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Scalable Quantum Computer Simulation on HPC Systems

Scalable Computing Systems and Applications in AI, Big Data and HPC

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Outline

1 Recap

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Why to Simulating Quantum Computing?

- Real Quantum Machines (QMs) are expensive for now
- Test different architectures QM architectures and experiment
- Develop algorithms for machines, which do not exist yet

Schrödinger's method or Linear-algebraic way

- Most utilized and common - Schrödinger's method
- Quantum states are vectors
- Unitary operations are matrices
- Mixed states can be represented as density matrices (positive, semi-definite, trace = 1)
- $O(2^n)$ complexity

[1] Young, Scese, and Ebnenasir, "Simulating Quantum Computations on Classical Machines: A Survey"

Quantum Volume (QV)

- Quantum Computer benchmark metric
- Defined by the largest well performing squeare circuit [1]
- E.g. 4x4 circuit, QV = 16 (2^4)

[1] Cross et al., “Validating quantum computers using randomized model circuits”

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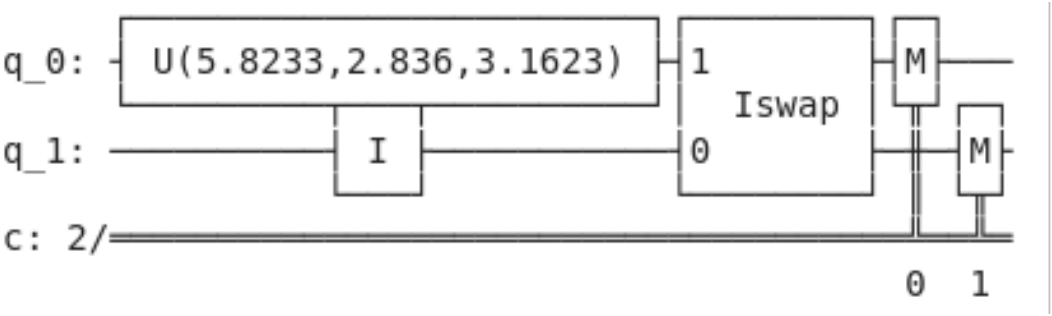
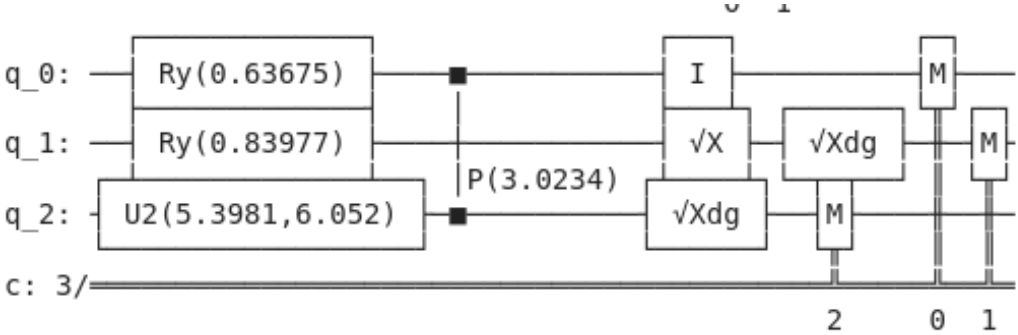
Quantum Computers - Quantum Volume

- QC with 20 qubits
- Start with 2 qubit circuit with depth 2
- Increase both number of qubits and depth until failure

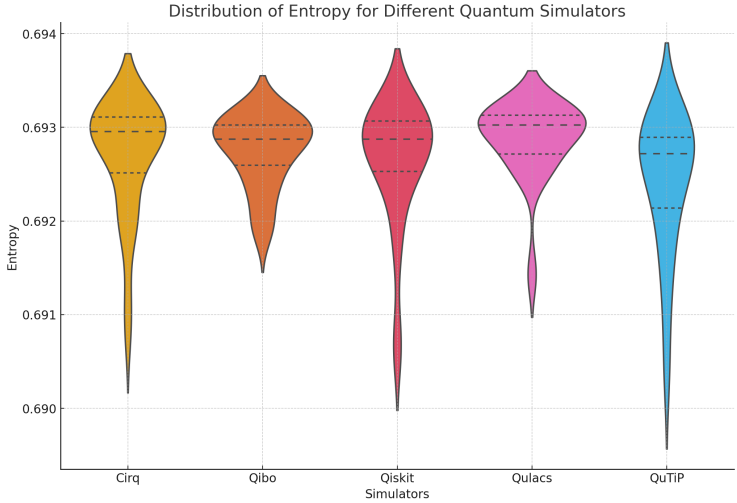
Square Circuits



Square Circuits



Why not on Simulators?



How to Benchmark a Simulator

- Is it as fast as a QC?
- Wall clock measurement for the same task
- Memory consumption for the same task
- Scalability

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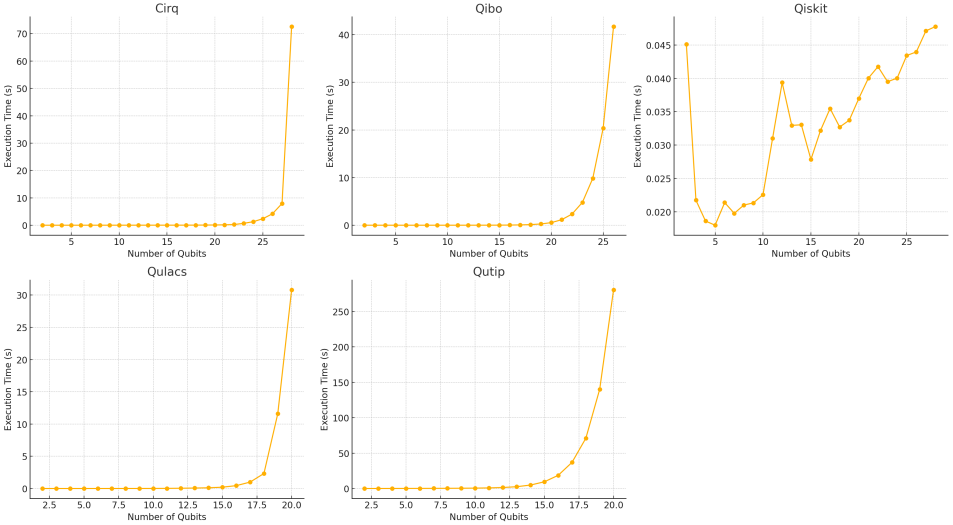
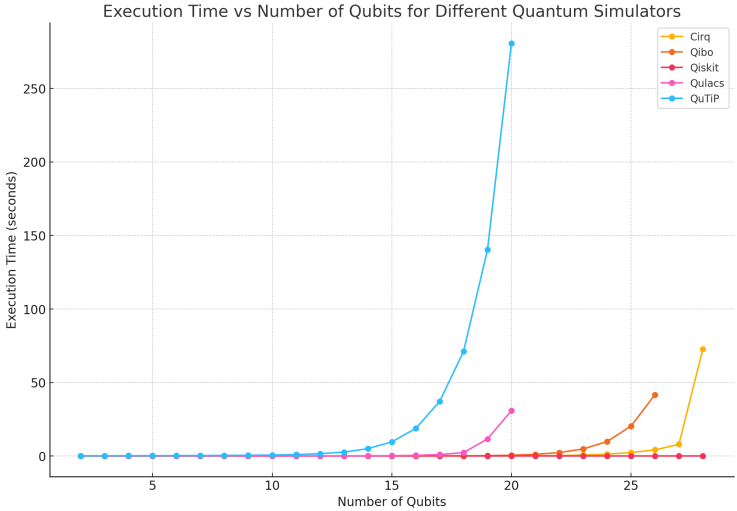
Wall Clock


Cirq
Execution Time (s)
Number of Qubits
Qibo
Execution Time (s)
Number of Qubits
Qiskit
Execution Time (s)
Number of Qubits
Qulacs
Execution Time (s)
Number of Qubits
Qutip
Execution Time (s)
Number of Qubits

Wall Clock

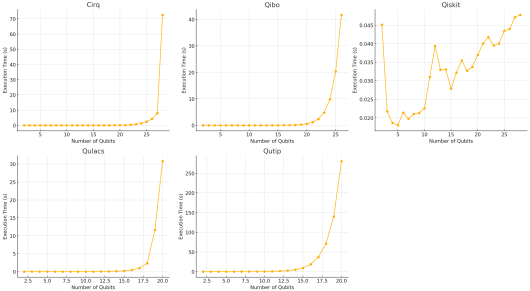

Execution Time vs Number of Qubits for Different Quantum Simulators
Cirq
Qibo
Qiskit
Qulacs
QuTiP
Execution Time (seconds)
Number of Qubits
0
50
100
150
200
250
5
10
15
20
25

Hardware

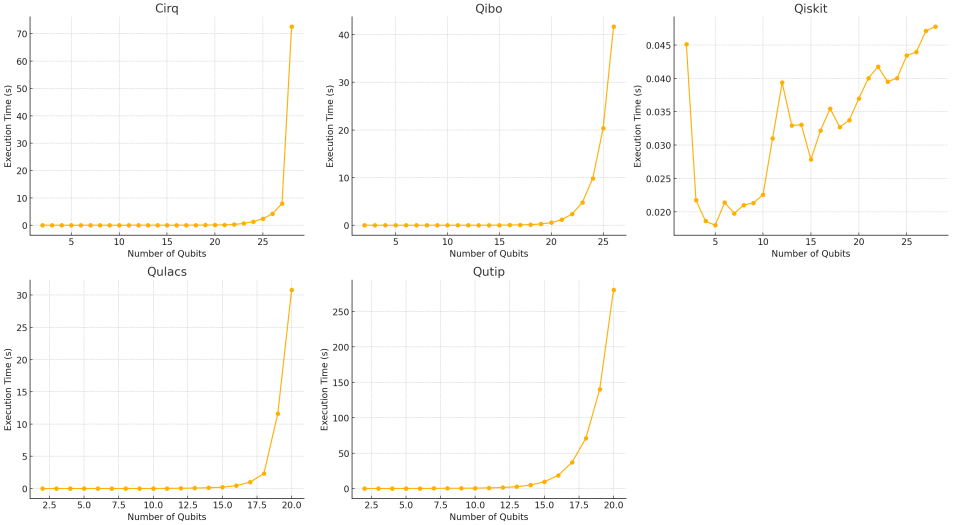
- AMD Ryzen 3 4300U
  - Cores/Threads: 4/4, 1 socket
  - Frequency: 1.4 - 2.7 GHz, boost enabled
  - Cache: L1: 256 KiB, L2: 2 MiB, L3: 4 MiB
- No Cluster yet
- No MPI yet

Insights

- Qiskit has limit of max qubits 28
- Qibo run out of memory starting from 27 qubits
- Qulacs has the best memory performance:
  - Uses 100% CPU - memory under-usage might be a symptom of CPU bottleneck
- In most cases, execution time doubles with +1 qubit - $O(2^n)$



Classical Computer Noise



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Plan

- Run MPI version on the cluster
- Benchmark parallelization
- Add more simulators
- Add more benchmarks (important)

References I

Cross, Andrew W. et al. “Validating quantum computers using randomized model circuits”. In: *Physical Review A* 100.3 (Sept. 2019). ISSN: 2469-9934. DOI: 10.1103/physreva.100.032328. URL: http://dx.doi.org/10.1103/PhysRevA.100.032328.

Young, Kieran, Marcus Scese, and Ali Ebnenasir. “Simulating Quantum Computations on Classical Machines: A Survey”. In: (2023). arXiv: 2311.16505 [quant-ph].