@zapatacomputing

# ZAPATA COMPUTING
# Challenges and opportunities in practical near-term quantum computers

June 5, 2019

ITU Workshop on Quantum Information Technology

Christopher Savoie, PhD, JD

Founder and CEO

@cjsavoie

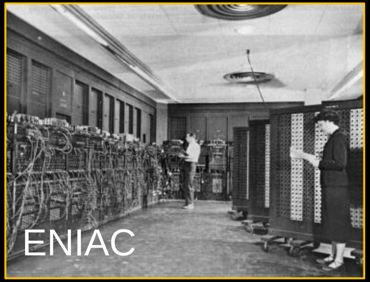
Abacus

Ball-and-disk integrator

***Special-purpose*** *computer for industrial measurements e.g. areas and volumes*

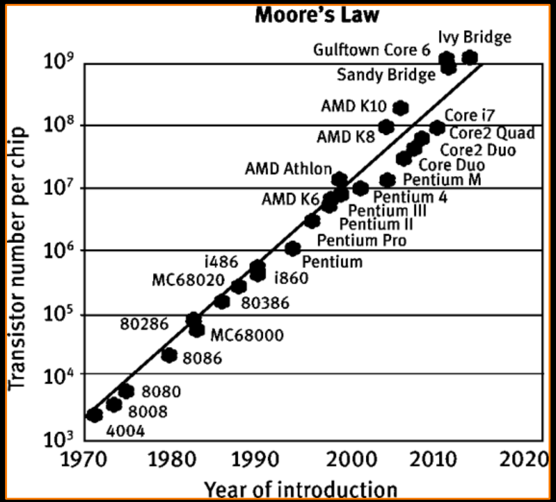
Alan Turing

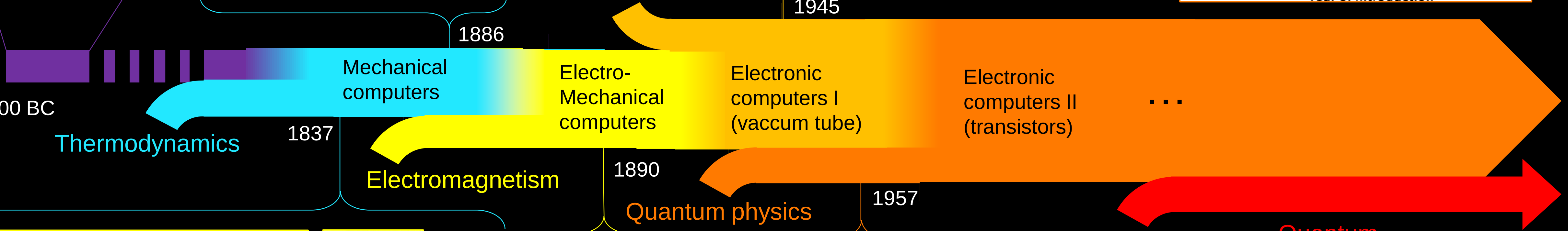
Theory of computation



John von Neumann

***General-purpose*** *computer that* ***significantly accelerated*** *Monte Carlo calculation over manual computation for Manhattan project*





2700 BC

Thermodynamics

1837

Mechanical computers

1886

Electromagnetism

Electro-Mechanical computers

1890

Quantum physics

1945

Electronic computers I (vaccum tube)

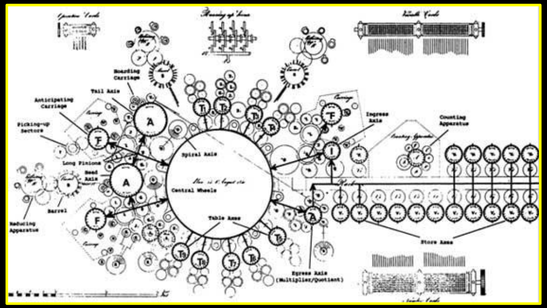
Electronic computers II (transistors)

1957

. . .

Quantum computation and quantum information

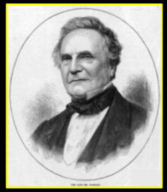
Quantum computers



Analytical engine

*Application: polynomial function evaluation*

*Failed due to limited funding and Babbage's own longevity*



Charles Babbage

Ada Lovelace

Tabulation machine

*Application: Data tabulation*

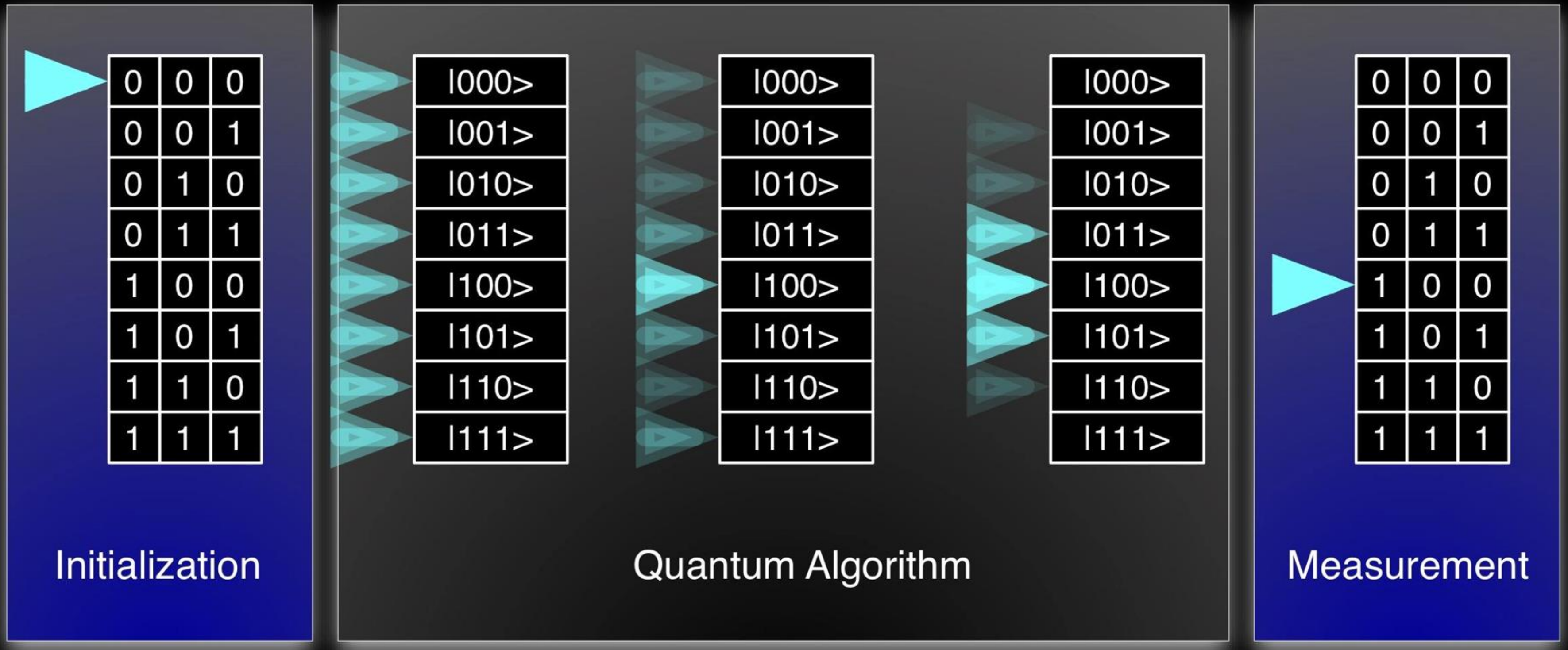
***Special-purpose*** *computer that demonstrated* ***clear advantage*** *over manual process for 1890 US census*

IBM 608

First commercial computer which is fully based on transistors

*"…****50 percent reduction in physical size*** *and a* ***90 percent reduction in power requirements*** *over comparable vacuum tube models…"*

# A **quantum computer** is a collection of qubits that can be coherently controlled to process quantum information



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Initialization

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Quantum Algorithm

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Measurement

8 states for 3 qubits

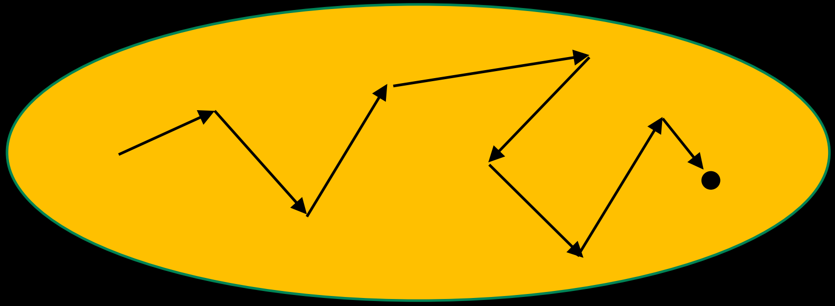
16 states for 4 qubits

32 states for 5 qubits

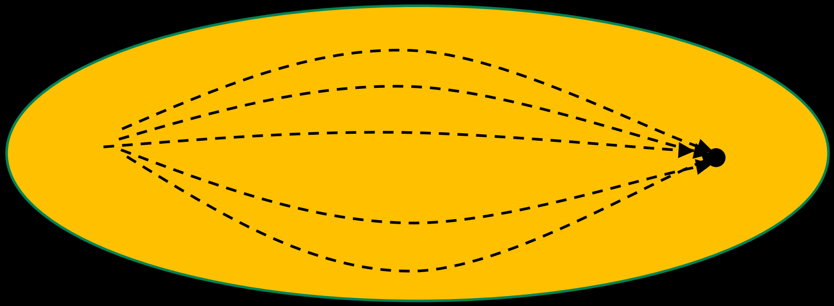
⋮

$2^{300}$ states for 300 qubits

Number of Hydrogen atoms in the Universe: $2^{285}$



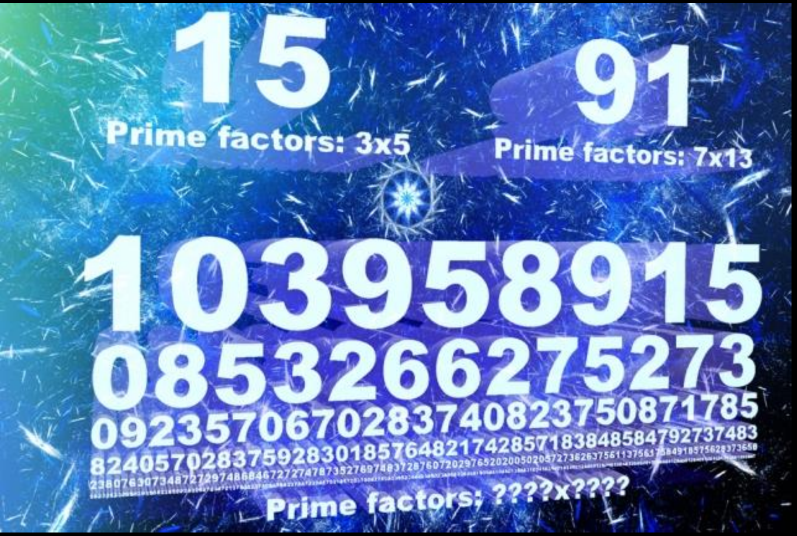
Classical computer



Quantum computer

### Integer factorization

Shor’s algorithm (1997)



### Information security

Potential threat to encryption protocols such as RSA, ECC

### Unstructured search

Grover’s algorithm (1996)

### Database

Brute-force search among a large number of items

### Quantum simulation

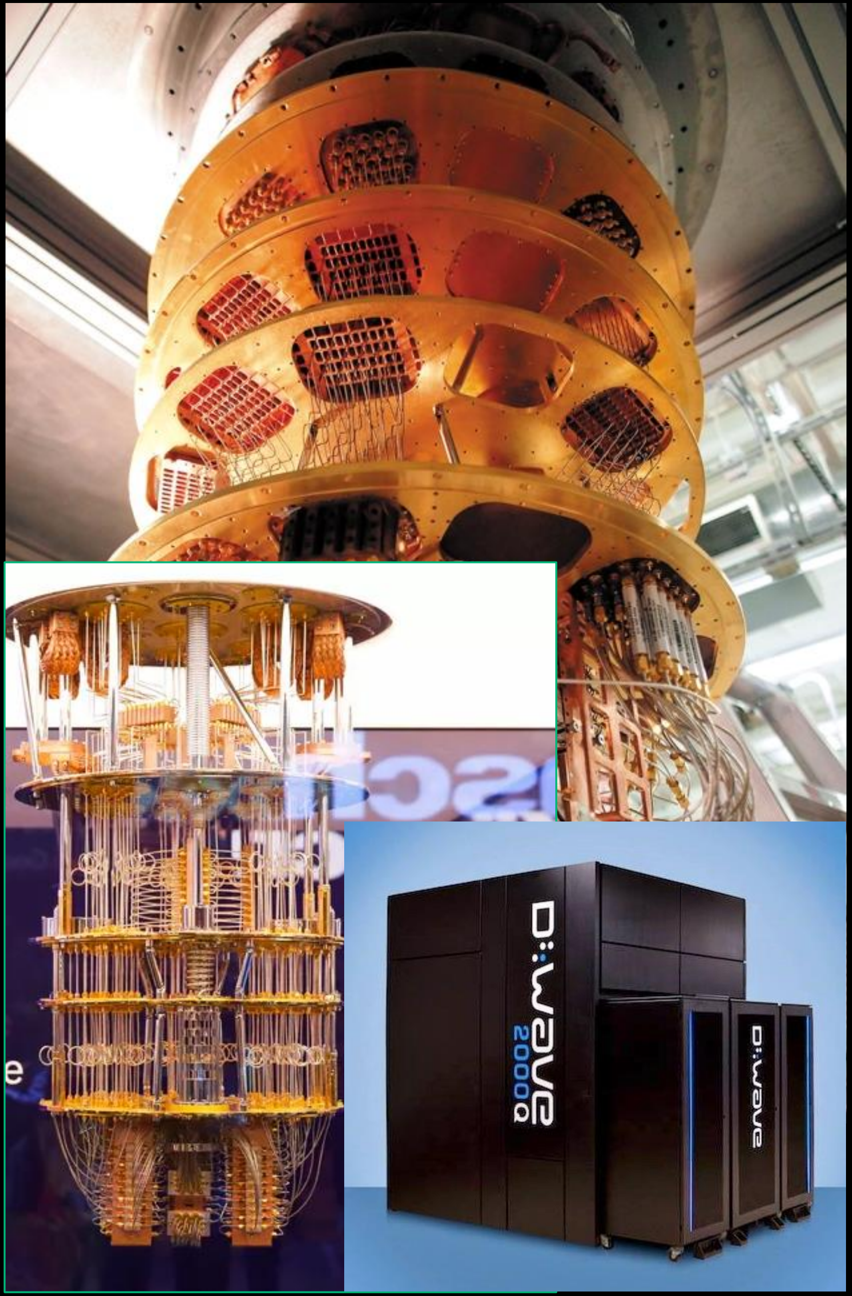
Aspuru-Guzik et al. (2005)

### Chemistry

Accurate calculation of molecular properties of drugs and materials

Shor, Peter W. "Polynomial-Time Algorithms for Prime Factorization and Discrete Logarithms on a Quantum Computer", *SIAM J. Comput*., 26 (5): 1484–1509, 1997
Grover, L.K. “A fast quantum mechanical algorithm for database search”, *Proceedings, 28th Annual ACM Symposium on the Theory of Computing*, p. 212, 1996
Aspuru-Guzik, A., A. Dutoi, P. J. Love, M. Head-Gordon. “Simulated quantum computation of molecular energies”, *Science*, Vol. 309, Issue 5741, pp. 1704-1707, 2005
Cao, Y., J. Romero, J. Olson, M. Degroot, P. Johnson, et al. “Quantum chemistry in the age of quantum computing”, *Chemical Review*. 2018. To appear.

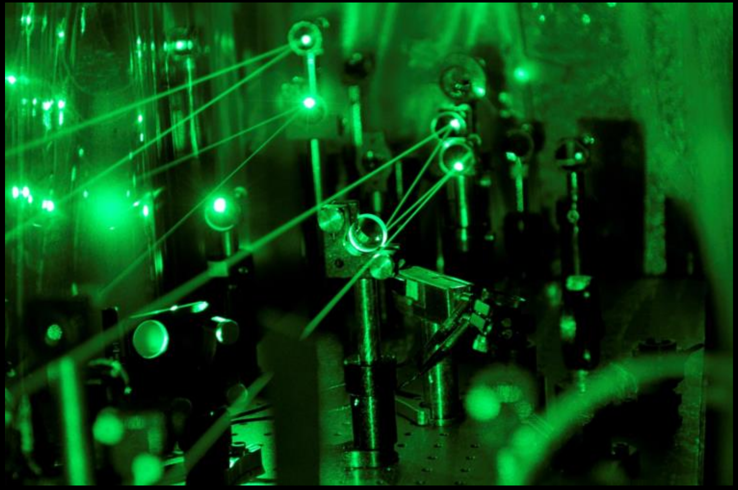
## Superconducting quantum computer



## Trapped ion quantum computer

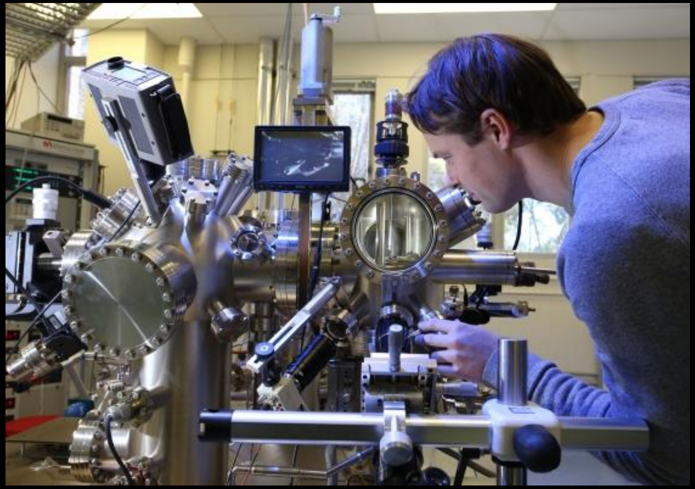
Source: © IQOQI / M. R. Knabl
The quantum computer uses
trapped calcium ions as qubits

## Photonic quantum computer



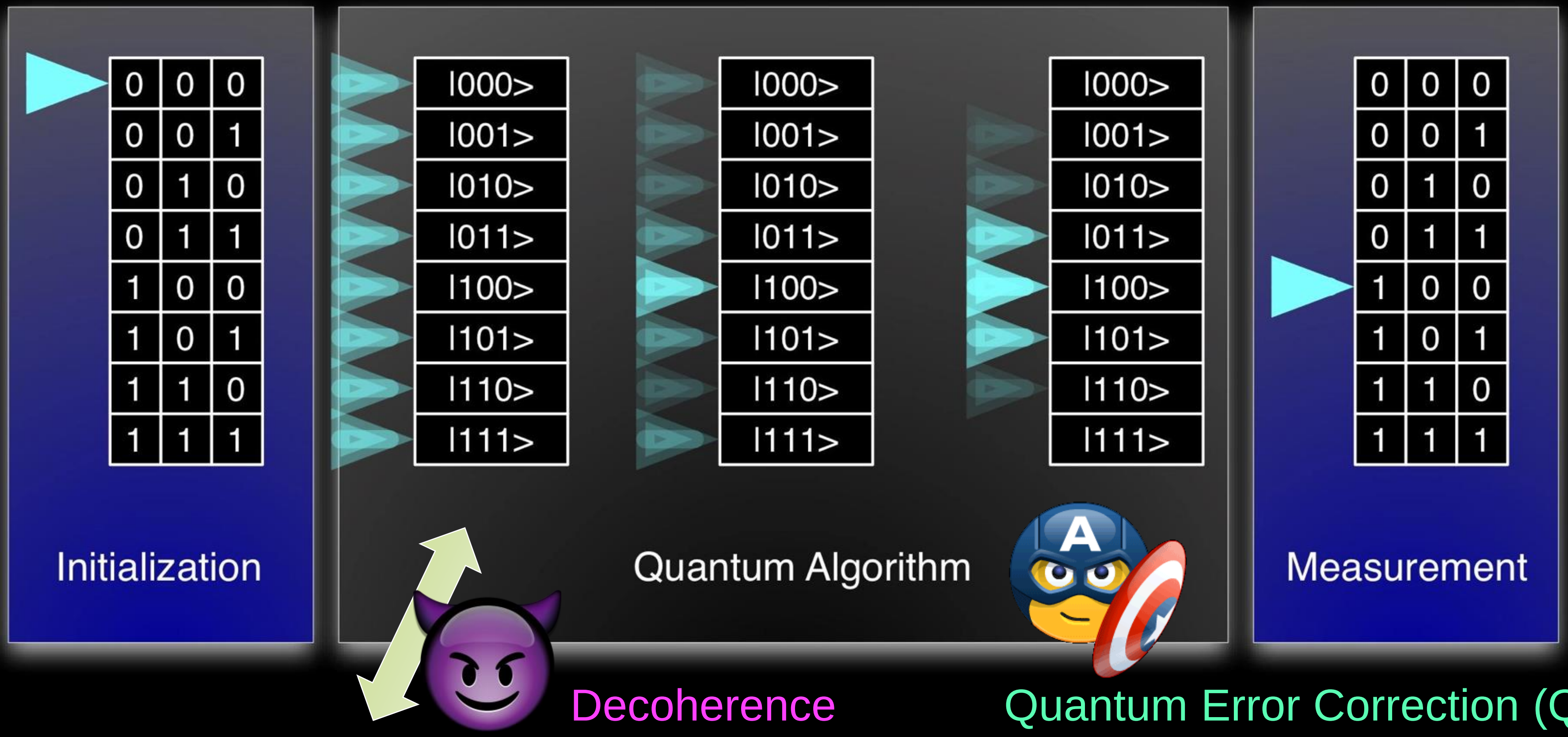
Credit: Zhejiang Daily

## Silicon-based quantum computer



Source: UNSW Sydney

…



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State-of-the-art QEC techniques require ~10000 physical qubits for each logical qubit

If the physical qubits are not too noisy, QEC can in principle allow for quantum computation of arbitrary duration, a regime known as fault tolerance

Environment

Decoherence

The physics of QC becomes classical

Quantum Error Correction (QEC)

Each logical qubit is encoded into multiple physical qubits

Resource estimate for quantum simulation problems of practical interest:

~1 million physical qubits, hours of QC

Current hardware: <100 qubits, ~0.001s

What useful applications can be found *before* scalable, fault-tolerant quantum computers are built?

Babbush, R, C. Gidney, D. W. Berry, N. Wiebe, J. McClean et al. ”Encoding Electronic Spectra in Quantum Circuits with Linear T Complexity", *Phys. Rev. X* 8, 041015 (2018)

# NISQ era

- Noisy Intermediate Scale Quantum (NISQ) devices
- Limited quantum computational resource
  - Qubit fidelity
  - Gate fidelity
  - Qubit connectivity
  - SPAM error

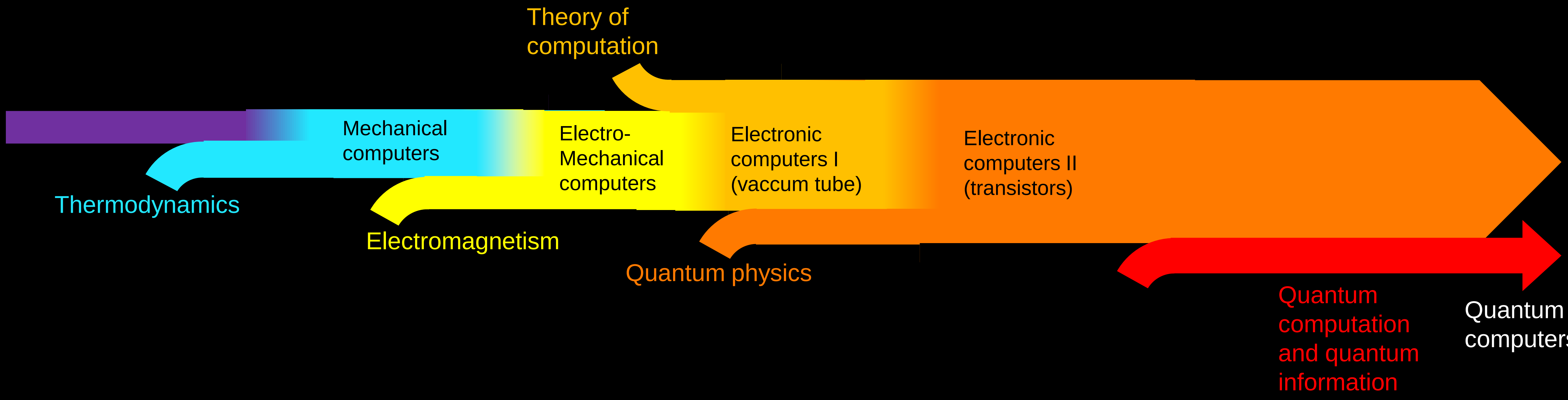
Builds on decades of quantum system and electrical engineering

- Need to optimize *all* layers of abstraction
  - Quantum algorithm
  - Quantum circuit
  - Compilation
  - Hardware instruction

Builds on decades of computer science and engineering

(Useful near-term quantum applications)

Preskill, J. " Quantum Computing in the NISQ era and beyond", *Quantum* 2, 79 (2018)



Theory of computation

Mechanical computers

Electro-
Mechanical
computers

Electronic
computers I
(vaccum tube)

Electronic
computers II
(transistors)

Thermodynamics

Electromagnetism

Quantum physics

Quantum
computation
and quantum
information

Quantum
computers

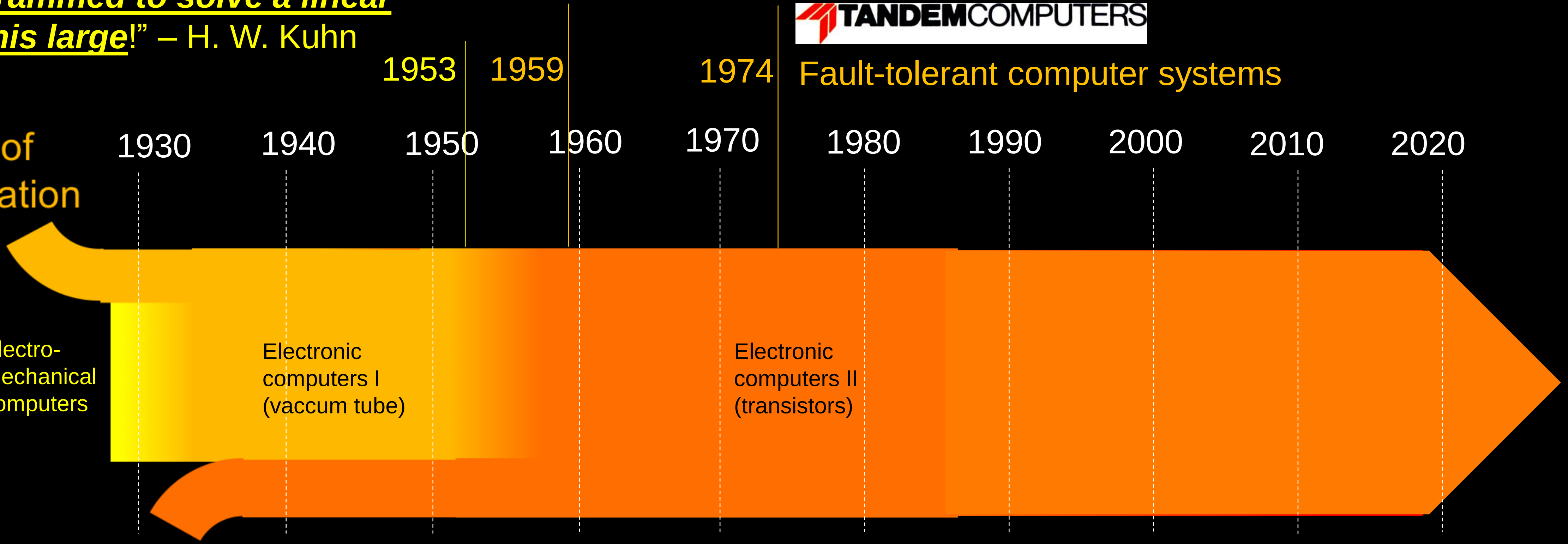
Theory of computation

Electro-Mechanical computers

Solving a 10 × 10 assignment problem with the simplex method on the SEAC, consisted of 256 Williamson cathode ray tubes, took 20 minutes. “In 1953, ***there was no machine in the world that had been programmed to solve a linear program this large***!” – H. W. Kuhn

“My Ph.D. thesis on computational quantum mechanics was done on the IBM 650, a 2000-word drum memory machine. I believe that ***the need to be very economical on this computer*** may have led to my early interest in optimal algorithms and computational complexity.” –J. F. Traub

TANDEMCOMPUTERS



Formal models of computation

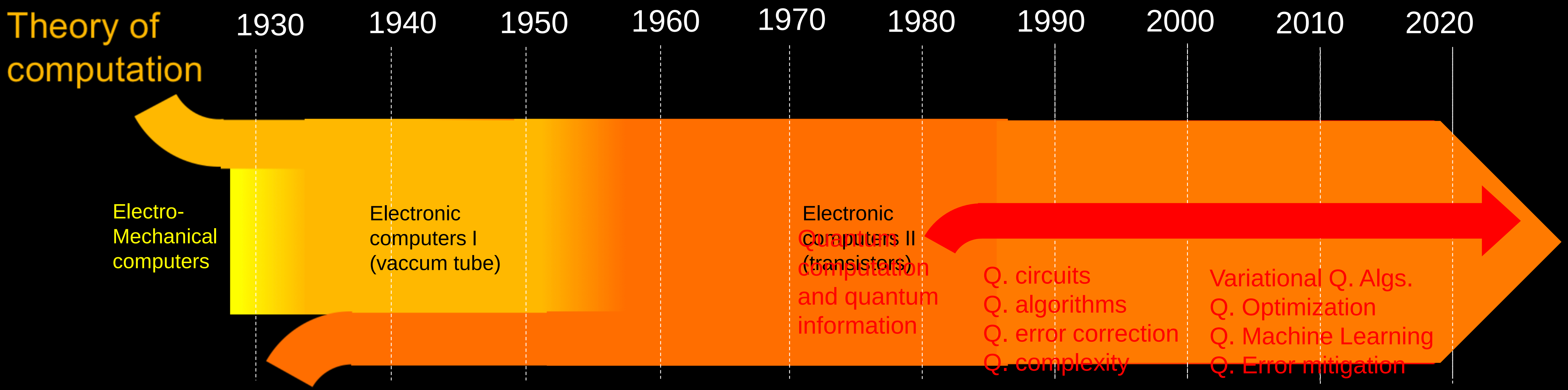
Programming languages
Language translators
Compilers
Operating systems
Computer architecture

Computational complexity
Algorithm & data structure

Networking
Parallel Computing

Machine learning

# Accelerated progress in quantum algorithm developments vs. classical computation



Theory of computation

1930 1940 1950 1960 1970 1980 1990 2000 2010 2020

Electro-
Mechanical
computers

Electronic
computers I
(vaccum tube)

Electronic
computers II
(transistors)

Quantum
computation
and quantum
information

Q. circuits
Q. algorithms
Q. error correction
Q. complexity
…

Variational Q. Algs.
Q. Optimization
Q. Machine Learning
Q. Error mitigation
…

Formal models of
computation

Programming languages
Language translators
Compilers
Operating systems
Computer architecture

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Algorithm & data structure

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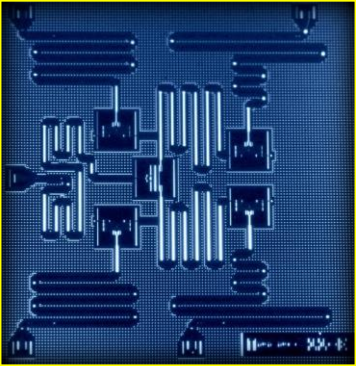
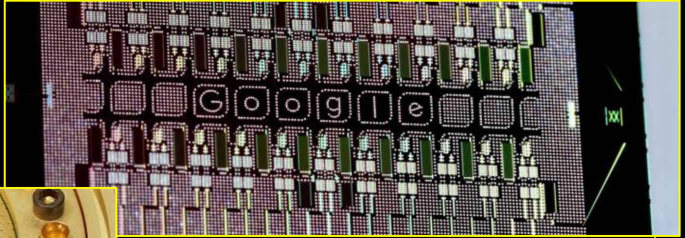
# NISQ era

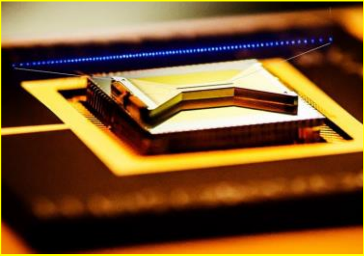


IBM 5-qubit processor
(Q Experience)

Rigetti 19Q device



Google 22-qubit Foxtail Xmon



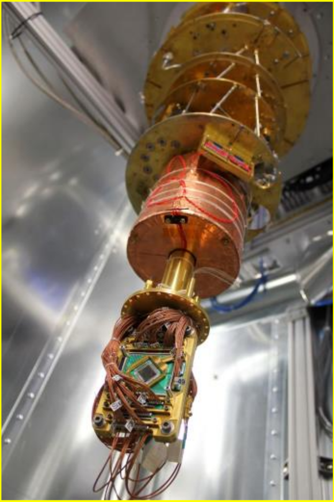
IonQ 11-qubit device

IBM System One (20 qubits)

2000 2010 2016 2020

2007 2011 2013 2015 2017 2018 2019

D-Wave 16-qubit
Orion quantum
annealer



D-Wave One,
128-qubits

D-Wave Two,
512-qubits

D-Wave 2X,
1152-qubits

D-Wave 2000Q,
2048-qubits

intel Honeywell

Alibaba Group
阿里巴巴集团

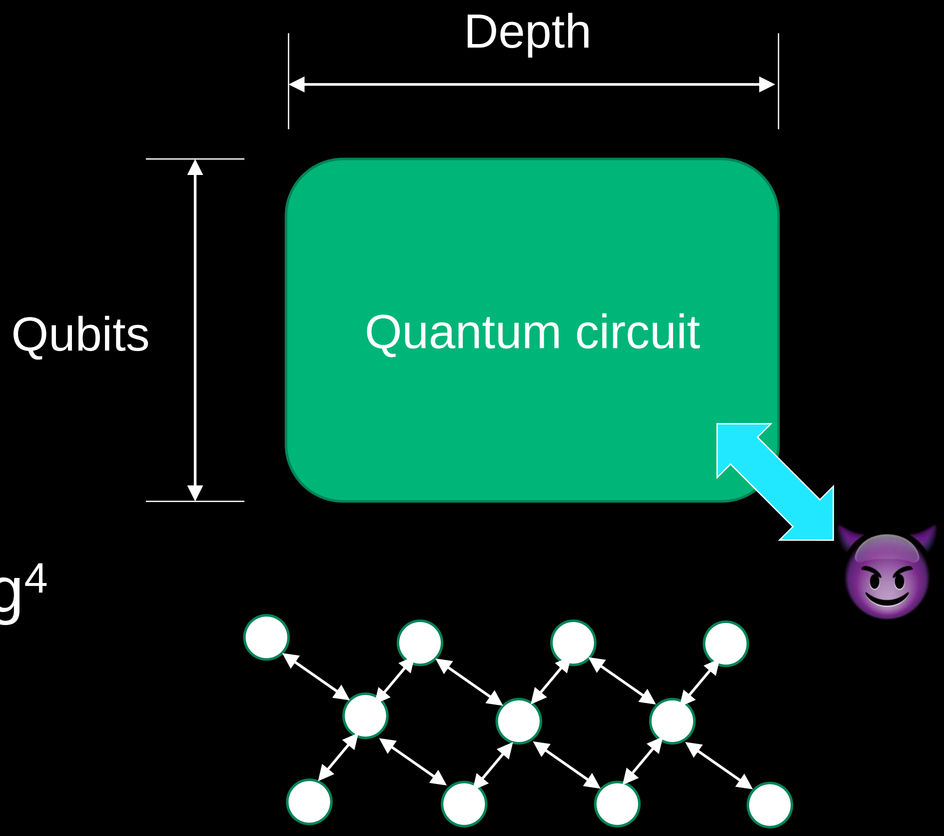
AQT QILIMANJARO

https://quantumcomputingreport.com/

# QC capability and performance metrics

It's not just about qubit counts.

- Qubit fidelity, gate fidelity
  - Quantum volume[1]
- Qubit connectivity
  - Ansatz expressive power in quantum chemistry[2] and supervised learning[3]
  - Embedding overhead in quantum annealing[4]
- Cost to reproduce classically
  - "Quantum supremacy" comparison[5]



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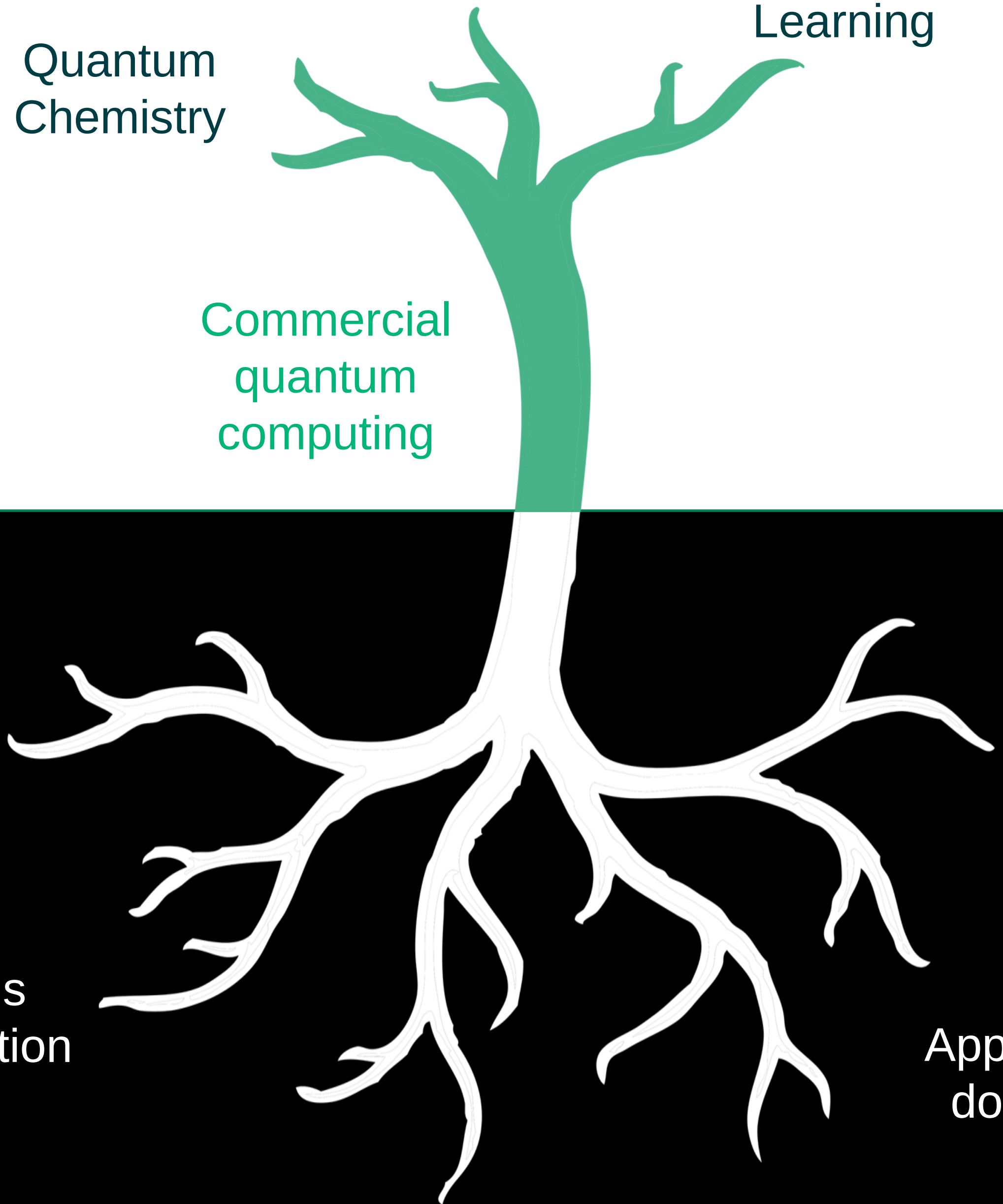
[1] Andrew W. Cross, Lev S. Bishop, Sarah Sheldon, Paul D. Nation, Jay M. Gambetta. 2018. arXiv:1811.12926 [quant-ph]
[2] A. Kandala, A. Mezzacapo, K. Temme, M. Takita, M. Brink, J. M. Chow, J. M. Gambetta. Nature 549, 242. 2017. arXiv:1704.05018 [quant-ph]
[3] D. Zhu, N. M. Linke, M. Benedetti, K. A. Landsman, N. H. Nguyen, C. H. Alderete, A. Perdomo-Ortiz, N. Korda, A. Garfoot, C. Brecque, L. Egan, O. Perdomo, C. Monroe. 2018. arXiv:1812.08862 [quant-ph]
[4] Z. Li, N. S. Dattani, X. Chen, X. Liu, H. Wang, R. Tanburn, H. Chen, X. Peng, and J. Du, (2017), arXiv:1706.08061 [quant-ph]
[5] Igor L. Markov, Aneeqa Fatima, Sergei V. Isakov, Sergio Boixo. 2018. arXiv:1807.10749 [quant-ph]



Industrial
Optimization

Machine
Learning

Quantum
Chemistry

Commercial
quantum
computing

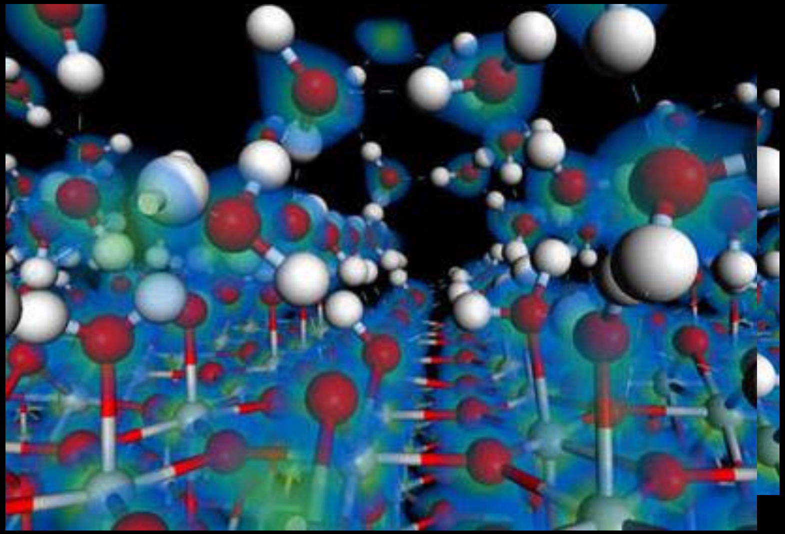
Software engineering

Quantum
hardware
engineering

Quantum algorithms
design & implementation

Application
domains

## Quantum simulation

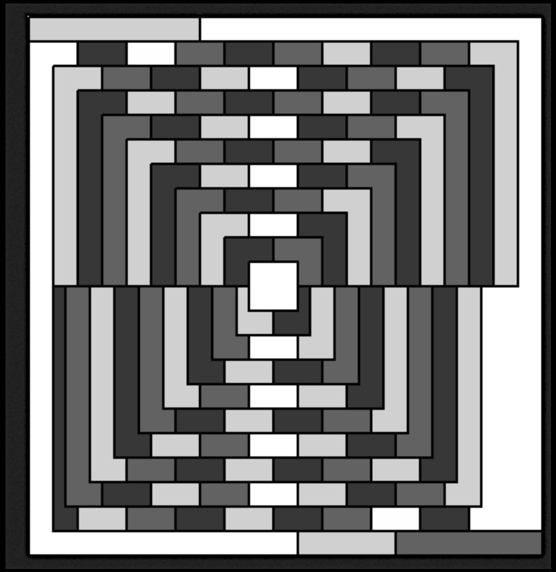


Variational quantum eigensolver

Hybrid quantum-classical simulator

Adiabatic quantum computing

## Combinatorial optimization



Q. Approx. Optimization Algorithm

Q. Alternating Operator Ansatz

Q. Annealing / Optical Ising machines

## Machine learning

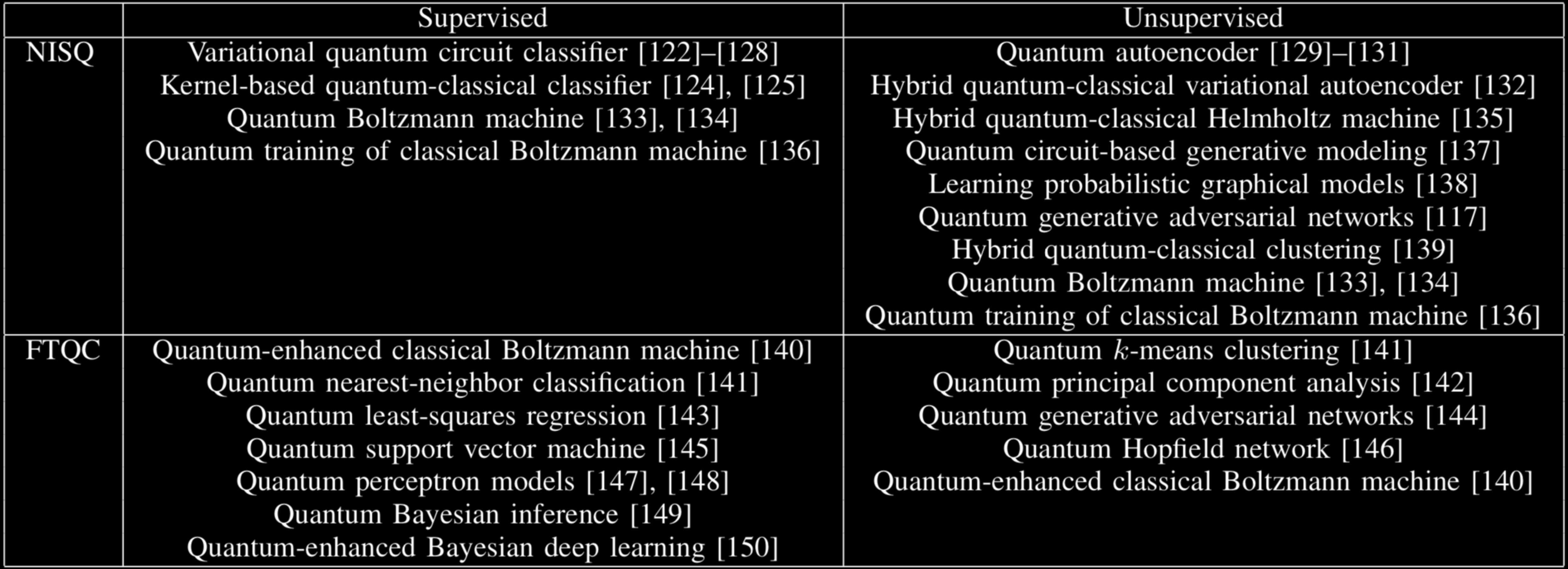
Variational circuit classifier

Kernel PCA

Quantum Boltzmann machine

Quantum autoencoder

Quantum GAN

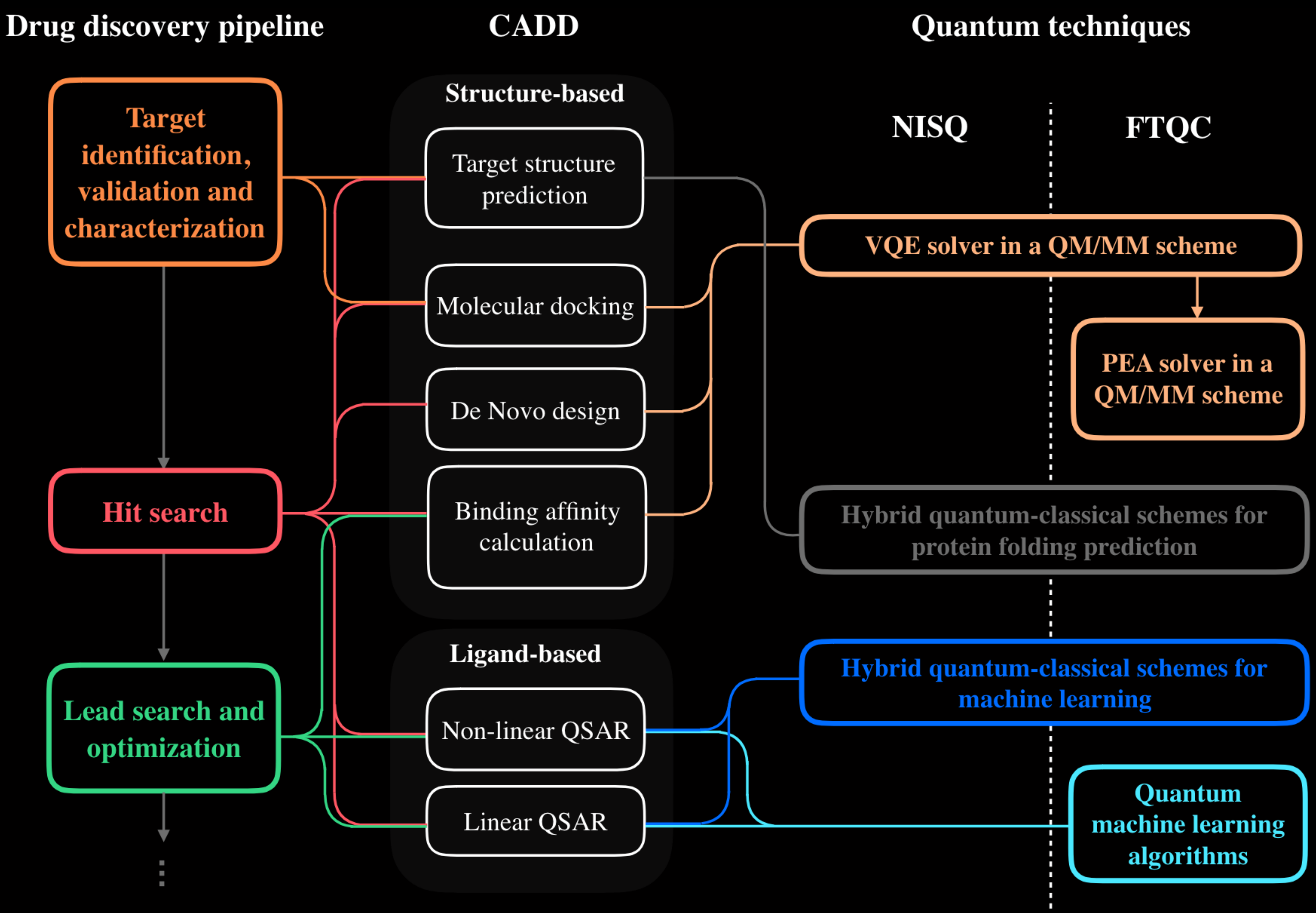


| | Supervised | Unsupervised |
|---|---|---|
| NISQ | Variational quantum circuit classifier [122]–[128]<br>Kernel-based quantum-classical classifier [124], [125]<br>Quantum Boltzmann machine [133], [134]<br>Quantum training of classical Boltzmann machine [136] | Quantum autoencoder [129]–[131]<br>Hybrid quantum-classical variational autoencoder [132]<br>Hybrid quantum-classical Helmholtz machine [135]<br>Quantum circuit-based generative modeling [137]<br>Learning probabilistic graphical models [138]<br>Quantum generative adversarial networks [117]<br>Hybrid quantum-classical clustering [139]<br>Quantum Boltzmann machine [133], [134]<br>Quantum training of classical Boltzmann machine [136] |
| FTQC | Quantum-enhanced classical Boltzmann machine [140]<br>Quantum nearest-neighbor classification [141]<br>Quantum least-squares regression [143]<br>Quantum support vector machine [145]<br>Quantum perceptron models [147], [148]<br>Quantum Bayesian inference [149]<br>Quantum-enhanced Bayesian deep learning [150] | Quantum $k$-means clustering [141]<br>Quantum principal component analysis [142]<br>Quantum generative adversarial networks [144]<br>Quantum Hopfield network [146]<br>Quantum-enhanced classical Boltzmann machine [140] |

Y. Cao, J. Romero, A. Aspuru-Guzik. *Potential of quantum computing for drug discovery.* IBM Journal of Research and Development. Vol. 62, Issue 6. 2018

| | | |
|---|---|---|
| High-tech | • Machine learning and artificial intelligence, such as neural networks<br>• Search<br>• Bidding strategies for advertisements<br>• Cybersecurity<br>• Online and product marketing<br>• Software verification and validation | IBM<br>Alibaba<br>Google<br>Microsoft<br>Telstra<br>Baidu<br>Samsung |
| Industrial goods | • Logistics: scheduling, planning, product distribution, routing<br>• Automotive: traffic simulation, e-charging station and parking search, autonomous driving<br>• Semiconductors: manufacturing, such as chip layout optimization<br>• Aerospace: R&D and manufacturing, such as fault-analysis, stronger polymers for airplanes<br>• Material science: effective catalytic converters for cars, battery cell research, more-efficient materials for solar cells, and property engineering uses such as OLEDS | Airbus<br>NASA<br>Northrop Grumman<br>Daimler<br>Raytheon<br>BMW<br>Volkswagen<br>Lockheed Martin<br>Honeywell<br>Bosch |
| Chemistry and Pharma | • Catalyst and enzyme design, such as nitrogenase<br>• Pharmaceuticals R&D, such as faster drug discovery<br>• Bioinformatics, such as genomics<br>• Patient diagnostics for health care, such as improved diagnostic capability for MRI | BASF<br>Biogen<br>Dow Chemical<br>JSR<br>DuPont<br>Amgen |
| Finance | • Trading strategies<br>• Portfolio optimization<br>• Asset pricing<br>• Risk analysis<br>• Fraud detection<br>• Market simulation | J.P. Morgan<br>Commonwealth Bank<br>Barclays<br>Goldman Sachs |
| Energy | • Network design<br>• Energy distribution<br>• Oil well optimization | Dubai Electricity & Water Authority<br>BP |

BCG -*The Next Decade in Quantum Computing—and How to Play*. May 2018



**Drug discovery pipeline**

**CADD**

**Quantum techniques**

**Target identification, validation and characterization**

**Hit search**

**Lead search and optimization**

**Structure-based**

Target structure prediction

Molecular docking

De Novo design

Binding affinity calculation

**Ligand-based**

Non-linear QSAR

Linear QSAR

**NISQ**

**FTQC**

**VQE solver in a QM/MM scheme**

**PEA solver in a QM/MM scheme**

**Hybrid quantum-classical schemes for protein folding prediction**

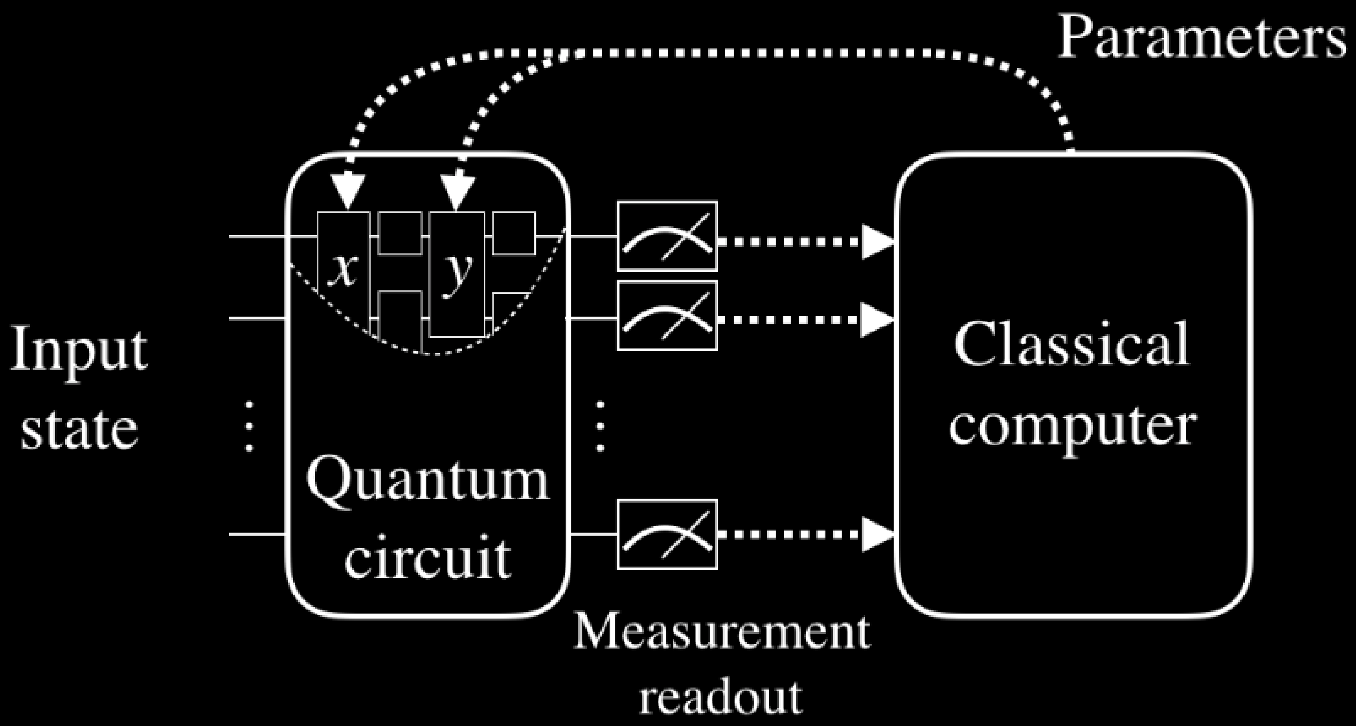
**Hybrid quantum-classical schemes for machine learning**

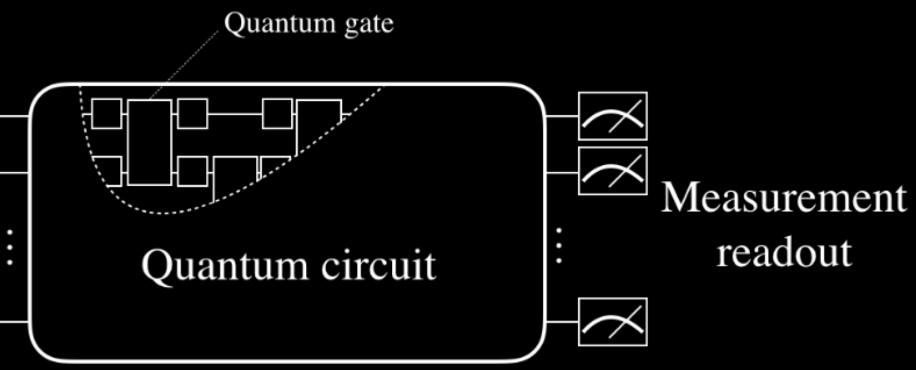
**Quantum machine learning algorithms**

Y. Cao, J. Romero, A. Aspuru-Guzik. *Potential of quantum computing for drug discovery.* IBM Journal of Research and Development. Vol. 62, Issue 6. 2018

# Near-term QC paradigm

Hybrid model that maximizes the use of both quantum and classical processors





# What can you do with existing devices?

Some examples of demo experiments run on hardware

| | Algorithm | # qubits | Circuit depth | Reference |
|---|---|---|---|---|
| ML | Variational circuit classifier | 2 | 3 | Partner app - Rigetti / Zapata[1] |
| ML / Chem | Quantum autoencoder | 2, 3 | <8 | Partner app - Rigetti / Zapata[1] |
| Chem | VQE for $H_2$ ground state | 2-4 | <7 | SC qubits (Google[2], IBM[3]), trapped ion[4] |
| Optimization | Factorization | 3 | <10 | IBM Hackathon - VQF[5] (Zapata) |
| QI | Mermin inequality violation | 3-5 | <15 | IBM Q Experience[6] |
| QI | Quantum info. scrambling | 7 | <10 | Trapped ion QC[7] |
| ML / Opt. | Clustering | 19 | 5 | Rigetti 19Q[8] |

[1] S. Sim, Y. Cao, J. Romero, P. D. Johnson, A. Aspuru-Guzik. 2018. arXiv:1810.10576 [quant-ph]

[2] P. J. J. O’Malley et al. *Phys. Rev. X* 6, 031007 (2016). arXiv:1512.06860 [quant-ph]

[3] A. Kandala, A. Mezzacapo, K. Temme, M. Takita, M. Brink, J. M. Chow, J. M. Gambetta. *Nature* 549, 242 (2017). arXiv:1704.05018 [quant-ph]

[4] C. Hempel et al. *Phys. Rev. X* 8, 031022 (2018). arXiv:1803.10238 [quant-ph]

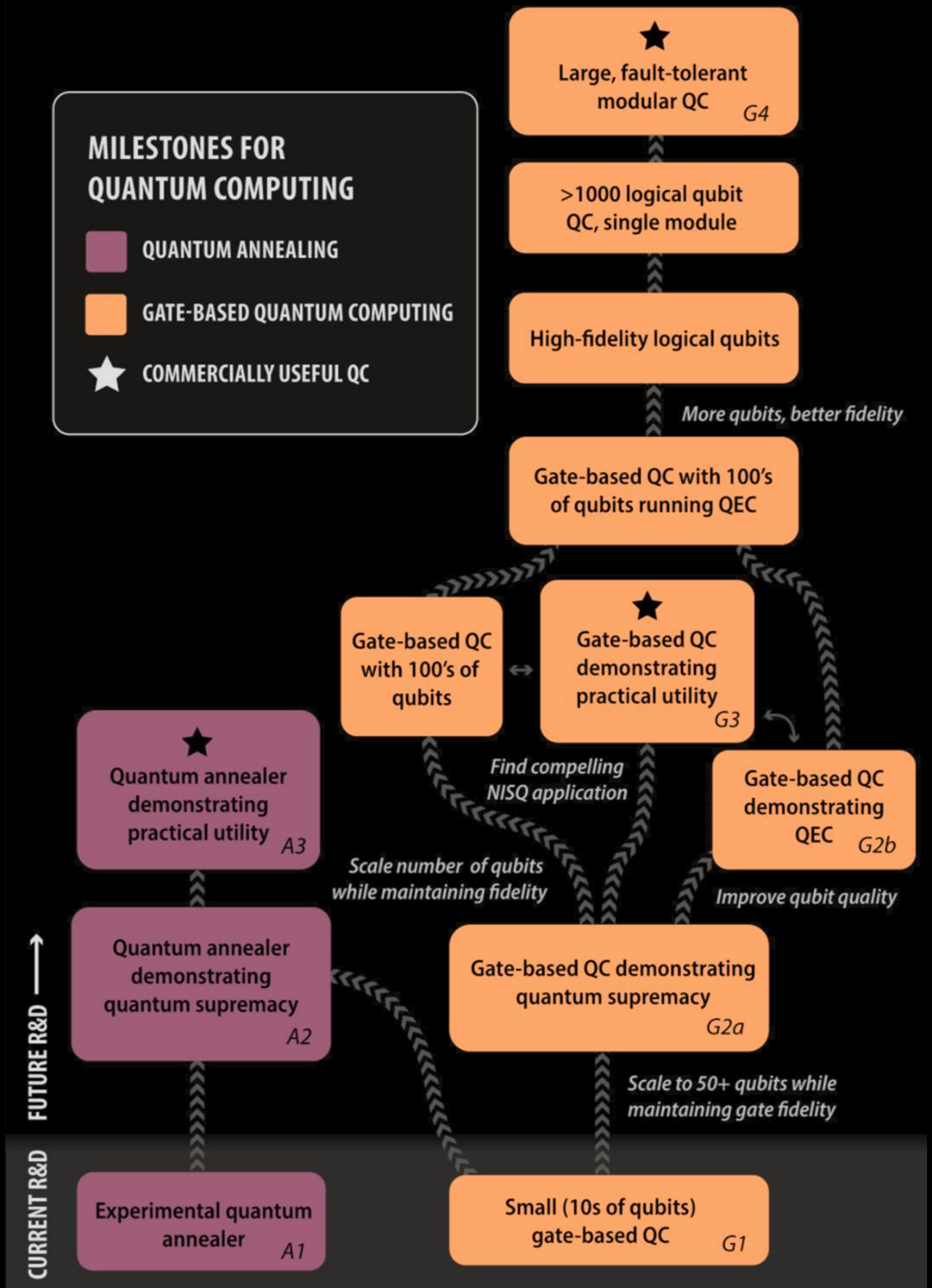
[5] E. R. Anschuetz, J. P. Olson, A. Aspuru-Guzik, Y. Cao. *Lecture Notes in Computer Science,* Vol. 11413, Ch. 7. 2018. arXiv:1808.08927 [quant-ph]

[6] Daniel Alsina, José Ignacio Latorre. *Phys. Rev. A* 94, 012314 (2016). arXiv:1605.04220 [quant-ph]

[7] K. A. Landsman, C. Figgatt, T. Schuster, N. M. Linke, B. Yoshida, N. Y. Yao, C. Monroe. *Nature* 567 61-65 (2019). arXiv:1806.02807 [quant-ph]

[8] J. S. Otterbach et al. 2017. arXiv:1712.05771 [quant-ph]

# QC milestones



National Academies of Sciences, Engineering, and Medicine. 2018. *Quantum Computing: Progress and Prospects*. Washington, DC: The National Academies Press. https://doi.org/10.17226/25196.

# Summary

Before general-purpose fault-tolerant devices mature, special-purpose noisy devices are already commercially relevant

Hardware and algorithm / theory co-evolve in moving the goal posts closer to each other

Government funding is crucial for sustaining the field in the early stage towards more commercial maturity

For quantum computing, we are building on decades of accumulation in science, technology and enterprise know-hows in classical computation. Timeline of progress will likely be accelerated significantly as a result.

More algorithmic innovation is needed to maximize the use of NISQ devices