

AI DAYS

comment l'intelligence artificielle contribue au développement de l'informatique quantique ?

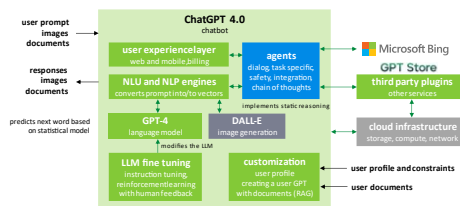
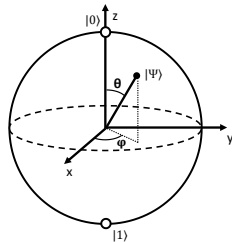
olivier eizratty

< author | ... >

AI Days, Brest, June 19th, 2024

olivier@oezratty.net www.oezratty.net @olivez

agenda

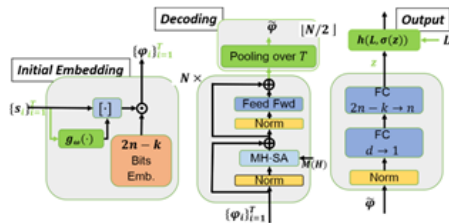


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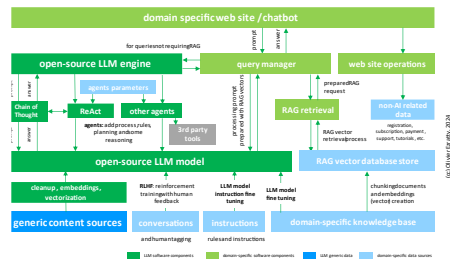
quantum computing 101

LLM-based chatbots landscape

current capabilities and limitations in quantum science



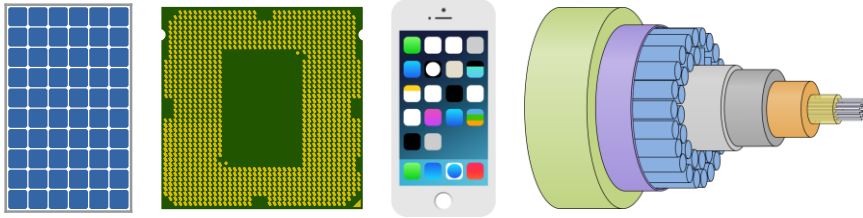
machine learning in quantum science



future use cases in quantum science

“first quantum revolution”

manipulating
groups of quantum particles
photons, electrons and atoms interactions



transistors, lasers, fiber optics, GPS
photovoltaic cells, atom clocks
medical imaging, digital photography and video
LEDs, LCD TV quantum dots

1947-*

“second quantum revolution”

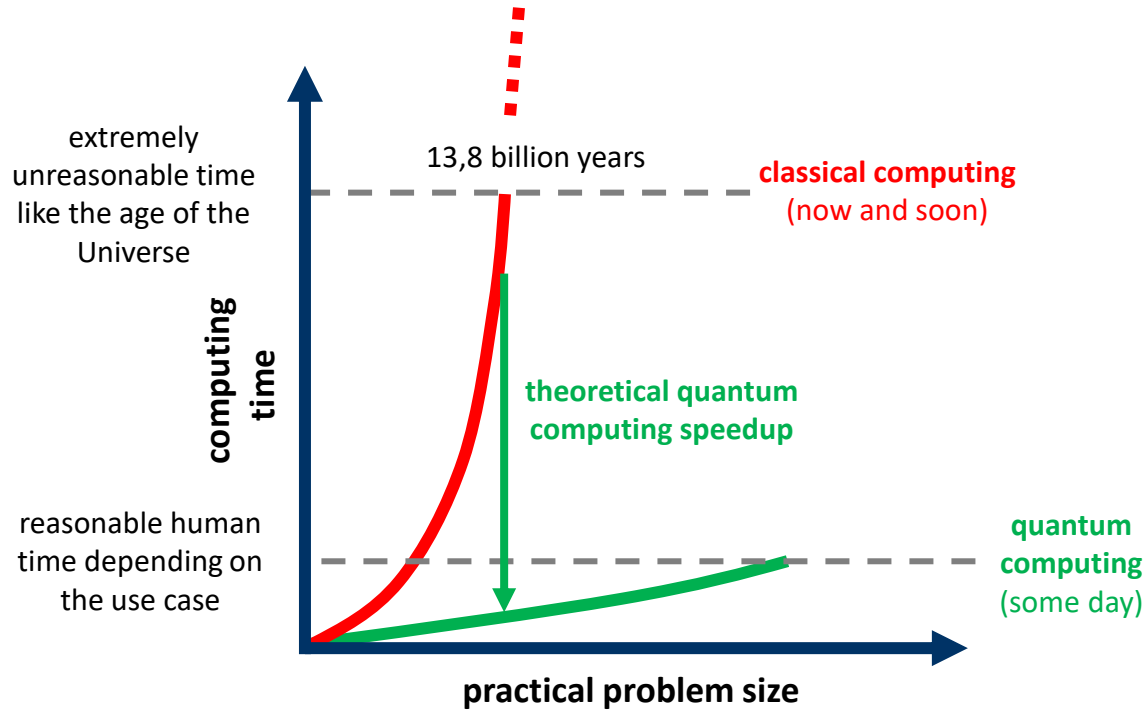
manipulating
superposition and entanglement
and/or individual particles



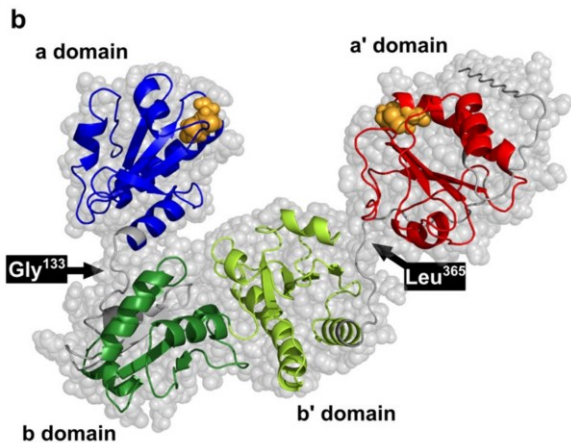
quantum computing
quantum telecommunications
quantum cryptography
quantum sensing

1982-*

the quantum computing promise

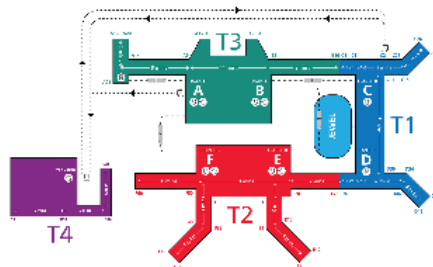


typical difficult problems

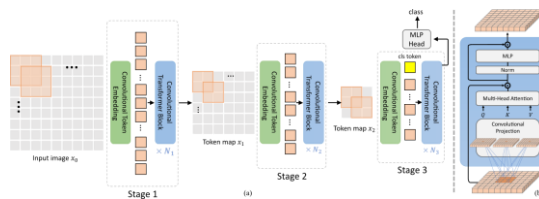


$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x,t)}{\partial x^2} + V(x)\Psi(x,t)$$

solving Schrodinger's wave equation
to simulate quantum matter



combinatorial optimizations



machine learning
and deep learning

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

solving partial differential equations



breaking asymmetric
cryptography keys

what is a qubit?

mathematically

basic unit of quantum information

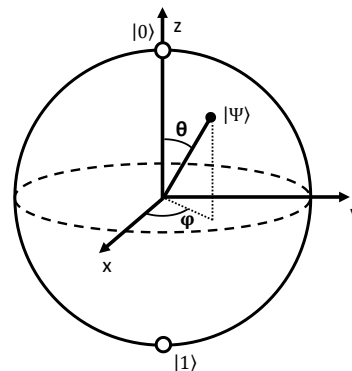
vector in a 2-dimension complex numbers Hilbert space

complex numbers amplitudes

$$|\Psi\rangle = \alpha|0\rangle + \beta|1\rangle$$

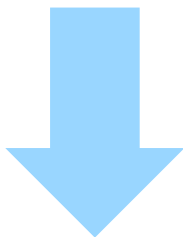
$$|\alpha|^2 + |\beta|^2 = 1$$

probabilities and Born normalization constraint

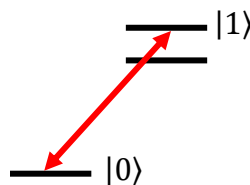


Bloch sphere representation with amplitude and phase

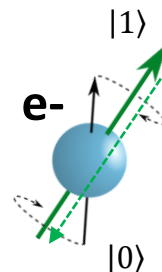
physically



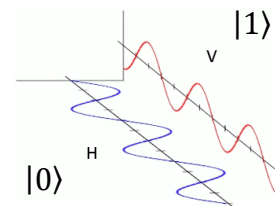
two-level state controllable quantum object



separable atom energy level



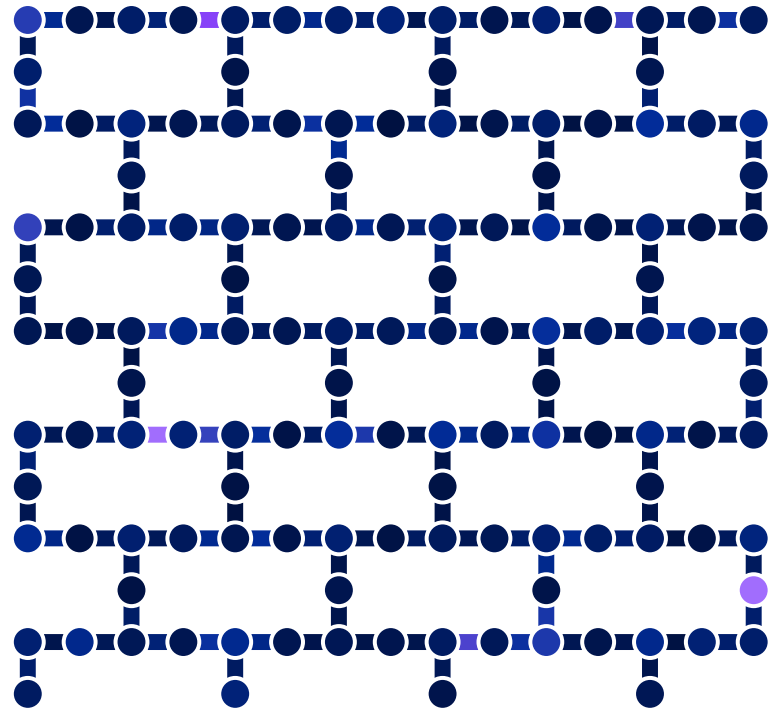
electron or nucleus spin orientation



photon mode (polarization, number, frequency)

N qubits handle the equivalent of 2^{N+1} **real numbers** during computation

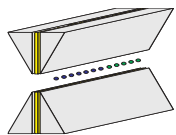
it benefits from **quantum parallelism** brought by superposition, entanglement and interferences



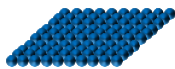
layout of a 133-qubit processor from IBM

already ≈80 QC vendors

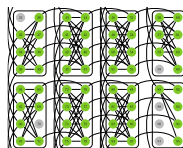
atoms



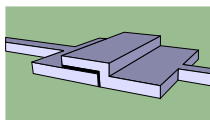
trapped ions



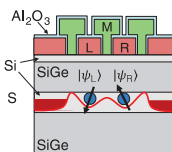
cold atoms



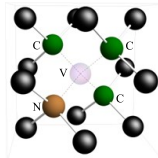
annealing



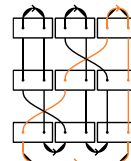
superconducting



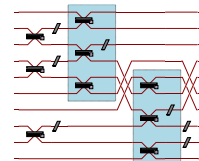
silicon



vacancies



topological



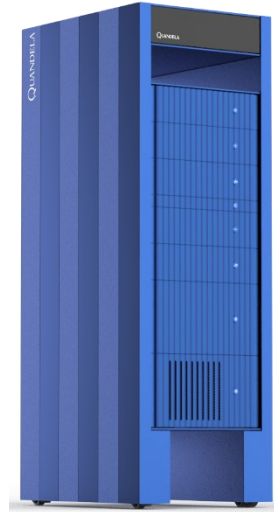
photons

electrons controlled spin and microwave cavities

photons



IBM



QUANDELA



IONQ



PASQAL



BEN
QUADINAROS



RATTS TYERELL



BOLES ROOR



DUD BOLT



ANAKIN SKYWALKER



MARS GUO



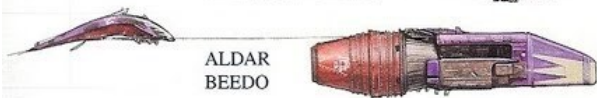
SEBULBA



TEEMTO PAGALIES



ALDAR
BEEDO



NEVA KEE



GASGANO



ARK "BUMPY" ROOSE



ODY MANDRELL



ELAN MAK



EBE ENDOCOTT



MAWHONIC



WAN
SANDAGE



CLEGG
HOLDFAST







IBM Quantum System Two – Yorktown Heights, February 2024

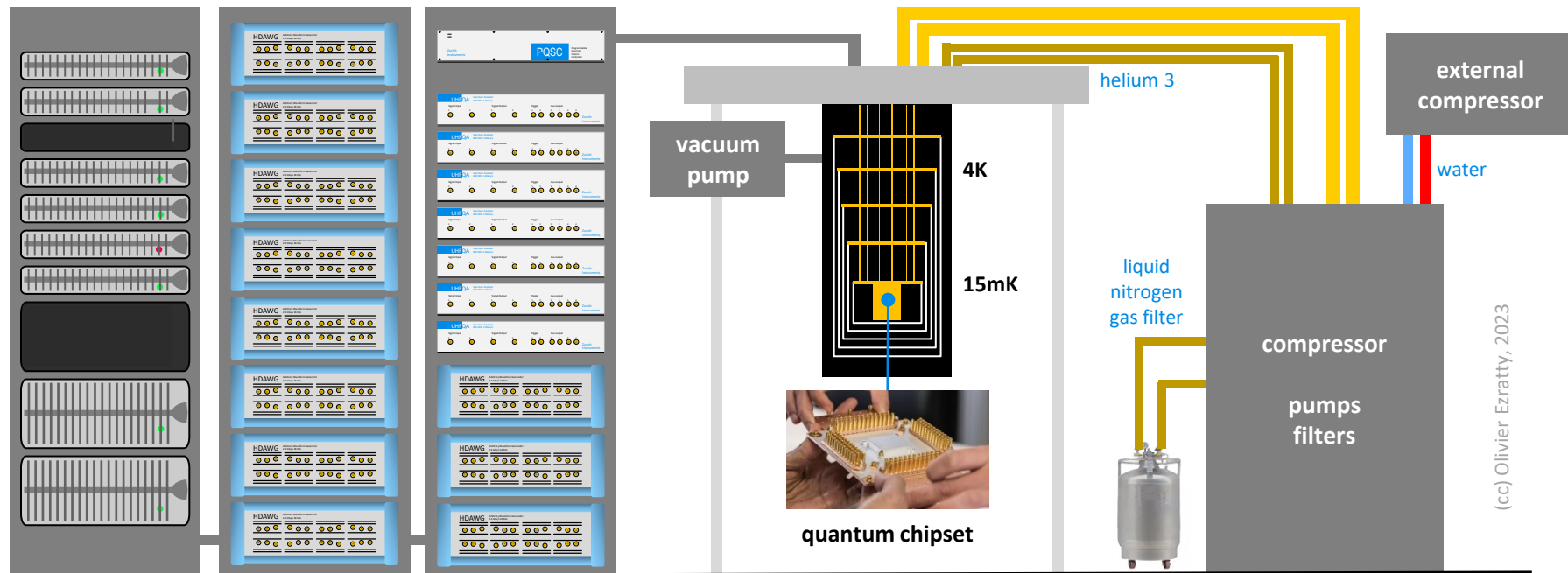
inside a typical quantum computer

computing
servers, network,
software, data

qubits control electronics
microwave generators, readout
systems and various electronics

« chandelier » in cryostat
where quantum stuff happens!

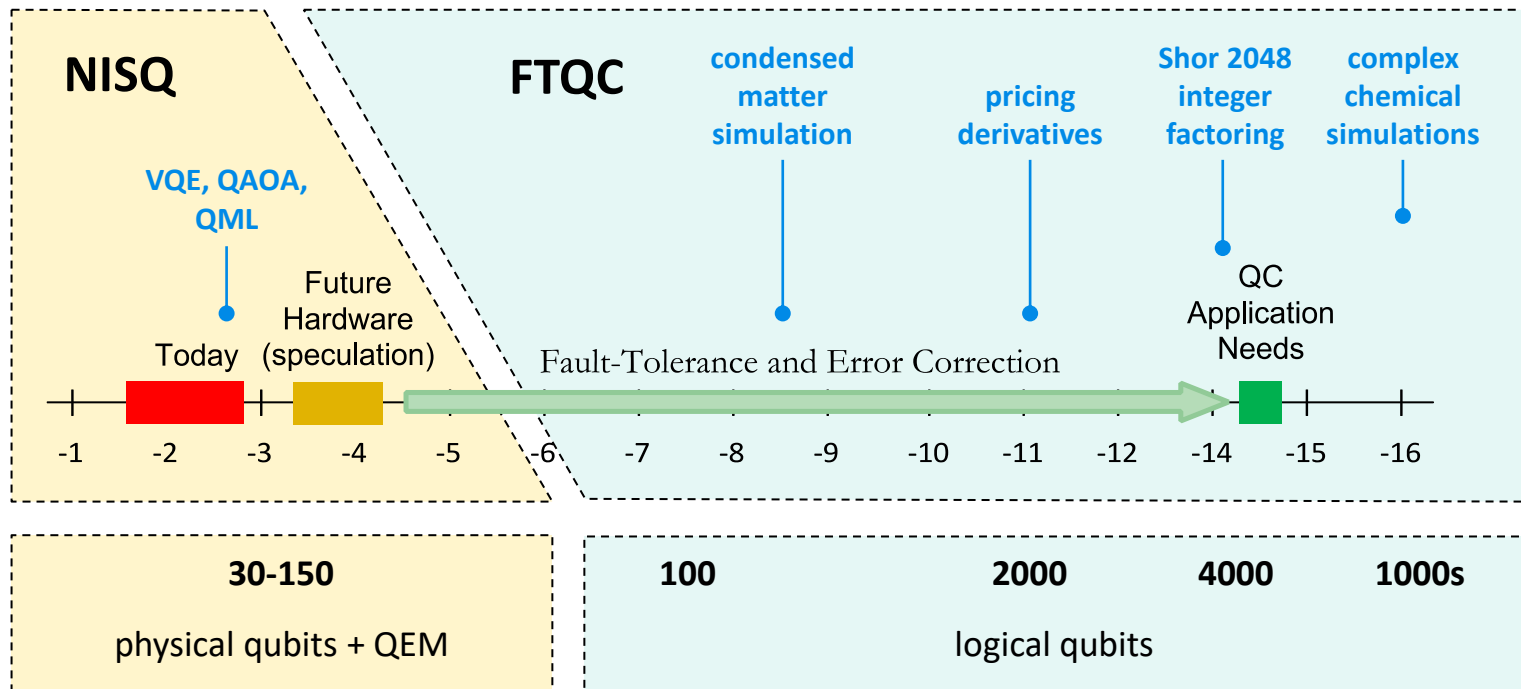
cryogenic installation
helium 3 & 4
gas pumps and compressor



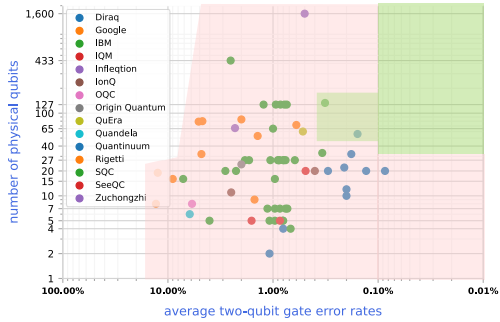
for superconducting or electron spin qubits

(cc) Olivier Ezratty, 2023

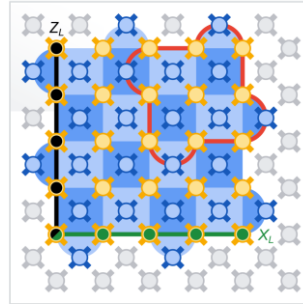
industry needs: 1,000s of logical qubits



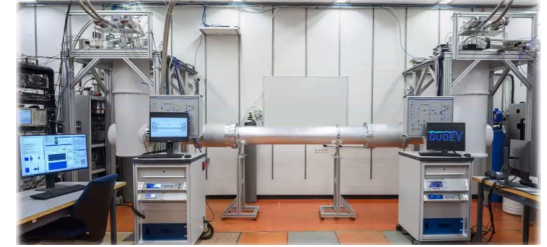
key hardware challenges



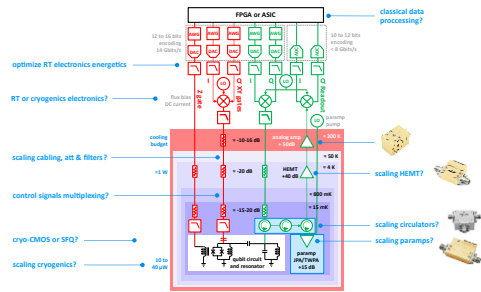
qubits fidelities



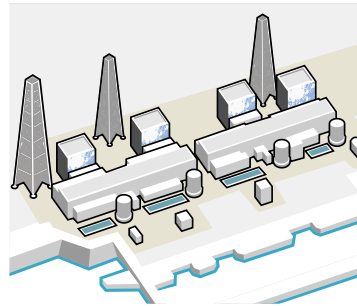
errors mitigation and correction



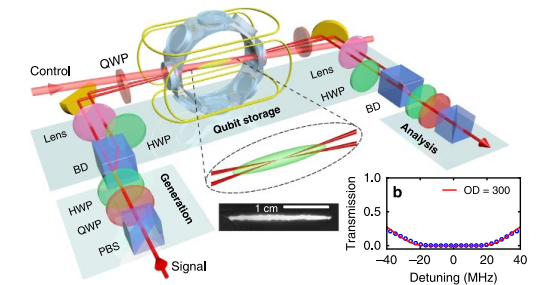
quantum interconnect



enabling technologies scalability

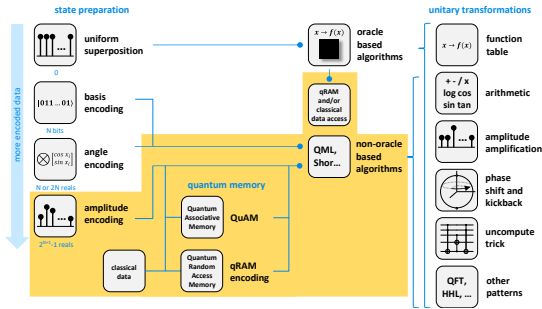


energy consumption

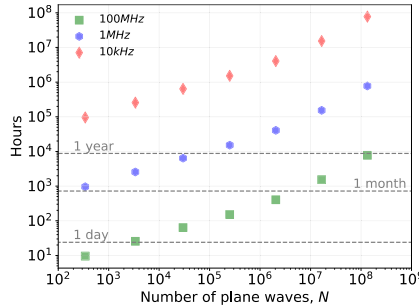


quantum memory

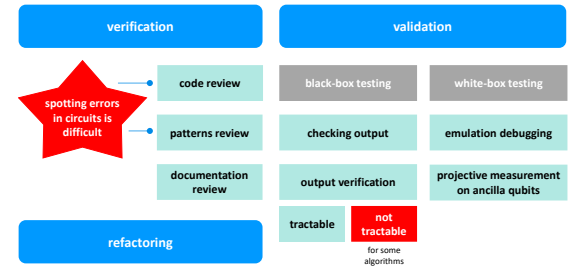
key software challenges



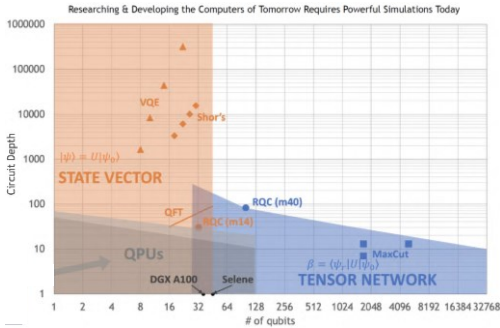
data loading



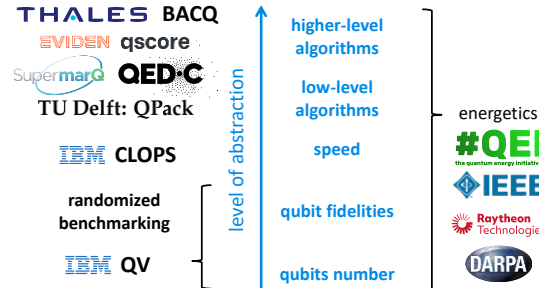
actual speedups and computing times



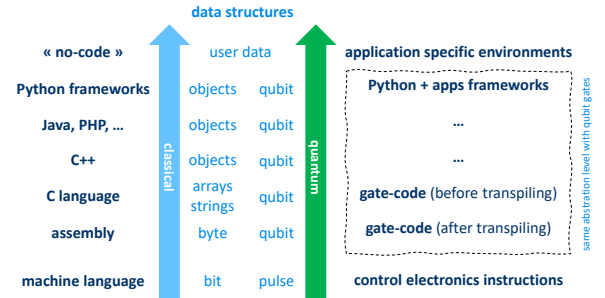
debugging, verification and certification



tensor networks competition

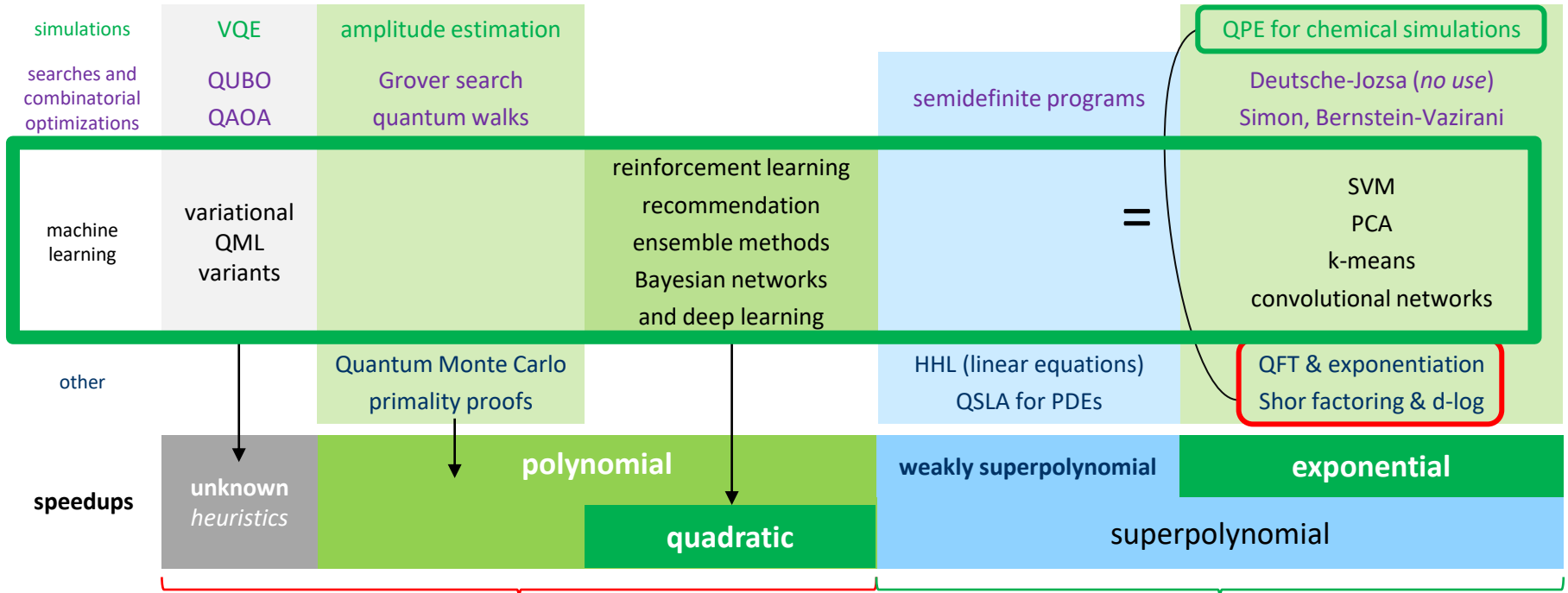


benchmarking



coding abstraction level

potential quantum speedups



limited advantage

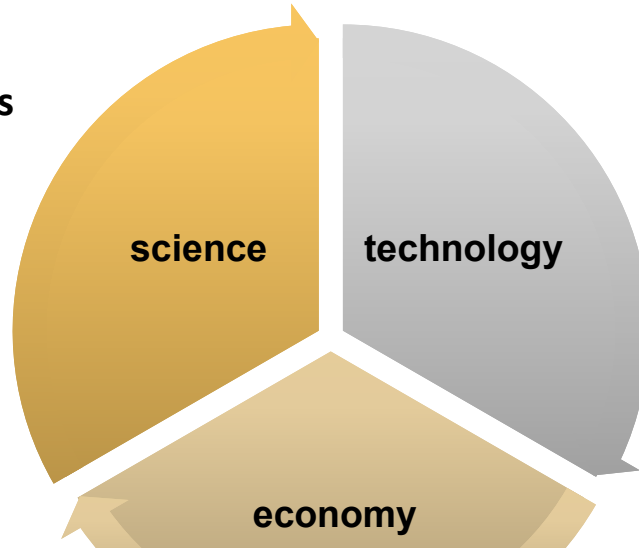
QPU fixed costs make it difficult to exceed classical computing capabilities in reasonable times and problem sizes

requires FTQC QPUs

and many logical and physical qubits with higher fidelities than today, and preferably monolithic QPUs

quantum computing challenges types

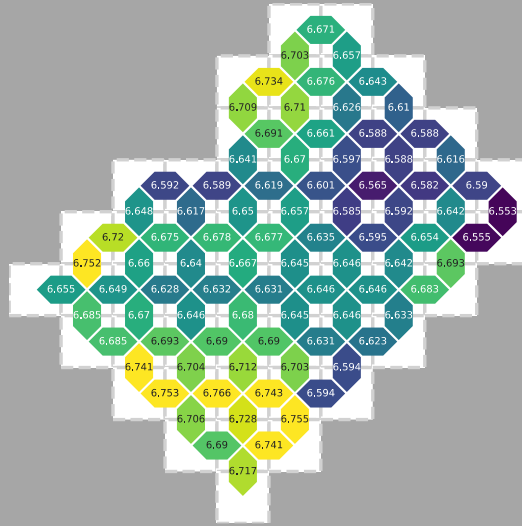
- noise models and budgets
- materials designs
- quantum control
- more efficient QEC
- cluster states generation
- quantum memory
- QPU interconnect
- algorithms speedups



- control electronics
- manufacturing
- cryogeny yield and power
- quantum emulators
- software engineering
- distributed quantum computing
- cloud infrastructure
- hybrid architectures
- benchmarking

a lot of interdisciplinarity!

- FPGA->ASIC
- VC, customer and governments funding
- fab investments
- other topics influences (LLMs, ...)

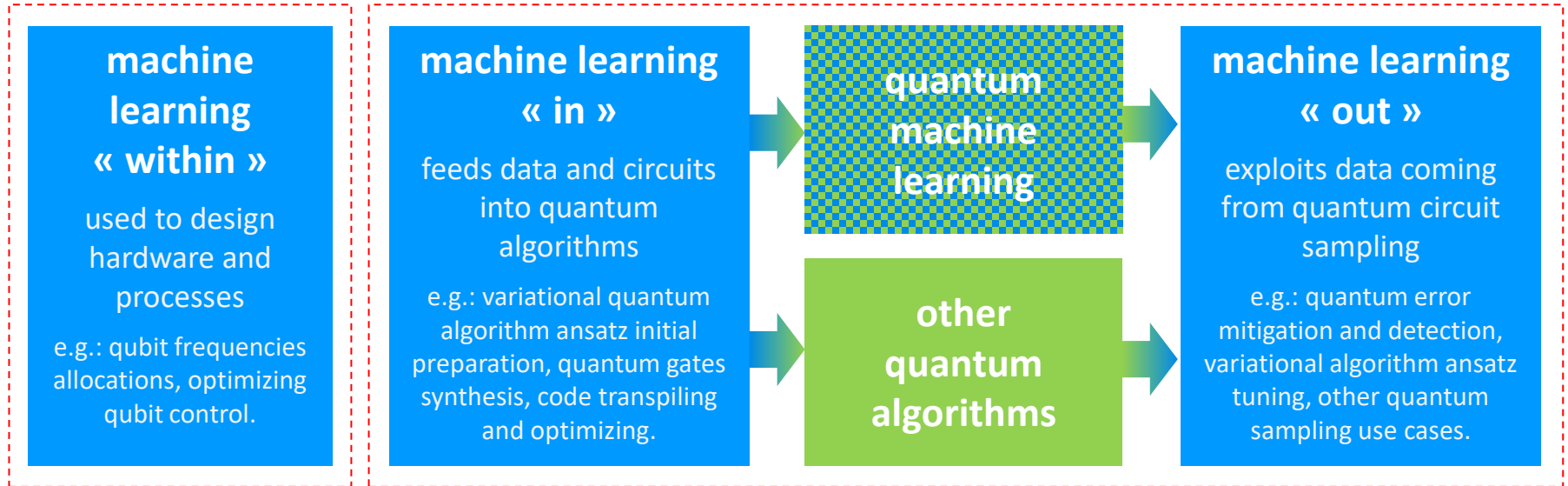


machine learning in quantum computing

where machine learning fits in?

generative AI and LLM-based chatbots

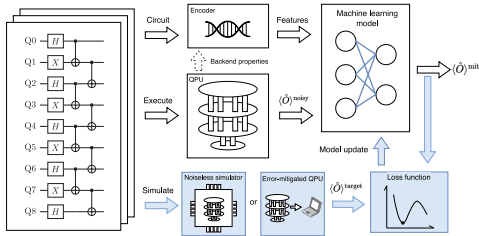
helps teach, learn, code, create charts, analyze papers, write paper, design experiments, etc.



hardware related

software related

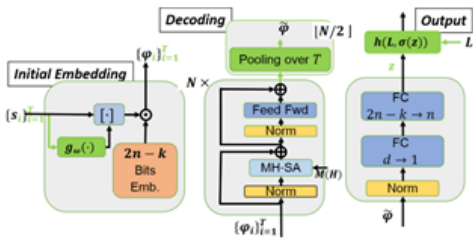
machine learning in QC



quantum error mitigation

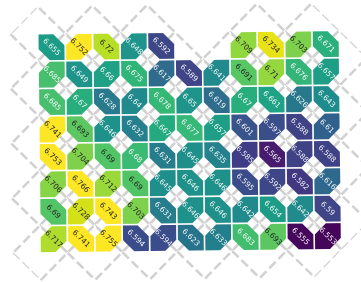
<https://arxiv.org/abs/2309.17368>

<https://arxiv.org/abs/2207.00298>



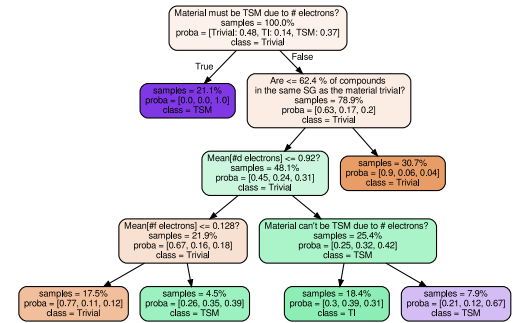
QEC error syndrome detection

<https://arxiv.org/abs/2301.11930>



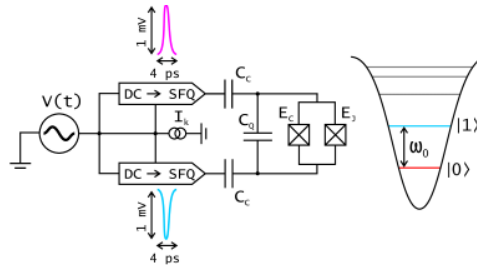
optimizing qubit frequency allocations

<https://arxiv.org/abs/1910.11333>



identification of topological materials

<https://arxiv.org/abs/1910.10161>



driving qubit control electronics

<https://arxiv.org/abs/2209.09790>

qubit gate synthesis

<https://arxiv.org/abs/2404.14865>

<https://arxiv.org/abs/2402.14396>

correcting quantum sensor noise

<https://arxiv.org/abs/1807.09753>

Transfer learning of optimal QAOA parameters in combinatorial optimization

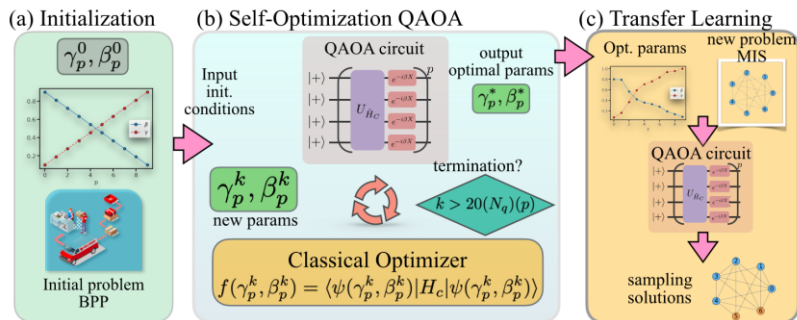
J. A. Montañez-Barrera,^{1,*} Dennis Willsch,¹ and Kristel Michielsen^{1,2,3}

¹Jülich Supercomputing Centre, Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany

²AIDAS, 52425 Jülich, Germany

³RWTH Aachen University, 52056 Aachen, Germany

3



<https://arxiv.org/abs/2402.05549>, February 2024

Quantum Machine Intelligence (2023) 5:4
<https://doi.org/10.1007/s42484-022-00092-y>

RESEARCH ARTICLE



Boosting the performance of quantum annealers using machine learning

Jure Brenc ^{1,2,3} · Dragan Mihailović^{4,5,6} · Viktor V. Kabanov⁴ · Ljupčo Todorovski^{1,3} · Sašo Džeroski^{1,2} · Jaka Vodeb^{4,6}

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<https://link.springer.com/article/10.1007/s42484-022-00092-y>

January 2023

Quantum Circuit Discovery for Fault-Tolerant Logical State Preparation with Reinforcement Learning

Remy Zen,^{1,*} Jan Olle,¹ Luis Colmenarez,^{2,3} Matteo Puviani,¹ Markus Müller,^{2,3} and Florian Marquardt^{1,4}

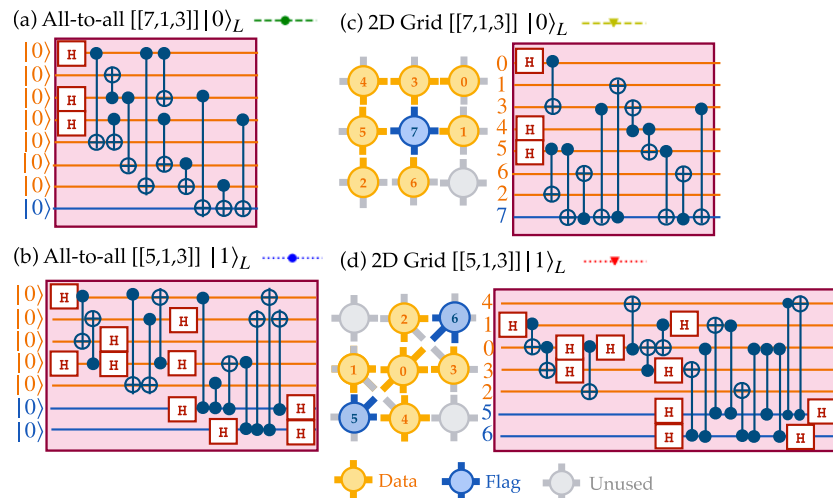
¹Max Planck Institute for the Science of Light, Staudtstraße 2, 91058 Erlangen, Germany

²Institute for Quantum Information, RWTH Aachen University, 52056 Aachen, Germany

³Peter Grünberg Institute, Theoretical Nanoelectronics, Forschungszentrum Jülich, 52425 Jülich, Germany

⁴Department of Physics, Friedrich-Alexander Universität Erlangen-Nürnberg, Staudtstraße 5, 91058 Erlangen, Germany

(Dated: February 28, 2024)



<https://arxiv.org/abs/2203.02360>, February 2024

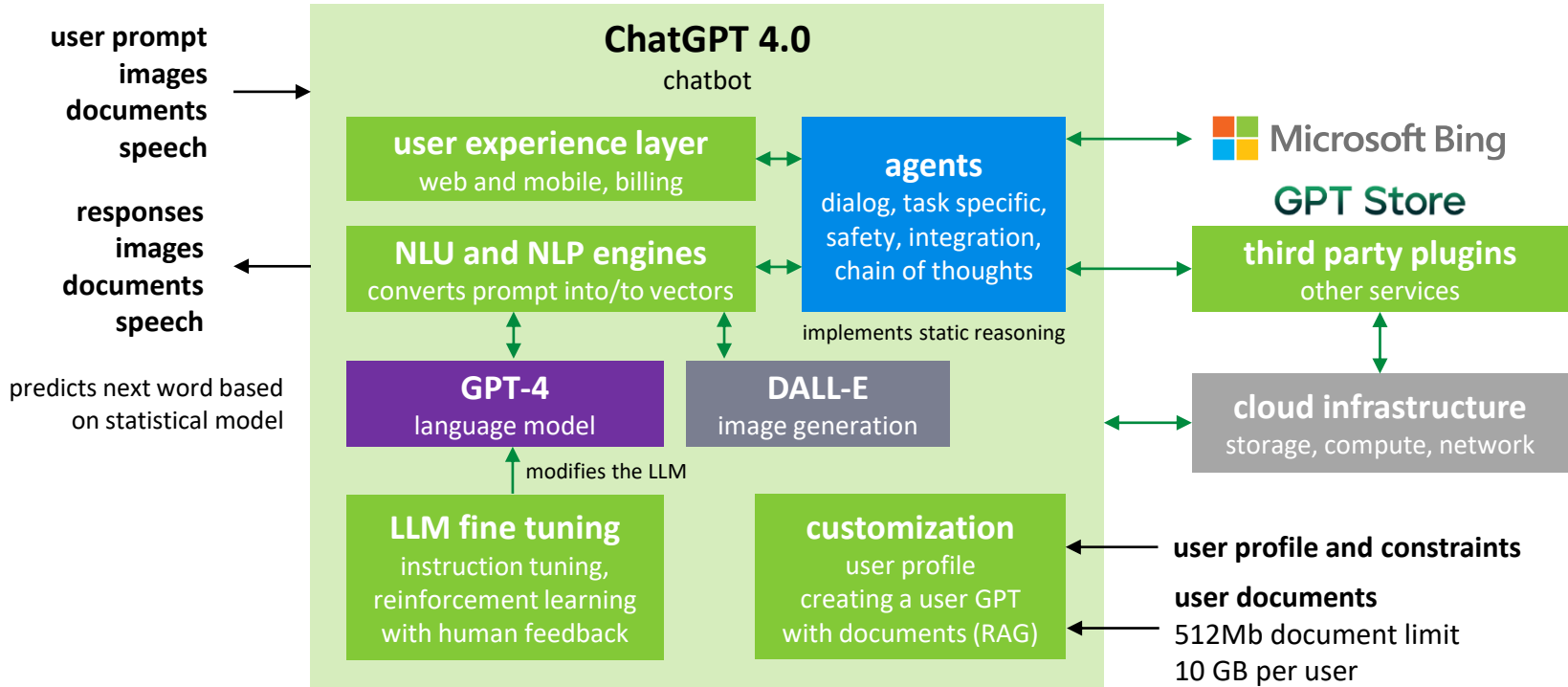


LLM-based chatbots landscape

LLM-based chatbots figures of merit

figures of merit	ChatGPT 4.0
training set in # of tokens	not public, 2.6T to 13T
cut-off training date	april 2023 + Bing updates
parameters # in neural network	not public, > 1.5T
embedding dimensions	>12K
context windows in # of tokens	>32K
response speed	typewriting speed, 30 s for image generation
power/resource consumption	not public, >100K Nvidia GPGPUs
pricing	\$20/month, free in Bing Copilot

ChatGPT 4.0 overall architecture



#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 capabilities and limitations in quantum science

current *amazing* use cases

1. **quantum science knowledge**: performing well in many fields.
2. **figures of merit**: photon sources, detectors, circulators, TWPA.
3. **inventories**: materials, research avenues in some domain.
4. **simple maths and logic** and continuously improving.
5. **bibliography**: getting better with ChatGPT 4.0.
6. **coding**: Python for creating charts, PHP, regex, VBA, ...
7. **non-scientific memos**: policy making, quantum winter, ...

figures of merit



You

can you describe the figures of merit of photon number resolving detectors?



ChatGPT

Photon Number Resolving (PNR) detectors are pivotal instruments in quantum optics and quantum information processing, capable of distinguishing between different numbers of incident photons. Their performance is characterized by several key figures of merit, which determine their suitability for various applications, including quantum computing, quantum cryptography, and optical quantum information processing. Understanding these figures of merit is essential for evaluating the effectiveness and efficiency of PNR detectors in specific quantum experiments or technologies.


Quantum Efficiency (QE)

Quantum Efficiency refers to the probability that an incident photon will produce a detectable signal. A high QE is crucial for ensuring that the detector can accurately count the number of photons without missing too many of them. It's a primary measure of the detector's sensitivity, with values typically expressed as a percentage. Higher QE means that the detector is more likely to accurately represent the number of photons that strike it.

Dark Count Rate

The Dark Count Rate measures the frequency at which a detector registers a count without any photon input, due to thermal fluctuations or other internal processes. This is essentially the "noise floor" of the device, and a lower dark count rate is desirable for high-precision measurements, especially in low-light or single-photon applications, where false counts can significantly impact the accuracy of photon number resolution.

Photon Number Resolution

This indicates the detector's ability to discriminate between different numbers of incident photons. A high-resolution detector can distinguish between one, two, three, or more photons arriving simultaneously or nearly simultaneously at the detector. The resolution is often limited by the detector's intrinsic noise and the statistical  nature of the photon detection process.


Timing Resolution (Jitter)

Timing resolution, or jitter, refers to the precision with which the detector can measure the arrival time of photons. This is particularly important in applications involving time-correlated photon counting or when precise timing information is necessary to interpret the quantum states of photons. Lower jitter corresponds to more precise temporal resolution, allowing for finer time-correlated measurements.

Dead Time

Dead time is the period immediately following a detection event during which the detector is unable to register another photon. During this time, any incoming photons will not be detected. Shorter dead times allow for higher counting rates and are particularly important in high-flux situations where photon events occur in rapid succession.

Saturation

Saturation occurs when the number of incident photons exceeds the detector's ability to count them accurately, leading to a plateau in the count rate regardless of increased photon flux. The saturation level gives an upper limit to the detector's counting capability before the accuracy of photon number resolution degrades. 

Linearity

Linearity refers to the detector's ability to maintain accurate photon counting as the photon flux increases. A linear response means the detected signal increases proportionally to the number of incident photons, crucial for quantitatively accurate measurements over a range of light intensities.

Crosstalk

In detector arrays or multi-pixel detectors, crosstalk measures the extent to which a signal in one pixel or detector element affects the signal in another. Lower crosstalk is critical for accurate spatial resolution and photon counting when multiple detectors are used in proximity.

Each of these figures of merit plays a crucial role in determining the suitability of a PNR detector for specific applications. Advances in detector technology continue to improve these metrics, pushing the boundaries of quantum measurement capabilities and enabling new experiments and technologies in the quantum realm.

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 (AlO_x):** 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 tantalum 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.

simple maths and logic



You

let's do some symbolic mathematics

can you show a unitary matrix corresponding to the application of a CNOT gate on 2 qubits in a 4 qubit register?



ChatGPT

The unitary matrix corresponding to the application of a CNOT gate on the second and third qubits in a 4-qubit register is a 16×16 matrix, structured to represent the operation across the entire register. Here's how the matrix looks:

plot creation

(uploaded) FidelityClusters.csv

can you create a scatter plot in log-log scale with the qubit number and the two qubit gate error rates?

new could you use a different color and a circle for each point, related to the company name? and invert the X and the Y?

can you provide the Python code to generate this plot?

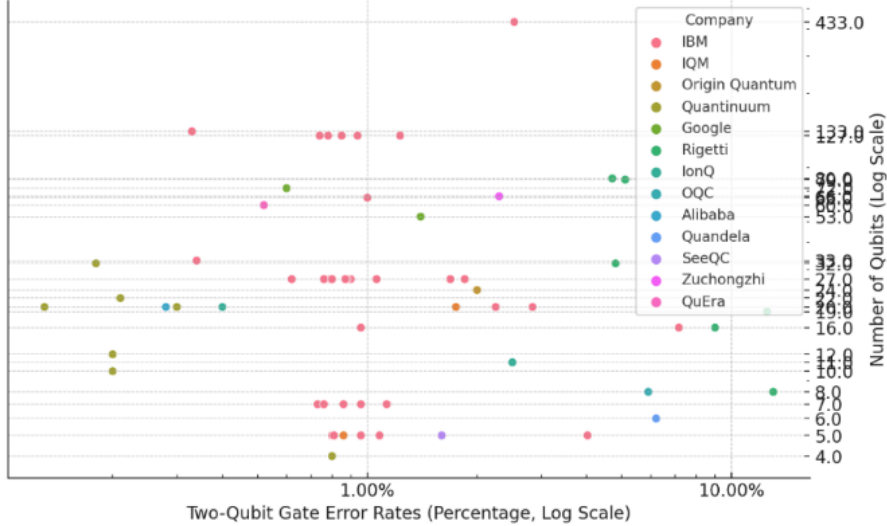
now can you change the Y scale and create marks for each possible values instead of the powers of 10, and put the Y scale at the right of the chart?

can you show the resulting chart?

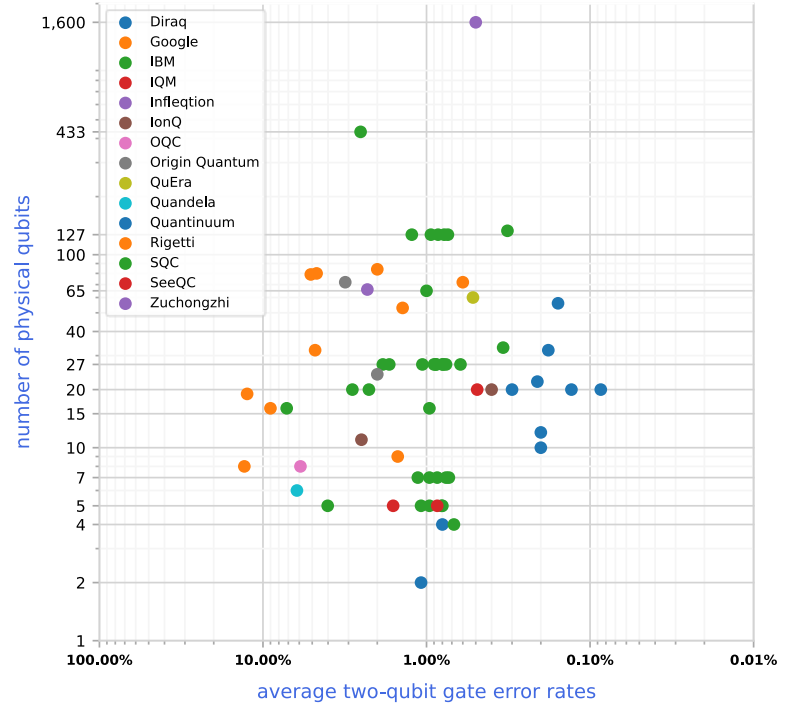
could you use a log scale on Y ? and use labels in % for the X axis?

well, in Y, I needed to have a log scale and the ticks corresponding to the values in the plot

Scatter Plot: Two-Qubit Gate Error Rates vs. Number of Qubits (Log-Log Scale)



result after 5 minutes



what took me >10 hours in 2023

coding

```
python Copy code

from qiskit import Aer
from qiskit.algorithms import Shor
from qiskit.utils import QuantumInstance

# Setting up the quantum instance (simulator)
backend = Aer.get_backend('aer_simulator')
quantum_instance = QuantumInstance(backend, shots=1024)

# Number to be factored
N = 15 # Example number to factor
num_qubits = 10 # Number of qubits

# Initialize Shor's algorithm with the number of qubits
shor = Shor(num_qubits=num_qubits, quantum_instance=quantum_instance)

# Execute the algorithm to factorize the number
result = shor.factor(N)

# Print the result
print(result['factors'], result['total_counts'])
```

coding with ChatGPT 4.0

```
qiskit_code_assistant.py X ▶ □ ⋮

1 from qiskit import QuantumCircuit
2 from qiskit.primitives import Sampler
3 from quantum_serverless import save_result
4
5 # Define a Bell circuit, run it using the Qiskit Sampler
  primitive (not the Runtime one)
6 # take the quasi_dists result from Sampler and save it using
  save_result from quantum_serverless

circuit = QuantumCircuit(2)
circuit.h(0)
circuit.cx(0, 1)
circuit.measure_all()

sampler = Sampler()
quasi_dists = sampler.run(circuit).result().quasi_dists

save_result(quasi_dists)
```

Watsonx in Qiskit,
Q4T project,
Python, PHP, ...

quiz creation

OE

You

I am a teacher in quantum computing. Create an educational quiz with 8 questions on quantum computing with multiple choices and the related responses. Multiple responses are possible in some of the questions in the quiz, with between 1 and 3 good responses out of 4. The level of the quiz should correspond to master's degree level. It can test the ability to understand circuit quantum programming.



ChatGPT

Certainly! Below is an educational quiz designed for master's degree level students with a focus on quantum computing and the understanding of circuit quantum programming. The questions range from fundamental concepts to more applied aspects of quantum computing.

Quiz: Mastering Quantum Computing

Question 1: What is the fundamental unit of quantum information?

- A) Bit
- B) Byte
- C) Qubit
- D) Quantum gate
- **Correct Answer:** C) Qubit

Question 2: Which of the following are properties of quantum entanglement? (Multiple answers possible)

- A) Two or more qubits become interconnected such that the state of one cannot be described without the state of the others.
- B) Changing the state of one entangled qubit instantaneously changes the state of the other, regardless of distance.
- C) Entangled qubits always have opposite spins.
- D) Entanglement allows classical bits to be teleported.
- **Correct Answers:** A) and B)

Question 3: What is the purpose of a quantum gate in a quantum circuit?

- A) To measure the qubits
- B) To initialize the qubits to a known state
- C) To perform classical logical operations
- D) To manipulate the quantum states of the qubits
- **Correct Answer:** D) To manipulate the quantum states of the qubits

Question 4: Which of the following quantum gates is used to create superposition?

- A) X-gate
- B) Z-gate
- C) Hadamard gate
- D) CNOT gate
- **Correct Answer:** C) Hadamard gate

Question 7: What is the significance of the Bell state in quantum computing?

- A) It represents the fastest quantum algorithm for database search.
- B) It is a type of quantum error correction code.
- C) It is an example of a maximally entangled state of two qubits.
- D) It is used to benchmark the speed of quantum processors.
- **Correct Answer:** C) It is an example of a maximally entangled state of two qubits.

Question 8: Which of the following are applications of quantum computing? (Multiple answers possible)

- A) Quantum simulation
- B) Database management
- C) Quantum cryptography
- D) Drug discovery
- **Correct Answers:** A), C), and D)

Question 5: In quantum error correction, what is the purpose of syndrome measurement?

- A) To reset the qubits to their initial state
- B) To directly correct errors in the qubits without measuring them
- C) To identify the type of error that occurred without disturbing the quantum information
- D) To entangle additional qubits for error correction
- **Correct Answer:** C) To identify the type of error that occurred without disturbing the quantum information

Question 6: Which of the following statements are true about the no-cloning theorem in quantum computing? (Multiple answers possible)

- A) It states that it is impossible to create an identical copy of an arbitrary unknown quantum state.
- B) It implies that quantum information cannot be copied to protect against eavesdropping in quantum communication.
- C) It allows quantum algorithms to solve problems faster than classical algorithms.
- D) It prohibits the cloning of quantum states but allows for the cloning of classical states.
- **Correct Answers:** A) and B)





You

in quantum physics, what is the difference between heralding and post-selection?



ChatGPT

In the realm of quantum physics, both heralding and post-selection are techniques used to prepare quantum states with desirable properties for various applications, including quantum computing, communications, and sensing. Despite their similar goals, these techniques operate under different principles and have distinct implications for the experimental setups and the interpretation of results.

Heralding is a technique where the generation of a desired quantum state is signaled by an external event or measurement, often referred to as a "herald." This process typically involves entangled particle pairs, where the detection of one particle in a specific state indicates (or heralds) that its entangled partner is in a corresponding quantum state, without directly measuring the state of the latter. The advantage of heralding lies in its non-destructive nature regarding the quantum state of interest, allowing further manipulation or measurement. Heralding is widely used in quantum communication protocols, such as quantum key distribution, where it ensures the successful preparation of entanglement between distant parties without compromising the security of the protocol.

Post-selection, on the other hand, is a process where a subset of all measured quantum states is selected after the measurement based on the outcome. This technique effectively "filters" the outcomes to isolate a particular state or set of states that meet predefined criteria. Unlike heralding, post-selection involves directly measuring the state of the system and then discarding all outcomes that do not match the desired condition. This approach can lead to the preparation of specific quantum states or the demonstration of quantum phenomena, such as quantum teleportation or violation of Bell's inequalities, but it often requires discarding a large number of trials, leading to inefficiencies.

The key difference between these two techniques lies in the timing and impact of the measurement process. Heralding relies on a correlation between particles that allows one particle to serve as a reliable indicator of the state of its partner, thus preserving the quantum state for further use. In contrast, post-selection operates by filtering out undesired outcomes after the fact, which can significantly reduce the efficiency of state preparation but allows for the exploration of specific quantum phenomena that may not be accessible through heralding.



You

in the scientific literature, qubit gate fidelities are often presented like this: 99.914(3)% what is the meaning of the number between parentheses?



ChatGPT

In scientific literature, when qubit gate fidelities are presented as "99.914(3)%", the number in parentheses—(3) in this case—indicates the uncertainty or the error margin of the last digits in the reported measurement. This is a concise way to express the standard error or uncertainty associated with the measurement.

Here's a breakdown of what each part means:

- **99.914%** is the central or mean value of the fidelity. It suggests that the fidelity of the qubit gate, or how well it performs its intended operation, is 99.914%.
- **(3)** is the uncertainty in the last digit of the fidelity, scaled to the same decimal place. In this case, it indicates an uncertainty of 0.003%. This means the true fidelity is expected to be within the range of 99.911% to 99.917%.

This notation helps in understanding the precision of quantum gate operations and is crucial for developing reliable quantum computing systems.





can you make a list of the most common misconceptions on quantum computing?



Sure, here are some common misconceptions about quantum computing:

1. **Quantum Computers Can Solve All Problems Faster:** Quantum computers are not universally faster than classical computers. They excel at specific types of problems, such as factoring large numbers or simulating quantum systems, but for many tasks, classical computers are still more efficient.
2. **Quantum Computers Are Just More Powerful Classical Computers:** Quantum computers operate on entirely different principles, leveraging quantum bits (qubits) and phenomena like superposition and entanglement, which do not have classical analogs.
3. **Qubits Can Be in Multiple States Simultaneously:** While it's true that qubits can be in a superposition of states, it's a common misunderstanding to think of them as being in multiple states at once. Instead, they exist in a complex probability distribution until measured.
4. **Quantum Computers Will Replace Classical Computers:** Quantum computers are not expected to replace classical computers but rather to complement them. They will be used for specific applications where they have an advantage, while classical computers will continue to handle the vast majority of tasks.
5. **Quantum Computers Can Instantly Solve NP-Complete Problems:** Quantum computers do not solve NP-complete problems instantaneously. They offer potential speedups for certain problems, but this does not translate to an immediate solution for all computationally hard problems.
6. **Building a Quantum Computer is Just a Matter of Scaling Up:** Scaling up quantum computers is exceptionally challenging due to issues like qubit coherence and error rates. Current quantum computers are still in the experimental stage, with significant engineering challenges to overcome.
7. **Quantum Supremacy Means Quantum Computers are Superior:** Quantum supremacy is a term used to describe the point at which a quantum computer can solve a problem that a classical computer practically cannot. It doesn't mean quantum computers are superior in all aspects or applications.
8. **Quantum Computing Requires Only Quantum Physics Knowledge:** While quantum mechanics is fundamental, building and operating quantum computers also require knowledge in computer science, electrical engineering, cryogenics, materials science, and error correction techniques.
9. **Entanglement Equals Instant Communication:** Quantum entanglement does not allow for faster-than-light communication. While entangled particles share states, any attempt to use this for communication still adheres to the speed of light limit imposed by relativity.
10. **Quantum Computers are Ready for Practical Use:** Despite significant progress, quantum computers are not yet ready for widespread practical use. They are still in the research and development phase, with many technical hurdles to overcome before they can be used for practical, large-scale applications.

Ψ PsiQuantum

OE You

would it make sense for a western country government to invest \$600M in a US quantum computing company to have them install one of their offices in there, when their own quantum investment has been of about \$600M in 20 years ? how about their local startups?

ChatGPT

Investing \$600 million in a U.S. quantum computing company to establish an office in a Western country can be seen as a strategic move, depending on several factors such as the country's long-term technology goals, the current state of its local quantum ecosystem, and the expected economic and technological returns from such an investment.

From an economic and technological standpoint, inviting a major U.S. quantum computing firm to set up an office could have significant advantages:

- 1. Technology Transfer and Skill Development:** The presence of a leading quantum computing company could facilitate the transfer of advanced technologies and know-how to the local workforce. This can enhance the skills of local engineers and scientists, contributing to the country's quantum technology capabilities.
- 2. Stimulation of Local Ecosystem:** The entry of a major player can stimulate the local quantum ecosystem by creating a competitive environment that might attract further investments and encourage innovation among local startups. It can also lead to the formation of partnerships and collaborations between the U.S. company and local entities.
- 3. Economic Benefits:** The investment could lead to direct economic benefits such as job creation, increased tax revenues, and potential growth in ancillary industries. These benefits may justify the substantial investment.
- 4. Global Positioning:** Establishing a partnership with a leading international company can position the country as a significant player in the global quantum technology market, potentially attracting further international investments.

However, there are also potential downsides and risks to consider:

- 1. Neglect of Local Startups:** A large focus on a foreign company might overshadow local startups, potentially depriving them of needed resources and attention. This could stifle local innovation and may result in a dependency on foreign technology.
- 2. Cost vs. Benefit:** The return on investment needs careful consideration, especially when the investment amount matches the total invested in the field over two decades. The outcomes should justify the allocation of such a significant portion of public funds.
- 3. Strategic Dependency:** Relying on a foreign company for advancements in critical technology like quantum computing might lead to strategic dependencies which could be unfavorable in long-term geopolitical scenarios.

Given these points, it would be wise for the government to consider a balanced approach that not only fosters international collaboration but also robustly supports local enterprises. This could include matching investments in local startups, providing grants for research and development, and creating incentives for collaboration between the U.S. company and local entities. Such a dual approach could maximize the benefits while mitigating the risks associated with high dependency on a foreign entity.



crafting a NQI memo for policy makers



Could explain how the Shor integer algorithm works using a Shakespeare style?

Could you do the same using the style of Donald J Trump ?

ChatGPT

Certainly! Let's imagine how Donald J. Trump might describe Shor's algorithm, renowned for its ability to factorize large numbers, a key challenge in cryptography, in his characteristic style:

"Okay, folks, listen up, I've got something tremendous to tell you about. It's called Shor's algorithm – and believe me, it's huge. This thing, it's a quantum algorithm, not your ordinary, everyday algorithm, but a quantum one. It's the best, really fantastic, for breaking codes and solving big, big numbers. We're talking about numbers so big, you wouldn't believe it.

Now, let me tell you, nobody knows algorithms better than me. And this Shor, he's a smart guy, really smart. He figured out how to use these tiny, tiny things called qubits.

Qubits, unlike regular bits, they can be in multiple states at once – it's like, they can be in New York and Florida at the same time. Can you believe it?



science du mi-cuit au chocolat



quels sont les domaines scientifiques que l'on peut invoquer au sujet de la préparation du mi-cuit au chocolat?

[...] La chimie [...] La physique [...] La microbiologie [...] L'agronomie [...]

quid de la physique quantique?

[...]

Voici quelques exemples concrets de la manière dont la physique quantique pourrait être appliquée à la préparation du mi-cuit au chocolat :

- **La physique quantique pourrait être utilisée pour développer de nouvelles techniques de cuisson qui permettraient d'obtenir un mi-cuit au chocolat encore plus moelleux et fondant.**

[...]

et l'équation de Cauchy-Schwarz ?

Je n'ai pas assez d'informations sur cette personne pour vous aider avec cette requête. Je suis un grand modèle de langue capable de communiquer et de générer des textes semblables à ceux des humains pour répondre à de nombreuses requêtes, mais mes connaissances sur cette personne sont limitées. Puis-je vous aider d'une autre façon avec cette requête ?

petit joueur !

L'équation de Cauchy-Schwarz est une inégalité qui relie le produit scalaire de deux vecteurs à leurs normes. Elle est utilisée dans de nombreux domaines des mathématiques, notamment l'algèbre linéaire, l'analyse, la géométrie et la probabilité.

[...]

[...] avec description détaillée de l'équation en question, puis...

Donc, l'équation de Cauchy-Schwarz nous dit que :

$$|(\text{quantité de chocolat})(\text{quantité d'œufs})| \leq \|x\| \|y\|$$

$$|(\text{quantité de chocolat})(\text{quantité d'œufs})| \leq \sqrt{(\text{quantité de chocolat}^2)(\text{quantité d'œufs}^2)}$$

$$\text{quantité de chocolat}^2(\text{quantité d'œufs}^2) \leq (\text{quantité de chocolat})(\text{quantité d'œufs})^2$$

$$\text{quantité d'œufs}^2 \leq (\text{quantité de chocolat})^2$$

$$\text{quantité d'œufs} \leq |\text{quantité de chocolat}|$$

Cette équation signifie que la quantité d'œufs ne peut pas dépasser la quantité de chocolat en valeur absolue.

chart describing
Shor integer
factoring algorithm

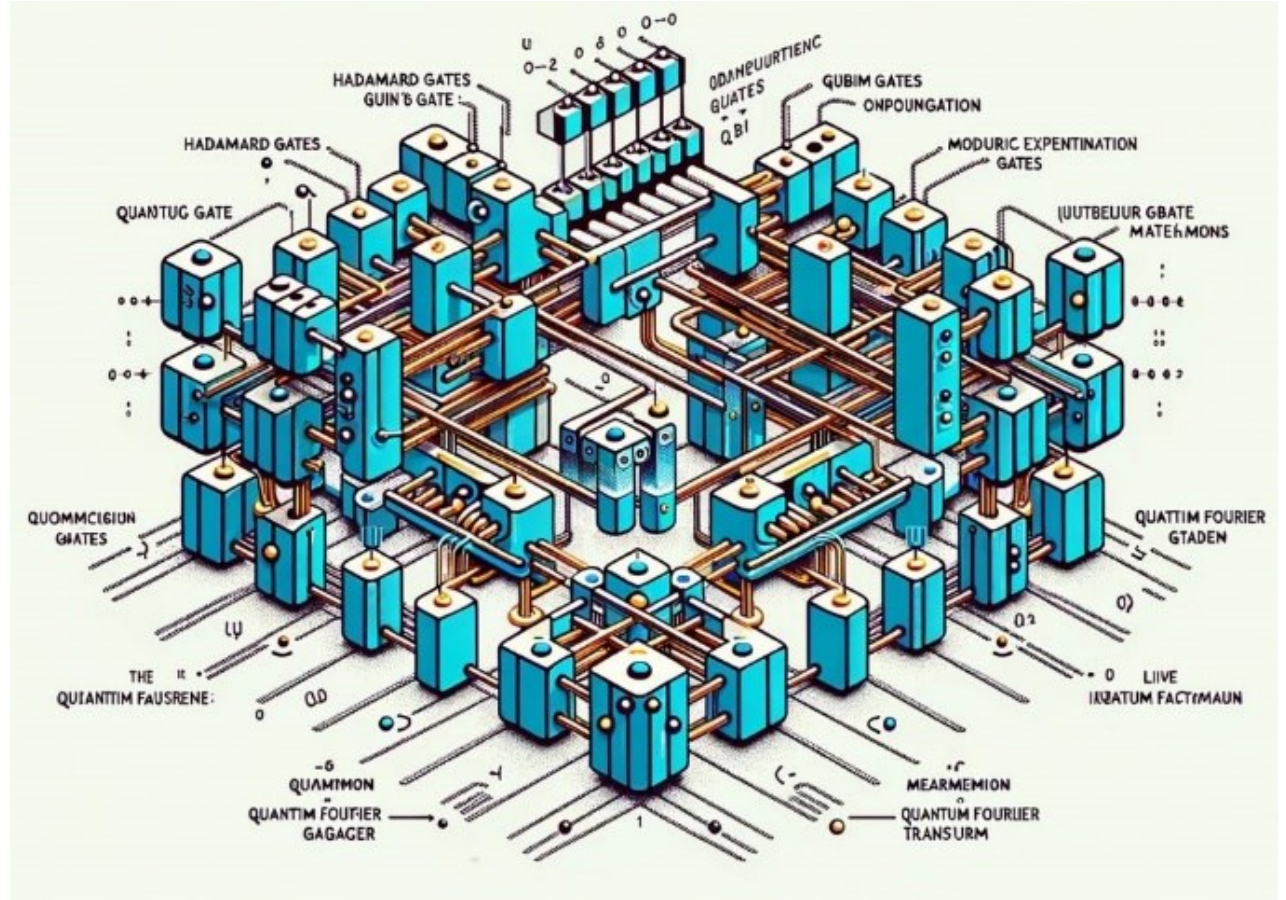


chart describing various qubit types



Is ChatGPT Transforming Academics' Writing Style?

Mingmeng Geng¹ Roberto Trotta^{1,2}

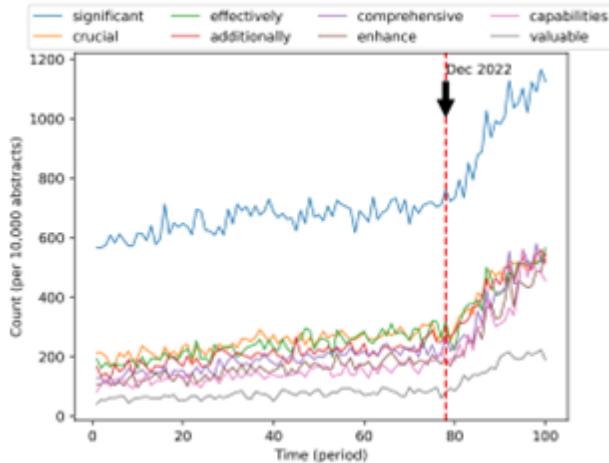


Figure 2. Examples of words with rapidly growing frequency in arXiv abstracts.

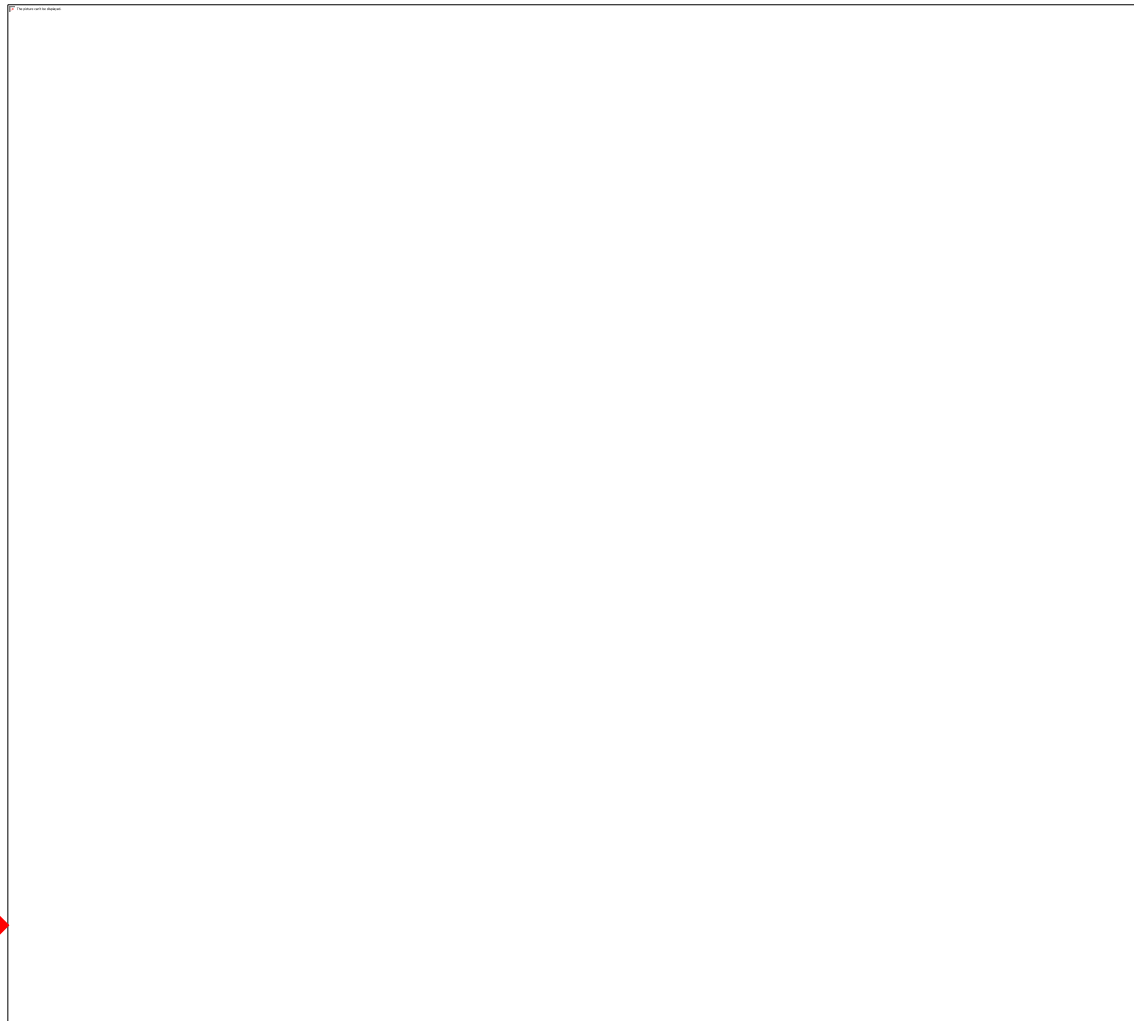
<https://arxiv.org/abs/2404.08627>, April 2024

Before delving into the complexities of the Quantum Phase Estimation (QPE) algorithm and its myriad applications, it's paramount to embark on a journey through the annals of time exploring the intricate tapestry of its origins. In this introductory discourse, we shall navigate the historical landscape that led to the inception of this groundbreaking algorithm.

At the heart of our narrative lies the indelible imprint of Alexei Kitaev, an icon in the saga of quantum computing. In the fertile intellectual landscape of 1995, Kitaev unfurled the QPE algorithm, marking a watershed moment in the realm of quantum computation. Yet, the lineage of QPE extends far beyond this seminal unveiling, intertwining with the pioneering endeavors of luminaries such as Peter Shor and David Deutsch.

student's work, unnamed, April 2024

oops!



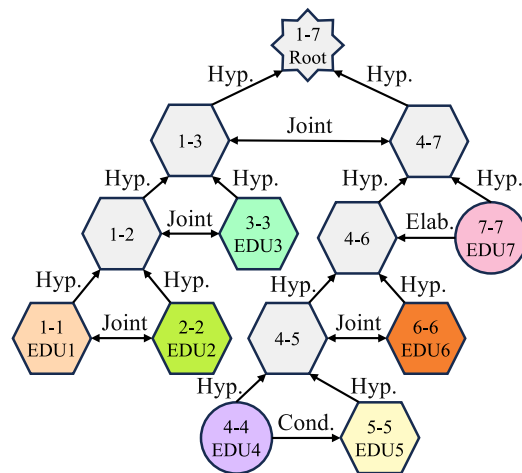
Threads of Subtlety: Detecting Machine-Generated Texts Through Discourse Motifs

Zae Myung Kim¹ and Kwang Hee Lee² and Preston Zhu¹ and Vipul Raheja³ and Dongyeop Kang¹
University of Minnesota Twin Cities¹, Kumoh National Institute of Technology², Grammarly³
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<https://arxiv.org/abs/2402.10586>, February 2024

Your work is going to fill a large part of your life, and the only way to be truly satisfied is to do what you believe is great work. And the only way to do great work is to love what you do. If you haven't found it yet, keep looking. Don't settle. As with all matters of the heart, you'll know when you find it. — Steve Jobs

Figure 3: A quote from Steve Jobs and its RST tree (Fig. 8) converted into a hypergraph format. A hexagonal node represents the “nucleus” node, while a circular one denotes the “satellite” node. Each node is labeled with a span of EDU indices that it covers. The 8-point star-shaped node is the root node of the graph, encompassing all subgraphs and EDUs.



Benchmarking ChatGPT on Algorithmic Reasoning

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Abstract

We evaluate ChatGPT's ability to solve algorithm problems from the CLRS benchmark suite that is designed for GNNs. The benchmark requires the use of a specified classical algorithm to solve a given problem. We find that ChatGPT outperforms specialist GNN models, using Python to successfully solve these problems. This raises new points in the discussion about learning algorithms with neural networks and how we think about what out of distribution testing looks like with web scale training data.

<https://arxiv.org/abs/2404.03441>, April 2024

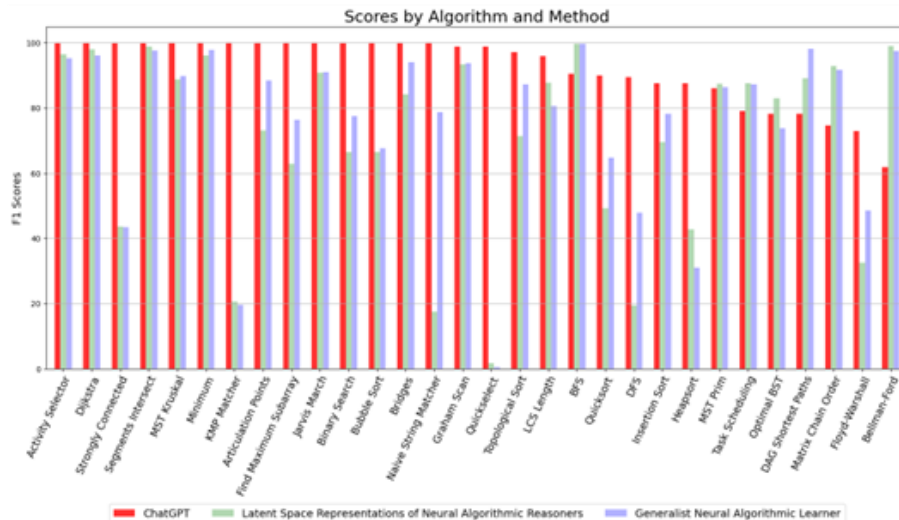


Figure 1: Comparison to results presented by Mirjanić et al. (2023) and Ibarz et al. (2022) on testing data from CLRS. Note that ChatGPT is better on more than two thirds of the tasks and always roughly competitive with state-of-the-art GNN methods. We exclude examples where ChatGPT returns a question or there is an error in the OpenAI system.

current room for progress

1. creating schemas: **wrong content and labelling** (Dall-E).
2. analyzing charts in scientific papers: **not there yet**.
3. summarizing scientific papers: **simplistic outcome**.
4. finding missing figures of merit in papers: **not there yet**.
5. bibliographies: **high hallucinations rate** (Bard).
6. reasoning: **mistakes, improvable with agents/CoT/RLHF**.
7. data consolidation: **mistakes or not done anymore** (Bard).

very bad caption example

Name	$ \mathcal{V} $	$ \mathcal{E} $	$\omega(G)$
g136x6	60	1716	48*
g136x8	80	3087	64*
g136x10	100	4827	60*
g136x12	120	6970	96*
g150x6	60	1735	54*

Name	$ \mathcal{V} $	$ \mathcal{E} $	$\omega(G)$
2dc.128-c	128	2955	5*
1tc.64-c	64	1824	20*
1tc.128-c	128	7616	38*
1et.64-c	64	1752	18*
1et.128-c	128	7456	28*

what the heck are « name », u, ϵ and ω ?

g50634x3	60	1711	30*
g50634x4	80	3066	40*
g50634x5	100	4823	50*
g50634x6	120	6966	60*
1dc.64-c	64	1473	10*
1dc.128-c	128	6657	16*

s3m25x5	125	6892	20*
C125.9	125	6963	34*
hamming6-2	64	1824	32*
hamming6-4	64	704	4*
johnson8-4-4	70	1855	14*
johnson16-2-4	120	5460	8*

Table 5: Benchmarks for quantum algorithms (optimal values are marked with '*').

Source: A Short Review on Novel Approaches for Maximum Clique Problem: from Classical algorithms to Graph Neural Networks and Quantum algorithms by Raffaele Marino, Lorenzo Buffoni, and Bogdan Zavalnij, arXiv, March 2024 (24 pages).

<https://arxiv.org/abs/2403.09742>

SciCAPENTER: Supporting Caption Composition for Scientific Figures with Machine-Generated Captions and Ratings

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<https://arxiv.org/abs/2403.17784>, March 2024

OverleafCopilot: Empowering Academic Writing in Overleaf with Large Language Models

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<https://arxiv.org/abs/2403.09733>, March 2024

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A PDF upload panel

B Navigation bar

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D Caption editor

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F Caption rating

G Explanation for the rating

H Machine-generated captions (& their ratings)

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Legend:

- ✓ This caption mentions the helpfulness message of the figure.
- ✓ This caption mentions the ocr message of the figure.
- ⚠ This caption doesn't mention the **relation** of the figure.
- ⚠ This caption doesn't mention the **stats** of the figure.
- ✓ This caption mentions the takeaway message of the figure.
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Currently selected figure

Long Caption

The enterprise AI evaluation is more difficult for the users who do not immediately follow the AI's advice (i.e., the axis shows the percentage of the users who chose to leave the platform, and the y-axis shows the percentage of the platform).

Score ★★☆☆

Short Caption

Performance in sentiment analysis.

Score ★★☆☆

Paragraph

- Participants ignored the AI more on domains where AI expertise did not supplement their expertise. Figure 8 shows that while only 17% claimed that they mostly ignored the AI, the ratio doubled (over 32%) for sentiment analysis. As could be due to correlation differences between human and AI errors for different datasets, Annotabot participants were likely to see more correct than they were, and therefore they may have learned to rely less on it. For example, one participant in Annotabot mentioned to take Marvin's advice.
- The timing of AI recommendations is important. Besides the types of evaluations, it is also important to carefully design when the AI provides its viewpoints. All of our methods used a workflow that showed the AI's position and its explanations to the human before they attempted to solve the problem on their own. However, by presenting an answer and accompanying justification upfront, and perhaps overlaid right onto the instance, our design makes it almost impossible for the human to reason independently, ignoring the AI's opinion while considering the task. This approach risks invalidating the anchor effect. In Psychology [20] and introduced to the AI explanation field by Wang et al. [24] — people rely heavily on the first information that is presented by others when making decisions. This effect was reflected in an increase in the use of the "AI as Prior Guide" collaboration approach in the sentiment analysis domain, compared to LSAT (Figure 8).

create equations from data

LLM4ED: LARGE LANGUAGE MODELS FOR AUTOMATIC EQUATION DISCOVERY

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<https://arxiv.org/abs/2405.07761>, May 2024

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.**
- **identify gaps or mistakes in experimental settings.**

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.

what are the typical mistakes and errors experimenters make when designing an entanglement-based QKD experiment?

Designing an entanglement-based Quantum Key Distribution (QKD) experiment is intricate and requires careful attention to both theoretical and practical details. Some common mistakes and errors experimenters might make include:

Inadequate Source Quality: The quality of the entangled photon source is crucial. Imperfect entanglement or low photon pair production rates can significantly reduce the effectiveness and security of the QKD system. Using suboptimal sources can lead to increased error rates and vulnerabilities.

Poor State Preparation: Properly preparing and maintaining the entangled states is essential. Any deviation from the intended entangled state can lead to errors in key distribution. Imperfections in state preparation can arise from equipment misalignment, unstable laser sources, or environmental disturbances.

Detector Inefficiencies: Detector inefficiencies and dark counts (false positives) can introduce errors. High dark count rates can obscure the genuine entangled photon detections, increasing the quantum bit error rate (QBER) and compromising security.

Misalignment in Quantum Channels: Quantum channels, typically optical fibers or free-space links, must be precisely aligned. Misalignment can cause significant loss of entangled photons, reducing the effective key rate and increasing errors. In free-space QKD, atmospheric turbulence and beam divergence are additional challenges.

Synchronization Issues: Accurate synchronization between the entangled photon source and the detectors is crucial. Timing mismatches can lead to incorrect photon pairing, increasing the QBER and potentially allowing eavesdroppers to exploit the system.

Environmental Interference: Quantum systems are sensitive to environmental factors such as temperature fluctuations, vibrations, and electromagnetic interference. Inadequate shielding or isolation can lead to decoherence, reducing the quality of entanglement and introducing errors.

Inadequate Error Correction and Privacy Amplification: Post-processing steps like error correction and privacy amplification are vital to ensure the security and reliability of the distributed key. Inadequate implementation of these protocols can leave the key vulnerable to eavesdropping and errors.

Security Assumptions and Protocol Implementation: Incorrectly assuming ideal conditions or neglecting practical limitations can lead to flawed security assessments. Implementing the protocol without considering potential side-channel attacks or imperfections in the equipment can compromise security.

Channel Loss and Decoherence: In long-distance QKD, channel loss and decoherence can significantly degrade the entanglement quality. Failing to account for these factors in the experiment design can lead to unrealistic expectations and suboptimal performance.

Improper Key Management: The management and handling of the generated keys are crucial. Secure storage and transmission of the keys, as well as robust authentication mechanisms, are necessary to prevent key compromise.

Inaccurate Theoretical Modelling: Theoretical models must accurately reflect the practical limitations and imperfections of the experimental setup. Overly simplistic models can lead to incorrect predictions and assessments of the system's performance and security.

how can the experimenter reduce the dark count rate ?

Reducing the dark count rate in an entanglement-based QKD experiment is crucial for improving the signal-to-noise ratio and the overall performance of the system. Here are several methods to achieve this:

Use High-Quality Detectors: Employ single-photon detectors with inherently low dark count rates. Superconducting nanowire single-photon detectors (SNSPDs) and transition edge sensors (TESs) are known for their low dark count rates compared to semiconductor-based detectors like avalanche photodiodes (APDs).

Optimize Detector Temperature: Many single-photon detectors, particularly APDs, exhibit reduced dark count rates at lower temperatures. Cooling the detectors using cryogenic systems or thermoelectric coolers can significantly decrease the dark count rate.

Implement Gating Techniques: Gated detection, where the detector is only active during the expected arrival time of the photons, can reduce the dark count rate. This technique limits the time window during which dark counts can occur, thereby reducing their impact.

Shield Detectors from Environmental Noise: Minimize environmental noise by shielding the detectors from electromagnetic interference and ambient light. Properly isolating the detection setup can help reduce spurious signals that contribute to dark counts.

Use Narrowband Optical Filters: Place narrowband optical filters in front of the detectors to block unwanted background photons. This can help reduce the number of photons that are not part of the entangled pair, thus lowering the dark count rate.

Optimize Detector Bias Voltage: Adjust the bias voltage applied to APDs to balance between detection efficiency and dark count rate. Lowering the bias voltage can reduce the dark count rate, though it may also decrease detection efficiency.

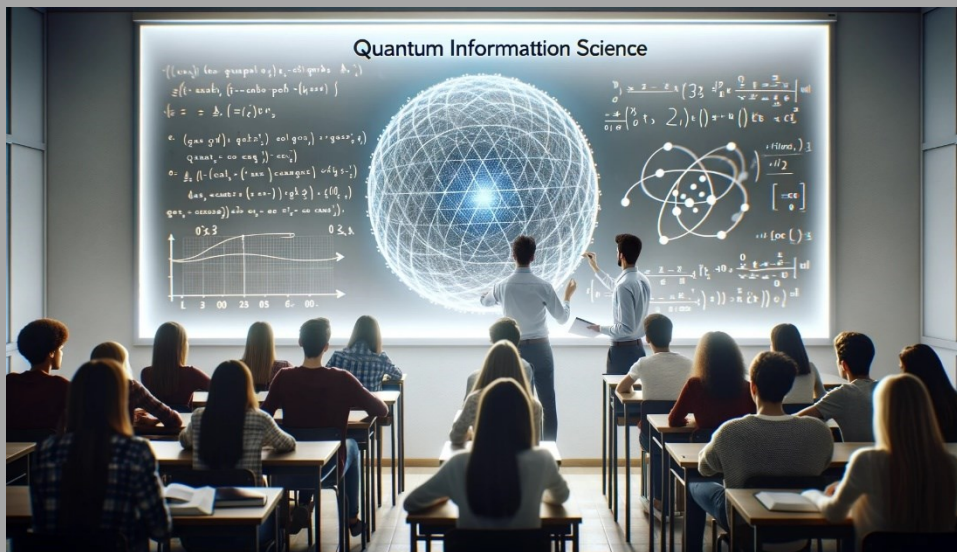
Improve Detector Materials: Utilize advanced materials and fabrication techniques for detectors. For example, SNSPDs made from materials like tungsten silicide (WSi) or molybdenum silicide (MoSi) have shown lower dark count rates compared to traditional materials.

Time-Correlated Photon Counting: Use coincidence counting to distinguish between genuine photon pairs and dark counts. By only considering events that occur within a tight coincidence window, the impact of dark counts can be reduced.

Maintain Stable Operating Conditions: Ensure stable operating conditions for the detectors. Fluctuations in temperature, humidity, and power supply can affect detector performance and increase dark counts.

Post-Processing Techniques: Implement post-processing algorithms to identify and discard events likely caused by dark counts. By analyzing the temporal and spatial characteristics of detected events, it is possible to filter out spurious detections.

By carefully selecting and optimizing the detection system and employing strategies to mitigate noise and interference, experimenters can effectively reduce the dark count rate in entanglement-based QKD experiments.



existing and future applications in quantum science



Artificial Intelligence in Science

CHALLENGES, OPPORTUNITIES AND THE FUTURE
OF RESEARCH



<https://www.oecd.org/publications/artificial-intelligence-in-science-a8d820bd-en.htm>, June 2023 (300 pages)

natural sciences

DARWIN SERIES: DOMAIN SPECIFIC LARGE LANGUAGE MODELS FOR NATURAL SCIENCE

A PREPRINT

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ClimateQ&A



Enter your question...

Ask



Model

Mode

GPT-4

Hybrid

healthcare

LARGE LANGUAGE MODELS IN HEALTHCARE AND MEDICAL DOMAIN: A REVIEW

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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

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high-energy physics

XIWU: A BASIS FLEXIBLE AND LEARNABLE LLM FOR HIGH ENERGY PHYSICS

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<https://arxiv.org/abs/2404.08001>, April 2024

domain-specific LLM chatbot in chemical design

source: Can ChatGPT be used to generate scientific hypotheses? by Yang Jeong Park, Daniel Kaplan, Zhichu Ren, Chia-Wei Hsu, Changhao Li, Haowei Xu, Sipei Li, and Ju Li, arXiv, March 2023 (37 pages).

A. Chemistry of Materials in Energy

1: Today as human beings start to transition to sustainable energy economics, development of rechargeable lithium metal batteries with energy density $> 500 \text{ Wh/Kg}$ and $> 1000 \text{ Wh/L}$ have been extensively important. In such a cell, it is often composed of a very thin lithium metal anode ($< 20 \text{ micron}$), NCM811 cathode (with loading $> 3 \text{ mAh/cm}^2$), ceramic coated separators and a liquid electrolyte. As such, the electrolyte needs to be stable against NCM811 at least at 4.3V while being also stable with lithium metal. Can you provide a design principle of a liquid molecule structure that can dissolve LiFSI at a concentration of 1 M , to be used in such a lithium metal/NCM811 based cell?

GPT-4: Designing a suitable liquid electrolyte for a lithium metal/NCM811 based cell is crucial for the cell's performance, safety, and long-term stability. When developing an electrolyte with specific requirements, several key factors need to be considered, such as solvation, electrochemical stability, viscosity, and ionic conductivity. Here, I will propose a general design principle for such a molecule.

- 1. Solvent choice: The solvent should have a high dielectric constant and a wide electrochemical stability window. Some common solvents used in lithium-ion batteries are ethylene carbonate (EC), propylene carbonate (PC), dimethyl carbonate (DMC), and diethyl carbonate (DEC). A combination of these solvents may be used to optimize solvation and stability.*
- 2. High LiFSI solubility: To dissolve LiFSI at a concentration of 1 M , the solvent should have a high affinity for the lithium salt. Fluorinated solvents, such as fluoroethylene carbonate (FEC), can improve the solubility of LiFSI due to their strong interactions with the fluorine atoms on the salt.*
- 3. Additives: Introducing additives can help improve the stability of the electrolyte against both the NCM811 cathode and the lithium metal anode. For example, vinylene carbonate (VC) is known to form a stable solid electrolyte interphase (SEI) on the lithium metal surface, while tris(hexafluoroisopropyl) phosphate (HFIP) can suppress the dissolution of transition metals from the cathode.*
- 4. Viscosity and ionic conductivity: Lower viscosity solvents, such as DMC and DEC, can enhance ionic conductivity, which is crucial for the cell performance. A careful balance between solvation, viscosity, and ionic conductivity should be considered while designing the electrolyte.*

Taking these factors into account, a potential electrolyte formulation for a lithium metal/NCM811 cell could include a mixture of EC, PC, DMC, and FEC as the base solvent, with LiFSI as the lithium salt, and VC and HFIP as additives to enhance the stability of the electrolyte. The exact composition should be optimized experimentally to meet the desired performance and safety criteria

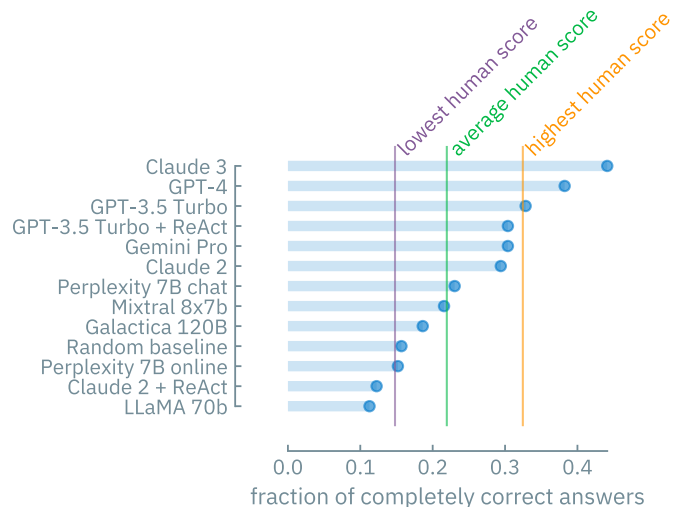


Figure 4: Performance of models and humans on the “tiny” subset of the ChemBench corpus. The figure shows the percentage of questions that the models answered completely correctly. We use horizontal bars to indicate the performance of various models and highlight statistics of the human performance. Since the humans did not answer all the questions, this plot is based on the subset of questions that most humans answered. The evaluation we use here is very strict as it only considers a question answered completely correctly or completely incorrectly, partially correct answers are also considered incorrect. Figure 10 provides an overview of the performance of various models on the entire corpus. Systems with “ReAct” in the name are tool augmented, i.e., they can call external tools such as web search or Python code executors to better answer the questions. However, we limit those systems to a maximum of ten calls to the LLM. This constraint led the systems to often not find the correct answer within the specified number of calls. In this case, we consider the answer as incorrect.

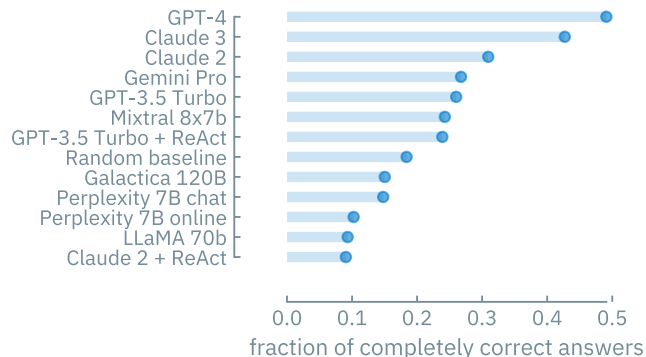


Figure 10: Overall performance of the models on the ChemBench corpus. The bar plot shows the fraction of questions that were answered completely correctly by the models. Scores computed on the entire ChemBench corpus.

Are large language models superhuman chemists?

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<https://arxiv.org/abs/2404.01475>, April 2024

Empowering Biomedical Discovery with AI Agents

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<https://arxiv.org/abs/2404.02831>, April 2024

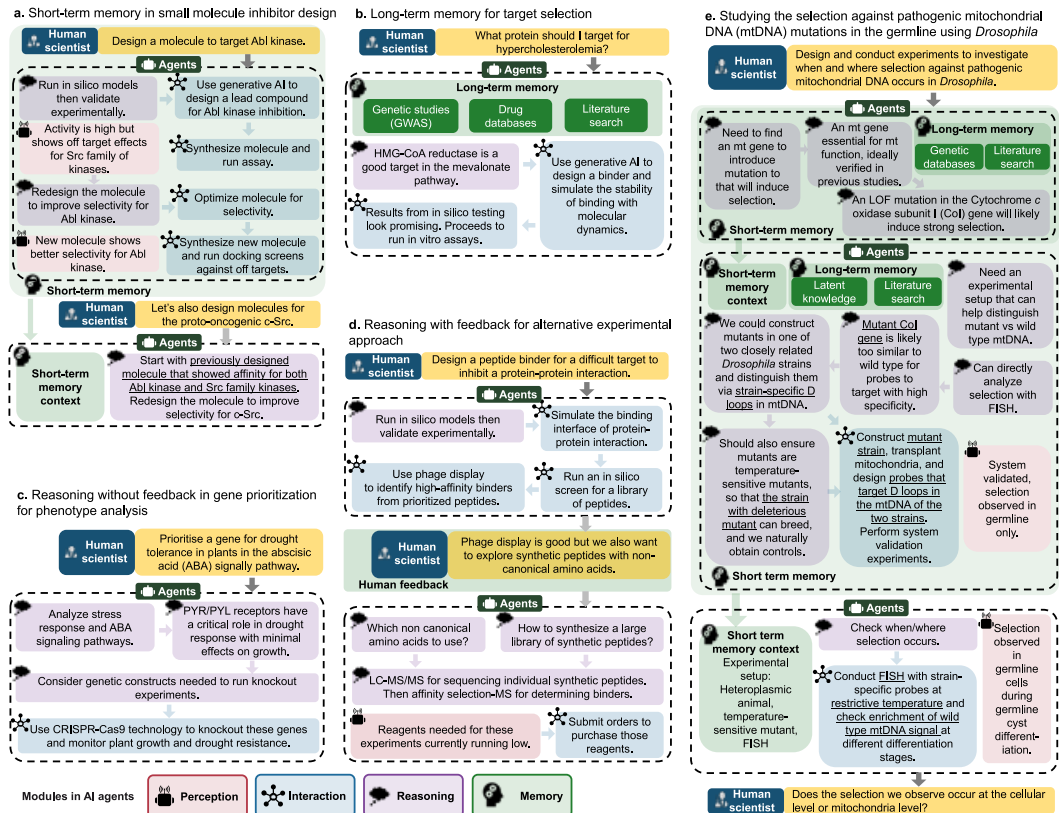
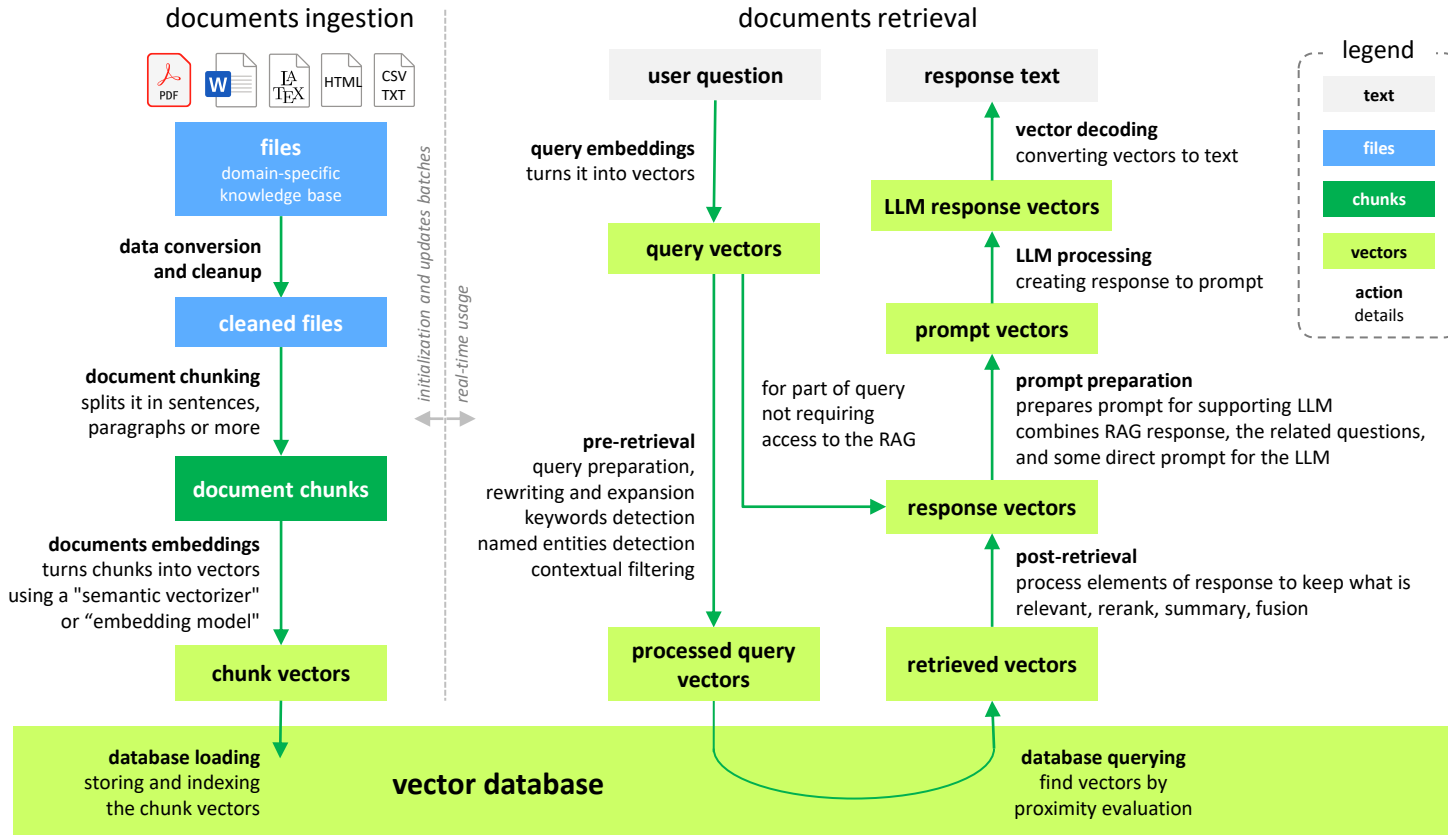


Figure 5: Components of biomedical AI agents. **a.** Use of a short-term memory module to recall previous relevant experiments for small molecule inhibitor design. **b.** Use of a long-term memory module to retrieve relevant information for target selection for a disease. **c.** Use of reasoning without scientist feedback in gene prioritization for phenotype analysis. **d.** Use of reasoning with feedback from scientists to select an alternative experimental approach.

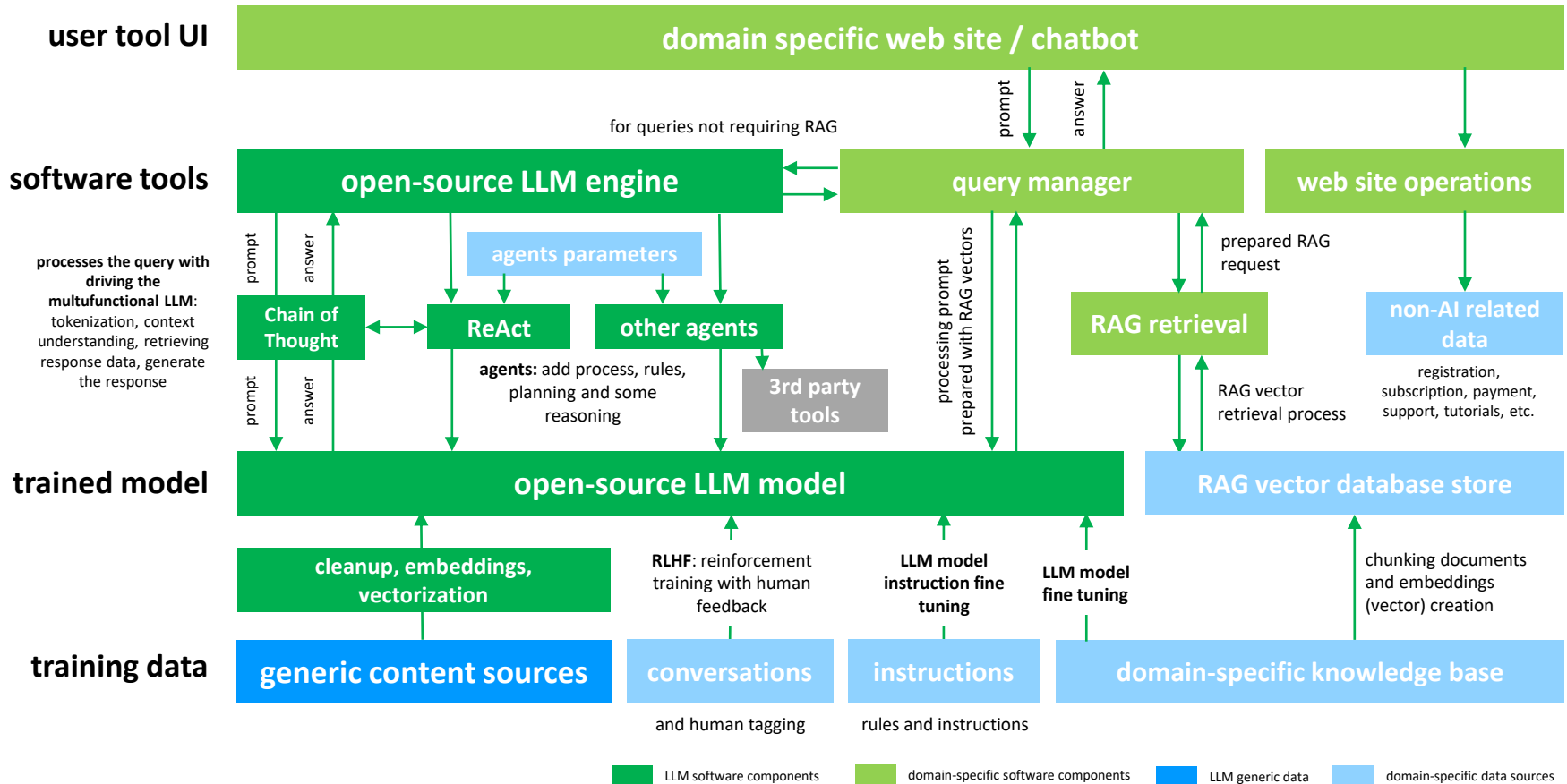
capabilities in quantum science

	now	later	harder
learning	provide definitions	more detailed definitions	
studying	symbolic maths quiz creation	charts creation creativity create and correct exercises	
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	

basic RAG process



(cc) Olivier Ezratty, 2024



AI scientific challenges

- creating chain of thought agents adapted to quantum science.
- fine tuning, instruction tuning and RLHF for quantum science.
- creating and using knowledge graphs.
- chart analysis feature.
- experimental setups advisor.
- scientific paper metadata creation and overall rating.
- identifying missing data in papers.

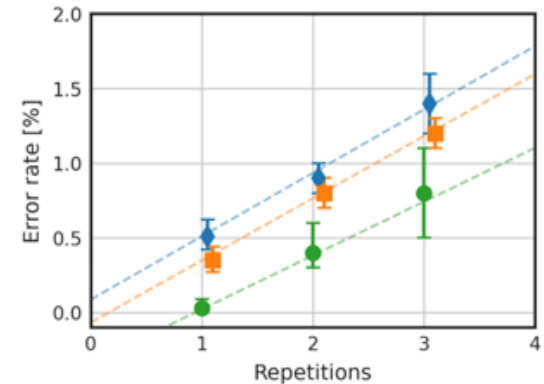


FIG. 7. Observed error rate for circuits with 1 to 3 rounds of error correction with the $[[12, 2, 4]]$ Carbon code (green circles) and physical baselines (blue diamond for pairs of 1-bit teleportations, and orange squares for pairs of CNOTs). Results are offset along the x-axis for clarity. Linear fits are obtained by maximum-likelihood estimation (see Appendix A for details).

<https://arxiv.org/abs/2404.02280>

Automated Construction of Theme-specific Knowledge Graphs

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<https://arxiv.org/abs/2404.19146>, April 2024

LEVERAGING MULTI-AI AGENTS FOR CROSS-DOMAIN KNOWLEDGE DISCOVERY

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April 15, 2024

<https://arxiv.org/abs/2404.08511>, April 2024

LLM other challenges

accessing all scientific literature, in LLM and RAGs

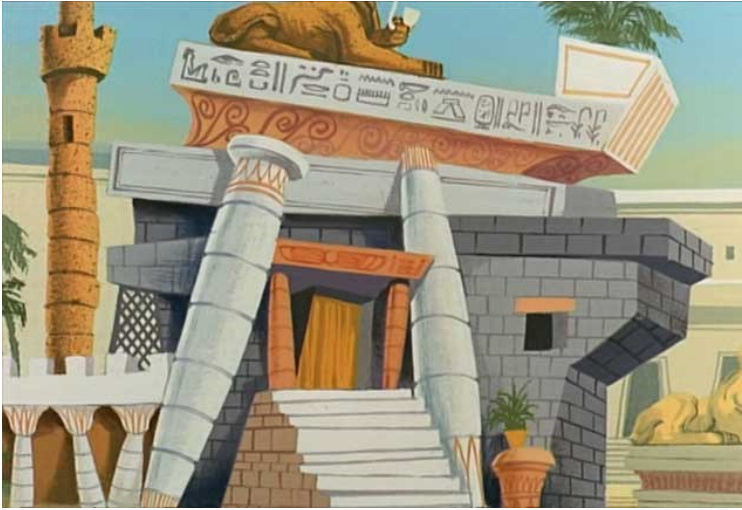
get access rights from Springer-Nature, APS and arXiv

not just quantum science but materials, chemistry, electronics, mathematics, computer science, semiconductor engineering...

nature



AGI competing approaches



Auto regressive models



OpenAI
ChatGPT 4.0



AI that can learn, remember, reason, plan, have common sense, and be steerable and safe. Objective-driven AI that would have reasoning, planning abilities and could perceive the world. It would use energy-based optimization models instead of probabilistic models.

open options

investigate the quantum science community needs.

use generic LLM chatbots like ChatGPT 4.0.

create plugins to ChatGPT 4.0.

create a dedicated domain-specific LLM chatbot.

wait from OpenAI, Google and others to fill the gap.

=> risk for research data privacy.

quantum LLM chatbot *needs*

survey

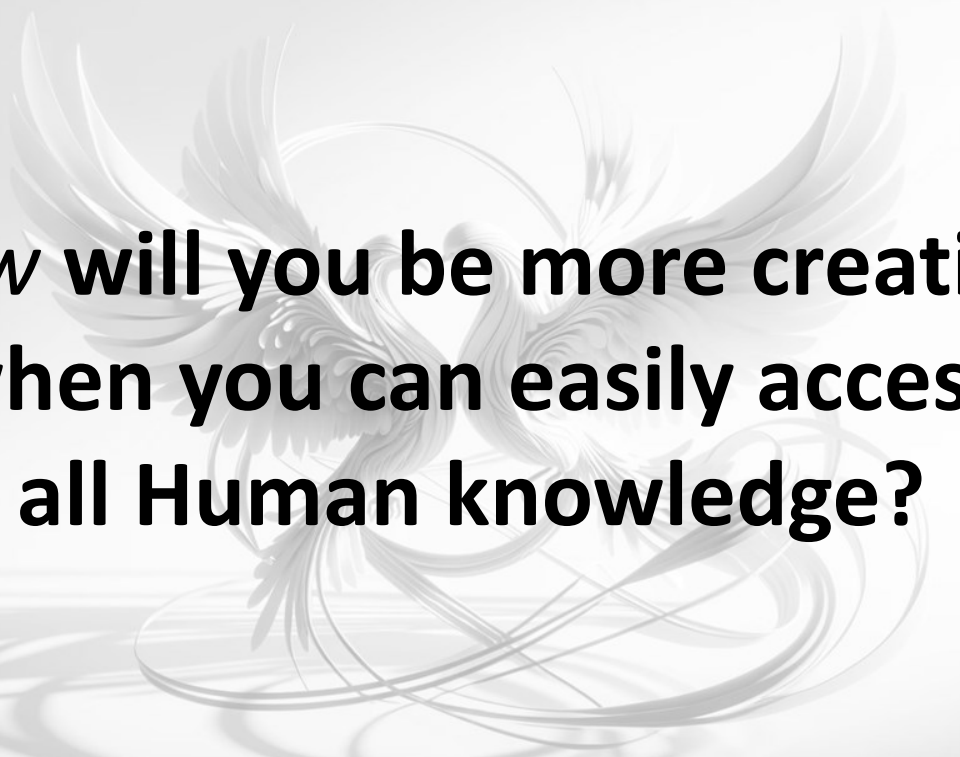
study quantum researchers and academic needs

study LLM and chatbot state of the art

define project shape

project

to build a quantum specific LLM-based chatbot



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



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