Building on belief

Life sciences research and quantum computing: The future is almost here

Abstract

The disruptive computational powers of quantum computing can provide the life sciences industry just the push it needs, especially in drug discovery and development. The laws of quantum mechanics have enormous potential not only in terms of providing speed but also in solving problems that were considered unsolvable till now. To that end, currently the life sciences industry is focusing on identifying appropriate use cases for quantum computing.

This paper discusses some of the key life sciences applications that quantum computing can revolutionize and discusses the way forward.

Application of quantum computing in life sciences

Unlike traditional computing, where bits denote 0 or 1, quantum bits or qubits in quantum computing can denote both 0 and 1 at the same time. While bits function independently, qubits interact with one another leading to exponential growth of states. That essentially means that quantum computers are not restricted to perform stepwise calculations but can compute a vast number of calculations simultaneously at a speed unimaginable with classic supercomputers. Given the incredible potential for innovation, quantum computing is expected to significantly disrupt the pharma and life sciences value chain (see Figure 1). Traditionally, research on small and large molecule properties and their interactions forms the basis of rational drug discovery. Quantum-inspired algorithms are expected to predict biochemical reactions better, as atomic and sub-atomic particles follow quantum principles.

Drug discovery	• Chemical simulations	• Chemical synthesis	• Molecular interactions	• Screening, QSAR	• Modeling and simulations, Molecular dynamics	• Genome sequence analysis: error checks, Sequence search	• Protein folding, structure and property prediction
Clinical development	• Dose response analysis	• Designing clinical trials	• Predicting adverse event reactions				
Diagnostics	• Medical image analysis, image reconstruction	• Quantum MRI	• Quantum sensore as miniaturized biomedical devices				
Therapy	• Precise radiation plan and dose	• Best therapy regimen	• Analysis of mega-data based on physiology, imaging, genomics, wearable technology, screening measures, patient records, environment measures for personalized medicine				
Information and insights	• Quantum NLP biomedical text mining and insights	• Knowledge synthesis					
Manufacturing and supply chain	• Supply chain optimizations	• Dynamic inventory allocation	• Logistics	• Risk modelling	• Process optimization for manufacturing	• IOT sensor data analysis	

Most compute-intense problems fall into three major categories – artificial intelligence (AI) and machine learning (ML), simulation, and optimization – where applying quantum computing returns immense value. Apart from this, there is also research focus on quantum technologies in imaging and cryptographic keys. Here we explore the potential use cases of quantum computing in these five areas of the life sciences industry.

Simulation

Simulating chemical reactions and interactions at molecular and sub-molecular levels is currently based on several approximations and assumptions due to compute infrastructure limitations. Industry segments like chemicals, materials, and pharmaceuticals, expect quantum developments to enable better predictive models of chemical or molecular synthesis and reactions based on simulations at molecular, atomic, and sub-atomic levels. Quantum computers can handle problems in estimating reaction rates and mechanisms[1] better than classical computers.

Humans have more than 20,000 genes, which are responsible for coding ~20,000 proteins. Further, each protein has ~100-200 variants. The Protein Data Bank currently has ~150,000 protein structures, of which ~46,000 are human proteins. Any chemical used as a drug can potentially bind to one or more of these 20,000 proteins, causing either beneficial or adverse reactions. The multiple molecular interactions between protein-protein, enzyme-substrate, protein-nucleic acid, drug-protein, and drug-nucleic acid play important roles in biological processes like signal transduction, transport, cell regulation, gene expression control, enzyme inhibition, and antibody-antigen recognition. Besides human proteins, there are proteins on pathogens and commensal microbes with which drugs can interact in human bodies. Quantum computers of the future are expected to accurately simulate these interactions. While today's quantum computers can simulate small molecules like hydrogen, lithium hydride, and beryllium hydride[2], this is a fairly smaller achievement in terms of molecule size and structural complexity. However, considering today's low-scale quantum computers, this is still quite an accomplishment.

Optimization

Quantum computing is expected to solve the classic traveling salesman problem (TSP) faster and with higher accuracy. Although in reality, the salesman wouldn't have to visit thousands of cities, this problem is relevant for solving several optimization issues across travel and transportation, supply chain, network infrastructure, air traffic control, work scheduling, financial services, and protein folding. Today's computers find it difficult to understand how real proteins fold into the shapes that help give them their function. In 2012, a Harvard research team reported the usage of quantum annealing to solve protein folding problems.[3] Quantum computing can address other optimization problems like molecular recognition, protein design, and sequence alignment. Researchers at the University of Southern California recently demonstrated the use of quantum processors to predict the binding of gene regulatory proteins to DNA.[4]

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[1] Annual Reviews, Simulating chemistry using quantum computers, May 2011, Accessed Oct 2021, https://www.annualreviews.org/doi/abs/10.1146/annurev-physchem-032210-103512

[2] Science, Quantum computer simulates largest molecule yet, sparking hope of future drug discoveries, Sep 2017, Accessed Oct 2021, https://www.sciencemag.org/news/2017/09/quantum-computer-simulates-largest-molecule-yet-sparking-hope-future-drug-discoveries

[3] Scientific Reports, Finding low-energy conformations of lattice protein models by quantum annealing, Aug 2012, Accessed Oct 2021, https://www.nature.com/articles/srep00571

[4] npj Quantum Information, Quantum annealing versus classical machine learning applied to a simplified computational biology problem, Feb 2018, Accessed Oct 2021, https://www.nature.com/articles/s41534-018-0060-8

The healthcare industry also faces operational-level optimization challenges like scheduling healthcare providers and deciding therapy regimens for cancer and other diseases. Minimizing damages to surrounding healthy tissues and organs during radiotherapy is a highly complex optimization problem with thousands of variables. Quantum computers have the potential to identify the most optimized and precise radiation and therapy plans after comparing all possible approaches.

ML and quantum computing

Running deep neural networks on huge datasets is constrained by the number of layers that current computing infrastructures can manage. Exponential scaling in compute power can support complex model building steps and allow real-time model building. With no lag in model building, AI systems can learn constantly in real time as new data is generated. Pharma research and development organizations are exploring AI and ML to understand disease mechanisms, identify biomarkers and targets, and predict compound properties, activities, and adverse reactions. It can also be used for de novo design and synthesis of small molecules, clinical trial analytics, image analytics for better diagnostics, and in analyzing literature, documents, and patents. Quantum computing can solve challenges like managing large datasets generated by high throughput systems, running compute-intensive analytics, and building effective ML models.

Imaging

The image capturing techniques for high-resolution images, CT-Scan, MRI, or HD videos generate large-sized files. Traditional image analysis relies on representing images pixel-by-pixel, needing enormous compute resources for high-resolution images. Quantum computing has the potential to revolutionize imaging and image processing through faster results. The potential to store N bits of classical information in log (2N) qubits will enable more granular-level imaging and image analysis that is unimaginable today. Image analysis of tissues, cells, and sub-cellular levels will transform how we diagnose, treat, and monitor diseases.

Case Western Reserve University (CWRU) and Siemens Healthcare have collaboratively developed a new approach for data acquisition, post-processing, and visualization, termed magnetic resonance fingerprinting (MRF).[5] This permits the simultaneous, non-invasive quantification of multiple important properties of a material or tissue and can revolutionize MRI-scan-based medical imaging with accuracy, speed, and predictive capacity. CWRU is also collaborating with Microsoft[6] to bring this to clinical reality with the help of quantum computing.

[5] Nature, Magnetic resonance fingerprinting, March 2013, Accessed Oct 2021, https://www.nature.com/articles/nature11971

[6] The Daily, Microsoft partners with CWRU on quantum computing, magnetic resonance fingerprinting, May 2018, Accessed Oct 2021, https://thedaily.case.edu/microsoft-partners-cwru-quantum-computing-magnetic-resonance-fingerprinting/

Cryptography

The current data encryption techniques are based on algorithms that are mathematically impossible to break by classic computers. However, quantum computers are expected to break into these encryptions easily with an exponential increase in compute power. As quantum computing can secure the key and data indefinitely with guaranteed unbreakable encryption, the National Institute of Standards and Technology (NIST) has begun focusing on providing quantum-based encryption techniques for the future[7]. The possibilities of applying quantum mechanics principles for developing un-hackable encryptions based on quantum key distribution is also underway.

Data is sacrosanct in the life sciences industry, both from the intellectual property (IP) perspective and for ensuring patient data privacy. The definition of Personal Identifiable Information is also evolving along with the new omics technologies. Protected access to medical records and secure data-sharing using quantum-based encryptions could be some of the earliest implementations of quantum computing in life sciences.

The way forward

Although the basic commercial quantum computing infrastructure is already available, we are nearing the large-scale operationalizing phase with accelerated innovations in hardware. Many big pharma companies have announced collaboration with quantum hardware or software players to evaluate Proofs of Concepts. A consortium, named QuPharm[8], has also been formed to work on identifying use cases and plan for precompetitive research in collaboration with Pistoia Alliance and Quantum Economic Development Consortium (QED-C).[9]

Identifying best-fit use cases and employing resources with quantum computing knowledge and skills are top priorities now. The more we understand life, the more we realize the complexities involved. Many of these complexities will unravel themselves with quantum-based advancements in computing and storage. Quantum computing could be the technology of the future that will enable accurate in silico de novo designing of efficacious and safe drugs.

[7] National Institute of Standards and Technology, NIST's Post-Quantum Cryptography Program Enters 'Selection Round,' July 2020, Accessed Oct 2021 https://www.nist.gov/news-events/news/2020/07/nists-post-quantum-cryptography-program-enters-selection-round

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Awards and accolades

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