UANTUM COMPUTING

Accelerating Biology 2020

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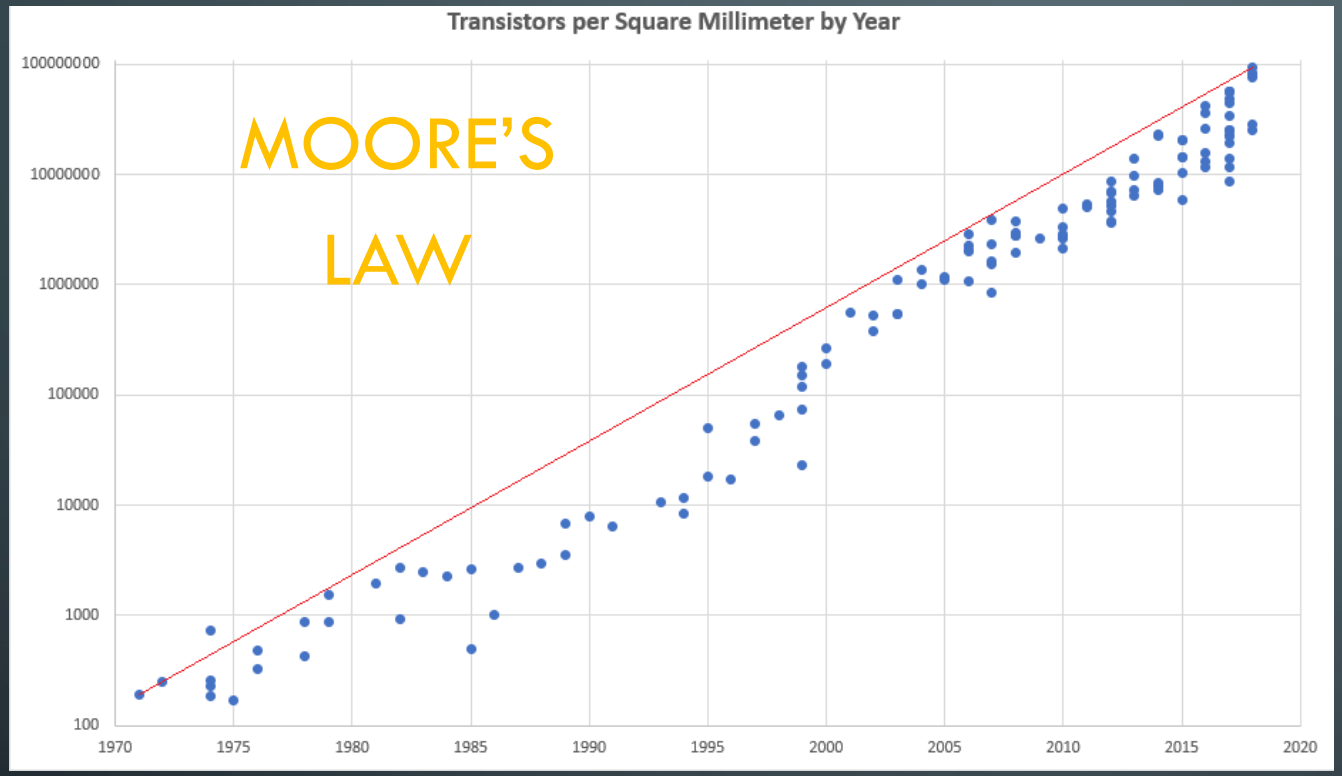
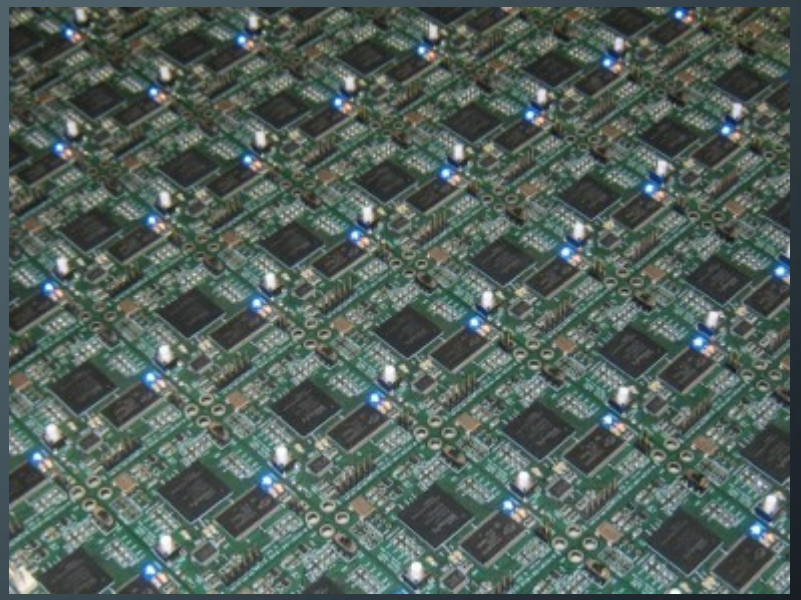
FUSS ABOUT "QUANTUM COMPUTING" ?

Classical computers have been around a long time, and in fact have only gotten faster with time. So what's the big deal about quantum computers? Why not build a faster classical computer? It seems to have worked out so far!

- Do quantum computers exist? Where can I ~~buy~~ find one?
- But I don't know quantum mechanics?
- Why should I care about quantum computing anyway?
- Does anyone use it?
- Is there a real case for using it? For HPC?

TODAYS COMPUTERS



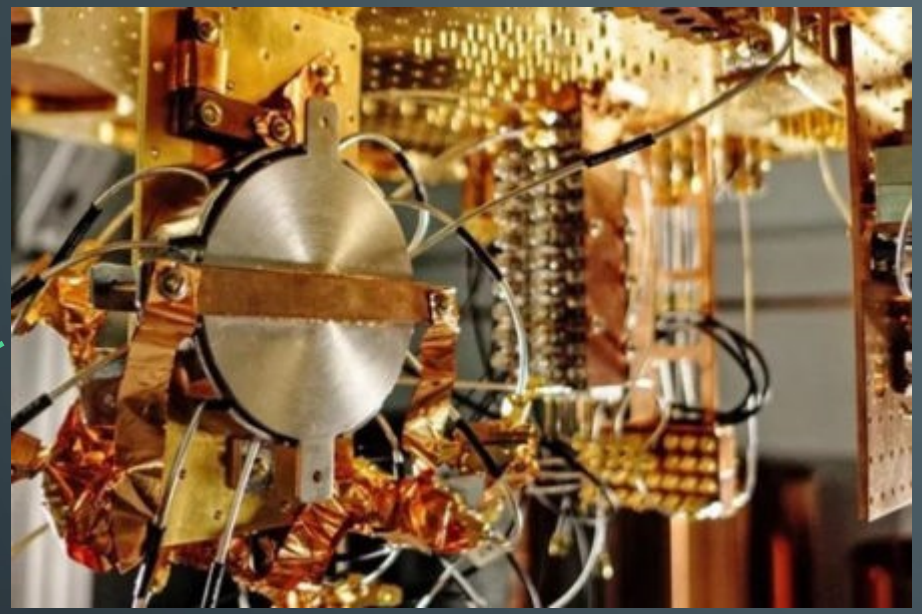


Todays chips ~ 45nm
Visible light ~ 400nm+
Quantum effect at nanoscale

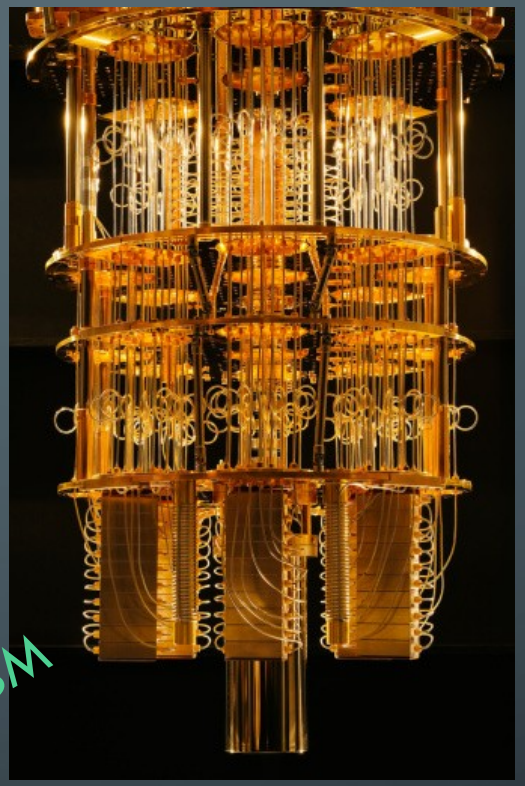
Parallel computing is nice …
But challenging, synthetic &
not applicable everywhere

TODAYS QUANTUM ~~COMPUTERS~~ SERVERS

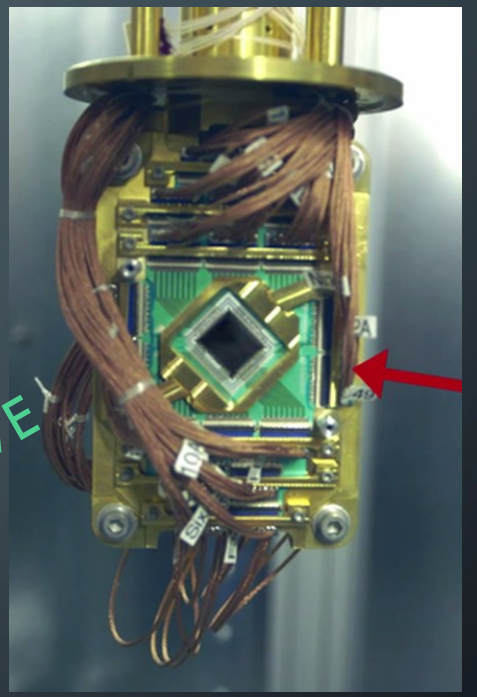
GOOGLE



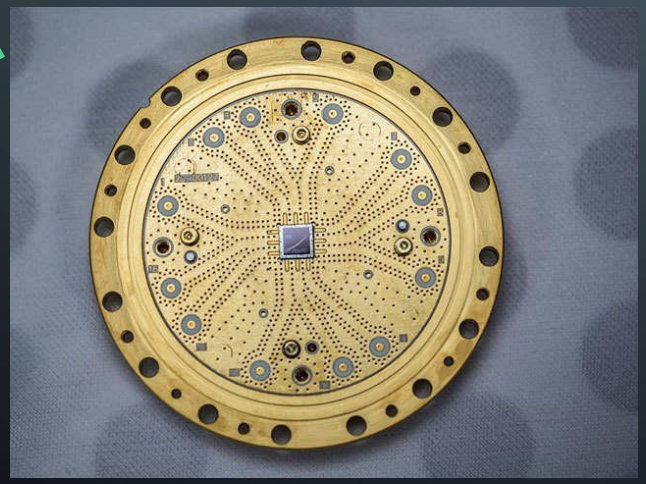
IBM



DWAVE

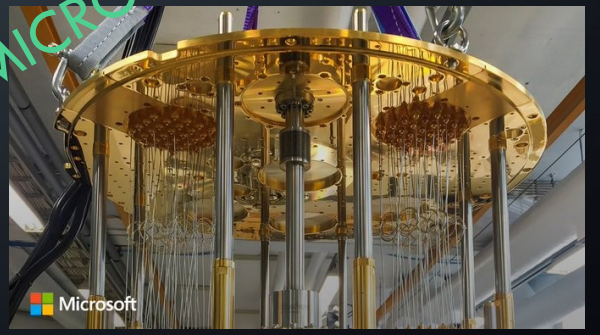


RIGETTI



IONQ

MICROSOFT



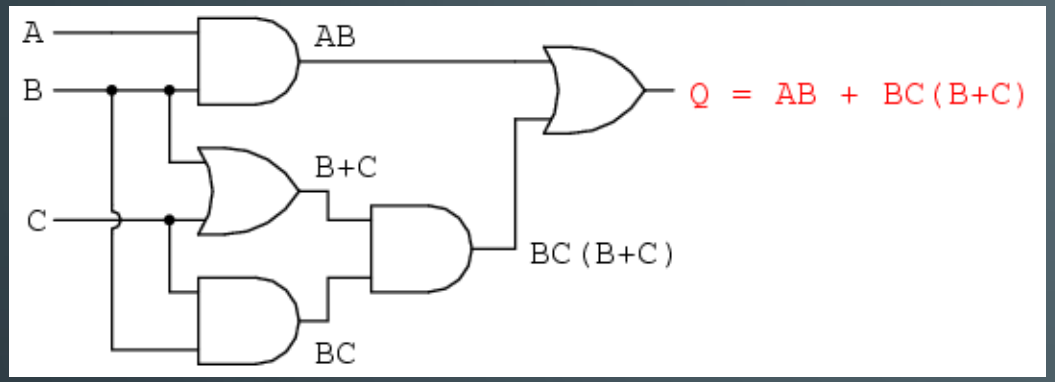
QUBIT COUNTER

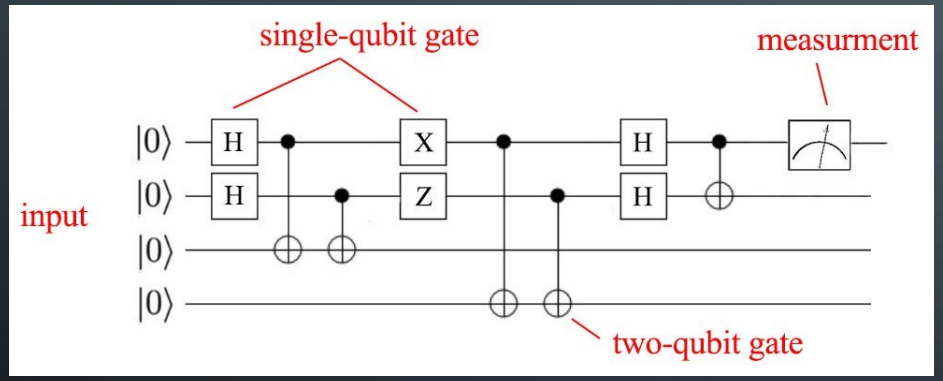
https://quantumcomputingreport.com/

Intel	Gate	Superconducting	49
Google	Gate	Superconducting	53/72
IBM	Gate	Superconducting	53
Rigetti	Gate	Superconducting	32
USTC (China)	Gate	Superconducting	10
IonQ	Gate	Ion Trap	11
IQOQI/Univ. Ulm/Univ. Innsbruck	Gate	Ion Trap	20
NSF STAQ Project	Gate	Ion Trap	N/A
Intel	Gate	Spin	26
Silicon Quantum Computing	Gate		
CEA-Leti/INAC/Institut Néel	Gate		
Univ. of Wisconsin	Gate	Neutral Atoms	49

D-Wave	Annealing	Superconducting	2048
iARPA QEO Research Program	Annealing	Superconducting	N/A

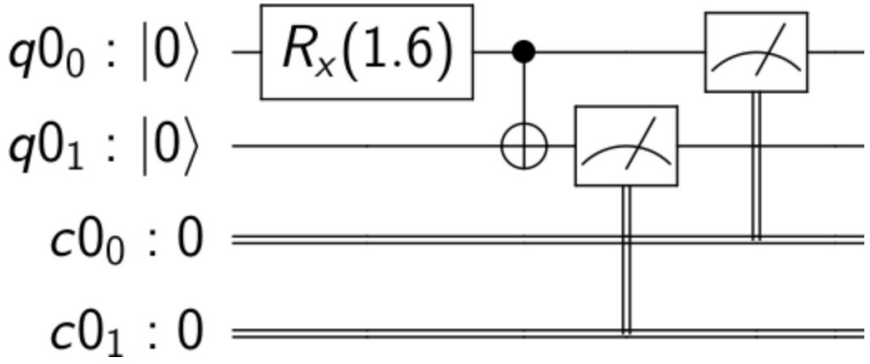
WRITING QUANTUM PROGRAMS (GATE MODEL)





In [7]:
```
from qiskit import QuantumRegister, ClassicalRegister, QuantumCircuit
from qiskit.tools.visualization import circuit_drawer
import numpy as np

qr = QuantumRegister(2)
cr = ClassicalRegister(2)
qp = QuantumCircuit(qr,cr)

qp.rx( np.pi/2,qr[0])
qp.cx(qr[0],qr[1])

qp.measure(qr,cr)

circuit_drawer(qp)
```

Out[7]:



DESIGNING QUANTUM PROGRAMS (GATE MODEL)

Physics-free QC = Linear algebra + Probability

Basic variable: qubit – 2 dimensional complex vector
E.g., 5 qubits ≡ $2^5 = 32$ dimensional complex vector
(similar to a randomized algorithm with 5 random bits)

Basic operation:
(1) 1 qubit evolution – 2 x 2 unitary matrix
E.g., 5 qubit evolution – multiply by 32x32 unitary matrix
(similar to stochastic matrices for randomized algorithms)

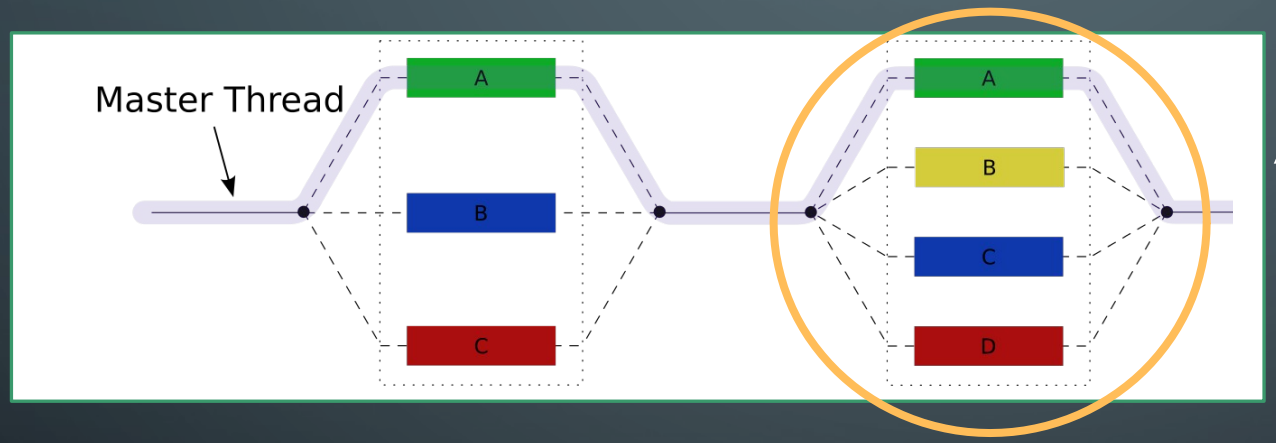
(2) 1 qubit measurement – 2 x 2 Hermitian matrix

PRINCIPLES OF QUANTUM COMPUTING

Random bit b : state is logical-0 (TAIL) OR logical-1 (HEAD)

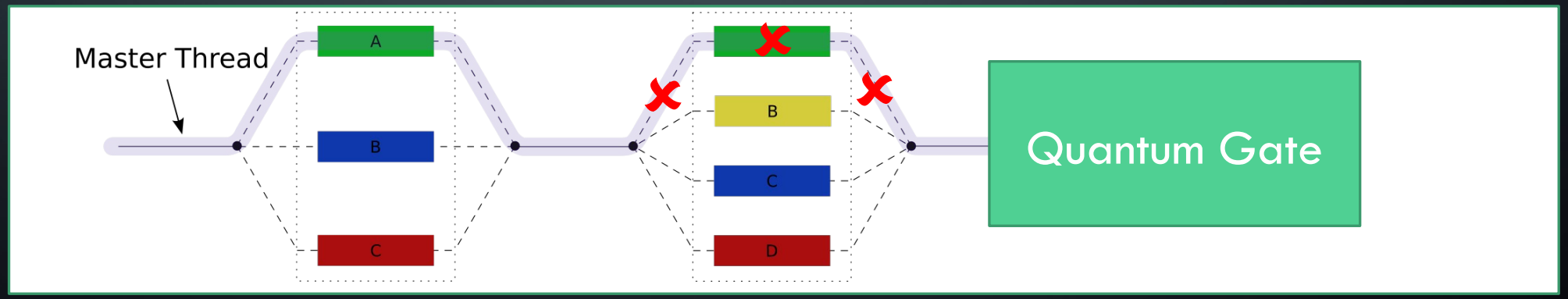
Qubit b = $\rangle - \rangle$: superposition of logical-0 AND logical-1

Qubit b = $\rangle - \rangle$: states can interfere destructively



Probability of each task
A, B, C, D =

Probability of each task
B, C, D =



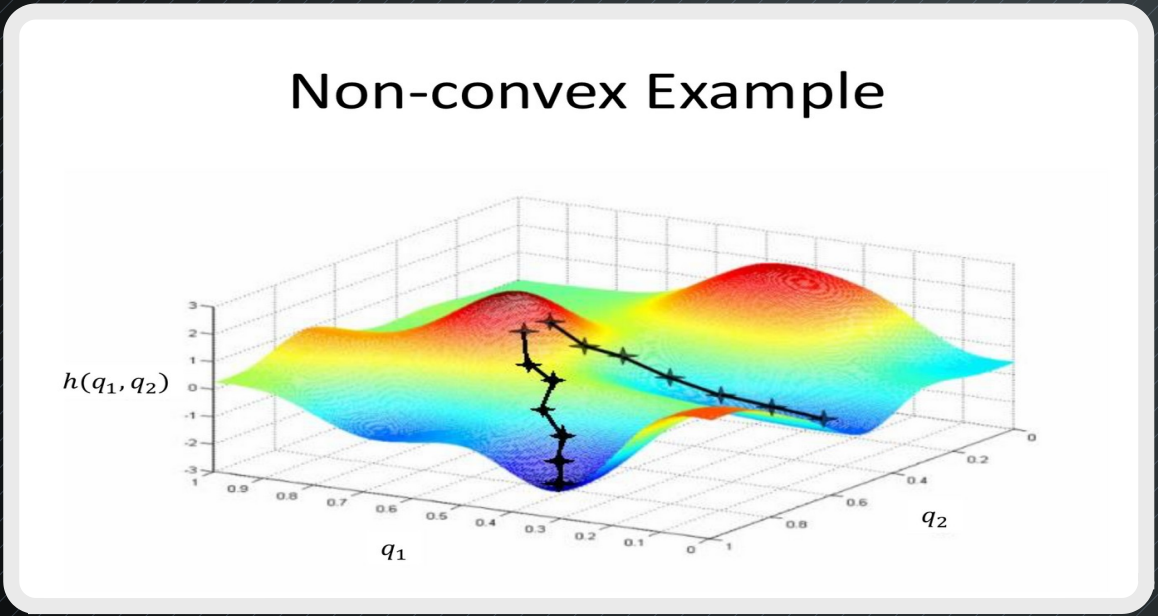
LINEAR SYSTEM OF EQUATIONS Ax=b

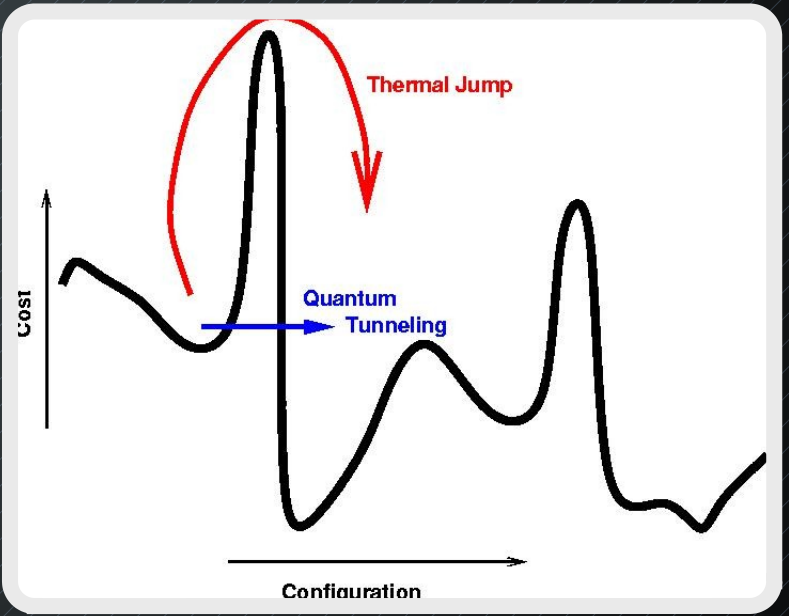
- **Find x:** Given N equations represented in the matrix form Ax=b. We are interested in the result of a scalar measurement M on the solution vector x, instead of the values of the solution vector itself.

Classical Complexity (Conjugate Gradient Descent Method)	Quantum Complexity (Harrow Hassidim Lloyd (HHL) Algorithm)

- Sparsity s: Ratio of the number of zero elements to the number of non-zero elements in the matrix
- Precision: Precision to the solution x
- Condition Number k: Ratio of maximum and minimum singular values of a matrix

QUANTUM ANNEALING





- Quantum annealing is similar to classical or simulated annealing, where thermal fluctuations allow the system to jump between different local minima in the energy landscape. As the temperature is lowered, the probability of moving to a worse solution tends to zero.

- In quantum annealing, these jumps are driven by quantum tunneling. This process explores the landscape of local minima more efficiently than thermal noise, especially when the energy barriers are tall and narrow.

QUANTUM ANNEALING

DNA sequences of length 12	Affinity of a TF
ACTAAGTACAAT	4.95
TTCCTATCCTGC	2.12
…	…

- Predict affinity of an unseen sequence.

- D-Wave system performed comparably or slightly better than classical counterparts for classification when the training size is small. (*Quantum annealing versus classical machine learning applied to a simplified computational biology problem, npj Quantum Information, (2018)*)

- It has been demonstrated that the feature weights obtained by DW reflect biological knowledge. This gives some confidence that quantum annealing (QA) is learning relevant biological patterns from the data.

A FEW STRING PROBLEMS

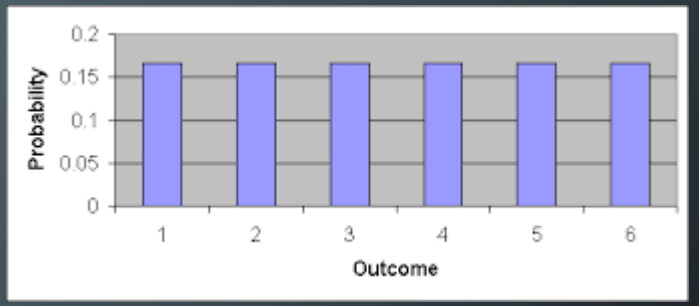
- Given a dictionary of n DNA sequences of length k each, find the most frequent one.
  (Best classical method uses a trie)
- Given a dictionary of n DNA sequences of length k each, sort the strings in some order.
  (Best classical method uses radix sort)
- Given a dictionary of n DNA sequences of length k each, and m query sequences of length k, determine if each query sequence is in the dictionary.

arXiv: 7 Jan 2020

REPEATED SAMPLING ≡ AMPLITUDE AMPLIFICATION

Problem: Find if dictionary contains sequence S

(*) X = RANDOM sequence from dictionary
If X = s: stop
Else: repeat and goto (*)



X is sequence 1 OR
X is sequence 2 OR
X is sequence 3 OR
…

Expected number of samples = 1/(size of dictionary)

Grover's search algorithm (*aka.* Amplitude Amplification):

Repeated sampling on a superposition of states, with –ve "possibility"

After expected $1/\sqrt{(\text{size of dictionary})}$ samples, X = S if S is present

MORE USE CASES OF QUANTUM COMPUTING

(did not cover quantum cryptography & quantum communication – some other day)

PORTFOLIO OPTIMIZATION on D-Wave

SPIN QUANTUM NUMBER determination (Chemistry)

LOWEST ENERGY EIGENVALUE of a Heisenberg model on a lattice

SIMULATION OF HYDROGEN MOLECULE by Google
(simulation of quantum-mechanical systems was the initial motivation of Richard Feynman to propose a quantum computer)

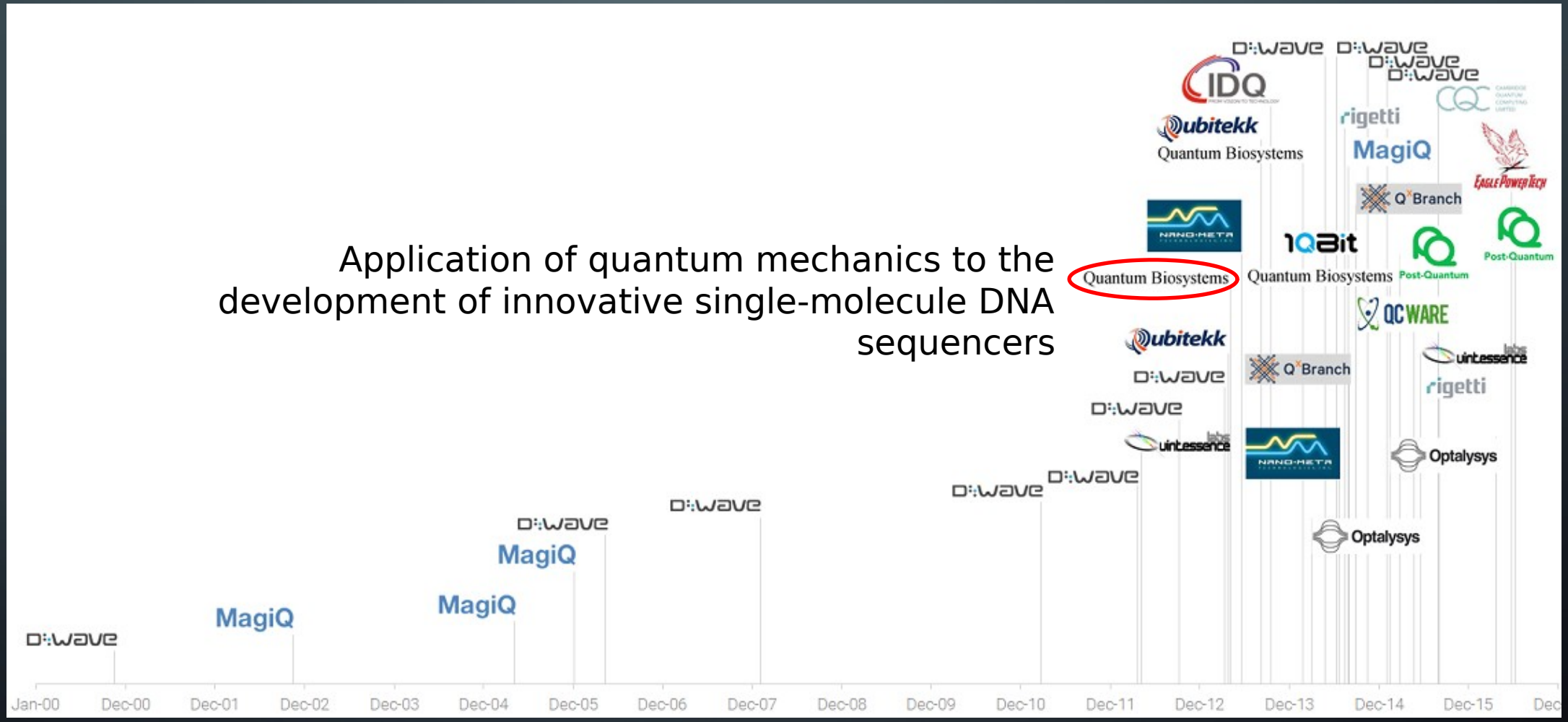
TRAFFIC OPTIMIZATION & EXPLORE MATERIAL STRUCTURE FOR E-VEHICLE BATTERY by Volkswagen Group and Google

GARTNER : EMERGING TECH. (2019)

1. AI cloud services
2. Autotion of ML
3. Augmented intelligence
4. Explainable AI
5. Edge AI
6. Reinforcement learning
7. Quantum Computing … has the potential to make significant contributions to the areas of systems optimization, machine learning, cryptography, drug discovery, and organic chemistry. Although outside the planning horizon of most enterprises, quantum computing could have strategic impacts in key businesses or operations.
8. AI Marketplaces

STARTUP FUNDING

Application of quantum mechanics to the development of innovative single-molecule DNA sequencers



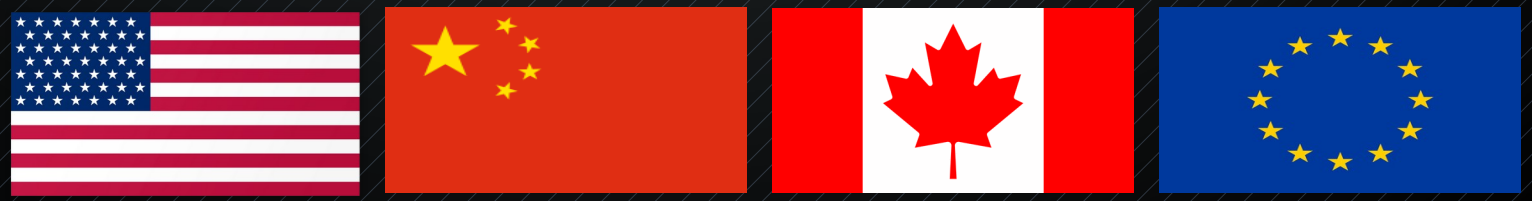
ERA OF QUANTUM COLD WAR ?

USA

- Penetrating Hard Targets (PHT): This project came into news from the NSA leak by Edward Snowden and the purpose is to build a Quantum Computer capable of breaking current encryption mechanisms. The current progress is unknown.
- On December 21, 2018, the National Quantum Initiative Act was signed into law by President Donald Trump, establishing the goals and priorities for a 10-year plan to accelerate the development of quantum information science and technology applications in the United States.

CHINA

- The latest reported record distance for quantum teleportation is 1,400 km (870 mi) by the group of Jian-Wei Pan using the Micius satellite for space-based quantum teleportation. With Micius, Chinese researchers are attempting to use photonic quantum technology to develop new forms of secure communications that would be unbreakable.
- It is reportedly investing $10bn in building the National Laboratory for Quantum Information Sciences in Hefei.



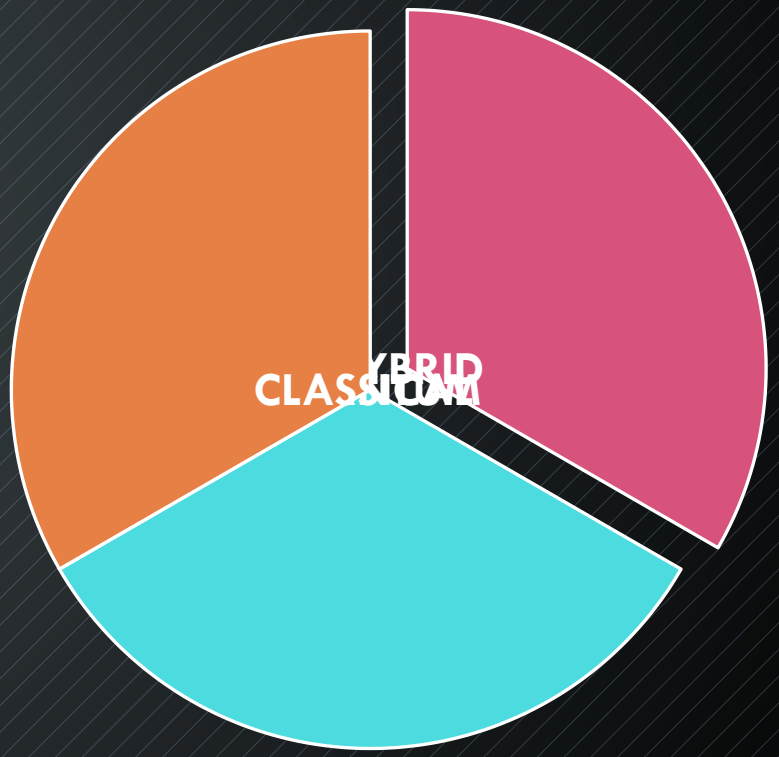
INDIA BUDGET 2020 SPEECH

63 (5). The government proposes to provide early life funding, including a seed fund to support ideation and development of early stage Start-ups.

Quantum technology is opening up new frontiers in computing, communications, cyber security with wide-spread applications. It is expected that lots of commercial applications would emerge from theoretical constructs which are developing in this area.

It is proposed to provide an outlay of ` 8000 crore over a period five years for the National Mission on Quantum Technologies and Applications.

FUTURE



Interesting! And accessible.

Worth investing time and effort (and money).

Best part : no clear winner application as of now.

Quantum Computing Group, IIIT Delhi

- Quantum algorithms for …
  - Optimization problems
  - Cryptography problems
- Quantum random number gen.
- Fault analysis of quantum circuits

"When you change the way you look at things, the things you look at change"

- Max Planck

(Father of Quantum Mechanics)

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