

Quantum Computers

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The topic of quantum computers has created quite a buzz in recent years. In 1998, Isaac Chuang, Neil Gershenfeld, and Mark Kubinec had constructed the first-ever quantum computer. Upon creation, the computer had been operating on just two quantum bits (qubits). In 2007, Canadian startup D-Wave created the 28-qubit computer, paving the way for the industry's present computing power. Nowadays, scientists can build up to 1,121-qubit computers.

It is a common misconception that quantum computers are just a better version of basic computers when, in reality, they are something completely different. Rather than bits, a quantum computer operates on qubits, which can exist in two states: a low-energy wave and a high-energy wave. When a quantum computer operates, these states interact and create constructive or destructive waves, which help solve complex problems like optimization. While a basic computer must try all possible options to find solutions, a quantum computer analyzes waves to find the most likely answer. Due to this efficiency increase, quantum computers are highly adept in finding structure within tons of data. For example, a quantum computer with around 1 million qubits could potentially hack into RSA Encryption, which secures most online financial transactions. This would involve using Shor's algorithm to efficiently find the prime factors of large numbers. While a powerful quantum computer could theoretically decrypt secure data in a matter of hours, the same task would take billions of years for a normal computer. Fortunately, this level of quantum computing decryption has not yet been developed, but experts at Google predict it could be done by 2030.

Another example of analyzing vast amounts of data using quantum computers is the simulation of nature. Fundamentally, life obeys quantum physics on a molecular level, so quantum computers can be easily applied. These new machines will allow scientists to simulate molecules and their different combinations to understand materials' properties and interactions. In this respect, quantum computers will make the process of creating new materials much more efficient, as scientists will not need to experiment with different molecules and observe the results; rather, they can quickly browse all possible combinations and ascertain their properties. Although scientists have developed techniques such as Monte Carlo Simulation and Density Functional Theory to develop new materials,

the molecular behavior models rely on approximations made by classical computers that often lose accuracy in real-world experiments. Quantum computers, by simulating molecular interactions with much greater precision, can overcome this issue and accelerate the development of new materials.

To simulate molecules, we typically need one qubit per electron orbital. However, due to limitations in qubit quality, practical simulations often necessitate more qubits than the number of orbitals. For instance, to simulate hydrogen with only one electron orbital, scientists would need around 56 qubits, as simulated by Google in 2016. Similarly, lithium hydride (LiH) and beryllium hydride (BeH₂) were both simulated in 2017 by IBM, followed by a simulation of water (H₂O) that was done in 2019 by IONQ.

Quantum computers will be able to solve many daily issues. Take fertilizer production, for example. Currently, fertilizer is produced using an energy-consuming method called the Haber-Bosch process, taking out nitrogen from the air. Unfortunately, this results in a huge amount of carbon dioxide emissions. Likewise, Ferredoxin, a catalyst used by bacteria, performs the same extraction of nitrogen from the air more efficiently and with less energy, though the process still produces a similar level of carbon dioxide. To solve this problem, quantum computers with around 200,000 qubits could be used to model a potential solution for an eco-friendlier way to fixate nitrogen, even though the quantum mechanics of these chemical reactions are not yet fully understood.

Innovations in quantum computing also affect progress in the medical field. Currently, to develop a new pharmacy product, scientists need an in-depth understanding of the interaction between the drug's molecules and biological molecules. However, getting to that point of understanding can be both time and money-consuming. Traditional computers have helped a lot with simulations and calculations, but some of the quantum interactions remain too complex. Quantum computers allow us to simulate systems directly and efficiently, providing more data and insights for drug design. Researchers from Imperial College London, Zhejiang Lab, and the University of Science and Technology of China successfully developed a Gaussian Boson Sampling (GBS), a special-purpose model of photonic quantum computation. They also applied quantum computing to two crucial drug design methods: Molecular Docking and RNA Folding Prediction. Dr. Raj Patel from Imperial College London, said, "Quantum computing can simulate interactions between molecules more

authentically, enabling us to predict the activity and safety of drug molecules more precisely during the drug design stage. This technology can also accelerate high-throughput screening of drugs, handle previously elusive complex biological systems, such as protein complexes, and promote cross-collaboration between physics, computational science, biology, and pharmacology.” (Patel, 2023) All of these innovations and developments testify to a bright future with a number of considerable breakthroughs in the area of medical treatment.

Lastly, quantum computers can also be used for military technologies. Quantum computers have the ability to provide secure communication without eavesdropping and information leakage. They can also identify patterns and forecast future events by analyzing existing data, making the military strategizing process more effective. Unfortunately, quantum computers can also easily help create new, more potent weapons, if they fall into the wrong hands. Therefore, it is crucial for decision-makers to understand the potential risks of using quantum computing in the military. Future studies might entail establishing standards for the ethical application of quantum computing.

To summarize, the main goal of developing quantum computers is to learn about ourselves and the world around us. This will lead to a myriad of new innovations in all spheres, whether in chemistry, ecology, healthcare, or the military. However, it is essential to always remember the dangers and restrict any inhumane use of these powerful quantum computers.

Bibliography:

World Economic Forum (2019) 'Quantum leap: why the next wave of computers will change the world', available from:

<https://www.weforum.org/agenda/2019/10/quantum-computers-next-frontier-classical-google-ibm-nasa-supremacy/#:~:text=In%201997%2C%20the%20first%20tiny,qubit%20quantum%20computer%20in%202007>

Holton W. (2024) 'quantum computer', available from:

<https://www.britannica.com/technology/quantum-computer#:~:text=In%201998%20Isaac%20Chuang%20of,data%20and%20output%20a%20solution>

Pasternack A. (2024) 'IBM built the biggest, coolest quantum computer. Now comes the hard part', available from:

<https://www.fastcompany.com/90992708/ibm-quantum-system-two#:~:text=That%20quest%20culminated%20last%20month,chip%20yet%2C%20with%201%2C121%20qubits>

Lichfield G. (2020) 'Inside the race to build the best quantum computer on Earth', available from:

Yu S. (2023) 'Towards using quantum computing to speed up drug development', available from:
<https://www.imperial.ac.uk/news/248638/towards-using-quantum-computing-speed-drug/#:~:text=transformations%20and%20advancements.-,Quantum%20computing%20can%20simulate%20interactions%20between%20molecules%20more%20authentically%2C%20enabling,during%20the%20drug%20design%20stage>

Quantum Flagship (2024) 'Fertilizer and other quantum computer chemistry', available from:

<https://qt.eu/applications/fertilizer-and-other-quantum-computer-chemistry>

Ghamari P. (2023) 'Quantum Computing and the Future of Military Technology', available from:

<https://www.linkedin.com/pulse/title-quantum-computing-future-military-technology-pooyan-ghamari#:~:text=Another%20potential%20use%20for%20quantum,to%20cutting%20edge%20drone%20technology>

Cleo Abram (2023) 'Quantum computers, explained with MKBHD', available from:

<https://youtu.be/e3fz3dghN44?si=PMBouUep3YQ8TxLY>

Domain of Science (2020) 'Quantum Simulation Explained in 9 Slides', available from:

<https://youtu.be/kD370qyxTyw?si=3Ebe55mCWaREQL5a>