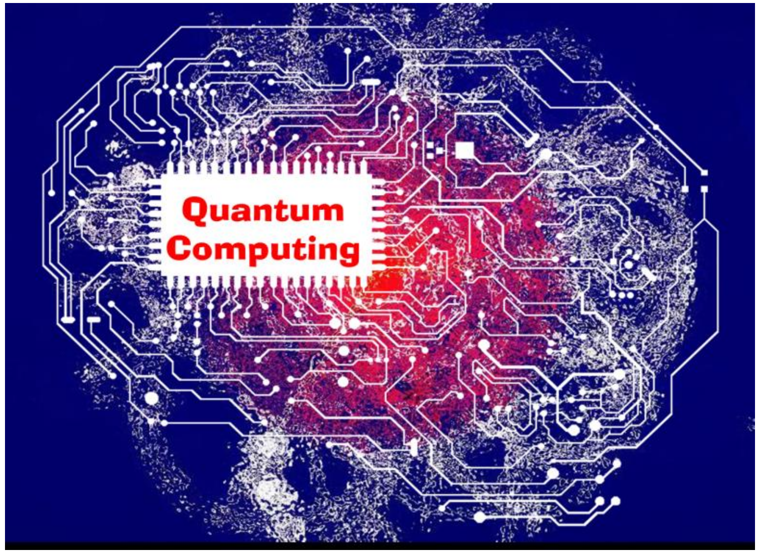
> Technology Practice

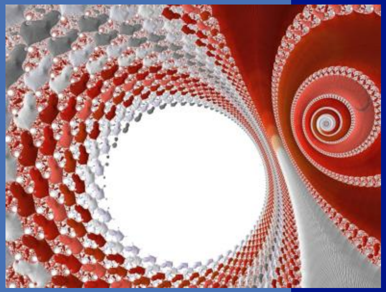


Bristlecone, the 72-qubit quantum chip, Google

Accelerating Drug Discovery with Disruptive Technologies : Quantum Computing

Dr. Bhushan Bonde

UCB Pharma



Inspired by patients.
Driven by science.

Why Quantum Computing?

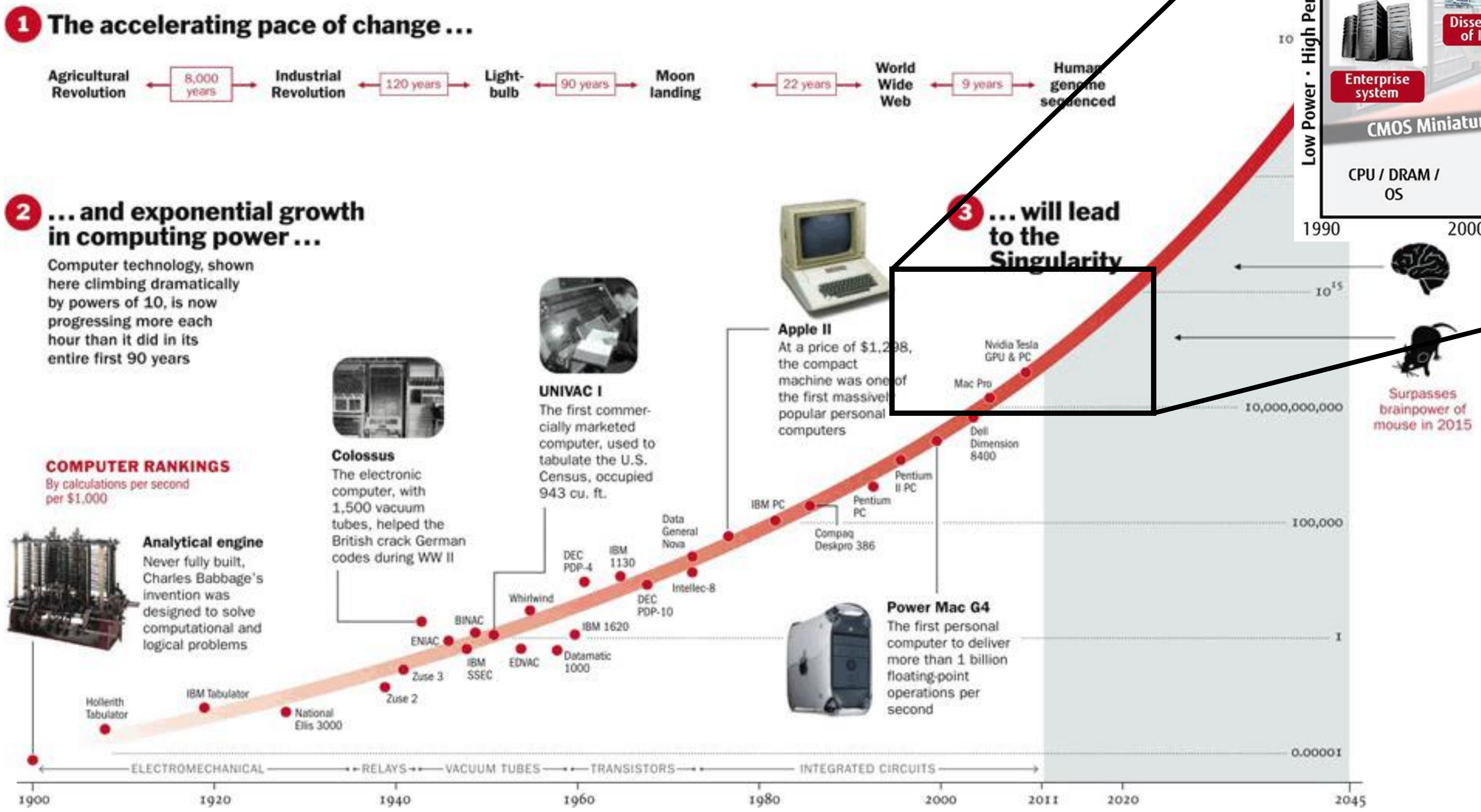
Chess (Shatranj) discovery

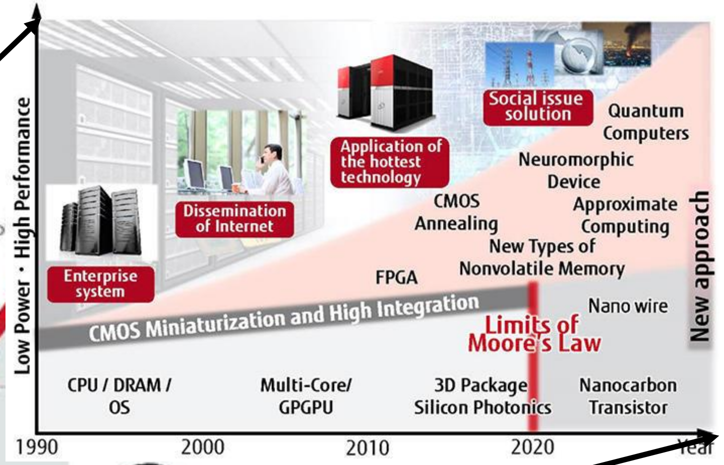
$$1 + 2 + 2^2 + 2^3 + \cdots + 2^{63} = 2^{64} - 1$$

18,446,744,073,709,551,615

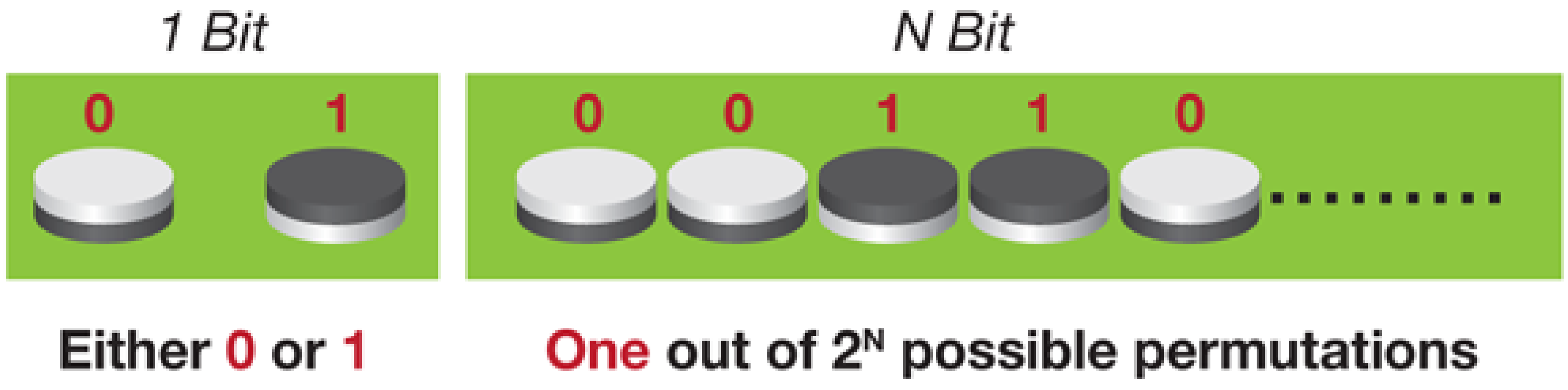
"….. speed, memory, and processing capacity of any possible future computer equipment are limited by specific physical barriers: the light barrier, the quantum barrier, and the thermodynamical barrier." …1965 quote by Prof. Hans-Joachim Bremermann (1926–1996)

Computing - scale

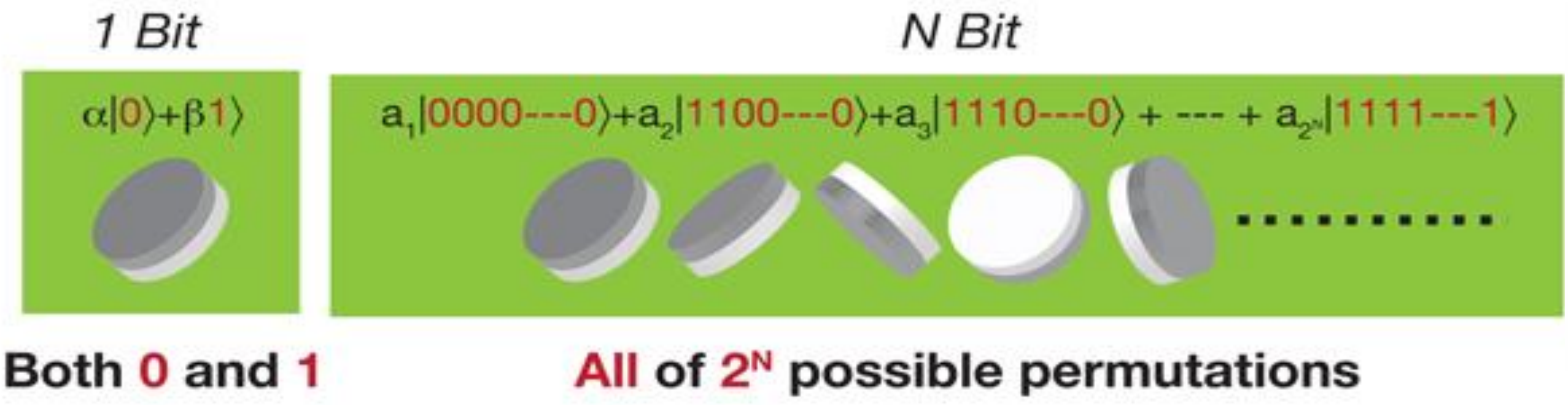




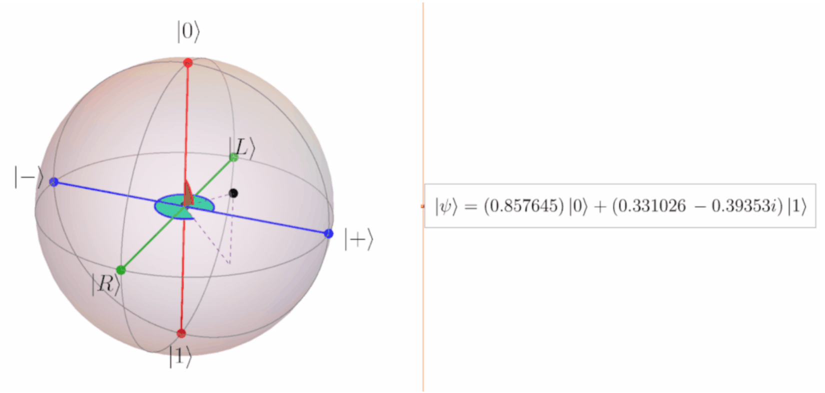
Bit vs Qubit



1 Bit
N Bit
0 1
0 0 1 1 0
Either 0 or 1
One out of 2N possible permutations

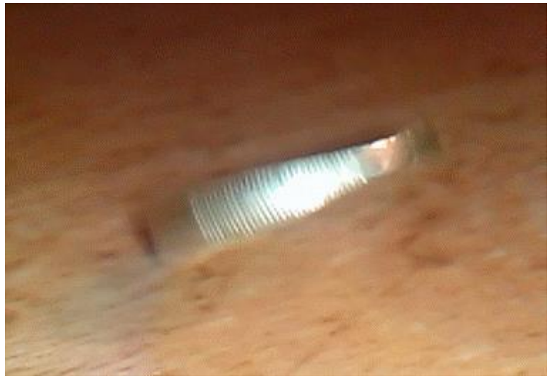


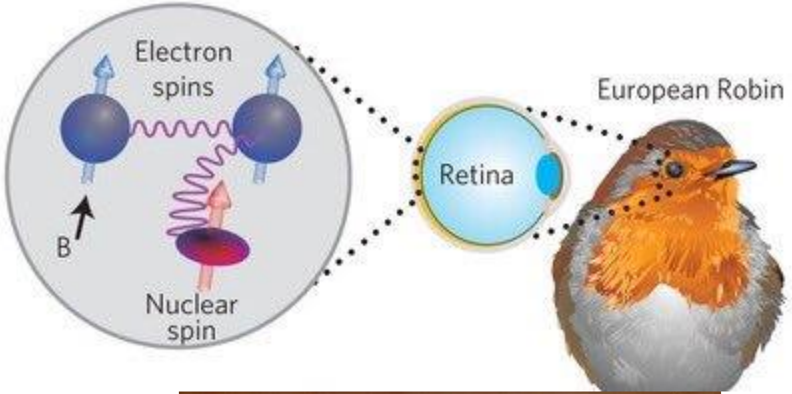
1 Bit
N Bit
α|0⟩+β1⟩
a1|0000---0⟩+a2|1100---0⟩+a3|1110---0⟩ + --- + a2N|1111---1⟩
Both 0 and 1
All of 2N possible permutations

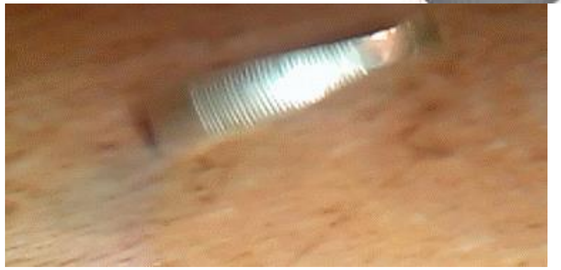


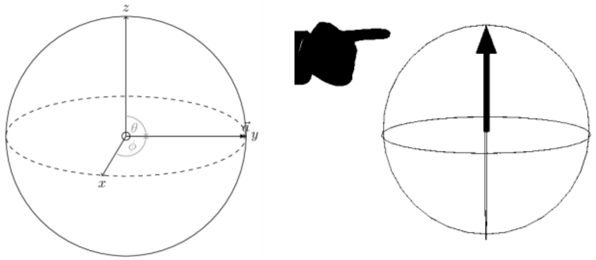
|0⟩
|1⟩
|L⟩
|R⟩
|−⟩
|+⟩
|ψ⟩ = (0.857645) |0⟩ + (0.331026 − 0.39353i) |1⟩

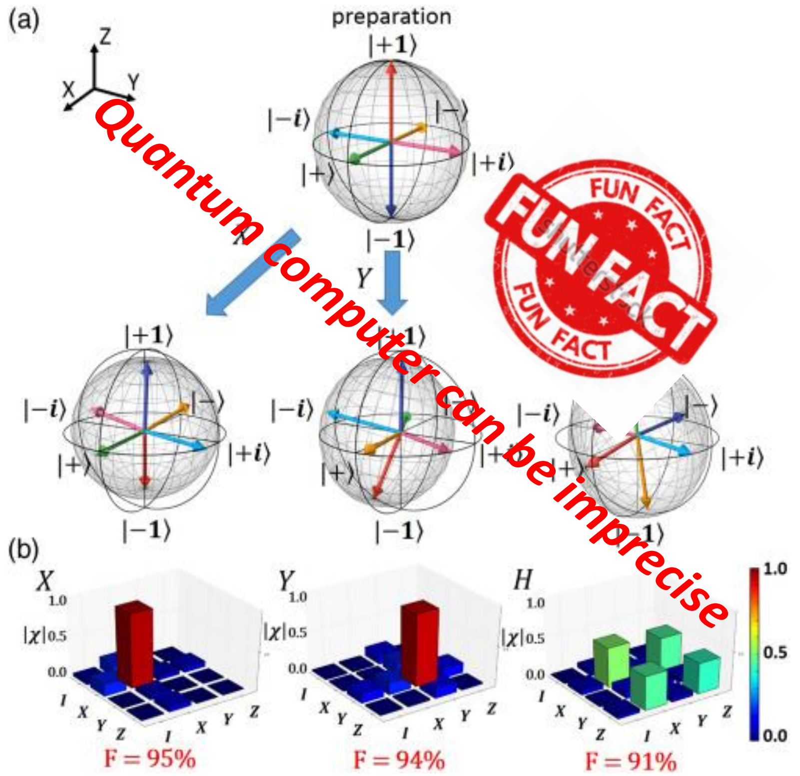
Basics of Quantum Computer









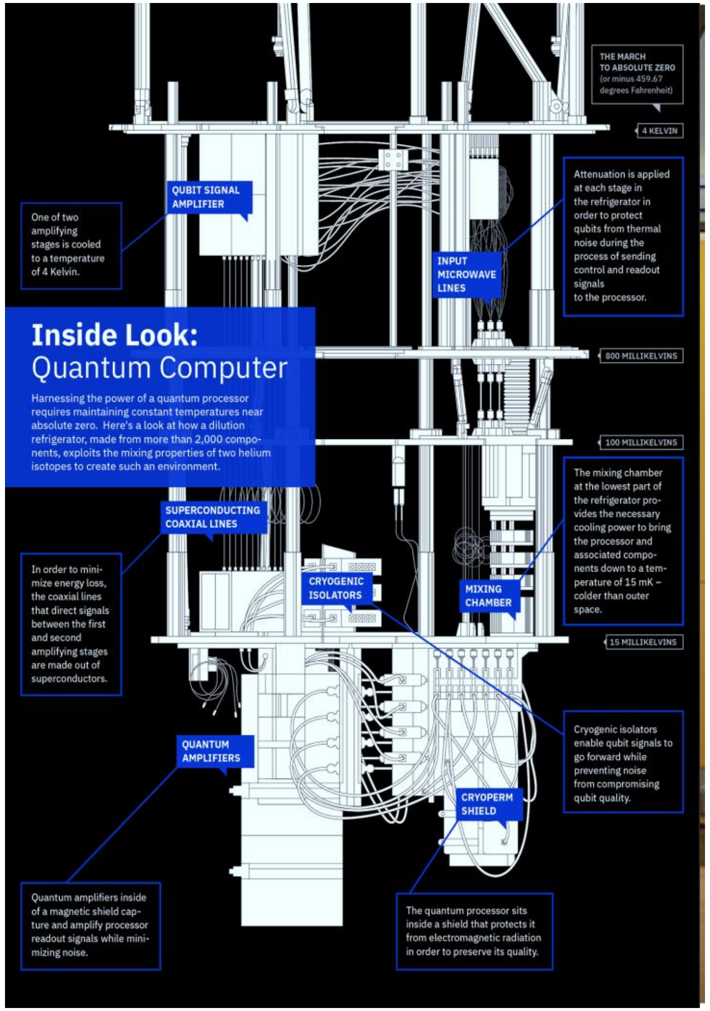


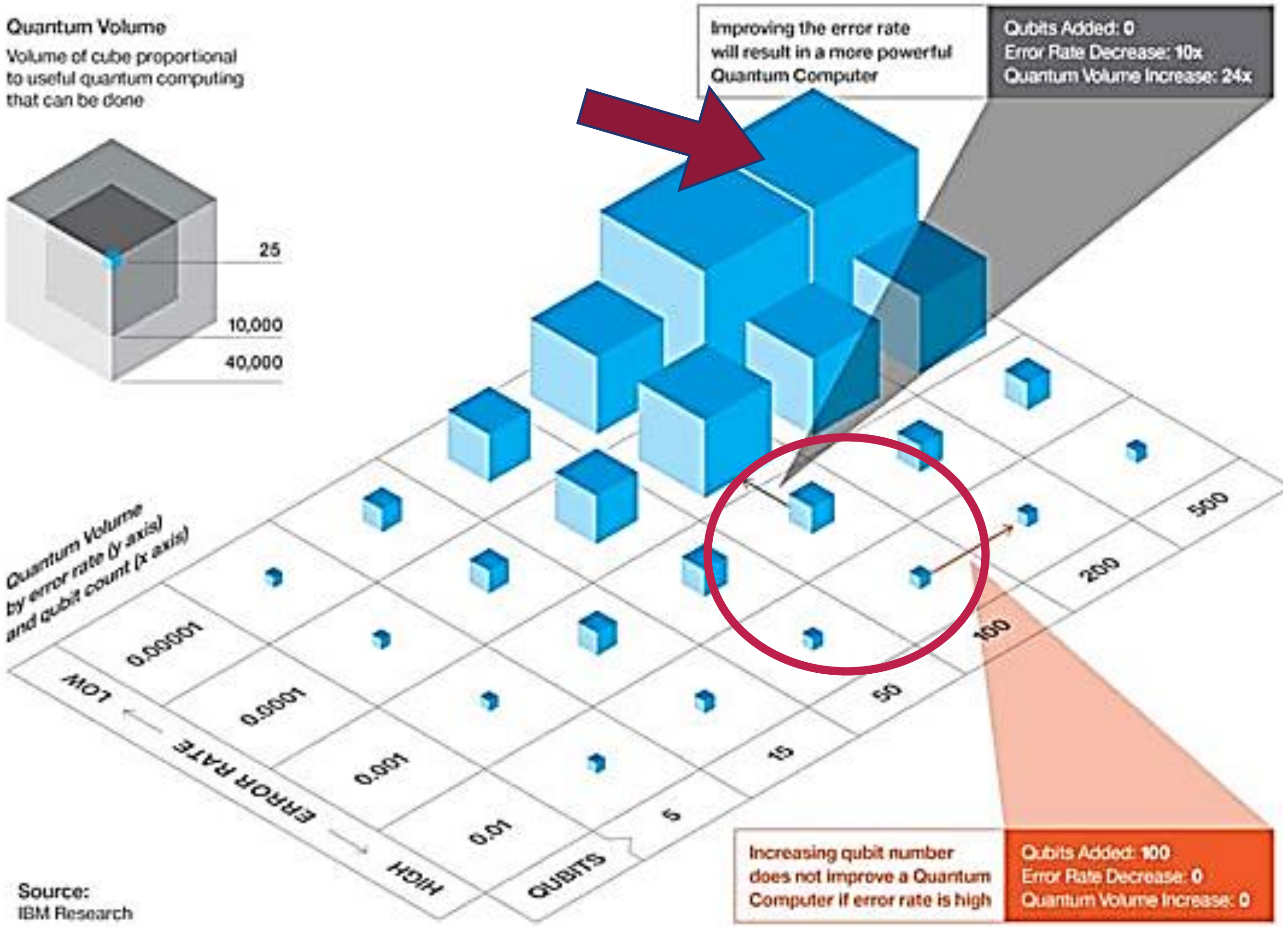
Superposition

Entanglement

Error Rate/Probability

Quantum Computer

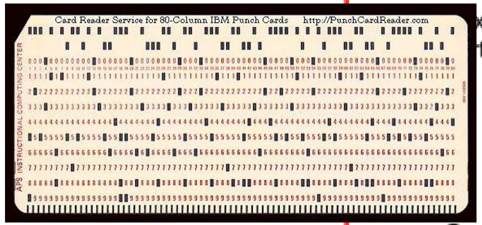




Accessing Quantum Computer

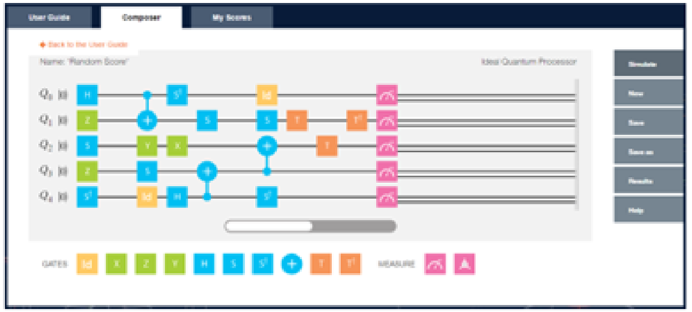
1\. Problem to solve

* similar to compilation in classical computing (e.g. compile C++ code)



Quantum circuit for idealized hardware

2\.

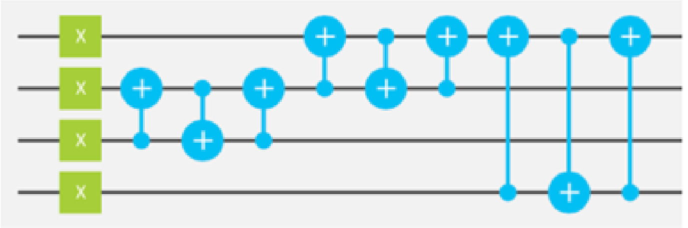


xample generated with Qiskit/QASM Editor/Composer to
rtray a quantum circuit for an ideal quantum processor

Compile

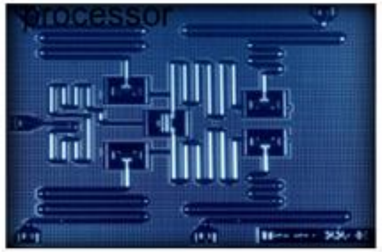
Quantum circuit for real hardware

3\.



* subject to hardware constraints
* adds additional gates (swap) to satisfy the hardware constraints

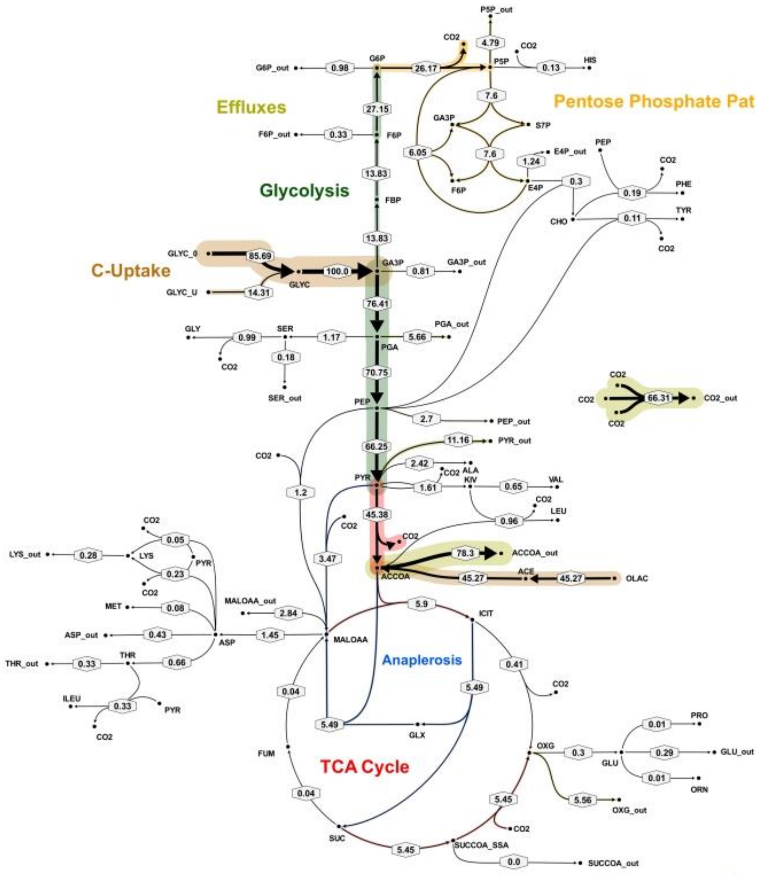
4\. Quantum processor



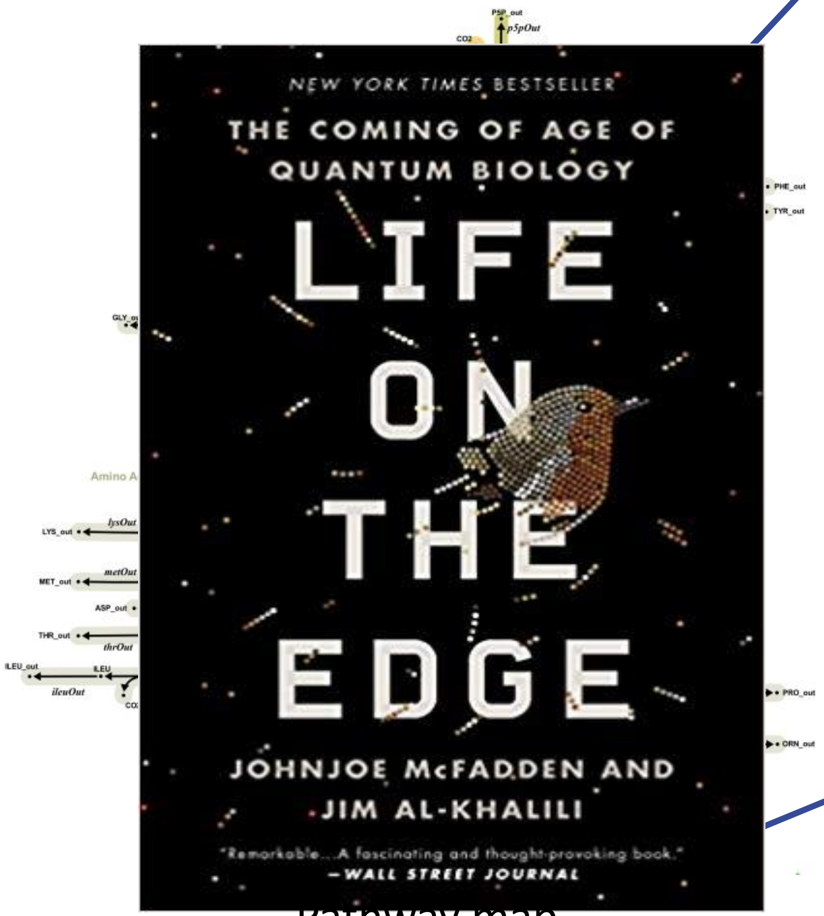
Healthcare, Medicine & Materials

Untangling the complexity of molecular and chemical interactions leading to the discovery of new medicines and materials

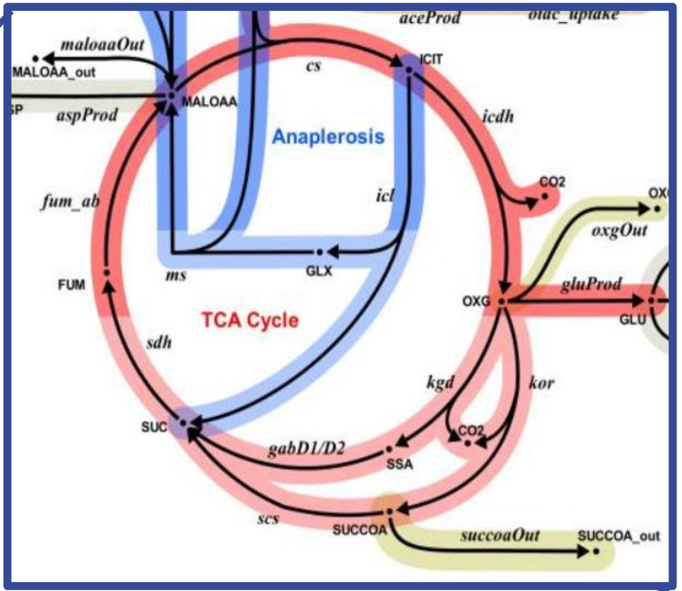
QC: Solving Computational Biology



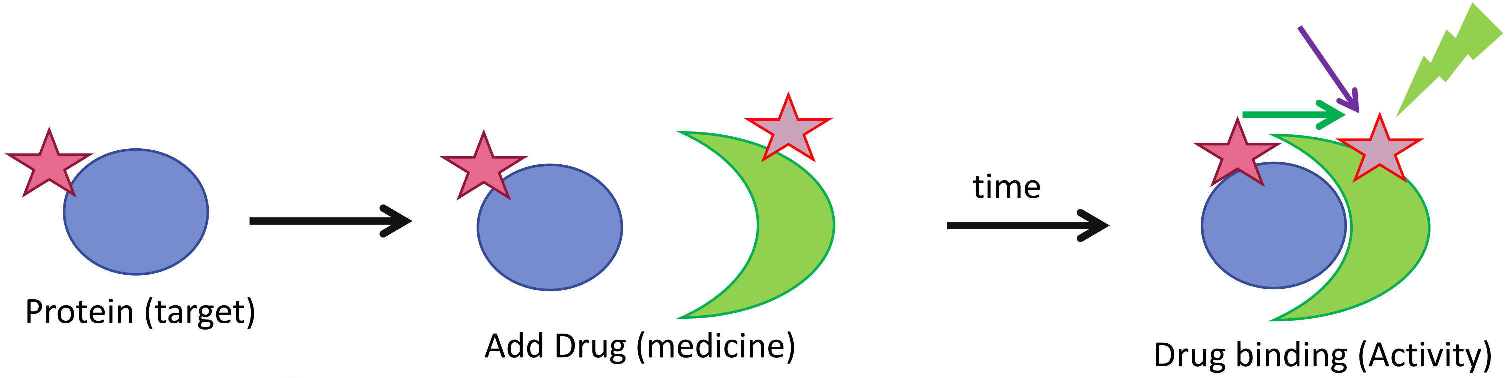
Pathway map
In vitro M. TB

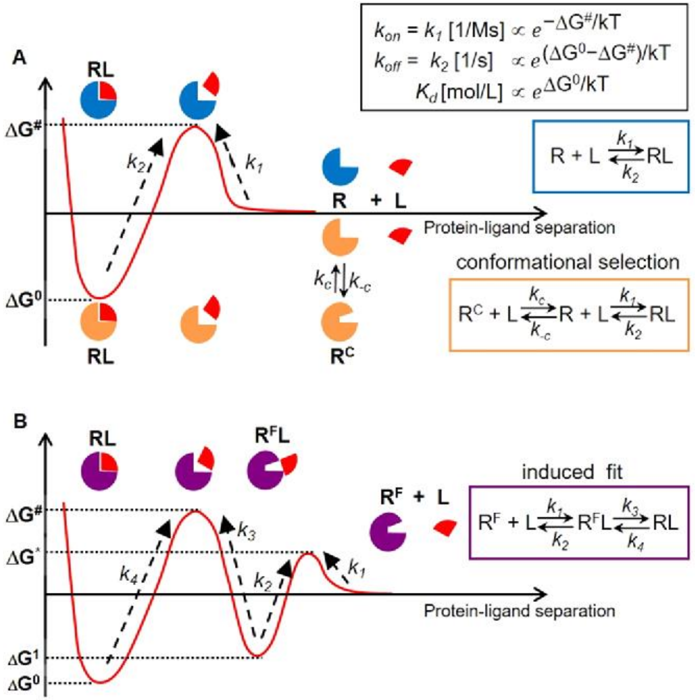


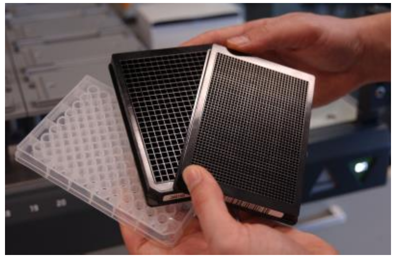
Pathway map
In vivo M. TB



UCB QC: Drug Activity prediction







Conventional (binary) computing:

- Solve simultaneously ~ 1200 differential equations
- Uses 200-300 processor cores and 100 -250 GB RAM.
- Time: ~ 3 to 15 days/experiment based on Algorithm (MC, SPO etc)

Quantum Computing:

- 4-5 Qubit -> solve in parallel -> min to hr. with IBM Q multiple runs
- 20 Qubit (not performed yet)-> quicker and larger data handling.
- Higher Qubit (~70-100) -> n-dim optimisation, accurate and fast results in seconds, real time experiments in the lab
- Handles multiple 1048 well plates data in parallel.

Healthcare, Medicine & Materials

Untangling the complexity of molecular and chemical interactions leading to the discovery of new medicines and materials

Supply Chain & Logistics

Finding the best solutions for ultra-efficient logistics and global supply chains, such as optimizing fleet operations for deliveries during the holiday season

Financial Services

Finding new ways to model financial data and isolating key global risk factors to make better investments

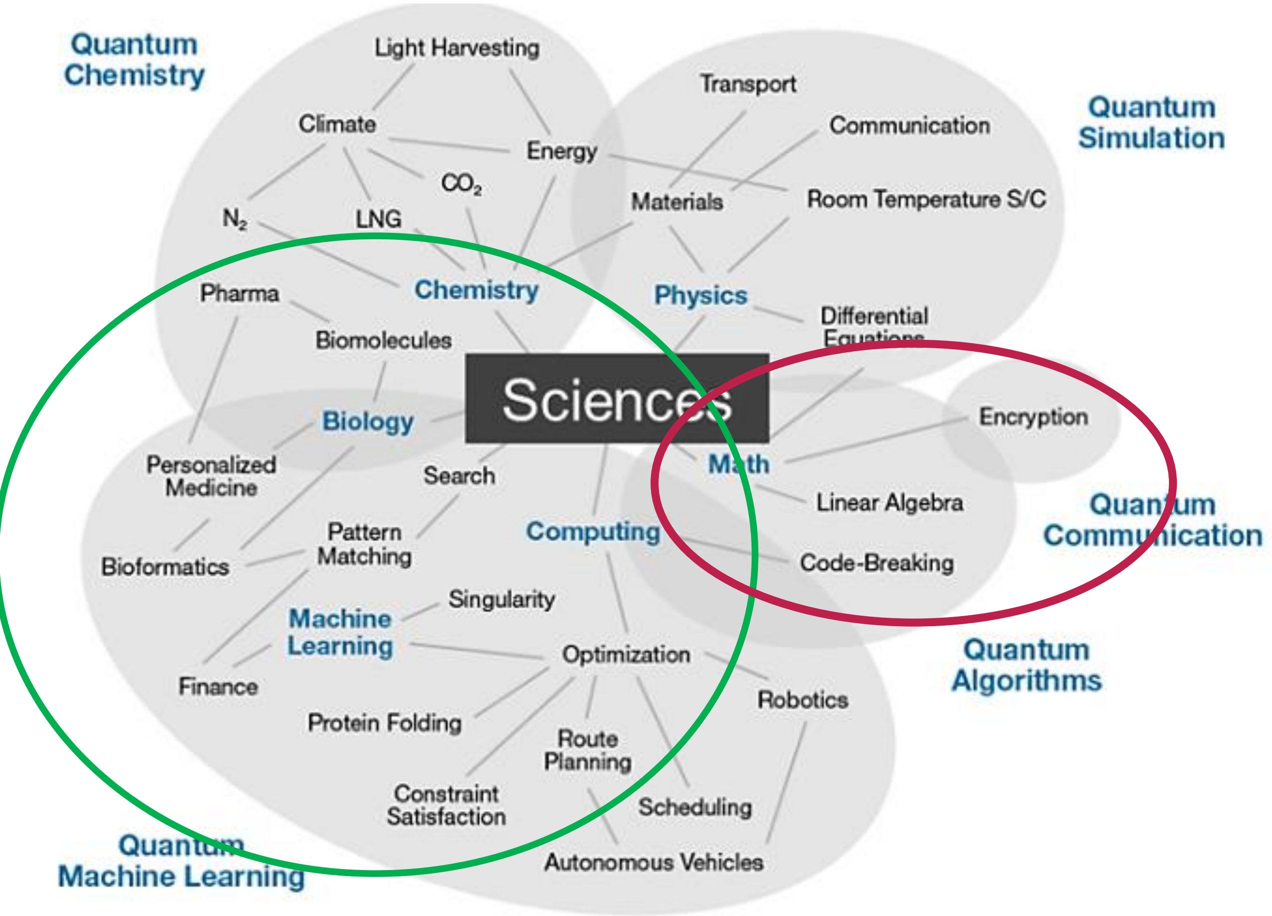
Artificial Intelligence, Machine Learning

Making facets of AI such as machine learning much more powerful when data sets are very large, such as in searching images or video

Data search, encryption and security

Enabling faster data searching and sorting in big data
Using quantum-safe (qubit) encryption algorithms

Algorithm and Application Domains



- Quantum Fourier Transform, Bernstein-Vazirani algorithm, Deutsch-Josza algorithm[1]
- Hidden Shift algorithm[2] – M. Roetteler (Microsoft)
- Grover's algorithm[4] – D. Maslov (NSF)
- Fault-tolerant quantum error detection[3] – K. Brown (Georgia Tech.)
- Quantum game theory and Nash equilibria[5] – N. Solmeyer (Army Research Lab)
- Renyi entropy measurement of a Fermi-Hubbard model system[6] – S. Johri (Intel)
- Quantum scrambling and out-of-time-order correlators[7] – N. Yao (UC Berkeley)
- Quantum machine learning[8] – A. Ortiz (NASA)
- Neural-network-based qubit readout[9] – A. Seif (QuiCS/UMD)
- Bacon-Shor quantum error correction codes[10] – T. Yoder (Harvard)
- Quantum Approximate Optimization (QAOA) of critical states[10] – T. Hsi Omar Shehab eh
- Deuteron VQE[11] – R. Pooser (Oak Ridge)

1) S. Debnath et al. Nature **536** (2016)
2) NML et al., PNAS **114**, 13 (2017)
3) NML et al., Sci Adv. **3**, 10 (2017)
4) C. Figgatt et al., Nat. Communs. **8**, 1918 (2017)
5) N. Solmeyer et al., QST **3** 045002 (2018)
6) NML et al., Phys. Rev. A **98**, 052334 (2018)
7) K. A. Landsman et al., arxiv 1806.02807
8) D. Zhu et al., arXiv 1812.08862 (2018)
9) A. Seif et al., J. Phys. B **51** 174006 (2018)
10) Ho, Wen Wei & H. Hsieh, Timothy. (2018).
11) E Dumitrescu et.al., Phys. Rev. Let 120, 210501 (2018) and Shehab et al. arXiv:1906.00476v1 (2019)

Industrial Landscape

IBM
D-Wave The Quantum Computing Company™
Google
Microsoft
rigetti
Silicon Quantum Computing

		IBM	rigetti		D-Wave	Google
HARDWARE	TECHNOLOGY	Quantum gates	Quantum gates	Coherent quantum annealing	Quantum annealing	Quantum gates
	QUBIT QUALITY REQUIRED	Very high	Very high	High	High	Very high
	QUANTUM GATES	Necessary	Necessary	Not used	Not used	Necessary
	QEC*	Essential	Essential	Not essential	Not essential	Essential
	NEAR-TERM APPLICATION	No, QEC needed	No, QEC needed	Yes	Yes	No, QEC needed
	QUBIT NUMBER FOR QUANTUM ADVANTAGE	10^6 - 10^7	10^6 - 10^7	100 - 1000	Unclear	10^6 - 10^7
	UNIVERSAL QUANTUM COMPUTATION	Short-term: No Long-term: Yes	Short-term: No Long-term: Yes	Short-term: No Long-term: Yes	Short-term: No Long-term: Unclear	Short-term: No Long-term: Yes
PLATFORM	QUANTUM COMPUTING IN THE CLOUD	Yes	Yes	Yes	Yes	Undefined
	QUANTUM LANGUAGE	QISKit	Forest	Qibo	Qbsolv	Unknown
	CODEBASE LANGUAGE	Python	Python	Python	Python	Python
	COMPATIBLE WITH OTHER PLATFORMS	No	No	Yes, compatible with all other QC	No	No
	TARGET USERS	Big corporations, research centers	Undefined	Any user	Big corporations, research centers	Undefined
	PRICE	Expensive, but some free services	Undefined	Affordable cost	Expensive	Undefined
	FREE SERVICES	Yes	Yes	Yes	No	No
	COMMUNITY FOCUSED	Yes	Yes	Yes	No	No
	OPEN ACCESS TO QA** LIBRARIES	No	No	Yes	Yes	No
	REWARDS TO QA DEVELOPERS	No	No	Yes	No	No

*QEC: Quantum Error Correction
**QA: Quantum Algorithms

FUN FACT

Bristlecone, the 72-qubit quantum chip, Google

Software & Consultants

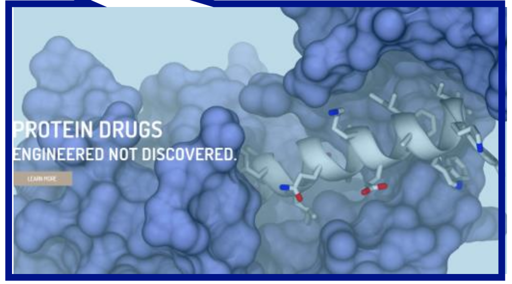
Quantum Consultants
Atos
Entanglement Partners
accenture
1QBit
Zapata Computing
CQC Cambridge Quantum Computing Limited
Q^x Branch
ENTROPICA LABS Quantum computing, at your service
quantum benchmark
QC WARE
ProteinQure
NETRAMARK
Artiste-qb.net
Qu & Co
EVERETTIAN
Q-CTRL
BRA-KET SCIENCE
QILIMANJARO
EeroQ
STRANGE WORKS
⟨Qubit|Era⟩
HORIZON QUANTUM COMPUTING
RIVER LANE RESEARCH

Biogen : Drug repurposing (1QBIT/Accenture)

FUN FACT

Enabling Technologies

Qubitekk
BlueFors
Leiden Cryogenics Leader in Low Temperature Techniques
Oxford Cryosystems
Zurich Instruments
ANYON
intel
KEYSIGHT TECHNOLOGIES
Signadyne
Raytheon BBN Technologies
QUANDELA
Metempsy
HYPRES
SPICE LABS
Delft Circuits quantum computing hardware
JANIS



Quantum Advantages & Challenges

Advantages:

- **Parallel computing** without parallel hardware
- Maximum of parallel processes: **simultaneously processing** the whole input
- New paradigm shift: Possible to find the best optimal solution, which is impossible to achieve for a given problem

Challenges:

- **Probabilistic** nature of quantum physics in measurement, readout, sampling
- **Early stage of Quantum** computing, need further development in problem abstraction
- Need **newer algorithms** development
- No **quantum memory** (yet?)
  - Quantum data storage discovered

Age of Quantum Computer … is here!!!

Quantum computers will not replace classical computers

- Solve classical computing limiting problems - processing power, time, energy and efficiency

Quantum computing has the potential of largest “new” technology

- Over the next decade, will solving the complex problems in various technology sector,
- Particle/Material research, Next Gen Batteries, Green Fertilizers, Weather forecasting …

Quantum-safe security will play a crucial role for data encryption

- Secure data/internet communication

Quantum computers will accelerate drug discovery and health solutions

- 3D Molecular conformation and chemical structure search from all known chemical compounds

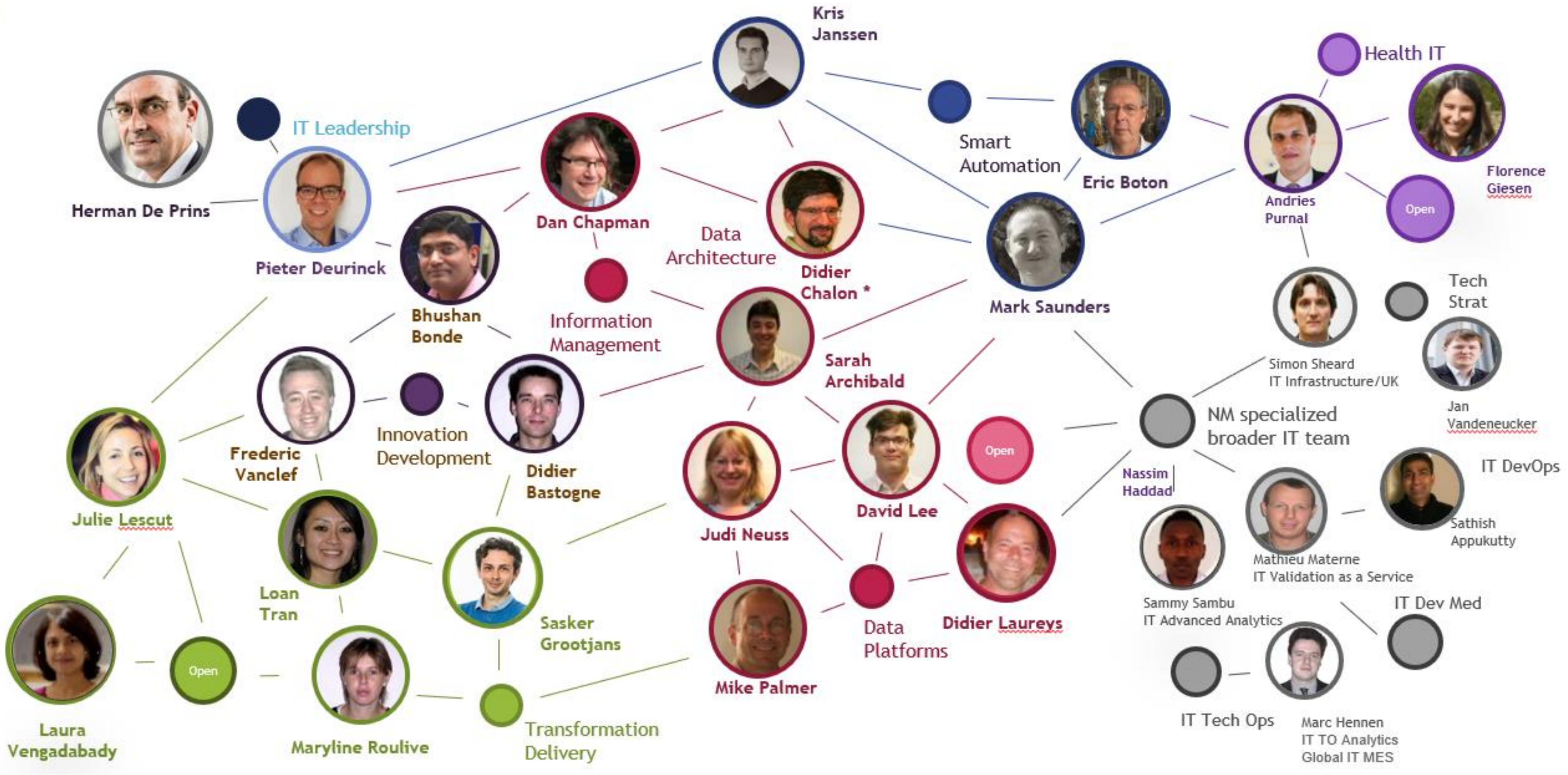
Quantum optimization will enable AI and Machine learning algorithm

- Perform better learning, promising to achieve the performance of biological brain

Acknowledgements

UCB IT Early Solutions Innovation Development

Daniel Chapman
Kris Jansson
Pieter Deurinck
Herman De Prins



Thank you