Quantum-Centric HPC: Motivation, Application, Facilitation

RMACC HPC Symposium

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Arizona State University
May 14, 2026

Outline:

Quantum-Centric HPC QCHPC (QCSC):

What, Why, How?

Recent Algorithmic Advances

Specific Use Cases

RMACC Community Experiences

Quantum Collaborative

The **Quantum Collaborative** at Arizona State University connects top scientific programs, initiatives, facilities, leading Quantum Information Science and Technology (QIST) talent, and industry partners to advance quantum information science, train the quantum workforce of tomorrow, and drive U.S. quantum economic advantage.

quantumcollaborative.org

Current Partners

Together we are realizing the promise of quantum technology.

Academic

Tecnológico de Monterrey

University of Wyoming

Virginia Tech

UTSA The University of Texas at San Antonio™

Purdue University

National laboratories

Sandia National Laboratories

Oak Ridge National Laboratory

Initiatives

Qubit x Qubit

¡MIRA!

Industry

Quantinuum

IBM

Dell

EY Building a better working world

Quantum AI

Cox

zayo

cisco

cr8dl.ai

SandboxAQ

QC Summit 2023

Some goals:

- Collective innovation
- Community growth
- Social impact

Some stats:

- 32 Proposals Submitted
- $452,383 Seed Fund Awards

Quantum Collaborative Stats To Date:

Seed Fund Numbers:

Seed Fund Project Proposals:	
Submitted:	47
Approved:	21
Declined:	26

Project Status:	
Completed:	11
Active:	4
Upcoming:	6

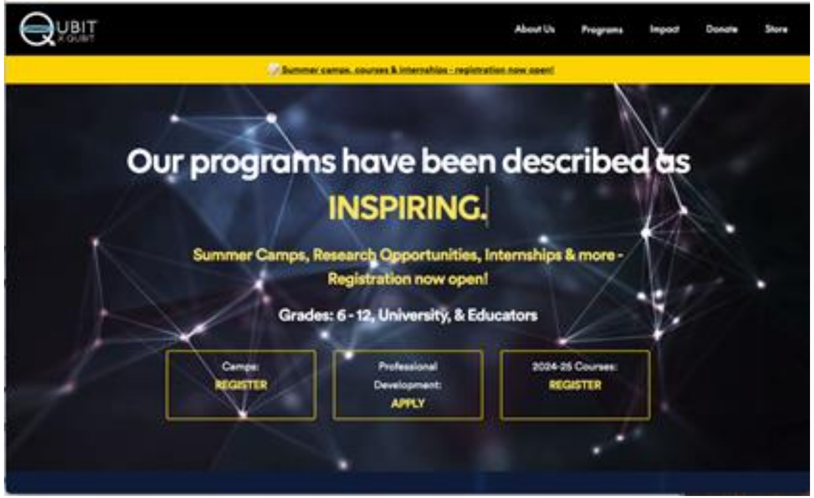
Federal Funding Proposals:	
Number of Awards:	17
Fed Dollars Awarded:	$30,199,515.00

Steering Committee Efforts:

Steering Committee:	Use Cases or Projects:
Quantum Computing and Simulation	Quantum Error Mitigation Supply Chain Optimization Quadratic Integer Programming Problems
Quantum Sensing and Metrology	QMed: Center for Quantum Medical Diagnostics
Quantum Networking and Communications	Quantum Networking Laboratory (moved to Purdue)
Education and Workforce Development	Partnerships with community colleges, ¡MIRA! SPaRQS; NSF Cybertraining grant

Education and Workforce Development

Qubit By Qubit



Summer camps, courses & internships - registration now open!

Our programs have been described as

INSPIRING.

Summer Camps, Research Opportunities, Internships & more - Registration now open!

Grades: 6 - 12, University, & Educators

¡MIRA! SparCQS →


SparQS Mobile Lab

Designed to be fun, engaging, welcoming, and inclusive.

Changing who has access to STEM!

Quantum Computing: the Motivation

Simulation of quantum systems:

- Difficult to simulate a quantum system on a classical computer
- Use quantum system to model another quantum system (simulator operates with principles of quantum mechanics)
- Richard Feynman: "Nature isn't classical, dammit, and if you want to make a simulation of Nature, you'd better make it quantum mechanical..."

Quantum Computing: the Inspiration

- Introduction of HPC and subsequent advancement:
  - explosive impact on computational research
  - combination of Moore’s Law and Dennard scaling reaching limit
- QC: potential to solve classically intractable problems:
  - complexity barriers
  - unrealistic runtimes
- Scaling of computational power:
  - classical: linear w number of transistors
  - quantum: exponential w number of coherent qubits

QC vs Classical Computing

Feature:	Classical Computing:	Quantum Computing:
Basic unit of information:	Bit (can be 0 or 1, on or off)	Qubit (can be 0, 1 or superposition of these states)
Circuit behavior:	Classical physics (calculus, electricity and magnetism, fluid dynamics)	Quantum mechanics (superposition, entanglement, interference)
Computation output:	Deterministic	Non-deterministic

Quantum Algorithms:

- **Shor's algorithm:** Exponential speedup in factorization
- **Grover's algorithm:** Quadratic speedup for unstructured search
- **Quantum walks-based algorithms:** Exponential and polynomial speedups
- **Quantum annealing:** Combinatorial optimization problems

Example Implementations of Quantum Algorithms in Research Computing

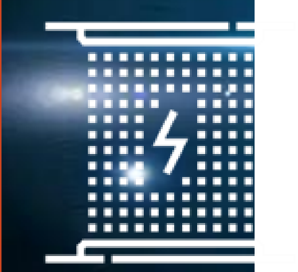
Optimization:

- Materials Discovery
- Combinatorial Optimization (e.g. Supply Chain scenarios)
- Pharmaceutical Applications (Drug Discovery)

Algorithms:

- Grover’s Search Algorithm
- QAOA (Quantum Approximate Optimization Ansatz)
- QUBO (Quadratic Unconstrained Binary Optimization)

Example Implementations of Quantum Algorithms in Research Computing



Cryptography:

- Quantum Key Distribution (QKD)
- Post-quantum Cryptography (PQC)

Quantum Machine Learning:

- Enhances many computational paradigms
- Quantum error mitigation
- Photovoltaic fault-detection

High-Level Quantum Stack

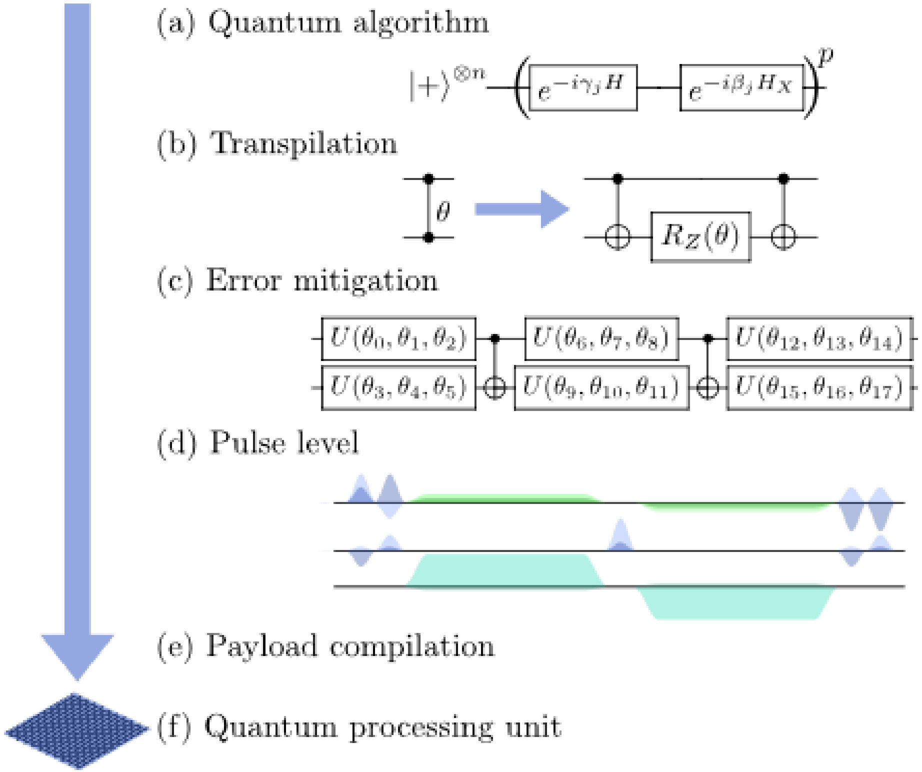


Figure 5. High-level summary of the quantum stack. (a) A quantum algorithm, including an encoding of decision variables in qubits and any hardware-guided problem simplifications, results in a high-level quantum circuit. (b) The instructions in this circuit are then transpiled to hardware native instructions. (c) Error mitigation methods, such as PEC, are often encoded as circuit instructions. (d) At the pulse-level, circuit instructions are represented by the physical pulses that are played on the qubits. (e) Finally, the circuit is compiled into machine-executable waveforms, (f) that are run on the quantum processor.

Abbas.arXiv.qPH.2312.02279v1.2023

Speedup Descriptions:

Quantum Utility:

- **NISQ** (Noisy Intermediate-Scale Quantum) era (100+ qubits)
- reliable calculations at a scale beyond the reach of brute-force classical methods
- serve as valuable, useful research tools

Quantum Advantage:

- perform **real-world** calculations faster than can be achieved classically
- commercially useful; real data and data volumes, constraints, goals

Quantum Supremacy:

- perform **any** calculation faster than can be achieved classically
- can be demonstrated on any problem, regardless of usefulness

Fault Tolerance:

“A system is fault-tolerant if it can continue to perform despite parts failing[2].”

Quantum circuits are reliable despite inevitable imperfections in qubits and gates.

NISQ era → FTQC: logical and physical qubits and gates are connected and controlled such that the 10000x gap required to reach FTQC from NISQ era is achieved[3].

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[2] https://www.ibm.com/docs/en/tpmfi/7.1.1.14?topic=security-fault-tolerance

[3] https://quantumcomputingreport.com/fault-tolerant-quantum-computing-will-deliver-the-transformative-promise-of-quantum-computing-part-1/

Limitations of NISQ-era Quantum Computers

NISQ: Noisy Intermediate-Scale Quantum (era):

- Qubit coherence times (relaxation and dephasing)
- Bottleneck when circuit duration ~ qubit coherence time
- Qubit connectivity (SWAP gates)
- Quantum circuit width and depth:
  - Number of qubits, max path length from init to measurement
  - Quantum error mitigation and correction (QEM/QEC)
  - FTQC: Need ~ 1000 physical qubits for 1 logical qubit (QEC)
  - Need millions of ‘reliable’ qubits

Limitations of NISQ-era Quantum Computers

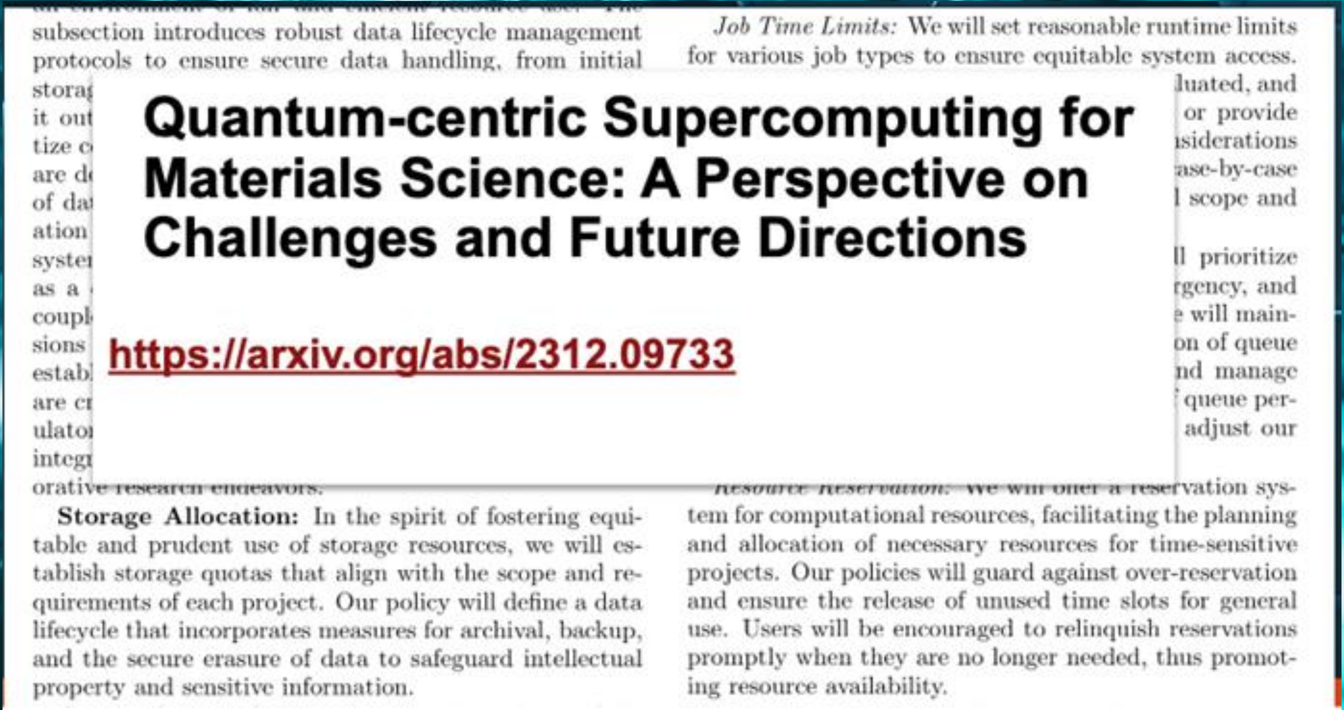
NISQ: Noisy Intermediate-Scale Quantum (era):

- Mapping to quantum computers engenders deep circuits
  - large number of measurements
    - high sensitivity to errors
    - substantial overhead incurred
  - excessive runtimes
- Enlist classical distributed computing to perform all but core, intrinsically quantum component of workflows

Quantum-Centric HPC

Quantum-centric Supercomputing for Materials Science: A Perspective on Challenges and Future Directions

https://arxiv.org/abs/2312.09733



subsection introduces robust data lifecycle management protocols to ensure secure data handling, from initial
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Storage Allocation: In the spirit of fostering equitable and prudent use of storage resources, we will establish storage quotas that align with the scope and requirements of each project. Our policy will define a data lifecycle that incorporates measures for archival, backup, and the secure erasure of data to safeguard intellectual property and sensitive information.

Job Time Limits: We will set reasonable runtime limits for various job types to ensure equitable system access.
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Resource Reservation: We will offer a reservation system for computational resources, facilitating the planning and allocation of necessary resources for time-sensitive projects. Our policies will guard against over-reservation and ensure the release of unused time slots for general use. Users will be encouraged to relinquish reservations promptly when they are no longer needed, thus promoting resource availability.

QCHPC in Research Computing

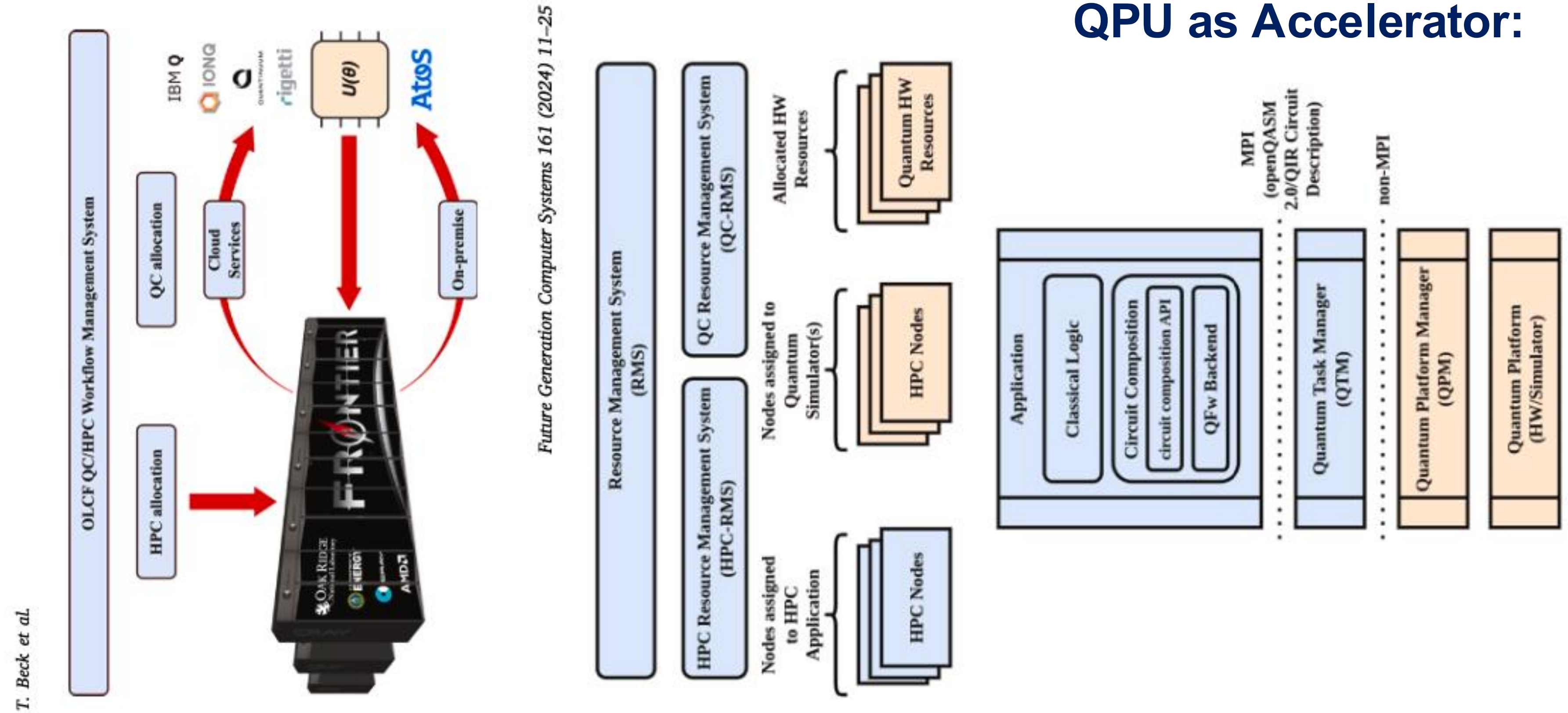
Computational Accelerator:

Quantum-centric HPC:

- QPUs play role similar to that currently played by GPUs
- Hybrid QC/HPC: QPU-performant code sections: off-load to cloud or on-premise hardware
- Circuit cutting designs to meet NISQ constraints

QCHPC Integration Framework

QPU as Accelerator:



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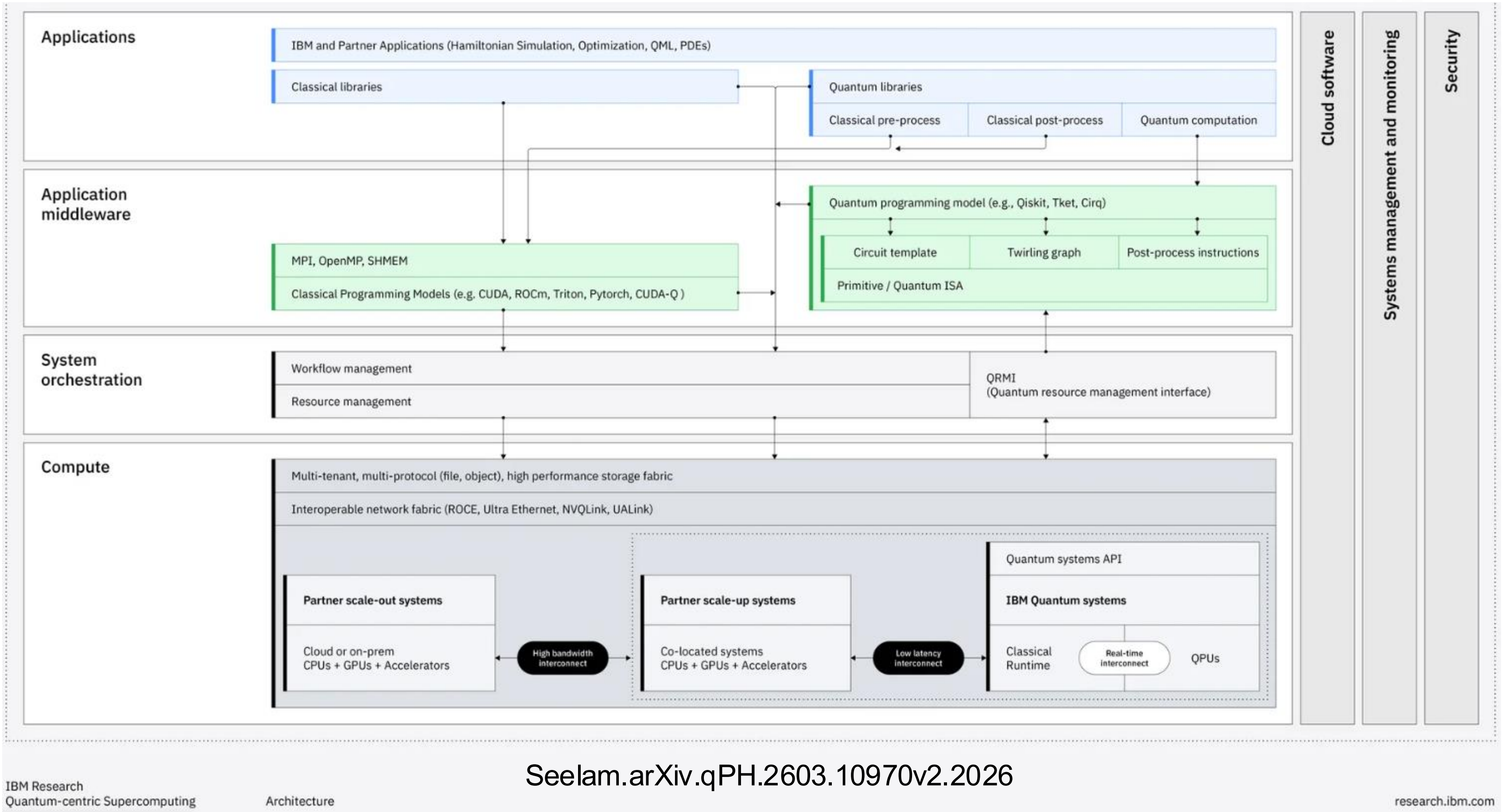
QCSC IBM Architecture



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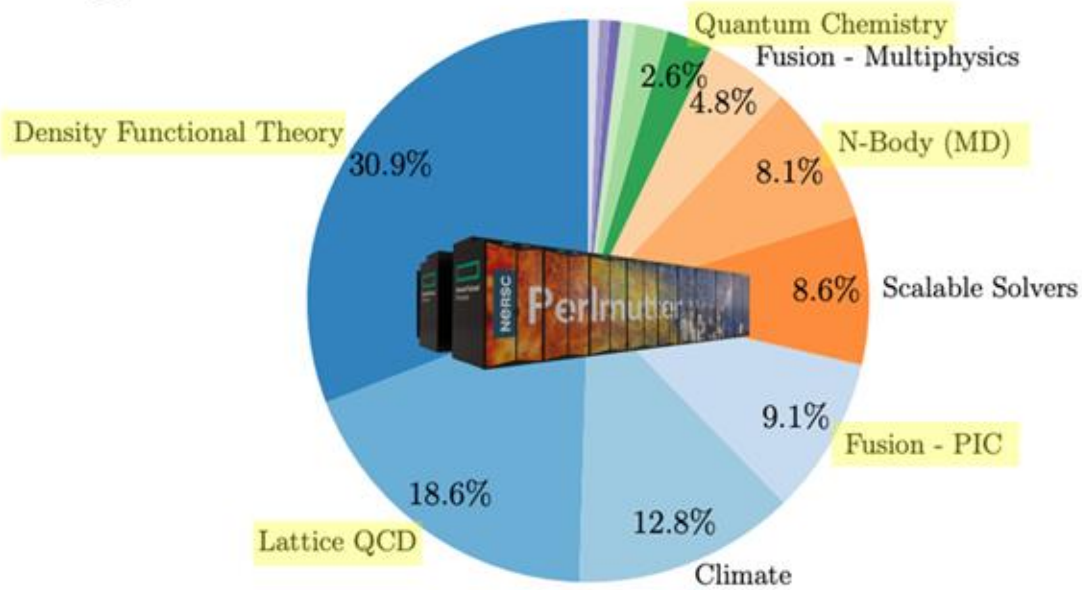
Hybrid Quantum/Classical Algorithms:

- **Quantum Approximate Optimization Algorithm (QAOA):** find approx solns to cmplx combinatorial opt
- **Variational Quantum Eigensolver (VQE):** find ground state/min energy of quantum system
- **Sample-based Quantum Diagonalization (SQD):** find eigenvalues and eigenvectors of quantum operators (classical post-processing technique)
- **Operator BackPropagation (OPB):** reduce circuit depth for measuring observables

>50% of NERSC workloads are applicable for HPC+QC



NERSC: National Energy Research Scientific Computing Center

Camps, D., Rrapaj, E., Klymko, K., Kim, H., Gott, K., Darbha, S., Balewski, J., Austin, B., & Wright, N. J. (2025). Quantum computing technology roadmaps and capability assessment for scientific computing: An analysis of use cases from the NERSC workload. arXiv preprint arXiv:2509.09882. https://arxiv.org/abs/2509.09882

QCHPC: Q Chem: Electronic Structure

Recent research from IBM, RIKEN, University of Michigan:
A. Shajan et. al., Jan 2026:

- Implements **fragment-based QCSC workflow** for molecular ES calculations
- Predicts relative energies of two conformers of **303-atom** miniprotein (Trp-cage)

- Uses **EWF formulation** to improve upon existing DMET-based approach
- Integrates SQD and FCI solvers for **quantum-centric portion**
- Deploys CCSD and MP2 solvers during **classical calculations**
- Older methods used VQE in combination with wavefn embedding methods
- **Use of VQE limits** ability to scale

Shajan.arXiv.qPH.2512.17130v2.2026

QCHPC: Q Chem: Electronic Structure

Recent work from IBM, RIKEN, Cleveland Clinic:
Merz et. al., May 2026:

- **Scales up** previous work from **303 atoms to 12635 atoms**
- Calculates electronic structure of pair of large protein-ligand complexes
    - Molecules: T4-Lysozyme and Trypsin
    - **> x 210 accuracy** over the Trp-cage calculations
    - **40 x increase in system size** compared to Trp-cage
- Largest HQC ES calculation to date (12635 atoms, 31795 orbitals)
- Two 156-qubit QPUs (using up to 94 qubits)
- Running > 100 hours
- Executing 9200 circuits
- Collecting 1.3 x 10^9 samples

Shows QC is useful for real world QChem!

https://www.ibm.com/quantum/blog/cleveland-clinic-riken-chemistry
Merz.arXiv.qPH.2605.01138v1.2026

QCHPC: Quantum Optimization

Combinatorial Optimization:

- **Searches** for an optimum object in a finite collection of objects
  - Collection has precise representation
  - Number of objects is enormous
- Can be **intractable** for classical algorithms at small problem sizes:
- Multiple **heuristic approaches** known, can be executed and tested
  - Increases possibility of NISQ performance prevailing in certain cases
  - Allows for exploration of instances of quantum advantage
- **Example:** vehicle-routing problem: **hybrid approach**
  - Solve vehicle-customer assignment classically
  - Solve TSP portion with quantum optimization

Koch.IBMOptWG.arXiv.qPH.2504.03832v1.2025

QCHPC: Quantum Optimization

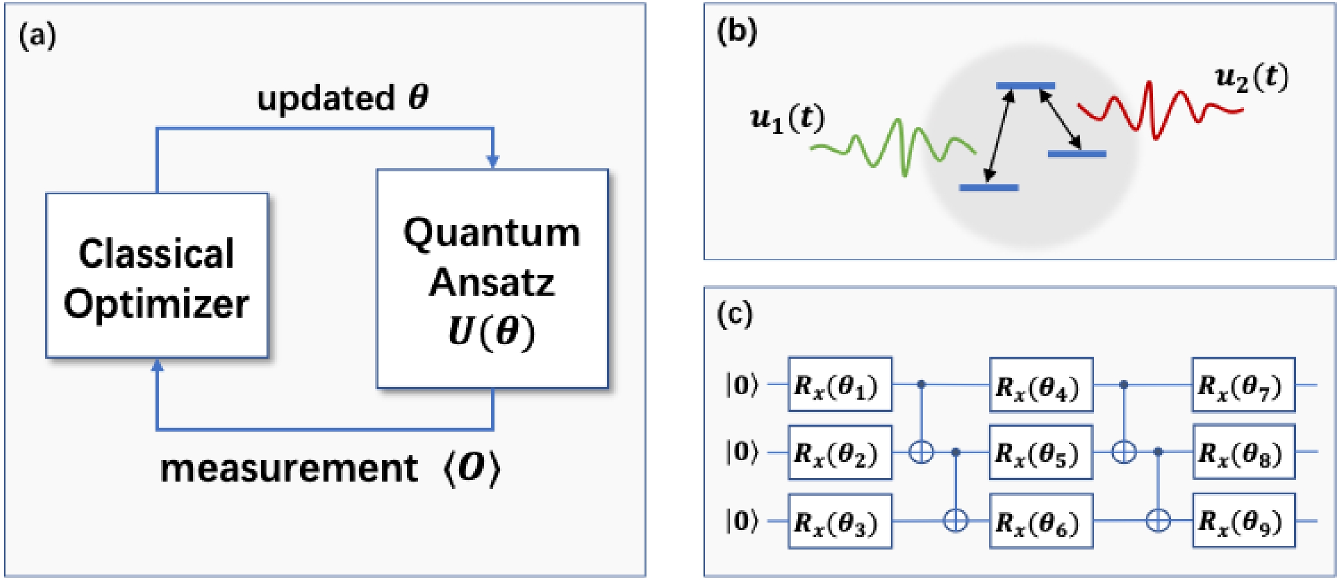


Figure 1: (a) The general setup of hybrid quantum-classical optimization system; (b) the optimization of classical fields in the control of a molecule or other modest sized quantum system; (c) the training of variational quantum circuits using a classical optimizer.

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Vehicle Routing Output

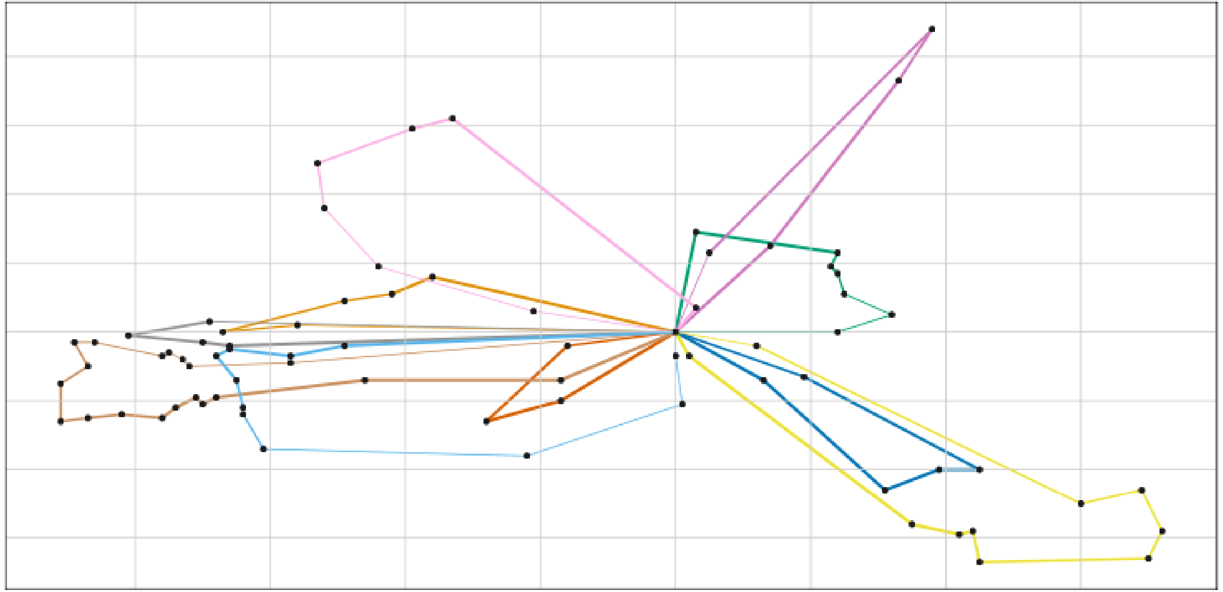


Figure 15: (Routing) Example instance *tai75a* (75 customers, 10 vehicles) from the Rochat and Taillard dataset [RT95] and optimal solution as obtained from CVRPLIB [LOQ]. Each line color represents the route of one vehicle between the customers (•) starting and ending at the central depot (■). The thickness of a line indicates the remaining capacity of the corresponding vehicle along the route. This example demonstrates the combinatorial complexity of finding the best route among all possible routes while fulfilling capacity constraints.

Koch.IBMOptWG.arXiv.qPH.2504.03832v1.2025

QCHPC: AI for QC

- AI can **optimize the distribution of tasks** between quantum and classical processors
- ML can **predict and correct quantum computation errors** (QEC)
- AI can **automate quantum device calibration**, and dynamically adjust control parameters (system stability)
- AI can be used to **efficiently allocate qubits**, optimize scheduling and compilation of q tasks
- AI can **develop sophisticated benchmarking tools** among quantum devices and algorithms
- AI techniques can **improve the training of QML models**

https://www.mckinsey.com/capabilities/mckinsey-digital/our-insights/tech-forward/enabling-the-next-frontier-of-quantum-computing

QCHPC: QC for AI

- Quantum algorithms **speed up data processing** and computations essential for enabling AGI
- Quantum algorithms **handle optimization problems more efficiently** than classical algorithms, boosting AGIs advanced reasoning and decision-making tasks
- QML **accelerates AI learning processes**, crucial for AGI's adaptability across diverse tasks and environments
- ‘Quantum parallelism’ **speeds up AGI's training and inference stages**, improving information analysis and synthesis
- Quantum algorithms **excel with complex, high-dimensional data**, providing tools for AGI to process and understand intricate information

https://www.mckinsey.com/capabilities/mckinsey-digital/our-insights/tech-forward/enabling-the-next-frontier-of-quantum-computing

QC for AI:

AI Genre:	Purpose:	Use Case:	Outcome:
LLMs	complement classical LLMs in parameter-efficient tuning	fine-tune billion-parameter AI model the system-generated hundreds of parallel quantum tasks per batch and leveraged hybrid processing to optimize output.	even after reducing model parameters by 76%, training effectiveness increased by 8.4% like equipping a classical model with a 'quantum engine'

Anhui QC Engineering Research Ctr, China
72-qubit superconducting QC: Origin Wukong

Quantum Working Group Alliances

Collaborative Quantum Research Efforts Hosted by IBM, by Invitation

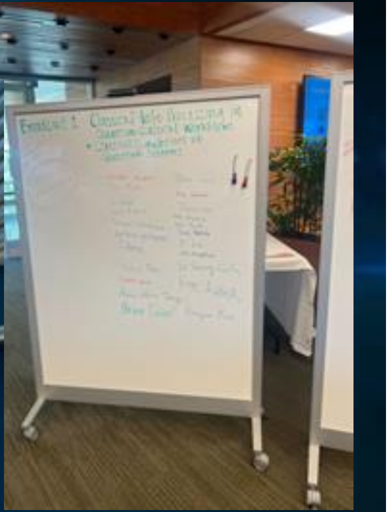
Benefits:

- Industry/university/national labs bringing experiences, knowledge together;
- Intense, focused brainstorming to re-energize or kick-start research with societal impacts
- Organized plan with expectations for outcomes

ASU Participation to Date:

- **Quantum-centric HPC** initial meeting: Chicago, 2023
    - QCHPC Materials Science focus
    - Paper produced (Torey, Doug co-authors)

Quantum Computing Materials Science: Almaden Working Group:



Quantum Working Group Alliances

Collaborative Quantum Research Efforts Hosted by IBM, by Invitation

ASU Participation to Date:

- **Quantum Sustainability Working Groups (JSC)**
    - Subgroup: quantum chemistry
        - Sustainable materials discovery for
        - Battery composition, concrete manufacturing
    - Subgroup: semiconductor supply chain
        - Fabrication process
        - Logistics (vehicle routing, inventory control)
    - Jouvence, 2024, Banff 2025
    - Member of JSC: overseeing all QSWG projects

Quantum Computing Sustainability: Jouvence Working Group:

Conclusions:

NISQ-era quantum computers:

- Have reached ‘utility scale’; close to ‘advantage’
- 100+ qubits (ex IBM): Heron: r1-133, r2-156, Eagle: r3-127
- Can offer meaningful contributions in many research areas

Integration with HPC platforms:

- Limitations of classical computers
- QPU as accelerator
- Other integration architectures
- Improve speed and/or accuracy
- Provide insight into previously intractable problems

References:

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- Merz.arXiv.qPH.2605.01138v1.2026
- Yamamoto.PRXQuantum.7.020319.2026

Thank you, and let's discuss!

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