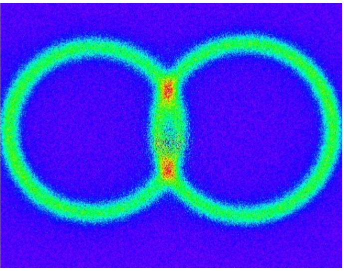
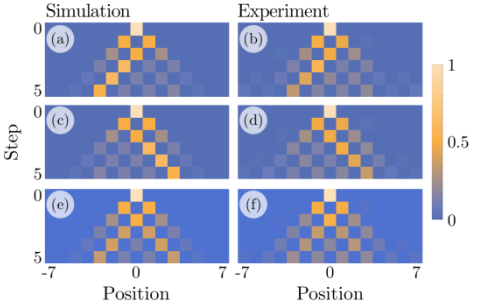
Quantum simulators for research and development of standards, benchmarking & validation

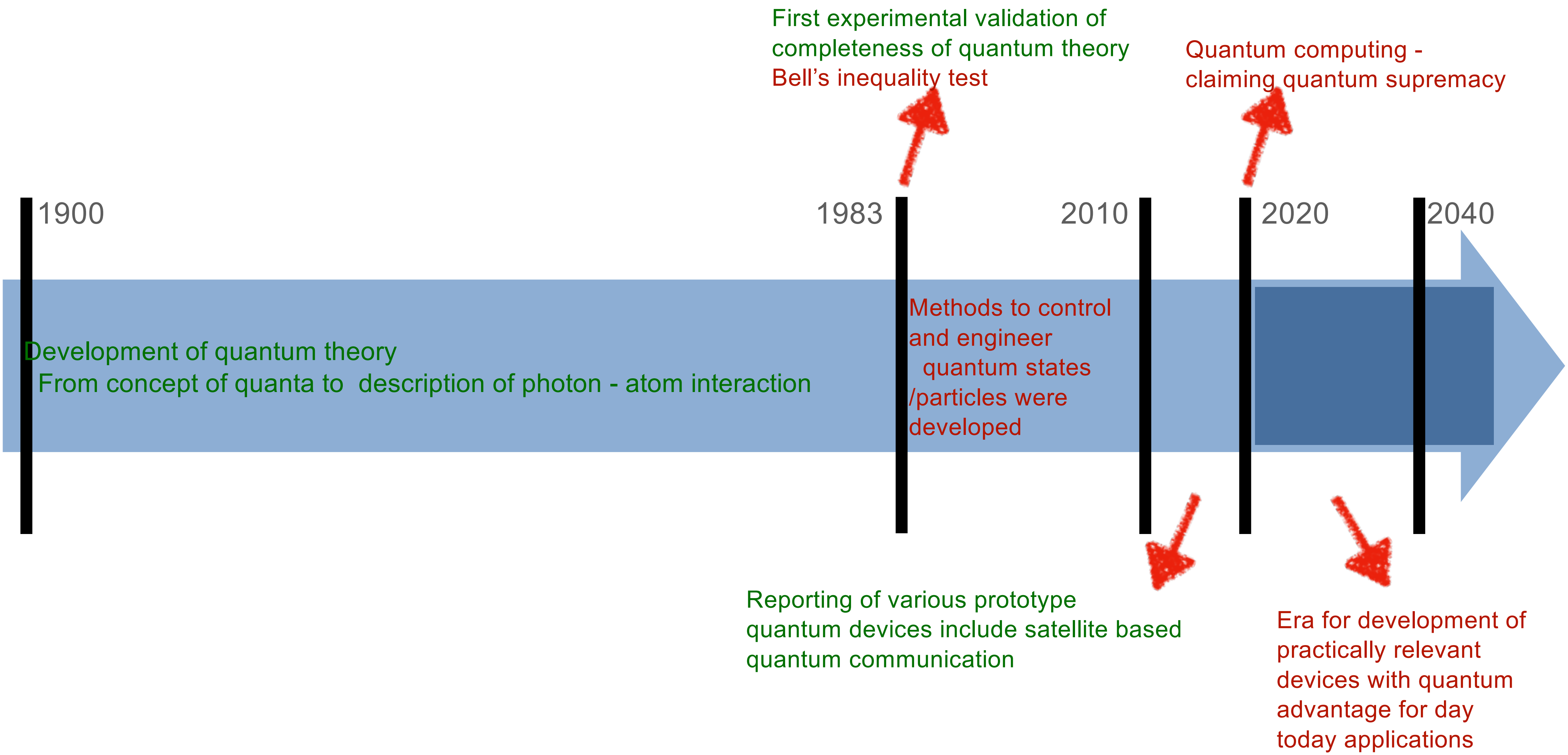


C. M. Chandrashekar

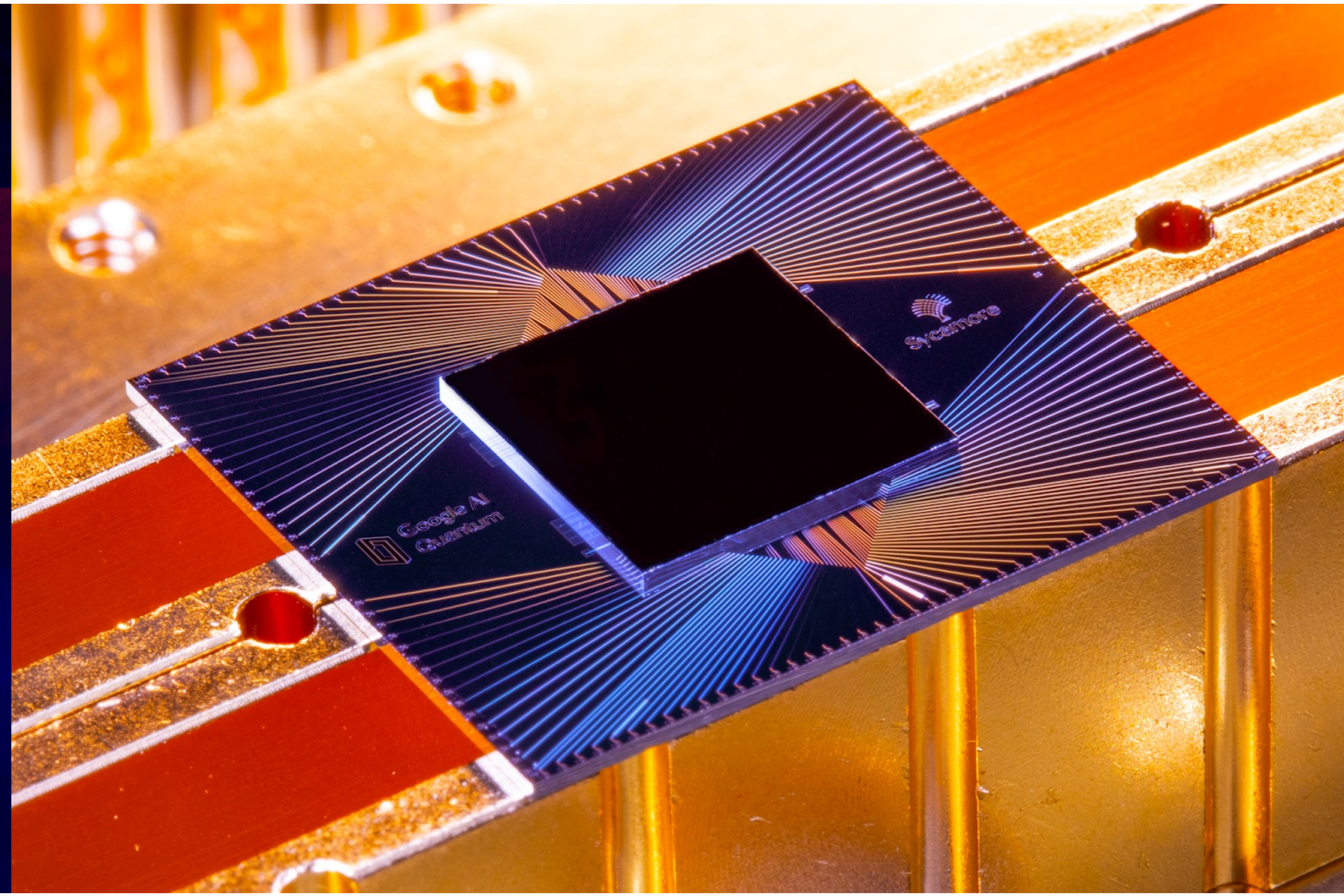
Quantum Optics and Quantum Information Processing Laboratory, IISc



Timeline - Quantum Mechanics to Quantum Technology



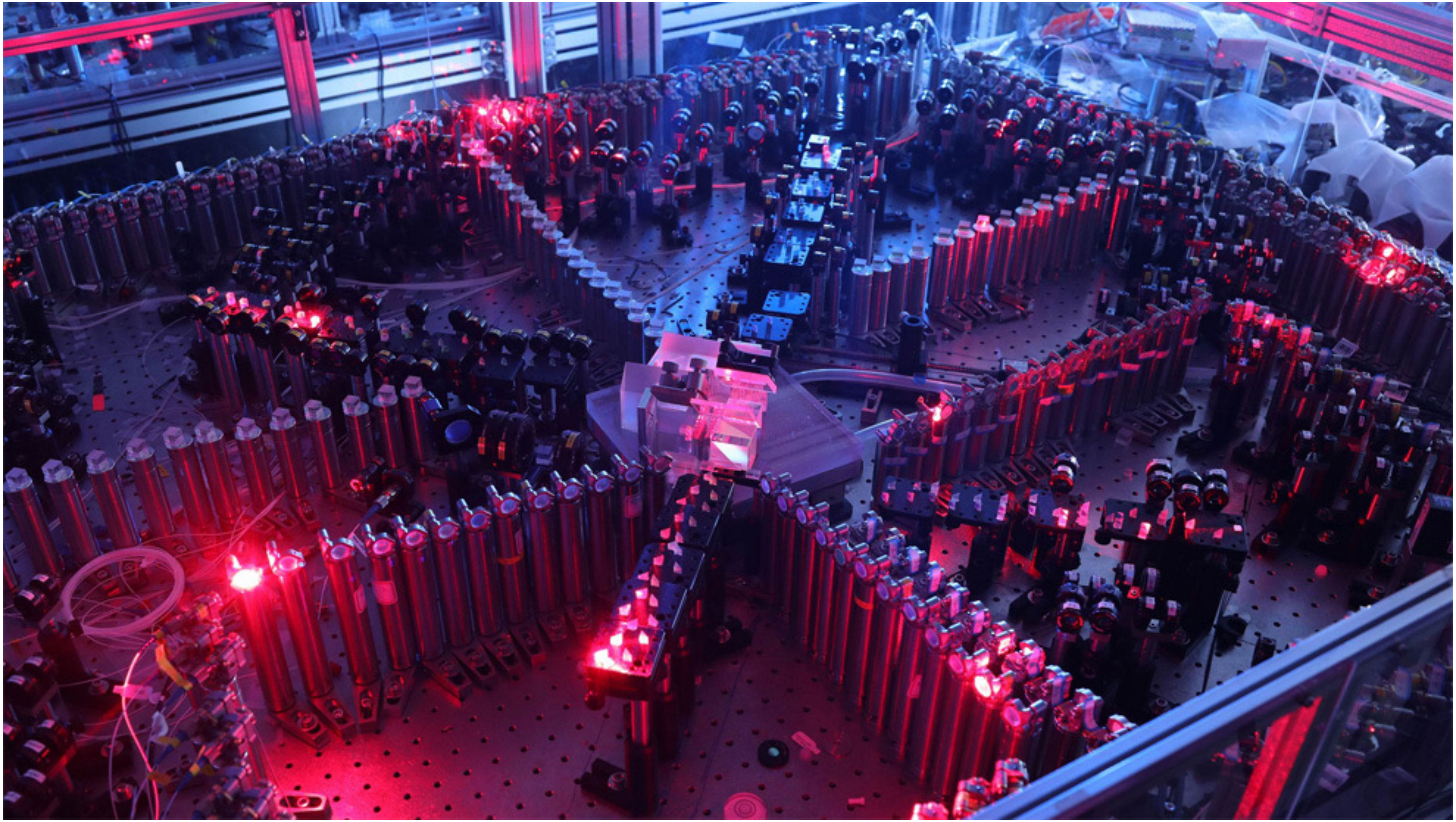
Quantum Supremacy



Nature, **574**, 505–510 (2019)

Sycamore – 53 qubit Superconducting Processor

Quantum Supremacy

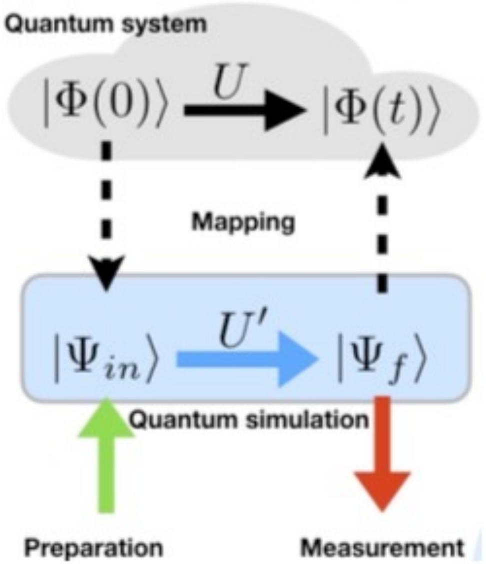


Science **370**, 1460–1463 (2020)

Optical circuit, maximum of 76 photons detected in one test and an average of 43 across several tests.

Quantum Simulation

Quantum Simulations use quantum methods to develop tools for solving challenging problems in basis sciences where quantum effects are prominent, in a range of fields, including physics, chemistry, biology and material sciences.



Main objective of quantum simulator:

- To harness controllable quantum evolutions in order to simulate other inaccessible complex quantum systems.
- To turn the exponential scaling of resources needed to simulate quantum systems on classical computers into a more favourable polynomial overhead on a quantum machine.

Computational Power of Qubits

Number of particles in quantum system	Superposition of quantum states	Number of bits needed to simulate quantum system
1	$\|0\rangle, \quad \|1\rangle$	$2^1 = 2$
2	$\|00\rangle, \|01\rangle, \|10\rangle, \|11\rangle$	$2^2 = 4$
3	$\|000\rangle, \|001\rangle, \ldots\ldots, \|111\rangle$	$2^3 = 8$
4	$\|0000\rangle, \|0001\rangle, \ldots\ldots, \|1111\rangle$	$2^4 = 16$
10	$\|0000000000\rangle, \ldots\ldots, \ldots\ldots$	$2^{10} = 1024$
30	$\|0000000000\ldots\ldots\rangle, \ldots\ldots, \ldots\ldots$	$2^{30} = 10737 \times 10^5$ 1G
50	$\|0000000000\ldots\ldots\ldots\rangle, \ldots\ldots, \ldots\ldots$	$2^{50} = 11259 \times 10^{11}$ 1P

Some examples

	Chemical formula	Classical bit	Qbits
Water	H_2O	10^4	14
Ethanol	C_2H_6O	10^{12}	42
Acetaminophen	$C_8H_9NO_2$	10^{36}	120
Caffeine	$C_{12}H_{22}O_{11}$	10^{48}	160
Sucrose	$C_8H_{10}N_3O_2$	10^{82}	274
Penicillin	$C_{16}H_{18}N_2NaO_4S$	10^{86}	286

Courtesy : IBM quantum

Digital and analog quantum simulation

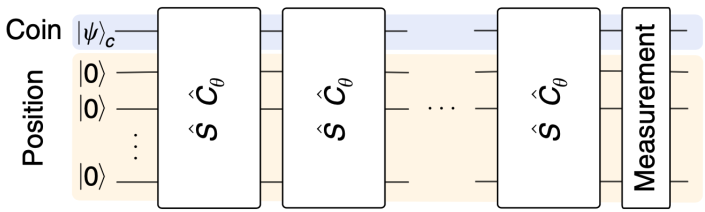
Digital Quantum Simulations : Decomposition of know Hamiltonian's of the complex quantum system into sum of local terms and approximating the combinations of discrete step-wise unitary operators with minimum errors is one of the standard way for arriving at operations scheme for digital quantum simulators. These operations will be in the form is computational gates on qubits which will approximate the time evolution of arbitrary local Hamiltonians.

Analog Quantum Simulations : Analog version represents an alternative approach that is not restricted to register of qubits and the dynamics are not necessarily build upon gates. A map is constructed that transfers the model of interest to the engineered dynamics of quantum simulators. This approach depends continuously on time and provides less flexibility due to their lack of universality.

Rev. Mod. Phys. 86, 153 (2014)

Digital quantum simulation

- **Dirac cellular automata**



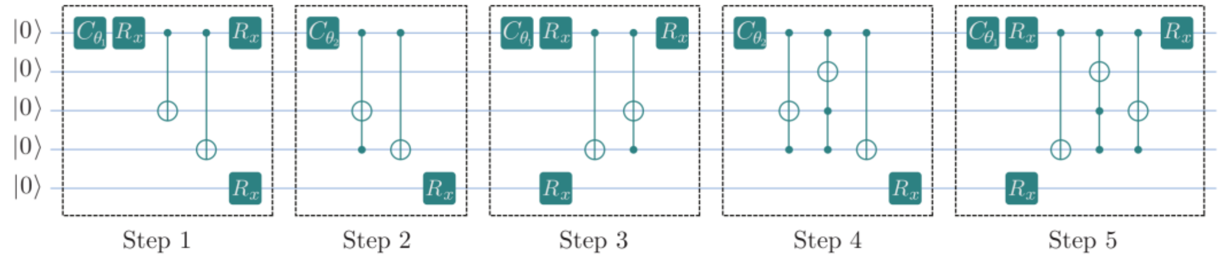
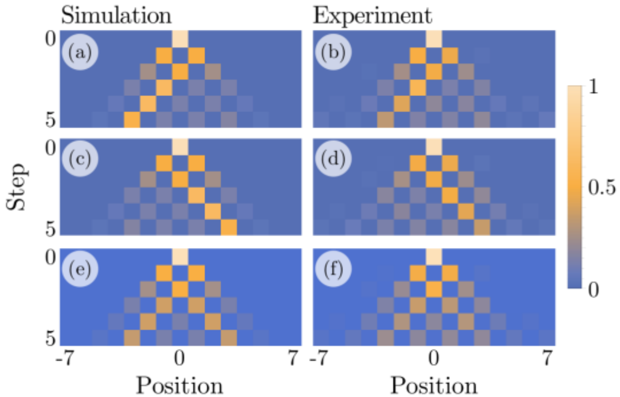


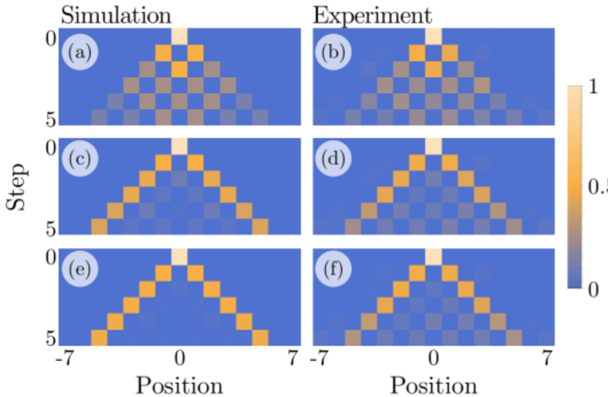
FIG. 2. Circuit diagram for a DQW. Each dashed-block describes one step in the quantum walk.

Table 1 Gate counting.

	DQW				DCA	
	$\|0\rangle_c/\|1\rangle_c$		$\|0\rangle_c + i\|1\rangle_c$		$\|0\rangle_c + i\|1\rangle_c$	
Step	R	XX	R	XX	R	XX
1	5	2	6	2	5	2
2	10	4	10	4	12	4
3	12	4	12	4	11	4
4	25	11	25	11	27	11
5	26	11	26	11	26	11
Total:	78	32	79	32	81	32

Number of single- and two-qubit gates per step and total number of gates after a 5-step evolution.





Trapped ions @ Maryland / IonQ

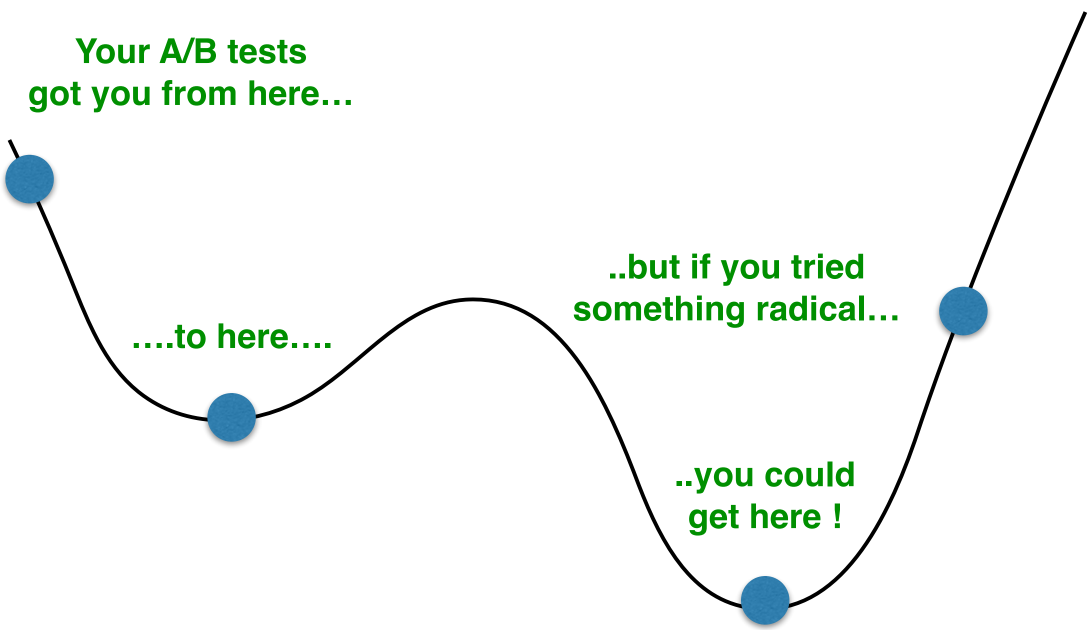
NATURE COMMUNICATIONS | (2020)11:3720

Analog quantum simulation

Solving optimization problems

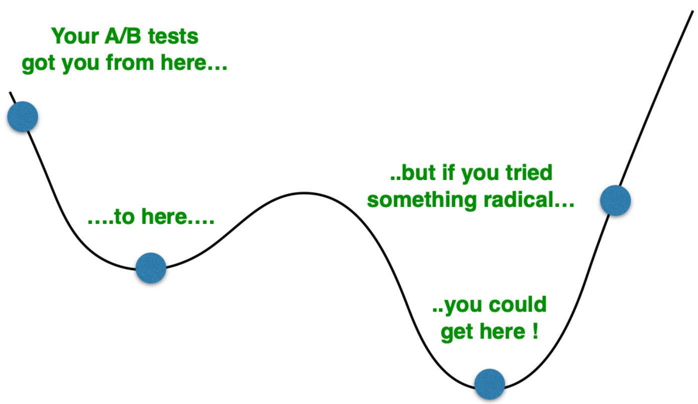
Goal of optimization problems :

- A general optimization problem is defined by **cost function**, seen as the **energy of a physical system**
- The goal is to find the global energy minimum, while avoiding local minima

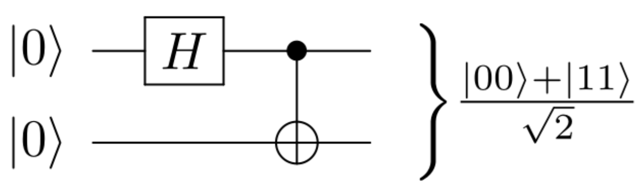


Broad Class of Quantum Processors

1. **Universal Quantum Computers (circuit-based processor)**
2. **Special task Quantum Computers (problem specific quantum simulator) – Optimization/ BS , Quantum annealing**
3. **Noisy Intermediate Scale Quantum (NISQ) Computers – Near-term devices**



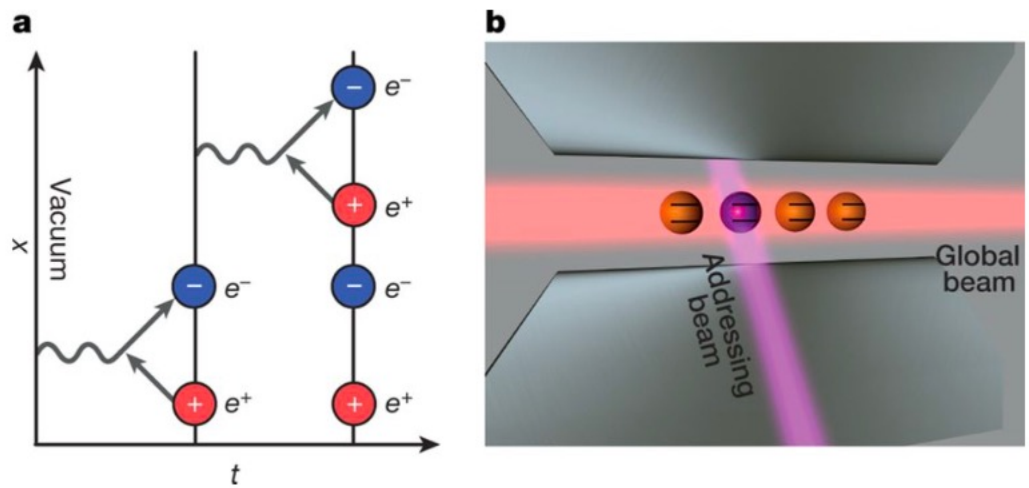
D-Waves global optimization problem



Operator	Gate(s)	Matrix
Pauli-X (X)	X	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
Pauli-Y (Y)	Y	$\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$
Pauli-Z (Z)	Z	$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
Hadamard (H)	H	$\frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$
Phase (S, P)	S	$\begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}$
$\pi/8$ (T)	T	$\begin{bmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{bmatrix}$
Controlled Not (CNOT, CX)		$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$
Controlled Z (CZ)	Z	$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$
SWAP		$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$
Toffoli (CCNOT, CCX, TOFF)		$\begin{bmatrix} 1&0&0&0&0&0&0&0 \\ 0&1&0&0&0&0&0&0 \\ 0&0&1&0&0&0&0&0 \\ 0&0&0&1&0&0&0&0 \\ 0&0&0&0&1&0&0&0 \\ 0&0&0&0&0&1&0&0 \\ 0&0&0&0&0&0&0&1 \\ 0&0&0&0&0&0&1&0 \end{bmatrix}$

Problems on NISQ / Near-term Q Computers

- **Real-time dynamics of lattice gauge theories using a four-qubit system** (quantum Monte Carlo methods describe equilibrium phenomena, no systematic techniques exist to tackle the dynamical long-time behaviour)



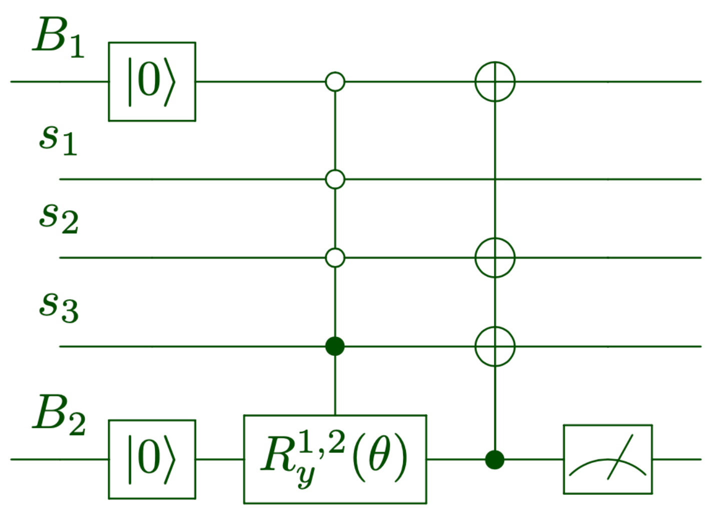
Coherent real-time dynamics of particle - antiparticle creation by realizing the Schwinger model on four $^{40}Ca^{+}$ ion qubit quantum computer.

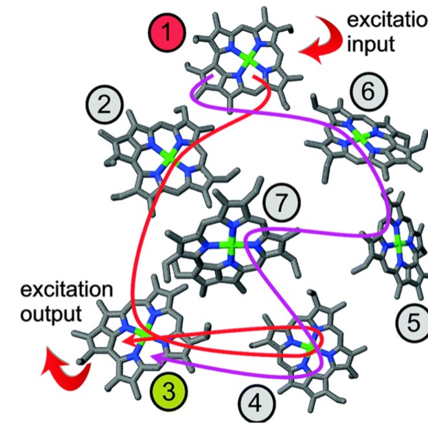
Real-time quantum simulations of non-Abelian lattice gauge theories ?

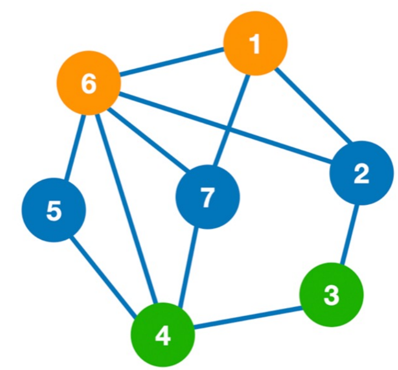
Nature 534, 517 (2016)

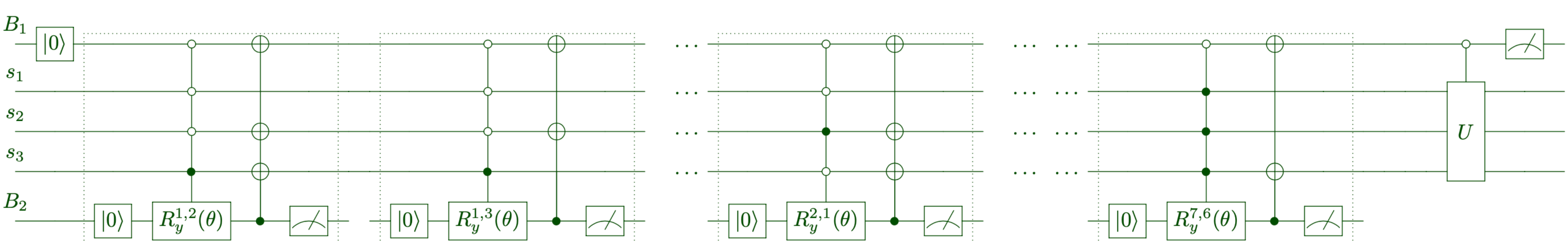
Problems on NISQ / Near-term Q Computers

- **Quantum circuit for environment assisted quantum transport (ENAQT) for FMO complex**





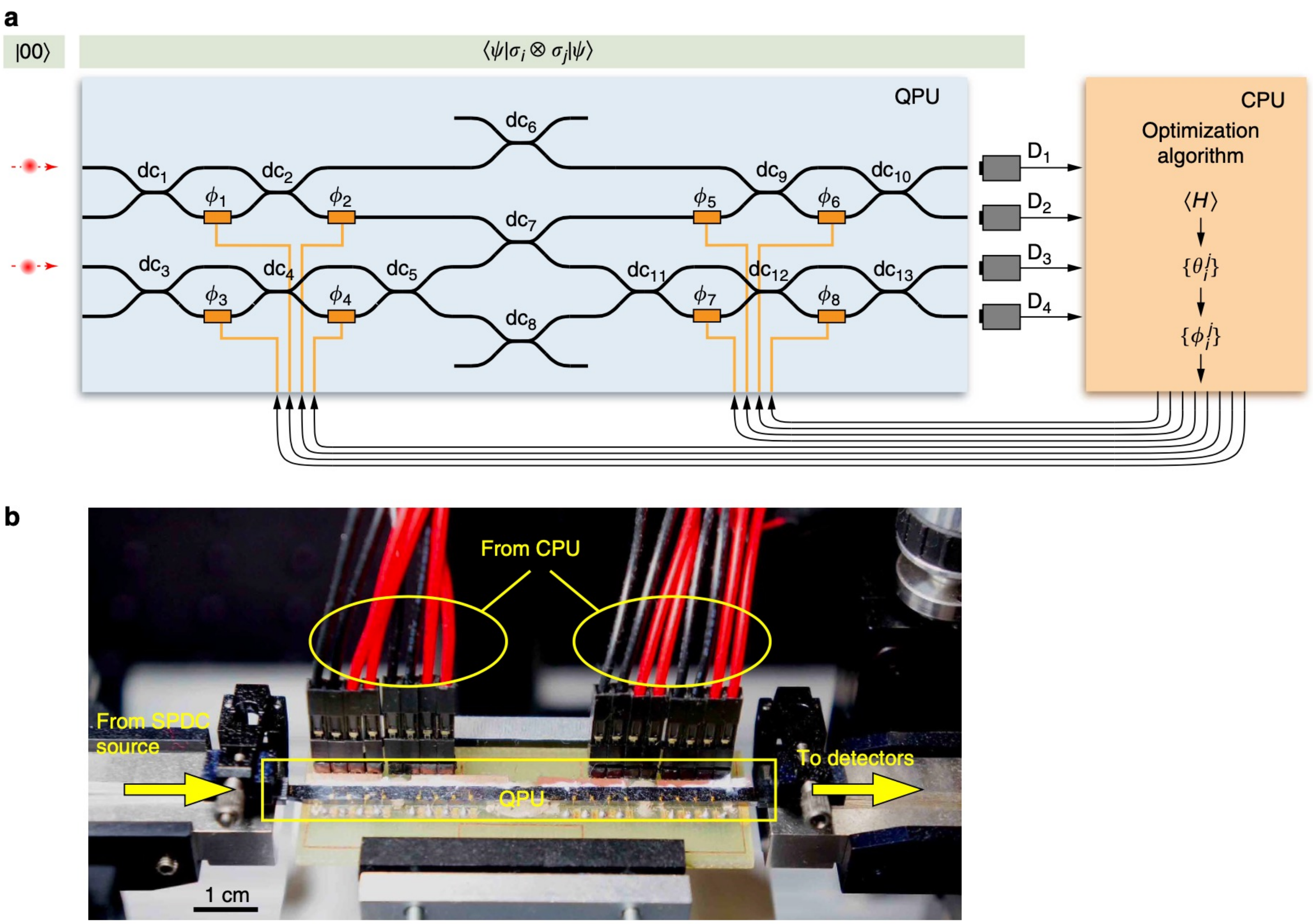




New J. Phys. **22** 123027 (2020)

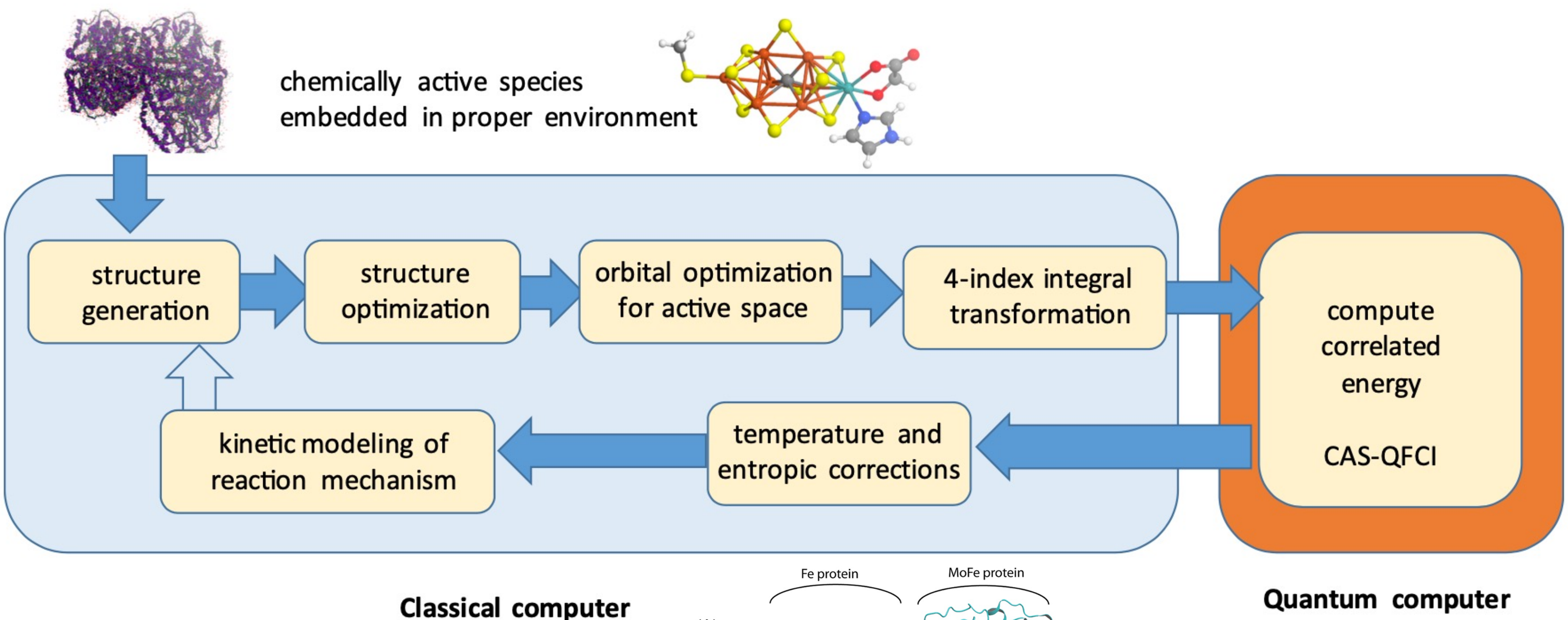
Variational Eigenvalue Solver (Classical – Quantum)

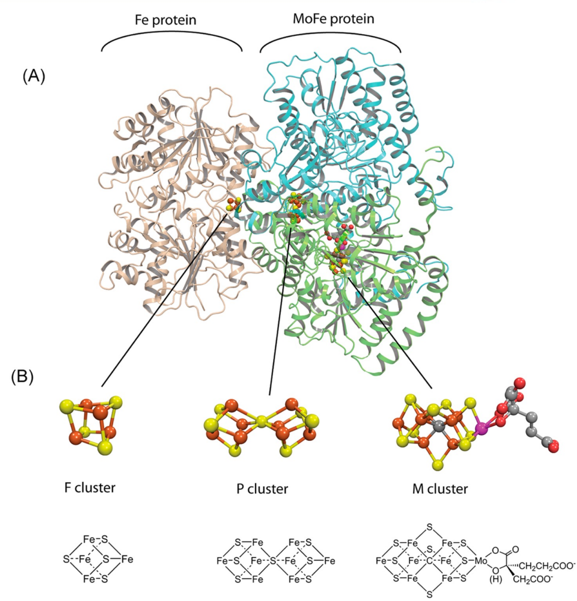
- **Calculating the ground-state molecular energy for He-H⁺**



Variational Eigenvalue Solver (Classical – Quantum)

- **Biological nitrogen fixation by the enzyme nitrogenase**





PNAS | **July 18, 2017** | vol. 114 | no. 29 | **7555–7560**

Quantum Simulator & Quantum Circuit Simulator

Quantum simulator

- Should demonstrate some quantum phenomena in use during its operations
  Ideally it will be a quantum system (quantum hardware - QPU)

- Should solve at least one problem of an other quantum system or simulate some features of an other quantum systems (need not be circuit based approach)

Quantum circuit simulator

- Classical processors designed to simulate quantum circuits. It is used as a test bed for quantum processors / quantum simulators

https://quantiki.org/wiki/list-qc-simulators

IBM quantum circuit simulators

Amazon bracket (40 qubit – 90 core processor)

IISc – CDAC QSim: Quantum Computer Simulator Toolkit

Approx. 150
C/C++ - 35
GUI – 15
Python - 15

With Amazon Braket, you have a choice of quantum circuit simulators to run and test quantum algorithms, including the free local simulator in the Amazon Braket SDK, and three fully managed on-demand simulators: State Vector 1 (SV1), Density Matrix 1 (DM1), and Tensor Network 1 (TN1). SV1 is a general purpose quantum circuit simulator, DM1 enables you to simulate the effect of noise on your circuits, and TN1 specializes in larger scale simulations for certain types of quantum circuits. All on-demand simulators automatically

Thank you