
CONCEPT PAPER

Hybrid Quantum AI for India

National community building, transformational applications and commercialisation

Proposed five-year research and capacity-building priorities for IAIRO

Collaboration context

IAIRO-Penn State collaboration and MoU, with potential collaboration with Amaravati Quantum Valley, IBM and others

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Purpose and proposed direction

This concept paper outlines a five-year direction for Hybrid Quantum AI in India. It proposes an IAIRO focus on foundational research, selected applications and research-capacity building, supported by the IAIRO-Penn State collaboration and potential engagement with additional partners.

The agenda combines quantum computing for AI with AI for quantum computing. The proposed priorities cover foundations and benchmarks, drug discovery and generative chemistry, weather and climate systems, quantum-device error correction and control, and an IAIRO-hosted summer institute.

What Hybrid Quantum AI means

Hybrid Quantum AI brings together quantum computing and artificial intelligence through two complementary directions.

Direction	Role in Hybrid Quantum AI
Quantum computing for AI	Employ quantum algorithms and hardware to advance machine learning, reasoning and optimisation.
AI for quantum computing	Use AI, especially machine learning, to support calibration, error correction, compilation and control of quantum devices.

The paper focuses on hybrid quantum-classical methods that use Noisy Intermediate-Scale Quantum hardware. These methods include variational quantum circuits, quantum annealing and quantum kernels. They have been explored across manufacturing, energy management, finance, aerospace, healthcare, climate and Earth sciences, and drug discovery (Klusck et al. 2024). In this paper, Hybrid Quantum AI refers specifically to systems and algorithms that combine classical computing resources with quantum computing capabilities.

Why this matters now

- 1. Real-device experimentation.** Advances in Noisy Intermediate-Scale Quantum hardware and software frameworks, including IBM Qiskit, PennyLane and Cirq, allow hybrid algorithms to be tested on quantum devices. Early proofs of concept report advantages in optimisation, pattern recognition and simulation without full fault tolerance (Klusck et al. 2024).
- 2. Alignment with demanding workloads.** AI and scientific workloads involving linear algebra, sampling, partial differential equations and optimisation align with areas studied in quantum computing. Quantum support-vector machines and quantum linear solvers suggest substantial, and in some cases exponential, speedups over classical counterparts (Rebentrost, Mohseni, and Lloyd 2014).
- 3. AI for quantum systems.** Machine learning offers ways to improve quantum-device fidelity through data-driven error mitigation and calibration, strengthening the utility of Noisy Intermediate-Scale Quantum machines (Pelofske, Bäertschi, and Eidenbenz 2022; Pokharel and Lidar 2024).

Five-year agenda at a glance

IAIRO proposes five connected priorities spanning foundational methods, application research, quantum-system operation and researcher development.

	Priority	Proposed work
1	Foundations and benchmarks	Reproducible hybrid-advantage demonstrations using benchmarked datasets, task-level metrics, parameterised circuits and quantum kernels.
2	Drug discovery and generative chemistry	Quantum electronic-structure simulation combined with AI-based active learning and molecular structure generation.
3	Weather, climate hazards and Earth-system modelling	Quantum linear solvers and sampling routines within machine-learning surrogates and hybrid digital twins.
4	Error correction, calibration and control	Deep-learning and reinforcement-learning methods for error mitigation, device calibration and tuning.
5	Research capacity	An IAIRO-hosted summer institute combining lectures, tutorials, demonstrations and hands-on laboratory sessions.

Detailed research priorities

1 Foundations and benchmarks for hybrid machine learning

Develop reproducible demonstrations of hybrid advantage using benchmarked datasets and task-level metrics. The work would examine parameterised quantum circuits, quantum kernels and auto-parameterised quantum-circuit models with provable expressivity and noise robustness for machine learning, natural language processing, generative modelling and large-scale inference.

2 Drug discovery and generative chemistry

Integrate quantum electronic-structure simulation, including the Variational Quantum Eigensolver and Quantum Phase Estimation, with AI-based active learning and molecular structure generation. Quantum simulation of molecular Hamiltonians and generative chemistry models may accelerate the synthesis-test loop for new molecules (Li et al. 2021).

3 Weather, climate hazards and Earth-system modelling

Embed quantum linear solvers and sampling routines within machine-learning surrogates for weather and climate systems. The proposed work would also develop hybrid digital twins that couple quantum physics-based models with classical neural emulators, supporting forecasting and scenario exploration (Rainjonneau et al. 2023).

4 Error correction, calibration and control

Apply deep learning and reinforcement learning to error mitigation and device tuning (Quetschlich, Burgholzer, and Wille 2023; Klusch et al. 2024). The work would build on Ghosh's lab's research on quantum optimisation and error correction using machine learning (Chatterjee, Das et al. 2025; Chatterjee, Ghosh et al. 2025).

5 Research capacity and community building

Establish an IAIRO-hosted summer institute led by quantum AI experts and domain specialists. The institute would combine lectures, tutorials, demonstrations of progress across the proposed themes, and hands-on laboratory sessions using quantum hardware and simulation platforms.

Existing expertise and collaboration

The proposed drug-discovery theme would build on Honavar's group's work on diffusion models for molecular structure generation and Ghosh's group's work on quantum methods for small-molecule drug discovery (Li et al. 2021). Ghosh and Honavar also have active collaborations involving jointly supervised PhD students at Penn State University.

IAIRO leads based at the University of Texas at Austin are working on weather and climate problems. Vasant Honavar and IAIRO team members also have experience organising summer research institutes for junior researchers in interdisciplinary fields.

Together, the five priorities connect foundational Hybrid Quantum AI research with application studies, quantum-system operation and national research-capacity building.