Quantum Computing Fundamentals and Simulation Techniques: A Survey

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Abstract

This survey paper provides a comprehensive examination of quantum computing fundamentals and simulation methodologies, focusing on quantum state representation, strong and weak simulation theories, and the integration of classical computing techniques. It highlights the transformative potential of quantum computing across various domains, such as chemistry, materials science, and finance, where quantum simulations offer unprecedented capabilities. The paper explores the challenges of simulating quantum computers on classical systems, emphasizing hybrid quantum-classical architectures and the inefficiencies of classical simulations. Key methodologies include tensor networks, decision diagrams, and advanced representation techniques, which enhance scalability and efficiency in quantum simulations. The survey also delves into quantum algorithm simulation, addressing the complexities of simulating large quantum circuits and proposing solutions like tensor-network quantum circuits and hybrid approaches. Additionally, it discusses the integration of classical algorithms in quantum simulations, which optimize performance and resource utilization. The paper concludes by outlining the current state and challenges of quantum computing, emphasizing the need for robust hardware and error mitigation strategies to unlock its full potential. Future directions include refining quantum algorithms, developing quantum-resistant cryptographic systems, and enhancing hybrid quantum-classical methods to address real-world challenges. By synthesizing these areas, the survey contributes to the ongoing discourse in quantum computing, offering insights into its current landscape and future trajectory.

1 Introduction

1.1 Significance and Impact of Quantum Computing

Quantum computing represents a significant advancement in computational technology, leveraging quantum mechanics to tackle problems unattainable by classical systems [1]. The limitations of classical simulations become evident as the number of qubits exceeds 50, highlighting the necessity for innovative simulation techniques within quantum computing [2]. Transitioning from fundamental research to practical applications necessitates the development of scalable qubit systems to enable large-scale quantum computation [3].

The influence of quantum computing spans multiple scientific and engineering fields, particularly in simulating complex quantum systems. In chemistry and materials science, quantum simulations can accurately model the behavior of interacting particles, thus advancing molecular chemistry. Moreover, the potential for exponential speedups in computational tasks positions quantum computing to revolutionize high-performance scientific computing and foster breakthroughs in applied mathematics [4].

In finance, quantum computing offers innovative solutions for complex problems such as derivative pricing and risk modeling, essential for optimizing financial operations [5]. As quantum algorithms

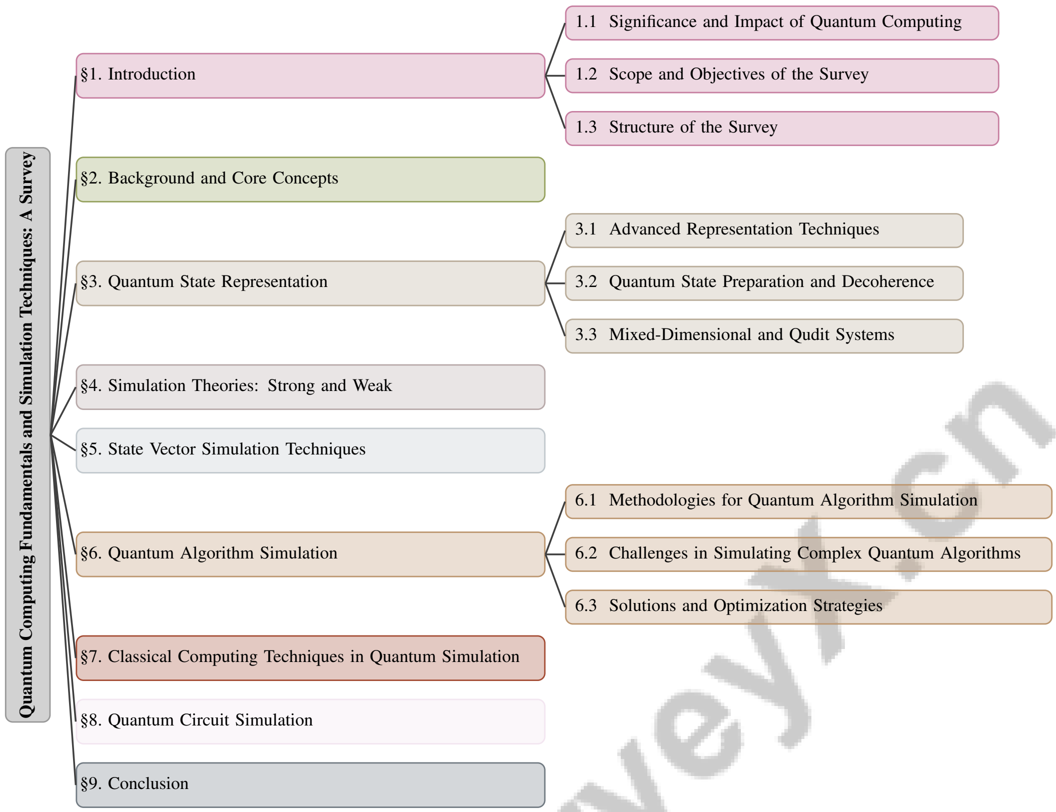

Figure 1: chapter structure

evolve, they promise to enhance computational capabilities, providing significant advantages in solving problems currently intractable for traditional supercomputers [6]. As these technologies mature, their transformative impact is anticipated to broaden, introducing new computational paradigms and solutions to intricate challenges.

1.2 Scope and Objectives of the Survey

This survey aims to provide a thorough examination of quantum computing, focusing on simulation techniques and theoretical frameworks crucial to this rapidly advancing field. A primary objective is to address the challenges of simulating quantum computers on classical systems, given the considerable demands on memory and computational resources [7]. This involves investigating the computational advantages of quantum algorithms, especially in solving complex optimization problems within energy systems, where classical algorithms face limitations [8].

The survey investigates the inefficiencies of classical simulations of quantum circuits and explores hybrid quantum-classical architectures designed to alleviate these issues [9]. It emphasizes the experiments conducted by the Google Quantum Team, particularly their work on sampling pseudo-random quantum circuits, a pivotal advancement in quantum circuit evaluation methods [10]. This exploration includes hybrid approaches that integrate classical and quantum resources, intentionally excluding purely classical simulation methods [11].

Additionally, the survey assesses the performance and accuracy of the Tensor Network Quantum Virtual Machine (TNQVM) in high-performance computing environments, highlighting its role in simulating quantum circuits [12]. It covers the fundamentals of quantum computing, its applications in chemical and biochemical engineering, and provides a bibliographic analysis of research trends in the field [13]. The survey underscores the limitations of existing classical numerical methods in simulating electronic structures and dynamics of molecular systems, reinforcing the need for a focus on quantum algorithms [14].

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The objectives further extend to exploring quantum simulations related to fundamental quantum fields of the Standard Model, including Quantum Chromodynamics (QCD) and electroweak interactions [15]. Moreover, the survey outlines the historical development of quantum computing, foundational concepts, mathematical models, applications in simulating quantum dynamics, quantum error correction, and future directions [16]. It also benchmarks the performance of the Intel Quantum Simulator (IQS) in cloud computing and high-performance computing (HPC) systems, contributing to the understanding of quantum algorithm simulation [17].

By addressing these areas, the survey aspires to present a comprehensive overview of the current state and future trajectories in quantum computing and simulation techniques, enriching the ongoing discourse in this transformative field. The rationale for topic selection encompasses the potential impact of quantum simulation on materials science, high-energy physics, and quantum chemistry [6], alongside the necessity for benchmarking and simulating quantum circuits on classical computers to enhance understanding of quantum computers and programs [1]. Additionally, the survey considers the modernization of classical software systems to facilitate their integration with emerging quantum computing systems, addressing the lack of systematic solutions for restructuring classical systems to accommodate quantum algorithms [18].

1.3 Structure of the Survey

This survey is systematically organized into key sections, each addressing distinct aspects of quantum computing and simulation techniques to provide a comprehensive understanding of the field. The introductory sections present foundational concepts of quantum computing, including quantum state representation and the core principles that underpin quantum simulations, setting the stage for advanced simulation methodologies and theoretical frameworks.

Research is categorized into three primary fields: stochastic modeling, optimization, and machine learning, examining specific quantum algorithms and their classical counterparts [19]. This categorization enhances comprehension of the diverse applications and potential of quantum algorithms in addressing complex problems across various domains.

Subsequent sections explore quantum state representation, emphasizing advanced techniques such as graph-based and geometric representations [20]. These discussions highlight the significance of efficient state representation and preparation, tackling challenges like decoherence and the representation of mixed-dimensional systems.

The discourse then transitions to simulation theories, differentiating between strong and weak simulation approaches while examining the theoretical foundations that support these methodologies. A comprehensive analysis of state vector simulation techniques follows, focusing on advanced methods such as quantum signal processing and tensor network approaches. This section includes practical applications of variational and reinforcement learning techniques, which are increasingly employed to enhance the efficiency and accuracy of simulations in various fields, including machine learning and quantum circuit simulation [21, 22].

The survey further investigates the methodologies and challenges associated with quantum algorithm simulation, proposing solutions and optimization strategies to improve simulation accuracy and efficiency. This exploration delves into the integration of classical computing techniques within quantum simulations, emphasizing hybrid quantum-classical approaches that effectively merge the computational strengths of both paradigms, particularly in teaching quantum principles to computer science students and refining classical simulation algorithms for complex quantum tasks [23, 24].

Finally, the survey concludes with an analysis of quantum circuit simulation techniques, focusing on classical methods for noise mitigation and error correction, alongside advanced tools such as Haskell-based and multi-GPU simulation environments. The framework categorizes quantum computing research into foundational theories, applications, and error correction mechanisms, delivering a comprehensive overview of the current landscape and future directions in quantum computing research [16]. This structured approach ensures an in-depth exploration of the field, equipping readers with a nuanced understanding of both theoretical and practical aspects of quantum computing.The following sections are organized as shown in Figure 1.

2 Background and Core Concepts

2.1 Foundational Concepts and Methods

Quantum computing introduces a novel computational paradigm by leveraging quantum mechanics principles such as superposition, entanglement, and coherence. Unlike classical bits, qubits can exist in superpositions, enabling concurrent computations, which is crucial for simulating complex quantum systems where classical simulations demand exponentially increasing resources [25, 26]. Entanglement allows interconnected qubits to influence each other regardless of distance, facilitating operations that surpass classical systems' capabilities, particularly in simulating many-body physics with intricate particle interactions [14, 27].

Quantum circuit simulation is a pivotal research area, employing techniques like array-based and decision diagram-based frameworks, each offering distinct advantages in performance and scalability [28]. The exponential memory requirement for classical storage of quantum states necessitates innovative simulation methods [26]. The Qubit Reorder Trick (QRT) optimizes simulation efficiency by minimizing unnecessary swap gates and optimizing qubit arrangements [3].

Emerging methodologies, such as deep learning architectures like Transformers, aim to represent quantum states as probability distributions, opening new possibilities for efficient quantum system simulation. Additionally, quantum algorithms for simulating Hamiltonian dynamics and eigenstates demonstrate the expanding applicability of quantum computing [14]. The integration of quantum and classical computing is exemplified by variational quantum algorithms (VQAs), which leverage noisy intermediate-scale quantum devices for practical applications [4]. Efforts are underway to modernize classical systems to operate alongside quantum systems, enabling the transition to quantum-enhanced computing environments.

These foundational concepts and methodologies address the complexities of quantum mechanics and showcase quantum computing's transformative potential. By harnessing superposition and entanglement, quantum computing can solve specific complex problems significantly faster than classical systems, unlocking breakthroughs in fields such as finance, pharmaceuticals, and materials science [29, 23, 30]. The continuing evolution of quantum technologies and algorithms expands the boundaries of achievable outcomes in quantum simulations, offering promising avenues for future research and application.

2.2 Quantum Complexity and Computational Models

Quantum complexity theory and computational models are crucial in advancing quantum computing, especially in simulation techniques. Quantum systems' unique properties, such as superposition and entanglement, present challenges that classical paradigms struggle to efficiently address [29]. This necessitates developing advanced computational models to fully exploit quantum computing's potential.

A major challenge is the efficient simulation of quantum circuits, particularly those using non-Clifford gates, which present exponential scaling difficulties due to their non-classical nature [31]. The classification of problems within BQP (Bounded-error Quantum Polynomial time) highlights the role of quantum computational models in solving problems intractable for classical algorithms. However, simulating large quantum circuits remains a significant hurdle due to resource constraints.

Simulating complex quantum systems, such as those in quantum chemistry, underscores the limitations of classical methods and the potential of quantum algorithms to provide efficient solutions [5]. For instance, simulating quantum circuits with up to 45 qubits poses substantial challenges for classical computers due to the exponential growth of computational requirements. Probabilistic simulations on classical systems are further complicated by non-positive quasi-probabilities associated with quantum states [32].

The Hamiltonian simulation problem, which involves approximating the unitary matrix governing a quantum system's time evolution, exemplifies the significance of quantum complexity. Minimizing query complexity and error is critical for optimizing simulations as qubit numbers increase [31]. Current quantum simulation methods often fail to fully harness quantum mechanics for simulating Hamiltonian dynamics.

Quantum circuit synthesis illustrates the complexities introduced by quantum computing. The constraints of qubit connectivity and decoherence complicate the synthesis of efficient quantum circuits, necessitating innovative approaches to overcome these challenges [13]. The exponential memory complexity of array-based quantum circuit simulators highlights the difficulties in simulating large-scale quantum systems, contrasting with more compact alternatives like decision diagrams.

The limitations of existing NISQ (Noisy Intermediate-Scale Quantum) devices, primarily due to noise and errors, impede their ability to achieve quantum advantage over classical optimization algorithms. This issue is exacerbated by the absence of common benchmarks for fair comparisons and the difficulties in evaluating performance across various quantum platforms [33]. Additionally, the exponential growth of computational state space with increasing qubit numbers, especially when accounting for noise effects, presents significant challenges in simulating gate-based quantum circuits.

Quantum complexity also impacts the application of error-correcting codes in quantum circuits, which often rely on labor-intensive manual processes and theoretical evaluations [5]. Furthermore, the inefficiency of gradient-based optimizers in variational quantum algorithms, particularly due to the vanishing gradient or barren plateau issue, becomes increasingly pronounced with more qubits.

Exploring computational models and complexity in quantum computing is essential for advancing simulation techniques. By systematically addressing the inherent challenges posed by quantum mechanics, including the no-cloning theorem and the intricacies of quantum entanglement, researchers can enhance the efficiency and scalability of quantum simulations. This advancement is crucial for unlocking significant breakthroughs across various scientific and technological domains, as the global market for quantum computing is projected to reach USD 1 trillion by 2035 [34, 30].

The exploration of quantum state representation techniques is crucial for advancing quantum simulations. As illustrated in Figure 2, this figure depicts the hierarchical structure of these techniques, categorizing advanced representation methods, state preparation and decoherence strategies, and mixed-dimensional systems. This visual representation not only clarifies the relationships among various methods but also highlights the key techniques and their contributions to enhancing the scalability and efficiency of quantum simulations. By providing a structured overview, the figure serves as a valuable tool for understanding the complexities of quantum state representation and its implications for future research.

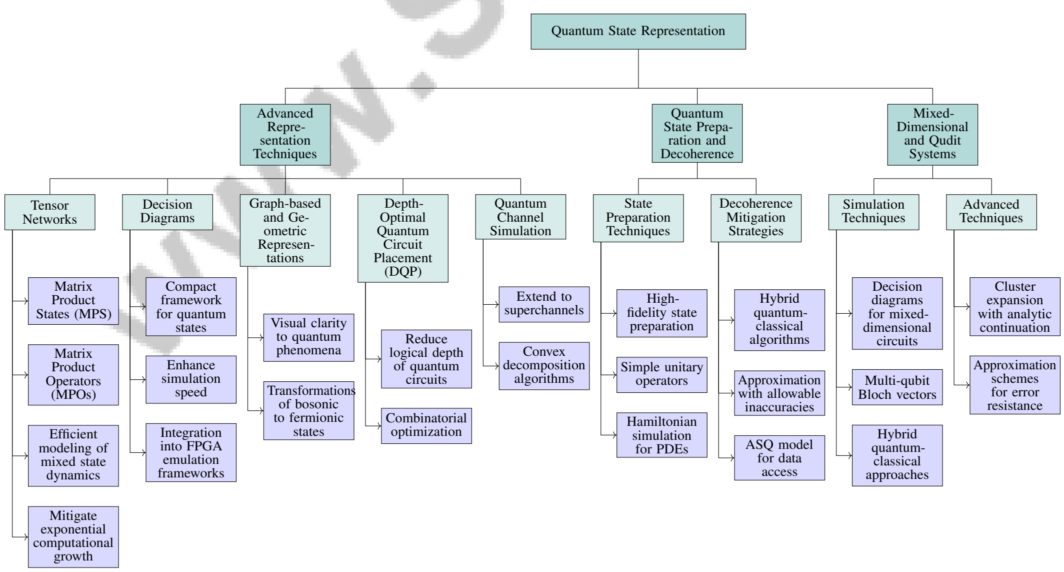

Figure 2: This figure illustrates the hierarchical structure of quantum state representation techniques, categorizing advanced representation methods, state preparation and decoherence strategies, and mixed-dimensional systems. It highlights the key techniques and their contributions to enhancing quantum simulations' scalability and efficiency.

3 Quantum State Representation

3.1 Advanced Representation Techniques

Advanced quantum state representation techniques are pivotal in enhancing the scalability and efficiency of quantum simulations, particularly in addressing the complexities inherent in Hilbert spaces and entanglement. Traditional state-vector approaches often falter under these demands, leading to the development of innovative methods such as tensor networks and decision diagrams. Tensor networks, including Matrix Product States (MPS) and Matrix Product Operators (MPOs), offer efficient modeling of mixed state dynamics in noisy quantum circuits, effectively mitigating exponential computational growth [24]. They are particularly effective in simulating one-dimensional noisy random quantum circuits.

Decision diagrams provide a compact framework for quantum states and operations, significantly enhancing simulation speed and reducing complexity [35]. Their integration into FPGA emulation frameworks ensures precise global phase maintenance during simulations, optimizing resource use.

Graph-based and geometric representations further bolster simulation efficiency by providing visual clarity to quantum phenomena. For instance, innovative transformations of bosonic to fermionic states with internal degrees of freedom exemplify advanced quantum state representation strategies [14].

The Depth-Optimal Quantum Circuit Placement (DQP) method leverages combinatorial optimization to reduce quantum circuits' logical depth while adhering to nearest neighbor constraints [36], highlighting algorithmic advancements' role in refining state representation.

Extending quantum channel simulation to superchannels via convex decomposition algorithms marks a significant innovation, enhancing complex quantum interaction simulations [37].

Collectively, these techniques—encompassing tensor networks, decision diagrams, and graph-based methods—offer robust frameworks for improving quantum simulations' scalability and efficiency. These advancements are foundational for developing sophisticated quantum algorithms and applications across diverse sectors, including finance, pharmaceuticals, and cybersecurity [38, 30, 4].

3.2 Quantum State Preparation and Decoherence

Quantum state preparation is crucial in quantum computing, involving initializing qubits into specific states necessary for algorithm execution. High-fidelity state preparation directly impacts quantum computation performance and accuracy. Decoherence, resulting from environmental interactions, presents a significant challenge by degrading quantum states. Hybrid quantum-classical algorithms like the variational quantum eigensolver (VQE) show promise in mitigating decoherence by leveraging classical resources to stabilize quantum computations [39, 29, 40, 41, 30].

Innovative techniques to enhance state preparation fidelity include implementing simple unitary operators exactly, optimizing quantum circuits, and minimizing single-qubit rotation errors [42]. Additionally, preparing quantum states to solve non-homogeneous linear partial differential equations through Hamiltonian simulation provides a structured framework for precise state initialization [43].

Decoherence necessitates robust mitigation strategies. Approximating quantum states with allowable inaccuracies while maintaining fidelity offers a viable solution for managing decoherence effects [26], balancing accuracy and computational efficiency.

The ASQ model introduces precision and probabilistic success into the data access framework, enhancing state preparation robustness by accounting for decoherence effects [28].

These techniques collectively address the dual challenges of quantum state preparation and decoherence, advancing quantum computing. Innovations such as quantum architecture search (QAS) and efficient circuit designs enhance state initialization fidelity, mitigate quantum noise, and optimize variational quantum algorithms (VQAs), facilitating reliable quantum computations and practical applications in quantum chemistry and data classification [44, 40, 45, 46, 47].

3.3 Mixed-Dimensional and Qudit Systems

The representation and simulation of mixed-dimensional systems and qudits present unique challenges and opportunities in quantum computing. These systems, extending beyond the conventional qubit framework, enrich state spaces and enhance quantum algorithms' computational power. Efficient simulation techniques are crucial for overcoming current physical implementation limitations and accelerating quantum algorithm exploration, promising substantial improvements in applied mathematics and scientific computing [4, 20].

Decision diagrams efficiently represent quantum states and operations, managing mixed-dimensional quantum circuits with reduced computational overhead [48], streamlining quantum state representation to handle increased complexity.

Another innovative technique uses multi-qubit Bloch vectors to represent n-qubit density matrices, simplifying quantum dynamics computations and enabling faster simulations [49]. This method leverages Bloch vectors' geometric properties for an intuitive framework for mixed-dimensional quantum systems.

Hybrid quantum-classical approaches classify states based on symmetry sectors, simplifying simulations and enhancing accuracy [50]. This focus on physically relevant states reduces computational complexity.

Combining cluster expansion with analytic continuation offers a promising strategy for simulating quantum dynamics in mixed-dimensional systems, efficiently capturing essential features of quantum interactions [51]. Integrating these advanced techniques enables more accurate and scalable simulations.

Approximation schemes leveraging quantum computations' error resistance offer a novel approach to creating compact quantum state representations [26], reducing resource demands for simulating mixed-dimensional systems and facilitating the exploration of larger, more complex quantum systems.

Advanced representation techniques for mixed-dimensional systems and qudits significantly enhance quantum simulations' scalability and efficiency, enabling the simulation of complex quantum circuits utilizing multiple information levels beyond traditional qubits. By addressing these systems' unique challenges, researchers unlock new computational capabilities and advance quantum technologies [20, 48].

4 Simulation Theories: Strong and Weak

4.1 Defining Strong and Weak Simulation Theories

Strong and weak simulation theories are pivotal for understanding quantum systems' computational capabilities and limitations. Strong simulation involves precise computation of probability amplitudes, crucial for high-precision algorithms like Shor's algorithm and quantum phase estimation, which demonstrate quantum superiority over classical methods in tasks requiring exact calculations. The Quantum Approximate Optimization Algorithm (QAOA) exemplifies strong simulation's utility in optimization problems where classical techniques fall short [4].

Weak simulation, on the other hand, focuses on sampling from a quantum system's probability distribution, requiring fewer computational resources. This approach is advantageous when exact amplitude calculations are unnecessary, facilitating efficient simulations aimed at sample generation. Weak simulation is especially pertinent in combinatorial optimization, where quantum superposition and interference offer performance enhancements over classical approaches [26]. The QuEST framework illustrates this by efficiently simulating generic quantum circuits using hybrid multithreading and distributed GPU acceleration.

Frameworks like QASMBench further clarify the distinction between strong and weak simulation by providing structured methodologies for assessing quantum algorithms' performance. These frameworks emphasize weak simulation's role in evaluating computational boundaries, showing how variational approaches—using parameterized trial states and classical optimization—effectively model noisy quantum circuits' dynamics. Hybrid simulation methodologies, such as those in CutQC, categorize quantum circuit evaluations into classical, quantum, and hybrid modes, integrating theoretical insights from complexity theory with practical considerations for current quantum devices.

This integration optimizes large quantum circuit evaluations, addressing the challenges posed by quantum processing units' (QPUs) demanding hardware requirements and the limitations of purely classical simulations [9, 52, 11].

The theoretical foundation of these simulation methodologies is informed by concepts like Rent's rule, which relates the number of interconnections to the number of components and has been adapted for quantum systems [3]. This adaptation is crucial for understanding quantum circuits' scaling behavior and their simulations.

Exploring strong and weak simulation theories offers valuable insights into quantum systems' computational potential, guiding the development of more efficient and scalable quantum algorithms. By tackling the complex challenges of quantum simulations, researchers can leverage unique quantum principles—such as superposition and entanglement—to significantly enhance quantum computer performance. This advancement facilitates rapid solutions to complex problems beyond classical capabilities and opens new applications across finance, pharmaceuticals, and materials science, driving innovation and economic growth in the evolving quantum technology landscape [38, 23, 30].

4.2 Theoretical Frameworks Supporting Simulation

Theoretical frameworks supporting strong and weak simulation theories in quantum computing are essential for advancing the field's understanding and capabilities. These frameworks are grounded in computational complexity principles and quantum systems' properties, providing a robust base for simulation techniques. A key aspect is the reliance on complexity-theoretic assumptions, highlighting classical simulations' challenges and supporting simulation theory development [29]. This perspective is critical for delineating the computational boundaries between classical and quantum systems, guiding the creation of efficient simulation algorithms.

Significant advancements include using stabilizer circuits, which enable compact quantum state representation and efficient simulation of operations. The Quipu framework exemplifies this by leveraging stabilizer circuits' properties to reduce computational overhead, facilitating more efficient quantum circuit simulations [53]. This approach effectively manages quantum simulations' complexities, enabling quantum state representation and manipulation without requiring exponentially large computational resources.

Additionally, integrating probabilistic models and decision diagrams enhances quantum simulations' efficiency. These methods streamline memory and computational requirements, particularly in noisy quantum environments [54]. Decision diagrams, in particular, offer advantages in memory efficiency and computational speed, providing a robust framework for simulating and verifying quantum circuits.

Moreover, developing weak simulation techniques that avoid reliance on exponentially-sized arrays marks a significant innovation, drastically reducing memory requirements and enabling efficient sampling from quantum states. This focus on efficient sampling expands quantum simulations' potential across various domains, including optimization and machine learning [55].

Frameworks supporting strong and weak simulation theories also address challenges posed by decoherence and the need for effective quantum error correction. As quantum systems scale, maintaining coherence and performing reliable computations become increasingly critical [16]. These frameworks incorporate strategies for mitigating decoherence and implementing error correction, ensuring quantum simulations' accuracy and reliability.

Collectively, these theoretical frameworks establish a solid foundation for developing quantum simulation theories by integrating diverse methodologies, such as scaffolded learning approaches for computer science students, advanced numerical techniques for quantum field theories, and innovative composite quantum simulation methods. This integration enhances understanding and application of quantum mechanics across various computational contexts [56, 23, 57]. By addressing quantum systems' inherent complexities and leveraging innovative techniques, such as stabilizer circuits and decision diagrams, these frameworks pave the way for more efficient and scalable quantum simulations, offering new insights and capabilities across a range of scientific and technological domains.

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5 State Vector Simulation Techniques

5.1 Quantum Signal Processing and Tensor Network Approaches

Quantum signal processing and tensor network methodologies are pivotal in enhancing the efficiency and scalability of state vector simulations in quantum computing. As quantum circuits expand in complexity with increasing qubits and gates, traditional methods struggle due to vast Hilbert spaces and intricate entanglement. Tensor networks, like Matrix Product States (MPS) and Projected Entangled Pair States (PEPS), effectively represent these entanglement properties, mitigating exponential computational demands [35]. Recent advances have optimized tensor network algorithms for GPU execution, reducing simulation time and improving accuracy. These techniques not only facilitate quantum circuit simulations for hybrid algorithms but also extend to machine learning and materials science, showcasing their versatility in advancing quantum technology [12, 21, 58, 59, 22].

Quantum signal processing enhances quantum state manipulation by reducing query complexity and improving simulation efficiency through piecewise polynomial approximations. This allows precise control over complex operations and sophisticated algorithm implementation. Quantum Random Access Codes (QRAC) further boost efficiency by mapping discrete features into fewer qubits, enhancing variational quantum circuit performance.

The Quantum Assisted Simulator (QAS) algorithm exemplifies innovative tensor network integration into quantum simulations. Utilizing a hybrid quantum-classical approach, QAS efficiently simulates quantum dynamics without classical feedback loops, circumventing issues like the barren plateau problem. Its compatibility with current NISQ hardware aids in tackling complex challenges, such as high-temperature superconductivity and drug design, more effectively than traditional methods [12, 51, 60, 22, 61]. Additionally, distributed simulation frameworks optimize communication and gate scheduling, overcoming classical hardware memory limitations for larger quantum system simulations.

The quantum superchannel simulation algorithm, employing convex decomposition of extreme superchannels, enhances simulation capabilities on experimental platforms [37]. This approach improves the simulation of complex quantum interactions, providing a robust framework for scaling quantum simulations.

The simulation path framework shows significant runtime improvements over traditional methods, emphasizing tensor network strategies' potential in decision diagram simulations [62]. By decomposing tasks into smaller, parallelizable subtasks, simulation efficiency is markedly enhanced.

These methodologies underscore the transformative potential of quantum signal processing and tensor network approaches in state vector simulations. They enable efficient simulation of large-scale quantum systems on classical computers, optimize quantum circuit designs, and advance machine learning applications across various domains [59, 21, 22, 58]. Leveraging these advanced techniques, researchers can achieve scalable and efficient quantum simulations, paving the way for significant advancements in quantum computing and its applications.

5.2 Variational and Reinforcement Learning Techniques

Method Name	Optimization Techniques	Simulation Frameworks	Scalability and Accuracy
QSAMC[14]	Quantum Algorithms Designed	Quantum Simulation Algorithms	Improved Computational Efficiency
QNO-HVA[63]	Quasi-Newton Methods	Quantum Emulator Qhipster	Improved Convergence Rates
PL[64]	Automatic Differentiation	Quantum Node Abstraction	Larger Quantum Circuit
LPAF[65]	Low Precision Arithmetic	Logarithmic Representation	Reduced Memory Usage
PQCS[2]	Partitioning Strategy	Independent Sub-circuits	Parallel Processing
SMQS[18]	-	-	-

Table 1: Overview of various methods integrating optimization techniques, simulation frameworks, and assessments of scalability and accuracy in state vector simulations for quantum computing. Each method is referenced with its key attributes, highlighting the advancements in computational efficiency and convergence rates. The table underscores the role of these methodologies in enhancing the performance of quantum simulations.

Variational and reinforcement learning techniques are crucial for enhancing state vector simulations in quantum computing, offering methodologies that improve efficiency and accuracy. Table 1 presents a comprehensive comparison of different methods employed in variational and reinforcement learning techniques, detailing their optimization strategies, simulation frameworks, and evaluations of scalability and accuracy in quantum computing. Variational methods, notably the Quantum Approximate Optimization Algorithm (QAOA), optimize energy systems by exploring large solution spaces efficiently. These techniques use parametrized quantum circuits to approximate quantum systems' ground states, minimizing energy functions through classical optimization [14]. Preconditioning techniques further enhance these methods by reducing ansatz depth, improving noise resilience and convergence rates [63].

Reinforcement learning complements variational methods by autonomously identifying optimal quantum circuit structures. Projective Simulation, for example, synthesizes quantum circuits to generate entangled states, automating quantum circuit design. This method optimizes ansatz structures for accurate ground energy estimates while maintaining low circuit depth [64].

Advanced simulation frameworks facilitate the integration of variational and reinforcement learning techniques into state vector simulations. Decision diagrams streamline quantum circuit simulations by applying approximations to reduce representation sizes, accelerating the simulation process [65]. This approach effectively manages the exponential growth of computational resources as circuit depth and qubit numbers increase [2].

Cluster expansion and shallow quantum circuit simulation techniques address challenges in 2D quantum dynamics, providing robust frameworks for simulating complex quantum phenomena. These methods use factorized tensor representations to reduce computational overhead and enhance simulation speed [66].

The QAS notably improves variational quantum algorithms (VQAs) by mitigating quantum noise and barren plateaus. The barren plateau problem complicates loss function optimization due to dimensionality challenges, a critical consideration in developing these algorithms. The transition from classical to hybrid systems using both classical and quantum computing capabilities exemplifies these techniques' potential in practical applications [18].

Integrating variational and reinforcement learning techniques into state vector simulations represents a significant advancement in quantum computing. These methodologies enhance the scalability and accuracy of quantum simulations by employing innovative graph-based representations that exploit redundancies in quantum states and operations. This facilitates larger quantum circuit simulations in reduced runtimes compared to traditional simulators and fosters novel quantum algorithms and applications. Consequently, these advancements offer profound insights that can transform various fields, including applied mathematics and scientific computing, positioning quantum computing as a pivotal technology for future breakthroughs across numerous sectors [23, 30, 20, 67, 4].

6 Quantum Algorithm Simulation

6.1 Methodologies for Quantum Algorithm Simulation

Simulating quantum algorithms is fundamental for advancing quantum computing, providing insights into their performance on classical systems. Various methodologies have emerged to optimize quantum algorithm simulation, addressing specific challenges and applications. Encoding optimization problems into quantum circuits demonstrates quantum algorithms' potential to solve complex tasks, particularly in linear algebra and optimization, achieving exponential speedups over classical methods [4]. Memory-Efficient Quantum Circuit Simulation (MEQCS) leverages amplitude-aware lossy data compression to significantly reduce memory requirements for quantum state amplitudes, enabling the simulation of deep circuits with up to 63 qubits using only 0.8 petabytes of memory while maintaining high fidelity [68, 69].

The integration of Quantum Random Access Code (QRAC) for encoding discrete features is pivotal for simulating quantum algorithms in classification tasks, reducing qubit requirements and enhancing frameworks like QuEST, a GPU-accelerated simulator supporting hybrid multithreaded and distributed environments. QuEST can simulate complex quantum circuits, including those with up to 38 qubits over 2048 compute nodes, showcasing strong and weak scaling efficiency compared to frameworks like ProjectQ and qHipster [9, 67]. Stochastic sampling and decision diagram (DD) representations facilitate the approximation of error effects in quantum circuit simulations, enhancing computational efficiency through probabilistic error modeling and compact state representations [70, 54, 71, 72, 26].

Efficient construction of circuits for single and double fermionic excitations is crucial for simulating quantum algorithms like the variational quantum eigensolver (VQE), which is significant for quantum chemistry applications. Collectively, these methodologies represent the forefront of quantum algorithm simulation, offering innovative solutions to scalability, efficiency, and practical applicability challenges. By leveraging techniques such as graph-based representations and efficient mapping methodologies, researchers can handle larger quantum systems with reduced runtime, advancing practical quantum applications and positioning quantum computing as a transformative force in scientific computing and applied mathematics [73, 23, 4, 20].

6.2 Challenges in Simulating Complex Quantum Algorithms

Simulating complex quantum algorithms poses significant challenges due to the exponential growth in computational resources required as qubit numbers increase, known as the curse of dimensionality. This scaling renders accurate simulations of larger quantum circuits infeasible using classical methods, as memory and processing requirements exceed practical limits [72]. A core obstacle is the exponential increase in memory usage with each additional qubit, making simulations beyond approximately 50 qubits impractical [32]. Limitations of current quantum hardware, including restricted qubit connectivity and noise, further complicate these challenges by introducing calibration errors and decoherence, undermining simulation accuracy.

The high number of CNOT gates required in existing simulation methods also limits fidelity and scalability, particularly on Noisy Intermediate-Scale Quantum (NISQ) devices [74]. These gates, essential for entangling qubits, introduce additional noise and errors that complicate the simulation of complex quantum algorithms. Furthermore, readout errors can lead to biased results, compromising simulation accuracy [33]. Despite these challenges, advancements in simulation methodologies, such as tensor networks and GPU acceleration, show promise in overcoming memory constraints and improving performance, achieving efficiencies up to 200,000 times faster than previous estimates [24].

Existing benchmarks often inadequately measure performance due to limitations in integration and optimization techniques within quantum circuit simulators [66]. While partitioning methods can enhance simulation efficiency, they may not be effective for circuits with high entanglement or depth beyond a certain threshold, where the overhead of partitioning may outweigh benefits [2]. Achieving low Rent exponents and enhancing extensibility is critical for developing scalable quantum processors, with shared control schemes offering significant potential [3].

Innovative approaches, such as the proposed simulation path framework, have demonstrated substantial runtime improvements by leveraging quantum characteristics. High-performance simulators like qFlex and the tensor-based simulator on the Sunway supercomputer have achieved remarkable results, reducing the time to simulate complex quantum circuits from thousands of years to mere seconds, while reaching peak performance levels of up to 4.4 Eflops. These advancements highlight the potential of such frameworks to simplify verification processes and achieve significant speedups compared to classical methods [75, 76, 4, 77]. Developing efficient simulation techniques and leveraging advanced computational resources will enable researchers to better manage the complexities of quantum systems, facilitating significant advancements in quantum computing applications.

6.3 Solutions and Optimization Strategies

Optimizing quantum algorithm simulations is crucial for enhancing efficiency and accuracy, especially as quantum systems grow in complexity. Tensor-network quantum circuits have shown significant potential in reducing computational overhead compared to classical methods [2]. Future research could focus on improving the scalability of these circuits by integrating sparse tensor methods and enhanced parallelization strategies, along with incorporating noise models for more realistic simulations [64].

The Quantum Subspace Expansion (QSE) method exemplifies advancements in hybrid quantum-classical approaches, effectively mitigating decoherence and enabling accurate determination of excited states [63]. This method underscores the importance of integrating classical and quantum resources to optimize simulations, particularly in managing noise and enhancing fidelity.

Circuit optimization techniques are critical for improving simulation performance. By minimizing the number of qubits required, these methods reduce memory requirements and enhance overall efficiency [78]. The character function decomposition method further improves the efficiency of classical simulations of quantum circuits, offering a novel approach to optimizing computational resources [72].

Innovative compression techniques, such as the lossy compression method introduced by Wu et al., significantly enhance compression ratios while maintaining acceptable fidelity, providing practical solutions for managing large-scale quantum circuit simulations [65]. Additionally, optimizing index arrangements for tensor contractions and exploring methods for rescaling quantum circuit data can further improve simulation efficiency without sacrificing accuracy.

The development of optimal contraction trees and improved ordering heuristics offers another avenue for enhancing tensor network simulation performance. By parallelizing algorithms and extending approaches to accommodate higher-order structures, researchers can achieve more efficient simulations [62].

Frameworks like HiSVSIM demonstrate significant improvements in simulation performance, achieving up to 3.9 times speedup as qubit numbers increase, showcasing effectiveness in handling large-scale quantum circuits. Future research could focus on enhancing the partitioning function itself, potentially leveraging ZX-calculus-based optimizations to improve partitionability and reduce runtime through advanced techniques like hierarchical partitioning for efficient simulation on multi-node GPUs, as well as mathematical methods to compress quantum operations and exploit parallelism in modern processors. Such approaches have shown significant performance gains in quantum circuit simulations, indicating a promising direction for accelerating computational efficiency in quantum algorithms like the Quantum Approximate Optimization Algorithm (QAOA) [79, 80, 81, 4].

By utilizing the adaptability of the LHRS to optimize the balance between qubit count and T gate count, its applicability across diverse quantum computing scenarios can be expanded. This flexibility allows for seamless integration into comprehensive quantum compilation workflows, ultimately leading to enhanced optimization and improved performance in solving complex industry-specific problems [76, 82, 40, 11, 67]. The Quipu framework's ability to efficiently simulate larger quantum circuits while maintaining global phases further exemplifies the potential for significant performance improvements through parallelization.

The various strategies highlighted in the references underscore the critical need for ongoing innovation in the development and optimization of quantum algorithm simulations, particularly given the transformative potential of quantum computing technologies to revolutionize high-performance scientific computing and applied mathematics. As researchers and industry leaders work to address scalability and performance challenges, these innovations will play a pivotal role in harnessing the capabilities of quantum processors, enabling breakthroughs that could significantly impact various computational disciplines and societal applications [44, 4]. Integrating advanced techniques and leveraging hybrid approaches will enhance the scalability and accuracy of quantum simulations, paving the way for breakthroughs in quantum computing applications.

7 Classical Computing Techniques in Quantum Simulation

7.1 Integration of Classical Algorithms in Quantum Simulations

Integrating classical algorithms into quantum simulations is essential for enhancing the performance and scalability of quantum systems, particularly within Noisy Intermediate-Scale Quantum (NISQ) devices. Classical techniques optimize resource utilization and enable efficient execution of quantum algorithms on limited hardware. Noise-aware optimizers, for instance, significantly improve the performance of variational quantum eigensolvers (VQE) by addressing quantum noise challenges [83]. Quasi-Newton optimization methods in hybrid variational algorithms demonstrate how classical approaches can enhance the efficiency of variational quantum circuits [63]. Platforms like PennyLane integrate variational quantum circuits with classical machine learning libraries, creating a fully differentiable quantum programming paradigm that optimizes circuit parameters [64].

Classical algorithms are crucial for improving memory efficiency and computational performance in quantum simulations, significantly reducing runtime and resource requirements. Techniques such as tensor network-based algorithms and lossy data compression have simulated quantum circuits with up to 63 qubits, minimizing memory usage to 16.5

Specialized toolkits for multi-GPU platforms, utilizing cache-aware optimizations and advanced data management strategies, underscore the significant role of classical algorithms in boosting simulation performance. Systems like Atlas and QTensor use hierarchical partitioning and dynamic mixed backends to efficiently simulate complex quantum circuits, minimizing communication costs and maximizing throughput, achieving performance improvements over two orders of magnitude compared to traditional methods [61, 81, 84]. This integration enhances computational efficiency, providing scalable solutions for managing complex quantum operations.

Incorporating classical algorithms into quantum simulations enhances performance and scalability while addressing challenges like noise mitigation and resource optimization. Advancements in quantum computing technologies are influencing scientific disciplines, enabling breakthroughs in applied mathematics, and potentially disrupting encryption methods, attracting substantial investment from industry leaders and government entities [23, 30, 4].

7.2 Enhancing Quantum Circuit Simulations with Classical Techniques

Enhancing quantum circuit simulations with classical techniques involves leveraging classical computing strengths to optimize performance and accuracy. Preconditioning methods in variational quantum linear solvers (VQLS) reduce the entanglement required for solving linear systems, although they may increase the entanglement needed for generating the preconditioned state [85]. Classical optimization algorithms are effectively integrated into quantum simulations, particularly in VQE problems like ethylene rotation, bond stretching, and Hubbard model simulations. These optimizers enhance performance in noisy environments by efficiently navigating parameter spaces, mitigating noise effects, and improving fidelity and convergence [83].

Classical techniques also play a crucial role in evaluating the environmental impact of quantum simulations. A method for calculating CO2e emissions considers the number of processors, average power per processor, simulation duration, carbon intensity, and power usage effectiveness [86]. This approach emphasizes integrating sustainability considerations into quantum simulation design and execution.

Integrating classical computing techniques into quantum circuit simulations significantly enhances computational efficiency and accuracy while addressing issues like noise mitigation and environmental impact. Recent advancements show that classical algorithms can simulate larger and deeper quantum circuits than previously possible, even under realistic noise conditions. A preliminary model indicates that simulating large quantum circuits can result in CO2e emissions 48 times greater than those from training a transformer machine learning model, highlighting the need to consider both performance and sustainability in quantum technology development [86, 52].

7.3 Hybrid Quantum-Classical Approaches

Hybrid quantum-classical approaches are pivotal in integrating quantum and classical computing, leveraging both paradigms' strengths to develop innovative solutions for complex computational tasks. The variational quantum eigensolver (VQE) exemplifies this synergy by addressing classically intractable eigenvalue problems, effectively minimizing coherence time requirements through combined quantum and classical resources. This methodology enhances simulation accuracy and mitigates decoherence errors, positioning hybrid approaches as frontrunners in achieving quantum supremacy over classical computation [34, 23, 41].

The Quantum Subspace Expansion (QSE) method illustrates the synergy between quantum and classical computation by combining variational state preparation with classical algorithms to explore excited states systematically [41]. This method underscores the potential of hybrid approaches in improving the accuracy and efficiency of quantum simulations, especially in applications requiring detailed exploration of quantum state spaces.

Incorporating classical neural networks within the quantum Generative Adversarial Network (qGAN) framework further demonstrates the effectiveness of hybrid approaches [45]. This integration allows for efficient training of quantum models, leveraging classical optimization techniques to refine quantum parameters and enhance overall simulation performance. The qGAN framework exemplifies how classical machine learning complements quantum computing, providing a robust platform for simulating complex quantum systems.

The Quantum Assisted Simulator (QAS) algorithm highlights the practical applicability of hybrid approaches, being compatible with current experimental capabilities and implementable on existing quantum hardware [60]. This compatibility ensures that hybrid techniques can be readily deployed, facilitating the transition from theoretical models to practical applications in quantum simulations.

Hybrid quantum-classical approaches represent a significant advancement in quantum computing, offering pathways to more efficient and scalable simulations. By leveraging the unique computational advantages of both quantum and classical systems, these innovative approaches are poised to revolutionize the simulation of intricate quantum phenomena, enhancing the performance and applications of quantum technologies across various sectors, including finance, pharmaceuticals, and high-performance scientific computing [19, 23, 30, 4].

8 Quantum Circuit Simulation

Addressing the challenges in quantum circuit simulation requires methodologies that improve reliability and performance, particularly through classical techniques for noise mitigation and error correction. These strategies are crucial in counteracting quantum noise and ensuring computational fidelity, thus advancing the accuracy and efficiency of simulations.

8.1 Classical Techniques for Noise Mitigation and Error Correction

Classical techniques enhance the fidelity of quantum circuit simulations, especially for variational quantum algorithms (VQAs) on noisy intermediate-scale quantum (NISQ) devices. Error mitigation and correction strategies balance circuit complexity and noise, improving robustness and trainability [40, 47, 87]. Amplitude-Aware Lossy Compression (AALC) exemplifies noise mitigation by optimizing memory usage while maintaining accuracy, crucial for large-scale quantum systems [68].

The QOPS compiler framework accelerates simulations through profile-guided optimization, reducing compilation time and enhancing efficiency [88]. Additionally, FTDD employs garbage collection and caching for dynamic memory management, optimizing performance in complex circuits [89]. Atlas enhances scalability by minimizing communication costs and maximizing parallelism [81]. Metrics from flexible simulation frameworks provide insights into noise mitigation, guiding robust methodology development [76].

These classical techniques are integral to advancing quantum computing by optimizing resources and improving simulation efficiency, addressing challenges in simulating complex quantum systems [44, 6, 8].

8.2 Decomposition and Tensor Network Techniques

Decomposition and tensor network techniques are essential for enhancing quantum circuit simulation efficiency and scalability. These methods optimize computational resources, addressing complexities in large-scale systems. Hybrid compression in full-state simulations integrates decomposition techniques for speed and memory optimization [90]. The Tetris algorithm reduces computational overhead by achieving linear complexity in rank simplification [89].

Atlas partitions circuits into subcircuits for single GPU simulation, maximizing resource utilization [81]. The QOPS framework uses profile-guided optimization to enhance speed and efficiency [88]. Combining decomposition and tensor network methods significantly reduces simulation times, leveraging modern GPUs for up to 12.5x acceleration [21, 22]. These methods address computational challenges, advancing quantum computing technologies.

8.3 Haskell-based and Multi-GPU Simulation Tools

Haskell-based and multi-GPU tools significantly advance quantum circuit simulation efficiency, managing large-scale system complexities. Haskell facilitates concise algorithm development with its strong type system and lazy evaluation, optimizing resource allocation and computational efficiency.

Haskell-based tools support high-performance environments like QuEST, managing decoherence and computational challenges [91, 67].

Multi-GPU tools enhance scalability by distributing tasks, reducing execution time. The QOPS framework leverages multi-GPU platforms for optimized simulations, outperforming traditional configurations [88]. Atlas demonstrates multi-GPU advantages, using up to 256 GPUs to maximize resources and reduce simulation time on the Perlmutter supercomputer [81].

Integrating Haskell-based and multi-GPU frameworks enables efficient hardware-accelerated simulations, enhancing quantum circuit analysis and supporting complex algorithm simulation. This progress facilitates quantum supremacy validation and new circuit design [91, 67, 61, 92]. These tools optimize resources and improve simulation efficiency, advancing quantum technologies and applications.

9 Conclusion

9.1 Current State and Challenges

Quantum computing is at a pivotal stage, showcasing substantial advancements while grappling with inherent challenges that shape its trajectory. The field promises transformative impacts, particularly in optimization and computational chemistry, where variational algorithms have shown promising capabilities in efficiently reaching ground states. Despite these advancements, practical deployment faces hurdles, notably in hardware limitations such as qubit coherence times and precision requirements essential for scalability. Quantum hardware remains a bottleneck, restricting the scope of computations that can be effectively executed. Although simulation tools have enhanced execution speeds, the need for advanced quantum hardware persists to support extensive circuits. Efforts to address these limitations include innovations like FPGA emulation frameworks, which improve execution speed and resource efficiency, paving the way for more practical quantum simulations.

Hybrid quantum-classical systems offer a solution to classical runtime and memory scalability issues, enabling the simulation of complex quantum circuits. However, high error rates and noise in quantum computations demand robust error mitigation strategies to ensure simulation accuracy. Noise-aware optimizers are crucial for leveraging hybrid algorithms on NISQ devices, enhancing the performance and reliability of quantum simulations. In quantum computational chemistry, while the potential for deeper insights into chemical systems is significant, current hardware constraints pose challenges. Similarly, the realization of quantum computing's benefits in finance relies on the development of more robust hardware. Visualization frameworks are advancing the understanding of quantum principles, yet the ability to simulate many variational algorithms classically raises questions about their non-classicality, highlighting the ongoing need for advancements in both hardware and algorithmic approaches.

9.2 Potential Applications and Future Directions

Quantum computing is poised to revolutionize numerous fields by addressing complex problems beyond the reach of classical systems. In optimization, techniques such as Quantum Signal Processing and Quantum Approximate Optimization Algorithms are central, and future research will likely refine these algorithms to improve gate fidelity and scalability for larger processors. Establishing industry-specific benchmarks will be critical for the practical implementation of quantum solutions. In cryptography, the emergence of quantum computing necessitates the development of quantum-resistant algorithms, with future efforts focusing on post-quantum cryptographic systems and exploring new mathematical problems for cryptographic applications.

Quantum networks present a significant frontier, requiring advancements in error correction, entanglement distribution, and integration with classical communication systems to realize their potential. In quantum circuit simulation, tools are expected to enhance performance for large circuits, with future improvements focusing on optimizing circuit analysis and automated transformations. The integration of tensor network methods for simulating density operators and approximating multi-qubit states presents promising research avenues. Optimizing decision diagram representations and sampling techniques could broaden the applicability of weak simulation methods.

The application of variational hybrid quantum-classical methods to larger systems and complex equations is another promising area, with a focus on optimizing ansatz and classical optimizers for speed-ups. Scaling unsupervised quantum machine learning methods to handle larger datasets and improving operation fidelity are crucial future directions. Research should also prioritize improving qubit coherence times, developing efficient algorithms suitable for NISQ devices, and exploring new physical platforms to enhance computation performance. The anticipated impact of quantum computing on various industries underscores the need for ongoing research to address existing challenges and limitations. Expanding benchmarks to include additional simulation techniques and optimizing methods for larger circuits will be essential.

The future of quantum computing holds immense promise, driven by continuous research and innovation. By addressing current challenges and exploring new applications, the field is poised to significantly impact science, technology, and industry, ushering in a new era of computational capabilities. Future research directions include enhancing frameworks for larger qubit sizes, integrating error-correcting codes, and incorporating error mitigation techniques. Exploring hyperfine interactions and adapting methods to include non-unitary effects in simulations will also be critical. In quantum chemistry, developing more robust algorithms, improving hardware, and investigating new applications remain priorities. Future research should enhance noise mitigation strategies, hybrid approaches, and explore additional problem classes that may benefit from quantum optimization. Optimizing communication patterns, exploring additional quantum operations, and implementing algorithms across various architectures represent further advancement areas. Hybrid approaches that leverage both paradigms to enhance efficiency and effectiveness in solving complex problems are also promising. Future research will focus on improving sampling strategies, reducing parameter space without compromising performance, and exploring applications beyond current algorithms. Developing new compression algorithms tailored for quantum state amplitudes and optimizing error bound selection processes to enhance performance and fidelity are also critical. Finally, optimizing resource requirements and minimizing errors for non-number-conserving simulations will be a focus, alongside developing robust statistical methods for comparing quantum and classical computing and exploring new architectures and algorithms to enhance computational capabilities.

References

[1] Kaitlin N. Smith, Michael A. Perlin, Pranav Gokhale, Paige Frederick, David Owusu-Antwi, Richard Rines, Victory Omole, and Frederic T. Chong. Clifford-based circuit cutting for quantum simulation, 2023.

[2] Zhao-Yun Chen, Qi Zhou, Cheng Xue, Xia Yang, Guang-Can Guo, and Guo-Ping Guo. 64-qubit quantum circuit simulation, 2018.

[3] David P Franke, James S Clarke, Lieven MK Vandersypen, and Menno Veldhorst. Rent's rule and extensibility in quantum computing. *Microprocessors and Microsystems*, 67:1–7, 2019.

[4] Matthias Möller and Cornelis Vuik. On the impact of quantum computing technology on future developments in high-performance scientific computing. *Ethics and information technology*, 19:253–269, 2017.

[5] Bela Bauer, Sergey Bravyi, Mario Motta, and Garnet Kin-Lic Chan. Quantum algorithms for quantum chemistry and quantum materials science. *Chemical Reviews*, 120(22):12685–12717, 2020.

[6] Andrew J Daley, Immanuel Bloch, Christian Kokail, Stuart Flannigan, Natalie Pearson, Matthias Troyer, and Peter Zoller. Practical quantum advantage in quantum simulation. *Nature*, 607(7920):667–676, 2022.

[7] Nader Khammassi, Imran Ashraf, Xiang Fu, Carmen G Almudever, and Koen Bertels. Qx: A high-performance quantum computer simulation platform. In *Design, Automation & Test in Europe Conference & Exhibition (DATE), 2017*, pages 464–469. IEEE, 2017.

[8] Akshay Ajagekar and Fengqi You. Quantum computing for energy systems optimization: Challenges and opportunities. *Energy*, 179:76–89, 2019.

[9] Wei Tang and Margaret Martonosi. Scaleqc: A scalable framework for hybrid computation on quantum and classical processors. *arXiv preprint arXiv:2207.00933*, 2022.

[10] Jack K. Horner and John F. Symons. What have google's random quantum circuit simulation experiments demonstrated about quantum supremacy?, 2020.

[11] Wei Tang, Teague Tomesh, Martin Suchara, Jeffrey Larson, and Margaret Martonosi. Cutqc: using small quantum computers for large quantum circuit evaluations. In *Proceedings of the 26th ACM International conference on architectural support for programming languages and operating systems*, pages 473–486, 2021.

[12] Thien Nguyen, Dmitry Lyakh, Eugene Dumitrescu, David Clark, Jeff Larkin, and Alexander McCaskey. Tensor network quantum virtual machine for simulating quantum circuits at exascale, 2021.

[13] Amirhossein Nourbakhsh, Mark Nicholas Jones, Kaur Kristjuhan, Deborah Carberry, Jay Karon, Christian Beenfeldt, Kyarash Shahriari, Martin P. Andersson, Mojgan A. Jadidi, and Seyed Soheil Mansouri. Quantum computing: Fundamentals, trends and perspectives for chemical and biochemical engineers, 2022.

[14] Mario Motta and Julia E Rice. Emerging quantum computing algorithms for quantum chemistry. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, 12(3):e1580, 2022.

[15] Christian W Bauer, Zohreh Davoudi, Natalie Klco, and Martin J Savage. Quantum simulation of fundamental particles and forces. *Nature Reviews Physics*, 5(7):420–432, 2023.

[16] John Preskill. Quantum computing 40 years later. In *Feynman lectures on computation*, pages 193–244. CRC Press, 2023.

[17] Gian Giacomo Guerreschi, Justin Hogaboam, Fabio Baruffa, and Nicolas PD Sawaya. Intel quantum simulator: A cloud-ready high-performance simulator of quantum circuits. *Quantum Science and Technology*, 5(3):034007, 2020.

[18] Ricardo Pérez-Castillo, Manuel A Serrano, and Mario Piattini. Software modernization to embrace quantum technology. *Advances in Engineering Software*, 151:102933, 2021.

[19] Dylan Herman, Cody Googin, Xiaoyuan Liu, Yue Sun, Alexey Galda, Ilya Safro, Marco Pistoia, and Yuri Alexeev. Quantum computing for finance. *Nature Reviews Physics*, 5(8):450–465, 2023.

[20] Alwin Zulehner and Robert Wille. Advanced simulation of quantum computations. *IEEE Transactions on Computer-Aided Design of Integrated Circuits and Systems*, 38(5):848–859, 2018.

[21] Marcos Díez García and Antonio Márquez Romero. Survey on computational applications of tensor network simulations, 2024.

[22] Feng Pan, Hanfeng Gu, Lvlin Kuang, Bing Liu, and Pan Zhang. Efficient quantum circuit simulation by tensor network methods on modern gpus, 2024.

[23] Anila Mjeda and Hazel Murray. Quantum computing education for computer science students: Bridging the gap with layered learning and intuitive analogies, 2024.

[24] Cupjin Huang, Fang Zhang, Michael Newman, Junjie Cai, Xun Gao, Zhengxiong Tian, Junyin Wu, Haihong Xu, Huanjun Yu, Bo Yuan, et al. Classical simulation of quantum supremacy circuits. *arXiv preprint arXiv:2005.06787*, 2020.

[25] Robert Gingrich, Colin P. Williams, and Nicolas Cerf. Generalized quantum search with parallelism, 1999.

[26] Alwin Zulehner, Stefan Hillmich, Igor L. Markov, and Robert Wille. Approximation of quantum states using decision diagrams, 2020.

[27] Adam Holmes, Sonika Johri, Gian Giacomo Guerreschi, James S Clarke, and Anne Y Matsuura. Impact of qubit connectivity on quantum algorithm performance. *Quantum Science and Technology*, 5(2):025009, 2020.

[28] Miguel Murça, Paul K. Faehrmann, and Yasser Omar. An access model for quantum encoded data, 2024.

[29] Aram W Harrow and Ashley Montanaro. Quantum computational supremacy. *Nature*, 549(7671):203–209, 2017.

[30] Roman Rietsche, Christian Dremel, Samuel Bosch, Léa Steinacker, Miriam Meckel, and Jan-Marco Leimeister. Quantum computing. *Electronic Markets*, 32(4):2525–2536, 2022.

[31] Sergey Bravyi, Dan Browne, Padraic Calpin, Earl Campbell, David Gosset, and Mark Howard. Simulation of quantum circuits by low-rank stabilizer decompositions. *Quantum*, 3:181, 2019.

[32] Juan Carrasquilla, Di Luo, Felipe Pérez, Ashley Milsted, Bryan K Clark, Maksims Volkovs, and Leandro Aolita. Probabilistic simulation of quantum circuits using a deep-learning architecture. *Physical Review A*, 104(3):032610, 2021.

[33] Benjamin Nachman, Miroslav Urbanek, Wibe A de Jong, and Christian W Bauer. Unfolding quantum computer readout noise. *npj Quantum Information*, 6(1):84, 2020.

[34] Angela Sara Cacciapuoti, Marcello Caleffi, Francesco Tafuri, Francesco Saverio Cataliotti, Stefano Gherardini, and Giuseppe Bianchi. Quantum internet: Networking challenges in distributed quantum computing. *IEEE Network*, 34(1):137–143, 2019.

[35] Andrea Pasquale, Andrea Papaluca, Renato M. S. Farias, Matteo Robbiati, Edoardo Pedicillo, and Stefano Carrazza. Beyond full statevector simulation with qibo, 2024.

[36] Debjyoti Bhattacharjee and Anupam Chattopadhyay. Depth-optimal quantum circuit placement for arbitrary topologies. *arXiv preprint arXiv:1703.08540*, 2017.

[37] K. Wang and D. S. Wang. Quantum circuit simulation of superchannels, 2023.

[38] Francesco Bova, Avi Goldfarb, and Roger G Melko. Commercial applications of quantum computing. *EPJ quantum technology*, 8(1):2, 2021.

[39] Yudong Cao, Jonathan Romero, Jonathan P Olson, Matthias Degroote, Peter D Johnson, Mária Kieferová, Ian D Kivlichan, Tim Menke, Borja Peropadre, Nicolas PD Sawaya, et al. Quantum chemistry in the age of quantum computing. *Chemical reviews*, 119(19):10856–10915, 2019.

[40] Article open.

[41] Jarrod R McClean, Mollie E Kimchi-Schwartz, Jonathan Carter, and Wibe A De Jong. Hybrid quantum-classical hierarchy for mitigation of decoherence and determination of excited states. *Physical Review A*, 95(4):042308, 2017.

[42] David Poulin, Alexei Kitaev, Damian S Steiger, Matthew B Hastings, and Matthias Troyer. Quantum algorithm for spectral measurement with a lower gate count. *Physical review letters*, 121(1):010501, 2018.

[43] Juan Miguel Arrazola, Timjan Kalajdzievski, Christian Weedbrook, and Seth Lloyd. Quantum algorithm for nonhomogeneous linear partial differential equations. *Physical Review A*, 100(3):032306, 2019.

[44] Amira Abbas, Andris Ambainis, Brandon Augustino, Andreas Bärtschi, Harry Buhrman, Carleton Coffrin, Giorgio Cortiana, Vedran Dunjko, Daniel J Egger, Bruce G Elmegreen, et al. Quantum optimization: Potential, challenges, and the path forward. *arXiv preprint arXiv:2312.02279*, 2023.

[45] Christa Zoufal, Aurélien Lucchi, and Stefan Woerner. Quantum generative adversarial networks for learning and loading random distributions. *npj Quantum Information*, 5(1):103, 2019.

[46] Adam Holmes and A. Y. Matsuura. Efficient quantum circuits for accurate state preparation of smooth, differentiable functions, 2020.

[47] Thomas Grurl, Christoph Pichler, Jürgen Fuß, and Robert Wille. Automatic implementation and evaluation of error-correcting codes for quantum computing: An open-source framework for quantum error correction, 2023.

[48] Kevin Mato, Stefan Hillmich, and Robert Wille. Mixed-dimensional quantum circuit simulation with decision diagrams, 2023.

[49] Qunsheng Huang and Christian B. Mendl. Efficient quantum circuit simulation using a multi-qubit bloch vector representation of density matrices, 2022.

[50] Natalie Klco, Eugene F Dumitrescu, Alex J McCaskey, Titus D Morris, Raphael C Pooser, Mikel Sanz, Enrique Solano, Pavel Lougovski, and Martin J Savage. Quantum-classical computation of schwinger model dynamics using quantum computers. *Physical Review A*, 98(3):032331, 2018.

[51] Yusen Wu, Yukun Zhang, and Xiao Yuan. An efficient classical algorithm for simulating short time 2d quantum dynamics, 2024.

[52] Jianxin Chen, Fang Zhang, Cupjin Huang, Michael Newman, and Yaoyun Shi. Classical simulation of intermediate-size quantum circuits. *arXiv preprint arXiv:1805.01450*, 2018.

[53] Héctor J. García and Igor L. Markov. Simulation of quantum circuits via stabilizer frames, 2017.

[54] Robert Wille, Stefan Hillmich, and Lukas Burgholzer. Decision diagrams for quantum computing, 2023.

[55] Just like the real thing: ast we.

[56] Junyu Liu and Yuan Xin. Quantum simulation of quantum field theories as quantum chemistry. *Journal of High Energy Physics*, 2020(12):1–48, 2020.

[57] Matthew Hagan and Nathan Wiebe. Composite quantum simulations. *Quantum*, 7:1181, 2023.

[58] Taylor L. Patti, Jean Kossaifi, Susanne F. Yelin, and Anima Anandkumar. Tensorly-quantum: Quantum machine learning with tensor methods, 2021.

[59] Diego Guala, Shaoming Zhang, Esther Cruz, Carlos A Riofrío, Johannes Klepsch, and Juan Miguel Arrazola. Practical overview of image classification with tensor-network quantum circuits. *Scientific Reports*, 13(1):4427, 2023.

[60] Kishor Bharti and Tobias Haug. Quantum-assisted simulator. *Physical Review A*, 104(4):042418, 2021.

[61] Danylo Lykov, Angela Chen, Huaxuan Chen, Kristopher Keipert, Zheng Zhang, Tom Gibbs, and Yuri Alexeev. Performance evaluation and acceleration of the qtensor quantum circuit simulator on gpus. In *2021 IEEE/ACM Second International Workshop on Quantum Computing Software (QCS)*, pages 27–34. IEEE, 2021.

[62] Lukas Burgholzer, Alexander Ploier, and Robert Wille. Simulation paths for quantum circuit simulation with decision diagrams, 2022.

[63] Gian Giacomo Guerreschi and Mikhail Smelyanskiy. Practical optimization for hybrid quantum-classical algorithms. *arXiv preprint arXiv:1701.01450*, 2017.

[64] Ville Bergholm, Josh Izaac, Maria Schuld, Christian Gogolin, Shahnawaz Ahmed, Vishnu Ajith, M Sohaib Alam, Guillermo Alonso-Linaje, B AkashNarayanan, Ali Asadi, et al. Pennylane: Automatic differentiation of hybrid quantum-classical computations. *arXiv preprint arXiv:1811.04968*, 2018.

[65] Santiago I. Betelu. The limits of quantum circuit simulation with low precision arithmetic, 2020.

[66] Chuan-Chi Wang. Queenv2: Future of quantum circuit simulation, 2024.

[67] Tyson Jones, Anna Brown, Ian Bush, and Simon C Benjamin. Quest and high performance simulation of quantum computers. *Scientific reports*, 9(1):10736, 2019.

[68] Xin-Chuan Wu, Sheng Di, Franck Cappello, Hal Finkel, Yuri Alexeev, and Frederic T. Chong. Amplitude-aware lossy compression for quantum circuit simulation, 2018.

[69] Xin-Chuan Wu, Sheng Di, Franck Cappello, Hal Finkel, Yuri Alexeev, and Frederic T. Chong. Memory-efficient quantum circuit simulation by using lossy data compression, 2018.

[70] Stefan Hillmich, Richard Kueng, Igor L. Markov, and Robert Wille. As accurate as needed, as efficient as possible: Approximations in dd-based quantum circuit simulation, 2020.

[71] Jingcheng Shen, Linbo Long, Masao Okita, and Fumihiko Ino. A reorder trick for decision diagram based quantum circuit simulation, 2022.

[72] Thomas Grurl, Richard Kueng, Jürgen Fuß, and Robert Wille. Stochastic quantum circuit simulation using decision diagrams, 2020.

[73] An efficient methodology for map.

[74] Efficient quantum circuits for q.

[75] Yong Liu, Xin Liu, Fang Li, Haohuan Fu, Yuling Yang, Jiawei Song, Pengpeng Zhao, Zhen Wang, Dajia Peng, Huarong Chen, et al. Closing the" quantum supremacy" gap: achieving real-time simulation of a random quantum circuit using a new sunway supercomputer. In *Proceedings of the international conference for high performance computing, networking, storage and analysis*, pages 1–12, 2021.

[76] Benjamin Villalonga, Sergio Boixo, Bron Nelson, Christopher Henze, Eleanor Rieffel, Rupak Biswas, and Salvatore Mandrà. A flexible high-performance simulator for verifying and benchmarking quantum circuits implemented on real hardware. *npj Quantum Information*, 5(1):86, 2019.

[77] Ales Kubicek, Athanasios Stratikopoulos, Juan Fumero, Nikos Foutris, and Christos Kotselidis. Tornadoqsim: An open-source high-performance and modular quantum circuit simulation framework, 2023.

[78] Lukas Burgholzer and Robert Wille. Advanced equivalence checking for quantum circuits. *IEEE Transactions on Computer-Aided Design of Integrated Circuits and Systems*, 40(9):1810–1824, 2020.

[79] Matthew Sutcliffe. Smarter k-partitioning of zx-diagrams for improved quantum circuit simulation, 2024.

[80] Yu-Cheng Lin, Chuan-Chi Wang, Chia-Heng Tu, and Shih-Hao Hung. Towards optimizations of quantum circuit simulation for solving max-cut problems with qaoa, 2023.

[81] Mingkuan Xu, Shiyi Cao, Xupeng Miao, Umut A. Acar, and Zhihao Jia. Atlas: Hierarchical partitioning for quantum circuit simulation on gpus (extended version), 2024.

[82] Andreas Bayerstadler, Guillaume Becquin, Julia Binder, Thierry Botter, Hans Ehm, Thomas Ehmer, Marvin Erdmann, Norbert Gaus, Philipp Harbach, Maximilian Hess, et al. Industry quantum computing applications. *EPJ Quantum Technology*, 8(1):25, 2021.

[83] Wim Lavrijsen, Ana Tudor, Juliane Müller, Costin Iancu, and Wibe de Jong. Classical optimizers for noisy intermediate-scale quantum devices, 2021.

[84] 0.5 petabyte simulation of a 45-.

[85] Aruto Hosaka, Koichi Yanagisawa, Shota Koshikawa, Isamu Kudo, Xiafukaiti Alifu, and Tsuyoshi Yoshida. Preconditioning for a variational quantum linear solver, 2024.

[86] Jinyang Li, Qiang Guan, Dingwen Tao, and Weiwen Jiang. Carbon emissions of quantum circuit simulation: More than you would think, 2023.

[87] Error mitigation for short-depth.

[88] Yu-Tsung Wu, Po-Hsuan Huang, Kai-Chieh Chang, Chia-Heng Tu, and Shih-Hao Hung. Qops: A compiler framework for quantum circuit simulation acceleration with profile guided optimizations, 2024.

[89] Qirui Zhang, Mehdi Saligane, Hun-Seok Kim, David Blaauw, Georgios Tzimpragos, and Dennis Sylvester. Quantum circuit simulation with fast tensor decision diagram, 2024.

[90] Xin-Chuan Wu, Sheng Di, Emma Maitreyee Dasgupta, Franck Cappello, Hal Finkel, Yuri Alexeev, and Frederic T. Chong. Full-state quantum circuit simulation by using data compression, 2020.

[91] Youssef Moawad, Wim Vanderbauwhede, and René Steijl. Transformations for accelerator-based quantum circuit simulation in haskell, 2022.

[92] Oumarou Oumarou, Alexandru Paler, and Robert Basmadjian. Fast quantum circuit simulation using hardware accelerated general purpose libraries, 2021.

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