OAK RIDGE National Laboratory

Quantum Computing User Program

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HPC Engineer – User Assistance

An overview of the purpose and structure of QCUP at ORNL managed by the Quantum Computing Institute.

ORNL is managed by UT-Battelle, LLC for the US Department of Energy

The Quantum Computing User Program is supported by the DOE Advanced Scientific Computing Research (ASCR) program office

U.S. DEPARTMENT OF ENERGY

Quantum Computing User Program

Enable Research

Provide a broad spectrum of user access to the best available quantum computing systems

Evaluate Technology

Monitor the breadth and performance of early quantum computing applications

Engage Community

Support growth of the quantum ecosystem by engaging with users, developers, vendors, and providers

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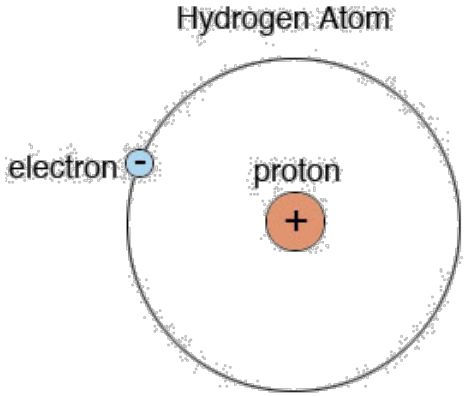
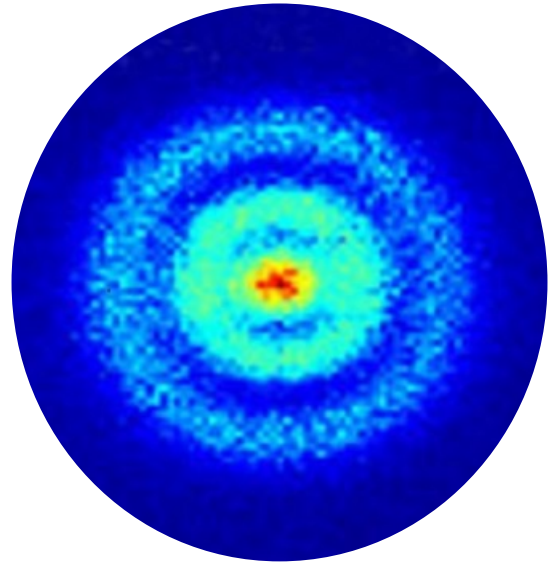
What is Quantum Computing?

- Quantum mechanical computation
  - In quantum mechanics, the *wave function* describes all knowledge about the system.
- Quantum computing manipulates the wave function to perform calculations.
  - Quantum dynamical control of the Hamiltonian corresponds to computation.

$$i\hbar \frac{\partial \Psi(t)}{\partial t} = H(t)\Psi(t)$$





Stodolna et al. PRL 110, 213001 (2013)

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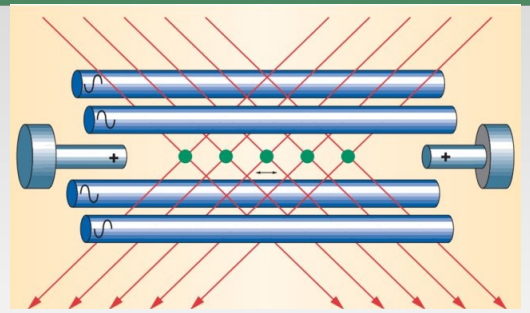
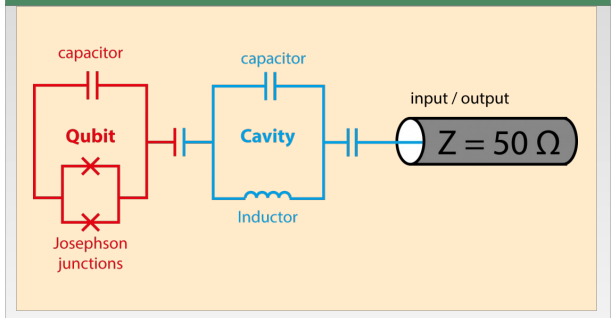
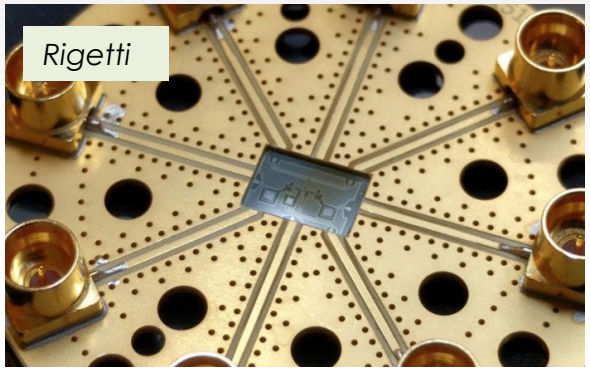
Many Types of Quantum Computing Technology

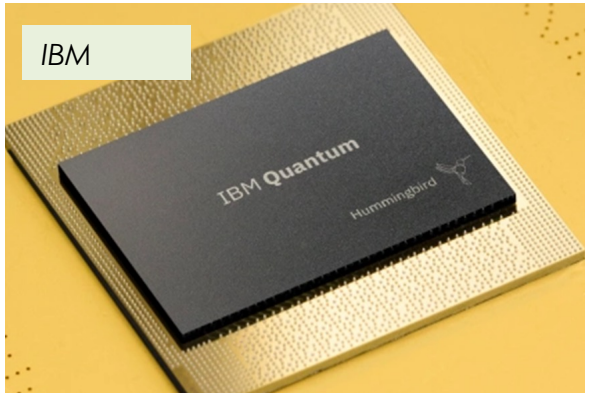
Atoms & Ions



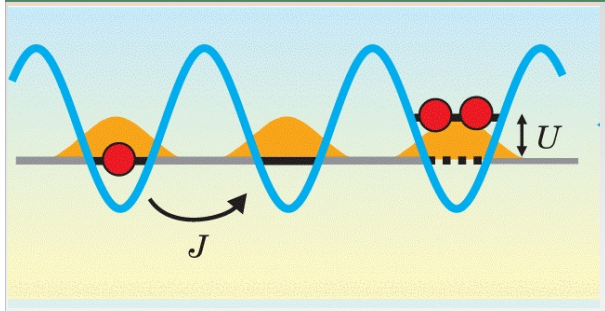
Superconductors

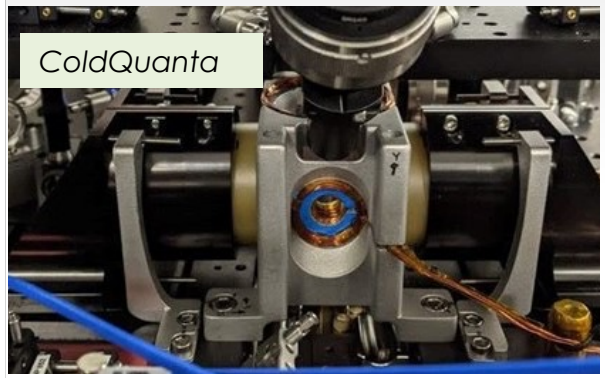


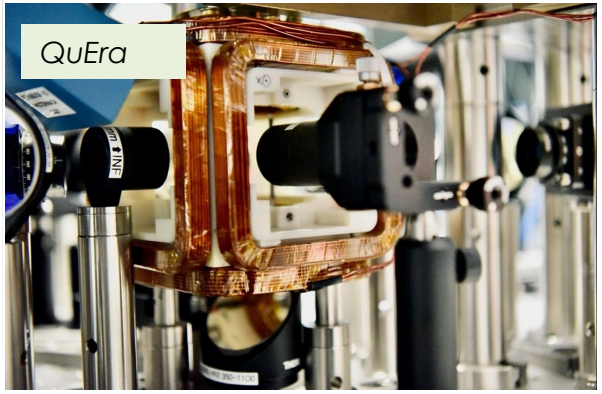




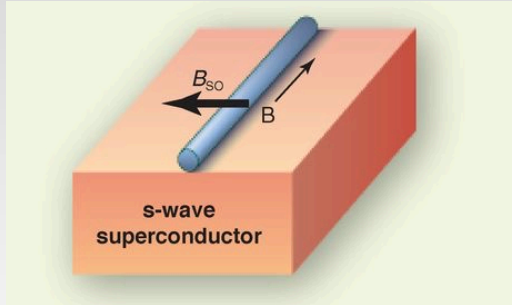
Neutral Atoms

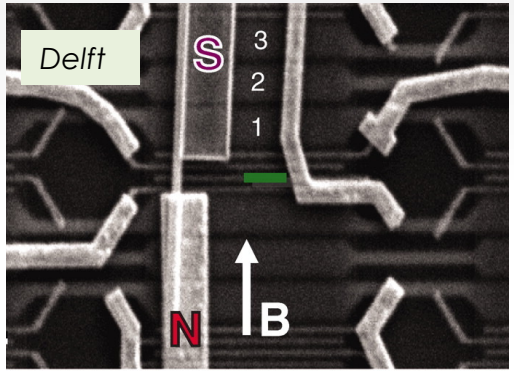


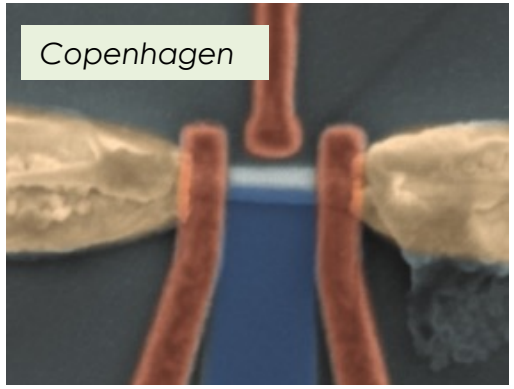




Topological Materials







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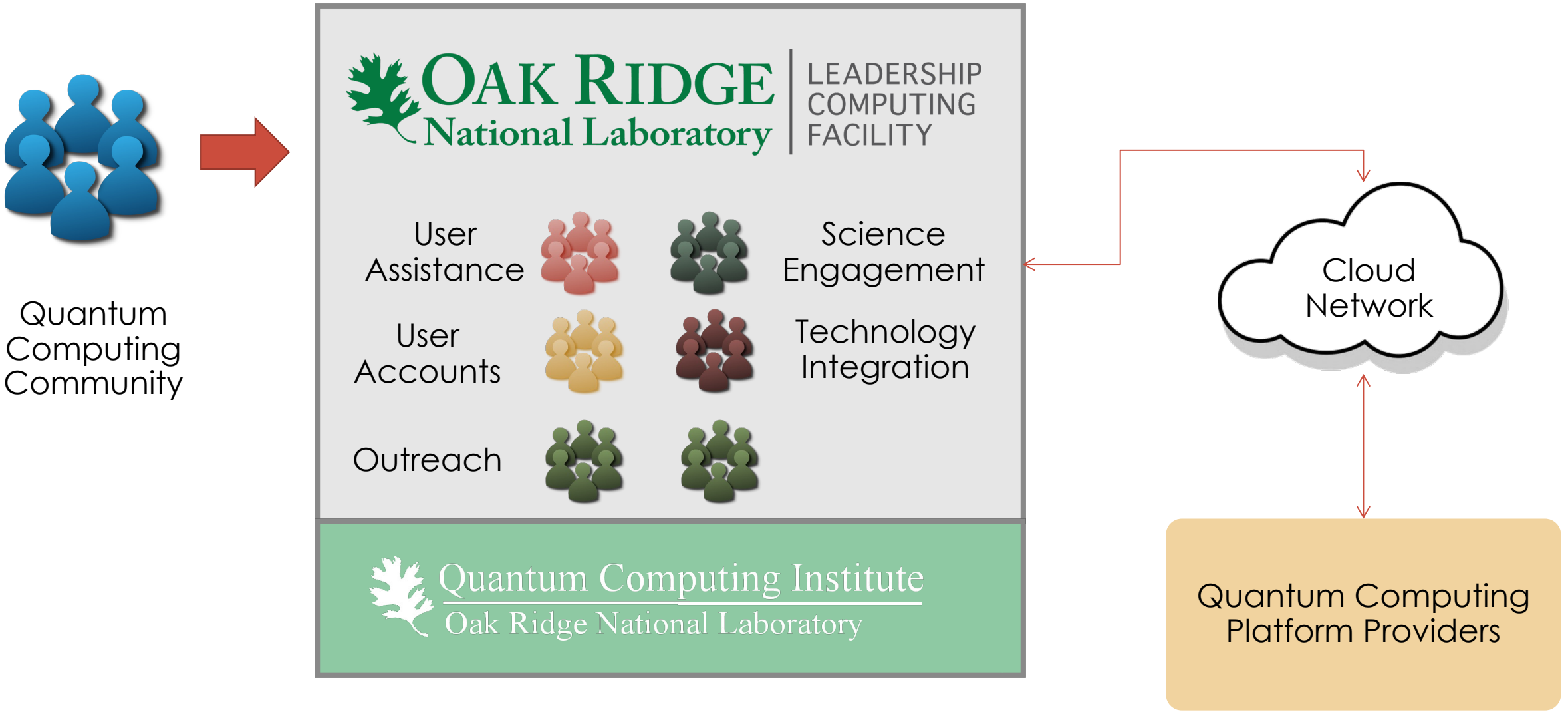
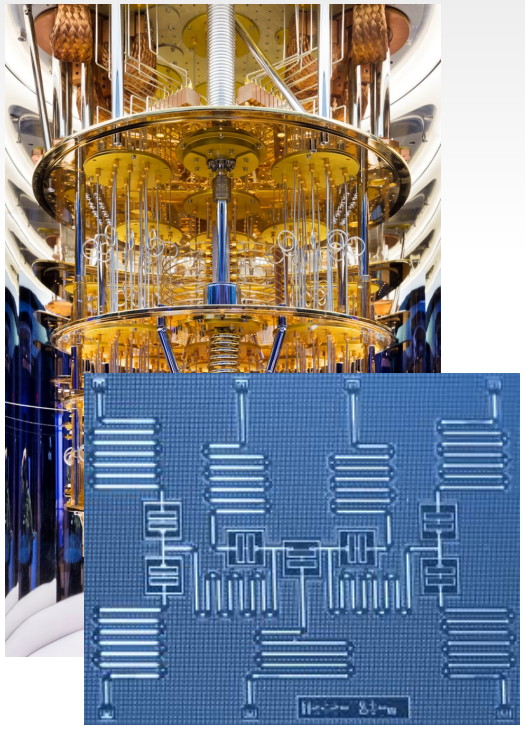
QCUP Operations Model: Cloud Access



Quantum Computing User Program Resources

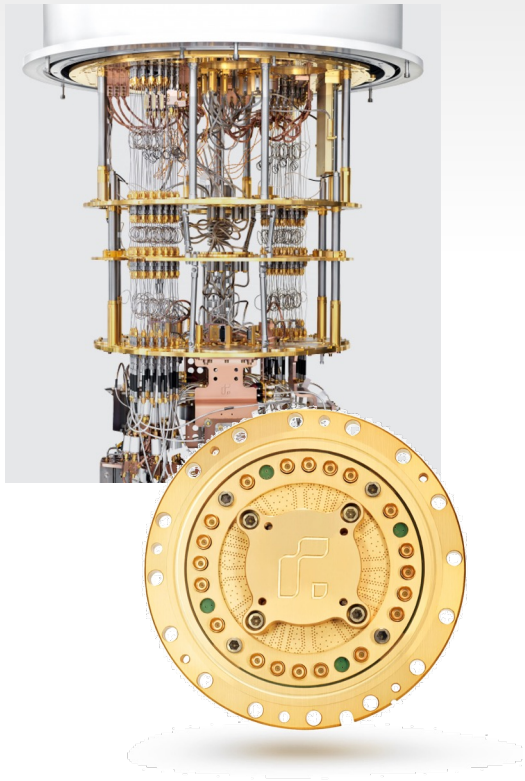
IBM

- General-purpose transmon systems provides up to 127 qubits



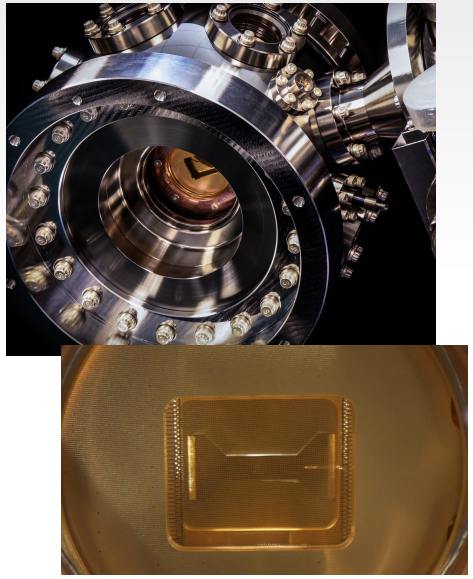
Rigetti

- General-purpose transmon systems provides up to 80 qubits



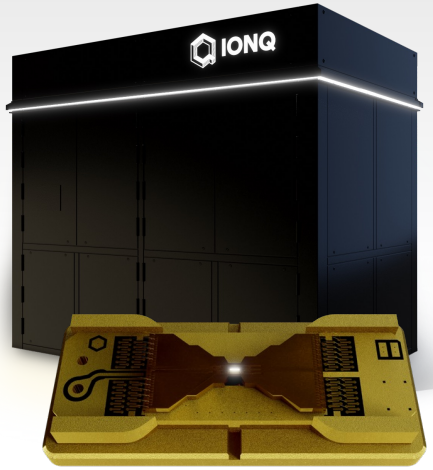
Quantinuum

- General-purpose ion trap systems provides up to 20 qubits



IonQ (pending)

- General-purpose ion trap systems provides up to 23 qubits

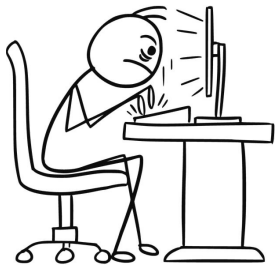


Total system count is 26

What are the steps to request access?

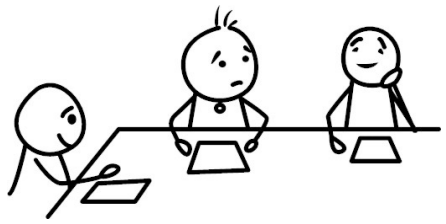
Project Request

- PI submits a proposal describing merit of idea and why it requires access to QCUP resources
- Online collects essential information
- Email notification of successful submission
- Available at olcf.ornl.gov



Project Review

- Quantum Resource Utilization Council (QRUC) receives proposals.
- QRUC reviews proposal for feasibility and merit.
- Additional review for export control, data sensitivity, user agreements



Project Award

- PI is notified that access to the system has been awarded.
- PI is notified of the allocation size, as warranted.
- PI receives unique project ID

User Request

- PI is evaluated as potential system user
- PI authorizes other user account requests
- Accounts vets users for export control, sensitive information, etc.
- OLCF notifies users of account creation.

Quantum Computing User Program Demographics

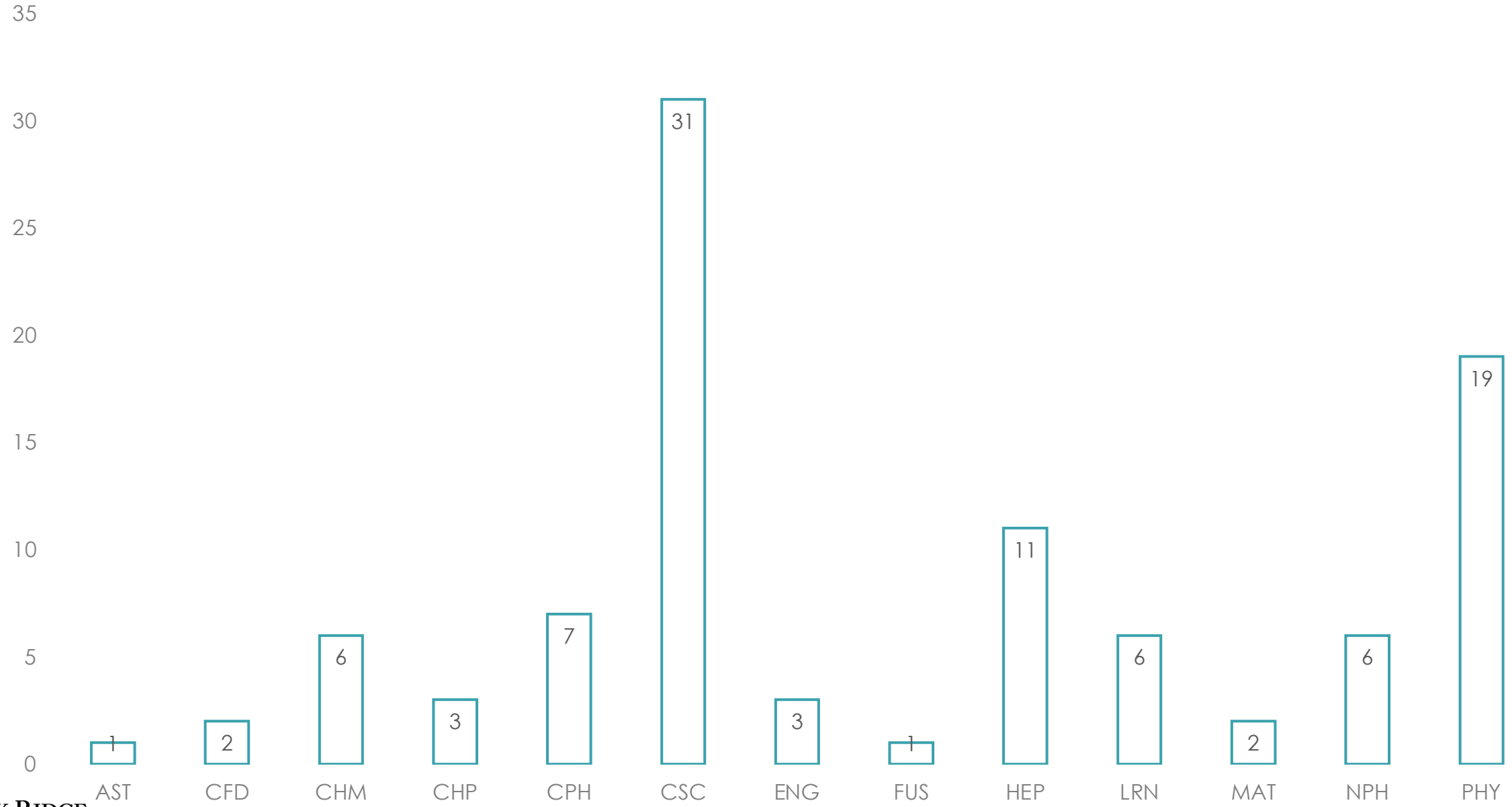
A Diverse User Base

- 400+ unique users across all systems for the program lifetime
- Users are from US national labs, universities, government, and industry
- Users range in quantum computing experience from novice to expert
- Teams consist of quantum computing expertise supported by application interests
- Teams use multiple programming languages and software environments

A Diverse Research Portfolio

- 46+ active projects across all systems
- Research teams funded by ASCR, BES, NP, HEP, NQI as well as other agencies
- Most projects focus on proof-of-principle demonstrations and/or new method development
- Some projects focus on application performance and/or benchmarking
- Some projects focus on device characterization, verification, and validation

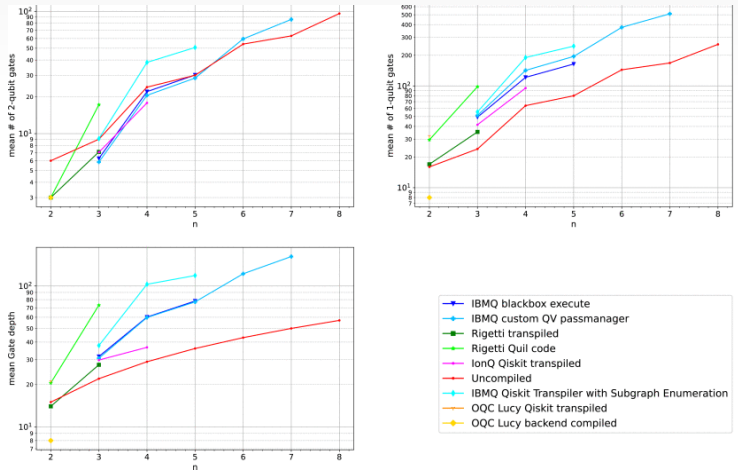
QCUP Projects by Category



Quantum Computing User Program Highlights

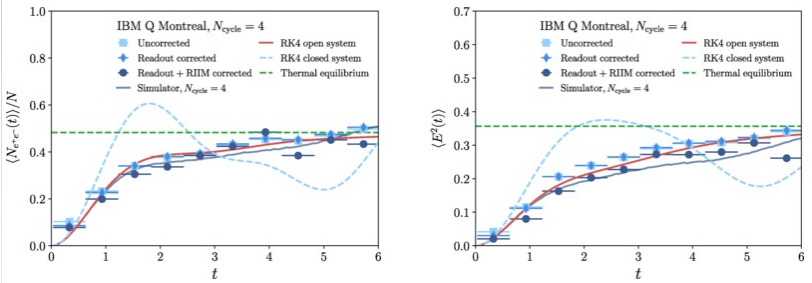
Computational Sciences

- Quantum volume in practice: What users can expect from NISQ devices
- Pelofske, E, et al., IEEE Transactions on Quantum Engineering, 3, 1-19 (2022).
- Used IBM, Rigetti, Quantinuum, and additional quantum devices to create quantum volume comparisons



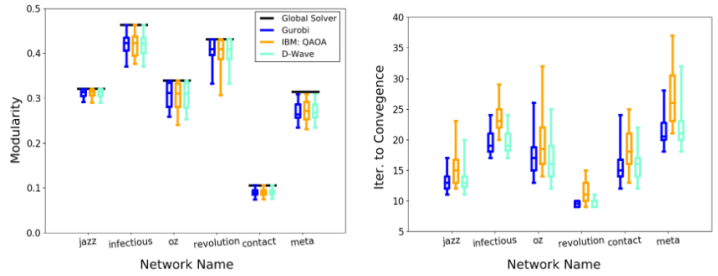
Quantum Volume circuit operations summary figures, with average single-submit, two-qubit, and SPAM operations.

- Quantum simulation of nonequilibrium dynamics and thermalization in the Schwinger model
- de Jong, Wibe A., et al. Physical Review D 106.5, 05450 (2022)
- Used IBM systems to simulate nonequilibrium dynamics of quantum field theories and the preparation of thermal states, setting benchmarks for future studies.



Results representing the first studies of quantum simulations of quantum field theoretical nonequilibrium dynamics and thermalization, where the quantum algorithm with four cycles gives a good approximation of the full result.

- Network community detection on small quantum computers
- R. Shaydulin et al., Advanced Quantum Technologies, 2 1900029 (2019)
- Used IBM and D-Wave to evaluate quantum and conventional optimization

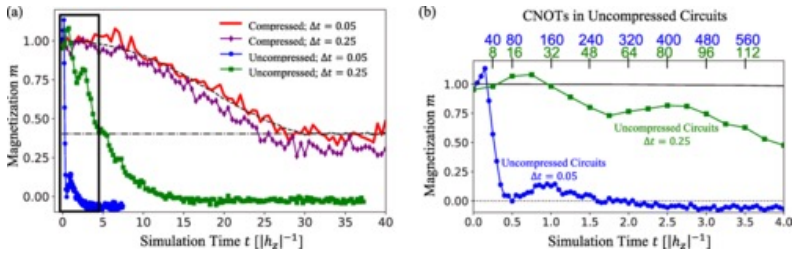


Modularity score for conventional and quantum methods for community detection

Quantum Computing User Program Highlights

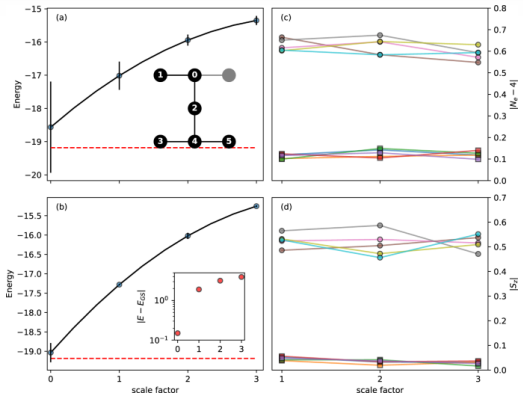
Physical Sciences

- Algebraic compression of quantum circuits for Hamiltonian evolution
- Kökcü, Efekan, et al., Physical Review A 105.3 (2022): 032420.
- Used IBM system to present and test an algorithm that compresses Trotter steps into a single block of quantum gates



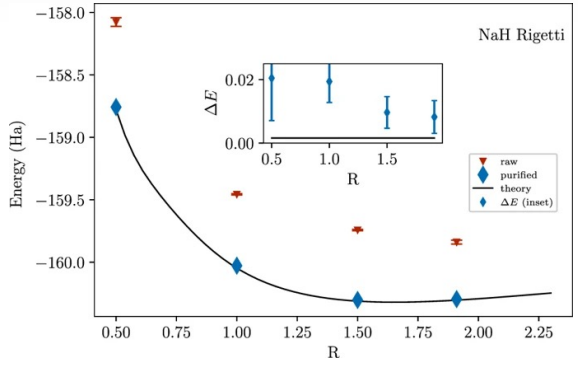
Simulation results from ibmq_Brooklyn comparing compressed circuits versus uncompressed circuits derived from standard Trotter decomposition. A five-qubit system is evolved under a time-dependent Hamiltonian.

- Comparative study of adaptive variational quantum eigensolvers for multi-orbital impurity models
- Mukherjee, Anirban, et al., Communications Physics 6.1, 4 (2023)
- Used IBM and Quantinuum systems to assess the gate depth and accuracy of variational ground state preparation



Calculations performed on a QPU (ibmq_casablanca), where each of the three transpiled measurement circuits for the model contain around 350 CNOT gates, demonstrating a two-fold increase over cases where qubit swapping was not used

- Quantum chemistry as a benchmark for near-term quantum computers
- A. J. McCaskey et al., npj Quantum Information 5, 99 (2019)
- Used IBM and Rigetti systems to test quantum chemistry calculations and compare methods

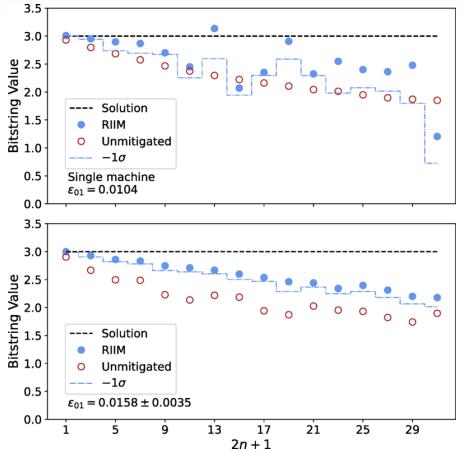


Raw and post-processed ground-state energy calculations for sodium hydride using Rigetti

Quantum Computing User Program Highlights

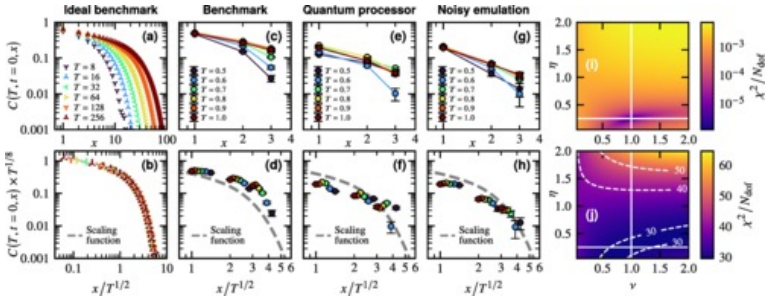
Other Sciences

- Computationally efficient zero-noise extrapolation for quantum-gate-error mitigation
- Pascuzzi, Vincent R., et al., Physical Review A 105.4 042406, (2022)
- Used IBM systems to improve the ability to mitigate noise via comparing and parallelizing zero-noise-extrapolation techniques



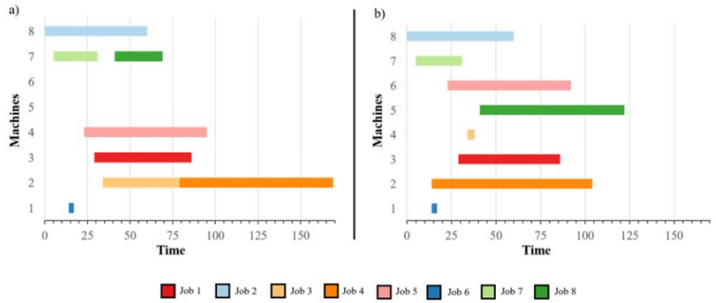
Comparison of a single-device to multiple devices for the case of the four-CNOT circuit with depolarizing gate noise

- Quantum criticality using a superconducting quantum processor
- Dupont, Maxime, and Joel E. Moore. Physical Review B 106.4, L041109, (2022)
- Used Rigetti to study a one-parameter noise-model to introduce and modify scaling laws to improve data analyses for extracting physical properties transparent to noise



Two-point correlation function calculations, comparing the emulations to actual simulation on quantum (Rigetti Aspen-9) hardware.

- Quantum computing based hybrid solution strategies for large-scale discrete-continuous optimization problems
- A. Ajagekar et al., Computers & Chemical Engineering 132, 106630 (2019)
- Use D-Wave system to test hybrid algorithms for optimization



Improvements in job shop scheduling using hybrid methods compared with commercial Gurobi solverv

QCUP Support and Engagement Teams

Accounts

- Manage project and user applications
  - Process online applications for resources
  - Vet accounts per DOE policies and processes
  - Initiate account creation with vendor support

User Assistance (UA)

- Engage with users and vendors for technical assistance
  - Primary point of contact for QCUP user assistance
  - Online messaging and queuing system, tickets
  - Technical documentation and training
  - Hackathons and development events

Software Services

- Integrate Quantum vendor APIs with the OLCF's existing software
  - Can manage quantum systems easily at an HPC center (user, project, quota management)
  - Users can apply for HPC and Quantum resources for the same project

Science Engagement

- Subject matter experts for quantum applications development
  - Liaisons with projects for scientific advances
  - One-on-one engagement driven by projects needs
  - Expertise in quantum computational methods and select disciplines
  - Evaluate quantum resource usage, best practices

Quantum Computing User Forum

Annual user meeting to highlight results and discuss common practices in the development of applications and software for quantum computing systems.

DATE
Next: July 2024

LOCATION
Oak Ridge National Laboratory

CONTACT
qcup@ornl.gov

www.olcf.ornl.gov/calendar/quantum-computing-user-forum

Important Links

- Overview page: https://www.olcf.ornl.gov/olcf-resources/compute-systems/quantum-computing-user-program/
- Documentation: https://docs.olcf.ornl.gov/quantum/index.html