How quantum computers will be able to save billions of lab animals

Previous decades have witnessed new developments and advancements in medical technologies, healthcare facilities, cures, treatments for various ailments, and the production of newer pharmaceuticals.
It is critical to ensure that treatments and medications do not have any hazardous or severe side effects on the Human Body.
We've made huge strides in terms of experimentation procedures, testing equipment for evasive substances, and virtual testing environments. However, hundreds of millions of animals are still employed in laboratories every year for drug testing, medical training, biological investigations, and even aesthetic testing. For the sake of experimentation, thousands of innocent animals have been killed in these studies. This method is Painful, Costly and Inefficient.

Dogs are one of the common test subjects(source)

Although these methods have proven reliable up to this point, recent research has been not less than a boon in demonstrating that utilising electrical simulations and Chemical Databases, we can simulate chemical reactions that occur inside the body. There exist plenty of databases containing information about properties of different molecules, which can be used for this purpose.
This implies that no physical living subjects are required for the experiment. This may appear to be relatively simple, it is not possible to accomplish on ordinary computers. Even super and cluster computers can't recreate the chemical events that occur inside the human body.

So is there a way to solve this problem?

Well, Quantum Computers have shown an exponential speed over classical computers. According to research, using these devices, it is feasible to replicate chemical reactions with a high degree of precision. The results of these computations will be used to determine which compounds are potentially detrimental or useful to our bodies.
This saves a lot of resources - time, money, and the misery that these poor living beings must endure.

What are we trying to simulate?

Chemical equations, as we all know, are made up of molecules, each of which has its own set of characteristics. These qualities will reveal everything we need to know about our medicine, from its efficacy to potential negative effects.
The ideal software for these simulations would take molecules from the chemical that is injected into the body and tell us the outcome of the reactions inside. These molecules can then be further analyzed as we will see later.

What would be the governing principle for this software?

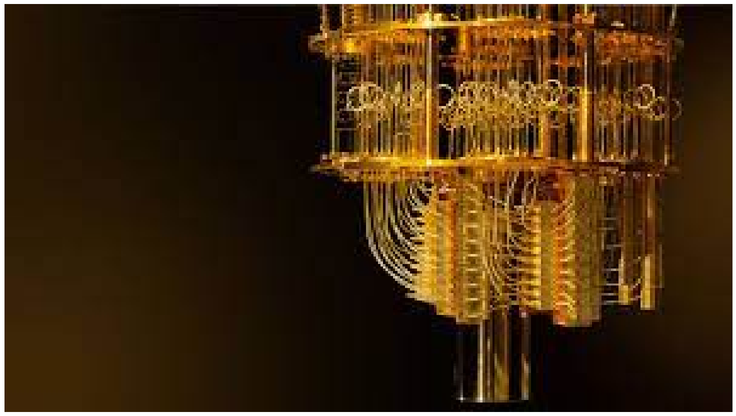
Quantum mechanical equations, such as the *Many-Body Schrodinger Equation*, will be solved at the atomic level, taking into consideration all of the molecules. The numeric values obtained from these computations will be compared with those in the database to see which molecules are produced as time passes. Scientists will examine the outcomes of our computations in order to advance pharmaceuticals that will be able to cure ailments and eliminate potentially dangerous drugs.

Let's take a deeper look into the Quantum mechanics of all this. The *Hamiltonian(H), the Wave Function,* and the *Energy of each State*, all of which evolve over time, make up the Schrodinger equation. The main element that defines our system is the Hamiltonian.
Our main goal is to find the Hamiltonian's eigen equations and eigenvalues. These are, respectively, the Wavefunction and the Energy. This is simple for a few atoms, but as the number of atoms grows, the number of terms inside the Hamiltonian grows exponentially, creating a gigantic mess that is unsolvable by conventional computers.

Here quantum computers come to the rescue !

Why are quantum computers better at simulating chemical equations than classical computers?

Perhaps because chemical equations can be predicted using Quantum Mechanical laws, and Quantum Computers have the word "Quantum" in their name. This answer is amusing yet incorrect, however the correct answer isn't far away.
Qubits, or quantum bits, are the most basic unit of quantum computers, and these qubits follow the laws of quantum mechanics which leads to the exponential speed up. These properties can be used by certain algorithms for modelling molecules. Variational Quantum EigenSolver is one such algorithm.



Quantum Computer(source)

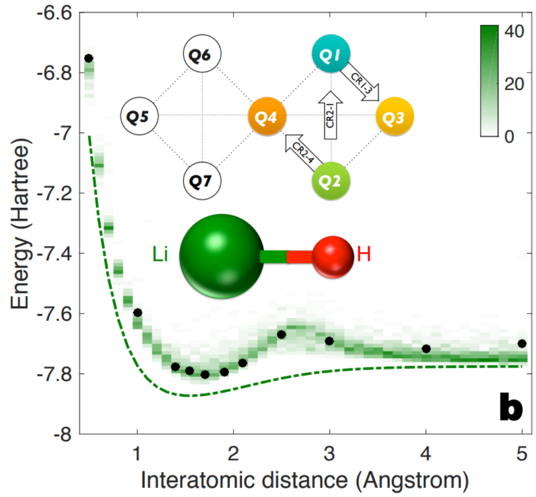
Variational Quantum EigenSolver

The Variational Quantum Eigensolver is one of the most powerful quantum algorithms and is used for determining a molecule's ground state. The fact that it has been able to achieve workable outcomes employing NISQ Devices is the key reason for its fame.

Quantum States are another name for the Wave Functions we discussed earlier. Quantum circuits can be used to represent these states. In VQE, we make a guess at a circuit that will be able to determine a molecule's quantum state; this circuit is called **ansatz**. The ansatz circuit is constructed using some fixed components and a few variable parameters. With each iteration, the parameters are tweaked in order to discover the lowest possible energy for our Quantum State (the most stable), which will reveal a lot about the molecule.

VQE is a fantastic Algorithm that has been used to model real-world molecules like LiH. Researchers were able to find the interatomic distance between lithium and hydrogen. It can run on Noisy Quantum Computers because it incorporates the best aspects of both classical and quantum computing. The ansatz or our guess quantum circuit is the quantum part, the classical part is where we optimize the parameters of our ansatz in order to get the ground state energy.

Despite the fact that we are still a long way from replicating chemical reactions inside human beings, VQE serves as confirmation that we are on the correct road and that quantum computers can really simulate Molecules.



Simulating the interatomic distance between the LiH molecule using VQE([Source]())

For a more depth intro to VQE look at this [research paper]()

Simualtions over Animal testing

One important consideration is that animal testing is fraught with controversy. Scientists reported in the Journal of the American Medical Association that medicines discovered in animals are not scalable to humans with identical conditions. In addition, diseases administered in laboratories are not the same as diseases that occur naturally in individuals.All of this debate makes animal testing even more implausible.

And, while it may seem impossible to completely eliminate animal testing, it is conceivable to supplement it with Quantum Computational Power, which will make the procedure faster, cheaper, and save many lives in the process

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