Quantum Computing

A gentle parachute from the 30 000ft overview

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Aspuru-Guzik Group

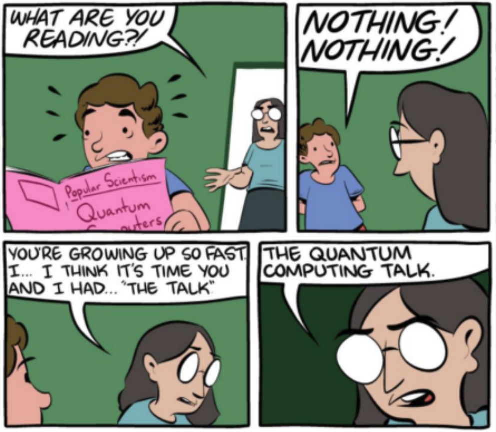





Popular science is rarely the full story

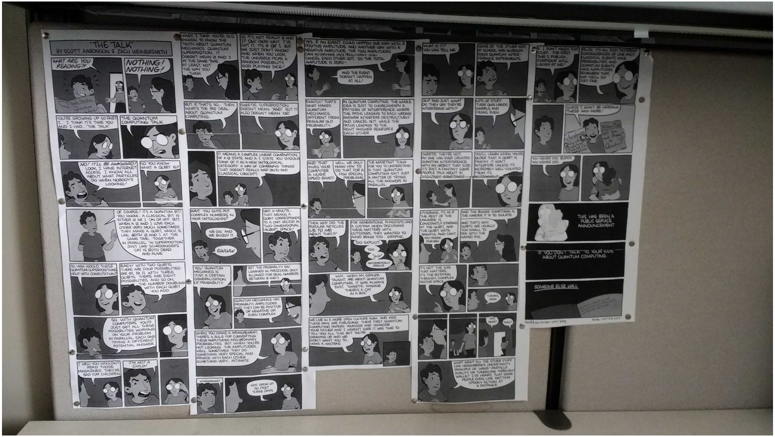
https://www.smbc-comics.com/comic/the-talk-3

Ask your friendly neighborhood theorist

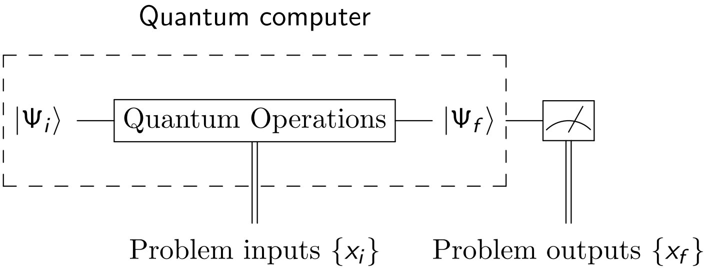


https://www.smbc-comics.com/comic/the-talk-3

Funny coincidence



Any device that uses quantum information to perform calculations



Any device that uses quantum information to perform calculations

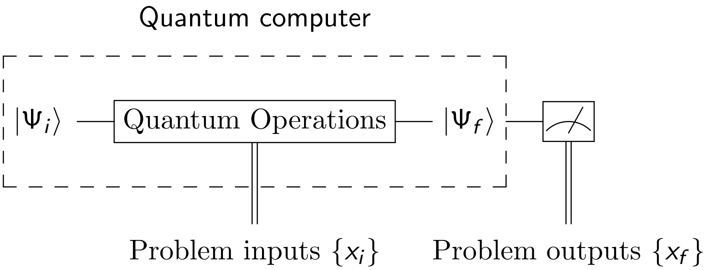
com·put·er
/kəmˈpyo͞odər/

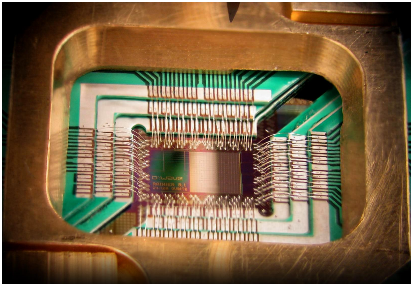
noun

an electronic device for storing and processing data, typically in binary form, according to instructions given to it in a variable program.

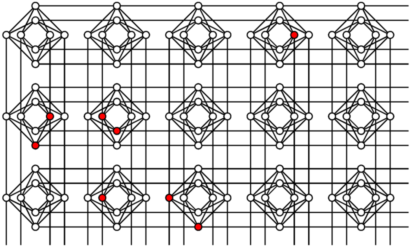
- a person who makes calculations, especially with a calculating machine.

Any device that uses quantum information to perform calculations





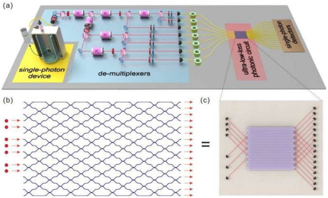
https://en.wikipedia.org/wiki/Quantum_annealing



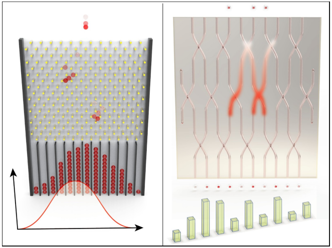
https://doi.org/10.1371/journal.pone.0172505

D'Wave

- $H = (1 - s)H_0 + sH_1(x_i)$
- start in easy $|\Psi_0\rangle$
- naturally go to hard $|\Psi_1\rangle$
- set parameters in H_1 once
- specific for optimization
- controversy about speedup



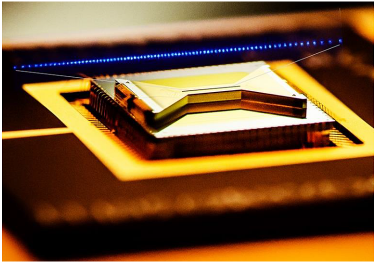
https://phys.org/news/2018-06-boson-sampling-photons-output-spite.html



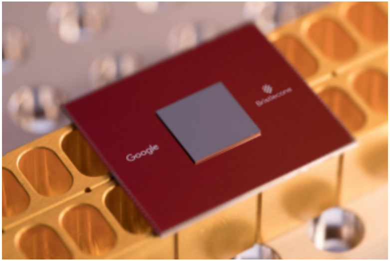
http://www.2physics.com/2013/03/experimental-boson-sampling.html

Boson sampling

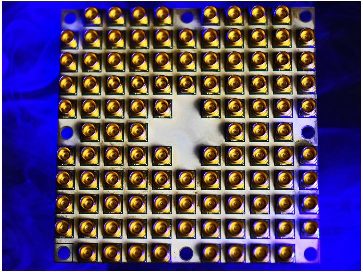
- quantum computer as sampler
- Proposed in 2011 by Aaronson
- Set parameters of circuit unitary U through optical elements
- sample from $\mathrm{perm}\,(U)$
- provably hard ($\#P$-hard)
- similar to Galton board



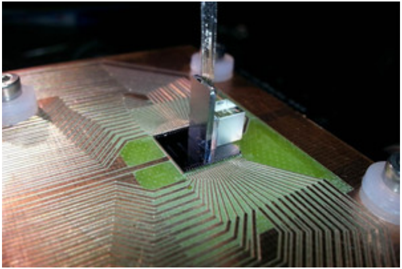
https://physicsworld.com/a/ion-based-commercial-quantum-computer-is-a-first/



https://ai.googleblog.com/2018/03/a-preview-of-bristlecone-googles-new.html



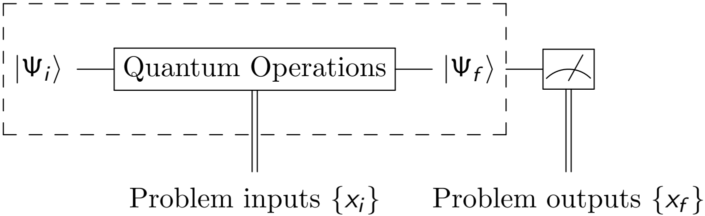
https://newsroom.intel.com/news/intel-advances-quantum-neuromorphic-computing-research/



https://www.tuwien.ac.at/en/news/news_detail/article/8946/

Any device that uses quantum information to perform calculations

Quantum computer



Digital (quantum) computing

Classical bits

- Express numbers base 2
  $47 = 101111$
- first non-trivial base
- with enough bits, represent any number
- easy to realize $\Rightarrow$ transistor

Quantum bit

- Expand wave function in basis vectors of 2-level systems
  $|\Psi\rangle = a\,|000\rangle + b\,|001\rangle + c\,|010\rangle + \dots$
- with enough qubits, represent any quantum system
- easiest to realize
  $\Rightarrow$ quantum control

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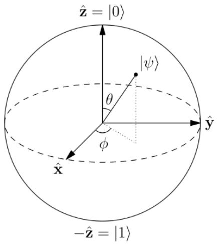


DiVincenzo requirements

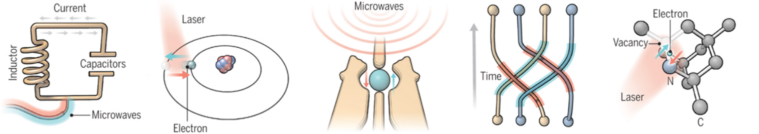
1. scalable wel characterizable
2. the ability to initialize the state of the qubits
3. long relevant decoherence times
4. a universal set of quantum gates
5. a qubit-specific measurement capability

Quantum specific

- entanglement $|\Psi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$
- superposition $|\Psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$

A bit of the action

In the race to build a quantum computer, companies are pursuing many types of quantum bits, or qubits, each with its own strengths and weaknesses.



	Superconducting loops	Trapped ions	Silicon quantum dots	Topological qubits	Diamond vacancies
	A resistance-free current oscillates back and forth around a circuit loop. An injected microwave signal excites the current into super-position states.	Electrically charged atoms, or ions, have quantum energies that depend on the location of electrons. Tuned lasers cool and trap the ions, and put them in superposition states.	These "artificial atoms" are made by adding an electron to a small piece of pure silicon. Microwaves control the electron's quantum state.	Quasiparticles can be seen in the behavior of electrons channeled through semi-conductor structures. Their braided paths can encode quantum information.	A nitrogen atom and a vacancy add an electron to a diamond lattice. Its quantum spin state, along with those of nearby carbon nuclei, can be controlled with light.
Longevity (seconds)	0.00005	>1000	0.03	N/A	10
Logic success rate	99.4%	99.9%	~99%	N/A	99.2%
Number entangled	9	14	2	N/A	6
Company support	Google, IBM, Quantum Circuits	ionQ	Intel	Microsoft, Bell Labs	Quantum Diamond Technologies
Pros	Fast working. Build on existing semiconductor industry.	Very stable. Highest achieved gate fidelities.	Stable. Build on existing semiconductor industry.	Greatly reduce errors.	Can operate at room temperature.
Cons	Collapse easily and must be kept cold.	Slow operation. Many lasers are needed.	Only a few entangled. Must be kept cold.	Existence not yet confirmed.	Difficult to entangle.

Note: Longevity is the record coherence time for a single qubit superposition state, logic success rate is the highest reported gate fidelity for logic operations on two qubits, and number entangled is the maximum number of qubits entangled and capable of performing two-qubit operations.

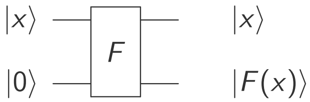
http://science.sciencemag.org/content/354/6316/1090.summary

Reversible computation

- all computations are unitary
- $U^{-1} = U^{\dagger}$
- problems with function evaluation

$$\begin{cases} U\left|x\right\rangle = \left|z\right\rangle \\ U\left|y\right\rangle = \left|z\right\rangle \end{cases}$$

$$\Rightarrow U\left(\left|x\right\rangle - \left|y\right\rangle\right) = 0$$



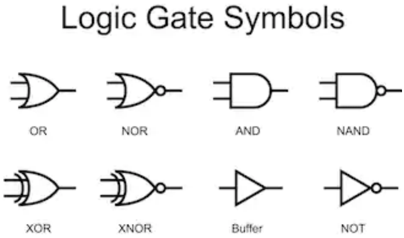
Quantum parallelism

- flip bits
- $00, 01, 10, 11$
- $\frac{1}{2}\left(\left|00\right\rangle + \left|01\right\rangle + \left|10\right\rangle + \left|11\right\rangle\right)$

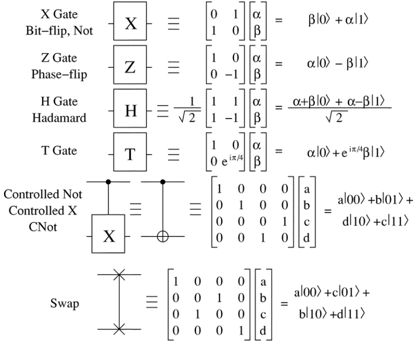
Measurement

- from quantum to classical
- projective $\Rightarrow$ collapse
- probability distribution

Classical bits



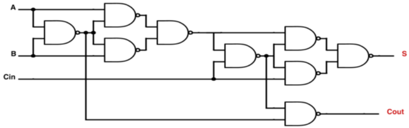
Quantum bit



https://ieeexplore.ieee.org/document/1263787?arnumber=1263787

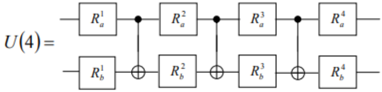
How many gates do you need?

Classical bits



- NAND and XOR are universal

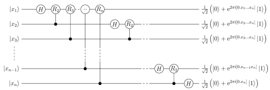
Quantum bit



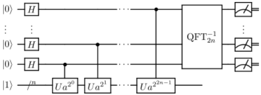
https://arxiv.org/abs/quant-ph/0602174

- single qubit rotation and CNOT ($\sqrt{\text{SWAP}}$) are universal
- different sets possible
- strongly depends on architecture

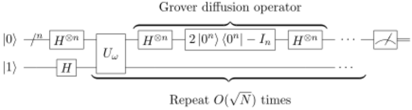
Using building blocks



https://en.wikipedia.org/wiki/Quantum_Fourier_transform



https://en.wikipedia.org/wiki/Shor%27s_algorithm

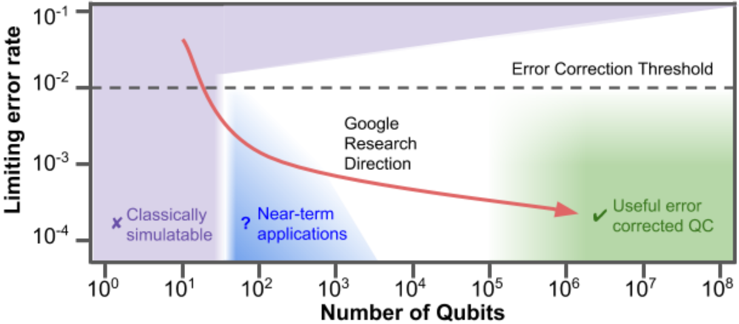


https://en.wikipedia.org/wiki/Grover%27s_algorithm

Speedups

- polynomial
- exponential
- heuristics
- oracles

NISQ = Noisy Intermediate Scale Quantum



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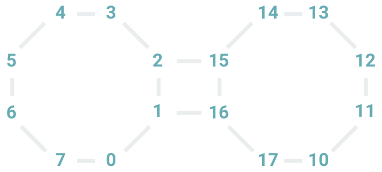
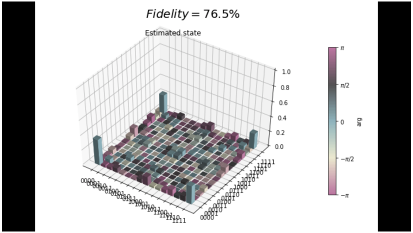
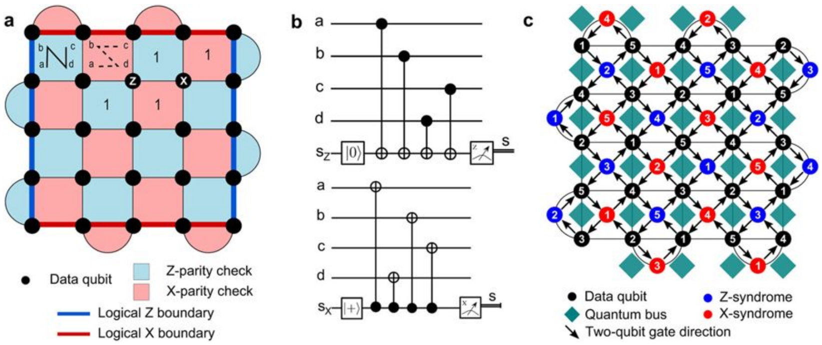


www.rigetti.com



Challenges

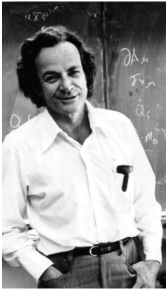
- connectivity
- decoherence
- qubit errors
- gate errors
- readout errors



https://www.nature.com/articles/s41534-016-0004-0

- redundancy but no-cloning theorem
- add ancilla qubits
- measure syndrome and adjust upon error
- huge overhead ± 1000 physical qubits per logical

Hamiltonian Simulation $|\Psi(t)\rangle = \exp(-iHt)\,|\Psi(0)\rangle$



Combination of algorithms

- State preparation
- Unitary evolution
- Phase estimation
- Amplitude amplification

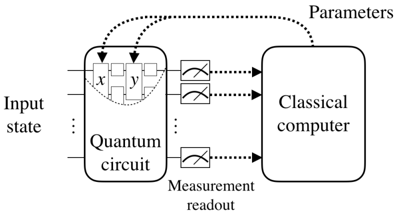
Resource estimates Fe_7MoS_9C

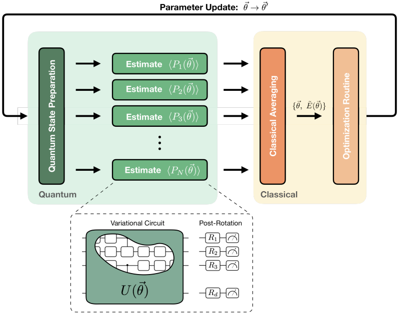
Structure	T gates	Cl. gates	Δt (10 ns)	Δt (100 ns)	Qubits
Quantitatively accurate simulation (0.1 mHa)					
Structure 1					
Serial	1.1×10^{15}	1.7×10^{15}	130 d	3.6 y	111
Nesting	3.5×10^{15}	5.7×10^{15}	15 d	4.9 mo	135
PAR	3.1×10^{16}	3.1×10^{16}	110 h	1.5 mo	1,982
Structure 2					
Serial	2.0×10^{15}	3.1×10^{15}	240 d	6.6 y	117
Nesting	6.5×10^{15}	1.0×10^{16}	27 d	8.9 mo	142
PAR	6.0×10^{16}	6.0×10^{16}	210 h	2.9 mo	2,024
Qualitatively accurate simulation (1 mHa)					
Structure 1					
Serial	1.0×10^{14}	1.6×10^{14}	12 d	3.9 mo	111
Nesting	3.3×10^{14}	5.6×10^{14}	1.4 d	14 d	135
PAR	3.0×10^{15}	3.0×10^{15}	11 h	4.6 d	1,982
Structure 2					
Serial	1.9×10^{14}	3.0×10^{14}	22 d	7.2 mo	117
Nesting	6.0×10^{14}	9.9×10^{14}	2.5 d	25 d	142
PAR	5.5×10^{15}	5.5×10^{15}	20 h	8.3 d	2,024

https://www.pnas.org/content/114/29/7555.abstract

$\Rightarrow$ Out of reach

Hybrid quantum classical algorithms





https://arxiv.org/abs/1812.09976

Year	Calculation	Citation	Number of qubits
1933	H_2	[74]	1
1950	Be	[76]	3, 4
1952	He	[77]	2
1955	He	[78]	2, 3
1956	BH	[41]	5
1956	H_2O	[41]	7
1957	LiH	[79]	3, 4, 5
1957	BeH^+	[79]	3, 4, 5
1960	Be	[82]	6
1960	CH_2	[83]	19
1963	H_2	[84]	3, 4, 5, 6
1966	HeH	[85]	3
1966	Li_2	[85]	3
1967	H_2O	[86]	10
1967	H_2O	[87]	24
1967	H_2O	[88, 89]	38, 39
1968	H_2O	[90]	39, 46
1968	Be	[91]	11
1969	Li, Be^+, B^{++}	[92]	9, 10
1969	BH, FH	[93]	12, 14
1970	H_2O	[94]	23

https://arxiv.org/abs/1208.5524

Architecture/ Platform	System-of-interest	Number of physical qubits	Year
Photonic chip	HeH^+	2	2014
Single trapped ion	HeH^+		2017
Superconducting processor (transmon qubits)	H_2	2	2016
Superconducting processor (transmon qubits)	H_2	2	2017
	LiH	4	2017
	BeH_2	6	2017
Ion trap processor (Ca^+ ions)	H_2	2	2018
	LiH	3	2018
Superconducting processor (transmon qubits)	H_2	2	2018
Silicon photonic chip	Two chlorophyll units in 18-mer ring of LHII complex	2	2018
Superconducting processor (transmon qubits) via Cloud	Deuteron	2-3	2018
Ion trap processor ($^{171}Yb^+$ ions)	H_2O	2-3	2019

https://arxiv.org/abs/1812.09976

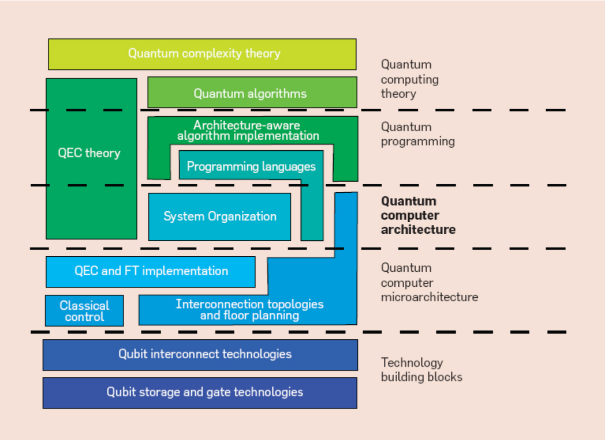
https://www.bbc.com/news/technology-12181153

https://www.research.ibm.com/ibm-q/

https://en.wikipedia.org/wiki/Summit_(supercomputer)

https://www.dwavesys.com

Many things need to work together

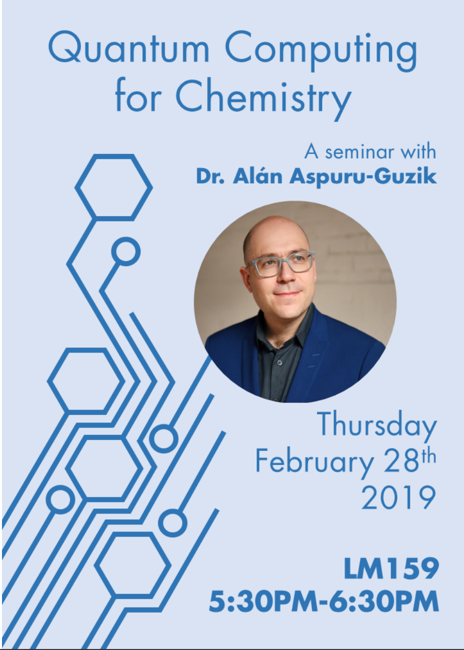


https://cacm.acm.org/magazines/2013/10/168172-a-blueprint-for-building-a-quantum-computer/fulltext

Thank you for your attention!

Further reading and self-promotion:
Quantum Chemistry in the Age of Quantum Computing
https://arxiv.org/abs/1812.09976

slides @ https://mfdgroot.github.io/


Quantum Computing
for Chemistry
A seminar with
Dr. Alán Aspuru-Guzik
Thursday
February 28th
2019
LM159
5:30PM-6:30PM