Quantum Computing for Personalized Immunotherapies in Neurological Autoimmune Diseases

Tashvi Pragnya Pasupulati

tashvi.pasupulati@gmail.com

Research Question: Exploring the potentials of quantum computing for personalized immunotherapies in neurological autoimmune diseases

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Abstract

Quantum computing offers transformative potential for the future of biomedicine and patient specific treatment plans by addressing the complexity and scale of patient-specific data. Neurological autoimmune diseases such as multiple sclerosis, neuromyelitis optica spectrum disorder, and autoimmune encephalitis present significant challenges to treat due to their different onset in patients and limitations of current immunotherapies. Quantum algorithms such as Variational Quantum Eigensolver, Quantum Approximate Optimization Algorithm, and Quantum Machine Learning enable precise molecular simulations, high-dimensional biomarker discovery, and integration of genomic, proteomic, and imaging data that would allow personalized treatments to individual immune signatures, as apposed to generalized treatments and simplified computational models. This review synthesizes recent progress in applying quantum computing to biomedical research and highlights its specific applications in neurological autoimmune diseases, ranging from drug discovery and biomarker identification to diagnostic imaging and adaptive treatment strategies. While current limitations in hardware scalability, error rates, clinical approval remain barriers, ongoing advances in quantum technology and cross-disciplinary collaboration are paving the way for quantum-enhanced personalized immunotherapies.

Introduction

In classical computers the smallest unit of information is known as a bit which exists in two possible states, either 0 or 1. However, in quantum computers the smallest unit of information is known as a quantum bit or a qubit. These qubits exist in what is called a superposition state where they can be both 0 and 1 at the same time with certain probabilities for each. For example a 3 bit classical system can represent one of 8 states at a time but a 3 qubit system can represent all 8 states at the same time. This parallelism makes it significantly faster compared to classical computers which process inputs one at a time.

Another quantum property is entanglement which is when two or more qubits are linked in a way that the state of one qubit is directly related to the state of the other(s) no matter how far apart they are. Entanglement allows the quantum computer to perform coordinated operations over multiple qubits allowing high efficiency compared to classical computers.

These properties are extremely valuable particularly in the medical field where researchers and physicians handle vast amounts of highly complex data such as a patient's full genome, highly intricate protein structs, and the dynamic activities of the immune system. Even a minor change in one component such as a genetic mutation can have a significant impact on biological processes. Classical computers struggle to analyze and connect all these factors in time to give truly individualized treatments and even with powerful artificial intelligence capabilities, these models still require to be simplified which limits their accuracy.

Quantum computers on the other hand use advanced algorithms such as Variational Quantum Eigensolver and quantum machine learning to detect the patterns between biological molecules in large medical datasets. This makes it possible to run more realistic and comprehensive molecular simulations regarding how a specific mutation may impact protein folding or how a new medication might interact with a protein, thereby improving individual treatment plans.

Neurological autoimmune diseases such as multiple sclerosis, neuromyelitis optica, and autoimmune encephalitis are particularly challenging to treat as they can be different in each patient. Personalized immunotherapy would allow the design treatments to each patient's unique immune profiles rather than using the same treatment for every patient. Quantum computing has the potential to analyze many types of patient data and simulate immune system interactions with medications in detail to help make therapies more accurate, faster to develop, and more suitable for individual needs.

This review looks at current research combining quantum computing and personalized immunotherapy, focusing on how these ideas could be used for neurological autoimmune diseases. It covers areas such as drug discovery, quantum algorithms, improving diagnosis, and optimizing treatment plans, while also discussing the challenges and future possibilities.

Methodology

The literature review was conducted using academic databases such as Pubmed, NIH, SpringerLink, and Google Scholar. Search terms included combinations of keywords such as "quantum computing," "neurological autoimmune diseases," "personalized immunotherapy," and "quantum algorithms in healthcare." Included sources were peer-reviewed journal articles and conference papers published between 2015 and 2025 to ensure coverage of the most recent advancements. Articles were selected if they addressed both quantum computing methods and biomedical or immunotherapy applications. Abstracts were screened for relevance, and after a full-text review, 13 key sources were selected for their depth, credibility, and applicability to the research objectives.

Overview of Quantum Computing in Biomedicine

Several important quantum algorithms such as Variational Quantum Eigensolver (VQE), Quantum Approximate Optimization Algorithm (QAOA), and Quantum Machine Learning (QML) are already being explored for biomedical research. The Variational Quantum Eigensolver is used to find the lowest ground state energy of a molecule which signifies the molecule's most stable structure. The molecule is converted into a hamiltonian which is an equation used to describe the molecule's energy. The VQE algorithm works by running the hamiltonian through a quantum circuit with adjustable parameters called an ansatz that is used to approximate the energy of the molecule according to its parameters. A classical computer is then used to adjust the ansatz parameters Ising optimization meteors such as gradient descent and the circuit is run again. This process repeats multiple times until the algorithm identifies the lowest possible energy. The Quantum Approximate Optimization Algorithm is another method to find the most optimal ground state energy of a molecule. For the QAOA, scientists model all the possible shapes and binding positions of a molecule as a mathematical graph where the nodes represent the possible configurations of a molecule and the edges represent the possible transitions between configurations. Each configuration corresponds to an energy score. This graph is then converted into a hamiltonian that maps out the molecule's energy landscape. The QAOA algorithm uses a quantum circuit with adjustable parameters to test all the configurations. a classical computer is used to adjust these parameters until the lowest ground state energy of the molecule is found. Quantum machine learning helps identify patterns that classical computers struggle with given the nature of the highly complex molecular data. Quantum machine learning uses information about molecules such as their atomic positions, bond angles, and electron interactions to convert them into quantum states through quantum feature mapping. This allows the quantum computer to identify all possible configurations of the molecule. Then a quantum algorithm such as a variational quantum classifier or quantum kernel method is trained to identify and explore many patterns in these quantum states in parallel. The trained algorithm is then used to predict drug candidates and optimize molecular structures faster and with more accuracy. Quantum algorithms and simulations are able to represent and predict binding affinities, reaction pathways, and conformational changes with high precision as they don't rely on approximations or classical molecular dynamics. When these algorithms are applied to datasets such as genomics, proteomics, transcriptomics, and metabolomics, they can process and correlate extremely high-dimensional data, revealing clinically significant biomarker patterns that may not have been revealed by classical methods. For example, quantum convolutional neural networks would be able to detect microcalcifications in mammograms or segment tumor boundaries in MRI scans faster. Such high-fidelity modeling methods will shorten lead optimization cycles, reduce having to rely on trial-and-error lab testing, and reduce cost and time in preclinical development.

Personalized Immunotherapy for Neurological Autoimmune Diseases

Personalized immunotherapy is an approach that could significantly enhance the management of neurological autoimmune diseases neurological autoimmune diseases are conditions where a person's immune system mistakenly attacks their own brain, spinal cord, or nerves. Some common examples of neurological autoimmune diseases are multiple sclerosis (MS), autoimmune encephalitis (AE), and neuromyelitis optical spectrum disorder (NMOSD). In multiple sclerosis the immune system damages the myelin around nerve fibers that allows signals to travel. When the myelin is damaged, the nerve signals slow down or stop which causes problems with movement vision and thinking. Every MS patient has lesions in different areas , size, and severity so a uniform treatment is ineffective to cure MS. In autoimmune encephalitis the immune system targets specific proteins on nerve cells causing confusion, memory problems, personality changes, seizures, or movement difficulties however symptoms can vary widely depending on the patient and the diagnosis can take time. Furthermore, many drugs struggle to cross the blood-brain barrier which limits how effectively they can reach the inflamed brain tissue. Neuromyelitis optica spectrum disorder is when the immune system creates antibodies that attack the optic nerves and spinal cord leading to vision loss, eye pain, problems with bladder or bowel control, muscle weakness and numbness. Many people with NMOSD have antibodies against the aquaporin-4 which helps with water movement in nerve cells. Current treatment for NMOSD focuses on reducing inflammation and preventing future attacks. The antibodies created by the immune system that target proteins in the brain for AE and NMOSD differ for each patient so the same treatment may not work for everyone.

Current therapies, such as monoclonal antibodies and broad-spectrum immunosuppressants, are able to reduce the disease activity but have side effects and are not able to address the full spectrum of immune dysregulation. For example these drugs don't completely address all the ways these immune diseases disrupt normal biological processes. they may block one pathway but still leave other harmful pathways open. A personalized approach using biomarkers from blood or spinal fluid would help identify the exact molecular activity happening in a specific patient's disease. Comprehensive immune profiling would help create a detailed map of a specific patient's immune system rather than assuming an autoimmune disease persists in every patient the same way. Furthermore, advanced neurological imaging would help spot the smallest and earliest sign of damage before systems get worse.

Quantum computing applications in personalized immunotherapy

Quantum computing enables high-fidelity molecular modeling, accelerating the design of targeted therapies for neurological autoimmune diseases. Quantum Support Vector Machines and data re-uploading classifiers can be used to screen extremely large chemical libraries to classify molecules based on chemical fingerprints faster compared to classical machine learning (Batra, 2021). This reduces the number of compounds that must be physically tested in a lab and hence allows researchers to quickly identify molecules that are more likely to interfere with immune processes such as an autoantibody binding to neuronal proteins. Furthermore, Variational Quantum Eigensolver and Quantum Phase Estimation can simulate molecules at a quantum mechanical level to help identify their lowest ground state energies and binding affinities between a drug and its biological target. Grover's search allows a quantum computer to find a desired item in an unsorted database much faster than a classical computer. By using grover's search researchers can explore chemical spaces more efficiently contributing to fragment-based drug discovery. For neurological autoimmune conditions, this could help identify small-molecule or peptide therapies that precisely target immune cell receptors or disrupt pathological protein–protein interactions without affecting normal brain function (Nałęcz-Charkiewicz, 2024). Biogen, Accenture , and 1QBit have collaborated to apply a quantum computer to model protein–ligand interactions in neurological drug discovery. The framework they created from identifying targets, modeling binding dynamics, and screening compounds can be directly applied to autoimmune neurology. Quantum simulations are also being used to model how antibodies are able to interact with nervous system proteins allowing for treatments to stop the immune system from damaging the central nervous system. These approaches mean that drug discovery could shift from trial-and-error screening toward data-driven, simulation-based design, shortening timelines and improving success rates for new therapies.

Quantum Convolutional Neural Network can be used to process RNA sequence data to detect subtle, non-linear relationships in gene expression that predict how a patient could respond to a particular therapy. In neurological autoimmune diseases predicting these immune checkpoint blockade responses even when those patterns are hidden in vast amounts of noisy data. could help predict which patients would respond properly to certain immunotherapies such as B-cell depleting agents or cytokine inhibitors (Nguyen, 2024). Researchers are able to categorize patients into biological subgroups like those with distinct cytokine signatures or immune cell profiles based on large-scale comics data and quantum-enhanced clustering and feature selection. This step is crucial in helping ensure that future clinical trials and treatments are targeted towards patients that are more likely to respond (Pal, 2024). Quantum Machine Learning models are able to integrate multiple data types such as genomic, transcriptomic, and proteomic to identify where genetic predisposition, environmental triggers, and immune dysregulation interact. QML's ability to process high-dimensional datasets without prohibitive computational cost allows for a richer, more precise picture of a patient's immune system, guiding drug selection and dosing. These can help advance precision medicine from a generalized approach to a predictive and individualized treatment approach.

Quantum Neural Networks can be used to process MRI and PET imaging data in order to identify subtle brain changes in Alzheimer's disease (Lal, 2025). This same approach can also be repurposed to detect early inflammatory or demyelinating lesions in the brain or spinal cord which may not be detected in conventional radiology. Quantum Principal Component Analysis can be applied to imaging datasets to reduce the number of features required to detect abnormalities while still preserving critical diagnostic information (Suvvari, 2025). This allows for faster and accurate image analysis. In neurological autoimmune diseases, this could mean identifying early neuroinflammatory activity before a patient experiences significant symptoms, making early intervention possible. For diseases such as multiple sclerosis early treatment intervention is more effective before irreversible nerve damage occurs. Quantum-enhanced imaging methods therefore have the potential to not only improve diagnostic accuracy but also shift the treatment window earlier.

Quantum annealing can help identify optimal combinations of immunotherapies for each patient by balancing multiple variables such as drug efficacy, side effects, and patient-specific immune profiles. This is particularly valuable in autoimmune neurology, where overtreatment can lead to dangerous immune suppression and undertreatment can allow disease progression. a hybrid quantum–classical systems could continuously adjust treatment protocols in real time based on patient monitoring data, such as immune cell counts, MRI results, or symptom changes before clinical relapse occurs. This could personalize not just the choice of therapy but also its timing and intensity allowing for proactive and adaptive medicine.

Current Limitations and Challenges

Current quantum computers face several challenges that limit their immediate impact. Quantum computers are extremely sensitive to environmental factors such as temperature changes, vibrations, and environmental noise. These factors can cause decoherence which is when the qubits lose their quantum states before the calculations are completed. This limits their accuracy and complexity in their calculations. Most currently available quantum processors are limited to only a few hundred qubits and not all are usable due to error rates. Complex biomedical datasets and simulations require thousands or millions of error-free qubits. Quantum computers also commonly work with classical computers to transfer data back and forth between the systems. This creates inefficiencies and compatibility challenges. While quantum algorithms identify promising personalized treatment strategies, work still needs to be done to move it into real world clinical practice such as compliance with ethical standards, cross-disciplinary collaboration, regulatory approval and large-scale trials.

Future Prospects

The future of quantum computing in personalized immunotherapies will depend heavily on advances in both hardware development and quantum algorithms. Current devices still struggle with decoherence, noise, and scalability challenges, but advancements in error correction, topological qubits, and hybrid quantum–classical workflows would allow clinically relevant simulations feasible. More specialized models such as improved variational solvers for molecular dynamics and quantum machine learning frameworks for multi-omic integration would allow more precision in drug discovery and biomarker identification. Pilot projects in neurological autoimmune diseases using quantum computing to simulate autoantibody–antigen interactions, predict patient responses to immune-modulating therapies, and optimize adaptive treatment schedules would not only demonstrate feasibility but also create critical datasets for validating quantum approaches in real clinical settings. Cross-disciplinary collaboration with quantum computer scientists, immunologists, neurologists, and bioinformaticians would help ensure that quantum computing does not remain a purely theoretical exercise, but instead becomes a practical tool for reshaping how complex immune-mediated neurological diseases are diagnosed and treated.

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