

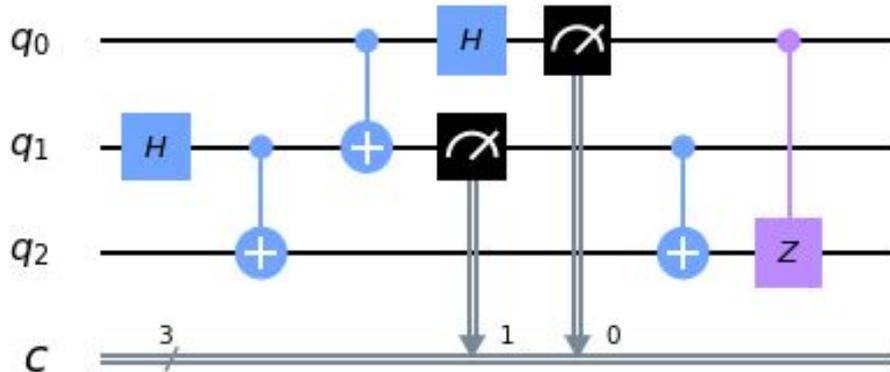
# Quantum Circuit Simulators

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February 18, 2021

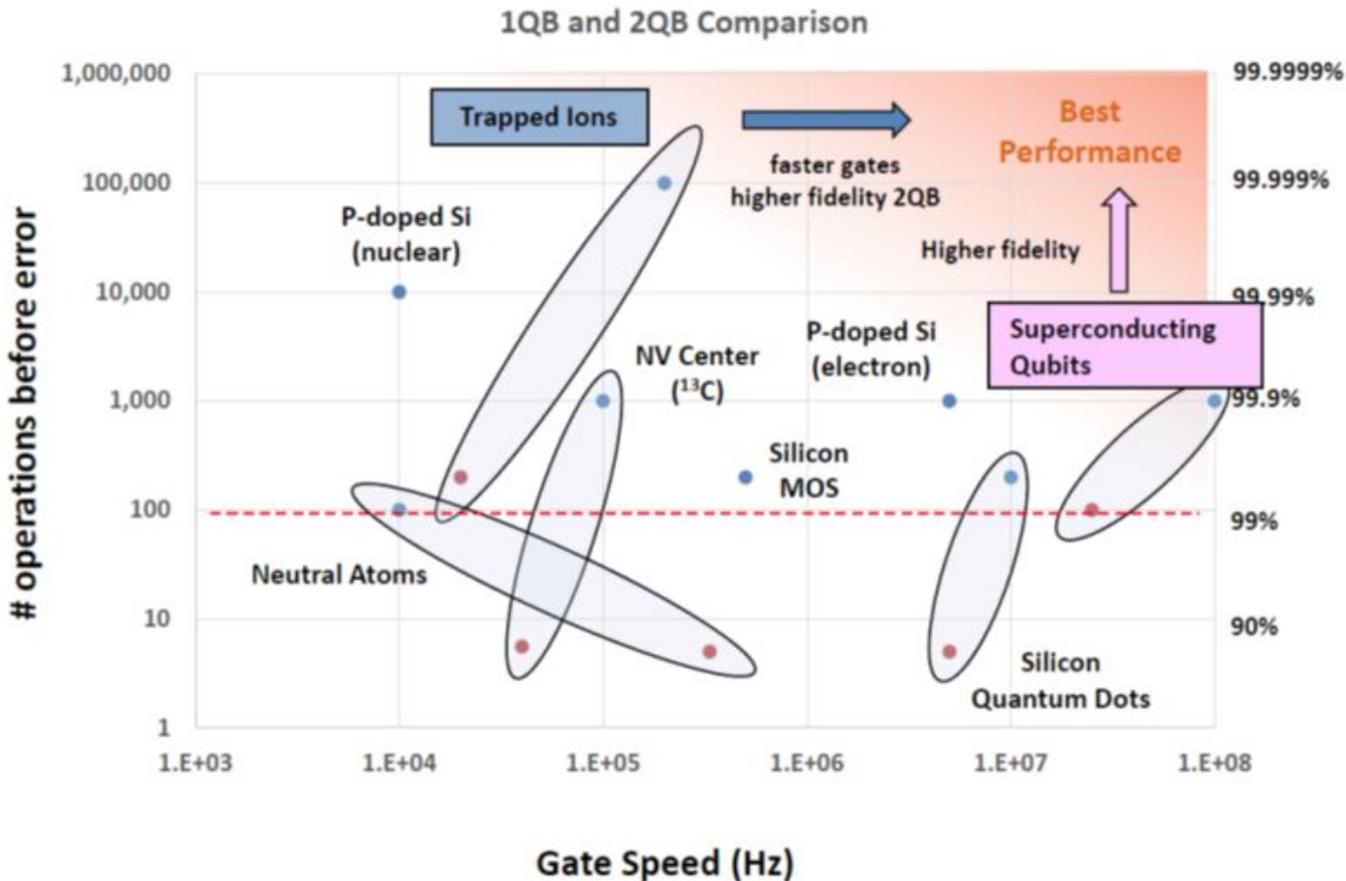
# What is a Quantum Circuit Simulator?



It is an universal quantum computer simulator which simulates the execution of quantum circuits with or without quantum noise

The input is a quantum circuit which is described using quantum assembly language (QASM)

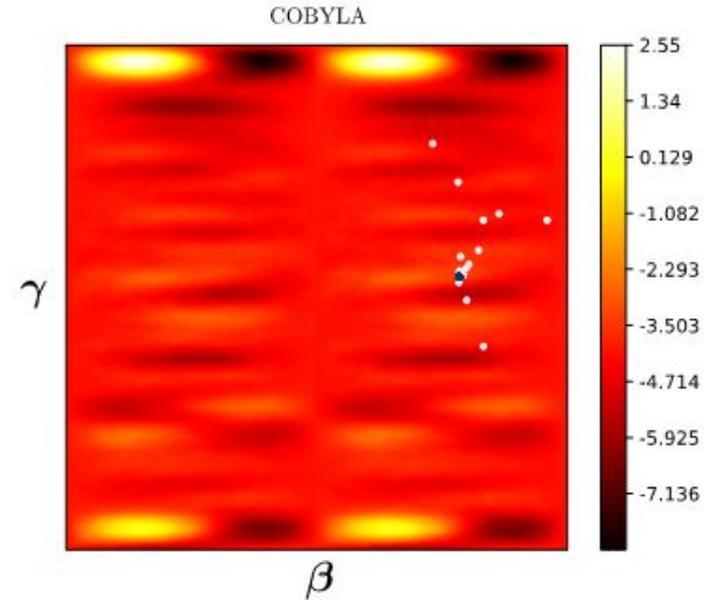
# Why we need quantum simulators?



Modern CPUs:  
~3 GHz, 100% fidelity

# Quantum Simulator Use Cases

- Verification of quantum advantage and supremacy claims
- Verification of large quantum devices
- Co-design quantum computers
- Energy efficiency studies of quantum computers
- Design of new quantum algorithms
- Finding parameters for variational quantum algorithms



# Argonne Simulators

Simulator	Advantages	Disadvantages
Intel-QS	highly scalable C++ HPC code (MPI/OpenMP), freely available from Git	under development, no documentation, lacking sophisticated error models
QuaC	time dynamics, scalable code, freely available from Git, error models	under development, poor documentations, depends on PETSc
Atos	robust commercial package, easy to use, excellent documentation, error models	not freely available, no MPI implementation

# Limitations of quantum simulators

Qubits	Memory	Time per operation
10	16 KB	Microseconds on a smartwatch
20	16 MB	Milliseconds on a smartphone
30	16 GB	Seconds on a laptop
40	16 TB	Seconds on a PC cluster
50	16 PB	Minutes on modern supercomputers
60	16 EB	Hours on <u>post-exascale</u> supercomputers?
70	16 ZB	Days on supercomputers in distant future?

# Quantum simulator types

First generation: store state vector or full density matrix

Limits: up to ~47 qubits

Second generation: tensor simulators (network contraction, MPS)

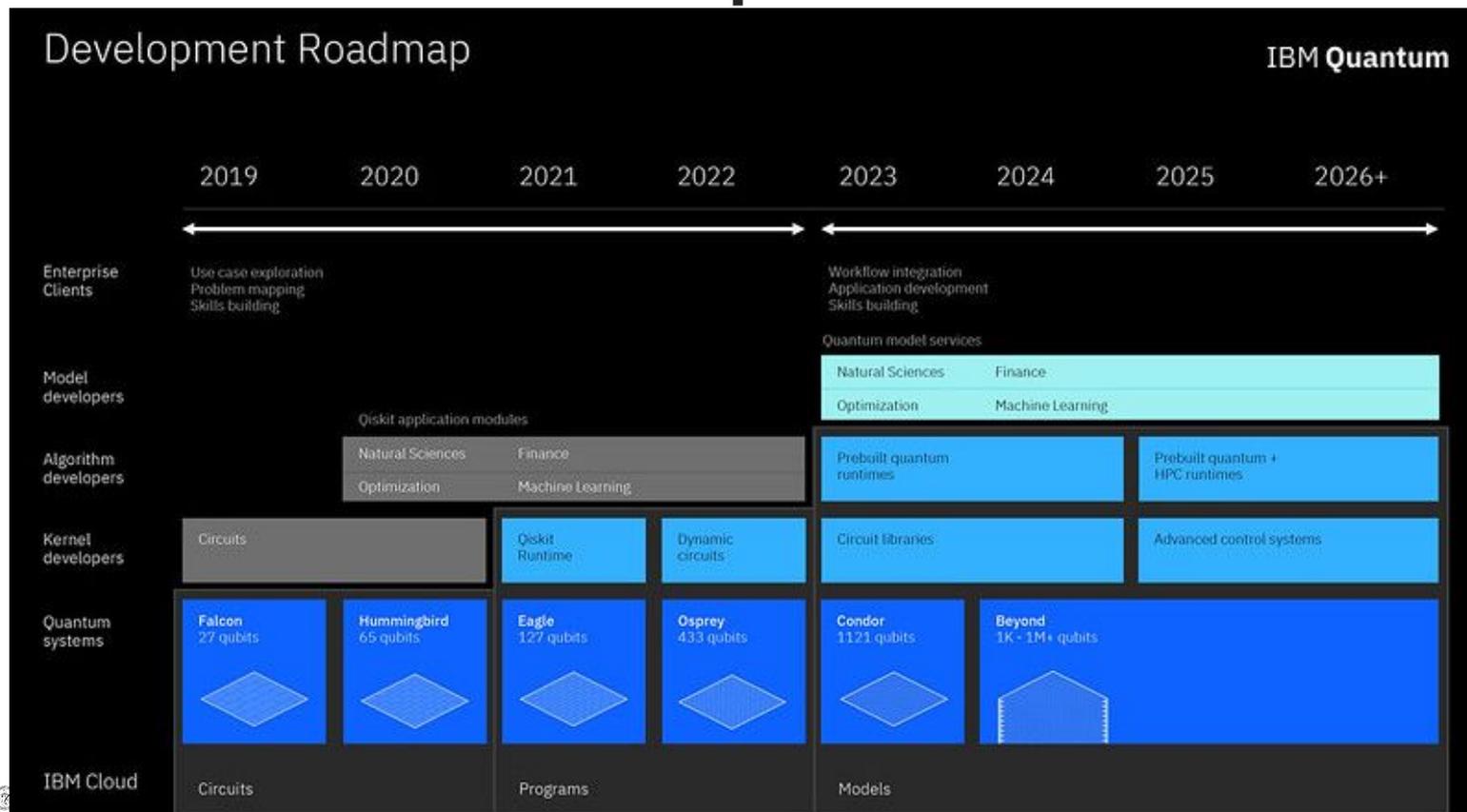
Limits: up to ~300 qubits

Third generation: approximate quantum simulators

Limits: 1,000+ qubits

Fourth generation: use small quantum computers to simulate large quantum computers

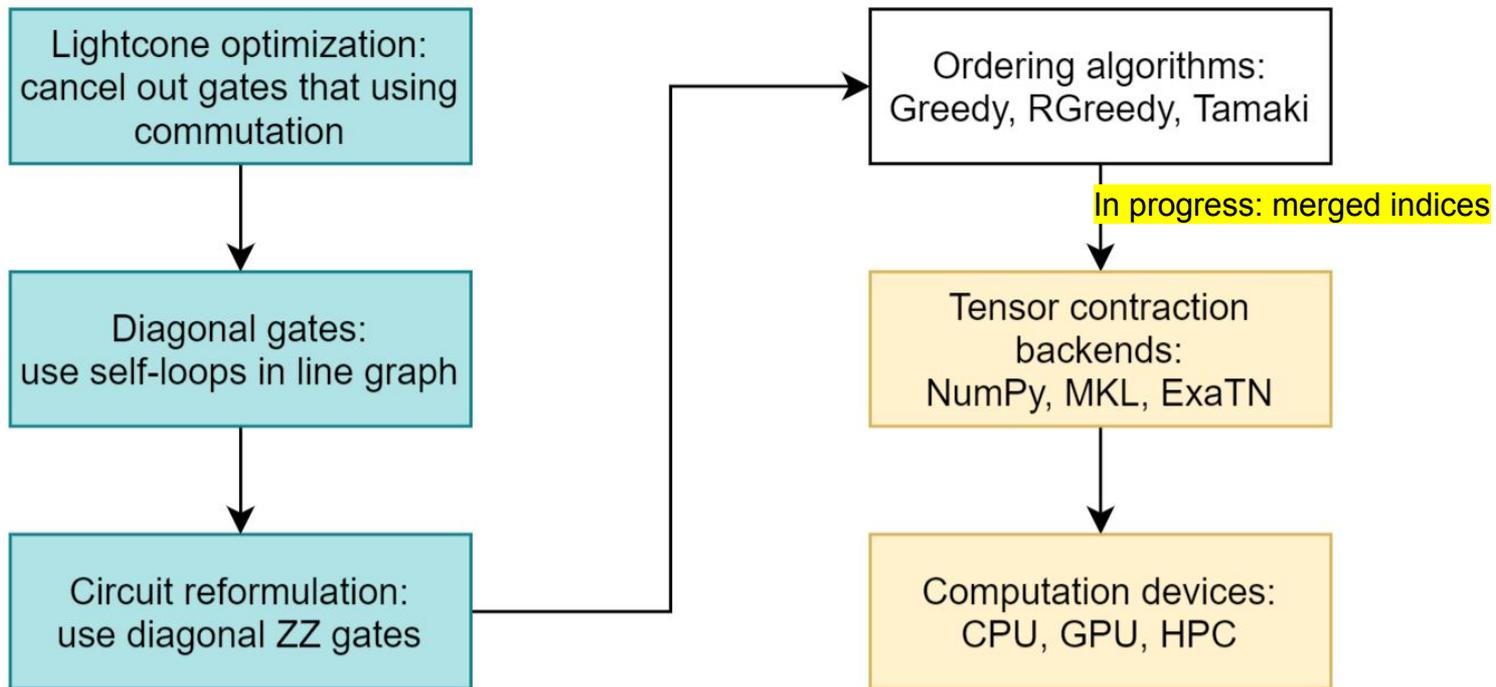
# IBM Quantum Roadmap



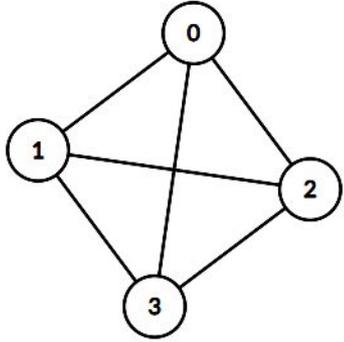
# Goals of the QTensor project

1. Open source quantum simulator based on tensor network contraction schemes
2. Easy to use and integrated in popular QIS frameworks like Qiskit
3. Fast simulation of certain types of circuits (QAOA and supremacy circuits)
4. Parallel distributed memory simulator designed to work on High Performance Computing (HPC) machines. In particular, it will run on exascale supercomputers Aurora and Frontier
5. Verification of quantum advantage using upcoming exa-scale supercomputer Aurora for DARPA projects

# QTensor Development



# QAOA circuit



Fully connected graph with 4 vertices and 6 edges. The corresponding circuit to solve MaxCut problem is below

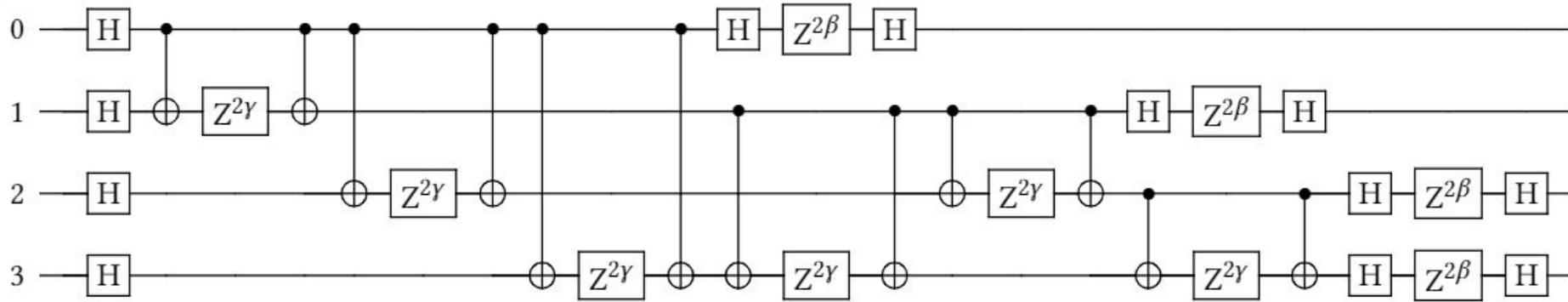
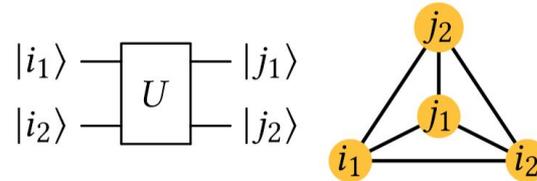
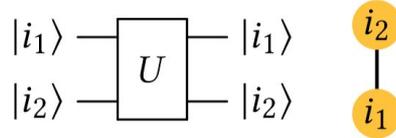
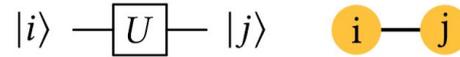


Figure 1:  $p=1$  depth QAOA circuit for a fully connected graph with 4 nodes.

# Line graph

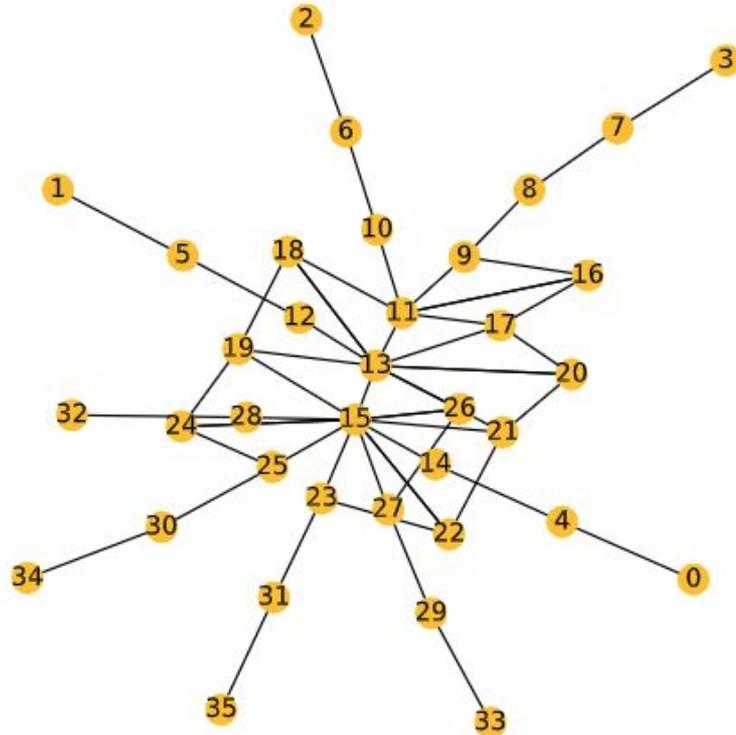


(a) Diagonal gates

(b) Non-diagonal gates

**Figure 2: Correspondence of quantum gates and graphical representation.**

# QAOA Tensor Network

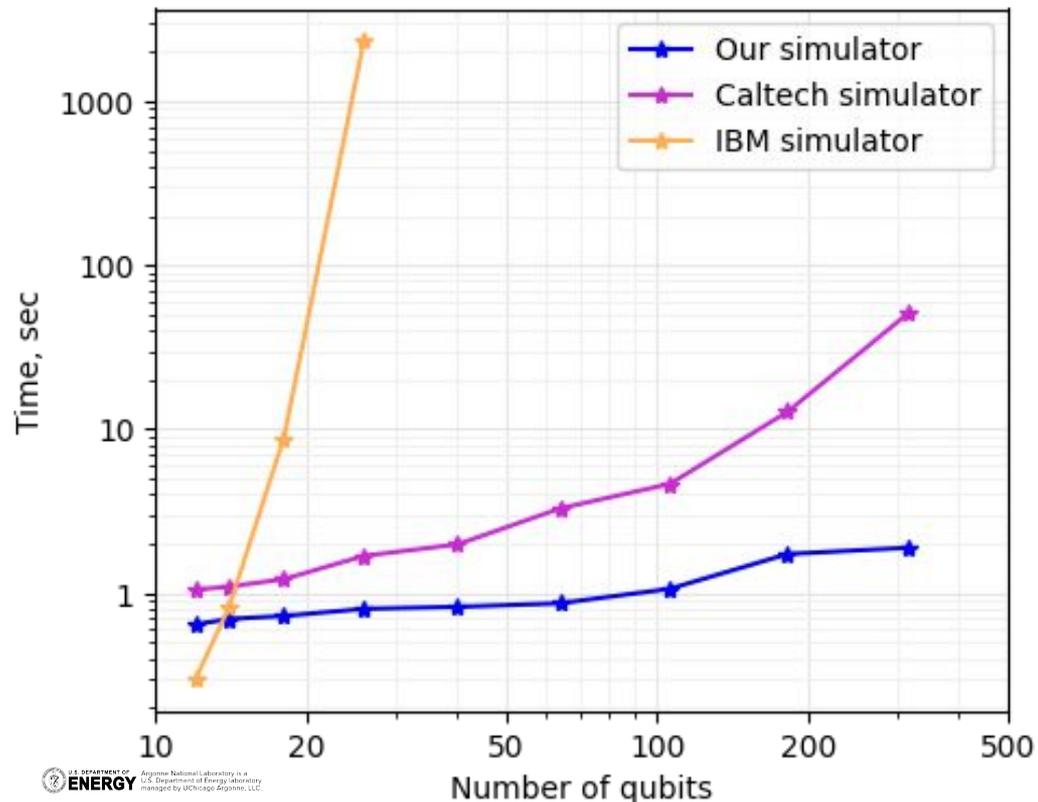


Graph representation of tensor expression of the circuit from previous slide. Every vertex corresponds to a tensor index of a quantum gate

The simulator contracts tensors in the optimal order

# QTensor: Energy Calculations

*Time for a quantum circuit simulation*



The problem to solve is  
MaxCut with QAOA for  $p=3$   
and  $d=3$  on one Intel Xeon  
CPU

# QTensor: Energy Calculations

	$d = 3$	$d = 4$	$d = 5$
$p = 1$	1.0	1.4	2.15
$p = 2$	1.71	4.01	7.44
$p = 3$	4	14.2	
$p = 4$	9.7		

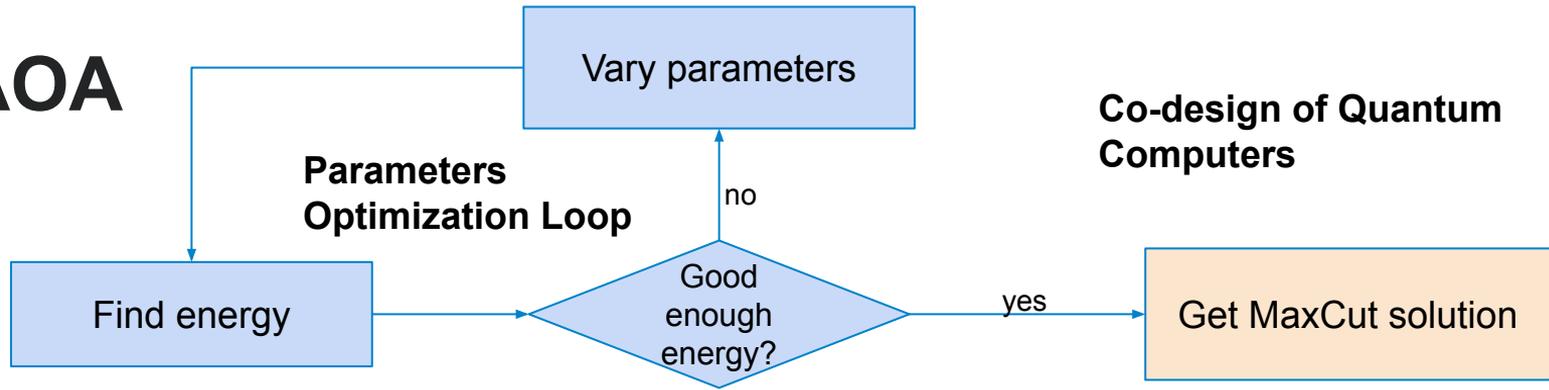
Table 1: QAOA Energy simulation time in seconds for 1000 node regular graphs. All calculations were done using QTensor simulator using NumPy backend on a single Intel Xeon Platinum 8180M CPU @ 2.50GHz with 56 physical cores.

# Parallel Simulations



We calculated the QAOA expectation value for a 1,000,000 qubit circuit with depth  $p=6$  in 1 hour and 20 minutes. The simulations were performed on the Theta supercomputer with 512 nodes.

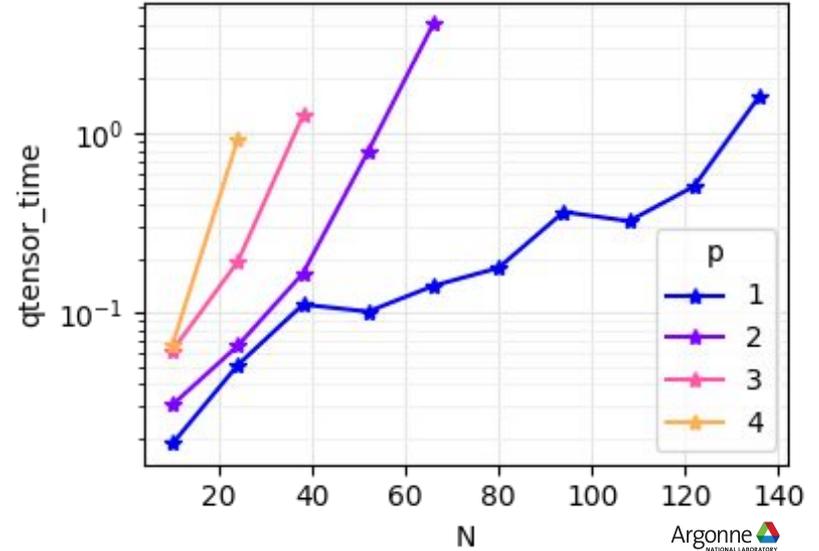
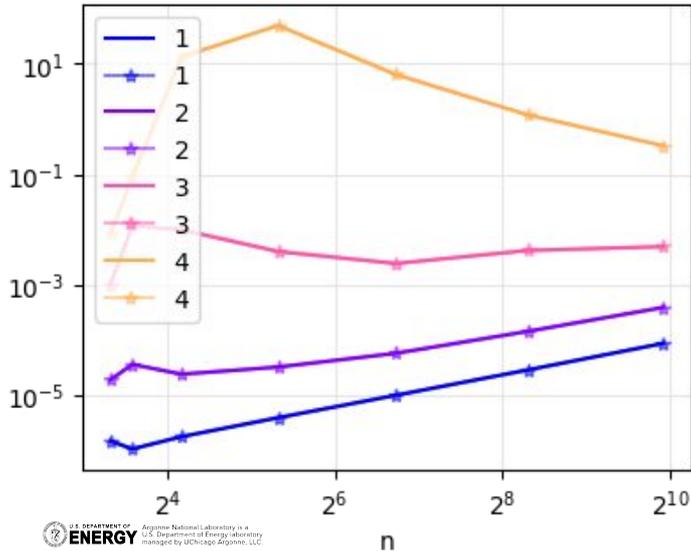
# QAOA



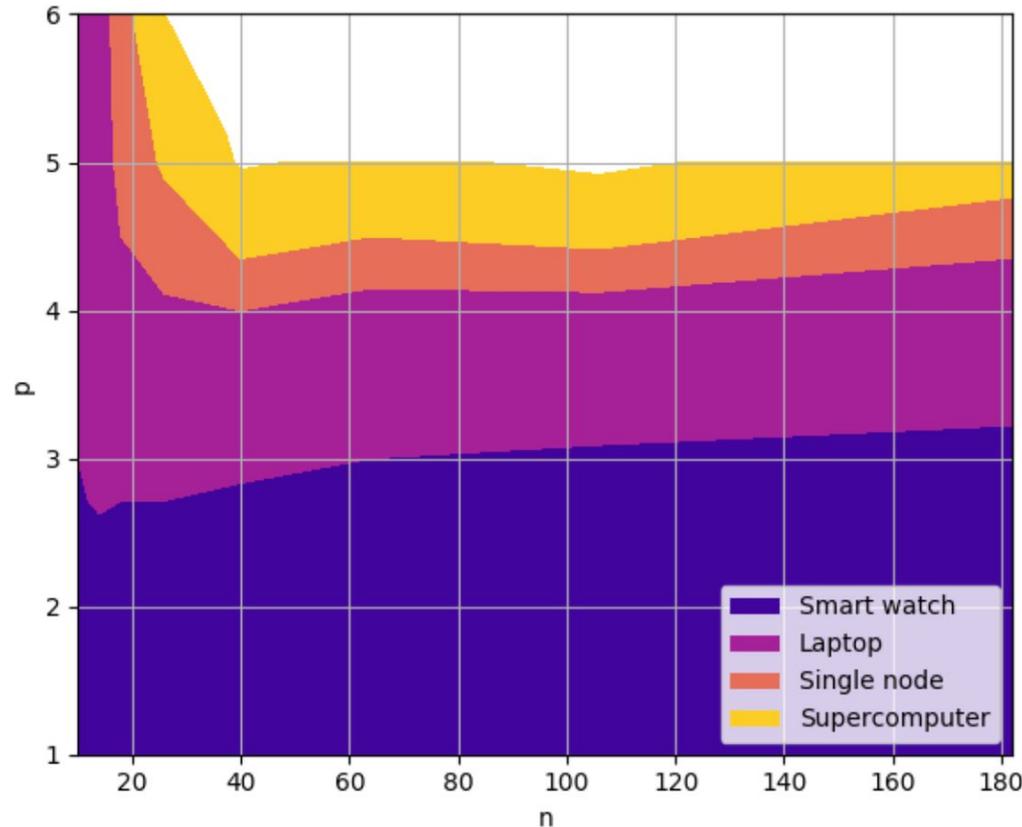
- Easy on classical

- Easy on quantum

Time estimate, seconds



# QTensor: energy expectation for QAOA



Testing limits of classical computing: the complexity of simulation quantum circuits classically as a function of  $n$  and  $p$  ( $n$ =number of qubits,  $p$ =depth of circuit)

This picture shows that for given  $p$  the runtime scales linearly with number of qubits. This is a promising result for demonstration of quantum advantage

# Quantum Simulator Use Cases: Simulation of Supremacy Circuits

Article | Published: 23 October 2019

## Quantum supremacy using a programmable superconducting processor

Frank Arute, Kunal Arya, [...] John M. Martinis 

*Nature* **574**, 505–510(2019) | [Cite this article](#)

**799k** Accesses | **693** Citations | **6025** Altmetric | [Metrics](#)

(CNN Business): Google claims it has designed a machine that needs only 200 seconds to solve a problem that would take the world's fastest supercomputer 10,000 years to figure out.

# Quantum Simulator Use Cases: Simulation of Supremacy Circuits

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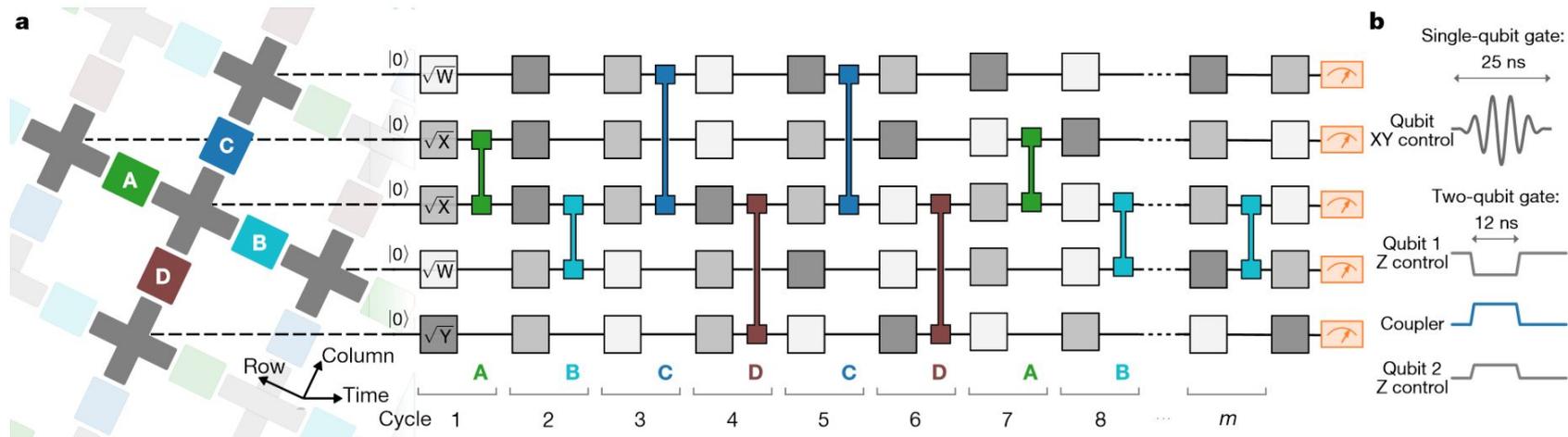
Quantum Computing

## On “Quantum Supremacy”

October 21, 2019 | Written by: Edwin Pednault, John Gunnels  
& Dmitri Maslov, and Jay Gambetta

“We argue that an ideal simulation of the same task can be performed on a classical system in 2.5 days and with far greater fidelity.”

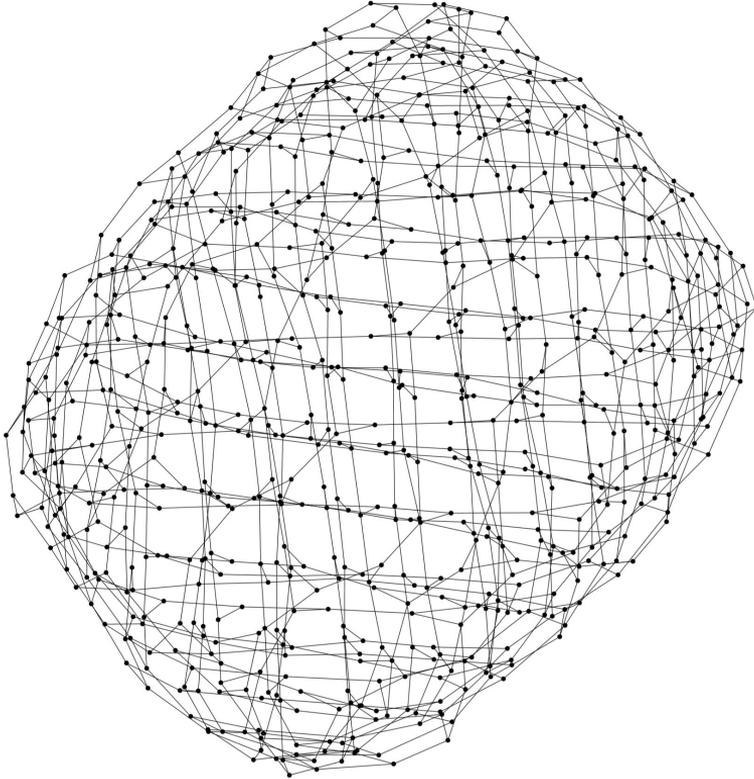
# Quantum Simulator Use Cases: Simulation of Supremacy Circuits



**Fig. 3 | Control operations for the quantum supremacy circuits. a**, Example quantum circuit instance used in our experiment. Every cycle includes a layer each of single- and two-qubit gates. The single-qubit gates are chosen randomly from  $\{\sqrt{X}, \sqrt{Y}, \sqrt{W}\}$ , where  $W = (X + Y)/\sqrt{2}$  and gates do not repeat sequentially. The sequence of two-qubit gates is chosen according to a tiling pattern, coupling each qubit sequentially to its four nearest-neighbour qubits. The

couplers are divided into four subsets (ABCD), each of which is executed simultaneously across the entire array corresponding to shaded colours. Here we show an intractable sequence (repeat ABCDCDAB); we also use different coupler subsets along with a simplifiable sequence (repeat EFGHEFGH, not shown) that can be simulated on a classical computer. **b**, Waveform of control signals for single- and two-qubit gates.

# Quantum Simulator Use Cases: Simulation of Supremacy Circuits



We estimated that the time to simulate with QTensor a million amplitudes of the Sycamore circuit could be brought down to minutes by using the Summit supercomputer

# Publications

1. Submitted to ACM Transactions for Quantum Computing  
**Tensor Network Quantum Simulator With Step-Dependent Parallelization**

DANYLO LYKOV, Argonne National Laboratory, USA

ROMAN SCHUTSKI, Rice University, USA

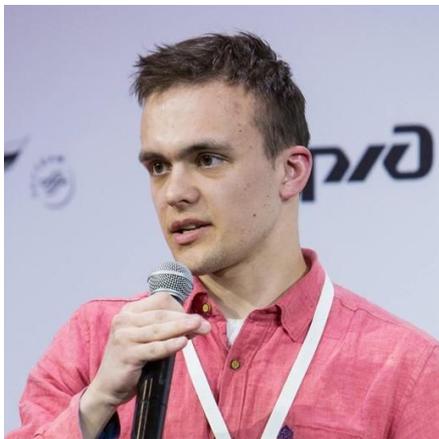
ALEXEY GALDA, University of Chicago Argonne National Laboratory, USA

VALERII VINOKUR, Argonne National Laboratory, USA

YURI ALEXEEV, Argonne National Laboratory, USA

2. In preparation the paper “QTensor: the fastest QAOA energy simulator” for NPJ Quantum Information
3. In preparation the paper for the 2nd International Workshop on Quantum Computing: Circuits Systems Automation and Applications (QC-CSAA)

# Quantum Simulator Team



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# Acknowledgements

<https://github.com/danlkv/QTensor>

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