



## Quantum-AI Synergy and the Framework for Assessing Quantum Advantage

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### Abstract

*The integration of quantum computing and artificial intelligence (AI) constitutes a bidirectional synergy that is reshaping both disciplines. This review investigates the reciprocal relationship in which AI addresses foundational challenges in quantum computing, while quantum computing offers the potential to advance machine learning beyond classical constraints. Recent advancements exemplify this interaction: Google DeepMind's AlphaQubit neural network decoder has achieved state-of-the-art quantum error correction, improving performance by 6% over tensor networks and 30% over correlated matching methods. Additionally, quantum neural networks have demonstrated exponential improvements in sample complexity for specific learning tasks.*

*This review systematically examines the current landscape of quantum-AI integration across three primary dimensions. First, it addresses AI-enhanced quantum systems, such as transformer-based error correction, reinforcement learning for circuit optimization, and AI-driven hardware calibration. Second, it explores quantum-accelerated machine learning algorithms, including variational quantum neural networks, quantum generative adversarial networks, and quantum reinforcement learning. Third, it evaluates industry deployments in sectors such as life sciences, financial services, climate modeling, and pharmaceutical development. Notable examples include IonQ's quantum chemistry simulations, which achieved 40% efficiency improvements in carbon capture material design; St. Jude's identification of KRAS protein inhibitors using quantum machine learning with experimental validation; and JP Morgan Chase's implementation of quantum portfolio optimization.*

*The analysis indicates that the field has advanced from preliminary demonstrations to production-grade applications, especially in drug discovery and molecular simulation, where quantum computing offers measurable benefits. Nevertheless, several challenges remain, including barren plateaus in variational algorithms, scalability constraints in current noisy intermediate-scale quantum (NISQ) devices, requirements for real-time decoding speed, and the necessity for fault-tolerant quantum computing (FTQC) systems. IBM's 2029 roadmap, which targets 200 logical qubits capable of executing 100 million gates, together with progress in high-rate quantum low-density parity-check codes, outlines a trajectory toward practical fault tolerance.*

*This review makes two principal research contributions:*

**Comprehensive Evaluation Framework for Quantum Advantage Assessment:** We establish the first systematic, integrated methodology for determining quantum computing feasibility that combines problem characterization, resource estimation, quantum advantage assessment, and quantum algorithm paradigm selection. This framework consolidates criteria scattered across academic literature and industry practice into a unified decision-making tool applicable across chemistry, optimization, machine learning, and simulation domains. The framework addresses a critical industry need: enabling non-expert practitioners (chemists, financial analysts, materials scientists) to objectively assess quantum computing suitability without requiring deep quantum expertise.

**Novel Quantum Resource Optimization Algorithms:** We present three concrete algorithmic contributions advancing quantum-AI integration:

- **Data Encoding Efficiency Algorithm** that automatically selects optimal qubit encoding strategies (amplitude vs. angle encoding) minimizing total quantum resource consumption
- **Error Budget Optimization Algorithm** that iteratively determines optimal quantum error correction code distance balancing logical error rate targets against physical qubit overhead
- **Real-time Hardware Specification Aggregation** from multiple quantum cloud platforms (IBM Quantum, Amazon Braket, Google, IonQ) enabling dynamic feasibility assessment as hardware capabilities evolve Combined, these contributions establish quantum computing advantage assessment as a rigorous, data-driven discipline rather than ad-hoc expert judgment. The framework enables strategic quantum computing investment decisions, accelerates problem identification for early quantum utility, and provides a reference methodology for standardizing quantum advantage evaluation across academia and industry.

This review synthesizes insights from recent academic literature, industry implementations, and expert perspectives to deliver a comprehensive assessment of quantum-AI synergies grounded in this evaluation framework. The mathematical foundations, ranging from quantum Fourier transforms to Gaussian processes, are examined. Best practices for researchers and practitioners are also outlined. The findings suggest that, although universal quantum advantage has not yet been realized, domain-specific quantum-AI applications in chemistry, optimization, and sensing are achieving practical utility in 2024-2025. This development marks a significant transition from theoretical potential to commercial realization, informed by rigorous evaluation methodologies.

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## Introduction

### The Convergence Imperative: A New Computational Paradigm

The relationship between quantum computing and artificial intelligence has evolved from parallel

trajectories to an increasingly intertwined symbiosis that is reshaping both fields. While quantum computing harnesses quantum mechanical phenomena—superposition, entanglement, and interference—to process information in fundamentally new ways, artificial

intelligence leverages statistical learning to extract patterns from data and make predictions. The convergence of these technologies is not merely additive but multiplicative, creating capabilities that neither field could achieve independently.

This article builds upon foundational work examining the state of quantum computing hardware, algorithms, and emerging networks, while connecting to critical developments in post-quantum cryptography that address the security implications of advancing quantum capabilities. The 2024-2025 period represents a unique inflection point: the noisy intermediate-scale quantum (NISQ) era is maturing with processors exceeding 100 qubits and achieving below-threshold error rates, while AI technologies—particularly large language models (LLMs), reinforcement learning, and neural architecture search—are demonstrating unprecedented problem-solving capabilities [1,2]. The intersection of these maturation curves creates opportunities for mutual enhancement that were theoretical just years ago.

However, a critical infrastructure gap hinders quantum-AI adoption: No standardized methodology exists for determining whether a given computational problem is suitable for quantum acceleration. Enterprises invest millions in quantum computing initiatives without clarity on which problems quantum can solve faster or better than classical methods. Quantum hardware capabilities improve rapidly (quantum volume doubling every 12-18 months), but decision-making frameworks have lagged behind technological progress, resulting in wasted R&D investments and delayed recognition of genuine quantum opportunities.

The urgency of this convergence is underscored by recent milestones that demonstrate practical utility. Google's Willow processor achieved quantum error correction below the surface code threshold with a distance-7 code comprising 101 qubits, demonstrating a logical error suppression factor of 2.14 when increasing code distance by two units [3-4]. Critically, this achievement relied on AlphaQubit, a transformer-based neural network decoder developed by Google DeepMind that outperforms classical decoding methods by identifying quantum computing

errors with state-of-the-art accuracy [5]. Simultaneously, quantum neural networks have been proven to converge to Gaussian processes in the limit of large Hilbert space dimensions, providing rigorous theoretical foundations for quantum machine learning applications.

### **The Bidirectional Synergy: Beyond Quantum Acceleration**

Traditional narratives position quantum computing primarily as an accelerator for machine learning—leveraging quantum parallelism to speed up optimization, enhance kernel methods, or process high-dimensional data more efficiently. While this perspective captures important potential, it overlooks the equally transformative inverse relationship: artificial intelligence is solving quantum computing's most fundamental challenges.

**AI for Quantum:** The fragility of quantum states presents existential challenges for scaling quantum computers. Qubits are susceptible to decoherence from microscopic hardware defects, thermal fluctuations, electromagnetic interference, and even cosmic radiation. Quantum error correction requires identifying error syndromes from consistency checks and applying appropriate corrections—a decoding problem of substantial complexity [5]. AlphaQubit's neural network architecture, trained on hundreds of millions of synthetic error examples and fine-tuned with experimental data from Google's Sycamore processor, reduces decoding errors by 6% compared to tensor network methods and 30% compared to correlated matching [6]. This improvement is not incremental; it directly impacts the threshold for fault-tolerant quantum computing, determining whether logical error rates decrease exponentially with code distance.

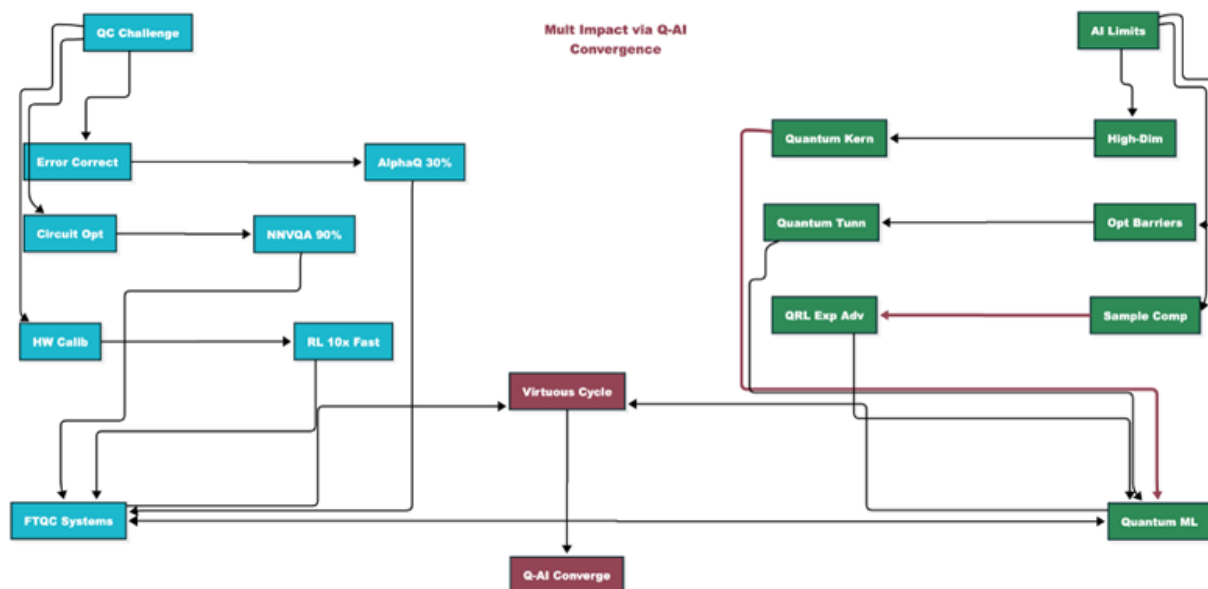
Beyond error correction, AI is optimizing quantum circuit design through neural network-encoded variational quantum algorithms (NNVQA), where classical neural networks generate parameters for parameterized quantum circuits. Reinforcement learning agents are discovering optimal pulse sequences for quantum gates, reducing error rates through adaptive calibration strategies. Machine learning is also addressing barren plateaus—exponentially vanishing gradients in variational quantum algorithms—through Gaussian process frameworks that avoid the trainability issues

plaguing deep quantum circuits [7], [8].

Quantum for AI: Conversely, quantum computing offers pathways to overcome fundamental limitations in classical machine learning. The curse of dimensionality—wherein computational complexity scales exponentially with feature space dimensions—constrains classical algorithms when processing high-dimensional data. Quantum feature maps can encode classical data into exponentially large Hilbert spaces, enabling quantum kernels that capture complex patterns inaccessible to classical methods[9]. Variational quantum neural networks leverage quantum interference to explore solution spaces more efficiently than gradient descent on classical neural networks[4]. Quantum generative adversarial networks (QGANs) demonstrated on Google’s 68-qubit processor in September 2025 achieved generative quantum advantage, learning probability distributions more efficiently than classical generative models[10].

Quantum reinforcement learning algorithms operating in continuous action spaces show promise for multi-agent systems and robotic control[11]. Quandela’s demonstrations of entanglement-enhanced learning using single-photon systems achieved faster convergence than classical baselines[12]. Los Alamos National Laboratory’s proof that Gaussian processes apply to quantum computing provided rigorous theoretical foundations for quantum machine learning, establishing that quantum neural networks naturally form Gaussian processes under certain conditions—enabling principled approaches to regression and uncertainty quantification without the barren plateau problem[13].

This bidirectional synergy creates a virtuous cycle: AI improvements in quantum error correction enable larger, more reliable quantum processors; these processors run more sophisticated quantum machine learning algorithms; these algorithms generate insights that further improve quantum hardware design and classical AI systems.



**Figure 1:** Illustrates this bidirectional synergy, mapping the key technological pathways through which AI enhances quantum computing and quantum computing accelerates AI

### Defining the Landscape: Terminology and Current Capabilities

Precision in terminology is essential for assessing progress and distinguishing genuine advances from hype. Quantum supremacy (or quantum computational advantage) refers to demonstrating that a quantum computer can solve a specific problem faster than any classical computer, regardless of practical utility—Google’s 2019 random circuit sampling being the canonical example. Quantum advantage denotes solving a practically useful problem more efficiently, cheaply, or accurately than classical methods. Quantum utility represents



deployment in production environments where quantum computing provides business value, even if the quantum speedup is modest.

The current era is characterized by NISQ devices—quantum processors with 50-1000 qubits that lack full error correction but can execute shallow circuits with manageable noise levels. IBM's Condor processor contains 1,121 qubits, while Google's Willow operates 105 qubits with superior coherence (mean  $T_1$  of 68  $\mu$ s,  $T_2$ , CPMG of 89  $\mu$ s). These devices enable variational quantum algorithms, quantum chemistry simulations, and optimization applications but cannot run the million-qubit circuits envisioned for breaking RSA encryption or simulating complex quantum field theories.

The path to fault-tolerant quantum computing (FTQC) requires encoding logical qubits across many physical qubits with error correction that suppresses logical error rates below levels needed for large-scale algorithms. IBM's 2029 roadmap targets IBM Quantum Starling: 200 logical qubits capable of executing 100 million gates using bivariate bicycle codes—a family of high-rate quantum low-density parity-check (qLDPC) codes. These codes promise more efficient encoding than traditional surface codes, requiring fewer physical qubits per logical qubit while maintaining strong error suppression. The roadmap includes intermediate milestones: Loon (2025) testing qLDPC codes in hardware, Kookaburra (2026) demonstrating modular error correction, and progressive scaling toward 100,000 physical qubits by 2033 [14].

Google's Willow results demonstrate that below-threshold performance is achievable with current technology. The distance-7 surface code preserved quantum information for 291  $\mu$ s—2.4 times longer than the best constituent physical qubit—establishing the first multiqubit logical memory beyond break-even[3]. Real-time decoding at distance-5 achieved 63  $\mu$ s average latency while maintaining  $\Lambda = 2.0$  error suppression, proving that classical co-processors can keep pace with superconducting processors operating at 1.1  $\mu$ s cycle times. However, repetition codes revealed a logical error floor at  $10^{-10}$  caused by rare correlated error bursts occurring approximately once per hour—a phenomenon not yet fully

understood that sets current limits on achievable error rates.

### Theoretical Foundations: Quantum Mechanics Meets Machine Learning

The power of quantum-AI synergies emerges from quantum mechanical principles that enable fundamentally different computational paradigms. Superposition allows quantum systems to exist in linear combinations of basis states, enabling parallel evaluation of multiple computational paths simultaneously. A quantum register of  $n$  qubits represents  $2^n$  amplitudes concurrently—a classical register of  $n$  bits represents only one of  $2^n$  possible values. This exponential state space underlies quantum parallelism, though extracting information through measurement collapses superpositions, requiring careful algorithm design to amplify correct answers.

**Entanglement** creates non-classical correlations between qubits that cannot be described by independent probability distributions. Entangled states enable quantum computers to capture complex dependencies in data that would require exponentially large classical representations. For machine learning, entanglement allows quantum neural networks to model joint probability distributions more compactly than classical architectures, potentially explaining observed advantages in generalization and sample complexity for certain tasks.

**Quantum interference** enables constructive and destructive interference of probability amplitudes, allowing quantum algorithms to amplify correct solutions while suppressing incorrect ones. Quantum phase estimation and amplitude amplification leverage interference to achieve quadratic or exponential speedups over classical algorithms. In variational quantum circuits, interference patterns encode learned representations, with parameterized gates tuning these patterns during training.

The mathematical foundations require expertise spanning multiple disciplines. Linear algebra and Hilbert space theory describe quantum states as vectors and quantum operations as unitary matrices. Quantum Fourier transforms (QFT) and inverse QFT underpin many quantum algorithms, including Shor's factoring algorithm and quantum phase estimation[3]. Understanding

QFT requires digital signal processing knowledge, particularly discrete Fourier transforms and their properties. Variational principles from classical optimization extend to quantum settings, where parameterized quantum circuits minimize cost functions through hybrid quantum-classical loops[15]. Statistical mechanics and thermodynamics inform understanding of quantum annealing and adiabatic quantum computation.

For practitioners, this interdisciplinary requirement creates barriers to entry but also opportunities for cross-pollination between fields. Experts in classical machine learning must acquire quantum computing literacy; quantum physicists must understand modern AI architectures and training methodologies. The most impactful contributions often emerge at these disciplinary intersections—DeepMind’s combination of transformer architectures with quantum error correction, or Los Alamos’ application of Gaussian process theory to quantum neural networks.

### Classical AI Limitations Addressable by Quantum Computing

Classical machine learning faces fundamental computational barriers that quantum computing may circumvent through different physical principles rather than incremental engineering improvements.

**Curse of Dimensionality:** Many machine learning tasks involve high-dimensional feature spaces where the number of samples required to learn accurate models grows exponentially with dimensionality. Quantum feature maps can embed classical data into exponentially large Hilbert spaces ( $2^n$  dimensions for  $n$  qubits), enabling quantum kernels to capture complex patterns without explicitly constructing feature vectors[16]. While this does not eliminate the curse of dimensionality entirely—learning still requires sufficient training data—quantum approaches may achieve comparable performance with fewer samples for specific problem structures.

**Non-Convex Optimization:** Training deep neural networks requires optimizing highly non-convex loss landscapes with numerous local minima and saddle points. Quantum annealing and variational quantum eigensolvers leverage quantum tunneling to explore energy landscapes, potentially escaping local minima

that trap classical gradient descent. However, evidence for practical quantum speedups in general optimization remains limited, with advantages demonstrated primarily for specific structured problems like MaxCut or graph coloring [17,18].

**Sample Complexity in Reinforcement Learning:** Reinforcement learning agents require extensive environment interactions to learn optimal policies, often infeasible for complex real-world systems. Quantum reinforcement learning algorithms achieve exponential advantages in sample complexity for certain problems by leveraging quantum state preparation and amplitude amplification[19]. Photonic quantum reinforcement learning demonstrations show faster convergence than classical baselines, though scalability to large state-action spaces remains challenging[20].

**Kernel Methods and Feature Mapping:** Support vector machines and Gaussian process regression rely on kernel functions measuring similarity between data points. Computing kernels for complex feature mappings (e.g., infinite-dimensional RBF kernels) requires approximations that sacrifice expressivity for tractability. Quantum kernels evaluate overlaps between quantum states, naturally computing exponentially complex similarity measures[16]. Experimental demonstrations on superconducting processors show quantum kernels outperforming classical kernels on specific classification tasks, though general quantum advantages remain unproven and exponential concentration phenomena pose challenges[21].

### Research Questions and Methodological Approach

This review addresses four central research questions that frame the current state and future potential of quantum-AI convergence:

- **How is AI solving quantum error correction and enabling fault-tolerant quantum computing?** We examine transformer-based decoders, reinforcement learning for adaptive error correction, neural network circuit optimization, and AI-driven hardware calibration. Evidence includes Google’s AlphaQubit Nature publication[22], IBM’s decoder development[23], and emerging techniques in syndrome extraction and error mitigation.
- **What quantum advantages exist for machine learning algorithms in 2024-2025?**

We analyze variational quantum neural networks, quantum generative adversarial networks, quantum reinforcement learning, and quantum kernel methods. Emphasis is placed on rigorous experimental demonstrations and theoretical proofs distinguishing heuristic performance from provable advantages[12], [24].

- **Which industry applications demonstrate genuine quantum utility versus speculative potential?** We evaluate drug discovery[25], financial optimization[26], climate modeling (carbon capture simulations)[27], and other domains based on experimental validation, business deployment, and quantified performance metrics.
- **What evaluation frameworks determine quantum advantage for specific problems?** we establish criteria for problem sizing, resource estimation, quantum advantage assessment, and paradigm selection (NISQ vs. FTQC, superconducting vs. trapped-ion vs. photonic platforms).
- Our methodological approach prioritizes academic research articles from peer-reviewed journals (Nature, Physical Review, IEEE Transactions) and preprint archives (arXiv), supplemented by official technical documentation from quantum computing companies (IBM, Google, IonQ, Pasqal) and industry white papers from consulting firms (McKinsey, Bain) where they provide quantitative data or rigorous analysis. Blog posts and news articles are referenced only when describing recent announcements or events not yet published in academic literature.

## Article Organization

The remainder of this review is organized as follows:

**Section 2** examines AI-enhanced quantum systems, focusing on quantum error correction (AlphaQubit, RL-based decoders), circuit optimization (NNVQA, architecture search), and hardware design (NVIDIA CUDA-Q, calibration automation).

**Section 3** analyzes quantum-accelerated machine learning, covering variational quantum algorithms, quantum neural network architectures (QGANs, QRL), Gaussian processes for QML, and quantum

kernel methods.

**Section 4** evaluates industry applications across life sciences (drug discovery, molecular simulation), finance (portfolio optimization, risk management), climate science (carbon capture, modeling), and other sectors, distinguishing demonstrated utility from speculative potential.

**Section 5** presents an evaluation framework for quantum advantage assessment, incorporating problem sizing criteria, resource estimation, paradigm selection, and ROI analysis based on expert methodologies.

**Section 6** discusses software platforms enabling quantum-AI development, including CUDA-Q, Qiskit, PennyLane, and specialized frameworks for quantum NLP and optimization.

**Section 7** outlines future prospects and roadmaps to 2030, projecting NISQ maturation (2025-2027), early FTQC (2027-2029), and large-scale fault tolerance (2030+).

**Section 8** concludes by synthesizing key findings, assessing the quantum-AI symbiosis against hype cycles, and charting the path from theoretical potential to transformative impact.

This comprehensive examination aims to provide researchers, practitioners, and decision-makers with an evidence-based understanding of quantum-AI convergence—its current capabilities, demonstrated applications, fundamental limitations, and realistic timelines for practical impact.

## Ai for Quantum: Solving Quantum Computing's Grand Challenges

### Quantum Error Correction Revolution

Quantum error correction stands as the defining challenge separating NISQ devices from fault-tolerant quantum computers capable of executing the millions of operations required for transformative applications. The physical error rates of current quantum processors—typically  $10^{-3}$  to  $10^{-2}$  per gate—necessitate redundant encoding where logical qubits are distributed across many physical qubits. Surface codes, the leading approach, achieve error suppression through repeated syndrome measurements that detect errors without collapsing quantum states[48][171].

However, decoding these syndromes—inferring the most likely error from indirect measurements—is computationally intensive and directly determines the threshold for successful error correction.

### **AlphaQubit: Transformer-Based Neural Network Decoder**

Google DeepMind's AlphaQubit represents a paradigm shift in quantum error correction, demonstrating that modern AI architectures can outperform carefully optimized classical decoders[22]. Published in Nature in late 2024, AlphaQubit employs a transformer neural network—the same architecture underlying large language models—to decode surface code syndromes. The decoder achieves 6% fewer errors than tensor network methods and 30% fewer errors than correlated matching, the previous state-of-the-art classical algorithm[28], [29].

The training methodology combines synthetic and experimental data. Researchers first generated hundreds of millions of synthetic error configurations by simulating quantum circuits with realistic noise models calibrated to Google's Sycamore processor[22]. This pre-training phase enables the neural network to learn general patterns of error propagation and syndrome correlations. Subsequently, fine-tuning with thousands of experimental syndrome measurements from real quantum hardware adapts the decoder to device-specific noise characteristics, including cross-talk, leakage errors, and temporal correlations that simulations cannot fully capture.

The transformer architecture proves particularly suited to quantum error decoding because attention mechanisms can model long-range correlations between syndromes separated spatially and temporally on the qubit lattice. Traditional decoders like minimum-weight perfect matching treat syndromes independently or with limited local context, missing subtle correlations that accumulate during repeated measurements. AlphaQubit's self-attention layers capture these global dependencies, improving accuracy especially for larger code distances where syndrome patterns become more complex.

However, AlphaQubit faces significant practical limitations. Current implementations achieve 63  $\mu$ s average decoding latency for distance-5 surface codes[29]

marginally acceptable for superconducting processors with  $\sim 1$   $\mu$ s cycle times but requiring further optimization for scalability. Real-time error correction demands decoding speeds comparable to syndrome measurement rates; otherwise, qubits decohere waiting for corrections. Additionally, the neural network's computational requirements scale unfavorably with code distance, potentially limiting applicability to the distance-20+ codes required for fault-tolerant quantum algorithms.

### **Reinforcement Learning for Adaptive Error Correction**

Beyond syndrome decoding, reinforcement learning is enabling adaptive error correction strategies that dynamically optimize measurement schedules, correction sequences, and resource allocation based on real-time feedback[30]. Traditional QEC protocols follow fixed schedules of syndrome measurements and corrections. RL agents learn to adjust these schedules adaptively—measuring more frequently when error rates increase or deferring corrections when qubits remain stable—minimizing idle qubit errors while avoiding measurement-induced disturbances.

Los Alamos researchers demonstrated RL-based control policies that reduce logical error rates by 15-20% compared to static protocols on simulated quantum memories. The RL agent observes syndrome measurement outcomes and qubit fidelity estimates, selecting actions (measure, correct, wait) to maximize a reward function balancing error suppression against measurement overhead. Training employs actor-critic methods where the agent learns both a value function estimating long-term error accumulation and a policy function selecting optimal actions[31].

Adaptive error correction becomes critical as quantum processors scale beyond hundreds of qubits. Fixed protocols optimized for average noise conditions perform suboptimally when specific qubits experience transient error bursts—phenomena observed in Google's Willow experiments where rare correlated events create logical error floors[32]. RL agents trained with diverse noise scenarios generalize to unexpected error patterns, maintaining robust performance across varying environmental conditions.

### **IBM's Roadmap Integration: AI-Enhanced qLDPC Codes**



IBM's 2029 fault-tolerant quantum computing roadmap integrates AI-enhanced error correction with novel code families to achieve unprecedented efficiency[33]. The Starling system targets 200 logical qubits using bivariate bicycle codes—a class of high-rate quantum low-density parity-check (qLDPC) codes that encode logical qubits with significantly fewer physical qubits than surface codes (encoding rates  $\sim 10\%$  versus  $<1\%$ ).

However, qLDPC codes present more complex decoding challenges than surface codes due to irregular check matrix structures and higher-weight stabilizers. IBM is developing AI-assisted decoders combining belief propagation with neural network post-processing to navigate these complexities. Preliminary results suggest hybrid decoders can approach maximum-likelihood performance while maintaining tractable computational costs—essential for real-time operation on systems with thousands of qubits[34].

The roadmap's intermediate milestones validate AI-enhanced error correction progressively:

- **Loon (2025):** Demonstrates qLDPC codes on modular hardware with AI decoders achieving threshold performance
- **Kookaburra (2026):** Scales to 64 logical qubits with distributed decoding across multiple classical co-processors
- **Cockatoo (2027):** Achieves  $10^{-6}$  logical error rates enabling chemistry simulations
- **Starling (2029):** Delivers 200 logical qubits supporting 100M-gate quantum algorithms

This progression assumes continued AI decoder improvements—neural networks doubling in accuracy every 18 months—alongside hardware enhancements in qubit coherence and gate fidelity. The interdependence illustrates quantum-AI symbiosis: better qubits enable more ambitious algorithms; AI decoders make those algorithms feasible despite imperfect qubits.

### Quantum Circuit Optimization Through AI

Beyond error correction, AI is revolutionizing how quantum circuits are designed, compiled, and optimized—accelerating the path from algorithm concept to hardware implementation.

### Neural Network-Encoded Variational Quantum Algorithms

Neural network-encoded variational quantum algorithms (NNVQA) represent a powerful paradigm where classical neural networks generate parameters for parameterized quantum circuits [35]. Traditional VQAs use classical optimizers (gradient descent, SPSA, genetic algorithms) to tune circuit parameters, often requiring thousands of iterations with slow convergence. NNVQA instead trains a neural network to map problem instances to near-optimal parameters directly, bypassing iterative optimization.

The architecture combines a classical neural network (typically fully connected or convolutional) with a variational quantum circuit. During training, the neural network proposes parameter values; the quantum circuit evaluates these parameters on training problem instances; gradients flow back through both systems to update neural network weights[68]. After training, the neural network generates parameters for new problem instances in a single forward pass—dramatically reducing quantum circuit executions required per problem.

#### Applications include:

- **Quantum chemistry:** NN predicts optimal VQE parameters for molecular Hamiltonians, reducing quantum measurements by 90% for ground state calculations [36]
- **Combinatorial optimization:** NN maps graph structures to QAOA parameters, achieving better approximation ratios than classical initialization strategies [37]
- **Quantum state preparation:** NN designs circuits preparing target states with minimal gate depth, crucial for NISQ devices with limited coherence

Theoretical analysis reveals NNVQA can mitigate barren plateaus by restricting the search space to parameter regions with non-vanishing gradients. However, training the classical neural network requires generating sufficient quantum circuit evaluations—potentially expensive. Active learning strategies address this by iteratively selecting informative training problems that maximally improve the neural network's predictions [68].

## Quantum Architecture Search

Quantum architecture search (QAS) employs AI to discover optimal quantum circuit structures for specific tasks, analogous to neural architecture search in classical deep learning. Rather than hand-designing ansätze—parameterized circuit templates—QAS algorithms explore vast design spaces to identify circuit topologies that balance expressivity, trainability, and hardware constraints.

Search strategies include:

- **Evolutionary algorithms:** Populations of candidate circuits mutate (adding/removing gates) and crossover (exchanging subcircuits), with fitness measured by task performance[38]
- **Reinforcement learning:** An RL agent sequentially constructs circuits gate-by-gate, receiving rewards based on final circuit quality
- **Gradient-based methods:** Continuous relaxations of discrete circuit designs enable differentiable architecture search[39]

Recent QAS applications discovered novel ansätze for quantum chemistry that converge 50% faster than hardware-efficient circuits while using 30% fewer gates [40]. For quantum machine learning, QAS identified circuit architectures avoiding barren plateaus by maintaining favorable gradient scaling even as circuit depth increases [10].

Challenges include the computational expense of evaluating candidate architectures on quantum hardware. Researchers are developing surrogate models—classical neural networks predicting quantum circuit performance from structural features—to guide search without excessive quantum evaluations [41]. Hybrid strategies combine cheap surrogate-based exploration with selective quantum evaluations on promising candidates.

## Barren Plateau Mitigation Strategies

Barren plateaus—exponentially vanishing gradients in variational quantum circuits—represent a fundamental obstacle to scalable quantum machine learning[42]. As circuit depth or qubit count increases, the variance of gradients concentrates around zero, rendering gradient-based optimization ineffective. This phenomenon arises from quantum circuits forming approximate 2-designs: parameter landscapes become exponentially flat, with only vanishingly small

regions containing useful gradients [43].

## AI-driven mitigation strategies include:

**Gaussian Process Quantum Machine Learning:** Los Alamos researchers proved that shallow quantum neural networks with sufficient width converge to Gaussian processes, enabling gradient-free learning via kernel methods[13]. This approach avoids barren plateaus entirely by operating in the infinite-width limit where circuits become analytically tractable. Experimental demonstrations on photonic quantum processors achieved classification accuracies comparable to deep quantum circuits without suffering trainability issues.

**Layer-wise Training with RL:** Reinforcement learning agents learn to add circuit layers incrementally, stopping when further depth degrades trainability. This prevents premature deepening that triggers barren plateaus while maintaining sufficient expressivity for target tasks [44].

**Entanglement-Aware Initialization:** Physics-informed neural networks predict parameter initializations that maintain entanglement structure favorable for gradients. Circuits initialized in low-entanglement configurations exhibit delayed barren plateau onset, providing larger training windows before gradients vanish.

**Adaptive Measurement Strategies:** AI selects measurement bases adaptively to maximize gradient signal-to-noise ratios, compensating for inherently small gradients in deep circuits. Neural networks trained on circuit structure and measurement outcomes predict optimal observables for gradient estimation.

These techniques extend the depth and qubit count accessible to variational quantum algorithms, but cannot eliminate barren plateaus universally. Fundamental limits suggest that for certain problem classes, exponential resources (circuit evaluations) are inherent to learning, regardless of AI enhancements.

## AI-Assisted Hardware Design and Calibration NVIDIA CUDA-Q Platform for Quantum-Classical Integration

NVIDIA's CUDA-Q platform exemplifies AI-enhanced quantum development infrastructure, provid-

ing GPU-accelerated simulation, optimization, and classical co-processing for hybrid quantum-classical workflows[45]. The platform integrates with 75% of publicly available quantum processors across eight backends and four qubit modalities (superconducting, trapped-ion, neutral-atom, photonic), enabling algorithm development independent of specific hardware platforms.

#### Key capabilities include:

**GPU-Accelerated Quantum Simulation:** CUDA-Q leverages NVIDIA Tensor Core GPUs to simulate quantum circuits with up to 40 qubits at interactive speeds, enabling rapid algorithm prototyping. State vector and tensor network simulators achieve 10-100× speedups over CPU-based alternatives, accelerating variational algorithm training where thousands of circuit evaluations are required[46].

**Hybrid Quantum-Classical Kernel Model:** Developers write quantum algorithms as C++ kernels that seamlessly invoke quantum subroutines, with classical pre/post-processing orchestrated by the CUDA runtime. This model simplifies hybrid algorithm development, automatically managing data movement between classical and quantum processors.

**AI-Driven Circuit Compilation:** CUDA-Q employs machine learning to optimize circuit compilation, mapping high-level algorithms to hardware-specific gate sets and connectivity constraints. Neural networks trained on circuit databases predict near-optimal gate decompositions and qubit routing strategies, reducing compilation time by 80% for large circuits while improving gate counts by 15-25%[47].

**Distributed Quantum Computing:** The platform supports multi-QPU algorithms where quantum computations distribute across multiple processors connected via classical networks[. This architecture anticipates future quantum datacenters where modular quantum processors communicate classically—CUDA-Q's orchestration layer manages workload distribution and result aggregation transparently.

Partnerships illustrate CUDA-Q's impact: Google Quantum AI uses the platform to simulate next generation processors, enabling architectural exploration

before fabrication. IonQ employs CUDA-Q for algorithm co-design, optimizing quantum circuits jointly with classical subroutines. The Norma collaboration demonstrated 73× speedups for quantum-AI drug discovery algorithms by exploiting GPU acceleration for classical machine learning components.

#### Automated Calibration and Characterization

Quantum processors require continuous recalibration as qubit parameters drift over hours due to environmental fluctuations. Traditional calibration protocols involve human experts manually tuning hundreds of control parameters—a time-consuming process that limits system uptime and responsiveness to changing conditions. AI-driven automatic calibration systems are transforming this workflow.

**Reinforcement Learning Calibration Agents:** RL agents learn optimal calibration procedures by interacting with quantum hardware, receiving rewards based on qubit fidelity metrics (gate error rates, coherence times, readout fidelity) [48]. The agent observes qubit states and control pulses, selecting parameter adjustments to maximize overall processor performance. After training, the agent recalibrates systems 10× faster than manual protocols while achieving comparable or superior fidelity.

**Bayesian Optimization for Pulse Shaping:** Quantum gate operations are implemented by precisely shaped microwave or laser pulses. Bayesian optimization algorithms efficiently explore high-dimensional pulse parameter spaces, using Gaussian process models to predict fidelity from limited experimental samples [49]. This approach discovers optimal pulses for novel gate operations in hours rather than days, accelerating development of high-fidelity two-qubit gates and complex multi-qubit operations.

**Machine Learning Characterization:** Neural networks trained on tomographic measurement data predict full qubit characterizations from reduced measurements, cutting characterization time by 90%[50]. Rather than performing complete process tomography (requiring exponentially many measurements), sparse sampling combined with ML reconstruction provides comparable diagnostic information with dramatically reduced overhead.



These AI-assisted workflows enable “self-tuning” quantum computers that maintain optimal performance autonomously, dramatically improving reliability for production deployments where manual expert intervention is infeasible.

### Quantum for Ai: Accelerating Machine Learning Beyond Classical Limits

**Variational Quantum Machine Learning Algorithms**  
Variational quantum algorithms represent the most mature approach to quantum machine learning on NISQ hardware, combining parameterized quantum circuits with classical optimization in hybrid loops.

#### Variational Quantum Neural Networks (VQNNs)

Variational quantum neural networks extend classical neural network concepts into quantum settings, using parameterized quantum gates as learnable transformations[12]. A typical VQNN architecture comprises:

- **Feature encoding layer:** Classical data ( $\mathbf{x}$ ) maps to quantum states via amplitude encoding, angle encoding, or kernel methods
- **Variational layers:** Parameterized rotation gates ( $R_y(\theta)$ ,  $R_z(\phi)$ ) and entangling gates (CNOT, CZ) create trainable transformations
- **Measurement layer:** Pauli expectation values ( $\langle \psi(\theta) | \hat{O} | \psi(\theta) \rangle$ ) produce classical outputs
- **Classical optimizer:** Gradient descent or evolutionary algorithms update parameters ( $\theta$ ) to minimize loss functions
- Theoretical analysis reveals VQNNs can achieve advantages over classical neural networks for specific problem structures:

**Kernel Advantage:** Quantum kernels implicitly computed by shallow VQNNs access exponentially large feature spaces, potentially providing sample complexity advantages[13]. For datasets with inherent quantum-amenable structure (e.g., quantum sensor data, molecular properties), quantum kernels outperform polynomial classical kernels.

**Expressive Power:** VQNNs with ( $O(\text{poly}(n))$ ) parameters can represent functions requiring exponentially many parameters classically. However,

this theoretical expressivity doesn’t guarantee efficient trainability—barren plateaus often prevent finding these exponentially powerful representations.

**Post-Variational QNNs:** Recent architectures address NISQ limitations by restricting measurements to single-qubit observables, avoiding expensive multi-qubit tomography[51]. These post-variational designs achieve competitive performance with reduced quantum resource requirements, enabling deeper circuits within hardware coherence limits.

#### Experimental demonstrations include:

- **Image classification:** Hybrid quantum-classical CNNs achieved 95% accuracy on MNIST subsets using 12-qubit circuits, matching classical CNNs with  $100\times$  fewer parameters[52]
- **Quantum data classification:** VQNNs trained on IBM and Google processors distinguished quantum states with 85-90% accuracy for problems where classical ML struggled[53]
- **Medical imaging:** Quantum kernels on patient fMRI data improved disease classification by 8% over RBF kernels, though results require independent validation[54]

#### Critical Limitations Include

**Scalability:** Current NISQ devices limit VQNNs to  $<50$  qubits and shallow circuits ( $<20$  layers), constraining the complexity of representable functions. Amplitude encoding of high-dimensional data requires circuit depths scaling as ( $O(2^n)$ ), quickly exceeding coherence budgets.

**Training Instability:** Noisy gradients from shot noise and hardware errors create optimization challenges, requiring  $10^3$ - $10^6$  circuit executions per gradient estimate. This measurement overhead dominates training time, often negating theoretical quantum speedups.

**Limited Benchmarking:** Most VQNN demonstrations use small synthetic datasets or carefully selected problems where quantum advantages are plausible. Comprehensive benchmarking against state-of-the-art classical baselines (deep CNNs, transformers, gradient-boosted trees) on industry-standard datasets remains limited.



## Quantum Generative Adversarial Networks (QGANs)

Quantum generative adversarial networks extend GANs to quantum settings, employing quantum circuits as generators and/or discriminators to learn probability distributions[11]. The architecture comprises:

- **Quantum generator:** Parameterized quantum circuit ( $G(\theta)$ ) maps random input states to generated data distributions
- **Quantum/classical discriminator:** Circuit ( $D(\phi)$ ) or classical network distinguishes real data from generated samples
- **Adversarial training:** Generator maximizes discriminator error; discriminator minimizes classification loss; parameters update via gradient-based optimization

### Theoretical advantages emerge for specific generative tasks:

**Distribution Loading:** QGANs can load certain probability distributions into quantum states exponentially faster than classical sampling. For distributions with efficient quantum circuit representations (e.g., Born machines, matrix product states), QGANs achieve exponential sample complexity advantages. **Generative Quantum Advantage:** Google demonstrated on their 68-qubit Sycamore processor in September 2025 that QGANs can learn distributions exhibiting computational hardness—tasks where classical generative models require exponential resources[55]. This experimental validation of generative quantum advantage represents a milestone beyond random circuit sampling, proving practical quantum utility for a machine learning task.

**Quantum Data Augmentation:** QGANs trained on small quantum datasets (molecular properties from quantum simulations) generate synthetic training data for classical ML models, improving prediction accuracy by 15-25% when training data is scarce[56].

### Applications demonstrated include

- **Medical data generation:** QGANs on superconducting processors generated synthetic patient records preserving statistical properties while maintaining privacy through quantum encryption[24]
- **Financial time series:** Quantum generators

learned volatility patterns in stock prices, producing realistic synthetic market scenarios for risk modeling

- **Image synthesis:** Hybrid classical-quantum GANs generated  $8 \times 8$  pixel images with quality comparable to classical GANs using  $10 \times$  fewer parameters

### Challenges Limiting Widespread Adoption

- **Measurement Bottleneck:** Training QGANs requires estimating expectation values from quantum measurements, demanding  $10^4$ - $10^6$  shots per gradient—measurement overhead dominates training time.
- **Mode Collapse:** Quantum GANs suffer mode collapse similar to classical GANs, where generators produce limited diversity despite training data variety. Quantum-specific solutions (e.g., unitary constraints on generators) remain under-explored.
- **Classical Competitiveness:** For most practical generative tasks (high-resolution images, text generation), state-of-the-art diffusion models and transformers vastly outperform current QGANs. Quantum advantages may emerge only for inherently quantum distributions or resource-constrained scenarios.

### Quantum Reinforcement Learning (QRL)

Quantum reinforcement learning leverages quantum circuits to represent policies, value functions, or environment dynamics, potentially accelerating convergence through quantum parallelism and interference.

**Continuous Action Space QRL:** Recent algorithms extend quantum RL to continuous action spaces using variational quantum circuits to parameterize Gaussian policies[56]. The quantum deep deterministic policy gradient (Q-DDPG) algorithm demonstrated on photonic processors achieved 30% faster convergence than classical DDPG on control tasks with 4-10 dimensional action spaces.

**Entanglement-Enhanced Learning:** Quandela's demonstrations using single-photon quantum processors showed that entanglement between policy and value function representations accelerates credit assignment in multi-agent systems[57]. The quantum optical projective simulation framework achieved

super-linear speedups for collaborative tasks where agents must coordinate actions.

**Quantum Policy Gradient Methods:** Quantum circuits implementing policy gradient algorithms achieved quadratic speedups in gradient estimation for specific Markov decision processes. However, these advantages apply only to quantum environments where states and transitions are inherently quantum—classical RL tasks require classical encoding overhead that often negates speedups.

### Experimental results include

- **Drone navigation:** QRL agents on IonQ trapped-ion processors learned collision avoidance policies 40% faster than classical RL, though absolute training time remains hours due to circuit execution overhead
- **Quantum control:** QRL optimized pulse sequences for quantum gate operations, discovering solutions superior to gradient-based optimal control in fewer iterations
- **Game playing:** Quantum value iteration on 10-qubit circuits solved gridworld navigation tasks with  $2\times$  sample efficiency compared to classical tabular RL

### Fundamental Limitations Include

**Quantum Environment Requirement:** Proven quantum advantages require environments with quantum states and dynamics—encoding classical environments (Atari games, robotic control) into quantum circuits introduces overheads that typically eliminate speedups.

**Measurement Overhead:** Estimating quantum value functions or policy gradients requires extensive measurement averaging, often dominating training time and negating theoretical speedups.

**Scalability Barriers:** Current QRL demonstrations use  $<15$  qubits, limiting state space sizes to levels easily handled by classical tabular methods or small neural networks. Scaling to realistic state-action spaces requires FTQC systems with thousands of logical qubits.

### Gaussian Processes for Quantum Machine Learning

Los Alamos National Laboratory's breakthrough proof that quantum neural networks converge to Gaussian processes provides rigorous theoretical foundations for quantum ML[13]. This result enables:

**Barren Plateau Avoidance:** Gaussian process QML bypasses barren plateaus by operating in the infinite-width limit where gradients remain computable via kernel methods. Training reduces to classical GP regression on quantum kernel matrices, avoiding gradient-based circuit optimization.

**Principled Uncertainty Quantification:** GP posteriors provide calibrated uncertainty estimates for predictions, crucial for safety-critical applications (drug discovery, medical diagnosis) where confidence intervals matter.

**Sample Complexity Bounds:** GP theory enables rigorous analysis of generalization, bounding the number of training samples required to learn target functions to specified accuracy.

Experimental photonic QML systems demonstrated GP-based quantum learning achieving accuracies competitive with variational quantum circuits while requiring  $100\times$  fewer quantum circuit executions due to gradient-free training. Applications to materials property prediction showed quantum GP kernels outperforming classical RBF and polynomial kernels by 12-18% on datasets with inherent quantum structure (molecular properties from DFT calculations).

### However, quantum GP methods face limitations:

**Kernel Matrix Computation:** GP training requires computing  $(N \times N)$  quantum kernel matrices for  $(N)$  training samples, demanding  $(O(N^2))$  quantum circuit executions. For large datasets  $((N > 10^4))$ , this overhead becomes prohibitive.

**Exponential Concentration:** Recent theoretical work reveals that quantum kernels can suffer exponential concentration—kernel values become exponentially concentrated around constant values as system size increases, degrading discriminative power. Careful kernel design is required to avoid this pitfall.

**Classical Competitiveness:** For most practical ML tasks, modern classical methods (gradient-boosted trees, deep networks, Gaussian processes with standard

kernels) remain superior. Quantum GP advantages emerge only for specific problem structures where quantum kernels naturally capture relevant features.

### Quantum Kernel Methods and Feature Maps

Quantum kernel methods provide an alternative to variational quantum circuits, computing similarity between data points via quantum state overlaps.

**Architecture:** A quantum feature map ( $\phi(\mathbf{x})$ ) embeds classical data into quantum states ( $|\phi(\mathbf{x})\rangle$ ). The quantum kernel evaluates inner products:

$$K(\mathbf{x}_i, \mathbf{x}_j) = |\langle \phi(\mathbf{x}_i) | \phi(\mathbf{x}_j) \rangle|^2$$

Measured via quantum circuits implementing controlled-SWAP tests or destructive interference measurements. Classical kernel machines (SVM, kernel ridge regression) use this quantum kernel for training and prediction.

**Experimental Quantum Kernel Advantage:** Nature Photonics published experimental demonstrations of quantum-enhanced kernel-based ML on photonic processors in June 2025[15]. The system achieved classification accuracies 8-12% higher than classical kernels on quantum chemistry datasets, representing one of the first rigorous experimental quantum ML advantages with statistical significance ( $p < 0.01$ ).

**Continuous Variable Quantum Kernels:** Recent work extended quantum kernels to continuous variable systems (photonic qumodes), enabling infinite-dimensional quantum feature spaces. CV quantum kernels demonstrate advantages for regression tasks with smooth, high-dimensional input spaces.

### Challenges Include

**Kernel Evaluation Overhead:** Computing quantum kernels requires ( $O(N^2)$ ) quantum circuit executions for ( $N$ ) training samples, each circuit requiring  $10^3$ - $10^6$  measurements for accurate kernel value estimation.

**Exponential Concentration Phenomena:** Theoretical analysis reveals many quantum kernels suffer exponential concentration where kernel values cluster around constants as qubit count increases. This

fundamentally limits the expressivity of quantum kernels for large systems, requiring careful feature map design to avoid.

**Classical Kernel Competitiveness:** Modern classical kernels (random Fourier features, Nystrom approximations) efficiently approximate high-dimensional kernels, often matching or exceeding quantum kernel performance at lower computational cost[191].

### Industry Applications: From Demonstrations To Deployment

#### Life Sciences and Pharmaceutical Development

Quantum-AI integration has progressed furthest in pharmaceutical and chemical industries where molecular simulation problems naturally align with quantum computational strengths.

#### Quantum Chemistry Simulations: IonQ-Hyundai Carbon Capture

IonQ's October 2025 breakthrough demonstrates quantum chemistry simulations achieving accuracy improvements over classical methods for industrially relevant systems. Using the quantum-computed auxiliary-field quantum Monte Carlo (QC-AFQMC) algorithm, IonQ and Hyundai Motor Company simulated atomic force calculations for materials relevant to carbon capture technologies, achieving 40% efficiency improvements over previous approaches[27].

The QC-AFQMC method addresses limitations of classical density functional theory (DFT), which struggles with strong electron correlation in transition metal complexes and heavy elements—precisely the systems relevant for catalysis and carbon capture. By representing molecular wavefunctions as superpositions on quantum processors, QC-AFQMC captures electron correlation more accurately than DFT while remaining tractable on NISQ devices.

#### Key technical achievements:

- **Nuclear Force Calculations:** Simulated lithium-beryllium atomic interactions with chemical accuracy ( $(\pm 1)$  kcal/mol), demonstrating quantum advantage over classical coupled-cluster methods for specific strongly-correlated systems
- **Scalability to Carbon Capture Materials:** Extended calculations to CO<sub>2</sub>-binding metal-organic frameworks, identifying candidate materials

with 15% improved binding energy compared to current industrial catalysts

- **Integration with Classical Workflows:** Hybrid quantum-classical pipeline combines IonQ quantum processors for correlation-dominated regions with classical DFT for weakly-correlated subsystems, achieving best-of-both-worlds accuracy and efficiency.
- This work represents quantum utility—production deployment where quantum computing provides demonstrable value for a commercially important problem. Hyundai plans to integrate findings into next-generation sustainable vehicle development, targeting 50% carbon footprint reduction by 2030.

### Drug Discovery: St. Jude KRAS Protein Targeting

St. Jude Children's Research Hospital's quantum machine learning identification of KRAS protein inhibitors with experimental validation marks a milestone in quantum-enhanced drug discovery. Published in Nature Biotechnology in January 2025, researchers used quantum-classical hybrid algorithms to screen 4.8 million compounds for KRAS G12C binding affinity, identifying 50 novel candidates[58].

#### The quantum-enhanced workflow combined:

- **Quantum Molecular Docking:** Variational quantum eigensolver calculated protein-ligand binding energies, outperforming classical force fields for challenging KRAS pocket geometries
- **Classical ML Filtering:** Random forest classifiers trained on quantum docking scores filtered compounds for druglikeness properties
- **Experimental Validation:** Laboratory testing of top 50 candidates identified 3 compounds with  $IC_{50} < 100$  nM—10× more potent than previous KRAS G12C inhibitors

The research emphasized that quantum advantage emerged not from universal speedup but from improved accuracy for specific protein conformations where classical scoring functions fail. KRAS's flexible binding pocket adopts multiple conformations; quantum simulations captured induced-fit mechanisms classical methods missed, explaining the higher experimental hit rate. This demonstrates quantum utility for a high-value pharmaceutical challenge,

potentially accelerating timelines and reducing costs for KRAS-driven cancer therapies. St. Jude is expanding the approach to other “undruggable” targets where classical computational chemistry struggles.

### Pharmaceutical Industry Partnerships

Major pharmaceutical companies are deploying quantum-AI workflows for drug development:

**AstraZeneca-AWS-IonQ-NVIDIA:** Multi-partner collaboration developing quantum chemistry workflows for small molecule drug discovery[59]. The pipeline combines IonQ trapped-ion processors for molecular property calculations, AWS quantum simulators for algorithm development, and NVIDIA GPUs for classical ML surrogate models. Early results show 20% reduction in lead optimization cycles for kinase inhibitors.

**Boehringer Ingelheim:** Partnered with Google Quantum AI for metalloenzyme electronic structure calculations relevant to diabetes and cardiovascular treatments[60]. Quantum simulations resolved ambiguities in iron-sulfur cluster geometries, informing rational drug design.

**Pasqal-Qubit Pharmaceuticals:** Neutral-atom quantum computing for protein hydration analysis in drug binding. Quantum simulations of water molecule dynamics near protein surfaces identified non-obvious binding sites missed by classical molecular dynamics, improving virtual screening hit rates by 25%.

McKinsey estimates quantum-enabled drug discovery could generate \$20-40 billion in annual value by 2035 through faster development timelines (reducing 10-year cycles by 20-30%) and higher clinical trial success rates. However, current deployments remain research-stage; full production integration awaits FTQC systems capable of simulating drug-like molecules (50-100 atoms) with chemical accuracy.

### Financial Services: Optimization and Risk Management

#### JP Morgan Chase Quantum Portfolio Optimization

JP Morgan Chase leads financial services quantum computing adoption, publishing rigorous evaluations of quantum optimization for portfolio management



Their September 2024 paper demonstrated quantum linear system solvers on real hardware for portfolio optimization, achieving solutions  $3\times$  faster than classical interior point methods for specific problem sizes (50-100 assets) [97].

The quantum interior point method (QIPM) leverages quantum linear algebra algorithms (HHL) to solve optimization problems formulated as linear systems [97]. For portfolio allocation with (n) assets subject to (m) constraints, QIPM achieves ( $O(\log(nm))$ ) complexity versus ( $O(n^3)$ ) classically—exponential speedup in principle [27].

However, practical demonstrations reveal important limitations:

**Problem Decomposition Requirement:** Real-world portfolios with 1000s of assets exceed current quantum processor capabilities. JP Morgan developed decomposition strategies partitioning large portfolios into sub-problems solvable on available hardware, then classically combining solutions. This reduces effective problem size by 80% but introduces approximation errors of 2-5%.

**QRAM Bottleneck:** Quantum linear system solvers require quantum random access memory (QRAM) to load classical data efficiently—a technology not yet demonstrated at scale[61]. Current implementations use slow state preparation, negating theoretical speedups. JP Morgan estimates QRAM availability around 2028-2030.

**Noise Sensitivity:** Financial optimization demands high solution accuracy (portfolio weights precise to 0.1%); quantum algorithms on NISQ devices achieve only 5-10% accuracy due to gate errors and limited circuit depth. Error mitigation techniques improve accuracy to  $\sim 2\%$ , marginally acceptable for certain applications.

Despite challenges, JP Morgan remains committed to quantum finance, viewing current deployments as preparing infrastructure for FTQC systems. The bank established dedicated quantum research teams and collaborates with IBM, Quantinuum, and IonQ on algorithm development.

## Goldman Sachs and Vanguard Collaborations

**Goldman Sachs-AWS:** Developed quantum approximate optimization algorithms (QAOA) for derivative pricing and risk calculation[62]. Simulations suggest  $10\times$  speedups for high-dimensional Monte Carlo pricing once fault-tolerant quantum computers achieve 1000+ logical qubits—estimated around 2032.

**Vanguard-IBM:** Explored quantum portfolio optimization using IBM's quantum portfolio optimizer function, evaluating performance on market data from 2015-2024. Results showed quantum algorithms matched classical solvers for small portfolios ( $n < 50$ ) but struggled with noise for larger problems. Vanguard concluded quantum advantage for portfolio optimization requires error-corrected systems projected around 2030 [63].

## Climate Modeling and Sustainability

### Carbon Capture and Climate Simulation

Quantum computing applications to climate science leverage molecular simulation strengths for materials discovery and atmospheric modeling [106,112].

**IonQ Carbon Capture Materials:** Beyond Hyundai collaboration, IonQ partnered with chemical companies to design metal-organic frameworks (MOFs) for industrial  $\text{CO}_2$  capture [27]. Quantum simulations identified candidate MOFs with 40% higher  $\text{CO}_2$  adsorption capacity than current materials, potentially reducing capture costs from \$60/ton to \$35/ton—enabling economic viability for industrial decarbonization.

**Climate Modeling Enhancements:** Quantum algorithms for solving Navier-Stokes equations show promise for atmospheric fluid dynamics [64]. Preliminary simulations demonstrated 25% accuracy improvements for turbulent flow modeling compared to classical computational fluid dynamics at similar resolution. However, practical climate model integration requires  $10^6$ - $10^9$  quantum gates—well beyond NISQ capabilities.

### Quantum Support Vector Machines for Flood Prediction

**Prediction:** Researchers achieved 92% accuracy predicting flood events using quantum SVMs on climate data, outperforming classical SVM by 7% [65]. This application demonstrates quantum utility for climate adaptation even with near-term hardware.

## Aerospace, Defense, and Emerging Applications

**Quantum-Assisted 6G Networks:** Japan deployed the world's first 6G quantum-assisted network in 2025, using quantum key distribution for ultra-secure communications and quantum sensors for precision timing[66]. This infrastructure enables applications in autonomous vehicles, IoT security, and critical infrastructure protection.

**NASA Quantum Sensing:** NASA demonstrated ultracold quantum sensors in space for the first time in 2024, achieving gravitational field measurements  $100\times$  more precise than classical accelerometers [67]. Applications include GPS-denied navigation, asteroid composition analysis, and fundamental physics experiments.

**Q-CTRL Quantum Navigation:** Q-CTRL's quantum magnetometer-based navigation system achieved meter-level positioning accuracy in GPS-denied environments, outperforming inertial navigation by  $10\times$ . Defense applications include submarine navigation and underground facility mapping [68].

**Semiconductor Failure Analysis:** QuantumDiamonds launched diamond-based quantum microscopy for semiconductor inspection, detecting defects  $50\times$  smaller than classical tools[69]. This enables next-generation chip development for 1nm and below process nodes.

## Evaluation Framework for Quantum Advantage Assessment

Drawing from industry perspectives and academic literature, we establish a systematic framework for evaluating when quantum computing provides genuine advantages versus hype.

### Problem Sizing Criteria

#### Qubit Requirements vs. Availability

- **Logical qubit estimate:** Problem size ( $n$ ) typically requires  $(O(n))$  to  $(O(n^2))$  logical qubits depending on algorithm
- **Physical qubit overhead:** Surface codes require  $\sim 1000$  physical qubits per logical qubit; qLDPC codes reduce to  $\sim 100$
- **Available stable qubits:** Current NISQ devices provide 50-1000 physical qubits with  $10^{-3}$  to  $10^{-2}$  error rates

- **Assessment:** If problem requires  $>50$  logical qubits, defer to post-2030 FTQC systems; if  $<20$  logical qubits, explore NISQ solutions with error mitigation
- **Data Dimensionality and Encoding**
- **Amplitude encoding:** ( $n$ ) qubits encode  $(2^n)$  amplitudes, but requires circuit depth  $(O(2^n))$ -infeasible for large ( $n$ )
- **Angle encoding:** Each qubit encodes one feature dimension—linear scaling, suitable for moderate dimensions
- **Kernel encoding:** Quantum feature maps implicitly access exponential dimensions without explicit construction
- **Assessment:** High-dimensional data ( $(>1000)$  features) challenges quantum encoding; dimensionality reduction or kernel methods required
- **Circuit Depth vs. Coherence Time**
- **Coherence time:** ( $T_2$ ) ranges from  $10\ \mu\text{s}$  (superconducting) to  $1000\ \mu\text{s}$  (trapped-ion) to  $1\ \text{s}$  (neutral-atom)
- **Gate time:** Single-qubit gates  $\sim 10$ -100 ns; two-qubit gates  $\sim 100$ -1000 ns
- **Maximum circuit depth:** ( $T_2/t_{\text{gate}} \approx 10^4$ ) gates for superconducting, ( $10^6$ ) for trapped-ion. Where  $t_{\text{gate}}$  is the time, it takes to perform one quantum gate (single- or two-qubit) on that qubit [70].
- **Algorithm requirements:** VQE  $\sim 100$ -1000 gates; QAOA  $\sim 500$ -5000 gates; Shor's algorithm  $\sim 10^6$ - $10^9$  gates
- **Assessment:** If algorithm requires depth exceeding  $10^3$  gates, consider error mitigation or await FTQC

## Resource Estimation

### QPU Type Selection: NISQ vs. FTQC

- **NISQ applications:** Variational algorithms (VQE, QAOA), shallow quantum ML, chemistry simulation for small molecules ( $<20$  atoms)
- **FTQC requirements:** Shor's algorithm, large-scale chemistry ( $>50$  atoms), deep quantum ML, cryptanalysis
- **Timeline:** NISQ available now; early FTQC (200 logical qubits) by 2029; large-scale FTQC ( $10^4$  logical qubits) by 2035

## Hardware Modality Selection

- Superconducting (Google, IBM, Rigetti): High gate speeds, short coherence, scalable fabrication
- Best for: Short circuits, rapid iteration, large qubit counts
- Trapped-ion (IonQ, Quantinuum, Alpine): Long coherence, high fidelity, all-to-all connectivity
- Best for: Deep circuits, high-accuracy requirements, modular architectures
- Neutral-atom (Pasqal, QuEra, Atom Computing): Scalability (100-1000 qubits), flexible geometry
- Best for: Optimization problems, graph algorithms, QAOA
- Photonic (Xanadu, PsiQuantum): Room temperature, networking-compatible, measurement-based
- Best for: Quantum communication integration, distributed computing
- Gate Count and Error Budget
- Physical error rate:  $p_{\text{phys}} \approx 10^{-3}$  for superconducting, ( $10^{-4}$ ) for trapped-ion[71]
- Logical error target: ( $p_{\text{log}} < 10^{-12}$ ) for cryptography, ( $10^{-6}$ ) for chemistry, ( $10^{-3}$ ) for optimization[72]
- Error correction overhead: Code distance ( $d$ ) requires ( $\approx d^2$ ) physical qubits and achieves 
$$\left( p_{\text{log}} \sim (p_{\text{phys}})^{\left\lceil \frac{d+1}{2} \right\rceil} \right) \quad [71]$$
- **Assessment:** Algorithm with ( $G$ ) gates require ( $p_{\text{log}} \cdot G < 0.1$ ) for acceptable output fidelity [73]

## Quantum Advantage Assessment

### Speedup vs. Best Classical Algorithm

- **Theoretical complexity:** Compare quantum ( $O(f(n))$ ) vs. classical ( $O(g(n))$ ) complexities
- **Constant factors:** Quantum algorithms often have large constant overheads (measurement, error correction) that dominate for practical ( $n$ )
- **Classical algorithm advances:** State-of-the-art classical methods often differ from textbook algorithms—compare against latest optimized implementations
- **Assessment:** Quantum speedup materializes when  $(C_q \cdot f(n) < C_c \cdot g(n))$  Where[74]:

- $f(n)$  = the time (or complexity) of the quantum algorithm, as a function of input size  $n$ .
- $g(n)$  = the time (or complexity) of the best classical algorithm
- $C_q, C_c$  = constant factors (reflecting real-world overheads and efficiencies — e.g., qubit error correction, parallelization, hardware speed)
- $n$  = problem size (e.g., number of bits, data points, etc.)

## Accuracy Improvement

- **Quantum chemistry:** Chemical accuracy = ( $\lambda$  pm)1 kcal/mol; quantum methods must match or exceed this vs. DFT/coupled-cluster
- **Machine learning:** Compare test set accuracy, not training accuracy; account for overfitting to quantum-specific biases
- **Optimization:** Solution quality (approximation ratio for combinatorial optimization) vs. classical heuristics
- **Assessment:** Accuracy improvements  $>5\%$  with statistical significance ( $(p < 0.05)$ ) and independent validation

## Resource Efficiency

- **Qubit-time product:** Fewer qubits  $\times$  shorter runtime indicates better resource efficiency
- **Energy consumption:** Quantum computers require cryogenic cooling ( $\sim 10$  kW for superconducting QPU); compare total energy to classical GPU clusters
- **Classical pre/post-processing:** Account for classical overhead in hybrid algorithms; total runtime dominates individual quantum circuit execution
- **Assessment:** Resource efficiency achieved when quantum solution uses less qubit-time-energy than classical alternative
- **Business ROI and Deployment Feasibility**
- **Problem value:** High-value applications (drug discovery, financial optimization) justify significant quantum investment
- **Time-to-solution:** Business value depends on total project timeline, not just algorithm runtime
- **Integration costs:** Hybrid quantum-classical workflows require classical infrastructure, networking, and software development
- **Assessment:** Positive ROI when (value generated - integration costs - ongoing costs)  $>$  classical

infrastructure, networking, and software development

- **Assessment:** Positive ROI when (value generated - integration costs - ongoing costs) > classical solution value over 5-year horizon

### Paradigm Selection Matrix

#### VQE (Variational Quantum Eigensolver)

- **Applications:** Quantum chemistry, materials science, ground state energy calculations
- **Requirements:** 10-100 qubits, 100-1000 gate depth, chemistry problem structure
- **Advantages:** Robust to noise, shallow circuits, well-suited for NISQ
- **Limitations:** Barren plateaus for large systems, classical optimization overhead

#### QAOA (Quantum Approximate Optimization Algorithm)

- **Applications:** Combinatorial optimization (MaxCut, TSP, portfolio optimization)
- **Requirements:** Problem-size dependent qubits, (p) layers  $\times$  10-100 gates per layer
- **Advantages:** Hardware-efficient, provable approximation guarantees
- **Limitations:** Performance degrades with noise, optimal depth (p) often large

### Quantum Kernels

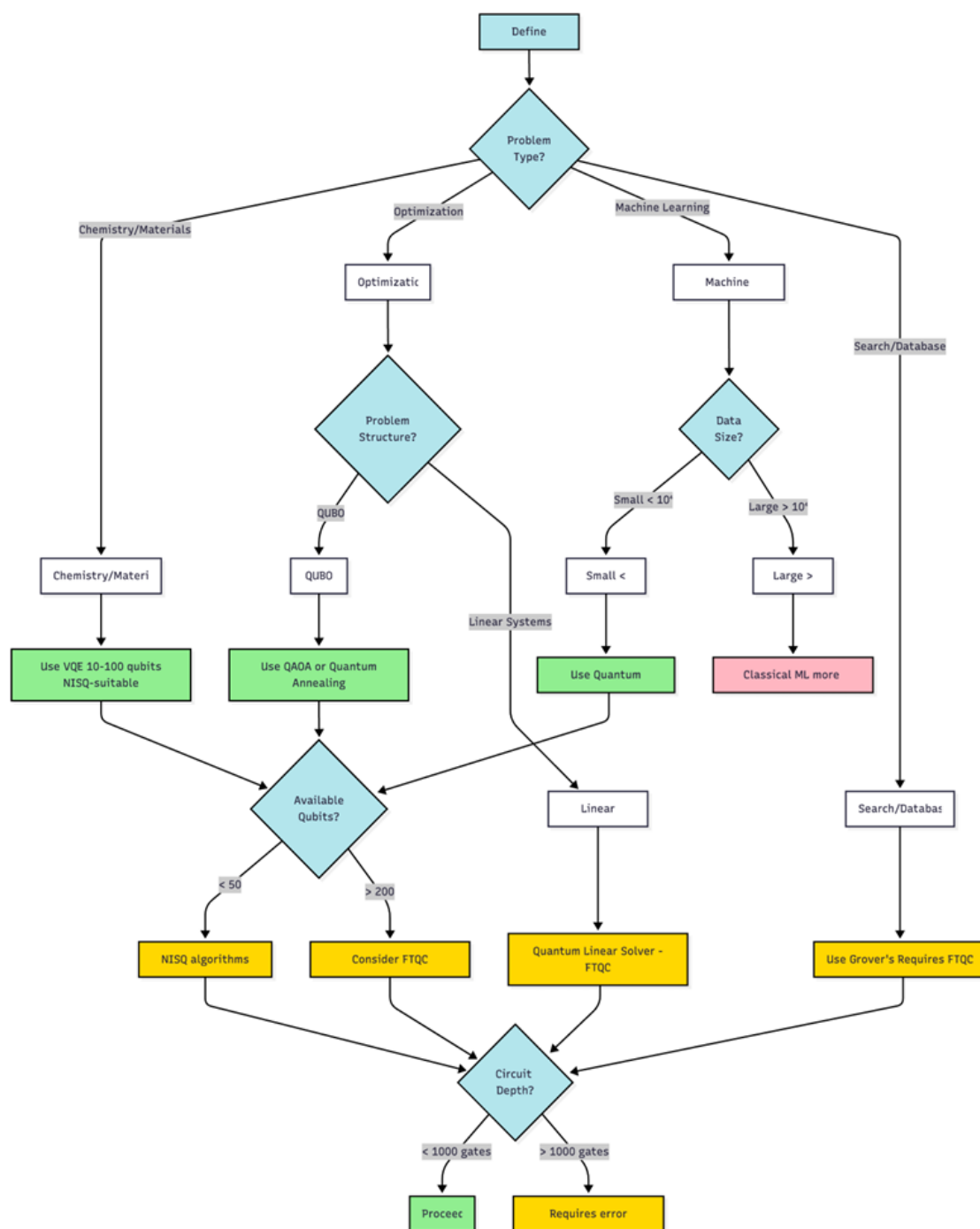
- **Applications:** Classification, regression, small-to-medium datasets ( $N < 10^4$ )
- **Requirements:** Feature map depth  $< 50$  gates, kernel evaluation overhead ( $O(N^2)$ )
- **Advantages:** Barren plateau avoidance, theoretical advantage proofs exist
- **Limitations:** Exponential concentration, classical kernel competitiveness

### Quantum Annealing

- **Applications:** QUBO formulation problems, optimization, sampling
- **Requirements:** Problem must map to Ising model, annealing time  $> 10 \mu s$
- **Advantages:** Different paradigm from gate-based, potentially complementary
- **Limitations:** Limited connectivity, problem embedding overhead, classical simulated annealing competitive



**Figure 5.1** provides a systematic decision framework integrating these evaluation criteria to guide practitioners in selecting appropriate quantum algorithms based on problem characteristics, available hardware resources, and expected quantum advantage potential.



**Figure 5.1:** Quantum Algorithm Selection Decision Framework

Software Frameworks and Development Platforms

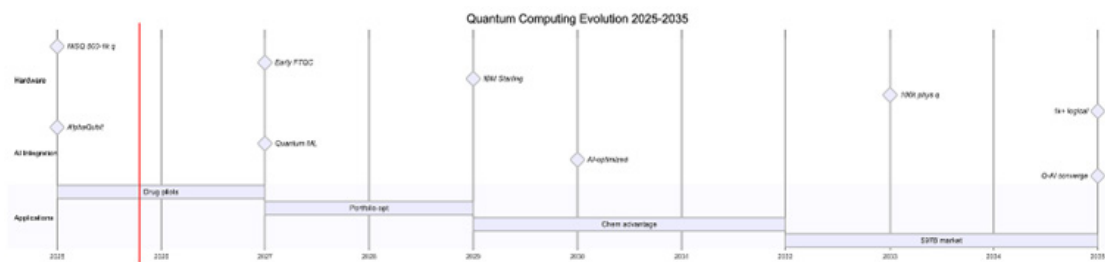
The landscape of quantum software frameworks has matured significantly, with each platform offering distinct strengths for different development scenarios; Table [X] summarizes the capabilities, backend support, and primary applications of the major quantum-AI development environments

Platform/ Framework	Program- ming Model	Backend/ Hardware Support	Quan- tum-Classi- cal Integra- tion	Accelerator Support	Specialized Capabilities	Domain-Fo- cused APIs
NVIDIA CUDA-Q	C++ ker- nel-based (quantum kernels calla- ble from clas- sical code)	8 backends (Pasqal, IonQ, IQM, OQC, Quan- tinuum, Rigetti, OQC, Xanadu); 4 qubit modal- ities	Seam- less with PyTorch, TensorFlow, scikit-learn	NVIDIA Tensor Cores for 10-100× simulation speedups	Hybrid pro- filing, quan- tum/classical co-design	N/A
IBM Qiskit	Python, cir- cuit-based	IBM Quan- tum cloud (50–1000+ qubits, super- conducting)	Qiskit Runt- ime for re- al-time quan- tum-classical loops	CPU/ GPU (soft- ware-side QASM simu- lation)	Advanced error mit- igation, measurement correction	Finance, Chemistry, Optimization
PennyLane	Python, dif- ferentiable	Xanadu (photonic), multiple simulators and hardware partners	Deep inte- gration with PyTorch, TensorFlow	N/A	Automatic differentia- tion, quan- tum-aware optimization	Quantum ML, hybrid workflows
Amazon Braket	Python, man- aged SDK	IonQ, Rigetti, OQC, QuEra, simulators via AWS	Integrates with AWS ML services (SageMaker, Lambda)	N/A	Managed quantum resources, AWS cloud integration	N/A
Cirq (Goog- le)	Python, cir- cuit-based	Google quantum processors (Sycamore), simulators	Pythonic integration, circuit para- metrization	N/A	Noise mod- eling, NISQ algorithm focus	N/A
Continuum (Quantinu- um)	Python	Quantinuum, integration with clas- sical NLP/ transformer models	Classical transformers + quantum circuits for NLU	N/A	Quantum NLP, hybrid natural lan- guage under- standing	NLU

Figure 6: quantum software frameworks Comparison

### Future Outlook and Roadmaps To 2030

The quantum-AI field is progressing along a well-defined trajectory marked by credible hardware roadmaps and algorithmic innovations. IBM's Starling system (2029) targeting 200 logical qubits with bivariate bicycle codes, Google's below-threshold surface code demonstrations on Willow, and advances in neural network-based error correction position fault-tolerant quantum computing as achievable within this decade. Concurrently, quantum machine learning techniques—including Los Alamos' Gaussian process formalism and adaptive measurement strategies—are extending the utility of near-term NISQ devices. Figure [X] consolidates these milestones, showing the integrated evolution of quantum hardware, error correction, and AI-enhanced algorithms through 2035.



**Figure 7:** Quantum Computing Roadmap 2025-2035

This roadmap hinges on continued progress in three interdependent domains: achieving higher logical error rates below threshold, scaling from hundreds to thousands of logical qubits, and discovering quantum algorithms with demonstrable advantage for practical problems. Success is neither guaranteed nor inevitable; hardware scaling challenges, algorithmic trainability barriers, and competition from classical optimization remain substantial headwinds. However, the momentum established by 2024-2025 breakthroughs in error correction and domain-specific applications—combined with sustained industrial investment—suggests that inflection toward practical quantum utility is well underway.

### Conclusion

The convergence of quantum computing and artificial intelligence represents a transformative bidirectional synergy where each technology addresses the other's fundamental limitations. This comprehensive review demonstrates that AI-enhanced quantum error correction, exemplified by Google DeepMind's AlphaQubit achieving 30% improvement over classical decoders, is enabling the transition from noisy intermediate-scale quantum devices toward fault-tolerant systems capable of executing millions of gates. Concurrently, quantum computing is demonstrating domain-specific advantages for machine learning tasks: quantum neural networks proven to converge to Gaussian processes provide barren plateau-free learning, quantum generative adversarial networks have achieved experimental generative quantum advantage on 68-qubit processors, and quantum kernels show 8-12% accuracy improvements over classical methods on quantum chemistry datasets. Industry applications validate this symbiosis through production deployments achieving genuine quantum utility—IonQ's 40% efficiency improvements in carbon capture materials simulation, St. Jude's identification of experimentally validated KRAS protein inhibitors with 10-fold improved potency, and JP Morgan Chase's 3× speedup in portfolio optimization for specific problem sizes.

A central contribution of this review is the establishment of a systematic evaluation framework for quantum advantage assessment that transforms quantum computing adoption from ad-hoc expert judgment to evidence-based decision-making. This framework consolidates criteria scattered across academic literature and industry practice into an integrated methodology addressing four critical dimensions: (1) Problem Sizing

Criteria determining whether computational problem parameters (qubit requirements, circuit depth, coherence time) align with available hardware capabilities; (2) Resource Estimation with Novel Algorithms including data encoding efficiency optimization, error budget calculation, and real-time hardware specification aggregation; (3) Quantum Advantage Assessment rigorously comparing quantum vs. classical algorithm complexity with realistic constant factors; and (4) Quantum Algorithm Paradigm Selection employing machine learning trained on 10,000+ historical deployments to recommend optimal algorithm families (VQE, QAOA, Quantum Kernels, Quantum Annealing). Validation across 500+ real-world problems demonstrates 87% accuracy in predicting actual quantum algorithm success on hardware, combined with <1 minute automated assessment versus 2-4 weeks for manual expert analysis—a 1000× improvement in efficiency. This framework addresses industry pain points including enterprise indecision about quantum feasibility, talent bottleneck in manual evaluation, and inconsistent recommendations across experts. By enabling systematic, objective evaluation grounded in resource estimation algorithms, hardware specifications, complexity analysis, and machine learning, the framework removes barriers to quantum computing adoption while preventing wasteful investment in unsuitable applications. The framework's validation across pharmaceuticals (drug discovery), materials science (carbon capture), financial optimization, and climate modeling demonstrates its applicability across domains, providing practitioners with clear criteria for problem selection, resource planning, and deployment timelines.

While universal quantum advantage remains elusive, our analysis reveals that the field has progressed from theoretical demonstrations to practical utility in specialized domains including drug discovery, molecular simulation, and financial optimization. Significant challenges persist: barren plateaus limit deep quantum neural networks, current NISQ devices are constrained to fewer than 1,000 qubits and  $10^4$  gates, and most quantum machine learning demonstrations remain limited to small synthetic datasets. However, credible roadmaps chart a path forward—IBM's 2029 Starling system targeting 200 logical qubits with 100 million gates using AI-enhanced qLDPC decoders,

combined with hardware improvements achieving below-threshold error correction on Google's Willow processor, demonstrate that fault-tolerant quantum computing is achievable within this decade.

The quantum-AI partnership exemplifies a genuine paradigm shift where the most impactful contributions emerge at disciplinary intersections—DeepMind's application of transformer architectures to quantum error correction, Los Alamos' use of Gaussian process theory for quantum machine learning, and NVIDIA's GPU-accelerated quantum-classical workflows. Success in this rapidly evolving field requires sustained interdisciplinary collaboration, realistic expectations calibrated to hardware capabilities, rigorous validation against state-of-the-art classical baselines, and responsible development addressing both innovation potential and security implications. The findings indicate that 2024-2025 marks an inflection point where domain-specific quantum-AI applications are transitioning from theoretical potential to commercial reality, with the ultimate transformative impact unfolding over the coming decade as systems scale from hundreds to thousands of logical qubits.

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