

Mini Review

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Quantum Computing will Revolutionize Chemical Analysis, Drug Discovery and New Material Design



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The latest Intel microprocessor, the Intel Core™ i9-9900K, has over 1.7 billion transistors. Misplacement of a single transistor could cause an error in a calculation and even good engineers make design errors from time to time. Building a new revision of a chip, testing, finding errors, fixing the errors, creating new masks, and building another chip can take months. And if there is any appreciable number of errors in the design, it would take centuries to make it error free. So, one of the tools that engineers rely to complete the design in a reasonable period of time is through computer simulation. By carrying out a computer simulation of a new design instead of building a revision and testing it, engineers can find and fix errors in a matter of minutes rather than months. And this can make such a large, complex design possible. Unfortunately, chemical, pharmaceutical, and material scientists are not currently able to do it like this. Because of the quantum mechanical interaction between elements in a molecule, the number of calculations that would be required to simulate even small molecules grows exponentially and the computation quickly become intractable. For example, in order to model the structure of penicillin would require a computer that contains something like 10^{86} classical bits, more than the number of atoms in the observable universe. Clearly, this is intractable. So, today's chemical researchers utilize computational chemistry programs which can only provide rough approximations and then they supplement them with a heavy dose of trial-and-error testing to see if it really works.

In developing a new drug, researchers may start with as many as 10,000 candidates and through a long and expensive process of laboratory, animal, and final human testing they may eventually get to the one or more that works. And the developing the new

drug can cost over \$1 billion and take over 10 years. So clearly there is a huge payoff if someone can find a better way. The road to this better way was first proposed by physicist Richard Feynman in the early 1980's who said "Nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy." His suggestion was to create a quantum computer that would leverage the principles of quantum mechanics to perform calculations in a new way. This leads to the possibility of simulating chemical interactions in a reasonable period of time and do for chemical and material design what Intel has been doing with microprocessors. In quantum computing there are two quantum mechanical phenomena discovered in the 1930's that can be leveraged to potentially create quantum computers with exponentially greater processing capabilities than classical computers. In a classical computer, the basic computational element is called a bit which can either be in the 0 or 1 state at any one time. Quantum computers are based upon computational elements called qubits which can be in the 0 state, 1 state, or a mixture of 0 and 1 at the same time. This ability to be in a mixture state is called superposition. The other key quantum mechanical phenomena is called entanglement. This is a strange phenomenon that Albert Einstein called "Spooky action at a distance" in which two qubits are linked so that if one of the qubit changes its state, the other will also change its state instantaneously. This can happen even if the two qubits are physically separated by many miles.

Over the past twenty years, scientists have started to develop computational devices that leverage these two properties to implement small quantum computers. And just as important computer scientists have started to discover algorithms that can

provide exponential speedups over classical computers that may provide the way for implementing some of chemical modelling that was previously intractable on a classical computer. The past five years have seen rapid development of such computers with major companies including IBM, Microsoft, Google, Intel and many small startup companies creating prototype systems. The state-of-the-art today includes quantum computers with 53 qubits in size available from both IBM and Google with an expected doubling in the number of qubits every one to two years. Scientists are estimating that the penicillin molecule that would have required 10^{86} classical bits could be simulated with a quantum computer that have 286 qubits. If the current pace of development holds, quantum computers of that size should be available later this decade. Within the past few years, a few algorithms and software libraries have been developed that use a capability called hybrid classical/quantum computing. This approach develops algorithms that utilize both classical and quantum computers to work together to solve a particular problem. Two algorithms that have been published that utilize this approach include the Variational Quantum Eigen solver (VQE) and also the Quantum Approximate Optimization Algorithm (QAOA). These algorithms have been designed to take advantage of the Noisy Intermediate Scale Quantum (NISQ) computers that will be available in the near term.

The implications for material science will be enormous. The ability to simulate a chemical reaction instead of discovering new compounds through trial and error and save billions of dollars as well as dramatically shortening the time to discovery. Not only

will quantum computer be used to help discover new materials, it may also be used on the manufacturing side to figure out ways of optimizing chemical processes to improve yields and minimizing the generation of undesirable manufacturing byproducts. The impact of quantum computing will be felt in a variety of industries. In the pharmaceutical area it will revolutionize drug discovery, in the automotive areas companies like Daimler is investigating the use of quantum computing to develop new battery chemistry for electric cars, there is even a company that is researching this approach to design better materials for OLED (Organic Light Emission Diode) screens for improved flat panel TVs. There is a lot of research on using this technology to fight climate change. Researchers have studied ways of using quantum computing to model the nitrogen fixation process to produce ammonia and replace the century old and high inefficient Bosch-Haber process which uses over 1% of the world's energy. Another key target is to find an efficient process for carbon sequestration to remove CO_2 from the atmosphere. And potentially, quantum computing modelling can help find new material for solar panels that will improve their efficiency and allow them to produce more electrical for a given amount of sunlight.

It is an exciting time right now for those working in quantum computing. Although it is still at a very early stage and some of the benefits will take several decades before they are realized, there is a lot of potential for it to positively change the world in the future and help solve many of the problems we face today.



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