

A Performance Model for Estimating the Cost of Scaling to Practical Quantum Advantage

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Economical and physical limits to Moore's scaling



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Signs of slowdown in Moore's scaling:

- cost per transistor flattening off?
- cost per fab going up?

. . .

 diminishing returns in process size improvements?

Opportunities for new approaches to computing



Improved energy efficiency through hardware specialization



New paradigms for computing

Why quantum computing for HPC?







What is **not** on the pie chart? Enabling the previously inconceivable with quantum technologies?

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When quantum computing for HPC?



How much will quantum computation cost?





Precisely worked out examples include:

•The main enzyme responsible for drug metabolism, cytochrome P450 (CYP), has unknown mechanisms of promoting oxidation, and simulating it will require 7.8 billion operations in 1434 logical qubits [Goings, Joshua J., et al. "Reliably assessing the electronic structure of cytochrome P450 on today's classical computers and tomorrow's quantum computers"]. In order to perform this many operations, each logical qubit will need to contain approximately 9745 physical qubits. This totals 109 billion gubit-seconds. (\$5.45B)

•The mechanism for biological fixation of nitrogen is a coveted chemical process that could significantly reduce the price and energy consumption of production of fertilizers, and it is based on the FeMo cofactor in a yet-not-understood process. This process can be simulated in a quantum computer with 2196 logical qubits in 32 billion operations [Lee, Joonho, et al. "Even more efficient quantum computations of chemistry through tensor hypercontraction".] This totals 448 billion qubitseconds. (\$22.4B)

•In order to factor a 2048 bit product of two primes, a quantum computer will require approximately 25 billion operations in 14238 logical qubits [Gidney, Craig, and Martin Ekerå. <u>"How to factor 2048 bit RSA integers in 8 hours using 20 million</u> noisy qubits."]. **This totals 432 billion qubit-seconds**. (\$21.6B)

\$5B-\$20B

All of these are **very** hard, very large problems!

How much would it cost to run the **first** scientifically relevant, classically-intractable calculation?

R. Stevens: A View of Post-Exascale Computational Science and the Emerging Mix of HPC, AI, and Quantum

Flowchart for quantum computing cost estimation



Two-dimensional Hubbard model

1 Quantum Problem

- Quantum physics model of interacting electrons on a square lattice with L² sites
- Complex phenomena such as metal-insulator transitions and superconductivity
- Applications in 2D materials
- Good approximate classical algorithms exist based on tensor networks and quantum monte carlo
 - They break down in certain difficult regimes that are of most interest
- General solution is classically hard and scales exponentially





Source: Geim, Nature (499) 419-425

Classical complexity:

- exact diagonalization memory: $\mathcal{O}(4^{L^2})$
- Quantum Monte Carlo: 13h on 3,456 CPUs (Fugaku) in "easy regime" for 8 x 8 lattice

Charlebois, Imada, PRX (2020)

Logical Quantum Resources for L² Hubbard Model

- Quantum phase estimation for computing ground state energy in "hard regime"
- $O(L^2)$ scaling of quantum algorithm \rightarrow exponential advantage over $O(4^{L^2})$ classical scaling
- Fixed relative error per lattice site leads to constant logical operations
- Perfect weak scaling

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Logical gates





Physical Resources for the Hubbard Model



Flowchart for quantum computing cost estimation



What does this cost?

Public Pricing data from Quantum Cloud Providers:

Technology	N _Q	Usage cost [\$/qs]
Superconducting	8-80	0.05
Ion Traps	~20	10
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Conclusions

- Developed new performance model to estimate cost of quantum computation
- Our resource and cost analysis projects that intractable quantum computation could be realized at \$1M not \$1B!
- Many caveats and uncertainties remain:
 - does pricing model scale linearly?
 - will future QC architectures be modular?
 - improvements in QEC and algorithms?



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