Quantum AI

Developing quantum algorithms for chemistry at Google

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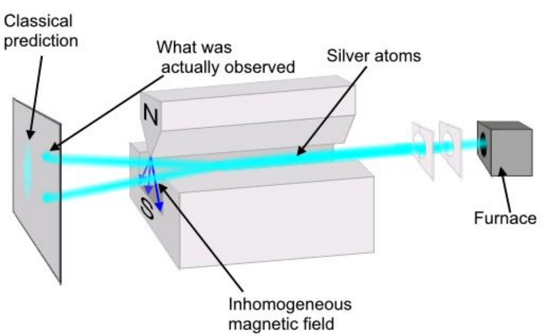
January 11, 2023

Google

Qubits and gates, briefly

Any 2-state quantum system is a qubit, $|\psi\rangle = a_0\,|0\rangle + a_1\,|1\rangle$



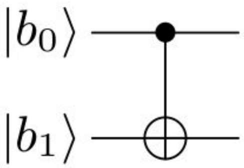
For 2 qubits, $|\psi\rangle = a_{00}\,|00\rangle + a_{01}\,|01\rangle + a_{10}\,|10\rangle + a_{11}\,|11\rangle$

N qubit systems requires $O(2^N)$ classical bits to represent

Information manipulated by controlled Hamiltonian evolutions

For instance, evolve 2 qubits under $H = (Z_0 - I_0) \otimes (I_1 - X_1)$ for time, $t = \pi/4$

$$e^{-iHt} : |b_0\rangle\,|b_1\rangle \mapsto |b_0\rangle\,|b_0 \oplus b_1\rangle$$



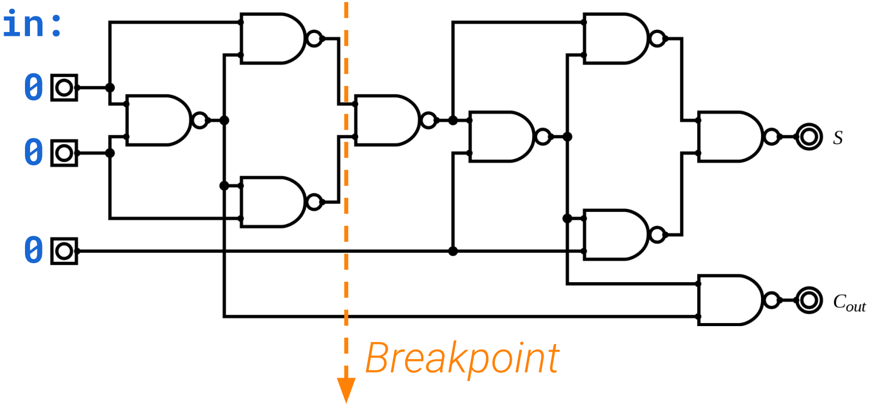
CNOT + single qubit rotations “universal” for all quantum dynamics / circuits

Quantum AI

Quantum circuits, briefly

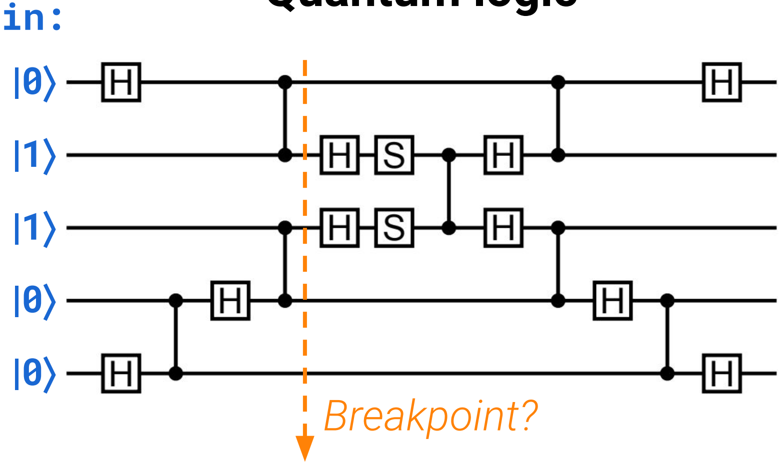
Use **different logic** to unlock new algorithms

“Classical” digital logic



1101

Quantum logic

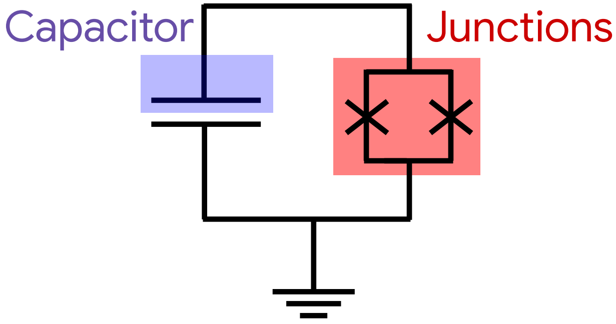


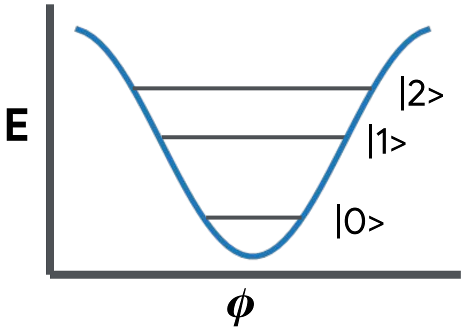
$|01100\rangle + |01101\rangle - |01110\rangle - |01111\rangle -$
$|11100\rangle - |11101\rangle + |11110\rangle + |11111\rangle$

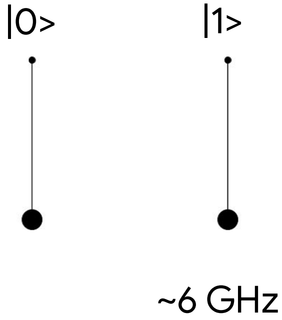
Linear superposition in high-dimensional space
Measurement **collapses** to one bitstring

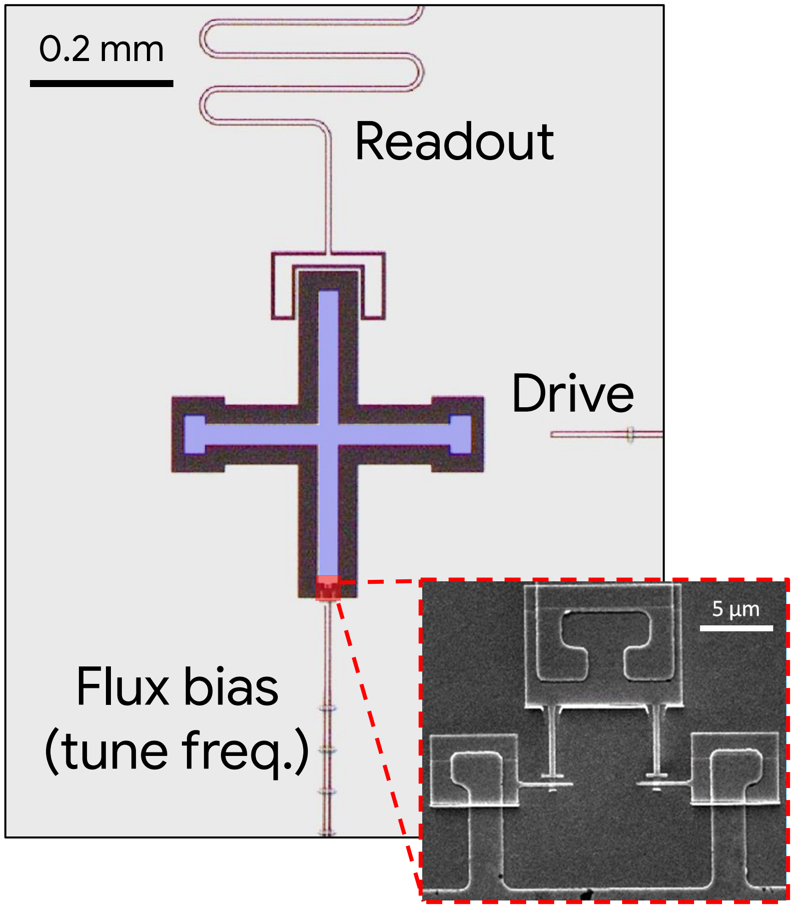
“Transmon” qubit

Nonlinear superconducting oscillator

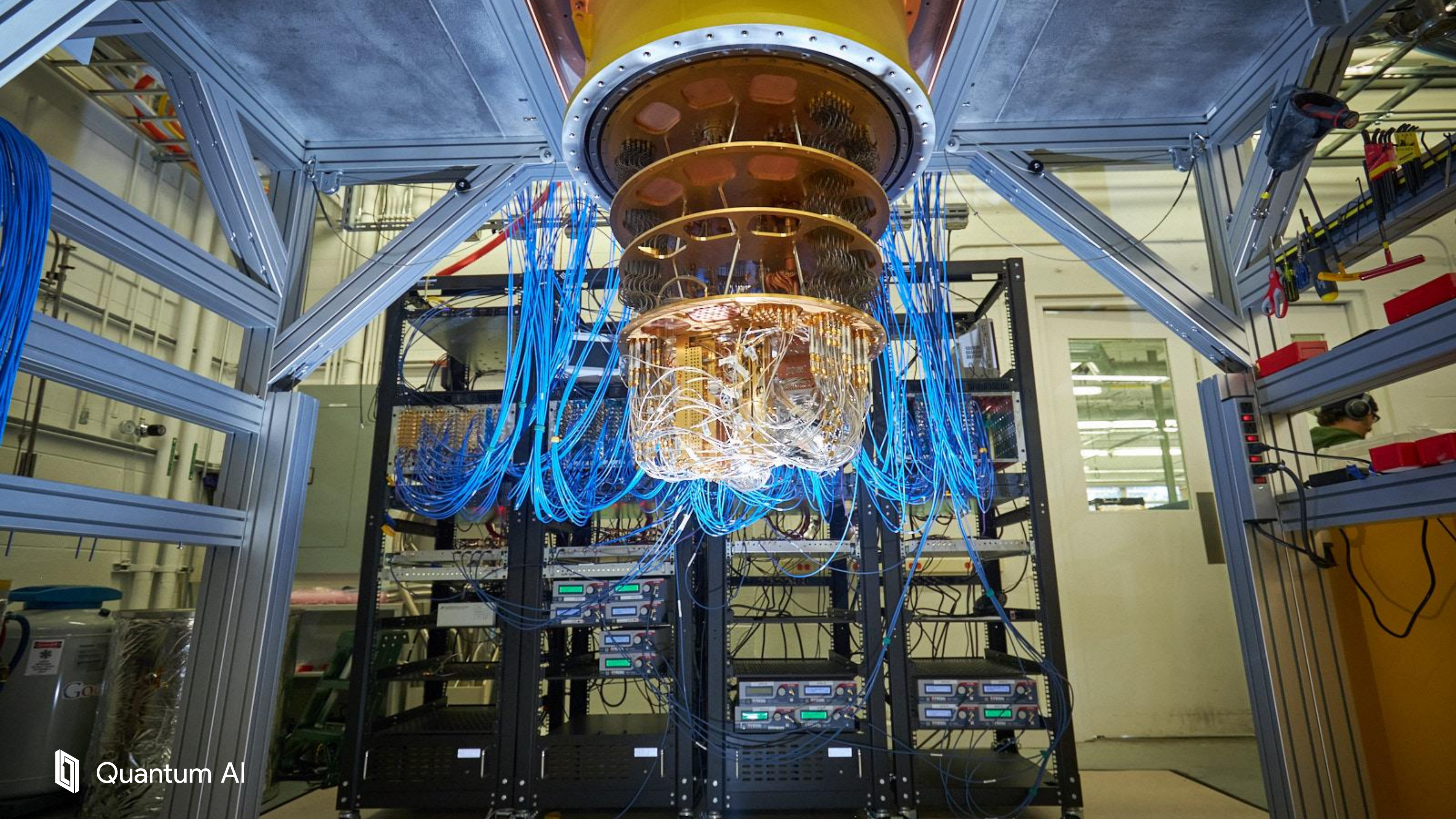








Quantum AI



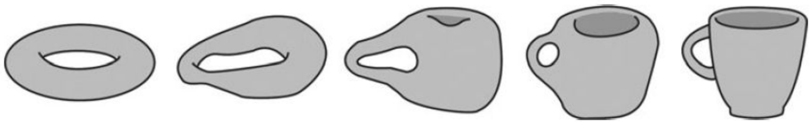
Quantum AI

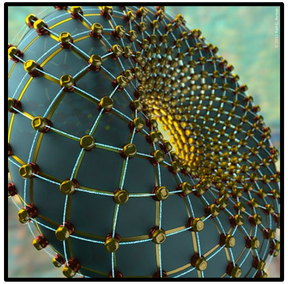
Fault-tolerance enables the quantum computer of our dreams

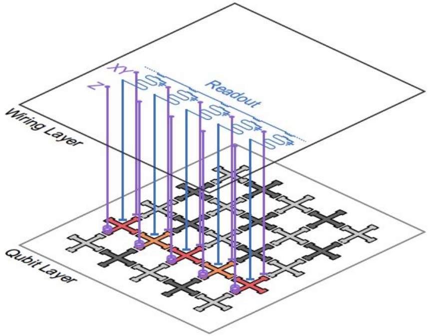
In early classical computers, logical bits were encoded in redundant physical bits:

$$|0\rangle = |000\rangle \qquad |1\rangle = |111\rangle \qquad |b_1, b_2, b_3\rangle \mapsto |\text{mode}\,\{b_0, b_1, b_2\}\rangle$$

Cannot copy qubits; popular idea is to encode information topologically

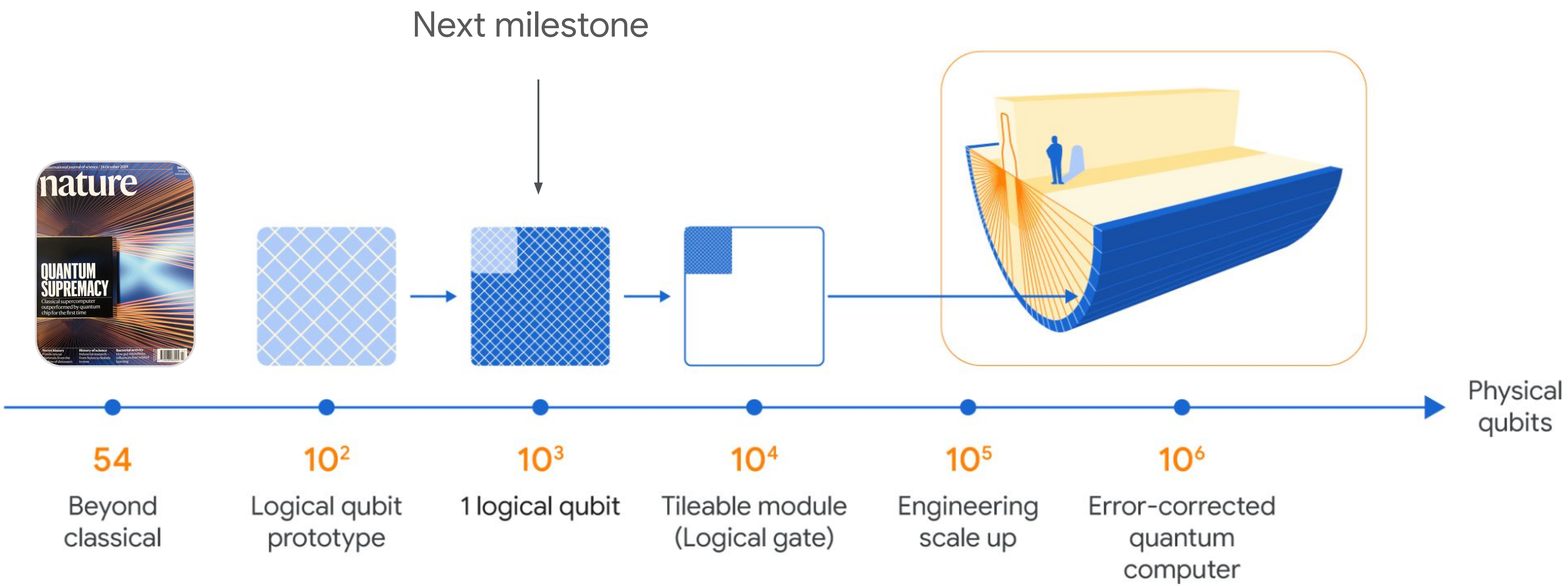






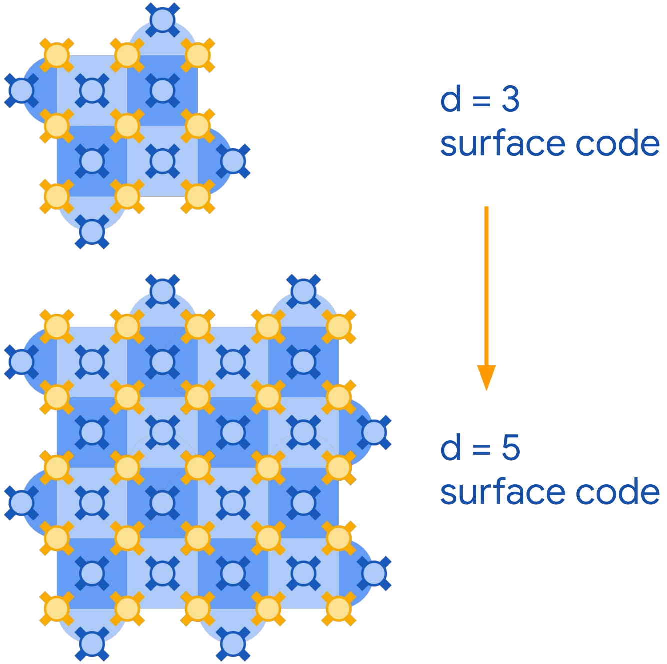
30 x 30 array of physical qubits in “surface code” has lifetime on order of millennia

Google’s roadmap to fault-tolerant quantum computing

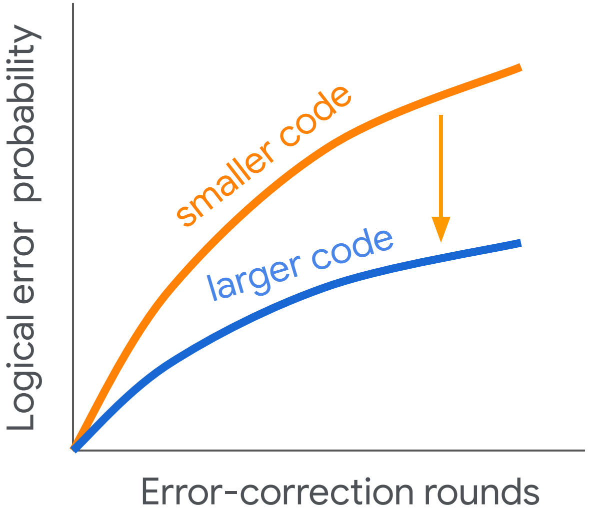


Milestone 2: Logical qubit prototype (plan)

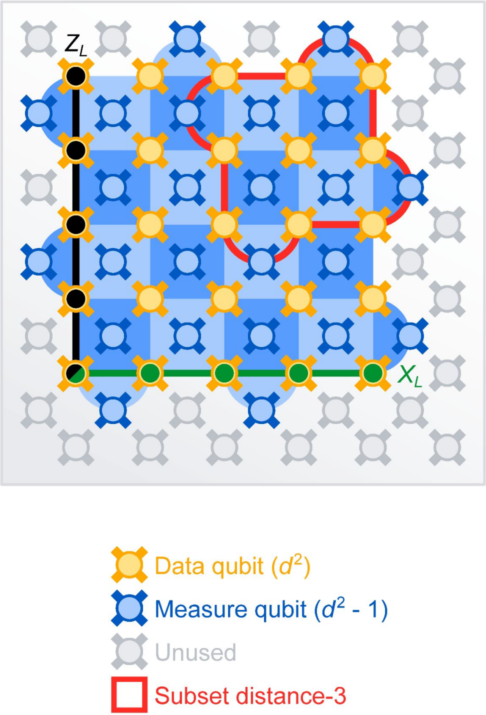
Run experiments to implement surface codes

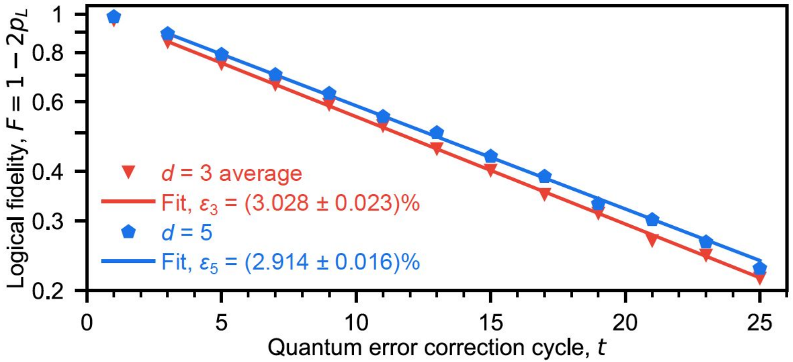


Analyze data and see if failure probability is lower with larger code



Milestone 2: Logical qubit prototype (experimental data)





Quantum AI

arXiv:2207.06431

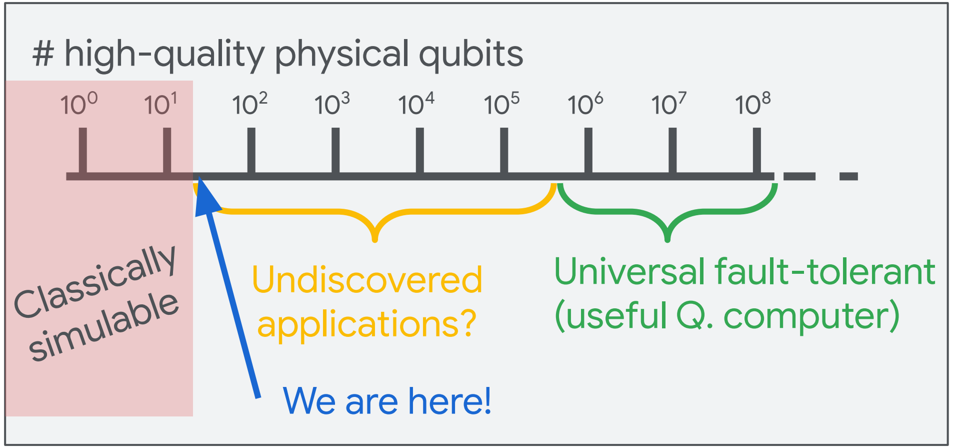
Quantum computers today

We are in the age of noisy intermediate scale (NISQ) quantum devices
We can run circuits on 50-100 qubits but errors severely limit circuit size

In 2019 Google team demonstrated beyond classical computation
i.e., we used our 54 qubit quantum computer to perform a well defined computational task that (was then) intractable on a classical computer

Ultimate goal is quantum error-correction
Has very large resource overheads

We'll have NISQ devices in the meantime
Will we be able to use such devices to achieve quantum advantage on a useful application?



Quantum AI

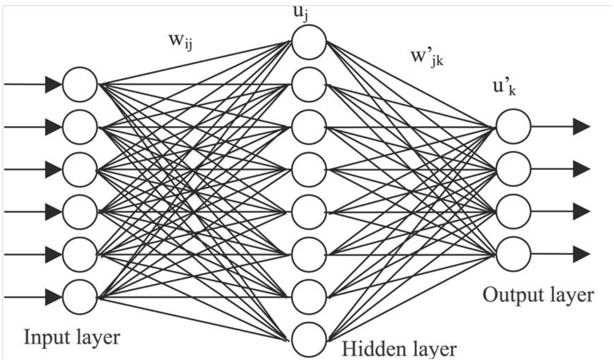
Quantum variational algorithms

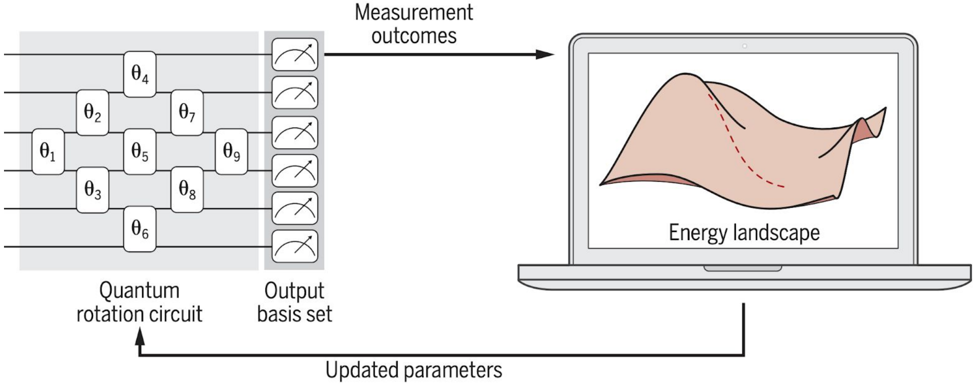
Quantum AI

Beyond classical experiments reveal that we can prepare extremely complex quantum states on existing hardware

But how do we make relevant states for an application?

Use a variational quantum algorithm - *Nat. Comm* 5, 421 (2014)
i.e., quantum circuits trained like a quantum neural network

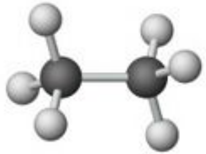




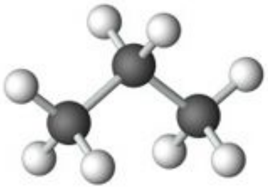
"Nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical" - Richard Feynman

Google AI Quantum

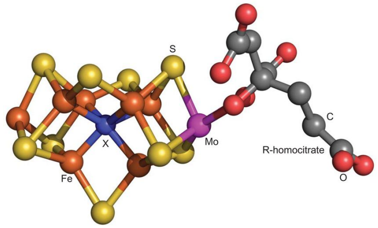
CPU seconds



CPU minutes



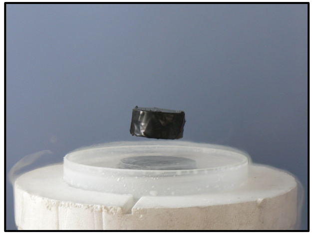
CPU days

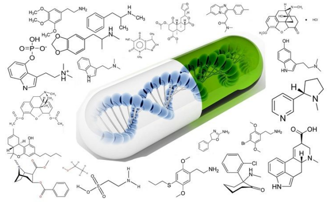


FeMoCo (intractable)

ammonia production
= 2% of world energy

The prospect of more efficient simulations is scientifically exciting and valuable!

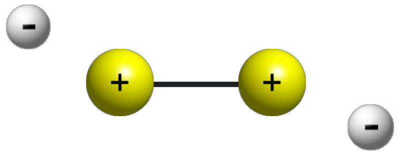




The molecular electronic structure problem

Goal is to solve for the energy of molecule

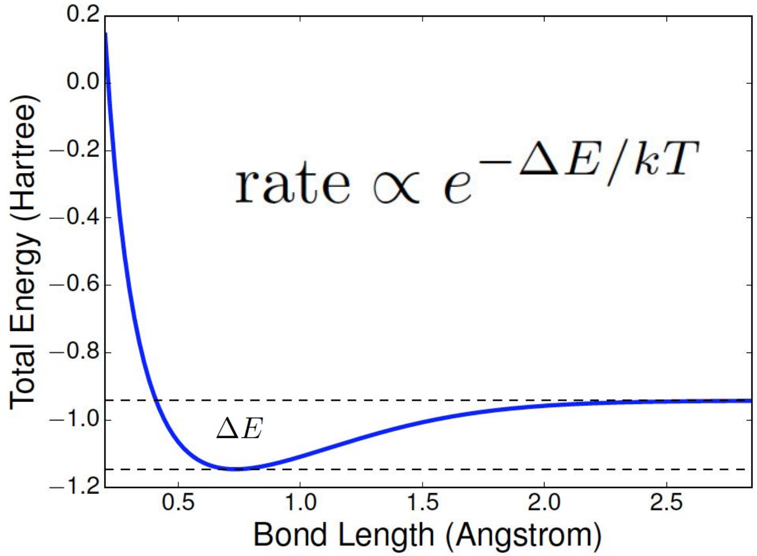
$$H = \hat{T}_{\text{nuc}} + \hat{T}_{\text{elec}} + \hat{V}_{\text{nuc-nuc}} + \hat{V}_{\text{nuc-elec}} + \hat{V}_{\text{elec-elec}}$$

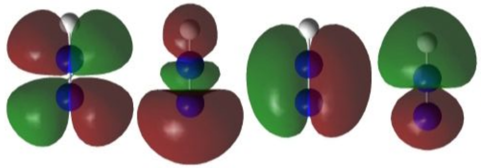


Energy surfaces allow us to understand reactions
Need chemical accuracy (1 kcal/mol) for rates

Such accuracy is often classically intractable
Especially for systems with strong correlation

To represent wavefunctions on computer one must discretize space (confine to basis)

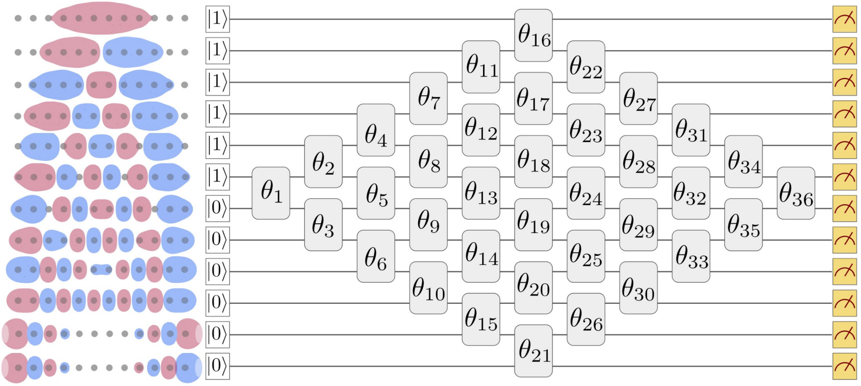


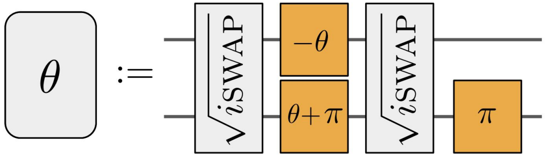


$$a_1\,|0011\rangle + a_2\,|0101\rangle + a_3\,|1001\rangle + a_4\,|0110\rangle + a_5\,|1010\rangle + a_6\,|1100\rangle$$

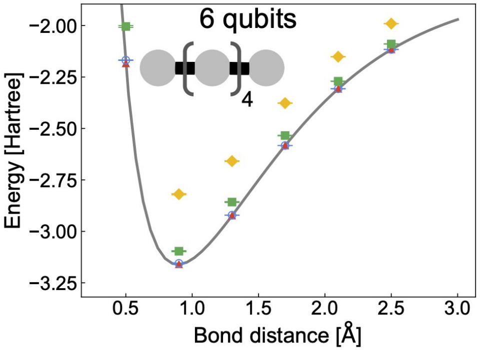
Realizing chemical variational algorithms

Science 369, 1084-1089 (2020)

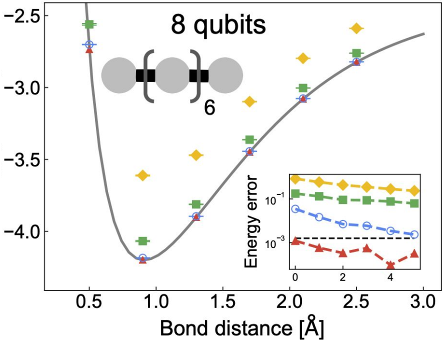




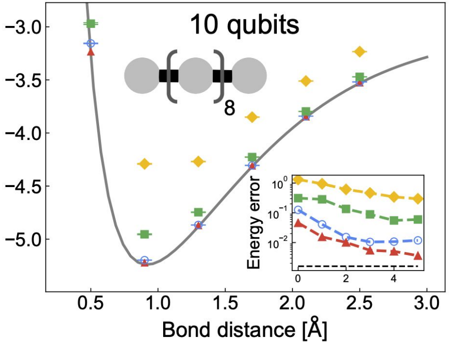
18 sqrt(iswap), 27 Rz



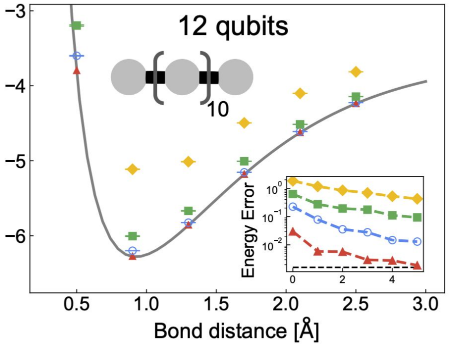
32 sqrt(iswap), 48 Rz



50 sqrt(iswap), 60 Rz



72 sqrt(iswap), 108 Rz



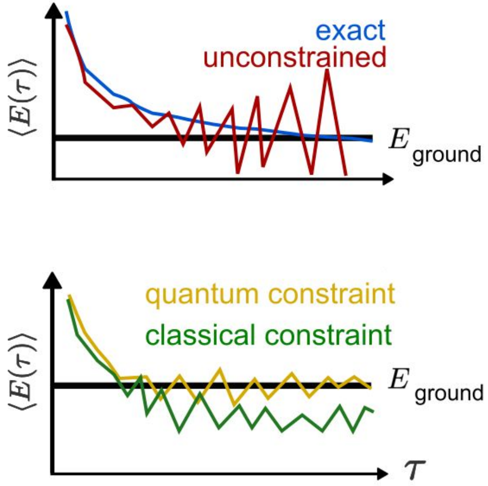
Quantum-Classical Hybrid Quantum Monte Carlo

Nature 603, 416–420 (2022)

quantum Monte Carlo
classically samples state via imaginary time evolution

the fermion sign problem
leads to exponentially high variance, but can be suppressed with a biasing constraint

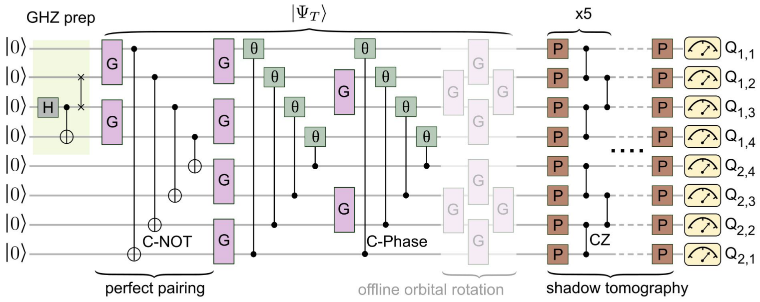
trial wavefunction from quantum computer
can apply this constraint without introducing high bias

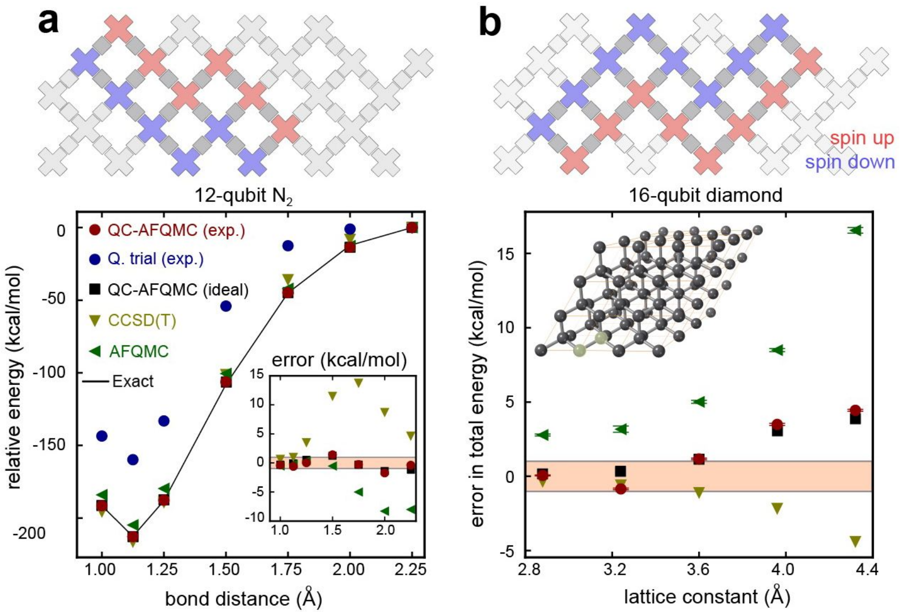


Quantum-Classical Hybrid Quantum Monte Carlo

Nature 603, 416–420 (2022)

The quantum processor makes a collection of randomized measurements of the **quantum trial wavefunction** to generate a **classical shadow**



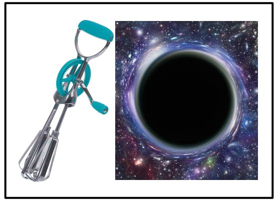


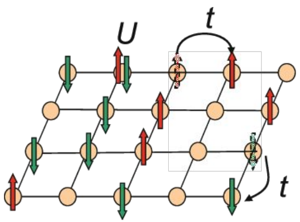
The energies from the Monte Carlo calculation driven by the quantum trial wavefunction are **highly accurate** (red circles) even though the bare trial wavefunction is not (blue circles)

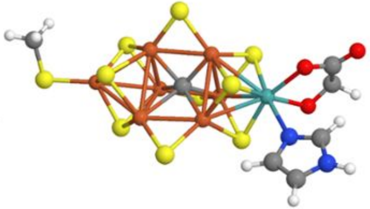
Quantum AI

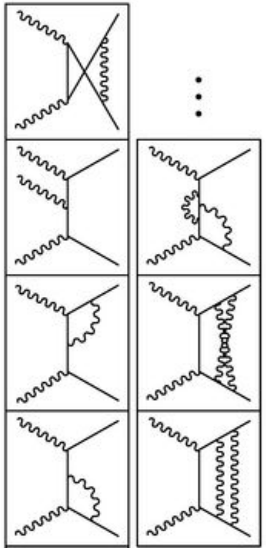
Quantum AI

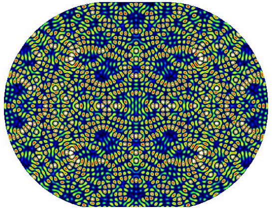
Spectrum of quantum simulation difficulty

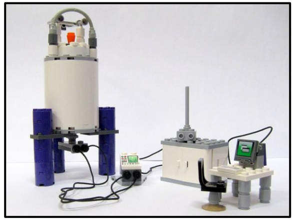












application difficulty

physical qubits required (with QEC)	25k-50k	50k - 250k	250k - 1MM	1MM - 5MM	???

Algorithms have rapidly improved!

Year	arXiv	First/Last Affiliations	Basis Set	Space Complexity	T Gate Complexity	T Gates for $N \approx 100$
2005	0604193	Berkeley	Arbitrary	$\mathcal{O}(N)$	$\mathcal{O}(\text{poly}(N/\epsilon))$	Unknown
2010	1001.3855	Harvard	Arbitrary	$\mathcal{O}(N)$	$\widetilde{\mathcal{O}}(N^{11}/\epsilon^{3/2})$	Unknown
2012	1208.5986	Haverford	Arbitrary	$\mathcal{O}(N)$	$\widetilde{\mathcal{O}}(N^{10}/\epsilon^{3/2})$	Unknown
2013	1312.1695	Microsoft / ETH Zurich	Arbitrary	$\mathcal{O}(N)$	$\widetilde{\mathcal{O}}(N^9/\epsilon^{3/2})$	$\sim 10^{20}$
2013	1312.2579	Haverford	Arbitrary	$\mathcal{O}(\eta \log N)$	$\mathcal{O}(\eta^2 N^8/\epsilon^{3/2})$	Unknown
2014	1403.1539	Microsoft / ETH Zurich	Arbitrary	$\mathcal{O}(N)$	$\widetilde{\mathcal{O}}(N^8/\epsilon^{3/2})$	Unknown
2014	1406.4920	Sherbrooke / Microsoft	Arbitrary	$\mathcal{O}(N)$	$\widetilde{\mathcal{O}}(N^7/\epsilon^{3/2})$	Unknown
2014	1410.8159	Harvard / Microsoft	Arbitrary	$\mathcal{O}(N)$	$\widetilde{\mathcal{O}}(N^6/\epsilon^{3/2})$	Unknown
2015	1506.01020	Harvard	Arbitrary	$\mathcal{O}(N)$	$\widetilde{\mathcal{O}}(N^5/\epsilon)$	Unknown
2015	1506.01029	Harvard	Arbitrary	$\mathcal{O}(\eta \log N)$	$\widetilde{\mathcal{O}}(\eta^2 N^3/\epsilon)$	Unknown
2016	1605.03590	ETH Zurich / Microsoft	Arbitrary	$\mathcal{O}(N)$	$\widetilde{\mathcal{O}}(N^6/\epsilon^{3/2})$	$\sim 10^{15}$
2018	1808.02625	Caltech / Google	Arbitrary	$\mathcal{O}(N)$	$\widetilde{\mathcal{O}}(N^{9/2}/\epsilon^{3/2})$	Unknown
2019	1902.02134	Macquarie / Google	Arbitrary	$\widetilde{\mathcal{O}}(N^{3/2})$	$\widetilde{\mathcal{O}}(N^4/\epsilon)$	$\sim 10^{11}$
2020	2007.14460	ETH Zurich / Microsoft	Arbitrary	$\widetilde{\mathcal{O}}(N^{3/2})$	$\widetilde{\mathcal{O}}(N^{7/2}/\epsilon)$	$\sim 10^{10}$
2020	2011.03494	Columbia / Google	Arbitrary	$\widetilde{\mathcal{O}}(N)$	$\widetilde{\mathcal{O}}(N^3/\epsilon)$	$\sim 10^9$

TABLE I. Best fault-tolerant algorithms for phase estimating chemistry in an arbitrary (e.g., molecular orbital) basis. N is number of basis functions, $\eta < N$ is number of electrons and ϵ is target precision. Gate counts here are for FeMoCo.

Year	arXiv	First/Last Affiliations	Basis Set	Space Complexity	T Gate Complexity	T Gates for $N \approx 100$
2017	1706.00023	Google / Caltech	Plane Waves	$\mathcal{O}(N)$	$\widetilde{\mathcal{O}}(N^{11/3}/\epsilon)$	Unknown
2018	1805.00675	Microsoft	Plane Waves	$\mathcal{O}(N \log(N/\epsilon))$	$\widetilde{\mathcal{O}}(N^2/\epsilon)$	Unknown
2018	1805.03662	Google	Plane Waves	$\mathcal{O}(N)$	$\mathcal{O}(N^3/\epsilon)$	$\sim 10^{10}$
2018	1807.09802	Google	Plane Waves	$\mathcal{O}(\eta \log N)$	$\widetilde{\mathcal{O}}(\eta^{8/3} N^{1/3}/\epsilon)$	Unknown
2019	1902.10673	Google	Plane Waves	$\mathcal{O}(N)$	$\widetilde{\mathcal{O}}(N^{5/2}/\epsilon^{3/2})$	$\sim 10^9$
2019	1912.08854	Maryland	Plane Waves	$\mathcal{O}(N)$	$\widetilde{\mathcal{O}}(N^2/\epsilon)$	Unknown
2020	2012.09194	Amazon	Plane Waves	$\mathcal{O}(N)$	$\widetilde{\mathcal{O}}(\eta^{8/3} N^{1/3}/\epsilon)$	$\sim 10^8$
2021	2105.12767	Google	Plane Waves	$\mathcal{O}(\eta \log N)$	$\widetilde{\mathcal{O}}(\eta^{8/3} N^{1/3}/\epsilon)$	$\sim 10^7$
2023	2301.01203	Google	Plane Waves	$\mathcal{O}(\eta \log N)$	$\widetilde{\mathcal{O}}(\eta^{7/3} N^{1/3}/\epsilon)$	Unknown

TABLE II. Best fault-tolerant algorithms for phase estimating chemistry in a plane wave basis. N is number of basis functions, $\eta < N$ is number of electrons and ϵ is target precision. Gate counts here are for $\eta = 40$.

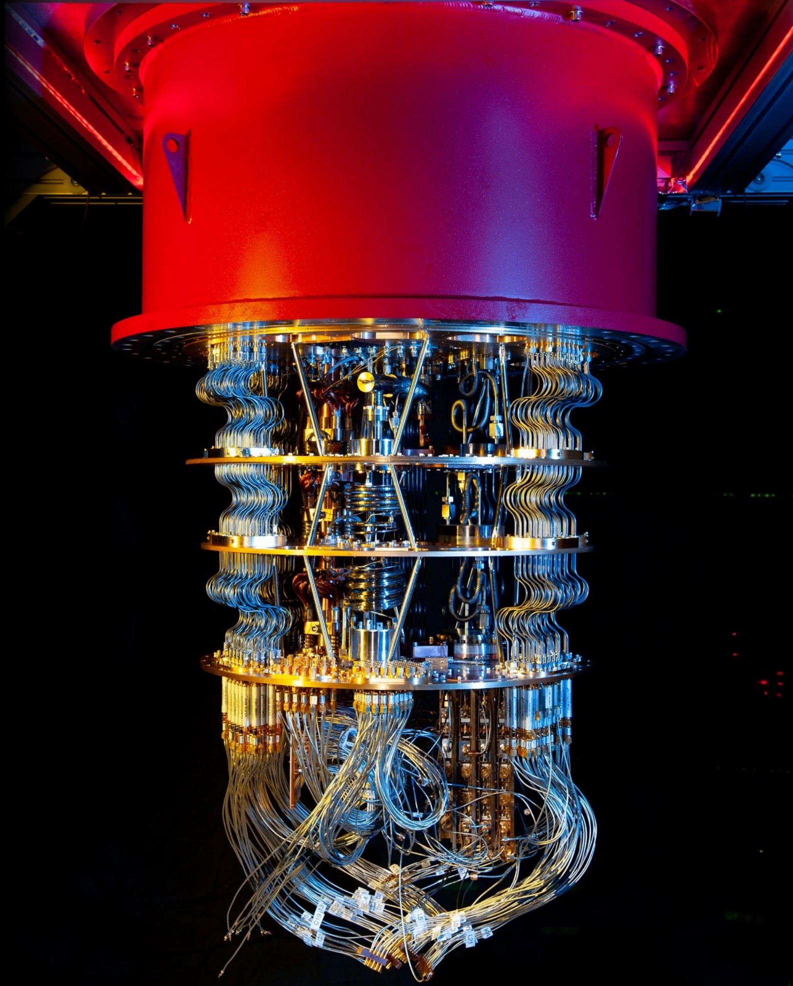
Google AI Quantum

Outlook

- It is still an open question whether quantum chemistry calculations will be feasible on NISQ devices
- QC-QMC allowed us to perform 16 qubit correlated calculation, surpassing VQE record in first experiment
- Error-correction requires many resources, methods are improving, and we are making hardware progress towards fault-tolerance

Thank you!

Quantum AI



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