

Quantum Computing in Healthcare and Medicines

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Abstract: As compare to the Classical Computer, Quantum Computer are more efficient, accurate and having high-performance quality which makes Quantum Computer to stand different. In Quantum Computer, the basic unit of information is qubits which exist in the superposition state whereas in Classical Computer, the basic unit of information is bits. When bits move from bits to qubits, it may help pharmaceutical research in the healthcare field, including studying how proteins fold, figuring out how molecules such as drugs and enzymes fit together, assessing the strength of interactions between a single biomolecule such as a protein or DNA and its ligand/binding partner such as a drug or inhibitor, and speeding up clinical trials. The idea of personalised treatment is made possible by the incredibly quick DNA sequencing capabilities of a quantum computer. Its efficiency and accuracy can enable the development of novel therapies option against Genetic Diseases. By carefully modelling, it can facilitate the creation of novel treatments and medications. The development of effective imaging systems with improved fine-grained clarity for real-time use by physicians is possible with quantum computers. Quantum computing holds promise for pharmaceutical research and development since it is useful for deciphering and reproducing intricate chemical and biological events.

Keywords: Quamtum computing, healthcare, classical physics, qubits, genetic diseases, Grover's algorithm

Introduction:

Classical Computers works on the phenomenon of Classical physics in classical physics the concept of "superposition" is describes as when two physical quantities are added together to give the third quantity which is totally different from the two original quantities that are being added. For example, constructive and destructive wave. Whereas Quantum Computers works on the phenomenon of Quantum mechanisms where Quantum superposition associates with quantum system it includes small particles like nuclei, proton, electron. Quantum systems can exist in a superposition state, and by measuring the system. It will collapse the superposition state into one definite classical state. For example, a coin is in the air it is the superposition of both heads and tails but when it lands it has definite state either tail or head.

In classical computers and digital computers, the basic unit of information is bit i.e., binary digits 0 or 1. The 1-bit is interpreted by computer hardware as an electrical current flowing through a wire, whereas the 0-bit is interpreted as an electrical current not flowing through a wire. One can consider these electrical signals to be "on" (the 1-bit) or "off" (the 0-bit). In Quantum Computer, the basic unit of information is qubits. Bits and qubits, both have two measurable states known as the 0 and 1 states. Qubits exist in a superposition state of 0's and 1's unlike classical bits. On a quantum computer, a qubit can now be used to execute some computations that would typically require performing each operation on 0 or 1 separately. It makes sense that this would speed up computations. When a qubit is measured, only one classical bits. All conceivable superpositions can be quantitatively represented using amplitudes. Amplitudes are crucial because they tell us probability of finding particle in specific state during a measurement.

Bloch sphere is the representation of qubits. Each spot on the Bloch sphere represents a unique superposition of a single qubit that may exist. The two measurable states of the qubit, 0 and 1, are represented by the top and bottom of the sphere, respectively. The qubit's present state is shown by an arrow on the Bloch sphere, which can point in any direction on the sphere's surface. The qubit is in a superposition state when the arrow is not pointed directly at the top or bottom of the sphere. For instance, a qubit measuring as 0 or 1 has a 50/50 chance of doing so anywhere near the equator. A certain state where the amplitudes can have various signs and be either real or imaginary numbers correlates to a specific point on the equator. A good visual aid for comprehending how a qubit might have an endless number of potential quantum states is the Bloch sphere shown in Fig 1.1. It does not apply to systems with two or more qubits and only represents one qubit.

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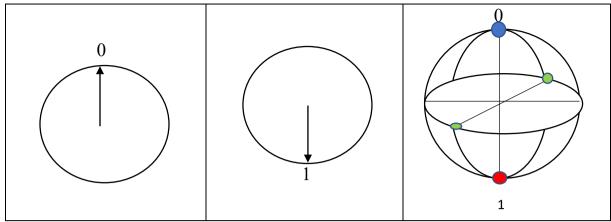


Fig 1.1 Representation of Qubits in Bloch sphere

As quantum computers are based on fundamentally different concepts than classical computers, they must be built from completely different technology, i.e. it is not possible to have a classical current in a superposition of both flowing and not flowing through a wire. Since quantum computing is still in its infancy, several different technologies could be used to create them. Superconductors are used in some technologies, optical systems in others, and molecules in still others.

A beam splitter divides a beam of light into two in classical optics by acting as a mirror that is only partially reflecting. 50% of the light intensity is transmitted and 50% is reflected using a 50/50 beam splitter. Traditionally, electric and magnetic fields have been thought of as the building blocks of a wave that makes up light. Yet another way to conceptualise light is as a stream of tiny particles known as photons. Despite having no mass, photons travel from one point to another at the speed of light. In a laser beam, photons are present. One photon can send at a time if laser's power lower. In the beam splitter experiment, both detectors would be activated simultaneously if the photon was split in half. The photon could not have broken up because only one detector activates at a time. The beam splitter is where the photon was either transmitted or reflected, and that's why we didn't know until it reached Detector 1 or 2. Up until it encounters the detectors, the single photon is in a superposition of the two states. It may seem like a semantic distinction, but this is significant because it represents two different ways that the cosmos behaves at the closest distances. Additionally, it will be crucial when the system becomes more intricate. Superposition state of photon shown below.

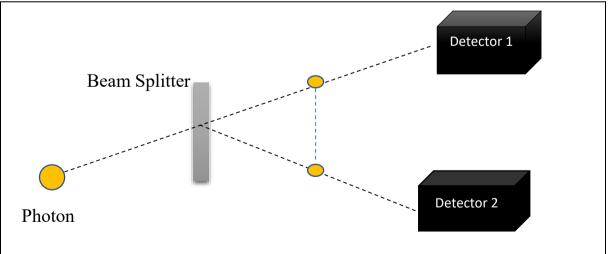


Fig 1.2: Photon is in Superposition state

Let the transmitted path be 0 (detector 1), and the reflected path be 1 (detector 2), Unfortunately, because quantum mechanics is intrinsically unpredictable, it is impossible to determine which detector will be turned on at any given moment. Due to the phenomena of superposition, a single qubit can be used by quantum computers to simultaneously process two bits of data. In fact, utilising photons as qubits, beam splitters to achieve superposition,

and pieces of glass that slow down photons along certain paths (phase shifters), it is conceivable to build a generalpurpose (also known as universal) quantum computer [1].

Another qubit prototype is an electron. An electron has numerous quantifiable characteristics, including energy, mass, and momentum. But we want to concentrate on a property with just two quantifiable values in order to make a qubit. Spin is a two-state characteristic of an electron. The electron has an inherent quantum mechanical characteristic known as "spin" much like the electron has a mass or charge. Although spin does not directly correspond to the electron physically rotating, the attribute was given that name because it can be mathematically expressed in a manner similar to orbital momentum. It was demonstrated by the Stern-Gerlach apparatus (SGA) that the electron spin may take only two values. The important thing to note in this situation is that the vertically oriented equipment (referred to as the z-direction by convention) only measures the spin as either up or down, not randomly oriented at any angle. A qubit can be represented by an electron's spin, which has two measurable states: 0 for spin up and 1 for spin down. The apparatus's orientation determines the "up" and "down" directions represent below in Fig 1.3.

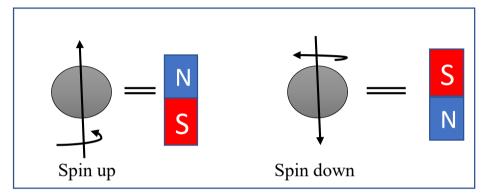


Fig 1.3: Electron spin in upward and downward direction and produce magnetic field

The z-direction is not fundamentally different from the x- or y-direction. Spin left or spin right would be measured by an SGA turned horizontally. Depending on whatever way the SGA was spun by 45°, the spin was either diagonally up or diagonally down. Traditionally, bar magnets with a vertical orientation in a horizontal magnetic field would land in the middle of the display. Although the spin cannot possible land in the centre, it can only be assessed as going left or right. The solution provided by quantum mechanics is for the electron to have a 50% chance of landing on either the left or the right. A spin-up electron is placed in a superposition condition of left and right when it passes through a horizontal SGA. The Stern–Gerlach experiment shows that qubits in superposition are an accurate description of how nature truly operates. Therefore, stimulating natural systems, such as the electrical characteristics of a molecule for use in drug design, understanding phyco-chemical properties of novel molecules (like protein, ligand), is an application of quantum computing.

Classical logic gates like OR, AND, NOT, and NAND are used in classical computers to manipulate bits. Quantum gates are used to control qubits in quantum computers. Depending on whatever gate is used, the states of the qubits change when it is applied to them. The gate gives instructions to rotate the qubit's arrow around the sphere in the Bloch sphere model. Quantum gates must be used to implement a quantum algorithm on a quantum computer. By measuring the qubit's state after a quantum algorithm has been run, the outcome is obtained. The way the qubit and quantum computer have been technologically implemented will affect how quantum gates are implemented in hardware. As an illustration, consider a spin-based qubit. The spin and hence the qubit state might then be changed using gates that are built utilising an external magnetic field.

A scientific phenomenon known as quantum entanglement happens when several qubits are correlated with one another. Entanglement can have peculiar and advantageous effects that might accelerate quantum computers relative to traditional computers. When qubits are "entangled," they can reveal secret quantum information that is unavailable in the classical world. The sharing of non-classical information between two or more quantum states is referred to as entanglement. Qubits or quantum states interacting with one another are the cause of this. Entanglement is produced by two-qubit gates, which act concurrently on two separate qubits. For this, the controlled NOT (CNOT) gate is widely employed.

The quantum computer uses a quantum algorithm to carry out tasks on some input qubits. Entanglement is used by Grover's algorithm, one of the two most well-known quantum computing methods, to explore databases more quickly than any classical computer can. The Deutsch-Jozsa Algorithm illustrates how quantum computers are

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capable of processing calculations more quickly than conventional computers. Parallelism is where quantum computers excel over traditional computers. A quantum computer can operate on all of the states concurrently since qubits can be in a superposition of states.

Today's Quantum Computers

There may be quantum algorithms that can speed up machine learning processes and effectively imitate molecules' quantum behaviour. As of 2018, businesses like IBM and Google have created various quantum computers with up to 72 qubits. Using Shor's technique, a 1024-bit contemporary encryption key might be factored with more than 5,000 qubits. In 2019, Google claimed to have achieved "quantum supremacy" by performing [2] the first quantum computation that a classical computer was unable to complete. A quantum computer can solve a problem that a traditional computer cannot, which is known as quantum supremacy. The issue's resolution might not, however, be useful in everyday life. It is crucial to understand that Google has achieved the quantum supremacy milestone, not the "quantum usefulness" one. On a 53-qubit quantum computer, Google completed their assignment in 200 s. They asserted that a conventional computer would require 10,000 years to complete the same operation. However, IBM soon after claimed that the operation could theoretically be completed in just 2.5 days using an enhanced classical supercomputing method [3]. When developing a quantum computer, various technical challenges could be encountered. Lasers can be used to create quantum computers. Random photons from the environment can also inadvertently enter the quantum computer, changing the quantum state unintentionally. This can happen if the quantum computer is exposed to the environment. "Noise" is the term for such unintentional changes. The quantum computer must be chilled to a temperature of about 450 degrees Fahrenheit, which is close to absolute zero, in order to limit the amount of these ambient photons. However, this is challenging. The necessity to maintain this low temperature increases as qubits are added. Additionally, as qubits are added, more lasers are required to interact with the qubits. Keeping several qubits in a confined area while also employing many lasers to create isolated interactions between them is technically challenging. Additionally, the likelihood that qubits will unintentionally interact with their surroundings increases with the number of qubits added. This interaction, known as decoherence, will ruin the system's quantum features. Governments and businesses are spending billions of dollars to make quantum computers a reality, though, considering how classical computers evolved from being the size of a room in the 1960s to an iPhone within a few decades. Quantum computers will eventually be used in addition to classical computers [4].

Application of Quantum Computers in Healthcare and Medicine

In the current highly connected IoT digital healthcare paradigm [5][6], which includes interconnected medical devices (such as medical sensors) that connected to the Internet or the cloud, quantum computing is particularly well suited to numerous compute-intensive applications of healthcare [7]. In addition to being advantageous for healthcare IoT, the enormous increase in computational power may also pave the way for quantum computers to make fundamental advancements in this field. When we move from bits to qubits, it may help pharmaceutical research in the healthcare field [8], including studying how proteins fold, figuring out how molecules such as drugs and enzymes fit together [9], assessing the strength of interactions between a single biomolecule such as a protein or DNA and its ligand/binding partner such as a drug or inhibitor[10], and speeding up clinical trials[11]. The idea of personalised treatment is made possible by the incredibly quick DNA sequencing capabilities of a quantum computer. Its efficiency and accuracy can enable the development of novel therapies option against Genetic Diseases. By carefully modelling, it can facilitate the creation of novel treatments and medications. The development of effective imaging systems with improved fine-grained clarity for real-time use by physicians is possible with quantum computers. Furthermore, it can resolve challenging optimisation difficulties related to creating the best radiation strategy for eliminating malignant cells while sparing the surrounding healthy tissues damage. A road to drug discovery and medical research will be opened up by quantum computing's ability to examine molecular interactions at the most fundamental level. Whole-genome sequencing requires a lot of time, but with the aid of qubits, whole-genome sequencing and analytics might be completed quickly. By using cuttingedge techniques to enable on-demand computing, redefine security for medical data, predict chronic diseases, and develop precise drugs, quantum computing might completely transform the healthcare sector.

For the study of complex omics datasets like metabolomics, transcriptomics, proteomics, and genomics, the finding and characterisation of biomarkers is essential. Increased feature space caused by these processes may result in complicated patterns and correlations that are nearly impossible to analyse using traditional computational techniques. Quantum computing could enable diagnostic insights during the diagnosis process, reducing the need for repeated diagnosis and therapy. This paradigm aids in delivering ongoing health monitoring and analysis for people. Additionally, it aids in performing meta-analysis for cell-level diagnostics to ascertain the optimal course of action at a particular moment. As a result, both patients and medical professionals may benefit from lower costs and expanded data-driven diagnoses.

Modelling atomic-level molecular interactions, which is required for medical research, is made possible by quantum computing for medical professionals. For diagnosis, therapy, medication discovery, and analytics, this will be very important. More than tens of thousands of proteins can now be encoded and their interactions with medications may be simulated, something that was previously impossible thanks to advances in quantum computing. In comparison to normal computing skills, quantum computing helps process this information orders of magnitude more effectively. Doctors may evaluate massive data sets and their permutations concurrently using quantum computing to find the most promising patterns. Gold nanoparticles can now be used in conjunction with established techniques, such as the bio-barcode assay, to detect disease-specific biomarkers in blood.

Molecular Stimulation

As opposed to classical computing, where integrated circuits control processing speed, quantum computers prefer to process data in a fundamentally unique manner using quantum bits. Contrary to classical computers, which are not built to take use of this phenomenon, quantum computers exploit the quantum entanglement phenomenon to store information instead of doing so in terms of 0s and 1s. Quantum computers can use machine learning (ML), optimisation, and artificial intelligence (AI) to run intricate simulations in the healthcare sector. Healthcare procedures frequently include intricate correlations and tightly coupled molecular structures with interacting electrons. For stimulating caffeine molecule classical computer require 10⁴⁸ bits whereas quantum computer require 200-300 quits. In this field, time is always the limiting factor, and processing needs for simulations and other operations expand exponentially with problem size.

Medical Image Analysis

Early disease detection could result in better prognosis, treatment, and cost savings in healthcare. For instance, it has been demonstrated in the literature that when colon cancer is detected early, the cost of therapy decreases by a factor of 4, but the survival rate could decline "by a factor of 9" [12]. While this is going on, the majority of diseases now treated and diagnosed are expensive, time-consuming, and have diagnosis errors of about 15-20% [13]. With computer-aided diagnostics advancing more quickly in recent years, the utilisation of X-rays, CT scans, and MRIs has become crucial. Noise, poor data quality, and replicability problems make diagnoses and treatments difficult under this circumstance. In this sense, image-aided diagnosis can be improved by quantum-assisted diagnosis, which has the ability to examine medical images and supervise processing processes like edge identification. While analytical methods are required for single-cell sequencing data and flow cytometry, the existing methodologies use single-cell procedures for diagnosis. These methods also call for sophisticated data analysis tools, especially when merging datasets from several methods. One of the primary issues in this context is the classification of cells based on their biochemical and physical characteristics. Although this categorization is crucial for important diagnoses like the separation of malignant cells from healthy cells, it necessitates a wide feature space and a much larger predictor variable. Such classifications and single-cell diagnostic procedures are made possible by quantum machine learning (QVM) techniques.

Personalized Medicine:

Precision medicine has been more prevalent during the past few years. Indeed, the pharmacokinetics, pharmacodynamics, and bioavailability of medications are all influenced by the heterogeneity of patients in terms of environment, clinical history, and genetic origin. Using omics data, "high resolution" snapshots of the underlying biology may be examined. As an illustration, it has been shown that the baseline properties of the tumour ecosystem, including its multi-omics landscape, influence how well breast cancer treatments respond [14]. Blockbuster medications, typically prescribed for conditions with high prevalence, saw success in recent decades, with total yearly sales exceeding US\$1 billion in the pharmaceutical industry [15]. However, the availability of personalised medications, such as cell and gene therapies, is expanding. As a result, almost a quarter of all FDA approvals in the previous seven years and 35% of approvals in 2021 will be for personalised medications [16]. The number of patients and the cost influence a molecule's total financial performance. Although the target populations for personalised medicines are frequently restricted, payers seem willing to authorise high list prices, particularly for one-time treatments. Zolgensma, a gene therapy licenced in May 2019 for pediatric spinal muscular atrophy injury, is the priciest medication on the market at the moment [17].

In order to reduce the time and expense of finding novel medicines and bringing them to market, as well as to personalise the therapies, artificial intelligence (AI) solutions are being employed. The abundance of biological and clinical data, however, makes it difficult for our available algorithmic and technological solutions to accurately and powerfully comprehend the complexity of human health. For instance, new computational

approaches would be required to fully utilise spatially-resolved transcriptome data, which contains information about the activity of genes inside a tissue [18].

In this situation, quantum computing could hasten the research and development of pharmaceuticals by more accurately modelling and forecasting the biological and clinical processes related to human health.

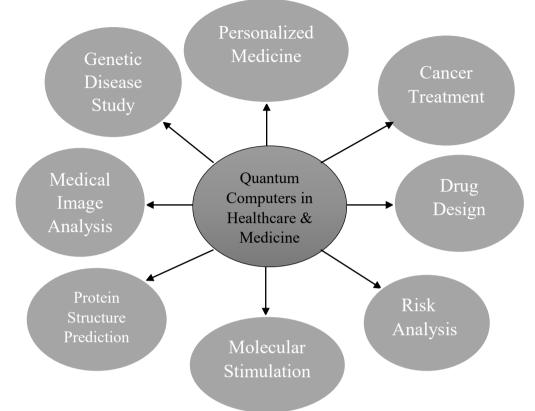


Fig 1.4: Application of Quantum Computers in Healthcare & Medicine

Risk Analysis

Health insurers can benefit from proactive assistance from the quantum computing as a service (QCaaS) with patient- and customer-focused solutions. A patient can have the health insurance that best suits them depending on their lifestyle and the environment in which they live by using the exact applications that the cloud-based QCaaS can give [19]. Traditional systems require a lot of time and money to profile risks. One can access the many possibilities fast and reduce the cost of risk profiling by using simulations and quantum computing to match it to the legal framework. This can assist health insurers with their underwriting and risk aggregation processes.

Protein Structure Prediction

The ability to infer a protein's three-dimensional form from its amino-acid sequence is one of the current drug discovery processes that is generating a lot of attention. The most traditional method for figuring out the protein structure is to explore each possible sequence one at a time. Finding the ideal protein structure for a particular sequence of amino acids may take this method several years. Machine learning is gradually becoming more popular, particularly with the release of Alpha Fold, a deep learning algorithm designed by Google's DeepMind to predict protein structures [20] and with recent developments made by Meta's teams that allow for faster but less accurate results [21]. The limitations of computer capacity, however, prevent machine learning from being used to explore protein structure. Protein structure prediction can be sped up and made more accurate by using quantum computing. The initial tests were performed to demonstrate the viability of creating such algorithms [22]. In order to expedite or completely do away with the drug candidate screening phase and reduce the cost of drug discovery while increasing accuracy, protein structure can be swiftly understood using quantum computing. This is made possible by the ability to learn the true behaviour and structure of a certain protein.

Genetic Diseases Study

Since quantum computing has advanced beyond experiments to enterprise-wide deployment in a select few industries, it has a wide range of possible applications. Recent years have seen the interesting results in a small number of industries. Following the tenets and characteristics of quantum theory, such as entanglement and superposition, it can enable the guess-and-practice based method of disease therapy with speedy fixes [23].

Recent study, "Implementation of a Hamming distance-like genomic quantum classifier using inner products on ibmqx2 and ibmq_16_melbourne" published in Quantum Machine Intelligence, Stefan Bekiranov, PhD, and colleagues describe the development of an algorithm that will enable researchers to study genetic diseases using quantum computers once there are much more powerful quantum computers to run it.

Bekiranov claims that the algorithm, a complicated collection of operating instructions, will aid in the creation of quantum computer algorithms and may eventually advance the field of genetic research [24].

Cancer Treatment

Radiation therapy has been utilised in the medical field for a long time to treat cancer and other tumors based procedures. Radiation therapy's primary objective is to reduce cancerous cells [25]. Patients have burning, dryness, and itching problems as a result of the ineffective attack on non-cancerous tissues, in addition to additional adverse effects including oral or joint disorders. Therefore, a method that can precisely target a specific cell that needs to be reduced in size and harmed is needed. In addition, it has been noted that many cancer patients struggled throughout Covid-19 as a result of the shift in attention to Covid-19.

Consideration is being given to some of the first quantum computing applications for patient modelling. For instance, based on genetic and chemical data, IBM claims that quantum machine learning might be used to enhance the prediction of the sensitivity of cancer cells to treatments [26].

The study of histone demethylases, which are involved in the transcription of genetic information contained in DNA, or comprehension of some particular cases of molecular recognition are two examples of approaches being developed by researchers to simulate with quantum computing biochemical systems that are intractable with classical algorithms on classical computers [27].

The transition from conventional machine learning to quantum-based models used in medicine has implications for another area of research. For instance, the Canadian startup Netramark accurately classified the subtypes of non-small-cell lung cancer by utilising quantum computing technologies [28].

Quantum algorithms may be used to research the human brain using data from genetics, genomics, neuroimaging, and deep behavioural phenotyping, as well as current efforts to employ quantum computers to model patients at the cellular, tissue, organ, and even behavioural level [29].

Quantum Compatibility of today's use case in the future

Regulatory restrictions, a lack of in-house knowledge, and a gap between data and AI and business teams hindered pharma businesses' adoption of Big Data, Big Data analytics, and AI. Clinical trial findings, which provide the foundation for market access authorisation, are a common source of operating data for pharmaceutical industry. However, a number of technologies have emerged and need to be embraced by the industry. These include Big Data, advanced analytics, and AI. The pharma industry's reluctance to adopt these technologies due to concerns about the reliability of AI-based solutions and their poor interpretability. Because of this, no "black box" technology could be employed for the studies that would later be used to support drug submissions or used in clinical practise. The pharmaceutical business is also very regulated. The implementation of Big Data and AI technologies was further hampered by a lack of internal expertise and potential scepticism over the dependability of AI-based solutions. Several pharmaceutical companies addressed this gap by working with internet behemoths, investing in niche start-ups, and setting up in-house data labs and data squads.

Digital efforts have typically been managed by IT and digital divisions. Therefore, it seems natural that these departments were the first to form AI and data teams. The earliest proofs of concept were successfully launched by small, divided teams. However, in order for AI initiatives to succeed, they must take into consideration the clinical and biological environment and be rooted in corporate interests. Additionally, new governance between IT and business teams was necessary for the robustification and industrialisation of use cases with actual business impact, particularly the beginning of cross-functional efforts.

Today, specialised divisions within pharmaceutical businesses are in charge of coordinating the implementation of AI and the shift to data strategy. One of the important trends aimed at laying strong foundations for the application of AI use cases with a measurable ROI is the building of data lakes and control towers.

The majority of the use cases that can be solved by quantum computing can already be partially solved by AI. In light of this, it is crucial to consider the possibility of the quantum advantage while developing data and AI strategy

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and governance in order to successfully exploit both approaches in tandem in the future and to prepare for the adoption of the newest technology.

For instance, AI has already made certain drug effect modelling possible. When applicable in the future, quantum computing might be used to accomplish the task more quickly or precisely while using more data points. Starting now, it is crucial to make sure that as much data as possible is gathered from real-world and digital clinical trials in order to get ready to embrace the quantum advantage.

IT Infrastructure Development with Future Quantum Advantage

High-performance computing (HPC) is the process of processing data in parallel to increase computer speed and carry out intricate calculations. HPC accomplishes these objectives by pooling computing resources, allowing even sophisticated applications to function effectively, dependably, and promptly in accordance with user demands and expectations. One of the most well-known instances of HPC is the supercomputer, which consists of numerous computers and processors operating in tandem to produce parallel processing and high performance. As a result, it performs better and uses significantly more power than a conventional computer. Scientists and engineers use supercomputers to tackle difficult computing jobs.

However, if the issue at hand exhibits a high level of complexity, some problems are too challenging even for supercomputers. As a result, complex issues involving many variables interacting in many ways are typically beyond the capabilities of supercomputers. For instance, simulating the actions of specific atoms within molecules is a difficult undertaking. In order to understand the behaviour of these proteins, it may be necessary to use quantum computers rather than supercomputers for activities like sorting through a sizable database of protein sequence. It is noteworthy that many HPC facilities intend to fund quantum computing in the near future to increase their hardware selection.

The use of high-speed computers for computationally demanding and data-intensive jobs is becoming more and more common nowadays, yet traditional computing is still the norm. The majority of projections state that quantum computers will become fully functional in the upcoming decade. Quantum cloud computing is a further development in technology that pharmaceutical businesses may find useful if they decide against investing in their own quantum computing infrastructure and instead prefer to access it over the cloud.

Future technological advancements will undoubtedly depend on a hybrid approach to computing, where businesses benefit from the adaptability of cloud-based HPC and the potent, specialised nature of hardware for quantum technology. Many feels that the debate over whether computing hardware will predominate in the future and the comparison of classical versus quantum computing are given too much weight. With both technologies being utilised to support big data projects and AI and ML applications, the future is probably going to be more complicated. It's unlikely that all current computers will be replaced by quantum ones. Quantum computers won't be required in many situations, and the hybrid model should suffice in others.

Conclusion

Quantum computing is projected to have numerous advantages for pharmaceutical research and development, including ones that go beyond time and money savings. Quantum computing holds promise for pharmaceutical research and development since it is useful for deciphering and reproducing intricate chemical and biological events. Essentially, it could signify a move towards more in-silico research, which would reduce the risk to clinical trial participants.

It would also be easier to select the best chemical for each patient depending on their genotype, endotype, socioeconomic status, and behavioural traits if multiple data sources were taken into account. Quantum computers have increased processing capacity and the potential to do calculations that are more sophisticated, which can advance personalised medicine. It is important to note that in order to fully utilise the capabilities of quantum computing, high-quality patient data would need to be available.

Longer ahead, pharmaceutical organisations can use quantum computing for purposes other than research and development, with improved supply chains and bioproduction being notable examples. Additionally, modelling intricate supply networks can aid in guaranteeing the consistency of component flow, helping to both prevent shortages and enable more adaptable production. Pharmaceutical industries need to start taking the potential of quantum computing into account in their operational and tactical decisions right now, even though quantum technology has to continue to advance.

The commercial potential of quantum computing is still being realised because it is a developing technology. In the mid- and long-term, quantum computing may play a significant role throughout the pharma value chain as the stability and quality of qubits rise as the technology is further developed. For statistical and advanced analysis, early adoption of quantum computing in addition to conventional and high-performance computing may be crucial for maintaining competitiveness.

References

[1] Knill, E.; Laflamme, R.; Milburn, G. J. (2001). A scheme for efficient quantum computation with linear optics. Nature. Nature Publishing Group. 409 (6816): 46–52.

[2] Arute, F., Arya, K., Babbush, R. et al. Quantum supremacy using a programmable superconducting processor. Nature 574, 505–510 (2019). https://doi.org/10.1038/s41586-019-1666-5

[3] Pednault, E., Gunnels, J. A., Nannicini, G., Horesh, L., Wisnieff, R., Leveraging secondary storage to simulate deep 54-qubit Sycamore circuits. arXiv:1910.09534. Posted October 21, 2019

[4] Theoretical physicists and computational scientists at Fermi National Accelerator Laboratory are working on improving algorithms and the foundations of quantum science in order to expand the problems that (near term) quantum devices can solve, e.g., https://qis.fnal.gov/quantum-computing-for-hep/

[5] A. Devi, V. Kalaivani, Enhanced BB84 quantum cryptography protocol for secure communication in wireless body sensor networks for medical applications, Personal and Ubiquitous Computing (2021) 1–11.

[6] S. Sadki, H. E. Bakkali, Towards negotiable privacy policies in mobile healthcare, in: Fifth International Conference on the Innovative Computing Technology (INTECH 2015), 2015, pp. 94–99.

[7] F. Fl"other, J. Murphy, J. Murtha, D. Sow, Exploring quantum computing use cases for healthcare (ibm expert insights) (2020).

[8] M. Zinner, F. Dahlhausen, P. Boehme, J. Ehlers, L. Bieske, L. Fehring, Toward the institutionalization of quantum computing in pharmaceutical research, Drug Discovery Today.

[9] L. Banchi, M. Fingerhuth, T. Babej, C. Ing, J. M. Arrazola, Molecular docking with gaussian boson sampling, Science advances 6 (23) (2020) eaax1950.

[10] R. Y. Li, R. Di Felice, R. Rohs, D. A. Lidar, Quantum annealing versus classical machine learning applied to a simplified computational biology problem, NPJ quantum information 4 (1) (2018) 1–10.

[11] V. V. Fedorov, S. L. Leonov, Combinatorial and model-based methods in structuring and optimizing cluster trials, in: Platform Trial Designs in Drug Development, Chapman and Hall/CRC, 2018, pp. 265–286.

[12] M. Birtwistle, Saving lives and averting costs? the case for earlier diagnosis just got stronger, cancer research uk. (September 22, 2014).

[13] H. Singh, A. N. Meyer, E. J. Thomas, The frequency of diagnostic errors in outpatient care: estimations from three large observational studies involving us adult populations, BMJ quality & safety 23 (9) (2014) 727–731.

[14] Sammut, S.-J., Crispin-Ortuzar, M., Chin, S.-F., Provenzano, E., Bardwell, H. B., MA, W., ... CALDAS, C. (2022). Multi-omic machine learning predictor of breast cancer therapy response. Nature, 601, 623–629.

[15] Schumaher, A., Hinder, M., Boger, N., Hartl, D., & Gassmann, O. (2022). The significance of blockbusters in the pharmaceutical industry. Nature Reviews Drug Discovery.

[16] Personalized Medicine Coalition. (2021). Personalized Medicine at FDA.

[17] FIERCE PHARMA. (2019, MAY 24). Novartis slaps \$2M-plus price tag on newly approved gene therapy Zolgensma—and cost watchdogs approve.

[18] Atta, L., & Fan, J. (2021). Computational challenges and opportunities in spatially resolved transcriptomic data analysis. Nature Communications, 12, 5283.doi:10.1038/s41467-021-25557-9

[19] Fairbank, J.F., Labianca, G. Joe, Steensma, H.K., Metters, R., 2006. Information processing design choices, strategy, and risk management performance. J. Manag. Inf. Syst. 23 (1), 293–319.

[20] Johan Jumper, R. E. (2021). Highly accurate protein structure prediction with AlphaFold. Nature: https://www.nature.com/articles/s41586-021-03819-2. [21] Zeming Lin, H. A. (2022, OCTOBER 31). Evolutionary-scale prediction of atomic level protein structure with a language model. bioRxiv: <u>https://www.biorxiv.org/content/10.1101/2022.07.20.500902v2</u>.

[22] Wong, R., & Chang, W.-L. (2021). Quantum Speedup for Protein Structure Prediction. IEEE TRANS NANOBIOSCIENCE, 20(3), 23-330. doi:10.1109/TNB.2021.3065051.

[23] Yuan, X., Yang, C., He, Q., Chen, J., Yu, D., Li, J., Zhai, S., Qin, Z., Du, K., Chu, Z., Qin, P., 2020. Current and perspective diagnostic techniques for COVID-19. ACS Infect. Dis. 6 (8), 1998–2016

[24] Kathuria, K., Ratan, A., McConnell, M. et al. Implementation of a Hamming distance–like genomic quantum classifier using inner products on ibmqx2 and ibmq_16_melbourne. Quantum Mach. Intell. 2, 7 (2020). https://doi.org/10.1007/s42484-020-00017-7

[25] Zheng, X., Sun, S., Mukkamala, R.R., Vatrapu, R., Ordieres-Mer'e, J., 2019. Accelerating health data sharing: a solution based on the internet of things and distributed ledger technologies. J. Med. Internet Res. 21 (6), 1–12.

[26] IBM Institute for Business Value. (2020). Exploring quantum computing use cases for healthcare. https://www.ibm.com/downloads/cas/8QDGKDZJ

[27] Cheng, H.-P., Deumens, E., Freericks, J. K., Li, C., & Sanders, B. A. (2020). Application of Quantum Computing to Biochemical Systems: A Look to the Future. Front Chem., 8, 587143. doi:10.3389/fchem.2020.587143

[28] Jain, S., Ziauddin, J., Leonchyk, P., Yenkanchi, S., & Geraci, J. (2020). Quantum and classical machine learning for the classification of non-small-cell lung cancer patients. SN Appl. Sci., 2, 1088. doi:10.1007/s42452-020-2847-4

[29] Emani, P. S., Warell, J., Anticevic, A., Beiranov, S., Gandal, M., McConnell, M. J., Harrow, A. W. (2022). Quantum computing at the frontiers of biological sciences. Nature Methods, 18(7), 701-709. doi:10.1038/s41592-020-01004-3

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