Amsterdam University of Applied Sciences

HBO-ICT SOFTWARE ENGINEERING

Solving Hard Scientific Problems Using Quantum Computers

Progress Presentation

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Quantum Computation and Information

Quantum computers take advantage of quantum mechanical effects such as superposition and interference to solve certain problems faster than classical computers.

Quantum Computation and Information: Qubits

- Unlike a classical bit, a qubit can be in superposition of 0 and 1.
- In a superposition, each state has an amplitude, which can be a negative or positive complex number.
- When we measure a qubit, it collapses to 0 or 1 randomly.
- The amount of amplitudes grow exponentially with the number of qubits: a n-qubit system requires 2^n amplitudes to describe the system.

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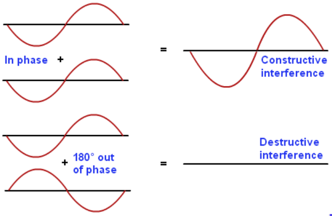
Quantum Computation and Information: Interference

“The goal in quantum computing is to choreograph a computation so that the amplitudes leading to wrong answers cancel each other out, while the amplitudes leading to right answers reinforce.” - Aaronson [1]



Quantum Computation and Information: Entanglement

Particles can interact and produce entangled states which show correlations in measurement outcomes.

Example: Bob and Alice share two entangled electrons with opposite spins. When Bob measures his electron to be spin up, Alice's electron must be spin down and vice versa.

Quantum Computational Complexity

- We describe running time of an algorithm as a function of the size of the input [4].
- We usually concentrate on the worst-case running time of an algorithm.
- Problems in class P: polynomial-time algorithms (“easy” problems) grow by some constant k given input size n: $O(n^k)$.
- Porblems in class NP: superpolynomial-time algorithms (“hard problems”), grow faster than $O(n^k)$, for example $O(2^n)$ or $O(n!)$.

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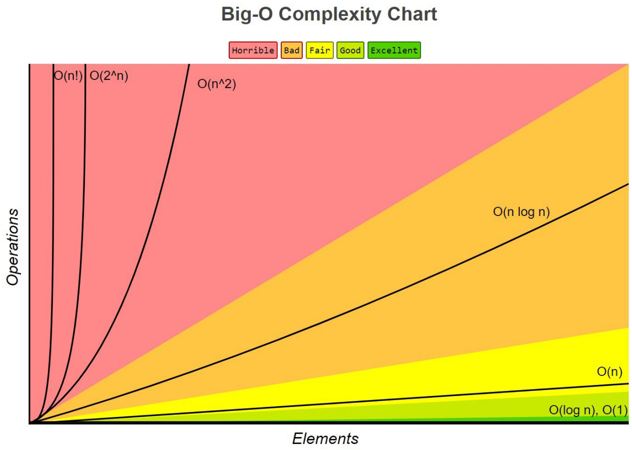
Quantum Computational Complexity



Quantum Computational Complexity

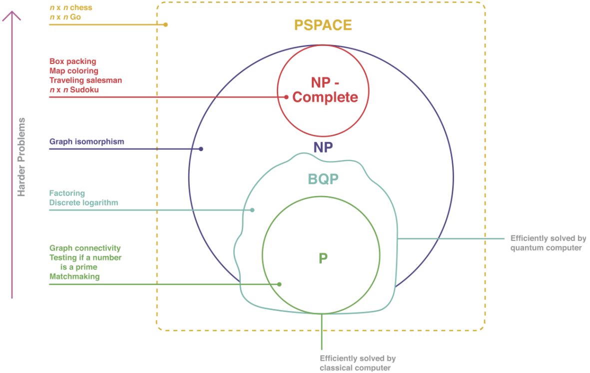


Figure: A diagram illustrating the hierarchy of several important complexity classes. Image by MIT OpenCourseWare.

Quantum Computational Complexity

Algorithm	Quantum Speedup	Technique
Factoring	Superpolynomial	[11]
Quantum Simulation	Superpolynomial	[12, 7, 3]
Searching	Polynomial	[6]
Constraint Satisfaction	Polynomial	[2]

Quantum Computing for Scientific Problems: Quantum Chemistry

Problem: find the minimum energy state of a molecule

- Since the founding of the field of quantum mechanics, we have been able to describe the state of a quantum-mechanical system by solving the Schrödinger equation [5].
- Applications in chemistry, biology, drug discovery, and materials science [8].

Quantum Computing for Scientific Problems: Quantum Chemistry

Problem: find the minimum energy state of a molecule

- Unfit for classical computers: quantum system grows exponentially with the number of particles - requires an exponential amount of classical bits to represent the quantum system.
- Quantum state's amplitudes grows exponentially with the amount of qubits — requires a linear amount of qubits to represent the quantum system.

Quantum Computing for Scientific Problems: Quantum Chemistry

Problem: find the minimum energy state of a molecule
Quantum algorithms for finding the minimum energy state of a molecule:

- Quantum Phase Estimation (QPE) algorithm — requires fault-tolerant quantum computer [9].
- Variational Quantum Eigensolver (VQE) — candidate for near-term quantum devices using iterative classical optimization [10].

Other Possible Scientific Applications for Quantum Computers

- Machine learning
- Cryptography
- Biology (genome sequencing)

[1] Scott Aaronson. “Quantum Computing Promises New Insights, Not Just Supermachines”. In: *Quantum Computing since Democritus*. Cambridge University Press, 2011. Chap. Quantum, pp. 109–131. ISBN: 9780511979309. DOI: 10.1017/cbo9780511979309.010.

[2] Andris Ambainis. “Quantum search algorithms”. In: (2005). arXiv: quant-ph/0504012.

[3] A. Aspuru-Guzik. “Simulated Quantum Computation of Molecular Energies”. In: *Science* 309.5741 (2005-09), pp. 1704–1707. ISSN: 0036-8075, 1095-9203. DOI: 10.1126/science.1113479.

[4] Thomas H Cormen et al. *Introduction to algorithms*. MIT press, 2009.

[5] David J. Griffiths and Darrell F. Schroeter. *Introduction to Quantum Mechanics*. Cambridge University Press, 2018-08. ISBN: 9781316995433, 9781107189638. DOI: 10.1017/9781316995433.

[6] Lov K Grover. "A fast quantum mechanical algorithm for database search". In: *Proceedings of the twenty-eighth annual ACM symposium on Theory of computing*. 1996, pp. 212–219.

[7] Seth Lloyd. "Universal quantum simulators". In: *Science* (1996), pp. 1073–1078.

[8] Sam McArdle et al. *Quantum computational chemistry*. 2018. arXiv: 1808.10402 [quant-ph].

[9] Michael A. Nielsen and Isaac L. Chuang. *Quantum Computation and Quantum Information. 10th Anniversary Edition*. 10th. New York, NY, USA: Cambridge University Press, 2009. ISBN: 9780511976667. DOI: 10.1017/cbo9780511976667.

[10] Alberto Peruzzo et al. "A variational eigenvalue solver on a photonic quantum processor". In: *Nat Commun* 5.1 (2014-07), p. 4213. ISSN: 2041-1723. DOI: 10.1038/ncomms5213.

[11] Peter W. Shor. "Polynomial-Time Algorithms for Prime Factorization and Discrete Logarithms on a Quantum Computer". In: *SIAM Rev.* 41.2 (1999-01), pp. 303–332. ISSN: 0036-1445, 1095-7200. DOI: 10.1137/s0036144598347011.

[12] Christof Zalka. "Efficient simulation of quantum systems by quantum computers". In: *Fortschritte der Physik: Progress of Physics* 46.6-8 (1998), pp. 877–879.