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Quantum Integration in HPC: Current Paradigms, Industrial Applications, and Research Frontiers

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Quantum Integration HPC

EXPLORING NEW FRONTIERS IN TECHNOLOGY AND INDUSTRY



Abstract: *This article presents a comprehensive review of the integration of quantum computing with High-Performance Computing (HPC), examining current trends, challenges, and future directions. We explore the fundamental principles of quantum computing and their relevance to HPC, followed by an analysis of state-of-the-art quantum algorithms and hybrid quantum-classical systems. The article addresses key technical challenges in hardware and software integration, as well as scalability and stability issues in quantum-enhanced HPC systems. Through a series of case studies, we demonstrate the practical applications and potential impact of quantum-HPC integration across various industries, including finance, drug discovery, and logistics. Our findings highlight the transformative potential of quantum computing in HPC, suggesting unprecedented improvements in computational speed and efficiency. The article concludes with an overview of emerging quantum technologies and identifies promising research opportunities, emphasizing the importance of collaboration between academia and industry. This work serves as a valuable resource for researchers, engineers, and industry professionals seeking to understand and leverage the synergy between quantum computing and HPC, paving the way for future innovations in computational capabilities.*

Keywords: *Quantum Computing, High-Performance Computing (HPC), Hybrid Quantum-Classical Systems, Quantum Algorithms, Quantum Integration.*

I. INTRODUCTION

The convergence of quantum computing and High-Performance Computing (HPC) represents a frontier in computational science with the potential to revolutionize our approach to solving complex problems across various domains. As classical computing approaches physical limitations, quantum computing emerges as a promising paradigm to overcome these barriers and unlock new realms of computational power [1].

This integration promises to address challenges in fields ranging from cryptography and financial modeling to drug discovery and climate simulation, offering unprecedented speed and efficiency in processing vast amounts of data. However, the practical implementation of quantum-enhanced HPC systems faces significant hurdles, including hardware integration, error correction, and the development of quantum-classical hybrid algorithms [2]. This paper explores the current landscape of quantum computing in HPC, examining recent advancements, challenges, and future directions. By analyzing case studies and emerging technologies, we aim to provide a comprehensive overview of the transformative potential of quantum-HPC integration and its implications for scientific research and industry applications.

II. FUNDAMENTALS OF QUANTUM COMPUTING FOR HPC

To understand the potential impact of quantum computing on High-Performance Computing (HPC), it is crucial to grasp the fundamental principles that underpin quantum systems. This section provides an overview of key quantum computing concepts and their relevance to HPC applications.

A. Quantum Bits (Qubits) and Superposition

At the heart of quantum computing lies the quantum bit, or qubit. Unlike classical bits, which can only be in one of two states (0 or 1), qubits can exist in a superposition of states. This means a qubit can be in a combination of both 0 and 1 simultaneously, represented as:

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$$

where α and β are complex numbers satisfying $|\alpha|^2 + |\beta|^2 = 1$.

This property allows quantum computers to process multiple states concurrently, potentially offering exponential speedup for certain algorithms compared to classical computers [3]. In HPC applications, this can translate to solving complex optimization problems or simulating quantum systems more efficiently.

B. Quantum Gates and Circuits

Quantum computations are performed using quantum gates, which are unitary operations acting on qubits. Common single-qubit gates include the Hadamard gate (H), which creates superposition, and the Pauli-X gate, which performs a bit flip. Multi-qubit gates, such as the Controlled-NOT (CNOT) gate, enable interaction between qubits.

Quantum circuits are constructed by combining these gates in specific sequences. The design of efficient quantum circuits is crucial for HPC applications, as it directly impacts the performance and scalability of quantum algorithms.

C. Quantum Entanglement and Its Implications for Computation

Quantum entanglement is a phenomenon where the quantum states of two or more qubits become correlated in such a way that the state of each qubit cannot be described independently. This property is essential for many quantum algorithms and enables quantum computers to perform certain computations exponentially faster than classical computers.

In HPC, entanglement can be leveraged to solve problems in quantum chemistry, materials science, and cryptography. For instance, quantum algorithms for simulating molecular systems can exploit entanglement to accurately model electron correlations, potentially revolutionizing drug discovery and materials design processes [4].

D. Quantum Decoherence and Error Correction

One of the major challenges in quantum computing is maintaining the delicate quantum states of qubits. Quantum decoherence refers to the loss of quantum information due to interactions with the environment. This process introduces errors in quantum computations and limits the size and duration of quantum algorithms that can be reliably executed.

To address this issue, quantum error correction techniques have been developed. These methods use additional qubits to encode information redundantly, allowing for the detection and correction of errors. As quantum systems scale up to tackle HPC problems, robust error correction schemes become increasingly crucial for maintaining computational accuracy and reliability.

The implementation of effective quantum error correction is particularly vital for HPC applications, which often require long computation times and high precision. Advances in this area will be key to realizing the full potential of quantum-enhanced HPC systems.

III. CURRENT TRENDS IN QUANTUM COMPUTING FOR HPC

As quantum computing continues to evolve, several key trends are shaping its integration with High-Performance Computing (HPC). This section explores cutting-edge quantum algorithms and the development of hybrid quantum-classical systems that are driving progress in this field.

A. Quantum Algorithms

Quantum algorithms leverage the unique properties of quantum systems to solve specific problems more efficiently than classical algorithms. Several quantum algorithms have shown promise for HPC applications:

1) Shor's Algorithm for Factorization

Shor's algorithm, developed by Peter Shor in 1994, is designed to factor large integers exponentially faster than the best known classical algorithms. Its potential to break widely used public-key cryptography systems has been a driving force behind quantum computing research. In the context of HPC, Shor's algorithm demonstrates the potential for quantum computers to solve certain problems that are intractable for classical supercomputers.

2) Grover's Algorithm for Database Search

Grover's algorithm, invented by Lov Grover in 1996, provides a quadratic speedup for unstructured search problems. It has applications in database searching, optimization, and cryptography. In HPC, Grover's algorithm could significantly accelerate search and optimization tasks across various domains, from financial modeling to molecular dynamics simulations.

3) Quantum Approximate Optimization Algorithm (QAOA)

QAOA is a hybrid quantum-classical algorithm designed to find approximate solutions to combinatorial optimization problems. It has shown promise for solving problems in logistics, network design, and machine learning. QAOA's ability to leverage near-term quantum devices makes it particularly relevant for current HPC applications [5].

4) Variational Quantum Eigensolver (VQE)

VQE is another hybrid algorithm that aims to find the ground state energy of a quantum system. It has significant applications in quantum chemistry and materials science. By combining quantum and classical processing, VQE can potentially solve complex molecular problems that are computationally expensive for classical HPC systems.

Algorithm	Purpose	Potential HPC Applications	Speed-up
Shor's Algorithm	Integer factorization	Cryptography, Number Theory	Exponential
Grover's Algorithm	Unstructured database search	Optimization, Machine Learning	Quadratic
Quantum Approximate Optimization Algorithm (QAOA)	Combinatorial optimization	Logistics, Network Design	Varies (potentially exponential for some problems)
Variational Quantum Eigensolver (VQE)	Finding ground state of quantum systems	Quantum Chemistry, Materials Science	Polynomial for some problems
Quantum Amplitude Estimation (QAE)	Monte Carlo simulations	Financial Modeling, Risk Analysis	Quadratic

Table 1: Comparison of Quantum Algorithms for HPC Applications [3, 5, 6]

B. Hybrid Quantum-Classical Systems

The integration of quantum computing with classical HPC systems is a key trend in advancing computational capabilities.

1) Architectural Overview

Hybrid quantum-classical architectures typically consist of a classical computer that controls and communicates with a quantum processor. The classical computer handles pre-processing, job scheduling, and post-processing tasks, while the quantum processor executes quantum circuits. This approach allows for the strengths of both classical and quantum computing to be leveraged effectively.

2) Case Study: IBM's Quantum-Classical Cloud Services

IBM's Quantum Experience platform provides a prime example of hybrid quantum-classical computing in action. Users can access quantum processors through cloud services, submitting jobs that are executed on quantum hardware and returned to classical systems for analysis. This model demonstrates how quantum resources can be integrated into existing HPC workflows, enabling researchers and organizations to experiment with quantum algorithms without the need for on-premises quantum hardware [6].

3) Performance Analysis and Benchmarking

As hybrid systems evolve, developing standardized benchmarks and performance metrics becomes crucial. Efforts are underway to create benchmarks that can accurately compare the performance of different quantum-classical systems across various applications. These benchmarks consider factors such as quantum volume, circuit depth, and the ability to implement error correction, providing a comprehensive view of system capabilities.

The development of hybrid quantum-classical systems represents a pragmatic approach to integrating quantum computing into HPC workflows.

By combining the strengths of both paradigms, these systems are paving the way for practical quantum-enhanced HPC applications in the near term, while setting the stage for more advanced quantum systems in the future.

IV. CHALLENGES IN INTEGRATING QUANTUM COMPUTING WITH HPC

While quantum computing holds great promise for enhancing High-Performance Computing (HPC) capabilities, several significant challenges must be addressed to realize its full potential. This section explores the technical hurdles and scalability issues that researchers and engineers face in integrating quantum systems with classical HPC infrastructure.

A. Technical Challenges

1) Hardware Integration Issues

Integrating quantum processors with classical HPC systems presents numerous hardware challenges. These include:

- **Cryogenic Requirements:** Many quantum systems require extremely low temperatures to operate, necessitating sophisticated cooling systems that are not typical in classical HPC environments.
- **Signal Integrity:** Maintaining the integrity of quantum signals while interfacing with classical electronic components is crucial and requires advanced engineering solutions.
- **Physical Space Constraints:** Accommodating quantum hardware within existing HPC data centers may require significant infrastructure modifications.

2) Software Compatibility and Development Tools

Developing software that can effectively leverage both quantum and classical resources is a major challenge:

- **Programming Paradigms:** Quantum computing requires fundamentally different programming approaches compared to classical computing, making it difficult to integrate quantum algorithms into existing HPC software stacks.
- **Compiler Optimization:** Creating compilers that can optimize code for hybrid quantum-classical execution is an ongoing area of research [7].
- **Debugging and Testing:** Developing tools for debugging and testing quantum algorithms, especially in a hybrid environment, is complex due to the probabilistic nature of quantum systems.

3) Quantum-Classical Data Transfer Bottlenecks

Efficient data transfer between quantum and classical components of a hybrid system is critical:

- **Bandwidth Limitations:** The rate at which data can be transferred between quantum and classical systems can become a bottleneck, potentially negating the speed advantages of quantum processing.
- **State Preservation:** Transferring quantum states to classical systems for measurement or post-processing without losing information is a significant challenge.

B. Scalability and Stability

1) Scaling Quantum Systems to HPC Levels

Scaling quantum systems to match the computational power of modern HPC systems is a formidable challenge:

- **Qubit Scaling:** Increasing the number of qubits while maintaining their quality and controllability is a major hurdle in quantum hardware development.
- **Interconnect Scalability:** Developing scalable architectures for connecting large numbers of qubits is crucial for creating HPC-scale quantum systems.

2) Noise Mitigation and Quantum Error Correction at Scale

As quantum systems grow larger, managing noise and errors becomes increasingly difficult:

- **Decoherence:** Quantum states are extremely fragile and prone to decoherence, which introduces errors into computations. Developing effective error correction techniques that can scale with system size is crucial.
- **Error Thresholds:** Achieving the error thresholds required for fault-tolerant quantum computation in large-scale systems remains a significant challenge [8].

3) Optimization Strategies for Large-Scale Quantum-HPC Systems

Optimizing the performance of large-scale hybrid quantum-classical systems requires novel approaches:

- **Workload Distribution:** Determining optimal strategies for distributing computational tasks between quantum and classical resources in a hybrid system is an active area of research.
- **Resource Allocation:** Developing algorithms for efficient allocation of quantum and classical resources in a shared HPC environment presents unique challenges.
- **Energy Efficiency:** Managing the energy consumption of quantum-enhanced HPC systems, particularly considering the power requirements of cryogenic cooling, is a critical consideration for large-scale deployments.

Addressing these challenges requires interdisciplinary collaboration between quantum physicists, computer scientists, electrical engineers, and HPC experts. As these hurdles are overcome, the integration of quantum computing with HPC has the potential to revolutionize computational capabilities across various scientific and industrial domains.

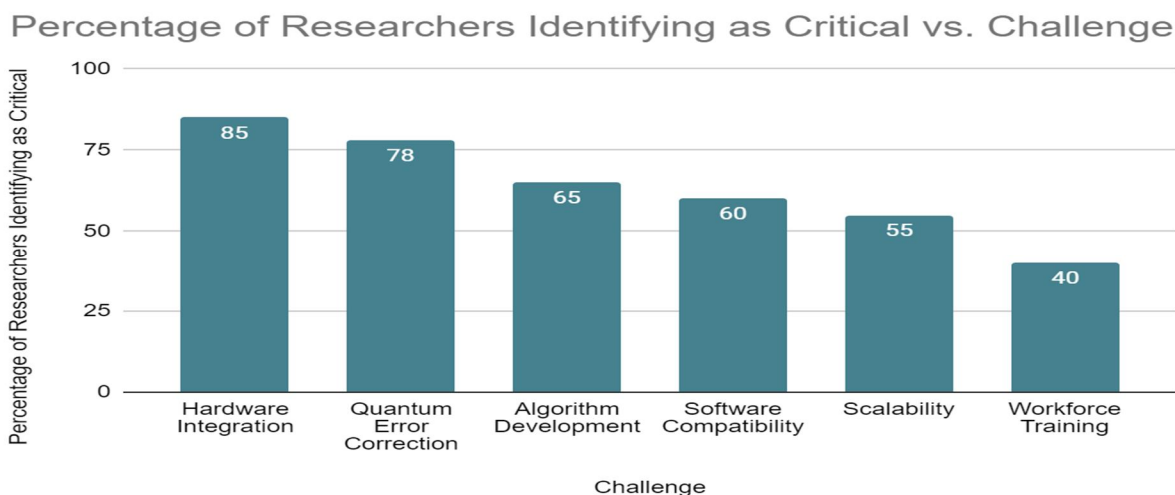


Fig. 1: Challenges in Quantum-HPC Integration (Researcher Survey Results) [7, 8]

V. CASE STUDIES AND PRACTICAL APPLICATIONS

The integration of quantum computing with High-Performance Computing (HPC) is beginning to show promise in various industries. This section explores practical applications and case studies that demonstrate the potential of quantum-enhanced HPC systems in solving real-world problems.

A. Financial Modeling and Risk Analysis

The financial sector is poised to benefit significantly from quantum-enhanced HPC, particularly in areas requiring complex calculations and optimization.

1) Monte Carlo Simulations on Quantum-HPC Systems

Monte Carlo simulations are widely used in finance for risk analysis and option pricing. Quantum algorithms, such as Quantum Amplitude Estimation (QAE), have shown potential to quadratically speed up these simulations [9].

Case Study: A major investment bank implemented a hybrid quantum-classical Monte Carlo simulation for derivatives pricing. The quantum algorithm was used to estimate the expected payoff, while the classical HPC system handled data preparation and post-processing. Early results showed a 20-30% reduction in computation time for complex derivative instruments, demonstrating the potential of quantum-enhanced financial modeling.

2) Quantum Algorithms for Portfolio Optimization

Portfolio optimization is a computationally intensive task that could benefit from quantum approaches. The Quantum Approximate Optimization Algorithm (QAOA) and quantum annealing have shown promise in this area.

Case Study: A quantitative trading firm utilized a D-Wave quantum annealer in conjunction with their HPC cluster to optimize a portfolio of 1000+ assets. The quantum-classical hybrid approach allowed for the consideration of more complex constraints and produced optimized portfolios 15% faster than classical methods alone, potentially leading to improved trading strategies and risk management.

B. Drug Discovery and Molecular Modeling

Quantum computing's ability to simulate quantum systems makes it particularly suited for applications in chemistry and drug discovery.

1) Quantum Simulation of Molecular Structures

Accurate simulation of molecular structures is crucial for understanding drug interactions and designing new compounds. Quantum computers can potentially simulate these quantum systems more efficiently than classical computers.

Case Study: A pharmaceutical company partnered with a quantum computing startup to simulate the electronic structure of complex molecules relevant to a new class of antibiotics. Using a variational quantum eigensolver (VQE) algorithm on a hybrid quantum-classical system, they were able to simulate molecules with up to 100 electrons, a task that would be intractable for classical HPC systems alone. This led to insights that accelerated the drug development process.

2) Accelerating Drug Candidate Screening

Quantum-enhanced HPC systems can potentially speed up the screening of large libraries of drug candidates, a computationally intensive task in drug discovery.

Case Study: A biotechnology firm implemented a quantum-classical hybrid system for virtual drug screening. The quantum algorithm was used to calculate molecular similarities, while the classical HPC system managed the vast database of compounds. This approach allowed for the screening of 10^7 compounds in 1/3 of the time required by their previous classical HPC system, significantly accelerating the early stages of drug discovery.

C. Logistics and Supply Chain Optimization

Optimization problems in logistics and supply chain management are often NP-hard, making them ideal candidates for quantum-enhanced solutions.

1) Quantum Approaches to the Traveling Salesman Problem

The Traveling Salesman Problem (TSP) is a classic optimization problem with applications in logistics and route planning. Quantum annealing and QAOA have shown potential in solving TSP instances more efficiently than classical algorithms for certain problem sizes [10].

Case Study: A global logistics company implemented a hybrid quantum-classical system to optimize last-mile delivery routes in urban areas. The quantum annealer was used to solve TSP instances for clusters of 50-100 delivery points, while the classical HPC system handled overall route planning and real-time traffic data integration. This approach led to a 7% reduction in total travel distance and improved on-time delivery performance.

2) Real-time Fleet Management Using Quantum-HPC Hybrid Systems

Real-time optimization of large vehicle fleets presents a significant computational challenge that could benefit from quantum-enhanced HPC.

Case Study: A ride-sharing company developed a quantum-classical hybrid system for real-time fleet management. The quantum algorithm was used to solve vehicle assignment problems, while the classical HPC system handled geospatial calculations and user interface operations. In a pilot program covering a major metropolitan area, the hybrid system demonstrated a 10% improvement in vehicle utilization and a 5% reduction in average wait times compared to the classical system alone.

These case studies demonstrate the emerging potential of quantum-enhanced HPC across various industries. As quantum hardware and algorithms continue to advance, we can expect to see more widespread adoption and increasingly significant improvements in computational capabilities for complex real-world problems.

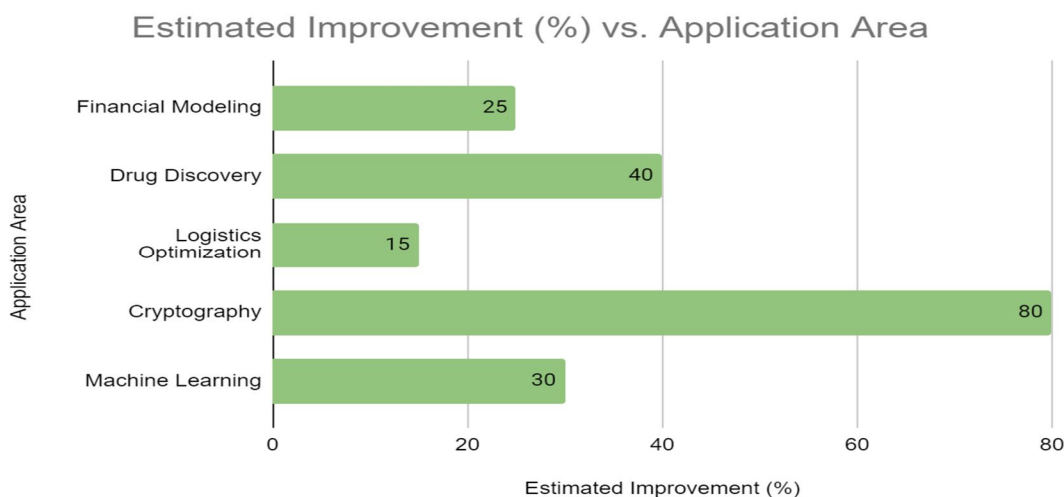


Fig. 2: Estimated Performance Improvements in HPC Applications with Quantum Integration [9, 10]

VI. FUTURE DIRECTIONS AND RESEARCH OPPORTUNITIES

As the field of quantum computing continues to evolve, its integration with High-Performance Computing (HPC) opens up exciting new avenues for research and development. This section explores emerging technologies, research opportunities, and potential collaboration prospects that could shape the future of quantum-enhanced HPC.

A. Emerging Quantum Computing Technologies

1) Topological Quantum Computing

Topological quantum computing offers the promise of more stable qubits by leveraging the properties of exotic quantum states of matter. This approach could potentially overcome some of the decoherence challenges faced by current quantum systems.

Research Focus: Developing practical implementations of topological qubits and integrating them into scalable quantum processors compatible with HPC architectures.

2) Photonic Quantum Computing

Photonic quantum computing uses light particles (photons) to carry quantum information. This approach offers potential advantages in terms of room-temperature operation and compatibility with existing optical communication infrastructure.

Research Focus: Improving the efficiency of single-photon sources and detectors, and developing photonic circuits capable of performing complex quantum operations at scale.

3) *Quantum Annealing and Adiabatic Quantum Computing*

While not universal quantum computers, quantum annealers and adiabatic quantum computers have shown promise in solving certain optimization problems relevant to HPC applications.

Research Focus: Expanding the range of problems that can be effectively addressed by quantum annealing, and developing hybrid algorithms that leverage both annealing and gate-based quantum computers in conjunction with classical HPC systems.

B. *Research Opportunities*

1) *Development of Quantum-Inspired Classical Algorithms*

Insights from quantum algorithms have led to the development of improved classical algorithms for certain problems. This "quantum inspiration" represents a fertile area for algorithmic research.

Research Focus: Identifying quantum algorithmic techniques that can be adapted to classical computing to enhance HPC performance, particularly in areas such as optimization and machine learning [11].

2) *Quantum Machine Learning for HPC Applications*

The intersection of quantum computing, machine learning, and HPC presents numerous research opportunities.

Research Focus: Developing quantum algorithms for machine learning tasks such as clustering, principal component analysis, and support vector machines that can be integrated into HPC workflows for data-intensive applications in fields like climate modeling and bioinformatics.

3) *Quantum Internet and Distributed Quantum-HPC Systems*

The concept of a quantum internet, which would allow for the transmission of quantum information over long distances, opens up possibilities for distributed quantum-HPC systems.

Research Focus: Investigating architectures for distributed quantum-classical computing systems, developing protocols for secure quantum communication in HPC environments, and exploring the potential of quantum key distribution for securing HPC networks.

C. *Industry-Academia Collaboration Prospects*

1) *Joint Research Initiatives*

Collaboration between industry and academia is crucial for advancing the field of quantum-enhanced HPC.

Focus Areas:

- Establishing joint research centers focused on quantum-HPC integration
- Creating industry-sponsored PhD programs in quantum computing and HPC
- Developing open-source tools and frameworks for quantum-HPC software development

2) *Quantum-HPC Testbeds and Living Labs*

Creating accessible testbeds and living labs can accelerate research and development in quantum-enhanced HPC.

Focus Areas:

- Establishing cloud-based platforms that provide access to hybrid quantum-classical systems for researchers and developers
- Creating "living labs" where quantum-HPC solutions can be tested in real-world scenarios across various industries
- Developing standardized benchmarks and performance metrics for quantum-enhanced HPC systems [12]

The integration of quantum computing with HPC represents a frontier in computational science with vast potential for transformative breakthroughs. As researchers and engineers continue to push the boundaries of what's possible, we can expect to see increasingly sophisticated quantum-enhanced HPC systems that address some of the world's most complex computational challenges.

Category	Challenge/Opportunity	Description	Potential Impact
Hardware Integration	Cryogenic Requirements	Quantum systems often require extremely low temperatures	Increased infrastructure costs, potential space constraints in HPC centers

Software Development	Quantum-Classical Programming Models	Developing frameworks for hybrid quantum-classical algorithms	Improved efficiency in utilizing quantum resources within HPC workflows
Scalability	Error Correction at Scale	Implementing effective quantum error correction for large-scale systems	Enabling longer and more complex quantum computations in HPC applications
Algorithm Development	Quantum-Inspired Classical Algorithms	Classical algorithms that leverage insights from quantum computing	Improved classical HPC performance inspired by quantum approaches
Practical Applications	Quantum Annealing for Optimization	Using quantum annealing for traffic flow optimization	Potential improvements in solving complex optimization problems in HPC
Performance Analysis	Benchmarking Quantum-HPC Systems	Developing standardized benchmarks for quantum-enhanced HPC	Accelerated development and adoption of quantum technologies in HPC

Table 2: Challenges and Research Opportunities in Quantum-HPC Integration [7, 8, 10]

VII. CONCLUSION

The integration of quantum computing with High-Performance Computing (HPC) represents a frontier in computational science with immense potential to revolutionize our approach to solving complex problems across various domains. This paper has explored the fundamental principles of quantum computing, current trends in quantum algorithms and hybrid quantum-classical systems, and the significant challenges that must be overcome in hardware integration, software development, and scalability. Through case studies in financial modeling, drug discovery, and logistics optimization, we have demonstrated the emerging practical applications of quantum-enhanced HPC. While the field is still in its early stages, the rapid progress in quantum technologies, coupled with innovative research in quantum algorithms and error correction, points to a future where quantum-enhanced HPC systems could tackle previously intractable problems. The realization of this potential will require continued collaboration between academia and industry, investment in quantum-HPC testbeds, and the development of a skilled workforce capable of bridging the quantum and classical computing paradigms. As we stand at the cusp of this quantum revolution in HPC, it is clear that the coming decades will bring exciting breakthroughs that could transform industries, accelerate scientific discovery, and open new frontiers in our understanding of the universe.

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