Quantum computing in the life sciences

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Emerging quantum computing technologies brings to mind thoughts of enhanced cybersecurity, improved financial modeling, artificial intelligence and traffic optimization. The applications of this new super computing technology is also changing the field of life sciences, including in genomics, drug designs and delivery and in overall patient care and dosage regimes.

Specific to the field of life sciences, the benefit of quantum computers is not necessarily in its speed or efficiency to perform a function, but in its ability to tackle computationally complex problems in a way that is far beyond the capabilities of classical computers. Both IBM and D-Wave have published reports outlining several use-cases of quantum computing in the life sciences. IBM suggests that the major challenges in the field include “understanding the relationships among sequence, structure, and function and how biopolymers interact with one another as well as with small organic molecules that are native to the body or designed as drugs”. D-Wave predicts that “the adoption of quantum computing could enable faster and more efficient identification of molecules with promising biochemical and therapeutic properties”.

Both IBM and D-Wave have developed technologies that were put to the test by multinational pharmaceutical company GlaxoSmithKline (GSK). GSK compared IBM’s approach to drug discovery using a method dubbed “gate-based quantum computers” with D-Wave’s method of “quantum annealing” in solving the codon optimization problem. In a nutshell, codon optimization is the process of selecting the combination of codons (where each amino acid in a protein sequence can be represented by as many as six codons), that maximizes the probability of the gene expression.

The solution to this problem in classical computers is limited by the size of the polypeptide chain for example. Although, in the classical setting, the problem could be solved on a small, non-realistic scale, scientist have not yet been able to solve the problem for large-scale, real-life applications in medicine.

The preliminary data of GSK’s comparison showed that the quantum annealing method presented by D-Wave, which offers close to two orders of magnitude more qubits than the gate-based method, is immediately applicable and promises to outperform classical methods at solving realistic optimization problems. However, IBM’s gate-based method comes up short in qubit count and the connections needed between qubits to solve the problem on a realistic biological scale. Although the gate-based method is not immediately applicable, it continues to show promise as developments in quantum computers are expected to present improvements in qubit count and connectivity.

Alongside GSK, smaller start-up pharmaceutical companies are also making use of the available quantum computing technologies in their drug discoveries. Menten.AI, a drug discovery company whose mandate is to create new drugs for indications with high unmet medical need, created the first protein design algorithm for quantum computers. In partnership with D-Wave, Menten.AI also created the world's first protein designed by a quantum computer. Most recently, the drug discovery company worked on several new peptides that can form proteins to be used in stopping the infection process of the SARS-CoV-2 spike glycoprotein (that is, peptides that can be used to prevent the spike protein from moving from a closed position to an open position where it can infect healthy cells). Menten.AI's development in the space has opened the door to the creation of new peptides that include not only natural amino acids, but also non-natural amino acids never used in nature.

These improvements in quantum technologies in the fields of drug discovery and genomics will undoubtedly flip classical methodologies and scientific processes on their head and will make way for more advanced solutions to classical problems. As the hardware technology and the algorithms improve, the potential benefits of quantum computing in drug discovery and genomics is limitless.

For more information on the changes in quantum computing in life sciences, please reach out to the authors.

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