International Journal of Scientific Research & Engineering Trends
Volume 12, Issue 2, Jan-Feb-2026, ISSN (Online): 2395-566X

Evaluating Quantum and Classical Computing Approaches in Modern Drug Discovery

R. Saniya Paul , Livistone S P, Dr. S. Sheeja
Department of Data Science, Sri Krishna Adithya College of Arts and Science, Coimbatore-41

Abstract- — Drug discovery is inherently complex and expensive with many requisites in terms of precision with respect to interactions' molecular modelling, biological activity prediction and chemical compounds optimisation. Classical computing methods have contributed substantially to the progress of computational drug discovery via molecular simulations, machine learning models and high-throughput virtual screening. However, challenges emerge from the exponentiality of molecular configuration space and the low efficiency of classical algorithms. Quantum computing as a new computing paradigm that offers a novel approach to computation based on various phenomena such as superposition and entanglement and therefore offers a way to overcome the previous limitations. This work presents a comparison of classical and quantum computing approaches in drug discovery with emphasis on their strengths and weaknesses, current progress and future prospects in different aspects of pharmaceutical research.

Keywords: Drug Discovery, Classical Computing, Quantum Computing, Molecular Modeling, Virtual Screening, Quantum Algorithms, Machine Learning in Drug Discovery, Computational Chemistry, Molecular Simulation, Pharmaceutical Research.

I. INTRODUCTION

Discovery of potential drugs is the process of finding candidate molecules that can interact with biological targets effectively while being safe and effective. With the increasing complexity of diseases and the rising demand for personalized medicine, computational methods have become indispensable for reducing time and cost in the early stages of drug development. Classical computing has enabled researchers to simulate molecular interactions, analyse biological data and predict drug behaviour using sophisticated algorithms and machine learning techniques. However, classical methods struggle to accurately model quantum mechanical interactions on a large scale, particularly for large and complex molecules.

In this context, quantum computing have emerged as a promising alternative that leverages principles of quantum mechanics to perform computations. Unlike classical bits, which can represent either a 0 or a 1, quantum bits can exist in multiple states simultaneously, allowing quantum computers to explore numerous possibilities concurrently. This unique capability has sparked tremendous interest in quantum computing for applications in computational chemistry and drug discovery. This paper presents a comparison of classical and quantum computing in drug discovery, emphasizing their strengths and weaknesses, current progress and future prospects in different aspects of pharmaceutical research.

II. BACKGROUND

Computational Drug Discovery

Computational drug discovery involves various methods designed to identify and validate potential drug molecules using computer-based models. The methods involved in computational drug discovery include molecular docking, molecular dynamics simulation, quantitative structure-activity relationship modelling, and virtual screening. By using computer models, it becomes possible to simulate the relationship between the drug molecule and the target. This increases the accuracy of the discovery of promising drug molecules, as the models are capable of simulating the relation of the molecules. Additionally, the models are cost-effective.

Fundamentals of Quantum Computing

It works on quantum bits that have the ability to be in multiple states at the same time due to the effect of superposition and entanglement. It has the ability to solve complex problems in a way that is more efficient compared to classical computation. For the case of chemistry, the algorithms involved in quantum computation include the Variational Quantum Eigen Solver and Quantum Phase Estimation. The algorithms target solving the electronic structure problem that represents the central problem of molecular simulation. It has the potential to solve the molecular energy problem with more accuracy compared to classical approximations.

III. CLASSICAL COMPUTING IN DRUG DISCOVERY

Classical computing has long been the workhorse of computational drug discovery. Molecular dynamics simulation is based on classical physics principles for the simulation of atom motion in time. This helps in deriving information about protein flexibility and ligand binding dynamics. Docking calculations assess possible binding modes based on scoring functions. The results of these calculations allow researchers to perform virtual screening of large compound libraries. Machine learning models based on experimental datasets also predict protein-target interactions.

Nonetheless, classical methods are inevitably confronted with several limitations. Molecular simulation algorithms become computationally prohibitive with increasing system sizes, while classical potential functions are inadequate in modelling certain quantum mechanical features, including electron correlations. Classical optimization heuristics might become stuck in suboptimal local minima, pushing the need to investigate other models of computation that can efficiently deal with complexity.

IV. QUANTUM COMPUTING IN DRUG DISCOVERY

Quantum computing brings in a complete new paradigm for the solving of computational chemistry problems by directly modelling quantum systems. Quantum algorithms will represent molecular wavefunctions more naturally, for which reasons the accurate calculation of both ground-state energies and reaction pathways will be possible. Especially Variational Quantum Eigen solver has recently gained much attention because of its compatibility with current noisy quantum hardware. Combining quantum circuits with classical optimization allows VQE to provide approximate solutions to molecular energy problems.

Besides quantum chemistry, quantum machine learning techniques are also being explored for other drug discovery tasks, including the classification and property prediction of molecules. This approach tends to take advantage of the high-dimensional feature space from quantum states to capture those patterns that may be challenging for classical models. Hybrid classical-quantum workflows appear particularly promising, as quantum processors can handle computationally intensive subproblems while the overall data processing and optimization are managed classically.

V. COMPARATIVE ANALYSIS OF CLASSICAL AND QUANTUM APPROACHES

Comparative analysis shows that traditional computing continues to be very efficient for large-scale screenings and data-modelling tasks. The approximations used in traditional computing restrict it to less accurate modelling of quantum interactions. Theoretical accuracy for the simulation of molecules is higher in quantum computing, which is currently limited by the noise level and the number of qubits in the hardware.

Although classical techniques are highly scalable and reliable, quantum techniques promise better accuracy for certain molecular calculations. Currently, the advantage offered by quantum calculations is largely theoretical or applicable only to small molecules. A mixture of both techniques can act as an intermediate solution because it provides scalability similar to a classical computer as well as accuracy similar to a quantum computer.

VI. ROLE OF QUANTUM COMPUTING IN LEAD OPTIMIZATION

Lead optimization is an essential component of drug discovery whereby promising compounds are improved. Traditional methods involve simulation and optimization guided by experimental feedback. This process is usually a tedious activity involving simulations that can be computer intensive. However, quantum computing has the potential of speeding up this process based on more accurate simulation of energy profiles in molecules. Quantum computers focus on the simulation of electronic interactions in molecules. This is an area where more light can be shed on structure-activity relationships of compounds. This will enable researchers to make suitable modifications on the structures of the compounds. This has the potential of shortening development timelines.

VII. QUANTUM ADVANTAGE IN EXPLORING CHEMICAL SPACE

Chemical space refers to the enormous number of possible chemical compounds and is astronomically large; this space cannot be systematically traversed by traditional means. Classical algorithms rely on heuristics and sampling methods to traverse this space; these algorithms often overlook optimal solutions. Quantum computing breaks new grounds for traversing this space by virtue of its quantum parallelism capabilities for exploring various molecular structures at once. Despite these nascent capabilities and their promise for sizeable

acceleration in smaller-scale systems on current devices, theory-scale calculations predict that quantum-aided search and optimization algorithms can offer massive boosts to the effectiveness of discovering new drug leads.

IX. IMPACT OF NOISY INTERMEDIATE-SCALE QUANTUM (NISQ) DEVICES

Current quantum computers belong to the family of Noisy Intermediate-Scale Quantum devices. They entail limited qubits. The devices can be noisy. The devices can only perform complex quantum circuits of limited depths. The devices can only be applied in proof-of-concepts of initial screening of small molecules. Research in the NISQ-era can be important. It promotes algorithm development. It also fosters the development of efficient hybrid models. An important part of work towards quantum advantage in drug discovery is knowing how meaningful information can be obtained from noisy quantum devices.

X. HYBRID CLASSICAL–QUANTUM DRUG DISCOVERY PIPELINES

Hybrid computing pipelines offer a viable way to integrate quantum computing capabilities with the traditional drug discovery process. In a hybrid setting, classical computers perform those tasks which are data intensive, like data preparation and machine learning inference, while quantum computers solve specific problems like optimization. This combination of both approaches allows one to exploit their strengths and overcome their weaknesses. The problem is that hybrid computing pipelines are best suited for the current state of technology and can be used to incrementally integrate quantum computing with the pharmaceutical industry.

XI. COMPARISON OF COMPUTATIONAL COST AND EFFICIENCY

Computational cost is an important aspect to consider in terms of determining the applicability of new technologies to drug discovery. Traditional simulation calculations tend to rely on high performance computing resources available in computer clusters. This results in substantial energy and economic costs. Quantum computing, which is currently a costly undertaking in terms of technological development, has tremendous potential in terms of lowering computational complexity. The future availability of scalable quantum computers could provide a cost-effective platform for simulating molecules from a standpoint of energy efficiency.

XII. SOFTWARE FRAMEWORKS AND TOOLCHAINS

Software frameworks are crucial in enabling quantum drug discovery research. On the classical side, molecular dynamics engines and cheminformatics libraries are mature and widely used. In contrast, quantum software ecosystems are evolving, with a set of frameworks designed to support quantum circuit design, simulation, and hybrid execution. For practical implementation, quantum software will have to be integrated into the classical drug discovery landscape. Standardization and interoperability among platforms will be crucially important in determining the speed of adoption at pharmaceutical companies.

XIII. BENCHMARKING CLASSICAL AND QUANTUM PERFORMANCE

It is imperative to carry out benchmarking of the quantum methods in relation to the classical methods used in drug development. This involves measuring the performance of the methods, including their accuracy, running time, scalability, among other parameters, on standardized datasets. Most of the existing methods of benchmarking have been limited to small molecules, mainly owing to the hardware limitations, such that it becomes hard to prove a quantum advantage.

XIV. ETHICAL AND SOCIETAL IMPLICATIONS

Quantum computation in the process of designing new drugs also involves certain societal implications. On the one hand, faster development of new drugs can ensure better access to life-saving medication. On the other hand, if quantum technologies are not accessible to all, the gap between the haves and have-nots can become wider. Additionally, there can also be threats to data security, as quantum technologies can easily compromise confidentiality.

XV. INDUSTRIAL ADOPTION AND REAL-WORLD FEASIBILITY

The pharmaceutical industry has recently started exploring quantum computing. This has been achieved in collaboration with technology companies and research institutions. Currently, industrial application of quantum computing is in the initial stages of determining its feasibility, as opposed to full implementation. This will assist in gaining knowledge about

potential areas of application and return on investment. However, large-scale implementation may take several years.

XVI. CHALLENGES AND LIMITATIONS

The widespread adoption of quantum computing in drug discovery is hindered by several challenges. Current quantum hardware suffers from noise, short coherence times, and limited qubit connectivity, which restrict the size of solvable problems. Additionally, quantum algorithms require further development to handle real-world pharmaceutical datasets effectively. Integration with existing classical workflows also presents technical and organizational challenges, requiring interdisciplinary collaboration between chemists, computer scientists, and quantum engineers.

XVII. FUTURE RESEARCH DIRECTIONS

Future research in quantum drug discovery is expected to focus on improving hardware reliability, developing error-corrected quantum systems, and designing domain-specific algorithms tailored to pharmaceutical problems. Hybrid classical–quantum frameworks will play a crucial role in bridging the gap between theory and practical application. As quantum technology matures, it is anticipated that quantum computing will significantly enhance molecular simulations, optimization tasks, and personalized medicine approaches.

XVIII. CONCLUSION

Quantum computing represents a transformative opportunity for drug discovery by addressing computational challenges that are difficult to solve using classical methods. While classical computing will continue to dominate current drug discovery pipelines, quantum computing offers the potential for breakthroughs in accuracy and efficiency. The most realistic path forward lies in hybrid computing models that integrate quantum algorithms into classical workflows. Continued research and technological advancements will determine the extent to which quantum computing reshapes the future of pharmaceutical innovation.

REFERENCES

1. 1.Aspuru-Guzik, A., et al., Simulated Quantum Computation of Molecular Energies, Science, 2005.
2. Cao, Y., et al., Quantum Chemistry in the Age of Quantum Computing, Chemical Reviews, 2019.
3. McArdle, S., et al., Variational Quantum Eigen solver, Reports on Progress in Physics, 2020.
4. Biamonte, J., et al., Quantum Machine Learning, Nature, 2017.