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REVIEW ARTICLE

Quantum Computing and Artificial Intelligence Convergence: Foundations for Scientific Innovation

Hassan Al-Sabah*[1], and Omar Al-Sharif[1]

Abstract. The convergence of quantum computing and artificial intelligence (AI) has emerged as a transformative paradigm with the potential to revolutionize scientific discovery across diverse domains, including materials science, pharmaceutical research, and computational chemistry. While classical computing and conventional AI have significantly accelerated data-driven research, they often face limitations in solving highly complex optimization, simulation, and molecular modelling problems due to computational constraints. Quantum computing introduces fundamentally new computational capabilities based on quantum mechanical principles such as superposition, entanglement, and quantum interference, enabling efficient exploration of complex solution spaces that are intractable for classical computers. When integrated with AI techniques, these capabilities provide powerful frameworks for accelerating knowledge discovery, predictive modelling, and decision-making in scientific research. This review presents the fundamental principles underlying Quantum-AI convergence, focusing on the foundational concepts of quantum computing, artificial intelligence, quantum machine learning, hybrid quantum-classical computation, and quantum optimization. The paper examines how these principles collectively establish a new computational paradigm capable of addressing scientific challenges with improved efficiency and scalability. By emphasizing theoretical foundations rather than application-specific implementations, this review provides researchers with a comprehensive understanding of the core concepts driving Quantum-AI convergence and its significance in enabling future scientific innovation.

Keywords: Quantum Computing, Artificial Intelligence, Quantum Machine Learning, Scientific Discovery, Materials Informatics, Drug Discovery

1* Department of Computer Science and Artificial Intelligence, College of Science
Kuwait University, Sabah Al-Salem University City (Shadadiya Campus), Safat, Kuwait.

1. Introduction

Artificial Intelligence (AI) has transformed scientific research by enabling computers to analyze vast amounts of data, recognize complex patterns, and support decision-making across numerous disciplines. Machine learning and deep learning algorithms have demonstrated remarkable success in image recognition, natural language processing, computational chemistry, materials science, and biomedical research, significantly accelerating scientific innovation [1], [2]. Despite these achievements, many scientific problems remain computationally challenging because of their enormous search spaces, nonlinear relationships, and combinatorial complexity. Conventional high-performance computing systems often require substantial computational resources and time to solve these problems, creating a growing demand for fundamentally new computing paradigms capable of overcoming these limitations [3].

Quantum computing has emerged as one of the most promising technologies for addressing computational problems that are beyond the practical capabilities of classical computers. Unlike classical computers that process information using binary bits, quantum computers utilize quantum bits (qubits) that exploit the principles of superposition, entanglement, and quantum interference to perform computations in fundamentally different ways [4], [5]. These quantum mechanical properties allow quantum systems to explore multiple computational states simultaneously, offering significant advantages for optimization, simulation, cryptography, and scientific modeling. Although practical fault-tolerant quantum computers are still under development, recent advances in noisy intermediate-scale quantum (NISQ) devices have accelerated research into hybrid quantum-classical algorithms suitable for near-term scientific applications [6].

The integration of quantum computing with artificial intelligence has given rise to the emerging field of Quantum Artificial Intelligence (Quantum-AI), which combines the strengths of both computational paradigms. Artificial intelligence provides sophisticated learning algorithms capable of extracting knowledge from complex datasets, while quantum computing offers enhanced computational capabilities for solving optimization and simulation problems that are difficult for classical processors [7]. Rather than replacing conventional AI methods, quantum computing complements them by accelerating selected computational tasks, enabling more efficient exploration of large solution spaces and potentially improving learning performance for certain classes of problems [8].

One of the primary motivations for Quantum-AI convergence is its potential to transform scientific discovery. Modern scientific research increasingly relies on computational modeling to investigate molecular interactions, material properties, biological processes, and chemical reactions. Many of these problems involve solving high-dimensional optimization tasks or accurately simulating quantum mechanical systems, which rapidly become computationally infeasible using classical approaches [9]. Quantum computing naturally represents quantum systems, making it particularly suitable for molecular simulation and electronic structure calculations. When combined with AI-driven predictive modeling, these capabilities offer new opportunities for accelerating scientific research and reducing experimental costs.

Materials discovery represents one of the most promising areas benefiting from Quantum-AI convergence. The development of advanced materials for renewable energy, electronics, aerospace, and sustainable manufacturing requires exploring enormous combinations of atomic structures and chemical compositions. Artificial intelligence has already demonstrated significant capabilities in predicting material properties from experimental and simulation data [10]. However, accurately modeling quantum interactions within complex materials remains computationally demanding. Quantum computing provides the theoretical capability to simulate these interactions more efficiently, enabling AI models to learn from more accurate quantum-generated data and thereby improving predictive performance.

Similarly, pharmaceutical research has witnessed substantial advances through AI-assisted drug discovery. Machine learning models are increasingly employed for virtual screening, molecular property prediction, protein structure analysis, and candidate drug optimization [11]. Landmark developments such as AlphaFold have demonstrated how AI can revolutionize structural biology by accurately predicting protein structures from amino acid sequences [12]. Nevertheless, predicting molecular interactions at quantum mechanical precision remains a significant computational challenge. Quantum computing offers the possibility of performing accurate molecular simulations that complement AI-based prediction models, potentially reducing both the time and cost associated with pharmaceutical development.

The convergence of quantum computing and AI is not limited to materials science and drug discovery. It represents a broader computational framework for scientific innovation, enabling researchers to integrate quantum simulation, optimization algorithms, machine learning, and data-driven reasoning into unified computational workflows. Hybrid quantum-classical algorithms, variational quantum circuits, quantum neural networks, and quantum optimization techniques have emerged as important research directions that combine the strengths of quantum and classical computing while accommodating the practical limitations of current NISQ hardware [6], [13]. These developments have established Quantum-AI as a rapidly growing interdisciplinary field involving computer science, quantum physics, mathematics, chemistry, engineering, and life sciences.

Understanding the fundamental principles underlying Quantum-AI convergence is essential for appreciating its transformative potential in future scientific research. Concepts such as qubits, quantum gates, quantum superposition, artificial intelligence, machine learning, quantum optimization, and hybrid quantum-classical computation form the theoretical foundation upon which Quantum-AI systems are developed. These principles not only provide new computational capabilities but also establish the basis for designing intelligent scientific systems capable of solving previously intractable problems with improved computational efficiency.

This paper presents a review of the fundamental principles of Quantum-AI convergence with emphasis on its role in enabling scientific discovery. It examines the foundational concepts of quantum computing, artificial intelligence, quantum machine learning, hybrid quantum-classical computation, and quantum optimization. By focusing on these theoretical principles, the paper provides a comprehensive understanding of how Quantum-AI convergence establishes a new paradigm for future advances in materials discovery, drug design, and broader scientific innovation.

2. Fundamental Principles of Quantum-AI Convergence

Quantum-AI convergence represents the integration of quantum computing and artificial intelligence to establish a computational framework capable of addressing complex scientific problems beyond the practical capabilities of classical computing. While quantum computing provides computational advantages through quantum mechanical phenomena, artificial intelligence contributes learning algorithms that extract knowledge from large and complex datasets. The convergence of these two paradigms establishes the theoretical foundation for next-generation scientific computing by combining quantum information processing with intelligent data analysis [14]. This interdisciplinary approach has attracted considerable attention in recent years because it offers new opportunities for accelerating optimization, simulation, and predictive modeling in scientific research [15].

2.1. Foundations of Quantum Computing

Quantum computing is fundamentally different from classical computing because it exploits the principles of quantum mechanics to represent and manipulate information. Classical computers encode information using binary bits that exist in one of two possible states, namely 0 or 1. In contrast, quantum computers utilize quantum bits (qubits), which can simultaneously exist in multiple states through the phenomenon of superposition [5]. This capability enables quantum computers to process many computational possibilities in parallel, thereby increasing computational efficiency for specific classes of problems.

Another defining characteristic of quantum computing is entanglement, a quantum mechanical phenomenon in which two or more qubits become strongly correlated regardless of the physical distance separating them [16]. Entangled qubits behave as a single quantum system, allowing complex computations that cannot be efficiently replicated using classical information processing. Entanglement serves as one of the primary resources enabling quantum computational advantage.

A third fundamental principle is quantum interference, which manipulates probability amplitudes to enhance correct computational outcomes while suppressing incorrect ones [5]. Together, superposition, entanglement, and interference form the basis of quantum algorithms capable of solving certain computational problems more efficiently than classical algorithms.

Quantum computation is performed through quantum gates, which manipulate qubit states analogously to logic gates in classical computers. Common quantum gates include the Pauli-X gate, Hadamard gate, Controlled-NOT (CNOT) gate, and phase gates. These gates collectively form quantum circuits capable of implementing complex quantum algorithms [17].

Despite their enormous computational potential, present-day quantum computers belong to the Noisy Intermediate-Scale Quantum (NISQ) era, characterized by limited qubit counts and susceptibility to environmental noise [6]. Consequently, many current Quantum-AI algorithms employ hybrid quantum-classical approaches that leverage existing quantum hardware while compensating for its limitations through classical optimization.

2.2. Principles of Artificial Intelligence

Artificial Intelligence refers to the capability of computational systems to perform tasks that traditionally require human intelligence, including learning, reasoning, pattern recognition, prediction, and decision-making. Modern AI is primarily driven by machine learning, where algorithms automatically learn relationships from data rather than relying on explicitly programmed rules [1].

Machine learning algorithms are generally categorized into supervised learning, unsupervised learning, semi-supervised learning, and reinforcement learning. Supervised learning utilizes labeled datasets to predict future outcomes, whereas unsupervised learning identifies hidden structures within unlabeled data. Reinforcement learning enables intelligent agents to optimize sequential decision-making through interaction with dynamic environments [18].

Deep learning, a specialized branch of machine learning, employs multi-layer artificial neural networks capable of automatically extracting hierarchical features from large datasets

[1]. These models have achieved remarkable success across image recognition, speech processing, natural language understanding, scientific imaging, and computational biology. However, their performance often depends on extensive computational resources, making efficient training and optimization increasingly challenging for large-scale scientific problems.

Artificial intelligence systems are fundamentally dependent on four major components:

- Data acquisition
- Feature representation
- Model learning
- Prediction and decision-making

These components collectively enable AI systems to identify complex nonlinear relationships within scientific datasets, making AI an indispensable tool for modern scientific research [10].

The convergence of AI with quantum computing seeks to improve these computational processes by accelerating optimization, enhancing feature representation, and enabling efficient exploration of high-dimensional solution spaces that are computationally expensive for classical algorithms [7], [19].

2.3. Quantum Machine Learning

Quantum Machine Learning (QML) represents the intersection of quantum computing and machine learning, aiming to improve learning algorithms through quantum computational principles [20]. Rather than replacing classical machine learning, QML combines quantum circuits with conventional optimization methods to construct hybrid learning systems suitable for current quantum hardware.

One of the central concepts in QML is the Variational Quantum Circuit (VQC), in which parameterized quantum gates are optimized using classical algorithms. During training, quantum circuits generate computational outputs while classical optimizers iteratively update circuit parameters to minimize prediction errors [21]. This hybrid learning framework has become one of the most practical approaches for NISQ devices.

Another important concept is the Quantum Neural Network (QNN), which extends neural network architectures into quantum computational spaces. Instead of conventional neurons, QNNs employ parameterized quantum operations capable of representing highly complex feature relationships through quantum state evolution [22].

Quantum feature mapping represents another important principle in QML. Classical input data are encoded into quantum states through specialized embedding techniques, allowing quantum computers to construct high-dimensional feature spaces that may improve classification performance for certain datasets [13]. This principle forms the basis of quantum kernel methods and quantum-enhanced support vector machines.

Recent research has also explored quantum reinforcement learning, quantum generative models, and quantum transfer learning, demonstrating the broad potential of QML for future intelligent computing systems [23]. Although large-scale practical advantages remain under active investigation, QML has established an important theoretical foundation for Quantum-AI convergence.

2.4. Quantum Optimization

Optimization lies at the core of numerous scientific and engineering problems, including molecular structure prediction, materials design, logistics, financial modeling, and machine learning. Many optimization tasks involve searching enormous solution spaces where conventional algorithms become computationally expensive as the problem size increases. Quantum computing introduces new optimization paradigms capable of exploiting quantum parallelism and probabilistic search mechanisms to improve computational efficiency for selected optimization problems [24].

One of the most significant developments in quantum optimization is the Variational Quantum Eigensolver (VQE). VQE is a hybrid quantum-classical algorithm that combines parameterized quantum circuits with classical optimization techniques to estimate the ground-state energy of molecular systems. Since many problems in computational chemistry and materials science involve determining minimum-energy configurations, VQE has become one of the most promising algorithms for near-term quantum computers operating in the Noisy Intermediate-Scale Quantum (NISQ) era [25]. The algorithm iteratively updates quantum circuit parameters using classical optimizers until the minimum energy state is obtained.

Another important optimization framework is the Quantum Approximate Optimization Algorithm (QAOA), which is specifically designed for solving combinatorial optimization problems. QAOA alternates between quantum evolution operators and classical optimization to identify high-quality approximate solutions for complex optimization tasks [26]. Applications of QAOA include graph optimization, scheduling, network design, portfolio optimization, and resource allocation.

Quantum search algorithms also contribute significantly to optimization. Grover's algorithm provides a quadratic speedup for unstructured search problems by amplifying the probability of desired solutions through repeated quantum interference operations [27]. Although Grover's algorithm does not solve every optimization problem exponentially faster than classical methods, it demonstrates how quantum computation can reduce computational complexity for specific search tasks.

Another important optimization approach is Quantum Annealing, which employs quantum fluctuations to identify low-energy solutions within complex optimization landscapes. Quantum annealing has been successfully applied to scheduling, route optimization, machine learning, and combinatorial optimization problems, particularly using specialized quantum hardware developed for optimization tasks [28].

Collectively, these optimization methods form the computational backbone of Quantum-AI convergence. By integrating quantum optimization with machine learning algorithms, researchers can develop intelligent systems capable of solving computational problems that are difficult or inefficient for conventional optimization techniques.

2.5. Hybrid Quantum-Classical Computing

Current quantum computers possess limited computational resources and remain susceptible to environmental noise and decoherence. Consequently, purely quantum computational workflows are not yet practical for solving most real-world scientific problems. Hybrid quantum-classical computing has therefore emerged as the dominant computational paradigm for current Quantum-AI research [6].

In hybrid computing, computational tasks are divided between classical and quantum processors according to their respective strengths. Classical computers perform data preprocessing, optimization, parameter updates, and result interpretation, whereas quantum processors execute computationally intensive operations involving quantum state evolution and probability estimation [15]. This collaborative approach enables existing quantum hardware to contribute meaningfully despite hardware limitations.

A typical hybrid Quantum-AI workflow consists of several sequential stages:

1. Scientific data acquisition and preprocessing.
2. Encoding classical data into quantum states.
3. Quantum circuit execution.
4. Quantum measurement.
5. Classical optimization of quantum circuit parameters.

6. Iterative convergence until an optimal solution is obtained.

This iterative optimization process forms the basis of many modern Quantum Machine Learning algorithms, including Variational Quantum Circuits and Quantum Neural Networks [21].

Hybrid architectures provide several important advantages:

- Efficient utilization of existing NISQ hardware.
- Reduced quantum circuit depth.
- Improved computational stability.
- Compatibility with established AI frameworks.
- Gradual integration of quantum technologies into existing computing infrastructures.

Because hybrid systems leverage mature classical computing resources alongside emerging quantum processors, they currently represent the most practical pathway toward large-scale Quantum-AI implementation.

2.6. Quantum-AI Principles for Scientific Discovery

Scientific discovery increasingly depends upon computational methods capable of analyzing complex systems involving enormous datasets, multidimensional parameter spaces, and nonlinear interactions. Quantum-AI convergence establishes a new computational framework that combines the predictive capabilities of artificial intelligence with the computational strengths of quantum information processing [20].

One important scientific principle underlying Quantum-AI is accurate quantum simulation. Many chemical and physical systems obey quantum mechanical laws that are difficult to simulate efficiently using classical computers. Quantum computers naturally represent quantum states, making them particularly suitable for molecular simulation, electronic structure calculations, and chemical reaction modeling [9]. Artificial intelligence complements these simulations by learning patterns from quantum-generated data, enabling faster prediction of material properties and molecular behaviors.

Another foundational principle is intelligent exploration of high-dimensional search spaces. Materials discovery often requires evaluating millions of possible atomic structures and chemical compositions before identifying promising candidates. Similarly, pharmaceutical research involves screening enormous molecular libraries to discover compounds with desirable therapeutic properties. AI algorithms efficiently prioritize candidate solutions, while quantum optimization provides new mechanisms for exploring complex solution spaces more effectively [10], [11].

Quantum-AI also supports scientific hypothesis generation, where machine learning models identify hidden relationships within experimental data while quantum computation performs detailed simulations that validate predicted hypotheses. This combination reduces experimental effort, accelerates scientific investigation, and improves decision-making throughout the research process.

Although current quantum hardware remains limited, the theoretical principles of Quantum-AI establish an important computational foundation for future scientific innovation. Continued improvements in quantum hardware, error correction, scalable quantum algorithms, and intelligent learning systems are expected to further strengthen this convergence in the coming decades [6], [15].

2.7. Summary

Quantum-AI convergence represents a significant advancement in computational science by integrating the complementary strengths of quantum computing and artificial intelligence. Unlike conventional computing paradigms, Quantum-AI exploits the quantum mechanical principles of superposition, entanglement, and interference alongside data-driven learning algorithms to solve computational problems that are difficult for classical systems [5], [15]. The combination of quantum information processing with intelligent learning establishes a new computational framework capable of supporting scientific research with improved efficiency and scalability.

The fundamental principles discussed in this review—including quantum computation, artificial intelligence, quantum machine learning, quantum optimization, and hybrid quantum-classical computing—collectively provide the theoretical foundation for next-generation scientific computing. While current quantum computers remain constrained by limited qubit counts, noise, and decoherence, hybrid computational strategies have demonstrated that practical Quantum-AI systems can already address selected optimization and simulation tasks using existing NISQ hardware [6], [21]. Continued advances in quantum hardware, scalable learning algorithms, and error-correction techniques are expected to further expand the capabilities of Quantum-AI systems in the coming years.

The convergence of these technologies has particular significance for scientific discovery. By enabling more accurate molecular simulations, efficient optimization of high-dimensional search spaces, and intelligent analysis of complex scientific data, Quantum-AI provides a promising computational foundation for accelerating research in materials science, computational chemistry, pharmaceutical development, and numerous other scientific disciplines [9], [10]. As quantum technologies continue to mature, Quantum-AI is expected to become an increasingly important component of future scientific computing infrastructures.

3. Conclusion

The convergence of quantum computing and artificial intelligence represents one of the most significant developments in modern computational science. Rather than functioning as independent technologies, these complementary paradigms combine quantum information processing with intelligent learning to establish a new framework for solving complex scientific problems. The fundamental principles discussed in this review—including qubit-based computation, quantum superposition, entanglement, quantum machine learning, hybrid quantum-classical computing, and quantum optimization—provide the theoretical basis for this emerging interdisciplinary field.

Unlike traditional computing systems that rely exclusively on classical processors, Quantum-AI utilizes quantum computational resources to complement advanced artificial intelligence algorithms. This convergence enables more efficient exploration of high-dimensional solution spaces, improved optimization strategies, and enhanced simulation of quantum mechanical systems. Such capabilities are particularly valuable for computationally intensive scientific domains including materials discovery, drug design, molecular simulation, and chemical modeling.

Although large-scale fault-tolerant quantum computers have not yet become widely available, significant progress has been achieved through Noisy Intermediate-Scale Quantum (NISQ) devices and hybrid computational approaches. Variational quantum algorithms, quantum neural networks, quantum optimization methods, and quantum-enhanced machine learning have demonstrated the feasibility of integrating quantum processors with classical AI frameworks. These developments provide practical pathways toward realizing Quantum-AI systems while overcoming current hardware limitations.

Future research is expected to focus on improving quantum hardware reliability, developing scalable quantum machine learning algorithms, enhancing quantum error correction, and establishing standardized software frameworks for Quantum-AI applications. As these challenges are addressed, Quantum-AI is likely to play a transformative role in enabling faster scientific discovery, improving computational efficiency, and accelerating innovation across multiple scientific and engineering disciplines. Consequently, understanding the foundational principles of Quantum-AI convergence is essential for researchers seeking to develop next-generation intelligent systems capable of addressing increasingly complex scientific challenges.

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