

Implementations of Quantum Computing in Medicine: Evidence from Drug Discovery, Genomics, and Medical Imaging

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Abstract. Quantum computing is becoming a revolutionary technology with vast applicability across many sectors, including medicine. As the medical science is in front of more complicated problems involving drug discovery, genomics, and disease modeling, the application of quantum computing opens doors to new opportunities. This paper also discusses specific uses of quantum computing in the healthcare domain: drug discovery, genomics and genetics, medical imaging, biomolecular simulations, and public health. The research also embraces how quantum algorithms improve drug discovery, genome data, and disease diagnosis with focus on improving techniques in medical imaging and biomolecular modeling. These include quantum machine learning, applying in personalized medicine, quantum simulations, for protein folding, and increased resolution of imaging techniques. As with all technologies, there are still numerous concerns associated with scaling such a tool, optimizing the employed algorithms, and maintaining the privacy of the patient's information and the security of this data. Its relevance is in the investigations conducted to show the applicability of current problems in medicine to quantum computing in order to spearhead more research and cooperation across various fields. Over time, quantum technologies' potential keeps emerging and consequently will revolutionize healthcare, enhance patient experience, and fuel pharmaceutical development.

Keywords: Quantum Computing, Drug Discovery, Genomics, and Medical Imaging.

1. Introduction

Scalar computing, where one data point is processed with each operation, has been at the essence of classical computing [1]. Over several decades, this philosophy has been instrumental in achieving advancements to technology that provided impacts in fields such as computed tomography, computational biology, and molecular modeling and drug design, among others. Nevertheless, as the amount and sources of data grew, the problems with scalar computing became evident. The rise of parallel computing offered a solution to this issue by allowing for the process of multiple data at once improving the rate of computation [2-4]. However, it is still difficult to overcome other issues related to the use of parallel and high-performance computing, especially due to quantum-level events in the medical field [5]. The arrival of quantum computing read a major shift as it was marked as. Quantum to classical computers differ majorly in that the former uses bits that can only be either 0 or 1 while the latter uses quantum bits or qubits which can be simultaneously in more positions. This makes quantum computers handle large volumes of data and do computation more effectively than what classical systems do [6-8]. The idea of quantum computing was first proposed in the latter half of the 20th century while its tangible use, particularly in the medical field, has only been realized within the last couple of years. Such issues have the capability of reforming the healthcare sector by solving issues that classical systems find difficult to deal with.

Currently, quantum computing has advances various areas in the medical field, including cancer, brain scans, as well as finding drugs. The following are key areas where quantum computing is having a profound impact. It is quite clear that quantum computing offers a solution for the enhancement of cancer diagnosis and subsequent treatment. It can simulate molecular interactions in a more accurate manner which enables the development of accurate therapies. For instance, quantum simulations enable scientists investigate how protein molecules fold in cancer cells, a key aspect regarding optimality of molecules in cancer drugs. An example is given of how quantum computing helps to find anticancer agents as a result of drug interactions at the molecular level [9]. Quantum computing

is improving neuroimaging by helping to make quicker and more precise interpretations of large brain scan data. Quantum algorithms enhance data analysis, including big data from functional MRI, to achieve improved diagnostic accuracy. Using quantum methods, it is possible to decrease interference in MRI and increase the definition and speed of imaging necessary to diagnose neurological diseases, including Alzheimer's disease at the initial stage [10]. In the case of drug discovery, it accelerates a series of molecular dynamics and quantum chemistry calculations which is crucial for creating new drugs. As a result, quantum simulations make possible the prediction of how molecules will interact, which is not easy for classical computers. There is the possibility of using quantum computing in solving the complex problems for pharmacology and reducing the time to find the potential drugs for the treatment of different diseases [11].

The potential transformative impact of quantum computing in solving medical challenges, from enhancing the accuracy of diagnosis to speeding up drug discovery, is evidenced by these recent advancements. Traditional computing systems are insufficient to solve the increasingly complex problems facing the medical field. Healthcare demand escalate with increased desire for faster and more accurate drug discovery, disease modeling and image. Quantum computing has the power to solve problems that are insurmountable with classical computing, providing the capability to work with extremely large amounts of data. The power of quantum computing to simulate molecular interactions, and to analyze large datasets at granular levels, makes it ideally suited as a new tool for transforming medical research and patient care. The goal of this study is to determine how quantum computing can be developed for use in medicine to address the issues facing us today and improve health outcomes. The transformative potential of quantum computing in medicine will be explored in seven parts of this study. The rest of the paper is organized as follows. In Sec. 2, introduction to the principles of quantum computing and demonstration of how it is applied in drug discovery, genomics, medical imaging, and disease modeling is discussed. Sec. 3 is a study on the application of quantum computing to drug discovery, presenting molecular docking, searching algorithms, and quantum machine learning. Sec. 4 focuses on its role in genomics and personalized medicine. Sec. 5 looks at its medical imaging advances. Sec. 6 contains a discussion of biomolecular simulations, and Sec. 7 is dedicated to the use of biomolecular simulations in public health. In Sec. 8, the limitations, challenges, and future directions of quantum computing in medicine will be finally addressed. Eventually, a brief summary is given in Sec. 9.

2. Principle of Quantum Computing

Quantum computing is a paradigm shift of computation based on quantum mechanics. Quantum computers, however, differ from classical computers, which use bits representing either 0 or 1. Superposition allows these qubits to be both 0 and 1 simultaneously. This unique property of quantum computers allows them to carry out a large number of calculations in parallel, giving rise to unprecedented computational benefits compared to classical systems. Another critical quantum concept is entanglement, where qubits become correlated, and the state of one qubit influences the state of another, regardless of distance. This interconnectedness is essential for performing operations using quantum gates, such as Hadamard and CNOT (controlled NOT), which manipulate qubits based on superposition and entanglement [4].

Preparing entangled photon states is crucial to the method of quantum computation. The ability to run quantum systems in parallel is dependent on these states. Spontaneous Parametric-Down Conversion (SPDC) is used to create entangled photon pairs, where a photon of a laser beam interacts with a nonlinear crystal to produce two entangled photons. Then these photon pairs are used for computation in quantum circuits. Entangled photons are usually sent through optical fibers or quantum channels to be processed by quantum gates. Quantum key distribution (QKD) protocols are shown to realize this technology, guaranteeing secure communications and cryptography.

Despite, its potential, quantum computing faces several challenges [6]:

- Decoherence and Noise: Quantum states are nevertheless very sensitive to external disturbances, which causes their decoherence, and eventually loss of the quantum information.
- Error Correction: Generating enough qubits necessary for effective quantum error correction is impractical with current systems, and thus making practical quantum computing challenging.
- Scalability: Due to its need for many qubits and complex infrastructure, building large scale quantum computers for real world application is still difficult.
- Quantum Software: For the most part, building algorithms that take advantage of a full quantum computer is still in its early stages.
- Cost and Hardware Development: For example, it is expensive to build stable quantum hardware, and it requires the hardware to be kept in extreme situations, such as nearly absolute zero temperature, to preserve quantum coherence.

It is these limitations that emphasize the requirement for further advancement to exploit the full potential of quantum computing.

3. Applications of Quantum Computing in Medicine: Drug Discovery

Quantum computing is poised to revolutionize the field of drug discovery. The quantum computers have the potential to revolutionise molecular simulations, enable faster optimization of drug candidates and predict biomolecular behaviour by using quantum mechanics. Below, one explores some of the more recent applications of quantum computing to drug discovery, particularly in the realm of molecular docking, quantum search algorithms, quantum machine learning, and a case study highlighting all these concepts.

Molecular docking refers to a kind of computation, which projects a drug molecule with its target protein. While effective, traditional methods can be time consuming and computationally expensive for large molecules or complex protein structures. These quantum computers, which can process a subset of possibilities all at once, could greatly reduce this process. Grover's algorithm and similar quantum search algorithms have been shown to nearly randomize searches of very large molecular databases. With this capability, a faster identification of possible drug candidates is possible which helps to better understand molecular interactions and that do away with the time spent with the traditional trial and error method. The application of quantum algorithms to accelerate molecular docking by identifying the optimal drug-target interaction are discussed [12]. The researchers showed that quantum search algorithms could predict a broader space of possible molecular configurations than classical algorithms, and that these better predictions could be made for predicting the efficacy of drug molecules.

Quantum machine learning (QML) is a fusion of quantum computations and machine learning approaches to facilitate the processing of big amounts of higher dimensional data more efficiently than possible on traditional computers. QML is applicable to the prediction of drug toxicity, analyzing large biological datasets, and by optimization of drug properties in drug discovery. The QML algorithms are able to process faster the molecular features and biological activity than traditional machine learning models, which demand large amounts of computer resources. Although more work is required, it is possible to build quantum enhanced machine learning models that can learn from molecular structures and then make predictions, for example, drug target interactions, with greater accuracy. They can also help to lessen the computational requirements for simulating how molecules behave in different environments. Others showed that quantum machine learning techniques can be applied to increase prediction ability of molecular properties and accelerate drug discovery [13]. The study combined quantum computing's capacity for working with large datasets with machine learning to demonstrate that QML could outperform standard models for predicting drug efficacy and safety.

An IBM and Pfizer collaboration on the use of quantum computing for the development of new drugs provides a compelling case study in quantum computing and drug discovery (seen from Fig. 1) [14]. Here quantum computers were used to simulate molecular interactions at a level that classical

computers could not achieve. The focus of their collaboration was to discover how quantum simulations could find promising drug candidates for diseases including cancer and infectious diseases. The case study showed how the quantum simulations could mimic complex molecular interactions, accelerating the early stage drug discovery process by allowing researchers to formulate and test a broad array of drug candidates in just a small fraction of the time. The researchers used quantum computers to simulate molecular dynamics, which enabled them to identify drug candidates that would otherwise be very hard to model using classical methods. This case study demonstrates that quantum computing can be used to perform large scale molecular simulation with advantages of accuracy and efficiency compared to traditional computational methods. It's becoming clear where quantum computers can really revolutionize drug discovery, particularly for complex diseases.

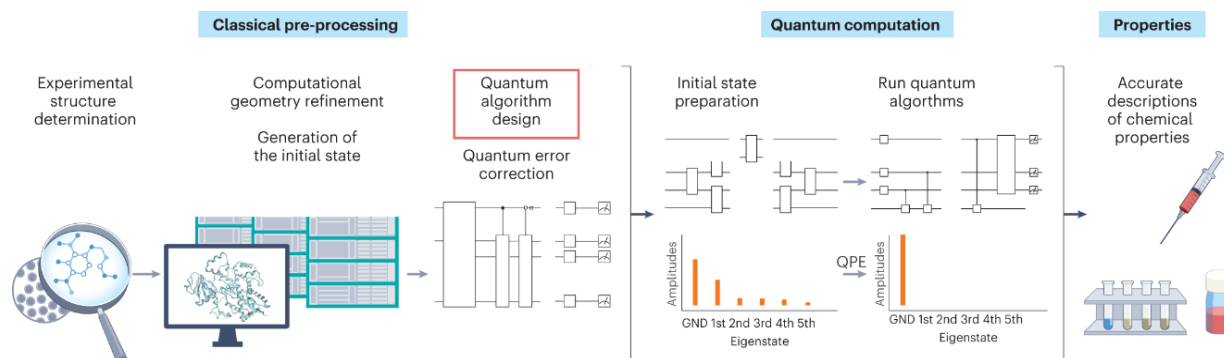


Figure 1. A sketch for quantum computing in drug discovery [14]

4. Applications of Quantum Computing in Genomics

Genomics is rapidly moving from its initial focus on simple sequencing to include computationally intensive processes that require eventual analysis by quantum computing. The use of quantum computers to handle genomic data is a natural application since genomic data involves gestating huge quantities of complex information and quantum computers are able to effectively and efficiently process this information than conventional components. In particular, below, genomic data analysis, quantum algorithms in gene sequence analysis, and the use of quantum computing in propelling personalized medicine are being discussed.

Genomic data analysis is a field that involves processing large datasets, that can be complicated and computationally intensive. The sheer scale of genomic data makes it impossible to work with using traditional computational methods, resulting in long processing times and inefficiency. By exploiting its ability to perform parallel computations, quantum computing provides an alternative that promises faster data processing and efficient analysis. Many of these stages of genomic data analysis, including sequence alignment, gene identification, and pattern recognition can be sped up with the help of quantum algorithms such as Quantum Fourier Transform and Grover's search algorithm. Scholars showed in a significant paper that quantum computing could drastically shrink the time needed to align and compare large genomic datasets; a crucial step in genomic research and applications [15].

Gene sequence analysis is the determination of the order of nucleotides contained within DNA molecule, a requisite to understand genetic variations and mutations. However, for runs on large datasets, gene sequence analysis methods like dynamic programming and hidden Markov models are often computationally expensive and use lots of resources. However, quantum parallelism and interference can be exploited to obtain more efficient algorithms for gene sequence analysis. Quantum inspired algorithms were used to accelerate the sequence matching process and increase genetic variation detection accuracy. Some study has shown that quantum algorithms facilitate faster discovery of gene mutations, something very important in genetic disease research as well as drug development [16].

Quantum computing also offers potential for saving lives in personalized medicine, in which patients receive medical treatment tailored to their unique genetic profiles. It is the ability to process large-scale genetic data at a previously unattainable speed that will lead to the discovery of genetic markers unique to one specific disease. Quantum computers can also be used to simulate how drugs may interact with different genetic mutations, helping to create more effective, personal treatment plans. Quantum computing could enable personalized medicine by helping to develop precision therapies which simulate complex biological systems and predict how genetic variation influences an individual response to treatment. Quantum computing can be utilized to predict the most effective treatment regimens for patients based on their genetic profiles, increasing the rate of success of precision therapies (seen from Fig. 2) [17].

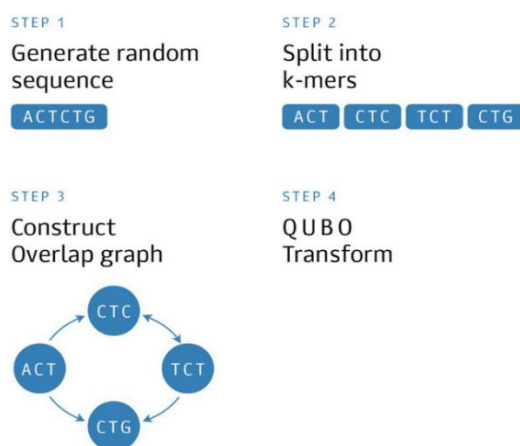


Figure 2. Quantum algorithms in gene sequence analysis [17]

5. Applications of Quantum Computing in Medical Imaging

Medical imaging is no exception among the fields that are taking strides towards quantum computing. Quantum technologies offer a unique opportunity to improve resolution, speed and accuracy in medical imaging techniques, in particular in Magnetic Resonance Imaging (MRI) and Computed Tomography (CT). The potential applications of quantum computers in MRI and CT imaging, quantum imaging technology, and how quantum computers are increasing imaging resolution and refocusing imaging speed are explored in this section.

Quantum imaging is a form of imaging that uses principles of quantum mechanics to generate highly precise microscopic (or subatomic) level images. Quantum imaging, on the other hand, unlike classical imaging methods that rely on light or some other electromagnetic wave detection, uses features of quantum phenomena such as entanglement and superposition to improve imaging capabilities. Quantum imaging can be more resolutional or more sensitive than classical methods by using quantum states such as entangled photons or squeezed light. Along with the recent development demonstrated the use of quantum imaging techniques can enhance the contrast and resolution of medical images. For instance, quantum enhanced optical imaging has the potential of resolving the minute differences in tissue properties that can be critical for early diagnosis of diseases like cancer. Quantum imaging also can help reduce the amount of radiation that is necessary to image, particularly important in medical imaging where patient safety is especially of concern.

MRI and CT imaging are just two useful tools for diagnosing several medical conditions, from neurological disease to cancer. Both methods, however, have the disadvantages of low imaging speed and resolution. For example, MRI typically requires a long time to collect detailed images in subjects with large or complex anatomy. While faster, CT imaging can return lower resolution and higher radiation exposure. However, Quantum Computing has the potential to vastly improve MRI and CT imaging alike by improving image reconstruction rates, processing algorithms, and the overall performance of imaging. Reconstructing MRI and CT images with greater precision and faster has applications for classical quantum algorithms such as quantum Fourier transforms and quantum phase

estimation. Some scholars illustrate that quantum computing could lead to improved MRI image reconstruction via quantum algorithms that reduce noise, improve resolution of images and thereby yield clearer and more accurate diagnostic information. Some of the key limitations in traditional medical imaging, like resolution of the image and the time it takes to scan, can also be addressed by quantum computing [18].

Quantum algorithms can be used to substantially speed up image reconstruction time, reduce noise in imaging data, and increase the clarity and sharpness of the resulting images. One example is quantum enhanced imaging that provides better resolution of detecting smaller lesions or abnormalities within organs and tissues. Medical imaging data can be processed more quickly and more accurately than using traditional methods through quantum algorithms such as quantum machine learning or quantum image processing. The concept would allow scans to potentially be completed more quickly and overall patient experience would be better, and doctors would be able to see clearer, more detailed images on which to base diagnosis. However, recent studies have shown that quantum computing can boost the resolution and accuracy of both MRI and CT scans. Applying quantum image processing could significantly improve the resolution of images recovered by CT or MRI and would accelerate the speed of reconstruction, which in turn would help to speed up diagnoses and improve treatment outcomes [18].

6. Applications of Quantum Computers in Biomolecular Simulation

Biomolecular simulation is a vitally important area of research, especially for protein folding, enzyme dynamics, and drug-target interactions. Typical computational methodologies are demonstrably slow and inaccurate when simulating large biomolecules, such as proteins and enzyme. Fortunately, quantum computing provides a novel way to cope with this by harnessing quantum algorithms to simulate complex molecular systems more efficiently and more precisely. In this section, quantum algorithms for protein folding problems, enzyme dynamics and quantum simulation, as well as drug target interaction simulation are discussed.

Protein folding is an important process of biology for which proteins are adopting a three-dimensional structure that is necessary for its regulation. Predicting protein folding is one of the most difficult theoretical problems in computational biology because there are a very large number of possible configurations for a protein chain. However, the complexity of these calculations makes traditional simulation methods, like molecular dynamics simulations, unable to predict protein structures accurately on a reasonable time scale. Protein folding problem has been addressed with quantum algorithms particularly quantum annealing and quantum machine learning. Using quantum annealing, researchers can use this technique to determine the lowest energy configurations of a protein structure and thereby predict what a protein can fold into in its functional form. Moreover, quantum machine learning algorithms are being developed to speed up and improve protein folding process prediction. Quantum algorithms can simulate protein folding processes with more efficiency and accuracy than classical methods can and it can help provide insight into (disease related) proteins [19].

The movement and interactions of enzymes with substrates in biochemical reactions are known as enzyme dynamics. For drug design as well as to understand metabolic processes, it is essential to understand enzyme dynamics precisely. However, calculation of enzyme dynamics with classical methods could be computationally and statistically expensive, especially for large enzymes with complicated structures. A more accurate and more efficient way to simulate enzyme dynamics is Quantum simulation. By simulating the quantum nature of enzymes, quantum computers can reproject electronic interactions between atoms between the enzyme and its substrate. Researchers apply quantum algorithms, such as the variational quantum eigensolver (VQE), to simulate enzyme reactions by approximately modeling the electronic structure of enzymes, shed light on enzyme catalysis and reaction mechanisms at a finer scale. A study demonstrated that quantum algorithms

can provide orders of magnitude improvements in understanding enzyme catalysis mechanisms, enabling new ways to discover drugs and engineer metabolism [20].

Developing effective treatments requires to understand the interactions between drugs and their target biomolecules. Like molecular docking, traditional computational methods struggle to simulate the binding of small molecules to large biomolecules like proteins and nucleic acids. Usually these interactions at the atomic level cannot be simulated accurately and quickly enough on classical computers. More accurate representations of molecular interactions can be provided by quantum computing in drug target interaction simulations. By simulating the electronic properties of both the drug molecules and their target biomolecules, quantum algorithms like quantum Monte Carlo and quantum machine learning can model interaction between drugs and their targets. This facilitates drug screening and allows researchers to explore how drugs bind to their targets, and to predict their efficacy before undergoing clinical trials. Others have shown that quantum computers can be used in place of simulating drug-receptor interactions to make faster and more precise binding affinity predictions [21]. These simulations will be useful for accelerating drug discovery process and designing an optimized drug as given in Fig. 3.

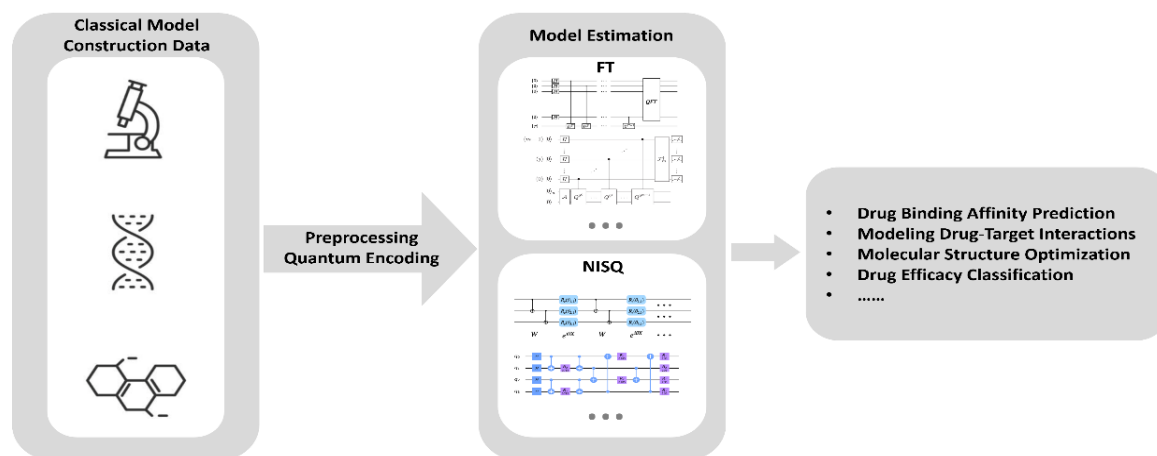


Figure 3. Quantum-machine-assisted drug discovery with survey and perspective [21]

7. Applications of Quantum Computers in Public Health

Quantum computing has the potential to revolutionize understanding and management of epidemic diseases, disease transmission models and vaccine development in a public health critical area. Quantum computing has the potential to process large amounts of data and simulate complex systems in a way that would not be possible with classical computing techniques, enabling the discovery of insights that would have been considered unfathomable using this type of computers earlier. In this section, how quantum computing may be used to model epidemic diseases, predict outbreaks and create vaccines is discussed.

Disease transmission models are fundamental for prediction of disease spread within populations, which is critical for the management of outbreaks and the prevention of disease spread wide. Classical computing approaches are employed to simulate disease spread in traditional epidemiological models. Nevertheless, these models can lead to excessive computational burden and fail to adequately describe complexities of real world scenarios for disease with highly dynamic behavior. On the other hand, quantum simulation can allow the modeling of interactions between any of the different factors that influence disease transmission: population movement, contact rates, environmental influences, etc. Disease transmission models that are simulated with higher precision and computational efficiency are being carried out with the use of quantum algorithms, such as quantum Monte Carlo and quantum annealing. They can help public health officials predict the course an epidemic might take and prepare to arrest its spread. A study showed how quantum computing could be used to simulate spread of an infectious disease such as influenza, within a population. Results indicated that

quantum simulation could capture interactions that were too complex to be revealed by classical methods, revealing insights into disease spread dynamics [22].

One of the most important aspects of epidemic management is the ability to predict potential outbreaks and develop effective control strategies. Classical predictive models often struggle with the inherent complexity and uncertainty of disease spread, especially when there are multiple factors interacting in non-linear ways, such as genetic variation, immunity, and environmental factors.

Quantum computing offers a new paradigm for predictive modeling. Quantum algorithms, particularly those based on quantum machine learning and optimization techniques, can process large datasets more efficiently and find patterns that are not immediately apparent with classical approaches. Quantum machine learning can identify correlations in large epidemiological datasets, which can help predict when and where an outbreak might occur. Additionally, quantum optimization can be used to devise the most effective control strategies, such as vaccination campaigns or social distancing measures, by analyzing different intervention scenarios and their potential outcomes. Some scholars investigated the application of quantum computing in predicting outbreaks of infectious diseases like COVID-19 [23]. They found that quantum algorithms could be used to forecast disease spread more accurately and provide real-time predictions, which would significantly improve response times during outbreaks.

Vaccine development is a lengthy and complex process that involves extensive research, testing, and clinical trials. Classical computational methods have been used to identify potential vaccine candidates, but these methods are limited in their ability to process large datasets and predict the effectiveness of new vaccines. Quantum computing, with its ability to simulate molecular interactions at the quantum level, offers a powerful tool for accelerating vaccine development. Quantum computers can model the interactions between antigens and immune system receptors with greater precision, identifying potential vaccine candidates more efficiently. Quantum machine learning can be used to analyze genetic sequences and predict how the immune system will respond to various pathogens. Moreover, quantum simulations can help researchers design more effective vaccines by simulating how the immune system might react to different antigenic structures, reducing the need for time-consuming trial-and-error processes. A recent study demonstrated how quantum computing could be used in the development of COVID-19 vaccines by simulating the spike protein of the virus and identifying potential binding sites for vaccine candidates [24]. The study showed that quantum computing could accelerate vaccine development by providing faster and more accurate simulations of viral proteins.

8. Limitations and Prospects

Quantum computing holds great promise for revolutionizing medicine, but several limitations must be addressed before its widespread application in healthcare. Current quantum processors are limited to a small number of qubits. For practical medical applications, such as drug discovery, genomics, and medical imaging, processors need to scale to thousands or millions of qubits. Advancements in qubit stability, error correction, and efficient quantum gates are essential for quantum computing to reach its full potential in medicine. While quantum algorithms show promise, their implementation in medical fields remains challenging. These algorithms need to be optimized for specific medical applications and real-time use, requiring collaboration between quantum scientists and medical professionals. Current algorithms are still in the developmental stage and must be adapted to medical requirements.

Quantum computing could render current encryption methods vulnerable, posing risks to sensitive medical data such as patient records and genetic information. Quantum-safe encryption techniques must be developed to ensure the security of patient data in a quantum-enabled healthcare system. Quantum computing is a resource-intensive technology, potentially leading to disparities in healthcare access. The high costs associated with developing and maintaining quantum systems could

widen the gap between developed and developing countries. Policymakers must ensure that quantum healthcare advancements are accessible to all populations.

Quantum computing could significantly accelerate drug discovery and personalized medicine. By providing deeper insights into biological systems, it may lead to breakthroughs in disease prevention and treatment. However, these advancements require continued progress in quantum hardware, algorithms, and integration with medical technologies. The Need for Interdisciplinary Collaboration: To unlock the potential of quantum computing in medicine, interdisciplinary collaboration is essential. Experts from quantum computing, healthcare, and policy must work together to develop solutions that address medical challenges and ensure ethical, equitable implementation. This partnership will be crucial for improving patient outcomes and advancing medical science.

9. Conclusion

To sum up, this study has explored the potential applications of quantum computing in medicine, focusing on areas such as drug discovery, genomics, medical imaging, biomolecular simulations, and public health. The results highlight the transformative potential of quantum technologies in solving complex medical challenges, from accelerating drug development to enhancing diagnostic imaging and optimizing personalized therapies. However, significant challenges remain in the scalability of quantum hardware, algorithm optimization, and ethical considerations such as data privacy and equitable access. Looking ahead, the future of quantum computing in medicine holds vast potential, but it is crucial to continue advancing both the technology and its integration with medical research. Further interdisciplinary collaboration between quantum scientists, healthcare professionals, and policymakers will be essential to unlock the full potential of quantum computing and ensure its responsible and widespread application in healthcare. The significance of this study lies in its exploration of the future of quantum technology in medicine, which could revolutionize patient care, healthcare delivery, and medical research. However, continued research and development are necessary to overcome current limitations and realize its transformative potential in the medical field.

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