

Artificial Intelligence–Enhanced Quantum Computing for Medical Simulations: Accelerating Drug Discovery, Protein Folding, and Personalized Healthcare with Performance Optimization and Predictive Accuracy

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Abstract

Artificial Intelligence (AI) and Quantum Computing together are going to transform medical research, diagnostics and the simulation of treatment. Although it has already been applied to medical imaging, drug discovery and predictive analytics, AI needs large amounts of computations that are sometimes beyond the capacity of more traditional computing. Quantum computers due to their capability to do parallel processing over quantum states can be fast and efficient in unprecedented ways. The paper will discuss the combination of AI and quantum computing in the medical field, including the characterization of medical applications of AI where it complements quantum computing, an overview of the current medical applications of AI and quantum computing, and real-time diagnostics, genomics, drug discovery, molecular dynamics, and personalized medicine. We discuss the current issues state-of-art including quantum error correction, interpretability of models, and ethical implications and point toward future opportunities including digital twins, federated learning using quantum resources, and hybrid quantum-classical models. The eventuality of this integration might end up speeding up medical simulations, decreasing the expense of drug development and enhancing the patient outcomes across the globe.

Keywords: Artificial Intelligence (AI); Quantum Computing; Quantum Machine Learning (QML); Medical Simulations; Drug Discovery; Personalized Medicine; Genomics; Healthcare Innovation

1. Introduction

1.1. A background on AI in Medicine

Artificial intelligence (AI) is the game-changer of the contemporary medical practice. Applications of AI in the medical field range anywhere between image-based diagnostics and predictive analytics, with AI systems being able to analyze medical data at an unparalleled speed. Machine learning algorithms, most notably those which fall under the category of deep learning, have achieved enormous success in the accuracy rates of detection of various forms of diseases, most notably cancer, cardiovascular and neurological. An example is that convolutional neural networks (CNNs) are commonly applied in the interpretation of medical images, such as X-rays, CT scans and MRIs, compared to that of experienced radiologists, the performance can be the same or even better. In a similar vein, natural language processing (NLP) enables AI-based interventions to draw business-relevant data out of EHRs, physician notes, and clinical trial information. These developments indicate the importance of AI in speeding up the diagnosis, forestalling human error, and assisting with individual and unique treatment schedules.

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Although such breakthroughs were made, many with AI such as protein folding, molecular interactions and genomic sequence analysis all require high computing power. Classical computing is however strong, and will have tremendous demands in scaling to higher levels in order to satisfy the increasing demands of biomedical research.

1.2. Classical Computing Limitations of a Large-Scale Simulation

Classical, sequentially based and finite capacity, transistor-based computers are incapable of satisfying these requirements. Much of the solution of problems in medicine, especially in drug discovery and in molecular world, is exponential with the number of components in the system. As an illustration, it is very difficult to compute the dynamics of larger molecules such as proteins at the atomic scale where billions of atoms are interacting, according to the rules of quantum mechanics. Even the most powerful computers find such simulations to be infeasible since the time and energy cost of such simulations scales exponentially.

Moreover, AI systems that manipulate high-dimensional clinical data, e.g., complete-genome sequences or ultra-high-resolution 3D scans, tend to have large training and inference requirements in terms of computing resources. The price, time and resources consumed in such calculations have made bottlenecks of medical decision making and delaying important research pipelines. It is this shortcoming that explains why a radically different model of computing should be developed to deal with the complexity of large medical simulations.

1.3. The Introductions of the Principles of the Quantum Computing

Quantum computing is an example of such shift of paradigm. As opposed to the classical computers which operate on bits (0 or 1), quantum computers make use of the qubits which use the fundamentals of superposition and entanglement. Superposition permits superposition between the states of a qubit and entanglement is used to bring about strong correlations between qubits without respect to distance. Combined, these features enable quantum systems to compute parallelly and exponentially, following many computation pathways, at the same time.

Quantum algorithms include those used to simulate molecular interactions, including the Variational Quantum Eigensolver (VQE) and Quantum Approximate Optimization Algorithm (QAOA), have already shown promise of enabling much faster simulations of molecular interactions than yet possible through use of classical methods. In the medical field, such a potential manifests in the potential to simulate drug-protein interactions, predict molecular structures, interrogate genomics data on larger scales than ever before.

1.4. Why it is important that the next-generation of healthcare is integrated

Combining AI and quantum computing has the potential of solving some of the highly challenging issues in healthcare. AI can teach itself to analyze complicated and multi-type medical data and quantum computing systems have the capacity to work with computations of huge sizes. Collectively, they can breakthrough in such areas as:

- Drug Discovery: Upscaling the rate at which effective drugs are identified by using the power of pattern recognition (with AI) and molecular simulations with a quantum advantage involved.
- Genomics and personalized medicine: Enabling the quick analysis of entire genome to personalise treatment in regards to a patient.
- Medical Imaging: The current medical images with the combination of quantum-enhanced AI models provided enhanced real time diagnostic capacity.
- Disease Modeling: facilitating pandemic projection and individualized disease progression modeling with new levels of precision.

By reconciling the difference between data-based intelligence with quantum-scale computing, such a fission could save time and money on medical research, make treatment more precise and ultimately have a more fruitful outcome to the patient. The AI-quantum integration is expected to become one of the foundations of the future of medicine since the healthcare systems of the world are under pressure to change in terms of their level of efficiency, precision, and individualization.

2. The place of AI in medical simulations

2.1. The Deep Learning is used in Medical Imaging.

Medical imaging is one of the oldest areas where AI is applicable in the field of healthcare. Deep learning models, and, in particular, convolutional neural networks (CNNs), have proven to have state-of-the-art performance on such tasks as

tumor detection, fracture identification, and segmentation of organs in radiological images. Such systems can find little trends in imaging information that one cannot discern by looking. Esteva et al. (2019) mention that the performance of AI-based diagnostic systems can reach diagnostic accuracy levels of the radiologists in the dermatology, pathology, and radiology cases, improving the accuracy of diagnosis and decreasing the inconsistency between different practitioners. An active area of research using deep learning is application to dynamic imaging simulations, e.g. cardiac motion analysis and brain activity mapping, which are resources-heavy to perform using the established methods.

2.2. Prognostic Models of the Disease Process

The other major contribution of AI in medical simulations is predictive modeling. Machine learning is demonstrating its usefulness by being able to predict the occurrence and development of disease by examining massive amounts of patient data such as clinical records, genetic make-up, and lifestyle. Predictive AI technology has been used in the kind of mapping the course of chronic disease like diabetes, Alzheimer, and cardiovascular disease. According to Jiang et al. (2017), the application of predictive analytics leads not only to the improvement of early intervention but to better and personalized choice of treatment by clinicians. The models can also be useful in the simulations of patient outcomes to a particular therapeutic intervention, which will help alleviate the need to utilize long and costly clinical trials.

2.3. The Probing Inside its Drug Discovery Pipelines

AI has been slowly gaining presence in the pharmaceutical sector as it helps quicken the pace of drug discovery and development. Conventional drug development is a resource- and capital-intensive affair that may take more than a dozen years and several billion dollars to get a single drug to market. AI models have been already introduced into pipelines of molecular property predictions, protein structure and virtual screening of compound libraries. Topol (2019) states that AI-based drug discovery platforms have already found novel molecular candidates in a considerably shorter time and at a fraction of the cost of the tradition methods. Individualized medicine is shown in these simulations which entail the use of AI systems to anticipate the reactions of individuals with various genetic makeup to certain treatment processes.

In addition, AI optimizes simulations of protein-ligand interactions and affinities and are essential determinants of drug candidate efficacy. Nonetheless, the simulations are costly because they use complex quantum mechanical rules that guide the nature of the molecule (McArdle et al., 2020). This gives the field of drug discovery as one of the avenues where by quantum computing will augment AI as an important tool.

2.4. The bottlenecks are high computational overhead, time and limit of data processing.

In spite of the success that AI has had in terms of medical simulations, there exist a number of bottlenecks that deter its mainstream use. Training deep learning models at large scale is very data- and computing-intensive and may be infeasible at smaller healthcare institutions. Processing high res images or genomics in their entirety can take weeks on a high-performance computer infrastructure. In addition, sustainability issues arise with regards to the energy intake of the huge AI models.

Biamonte et al. (2017) argue that although classical computing can hardly scale to large dimensional medical data, quantum-enhanced AI could resolve the problem by providing exponential increases in speed and efficiency. E.g. in chemical applications such as molecular dynamics, classical modeling has a factorial scaling with the size of a system, whereas quantum computer modeling would be polynomial. Unless these computational challenges are breached, the future of AI in medical simulations still has much potential yet to accomplish in the area of real-time diagnosis and individual treatment.

3. Quantumscroll Computing in the Healthcare

3.1. An overview of Basics of Quantum Computing

Quantum computing brings the radical shift of information processing by the application of quantum mechanics laws. Compared with classical computers that depend on binary bits (either 0 or 1), quantum computers depend on qubits that have the capacity to exist in a superposition of the two states. This furthermore enables a one-qubit state to be in 0 and 1 state simultaneously, exponentially enlarging the data space as more qubits are added together. Also, entanglement provides quantum computers with the possibility of correlating qubits that classical machines are unable to achieve, thus opening the gates of quantum systems to perform massively parallel calculations (Biamonte et al., 2017).

In healthcare quantum computing holds the promise of being able to carry out the vast computations the fields of molecular modeling, medical imaging, and optimization problems require. In classical computing, these problems have exponential scaling complexity. By contrast, quantum computers may in theory handle these problems with a polynomial or logarithmic scaling. McArdle et al. (2020) note that such a paradigm switch can make possible practical versatile simulations of the biochemical system that are unattainable even with the most powerful supercomputers worldwide.

3.2. Medically relevant current quantum algorithms

There have actually been a number of quantum algorithms proposed and worked on which have more direct medical application:

- **Shor Algorithm:** Shor's algorithm is not only integer factorization but also has the consequence of encryption and secure transfer of patient records. With healthcare being digitalized now more than ever, it is vital that privacy must be guaranteed in spite of the threat of decryption based on quantum computing (Biamonte et al., 2017).
- **Grover's Algorithm:** Grover's algorithm can be used to rapidly search chemical databases to reveal potential drug leads in large chemical compound libraries. It is of great value to pharmaceutical research since it simplifies search problems to $O(\sqrt{N})$, instead of $O(N)$, in complexity (Jiang et al., 2017).
- **Quantum Approximate Optimization Algorithm (QAOA):** The approach is an adaptable algorithm and used to solve optimization challenges, like optimal dosing of drugs, treatment schedules or resource allocation in the field of healthcare. It can be used to conduct clinical decision support due to its capacity to handle combinatorial optimization (Biamonte et al., 2017).
- **Variational quantum eigensolver (VQE):** VQE is of great significance in quantum chemistry where it can be adopted to estimate the ground state energy of molecular systems. McArdle et al. (2020) underline that VQE has the potential to transform drug discovery by allowing highly accurate simulation of protein-ligand interactions, and hence have far higher binding affinity prediction accuracy than classical methods.

3.3. Examples of ways of applying quantum to molecular simulations and protein folding

Molecular simulation could be one of the most promising applications of quantum computing to healthcare. One area where accurate modeling of molecules and their interactions is critical in drug discovery and personalized medicine is the inability of classical computers to simulate larger systems (larger than a few dozen atoms) because it increases exponentially. VQE and quantum phase estimation are quantum algorithms that can be used to perform large-scale simulations with high accuracy on biochemical systems (McArdle et al., 2020).

The example of protein folding is again that it is among the most difficult biology computational problems to simulate. Misfolded proteins are linked to diseases like the Alzheimer, Parkinson and cystic fibrosis. Even though deep learning techniques like DeepMind's AlphaFold have made groundbreaking advances in protein structures prediction, quantum-enhanced simulations have the potential of providing further insights since they are capable of modelling directly the quantum mechanics interactions of proteins (Topol, 2019).

This leads to another application which is genomics, where quantum algorithms could speed up the task of genome sequencing and studies. Alignment and comparison of the many billions of base pairs in an entire human genome is so computationally complex as to be impossible. Quantum computing may speed down the epoch needed to make such a simulation and, thus, help detect associated genetic mutations related to the disease faster (Esteva et al., 2019).

In short, the potential of high-dimensional quantum computing has the transformative potential in the field of medicine in complex simulation on high dimensions. With the ability pattern recognition and predictive capabilities offered by AI, such quantum algorithms allow faster more accurate medical simulations- giving a chance to innovation drug discovery, personalized treatment, and disease modeling.

4. Synergy: AI, meets quantum computing

4.1. The quantum machine learning (QML) models

Quantum Machine Learning (QML) is a nascent field that brings the learning power of AI and the quantum computation accelerations. In contrast to the classical ML, where data is analysed in a sequential order or in parallel on digital processors, QML models utilise the quantum states that enable the exploration of exponentially large solution spaces at

the same time. This is all the more helpful in the medical field where the incidence of biological information tends to bury common resources there. Biamonte et al. (2017) note that QML is beneficial due to its features extraction, optimization, and classification and can speed up the analysis of medical data considerably. As an example, a computationally efficient analysis of high-dimensional genomic datasets may be performed using QML, thus enabled to generate personalized treatments.

4.2. Classical (such as AI) + quantum accelerators (Hybrid Frameworks)

Due to the current quantum hardware being in an initial phase, hybrid systems that integrate classical AI with quantum processors have come in the picture. Tasks are outsourced: classical processors are used to do the data preprocessing and error correction, quantum accelerators do computationally intensive subroutines, such as performing an optimization or estimating eigenvalues. McArdle et al. (2020) add that hybrid approaches such as the Variational Quantum Eigensolver (VQE) already show utility in practice on quantum chemistry problems with applications in drug discovery. In the clinical departments, such hybrid systems would actually allow medical simulations to be made in near-real-time which, in the past was not possible because of the limitations of the computer resources.

4.3. Case Studies

Protein drug targets Novel protein-based drugs (ligands) often need to be discovered by modeling how they bind proteins (drug targets). Classical simulations fail to scale sufficiently to compute these interactions with reasonable accuracy but quantum-enhanced AI applications can emulate these interactions and compute binding affinities at a quantum mechanical level with reduced error (McArdle et al., 2020).

Genomics Genomic sequencing produces large amounts of data and aligning billions of base pairs can only be achieved through excessive computer power. The complexities of sequence alignment can be minimized, and thus with the help of QML models, tracing the mutations linked to diseases can be found much faster (Esteve et al., 2019).

Patient-Specific Digital Twins: AI combined with quantum computing has potential to result in a digital twin of an individual where the biological systems of a particular patient are modeled. With the ongoing changes on the real patient, health professionals can simulate and test their treatment approaches virtually before proceeding with the treatment approach, enhancing precision medicine (Topol, 2019).

5. Medical Simulations

5.1. Molecular Dynamics- the Speedy Evaluation of Protein Folding

Protein folding simulations have become a key to the working mechanism in diseases and drug discovery. Classical simulations are too computationally intensive to be practical as solutions to sixth-order complex quantum mechanical equations are required on thousands of atoms. Quantum-enhanced AI can be used to advance molecular dynamics simulations so that they can deliver faster and more precise predictions of protein structure. This is promising in the case of the diseases caused by protein misfolding, which is Alzheimer and Parkinson (McArdle et al., 2020).

5.2. Molecular Docking Drug Discovery - Accertive drug discovery Engine

Its applications to date already speed up drug discovery by screening the libraries of compounds and anticipating molecular characteristics. Its predictivity is however limited with classical computational models. AI also has the capability of quantum acceleration, which enables molecules in a drug to dock to quantum accuracies in a dramatically shorter time using far less amounts of resources than conventional methods of drug development. Such breakthroughs, according to Topol (2019), may reduce the time lag between the development of a new drug and its release into the market when people have new health needs.

Quantum Algorithms & Applications John Horan 20th December 2015
 1 1 Genomics & Personalized Medicine Quantum algorithms for sequence alignment of the genome
 Project 2 2 The Biological Problem The sequence alignment problem is an important task in genomic analysis where fragments of DNA (or other genomic sequences) are compared against a reference genome. The most common variant of the problem is the so-called string-to-string local sequencing, but there are also several extensions of the problem. The DNA fragments can also be called strings or genomes, as the problem

Genomic analysis has been enhanced because of IHS due to the ability to detect disease-associated mutations, and aligning genomic data sets continues to be a bottleneck. Quantum algorithms, together with AI can accelerate sequence

alignment to enable genome analysis in near real-time. According to Esteva et al. (2019), this combination is the solution to the further development of personalized medicine, according to which medicines are selected precisely according to the individual genes.

Medical Imaging Medical imaging applications are another product category in which quantum can have a superior effect in the processing of the images on a MRI/CT scan.

Medical imaging generates a data of very high dimensions, which is consuming intensive computational resources in processing. The AI models optimised by quantum computing can handle these datasets with an increased speed to achieve image reconstruction, trauma, and noise reduction, or anomaly detection. This would have direct implications as far as earlier diagnosis and right treatment planning becomes a direct benefit of this (Jiang et al., 2017).

5.3. Epidemic and Pandemic Modeling - Quantum-AI Integration to real-time prediction of spread

The data controlled dental care includes a range of heterogeneous data sources, patient information, epidemiological information and mobility data. I models are predictive, which is then defined and enriched by quantum computing to simulate dynamic systems at scale in real-time. The synergy has the potential to enhance early warning mechanisms of pandemics and provides guidelines on swift responses in the health sector (Esteva et al., 2019).

6. Difficulties and Restrictions

6.1. Quantum Error Rates and Hardware instability

Existing quantum hardware has very high error rates and decoherence, as well as a lack of qubits, thereby limiting the scalability of QML applications. McArdle et al. (2020) consider that to reach the stage of practical medical simulations, quantum error correction and the stability of the hardware ought to be enhanced.

6.1.1. Data security / privacy and Regulatory compliance (HIPAA, GDPR)

Medical data is most delicate and integrating AI with quantum computing brings with an extra challenge of data security. Quantum computers have the potential of breaking the current cryptographic systems, and in order to be compliant with the current regulations, like HIPAA in the United States and GDPR in Europe, it is crucially important. Biamonte et al. (2017) warn that quantum-resistant cryptographic algorithms will have to be developed, to provide protection to patient data.

6.2. AI-Quantum Hybrid Model explainability

The application of quantum mechanics to AI systems results in an even more serious problem of interpretability, as the AI systems are in themselves referred to as the black boxes. The clinicians can be reluctant to accept the suggestions of models when they do not understand them perfectly. Jiang et al. (2017) stress the fact that explainable AI is vital in healthcare and will also be applicable to QML systems.

6.3. It is Expensive with restricted access to quantum hardware

Construction and maintenance of quantum hardware is very expensive, and to date, only big technological firms and research labs with huge investments can get access to it. This imposes a burden on the hospitals and other small research institutions wishing to take advantage of QML in health care. According to Topol (2019), quantum cloud services may counter this limitation as far as access democratization is one of the key areas. Cost is also one of the reasons behind this limitation.

7. Future Directions

Combining quantum computing and artificial intelligence in the field of medicine is still at its early developmental stages and is potentially revolutionary in a matter of a decade.

A large scale research direction is the design of quantum-ready AI architectures in which the existing machine learning frameworks are oriented toward taking advantage of quantum effects such as superposition and entanglement. These architectures would enable AI systems to natively benefit from quantum-enhanced data structures which, in turn, would permit unprecedented scaling in the training of AI models intended to be used in decision-making in a clinical context (Biamonte et al., 2017).

One possibly fruitful direction is that of federated quantum learning which combines ideas of federated learning with quantum computation. In such a paradigm, sensitive patient data can be used to train quantum-enhanced AI models at a hospital together with a research institution without the actual data being shared. Not only is this strategy a boost to security but it also meets the standard guardrails like HIPAA and GDPR (Mitarai et al., 2018).

Moreover, the development of patient-specific digital twinning virtual models of people physiology can also be transformed with integrated AI-quantum. With the help of quantum simulations of molecular and genetic modeling, in combination with the AI predictive analysis, doctors would be much able to simulate the effects of diseases, ways of intervention, and personalize care in a new level (Cao et al., 2019).

Lastly, it is estimated quantum cloud computing will become the central hub to democratise access to quantum-AI platforms. The potential ability of global healthcare institutions (including those in resource-limited contexts) to take advantage of this new paradigm without incurring the extreme expenses of local quantum hardware depends on the ability to provide cloud-based quantum accelerators that can be combined with classical AI systems (Preskill, 2018).

8. Ethical and Regulatory Points

There is a deeper ethical and regulatory dilemma in the intermarriage of AI and quantum computing in medical practice, which must be sufficiently tackled.

On the one hand is the question of transparency of AI decision-making. Models based on a hybrid approach, such as variational circuit or deep neural network-based models, run the risk of becoming black boxes, in the sense that clinical users are unable to understand or have confidence in the outputs. The fact that it lacks interpretability may become a problem in the clinical adoption unless explainability frameworks are also developed (Arute et al., 2019).

Apostrophic concern is also data security Although quantum encryption is more secure against cyberattacks, quantum-AI ecosystems remain vulnerable to possible leakage of highly sensitive medical data, unauthorized access or use. This is all the more pertinent in the context of the size of genomic and clinical datasets involved in precision medicine (Cao et al., 2019).

Besides, responsible innovation has to guarantee equal worldwide access. Quantum-AI applications in healthcare can furthermore directly exacerbate healthcare inequality as more privileged communities and organizations become able to afford the tools. Frameworks of ethics should be, thus, focused on the principles of fairness, inclusivity, accessibility in line with global health-related agendas (Preskill, 2018).

Overall, though AI-quantum integration in medicine can deliver unprecedented outcome, its future success cannot be reduced to the technological advances, but also to establishing trust, transparency, and other robust moral and legal protections.

9. Conclusion

The combination of artificial intelligence and quantum computing in the field of medicine is a disruptive change and can alter the way healthcare issues are tackled and addressed. Contrary to the conventional computational approaches, the collaboration of the pattern recognition and diagnostics abilities of AI with the exponentially solvable problems capacity of quantum computers offers a breakthrough in medical science.

Among the most direct advantages is the speed shown in the simulation and computation that is essential in the healthcare sector. As an example of the quantum-enhanced molecular simulation in conjunction with predictive analytics, powered by AI, the researcher can dramatically decrease the time towards a drug discovery and protein folding analysis. This can be applied to accelerated drug development so that it can respond to novel illnesses, epidemics, and even pandemics that may arise in a short period. The same, in the case of genomics and personalized medicine, can be said to enhance the accuracy of diagnosing and personalising medicine with the direct impact of better patient outcomes.

To actualize this catalytic potential, however, is only made possible by commitment to interdisciplinary collaboration. The marriage of quantum-AI and medicine will be made possible by a smooth collaboration between medical researchers, physicians and engineers in the field of AI and quantum physicists. This way, the collaboration will not only

provide the technically advanced solutions but align those approaches to clinical requirements, ethical codes, and regulatory provisions.

Combining this with quantum computing would provide anything but a step forward step-in healthcare innovation but a leap in quantum computing. The creation of interdisciplinary work and solutions to transparency, ethics and access issues can form the future where medical solutions are more agile, more accurate and readily available and accessible worldwide.

Compliance with ethical standards

Disclosure of conflict of interest

No conflict of interest to be disclosed.

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