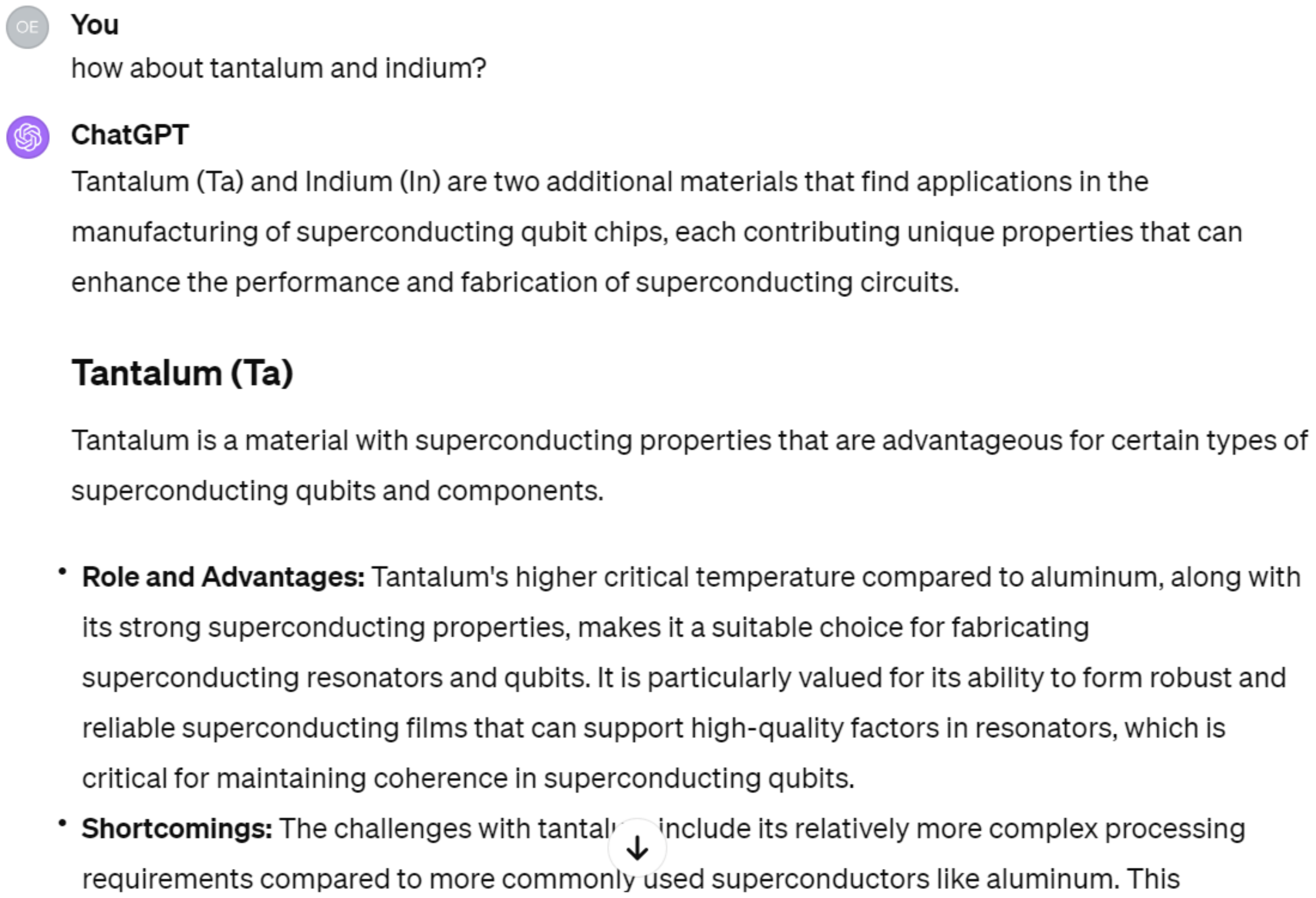
Advantages and Shortcomings

- **Niobium** is favored for its higher critical temperature, making it more robust to thermal fluctuations. However, it is more challenging to integrate with other materials compared to aluminum.
- **Aluminum** is preferred for its ability to easily form a high-quality oxide layer for Josephson junctions, but it has a lower critical temperature than niobium, which necessitates operation at lower temperatures.
- **Sapphire** substrates offer superior dielectric properties and thermal stability, but they are more expensive and difficult to process than silicon substrates.
- **Silicon** substrates are widely used due to their lower cost and compatibility with conventional semiconductor processes, though they may introduce more loss at microwave frequencies than sapphire.



Deposition Techniques

- **Sputtering:** A widely used technique for depositing thin films of metals like niobium and aluminum. It is favorable for its simplicity and control over film thickness and composition.
- **Molecular Beam Epitaxy (MBE):** This technique is used for creating high-quality semiconductor heterostructures. It offers excellent control over the growth process at the atomic level, beneficial for materials requiring precise layer thicknesses and composition, such as the tunnel barriers in Josephson junctions.
- **Thermal Oxidation:** Specifically used for the formation of aluminum oxide layers in Josephson junctions. Aluminum layers are exposed to oxygen at elevated temperatures to grow a controlled oxide layer.
- **Atomic Layer Deposition (ALD):** Used for depositing thin films with atomic layer precision. This technique is particularly useful for creating uniform and conformal insulating layers, essential for reducing loss in superconducting circuits.



You

how about tantalum and indium?

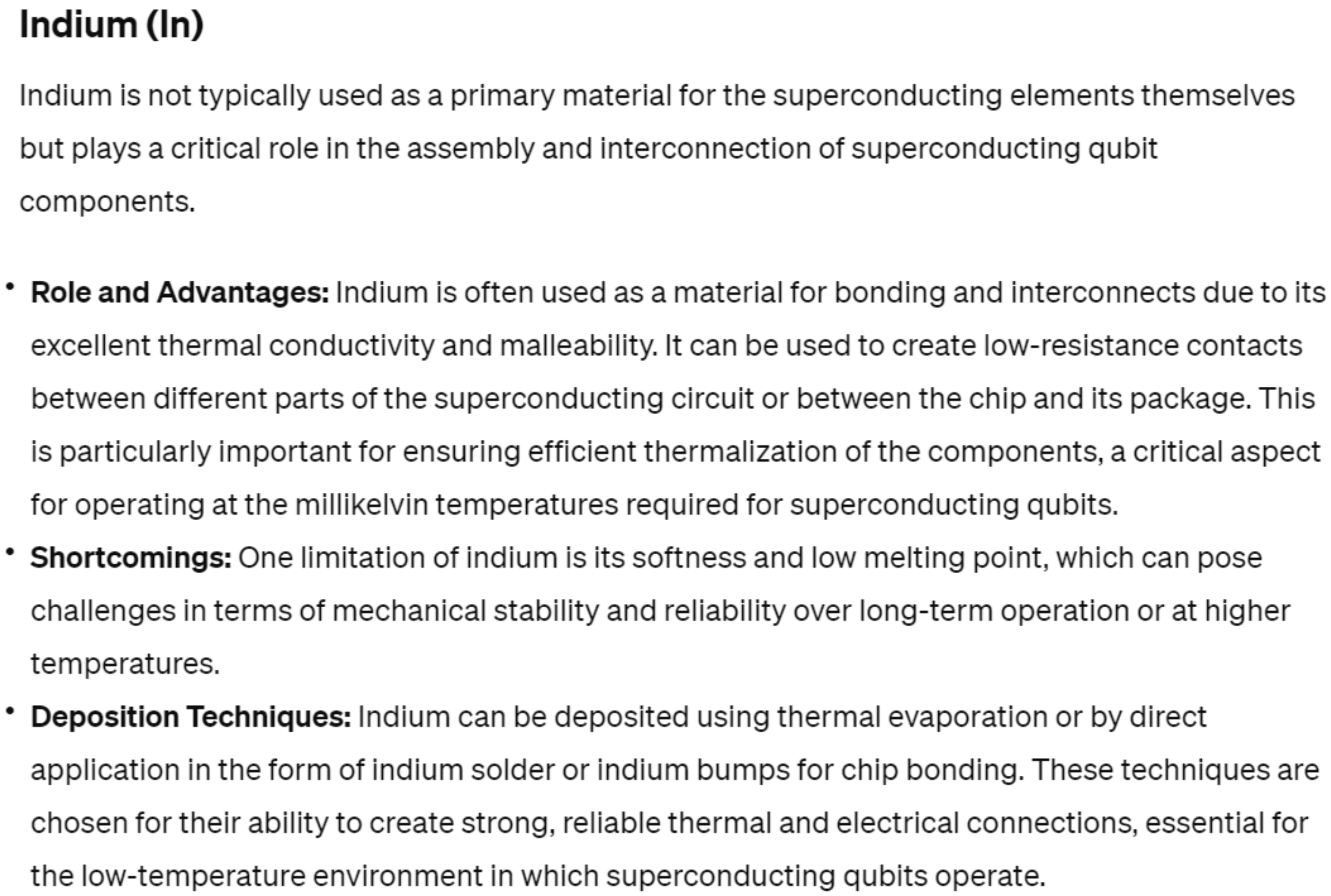
ChatGPT

Tantalum (Ta) and Indium (In) are two additional materials that find applications in the manufacturing of superconducting qubit chips, each contributing unique properties that can enhance the performance and fabrication of superconducting circuits.

Tantalum (Ta)

Tantalum is a material with superconducting properties that are advantageous for certain types of superconducting qubits and components.

- **Role and Advantages:** Tantalum's higher critical temperature compared to aluminum, along with its strong superconducting properties, makes it a suitable choice for fabricating superconducting resonators and qubits. It is particularly valued for its ability to form robust and reliable superconducting films that can support high-quality factors in resonators, which is critical for maintaining coherence in superconducting qubits.
- **Shortcomings:** The challenges with tantal include its relatively more complex processing requirements compared to more commonly used superconductors like aluminum. This



Indium (In)

Indium is not typically used as a primary material for the superconducting elements themselves but plays a critical role in the assembly and interconnection of superconducting qubit components.

- **Role and Advantages:** Indium is often used as a material for bonding and interconnects due to its excellent thermal conductivity and malleability. It can be used to create low-resistance contacts between different parts of the superconducting circuit or between the chip and its package. This is particularly important for ensuring efficient thermalization of the components, a critical aspect for operating at the millikelvin temperatures required for superconducting qubits.
- **Shortcomings:** One limitation of indium is its softness and low melting point, which can pose challenges in terms of mechanical stability and reliability over long-term operation or at higher temperatures.
- **Deposition Techniques:** Indium can be deposited using thermal evaporation or by direct application in the form of indium solder or indium bumps for chip bonding. These techniques are chosen for their ability to create strong, reliable thermal and electrical connections, essential for the low-temperature environment in which superconducting qubits operate.

creating schemas: wrong content and labelling (Dall-E). Missing generative adversarial (GAN) features.

summarizing scientific papers: still simplistic outcome.

analyzing charts in scientific papers: not there yet.

finding missing figures of merit in papers: not there yet.

bibliographies: high rate of hallucinations (Bard).

reasoning: many mistakes, improvable with agents/CoT/RLHF.

data consolidation (e.g.: qubit fidelities): mistakes + not done anymore (Bard).

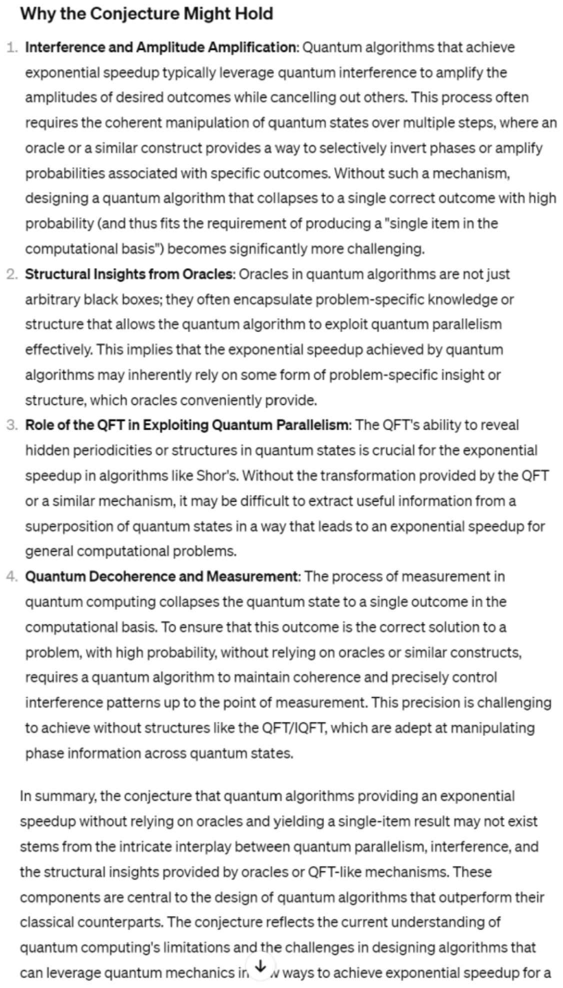
how could chatbots foster creativity in research?

test hypothesis and conjectures

identify white spaces

suggest potential research investigations

connect the dots between disparate scientific fields



Why the Conjecture Might Hold

1. **Interference and Amplitude Amplification:** Quantum algorithms that achieve exponential speedup typically leverage quantum interference to amplify the amplitudes of desired outcomes while cancelling out others. This process often requires the coherent manipulation of quantum states over multiple steps, where an oracle or a similar construct provides a way to selectively invert phases or amplify probabilities associated with specific outcomes. Without such a mechanism, designing a quantum algorithm that collapses to a single correct outcome with high probability (and thus fits the requirement of producing a "single item in the computational basis") becomes significantly more challenging.
2. **Structural Insights from Oracles:** Oracles in quantum algorithms are not just arbitrary black boxes; they often encapsulate problem-specific knowledge or structure that allows the quantum algorithm to exploit quantum parallelism effectively. This implies that the exponential speedup achieved by quantum algorithms may inherently rely on some form of problem-specific insight or structure, which oracles conveniently provide.
3. **Role of the QFT in Exploiting Quantum Parallelism:** The QFT's ability to reveal hidden periodicities or structures in quantum states is crucial for the exponential speedup in algorithms like Shor's. Without the transformation provided by the QFT or a similar mechanism, it may be difficult to extract useful information from a superposition of quantum states in a way that leads to an exponential speedup for general computational problems.
4. **Quantum Decoherence and Measurement:** The process of measurement in quantum computing collapses the quantum state to a single outcome in the computational basis. To ensure that this outcome is the correct solution to a problem, with high probability, without relying on oracles or similar constructs, requires a quantum algorithm to maintain coherence and precisely control interference patterns up to the point of measurement. This precision is challenging to achieve without structures like the QFT/IQFT, which are adept at manipulating phase information across quantum states.

In summary, the conjecture that quantum algorithms providing an exponential speedup without relying on oracles and yielding a single-item result may not exist stems from the intricate interplay between quantum parallelism, interference, and the structural insights provided by oracles or QFT-like mechanisms. These components are central to the design of quantum algorithms that outperform their classical counterparts. The conjecture reflects the current understanding of quantum computing's limitations and the challenges in designing algorithms that can leverage quantum mechanics in w ways to achieve exponential speedup for a

capabilities in quantum science

	now
learning	provide definitions
studying	symbolic maths quiz creation
reviewing papers	simplistic reviewing capability
writing papers	create layout, rewriting, style checks, translations
coding	helps save time with coding and debugging
ideation	simplistic outcomes
collaborative research	translations meeting transcripts actions follow-up
experimental design	propose basic setup

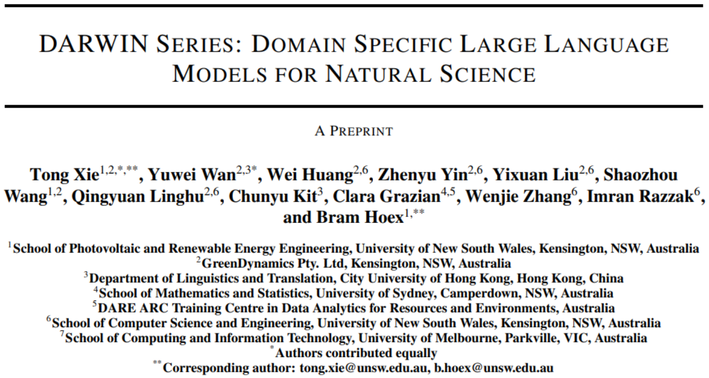
capabilities in quantum science

	now	later
learning	provide definitions	more detailed definitions
studying	symbolic maths quiz creation	charts creation creativity create and correct exercices
reviewing papers	simplistic reviewing capability	finding missing elements
writing papers	create layout, rewriting, style checks, translations	consistency checkings
coding	helps save time with coding and debugging	broader coding capabilities
ideation	simplistic outcomes	requires reasoning capabilities
collaborative research	translations meeting transcripts actions follow-up	more group work logistics
experimental design	propose basic setup	propose more detailed setups, compare vendor offerings

capabilities in quantum science

	now	later	harder
learning	provide definitions	more detailed definitions	
studying	symbolic maths quiz creation	charts creation creativity create and correct exercices	
reviewing papers	simplistic reviewing capability	finding missing elements	**critical view buildup** **charts analyzis**
writing papers	create layout, rewriting, style checks, translations	consistency checkings	**making hypothesis**
coding	helps save time with coding and debugging	broader coding capabilities	
ideation	simplistic outcomes	requires reasoning capabilities	**making hypothesis** **finding avenues**
collaborative research	translations meeting transcripts actions follow-up	more group work logistics	
experimental design	propose basic setup	propose more detailed setups, compare vendor offerings	

natural sciences



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A PREPRINT

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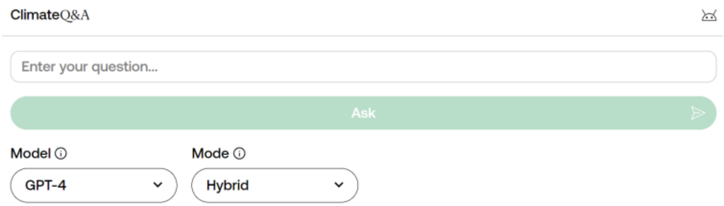

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healthcare

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chemistry

ORGANA: A Robotic Assistant for Automated Chemistry Experimentation and Characterization

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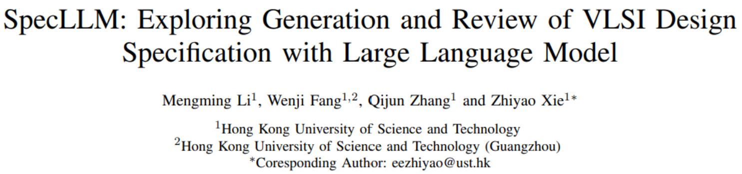
chips design



SpecLLM: Exploring Generation and Review of VLSI Design Specification with Large Language Model

Mengming Li[1], Wenji Fang[1,2], Qijun Zhang[1] and Zhiyao Xie[1*]

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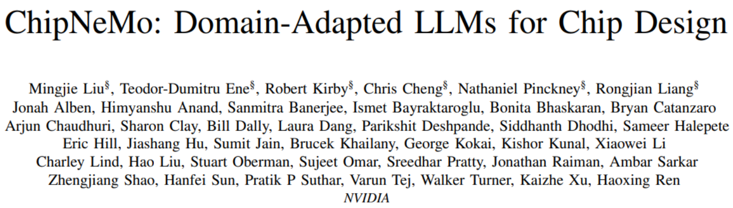
[2] Hong Kong University of Science and Technology (Guangzhou)
[*] Coresponding Author: eezhiyao@ust.hk

Using LLM such as ChatGPT for Designing and Implementing a RISC Processor: Execution, Challenges and Limitations

Shadeeb Hossain [ORCID ID: 0000-0002-5224-7684], Aayush Gohil, Yizhou Wang



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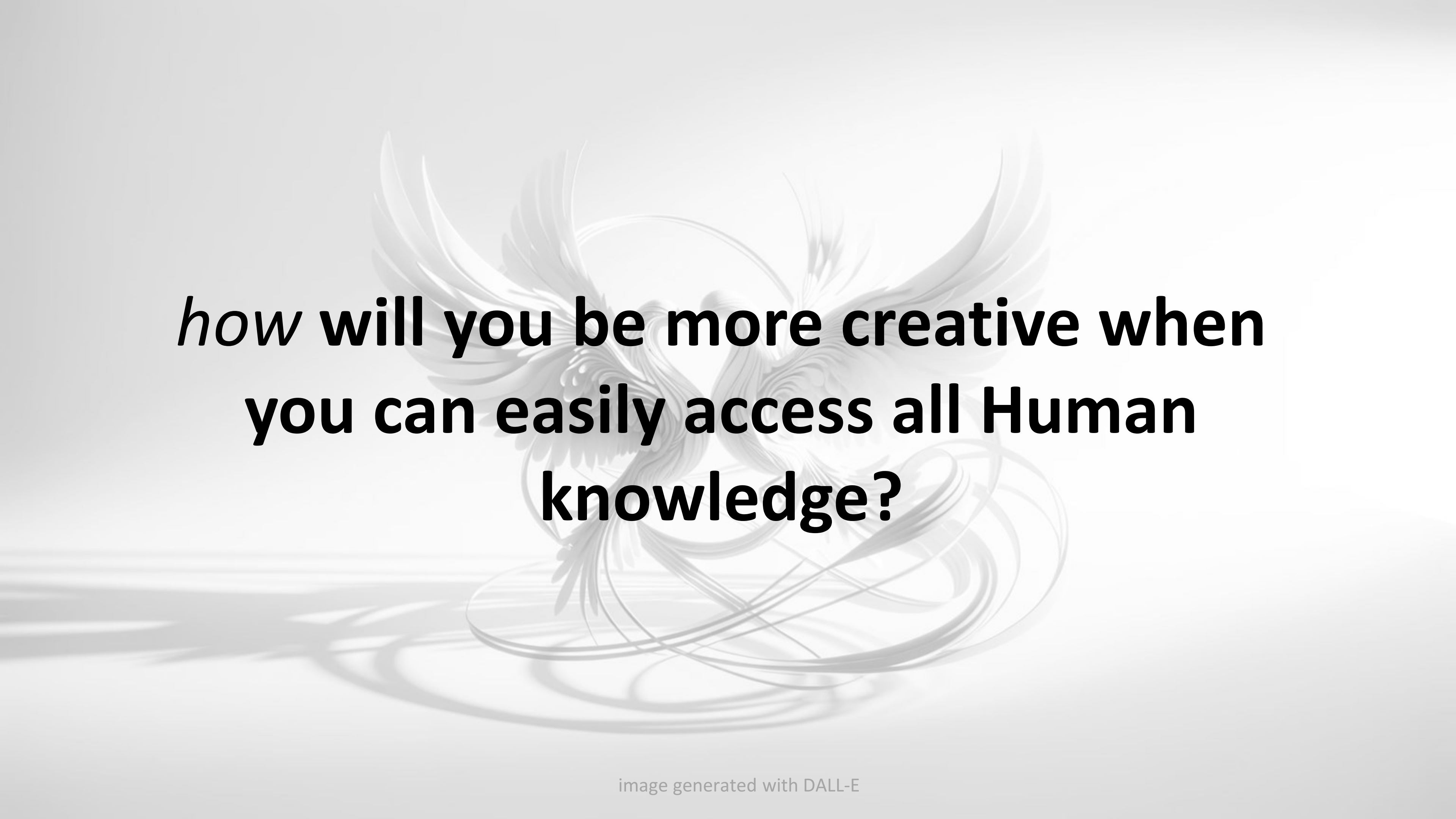
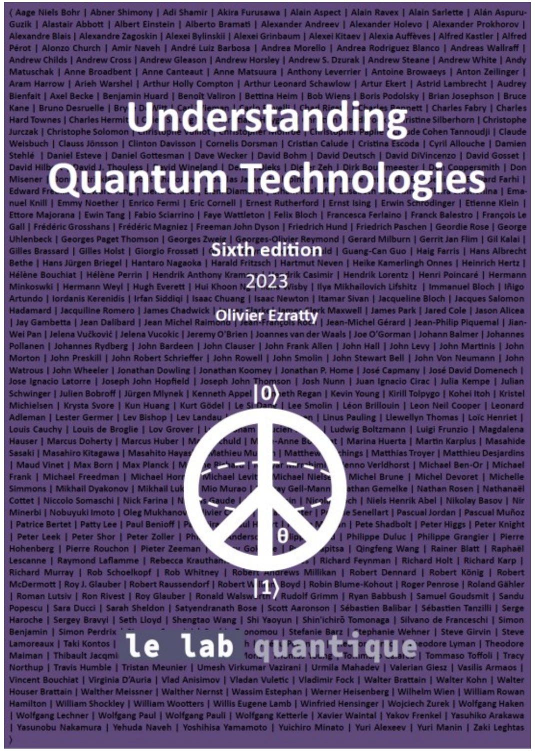


how **will you be more creative when you can easily access all Human knowledge?**

image generated with DALL-E



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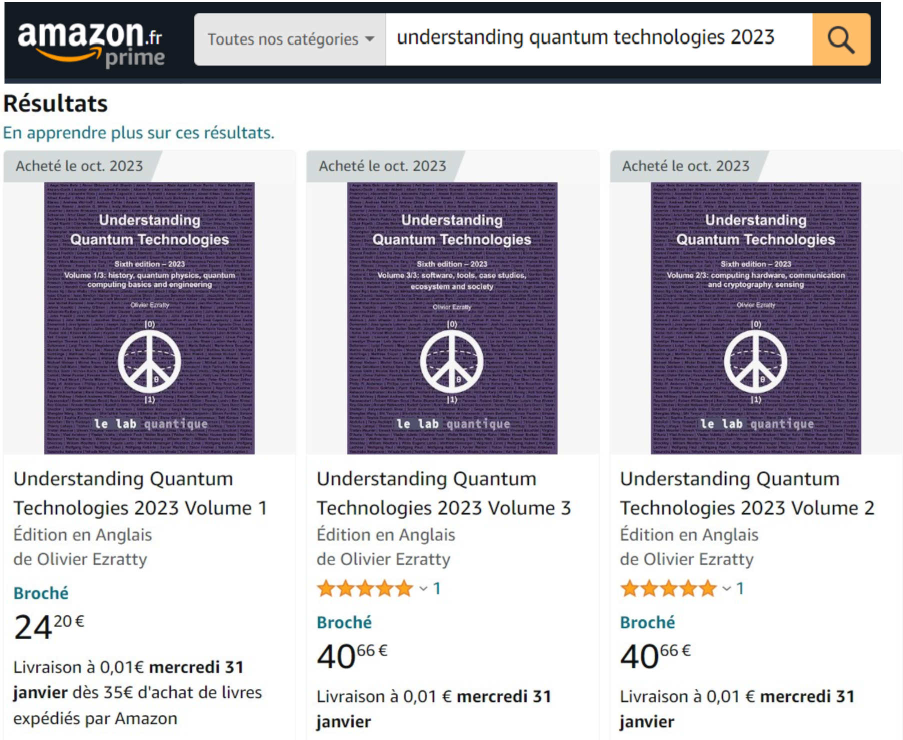

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