Webinars

An Overview of Quantum Computing

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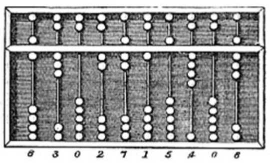
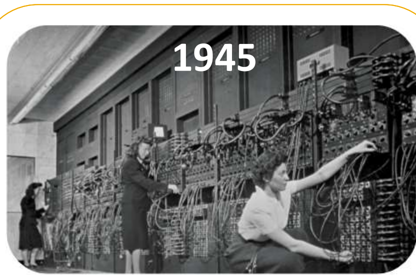


Abacus
First mentioned in a Chinese manuscript



ENIAC: The first general-purpose digital computer

Apple I: The first personal computer

Frontier: The first exascale computer

IBM System One: The first IBM quantum computer at a client site, Cleveland Clinic

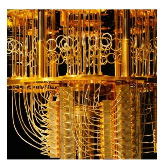
Which technology is the odd one out?

The consequences of mastering quantum computing … are no less significant than those faced by the scientists who lit up the New Mexico sky with the detonation at the Trinity test site 72 years ago.

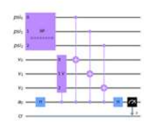
– Former U.S. representative Will Hurd (R-Tex) in 2017

Talk outline

Market & Investments



Hardware & Applications



Qubits, Gates & Circuits

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Three subfields within **Quantum Information Science**

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Quantum Computing

Some applications can greatly benefit from significant performance improvements, and there is potential for entirely new computing applications to emerge.

- Chemistry simulation
- Optimization
- Machine Learning

Quantum Communications

Enable secure transmission of quantum information over long distances, ensuring communications security, even in the face of unlimited quantum computing power.

- Scalable quantum repeater
- Quantum state teleportation

Quantum Sensing

Allow for measuring various quantities with significantly higher sensitivity than classical sensors.

- Atomic gravimetry & gradiometry for oil & gas exploration
- Logging borehole porosity

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Potential quantum technology market size by 2040

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Potential economic value from quantum computing

$620B–$1,270B

across four industries by 2035: chemicals, life sciences, finance, and automotive

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Source: Quantum Technology Monitor, McKinsey & Company, April 2023

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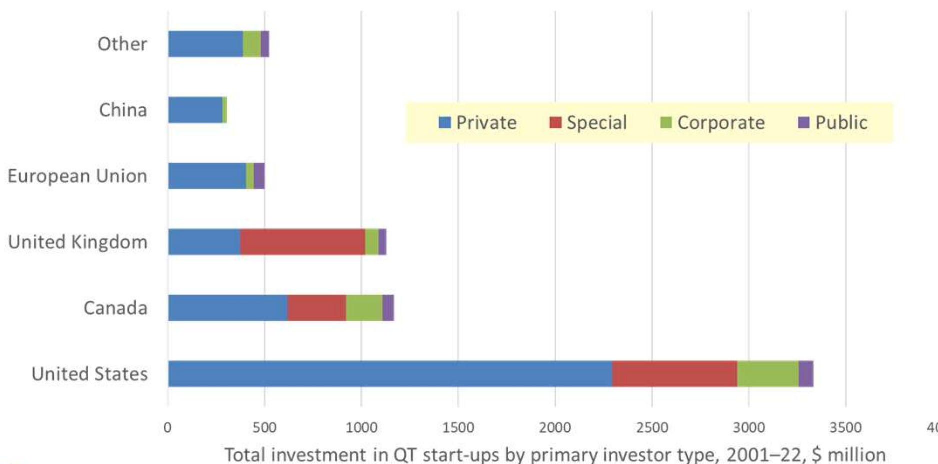
Private investments have fueled QT start-ups



Source: Quantum Technology Monitor, McKinsey & Company, April 2023

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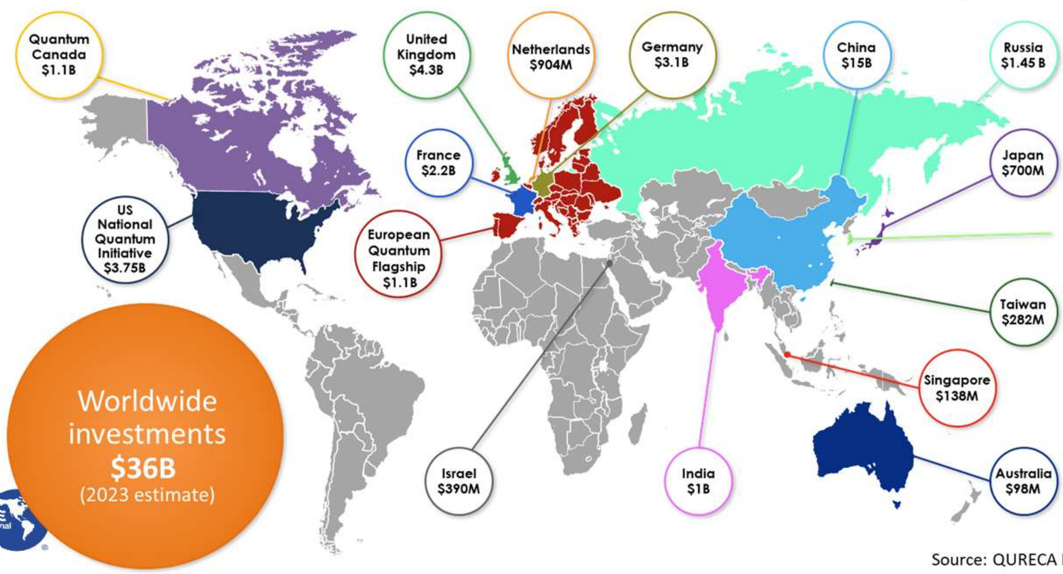
Public investments are ramping up



Source: QURECA Ltd.

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National Quantum Initiative became law in 2018

- "a coordinated Federal program to accelerate quantum research and development (R&D) for the economic and national security of the United States."
- NQI has launched 10 years of sustained effort.
- It authorizes NIST, NSF and DOE to strengthen Quantum Information Science (QIS) programs, centers, and consortia.
- FY2023 budget request is $844 million.

NIST

- Quantum Economic Development Consortium (QED-C)
- Two joint institutes with the University of Maryland
  - The Joint Quantum Institute (JQI)
  - The Joint Center for Quantum Information and Computer Science (QuICS)
- Quantum-based measurement technologies
- Since 2016, NIST has led an international competition-like standardization process for post-quantum cryptography (PQC)
  - Selected four candidate PQC algorithms in 2022

NSF

- Quantum Leap Challenge Institutes (QLCIs)
- Transformational Advances in Quantum Systems (TAQS) programs
- Center for Quantum Information and Control (CQuIC) – U. of New Mexico
- Center for Quantum Networks (CQN) – University of Arizona
- The NSF Quantum Foundry – UC, Santa Barbara and Montana State University/the University of Arkansas
- The Institute for Quantum Information and Matter (IQIM) – CalTech
- The MIT-Harvard Center for Ultracold Atoms (CUA)
- The Center for Integrated Quantum Materials (CIQM) – Harvard University
- Software-Tailored Architecture for Quantum co-design (STAQ) – Duke University
- Enabling Practical Scale Quantum Computing (EPiQC) – University of Chicago
- …

DOE

- DOE awarded $625 million over five years to establish five QIS Centers. This award was met with $340 million in contributions from the private sector and academia.
  - Q-NEXT · Next Gen Quantum Science and Engineering · Argonne National Lab
  - C2QA · Co-design Center for Quantum Advantage · Brookhaven National Lab
  - SQMS · Superconducting Quantum Materials and Systems Center · Fermi National Lab
  - QSA · Quantum Systems Accelerator · Lawrence Berkely National Lab
  - QSC · The Quantum Science Center · Oak Ridge National Lab

https://science.osti.gov/Initiatives/QIS/QIS-Centers

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QC may disrupt several industry segments soon

Economic value of quantum computing:

- + Incremental
- ++ Significant
- +++ Disruptive

Key Industry Segment	2025-30	2030-35
Oil and gas	+	++
Sustainable energy	+	+++
Chemicals	++	+++
Pharmaceuticals	++	+++
Automotive	++	++
Aerospace and defense	+	++
Advanced electronics	+	++
Semiconductors	+	++
Financial services	++	+++
Telecom	+	++
Media	+	+
Logistics	+	++

Source: Quantum Technology Monitor, McKinsey & Company, April 2023

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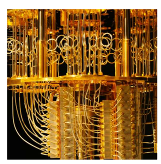
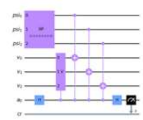
Talk outline

Market & Investments



Hardware & Applications



Qubits, Gates & Circuits

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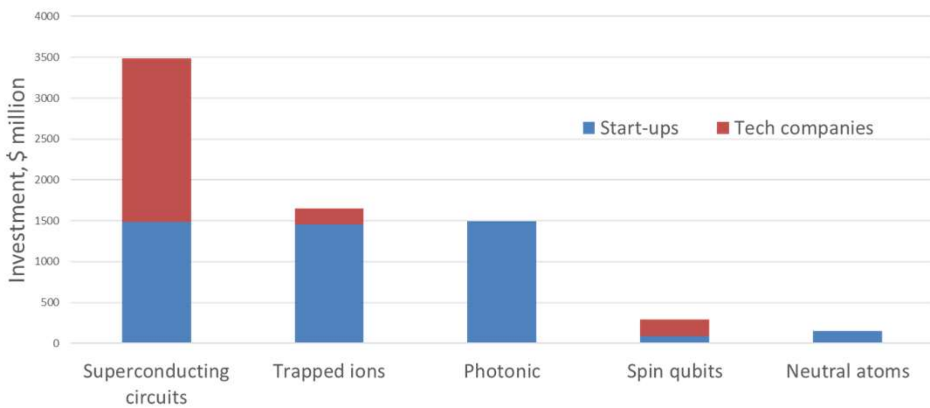
Several quantum computing hardware technologies are under development



Superconducting circuits	Trapped ions	Photonic	Spin qubits	Neutral atoms
IBM	IonQ	Xanadu	Intel	Atom computing
Google	Quantinuum	PsiQuantum		Quera
Alibaba				
AWS				

Source: Quantum Technology Monitor, McKinsey & Company, April 2023

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A **qubit** is a quantum system with two distinguishable states

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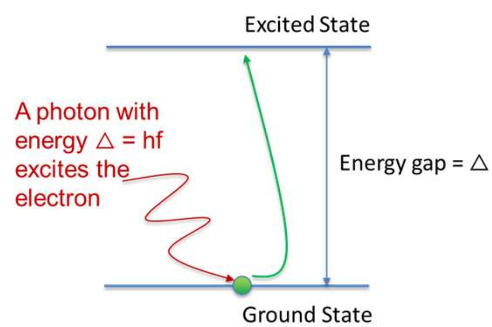
- The ground and excited states of a valence electron are a natural choice for a qubit:
  - **Neutral atoms,** trapped with optical tweezers
  - **Trapped ions** or charged atoms (e.g., Ytterbium-171), trapped in an oscillating electric field



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https://pennylane.ai/qml/demos_quantum-computing/

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A photon is another option for a qubit

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- Polarization qubit:
  - The photon's polarization is one way to define a qubit: horizontal polarization and vertical polarization.
- Path qubit:
  - The path a photon takes is another way to define a qubit: "here" and "there".

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https://uwaterloo.ca/institute-for-quantum-computing/quantum-101/quantum-information-science-and-technology/what-qubit

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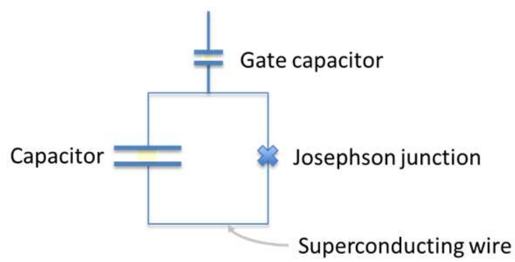
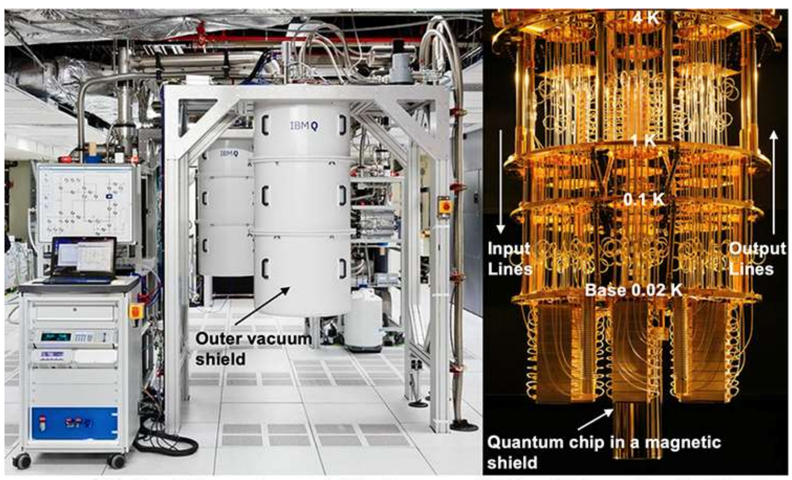
A manmade qubit is **Transmon**, an *artificial atom*



This is a quantum system with discrete energy levels.

Superconducting circuits must be maintained at 10 mK and shielded from vibrations, radiation etc.



Dilution fridge setup: outside view **Dilution fridge setup: inside view**

Source: IBM

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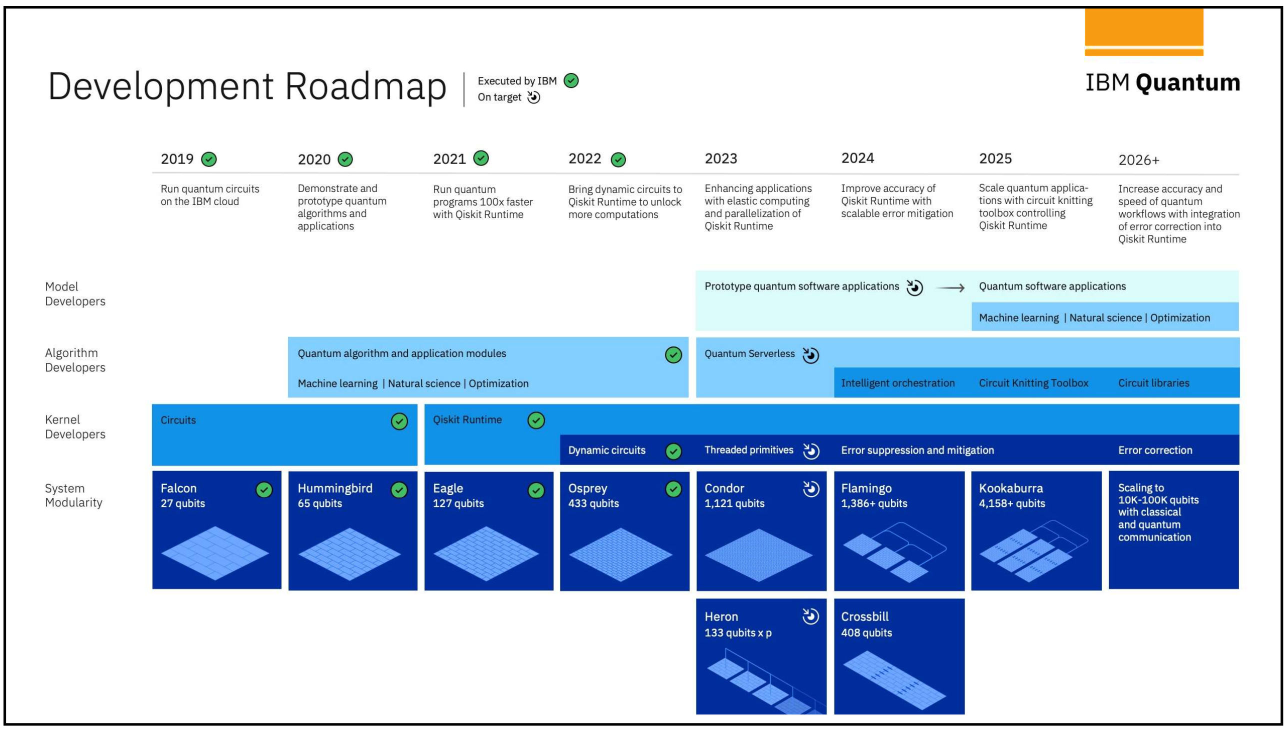
Development Roadmap
Executed by IBM
On target
IBM Quantum
2019
2020
2021
2022
2023
2024
2025
2026+
Run quantum circuits on the IBM cloud
Demonstrate and prototype quantum algorithms and applications
Run quantum programs 100x faster with Qiskit Runtime
Bring dynamic circuits to Qiskit Runtime to unlock more computations
Enhancing applications with elastic computing and parallelization of Qiskit Runtime
Improve accuracy of Qiskit Runtime with scalable error mitigation
Scale quantum applications with circuit knitting toolbox controlling Qiskit Runtime
Increase accuracy and speed of quantum workflows with integration of error correction into Qiskit Runtime
Model Developers
Prototype quantum software applications
Quantum software applications
Machine learning | Natural science | Optimization
Algorithm Developers
Quantum algorithm and application modules
Machine learning | Natural science | Optimization
Quantum Serverless
Intelligent orchestration
Circuit Knitting Toolbox
Circuit libraries
Kernel Developers
Circuits
Qiskit Runtime
Dynamic circuits
Threaded primitives
Error suppression and mitigation
Error correction
System Modularity
Falcon
27 qubits
Hummingbird
65 qubits
Eagle
127 qubits
Osprey
433 qubits
Condor
1,121 qubits
Flamingo
1,386+ qubits
Kookaburra
4,158+ qubits
Scaling to 10K-100K qubits with classical and quantum communication
Heron
133 qubits x p
Crossbill
408 qubits

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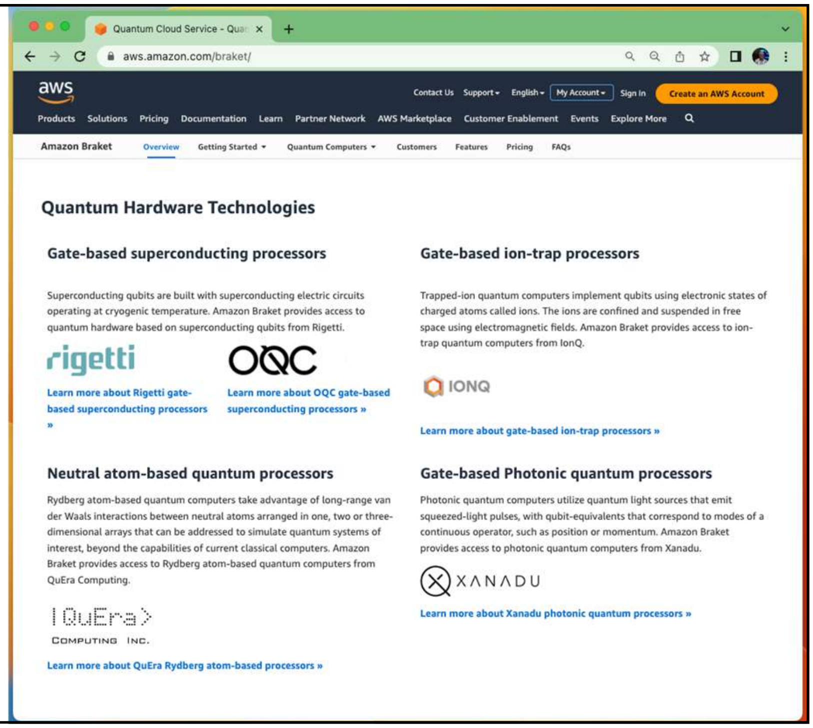
Quantum computers are available on the cloud

- Amazon Braket
- IBM Q
- Microsoft Azure



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Quantum Advantage has been demonstrated

Year	Organization	Quantum system	# of qubits	Comparing to supercomputer	Classical	Quantum
2019	Google, U.S.[1]	Sycamore	53	Summit	10,000 yr (2.5 days per IBM[2])	200 s
2020	U. of Science and Technology of China[3]	Jiǔzhāng	100	Sunway TaihuLight	2.5 B yr	200 s
2022	Xanadu, Canada[4]	Borealis	216	Fugaku	9,000 yr	36 µs
2023	U. of Science and Technology of China[5]	Jiǔzhāng		Frontier	600 yr	1.27 µs

1. Arute F et al. Nature, 2019. https://doi.org/10.1038/s41586-019-1666-5
2. Pednault et al. arXiv:1910.09534v2 [quant-ph] 22 Oct 2019
3. H.-S. Zhong et al. Science, 2020. https://doi.org/10.1126/science.abe8770
4. Madsen et al. Nature, 2022. https://doi.org/10.1038/s41586-022-04725-x
5. Yu-Hao Deng et al. arXiv:2304.12240v1 [quant-ph] 24 Apr 2023

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Practical algorithms with provable speedup exist

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Year	Inventors	Purpose	Speedup over classical
1994	Shor	Finding the prime factors of an integer	Exponential
1996	Grover	Unstructured search	Quadratic
2009	Harrow, Hassidim, Lloyd	Linear equation solver	Exponential

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Quantum computers: terrible and awesome*

- Quantum computers can't change what's computable
- Quantum operations are slow
- Quantum computers can do many calculations in parallel; yet a measurement yields only a *single, random outcome*

- To use effectively use QC clever algorithms are required
- Quantum advantage stems from far fewer operations required

* Nature briefing (2023). doi: https://doi.org/10.1038/d41586-023-01692-9

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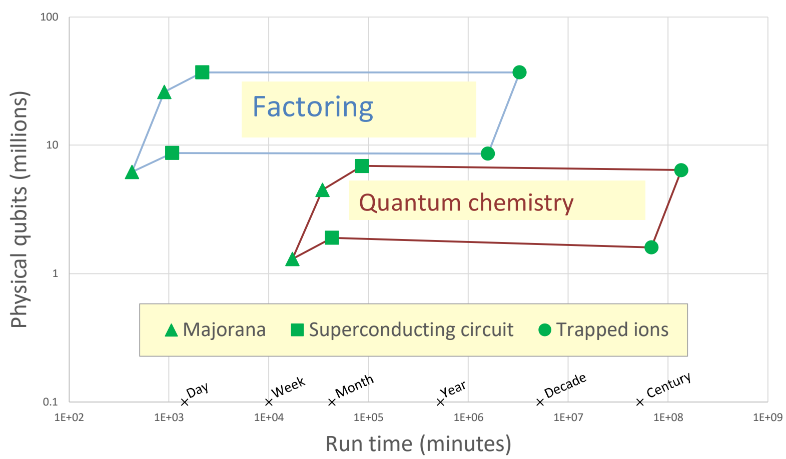
The algorithms with provable speedup require fault-tolerant qubits

- The physical qubits available today are noisy
- Quantum error correction (QEC) builds reliable logical qubits out of thousands of noisy physical qubits.
- A universal, fault-tolerant quantum computer could be 1 or 2 decades away

Over a million physical qubits may be required for practical applications



Beverland et al., arXiv:2211.07629v1 [quant-ph] 14 Nov 2022

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Near-term quantum advantage may come from heuristic algorithms running on NISQ computers

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- Today's computers are called Noisy Intermediate Scale Quantum (NISQ) computers
- Variational Quantum Eigensolver (VQE) for Quantum chemistry[1]
- Quantum Approximate Optimization Algorithm (QAOA)[2]
- Whether they will be able to surpass classical supercomputers is an outstanding question

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1. A. Peruzzo et al., Nat. Commun. 5, 4213 (2014)
2. Farhi E, Goldstone J, Gutmann S. arXiv:1411.4028v1 [quant-ph] 14 Nov 2014

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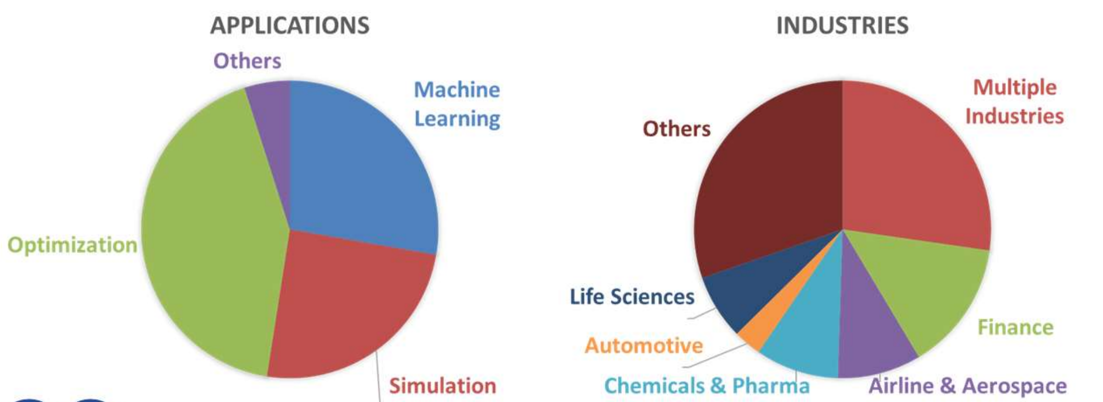
A 2022 survey shows many quantum computing projects being pursued by the industry



https://quantumconsortium.org/algorithms22/

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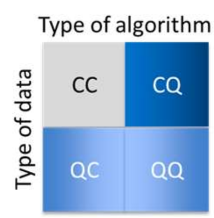
Optimization

- About 70% of the optimization projects in the 2022 survey used circuit-based computers, and the remainder used quantum annealing.
- Quantum annealing frames the optimization problem as the energy minimization of a quantum system; e.g., D-Wave[1].
- Quantum annealing and quantum circuit-based optimization explored for energy applications[2]
  - Locating energy facilities (solar, wind etc.) to minimize facility opening and transportation costs
  - Commitment of units to different loads/power demands minimizing the total operational costs
  - Heat exchanger networks in powerplants

1. https://www.dwavesys.com/applications
2. A. Ajagekar, F. You, Energy 179 (2019) 76–89

Quantum Machine Learning

- Main advantage: Quantum computers could represent complex structures that are hard to simulate classically
- Disadvantages: (1) I/O is generally difficult and slow (2) Vanishing gradients can make training difficult
- R&D in various ML areas
  - Quantum variational classification
  - Quantum kernel estimation
  - Quantum Generative Adversarial Networks



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Chemistry simulation

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- Quantum computers may one day revolutionize chemistry and materials science
  - Calculate molecules' energies and structures, model catalysis.
  - Design novel materials from the atom up.
- Variational quantum eigensolver (**VQE**) is suitable for NISQ computers[1]
  - Lithium superoxide (LiO_2) dimer rearrangement with applications to lithium-air (Li/O_2) batteries[2]
  - Binding energy of H_2 chains and the isomerization of diazene (H_2N_2) calculated using 12 qubits and 72 two-qubit gates[3]

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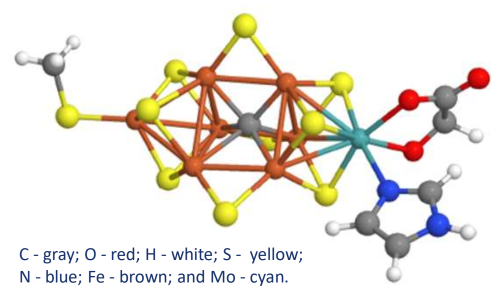
1. A. Peruzzo et al., Nat. Commun. 5, 4213 (2014)
2. Gao et al. arXiv:1906.10675 [quant-ph] (2019)
3. Rubin et al., Science 369, 1084–1089 (2020)

Iron molybdenum cofactor (FeMoco)

- NH_4 synthesis, which sustains 50% of the world's population and consumes 2% of its energy, requires high temperature and pressure (500°C/20 MPa)[1].
- Understanding biological N_2 fixation, which occurs at room T & P, could transform NH_4 synthesis industry
- The mechanism of FeMoco, responsible for N_2 fixation, could be simulated on a quantum computer in under 4 days[2]



C - gray; O - red; H - white; S - yellow; N - blue; Fe - brown; and Mo - cyan.

1. Reiher et al. PNAS 2017. www.pnas.org/cgi/doi/10.1073/pnas.1619152114
2. Lee et al. arXiv:2011.03494v2 [quant-ph] 11 Dec 2020

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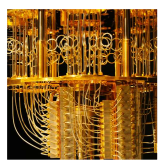
Talk outline

Market & Investments



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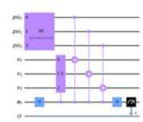

Qubits, Gates & Circuits

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The **bit** is a basic unit of classical information

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Physically, anything with two separate states can store 1 bit:

The flip of a coin	Heads	Tails
The state of a wire in a chip	Off	On
Spots of magnetism in a hard drive	North	South

Represented as a binary number **0** **1**

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Bit-strings encode information

The red-white pattern on the parachute of
Perseverance rover that landed on Mars in 2020

= Dare Mighty Things

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Information is manipulated with **Logic gates**

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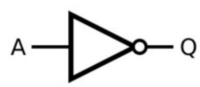
NOT



A	Q
0	1
1	0

AND

A	B	Q
0	0	0
0	1	0
1	0	0
1	1	1

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Logic gates form the basic building blocks of classical computation

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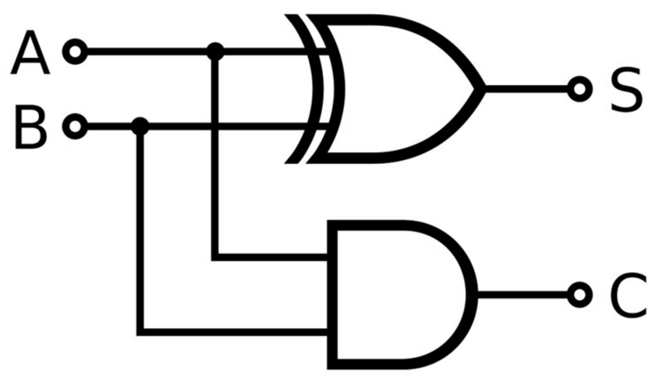
The **half adder** adds two single binary digits A and B, to give the sum (S) and carry (C).



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All classical computers are programmable implementations of logic gates

~10^9 Flops/s

...

1.6×10^{18} Flops/s

Frontier: The first Exascale supercomputer, Oak Ridge National Lab, 2022.

Axiom 1: Superposition principle

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The **qubit** is the fundamental unit of a quantum system, fully defined by its state vector.

The **basis states** of qubit are: $|0\rangle = \begin{pmatrix}1\\0\end{pmatrix}$ $|1\rangle = \begin{pmatrix}0\\1\end{pmatrix}$

A qubit can be in a state of **superposition** $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$,
where α and β are the **amplitudes**.

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State vectors are written in Dirac **bra-ket** notation

For example, in two dimensions,

$$\text{bra:} \quad \langle\psi| = (\alpha^* \quad \beta^*) \qquad \text{ket:} \quad |\psi\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

α and β are complex numbers, and * indicates the complex conjugate.

They form a finite-dimensional **Hilbert space**, an extension of 3D Euclidean space with a well-defined inner product:

$$\||\psi\rangle\|^2 = \langle\psi|\psi\rangle = \alpha^*\alpha + \beta^*\beta$$

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The **Born rule** provides the probability of detecting a specific state of the qubit

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$$P(|0\rangle) = |\alpha|^2 \qquad P(|1\rangle) = |\beta|^2$$

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

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The state of one qubit can be visualized as a point on a spherical surface called **Bloch Sphere**

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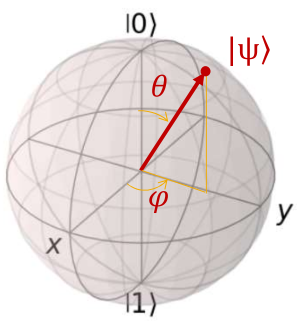

$$|\psi\rangle = \cos\frac{\theta}{2}\,|0\rangle + e^{i\varphi}\sin\frac{\theta}{2}\,|1\rangle$$

That is $\alpha = \cos\frac{\theta}{2}$, $\beta = e^{i\varphi}\sin\frac{\theta}{2}$

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No cloning theorem

An unknown quantum state's amplitudes α and β cannot be measured.

Copying a qubit is not possible!

Axiom 2: Quantum measurement

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When a qubit is measured, it yields a classical bit, 0 or 1.

The measurement can be in the computational basis $\{|0\rangle, |1\rangle\}$ or any of the infinitely many orthogonal bases.

Upon measurement, the qubit's state collapses to the observed state, e.g.,
Measuring $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$ in $\{|0\rangle, |1\rangle\}$ results in

$|\psi\rangle = |0\rangle$ with $|\alpha|^2$ probability or

$|\psi\rangle = |1\rangle$ with $|\beta|^2$ probability.

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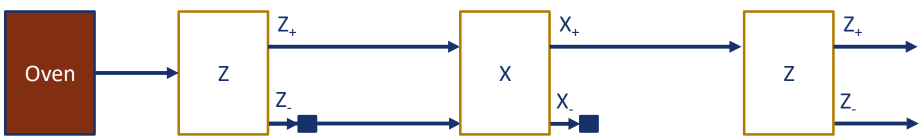
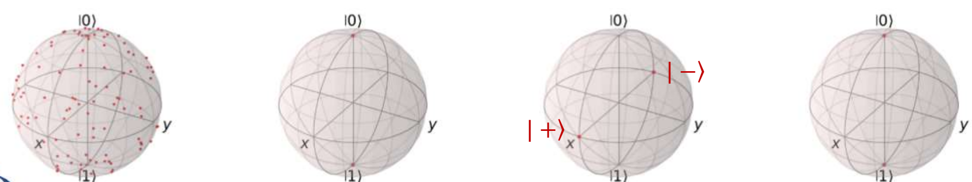
The first indication of qubits came in 1922 from the Stern-Gerlach experiment



Hot hydrogen atoms are beamed through magnetic fields.



Note: This multi-qubit system cannot be strictly visualized on a Bloch sphere.

Nielsen and Chuang (2010)

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Axiom 3: Unitary evolution

Quantum gates are the basic building blocks of quantum computation. They must be **unitary matrices** (U), which rotate or reflect the vector, preserving its length:

$$\mathrm{U}^{\dagger}\mathrm{U} = \mathrm{I}$$

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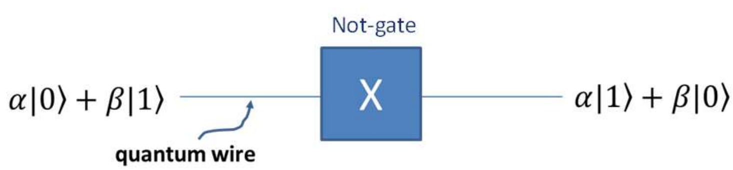
A basic **quantum circuit**



$$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} \beta \\ \alpha \end{pmatrix}$$

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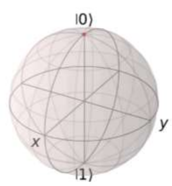
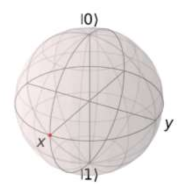
The commonly used **Hadamard** gate generates superposition states

$$|0\rangle \xrightarrow{\;H\;} \frac{|0\rangle + |1\rangle}{\sqrt{2}}$$

called $|+\rangle$ state

$$\frac{1}{\sqrt{2}}\begin{bmatrix}1 & 1\\ 1 & -1\end{bmatrix}\begin{pmatrix}1\\0\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}$$





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Quantum interference

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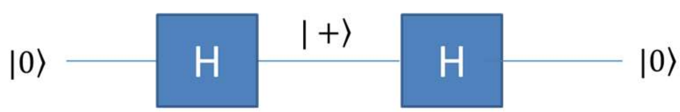
The probability of a state could become zero because quantum amplitudes take both positive and negative values, as opposed to classical probabilities that are always non-negative.

Sometimes a unitary transformation applied to a superposition state can *give a determinate state*



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Multi-qubit states

Multi-qubit computational basis states are tensor products; e.g.,

$$|10\rangle = |1\rangle \otimes |0\rangle = \binom{0}{1} \otimes \binom{1}{0} = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$$

The superposition in a 2-qubit system:

$$|\psi\rangle = \alpha_1|00\rangle + \alpha_2|01\rangle + \alpha_3|10\rangle + \alpha_4|11\rangle \text{ where } \sum_{i=1}^{2^2} |\alpha_i|^2 = 1$$

Representing superposition in an n-qubit system requires 2^n amplitudes!

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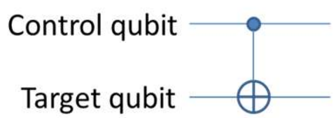
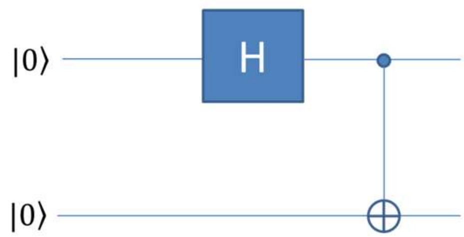
CNOT gate flips the target qubit based on the state of the control qubit



CNOT $\qquad |10\rangle \qquad |11\rangle$

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

Quantum entanglement

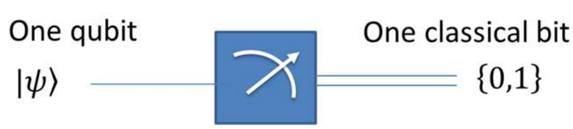


$$\frac{|00\rangle + |11\rangle}{\sqrt{2}}$$

This state, called the **Bell Pair**, can't be factored into a tensor product $|a\rangle \otimes |b\rangle$

Therefore, measuring one of the entangled qubits collapses the state of the other qubit regardless of how far apart the two qubits are!

Measurement is the final step of a quantum computation



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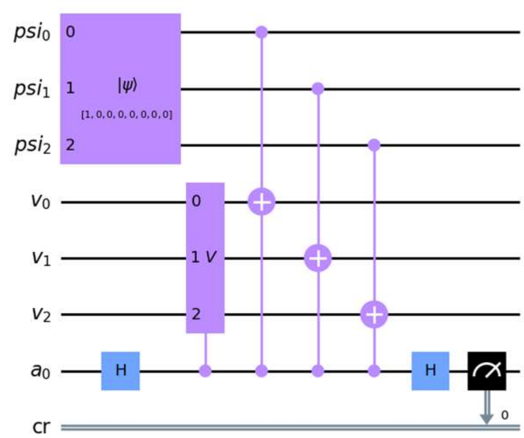
A quantum computation consists of three steps

1. Prepare the initial state

2. Apply a sequence of quantum gates



$$V|\psi|^2 = \frac{\#(0) - \#(1)}{\#(0) + \#(1)}$$

3. Obtain the result by measuring in the computational basis

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Deutsch-Josza algorithm

The first to demonstrate:

"The quantum computation solves the problem with certainty in exponentially less time than any classical deterministic computation."[1]

1. D. Deutsch and R. Jozsa, Proc. R. Soc. London, Ser. A, 439, 553 (1992).

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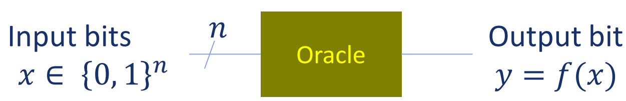
Deutsch-Josza – The task



We are given an Oracle (black box function) that outputs either

Constant: $y = 0$ for all inputs

or

Balanced: $y = 0$ for half the inputs and $y = 1$ for the other half

We are asked to determine whether the given Oracle is **constant** or **balanced.**

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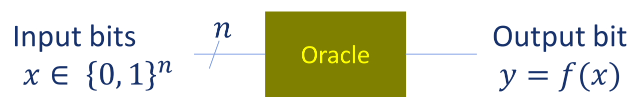
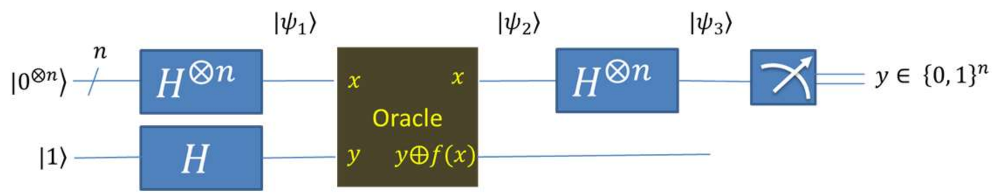
Deutsch-Josza – Classical algorithm



1. Input all zeros and read the output (say, it is 0)
2. Change a bit to create a new input
3. If the new output is 1 the Oracle is **balanced** → stop
4. Else
   a. If the number of iterations is $\frac{2^n}{2} + 1$ (the worst case), the Oracle is **constant** → stop
   b. Else go to step 2.

Deutsch-Josza – Quantum algorithm

Webinars



$$|\psi_1\rangle = \frac{1}{\sqrt{2^n}} \sum_{x \in \{0,1\}^n} |x\rangle \left(|0\rangle - |1\rangle\right)$$

$$|\psi_2\rangle = \frac{1}{\sqrt{2^n}} \sum_{x \in \{0,1\}^n} (-1)^{f(x)} |x\rangle \left(|0\rangle - |1\rangle\right)$$

$$|\psi_3\rangle = \frac{1}{2^n} \sum_{k \in \{0,1\}^n} \left[\sum_{x \in \{0,1\}^n} (-1)^{f(x)} (-1)^{x \cdot k} \right] |k\rangle$$

Quantum interference at work!

$$|\boldsymbol{\psi_3}\rangle = \begin{cases} |\mathbf{0}\rangle^{\otimes n} & \text{Oracle is constant} \\ else & \text{Oracle is balanced} \end{cases}$$

(Oracle is **constant**; Oracle is **balanced**)

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Deutsch-Josza – Quantum advantage

Number of Oracle calls for n = 50

Classical		Quantum
Best case	2	1
Worst case	**5.6×10^{14}**	

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Summary

- Quantum computing is expected to cause disruptions in multiple industries within the next 15 years.
- Rapid advancements are occurring in hardware tech and applications – chemistry, optimization, & machine learning.
- Quantum computing derives its power from phenomena – *superposition, entanglement, & interference* – not found in classical systems.

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