Oak Ridge Leadership Computing Facility Quantum Computing User Program

Travis S. Humble
Oak Ridge National Laboratory

Oak Ridge National Laboratory

Oak Ridge Leadership Computing

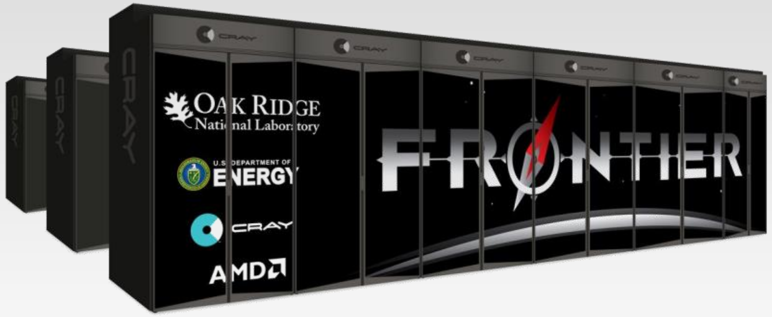
TITAN

Cray XK7, 18,688 Nodes
16-core AMD Interlagos + K20X
17 PFLOPS, 8.2 MW,
#1 TOP500 (2012)

SUMMIT

IBM, 4,600 Nodes
2 Power9 + 6 NVidia Volta
144 PFLOPS, 9.7 MW,
#1 TOP500 (2018-19)

FRONTIER



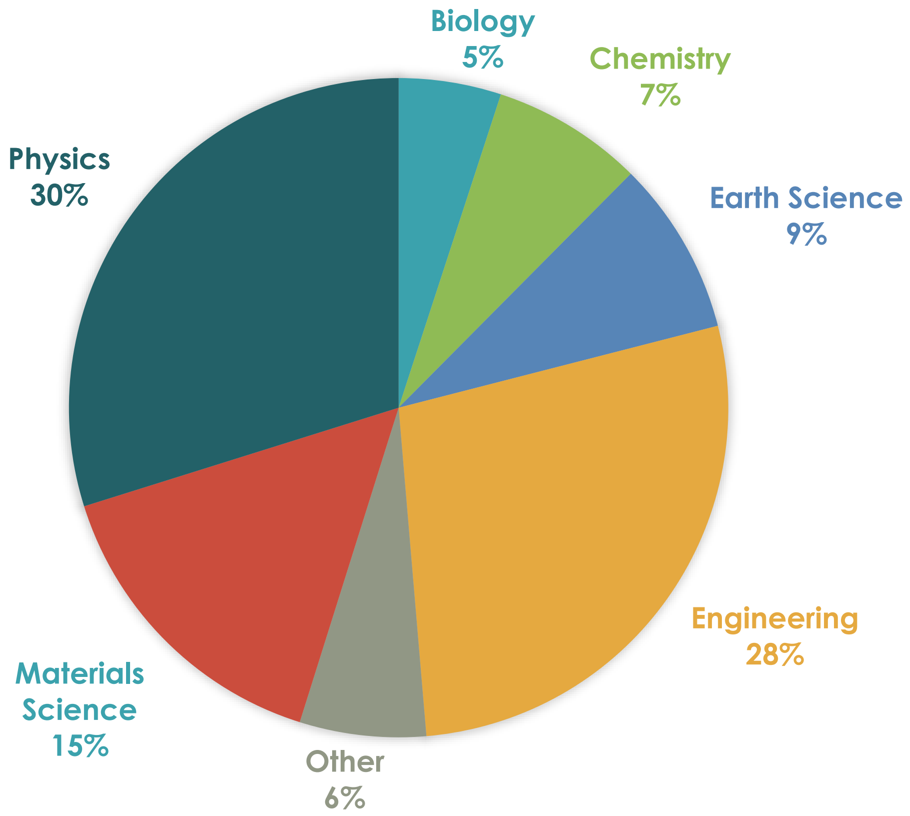
CRAY, 100 Cabinets
1:4 AMD EPYC : Radeon Instinct
1.5 EXAFLOPS
Expected 2021

Scientific discovery and energy security depend on advances in computational capability

Large-Scale Scientific Computing

- Computing for scientific and engineering problems and the science of doing such computations
- Modelling and simulation challenges generate hardware requirements, while hardware constraints spur new methods
- Example: Monte Carlo sampling using GPU-accelerated compute nodes

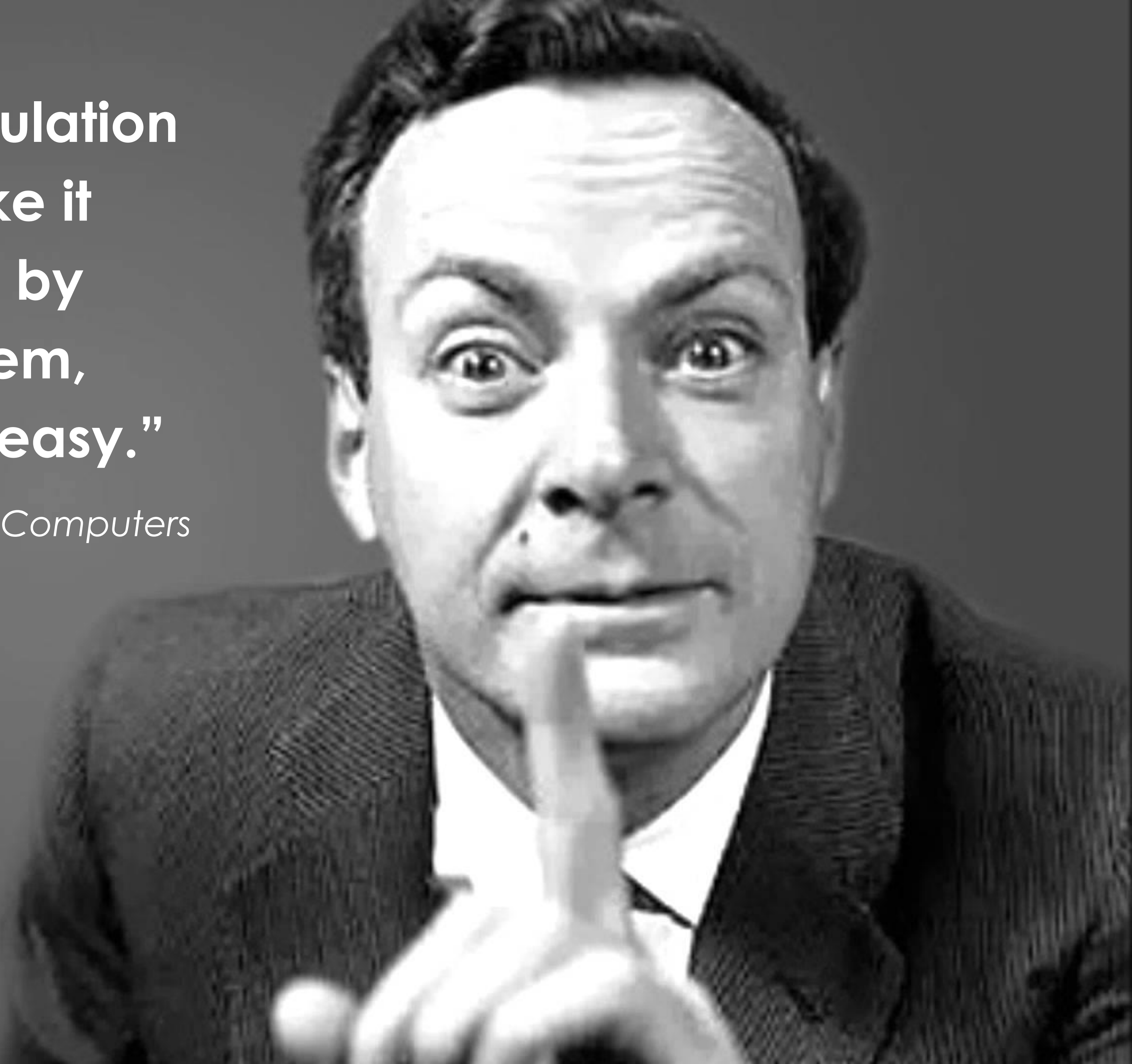
2019 INCITE Allocations by Category



“If you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it’s a wonderful problem, because it doesn't look so easy.”

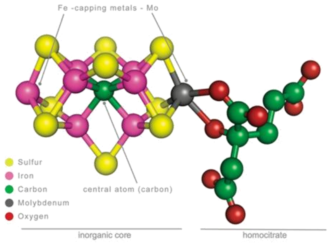
Richard Feynman, *Simulating Physics with Computers*

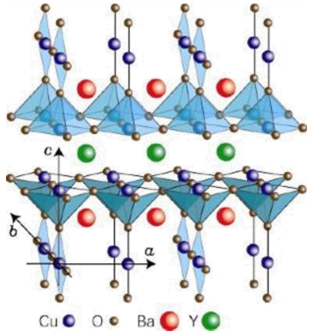
(1982)

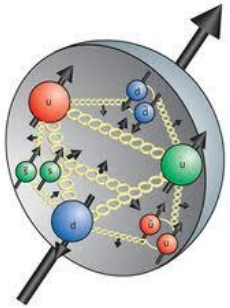


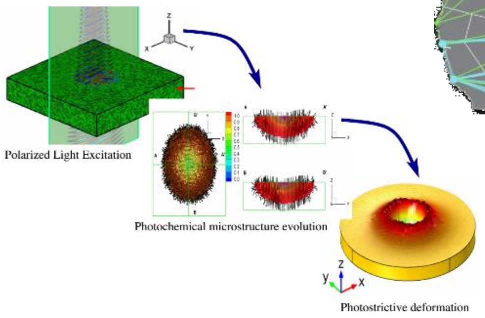
Scientific Applications of Quantum Computing

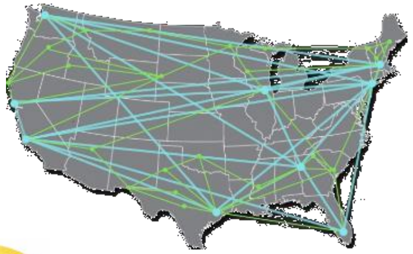
- Algorithms in the quantum computing model have been found to take fewer steps to solve problems
  - Quantum Simulation
  - Partition Functions
  - Discrete Optimization
  - Machine Learning
  - Factoring
  - Unstructured Search
  - Eigensystems
  - Linear Systems
- Several physical domains motivate quantum computing as a paradigm for scientific computing
  - High-energy Physics
  - Materials Science
  - Chemistry
  - Biological Systems
  - Artificial Intelligence
  - Data Analytics
  - Planning and Routing
  - Verification and Validation



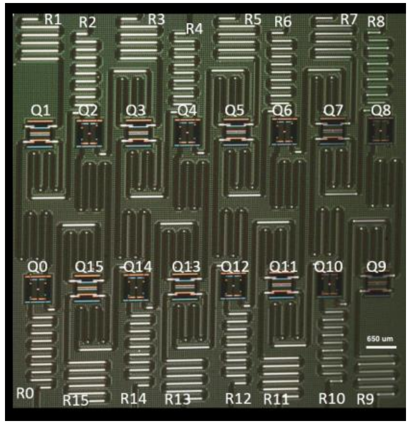




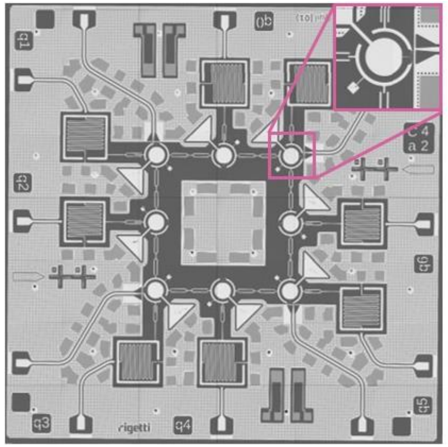




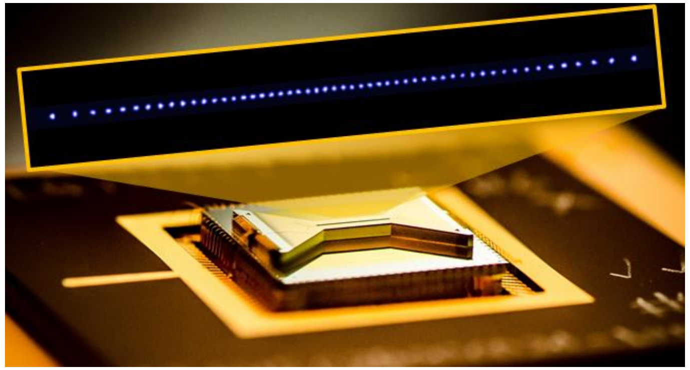
Quantum Processing Units



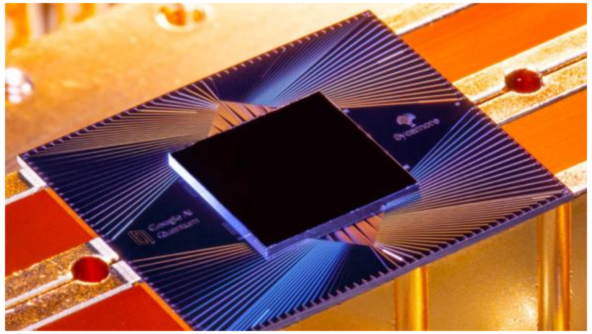
Superconducting chip from IBM



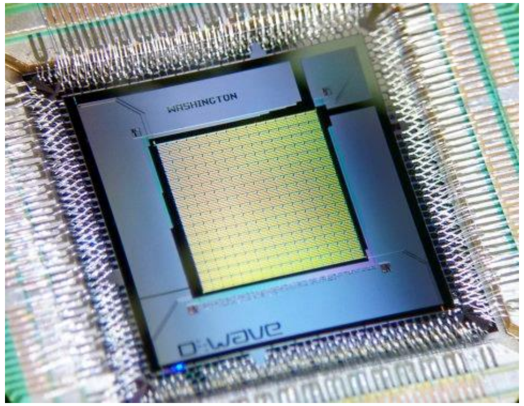
Superconducting chip from Rigetti



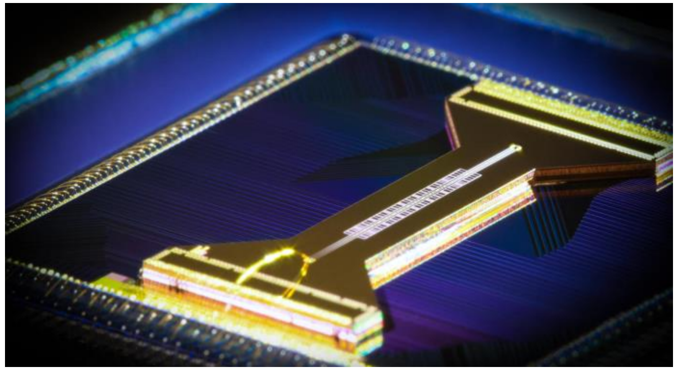
Ion trap chip from ionQ



Superconducting chip from Google



Superconducting chip from D-Wave Systems



Ion trap chip from Honeywell Quantum Solutions

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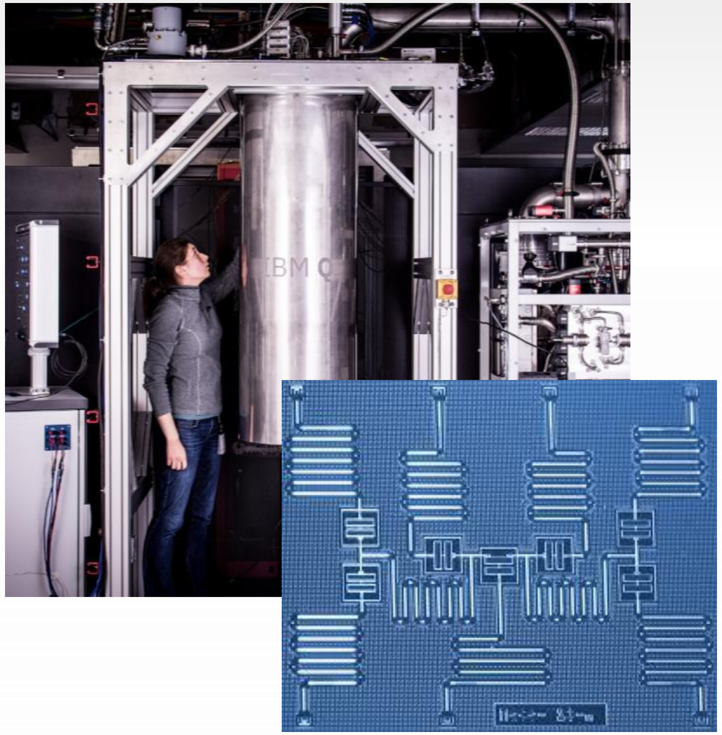
Quantum Computing Resources

D-Wave

- DW special-purpose annealing systems provides 2048 qubits

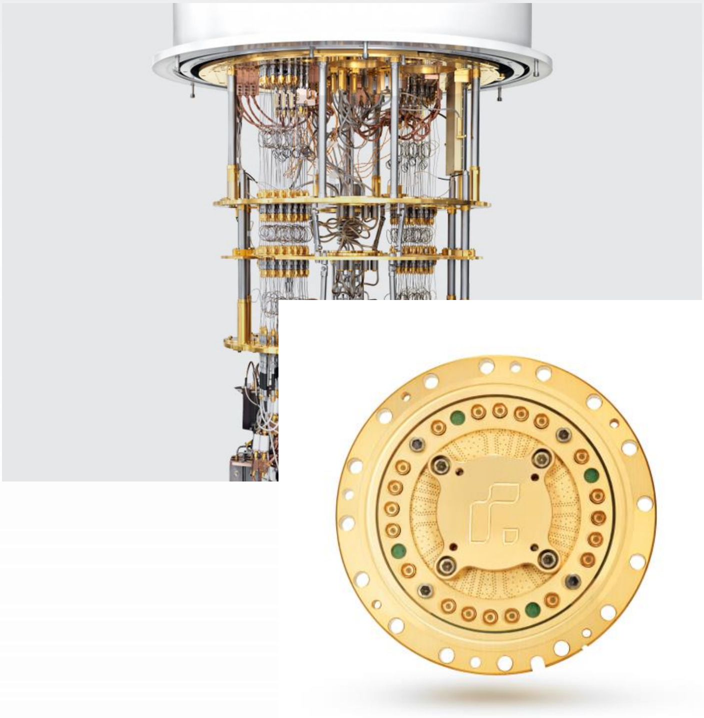
IBM

- IBM general-purpose gate system provides 53 qubits



Rigetti

- Rigetti general-purpose gate system provides 28 qubits



Quantum Computing User Program

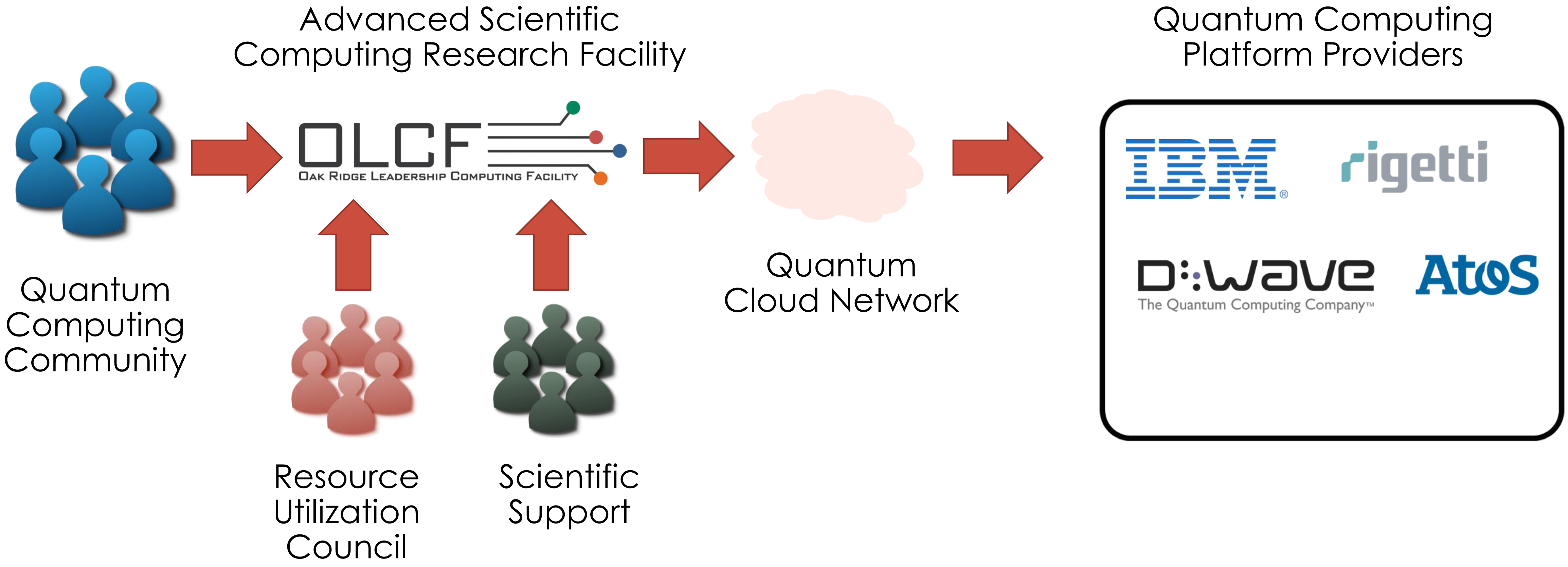
Enable User Access to Quantum Computing Resources

- Merit-based review and user agreements facilitate access to the computing resources.
- The user program is managed by the Oak Ridge Leadership Computing Facility to provide access to quantum computing resources.
- The user program is supported by the Department of Energy, Office of Science, Advanced Scientific Computing Research program office.

Evaluate Scientific Quantum Computing Use Cases

- How do users integrate quantum computing with scientific computing?
- The user program supports the Office of Science QIS research portfolio.
- This includes support for research funded by SC program offices:
  - Advanced Scientific Computing Research
  - Basic Energy Sciences
  - Biological Environmental Research
  - High-energy Physics
  - Fusion Energy Sciences
  - Nuclear Physics

OLCF Quantum Computing User Program Model



Current Quantum Computing Resources

IBM

- Technology: Superconducting qubits
- Capacity: 53 qubits
- Gate model
- Systems: 14

D-Wave

- Technology: Superconducting qubits
- Capacity: 2048 qubits
- Annealing model
- Systems: 2

Rigetti

- Technology: Superconducting qubits
- Capacity: 28 qubits
- Gate model
- Systems: 1

Atos

- Technology: Numerical simulators
- Capacity: 30 qubits
- Gate model
- Systems: 1

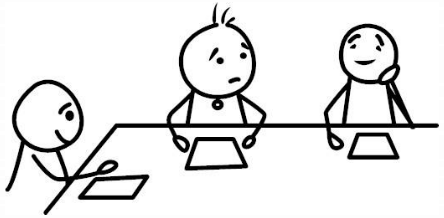
What are the steps to program access?

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

- OLCF Resource utilization council (RUC) receives proposals.
- RUC reviews proposal for feasibility and merit.
- OLCF review includes export control review, 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
- OLCF vets users for export control, sensitive information, etc.
- OLCF notifies users of account creation.

How does a PI get access?

PI initiates request

- PI visits online form at olcf.ornl.gov
- PI provides identifying information
  - Name and Contact Information
  - Citizenship Status
  - Employer and Funding Source
  - Project Details
  - Research Area
  - Resource Request
  - Duration (6 months)
  - Description of Work
  - Narrative (3 paragraphs)
  - Performance Summary
  - Data Management Plan
  - …

PI receives notification email

- PI receives email from OLCF notifying approval of project by RUC
- Email specifies resource and period of performance for access
  - 6 months
- Email notifies PI that project will next undergo export control review

PI receives approval email

- PI receives email notifying final approval by OLCF
- Email provides information about:
  - Host Access
  - User Account Requests
- Acknowledgements
  - This research used quantum computing resources of the Oak Ridge Leadership Computing Facility, which is a DOE Office of Science User Facility supported under Contract DE-AC05-00OR2272
- Email from OLCF completes project request procedure

How does a user get access?

User initiates requests

- User visits online form at olcf.ornl.gov
- User provides identifying information
  - Name
  - Contact Information
  - Residence
  - Citizenship Status
  - Employer
  - Funding Source
  - Project ID
  - Description of work
  - Data classification
  - Policy acceptance

PI approves request

- PI receives email from OLCF
- PI concurs user is member of designated project ID

OLCF evaluates user

- Check for existing user account
- Check for existing user agreement
- Check for nationality restrictions
- Check for employer restrictions
- Check for project restrictions
- …

OLCF notifies user

- User receives email from OLCF approving access to project ID
- Email includes instruction for vendor access agreements
  - Vendor specific agreements may apply for system access
- Email includes contact for OLCF User Assistance Center

Quantum Computing User Program Demographics

A Diverse User Base

- 130+ unique users across all systems
- 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

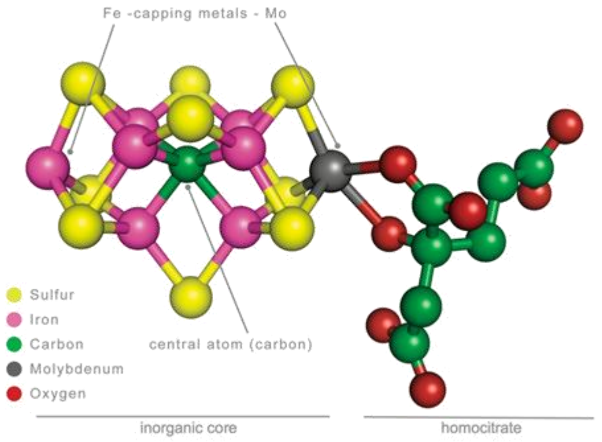
A Diverse Research Portfolio

- Research teams funded by ASCR, BES, and HEP as well as other program offices
- 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

Use Cases for Scientific Quantum Computing

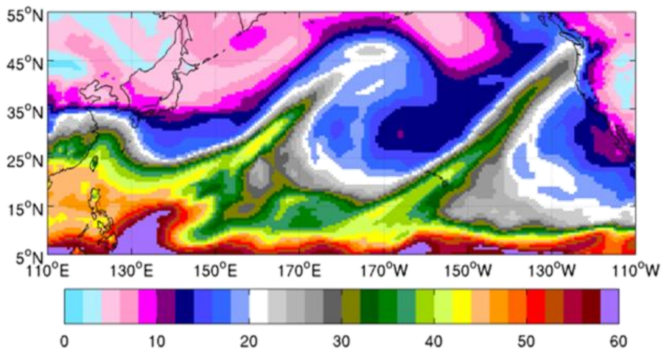
Physical Sciences

- Chemistry, Materials, High-Energy Physics, Nuclear Physics, Fusion



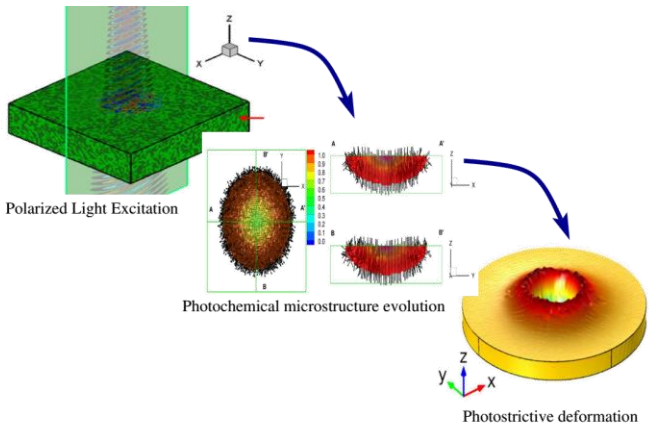
Data Sciences

- Artificial Intelligence, Machine Learning, Inference and Mining



Applied Sciences

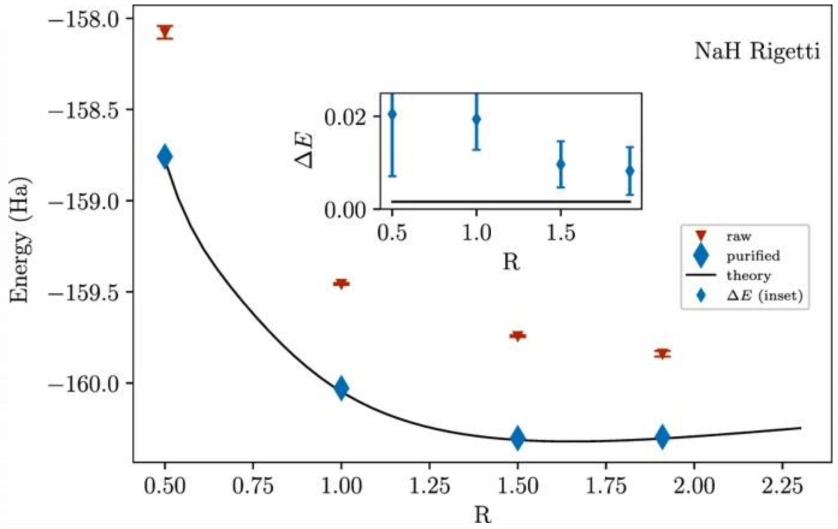
- Optimization, Engineering, Verification and Validation, Energy Sciences



Quantum Computing User Program Projects

Physical Sciences

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



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

Applied Sciences

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

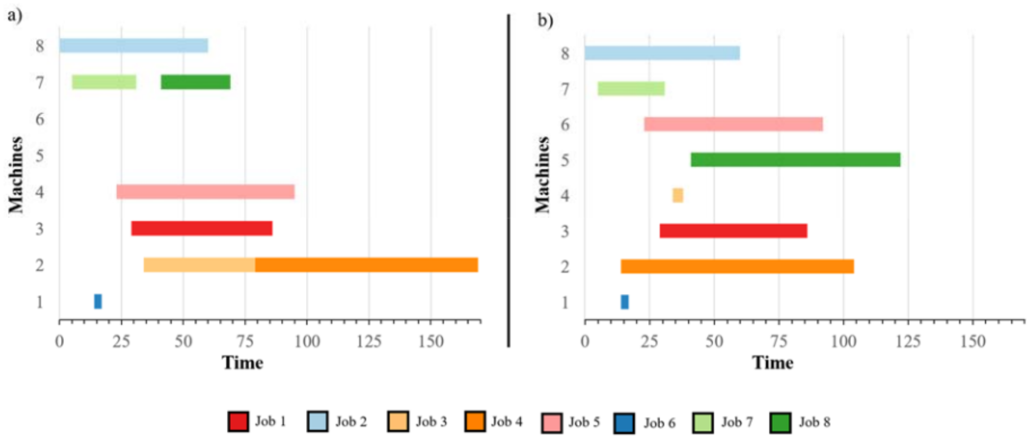
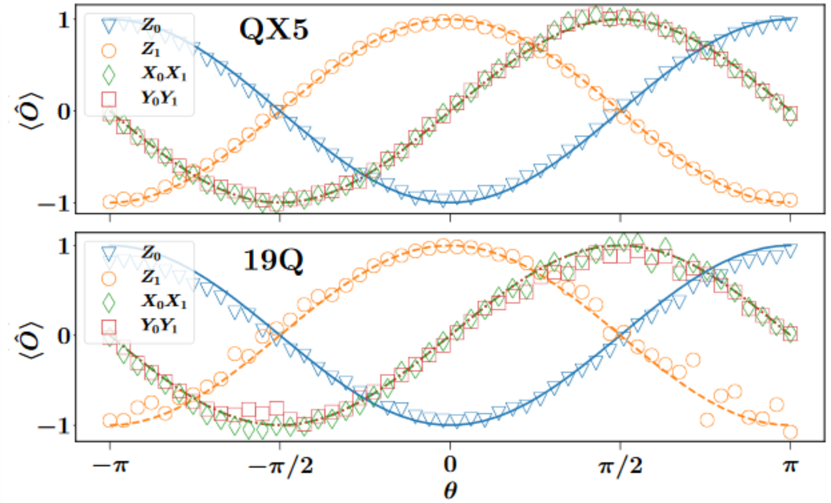


Figure 4. Gantt charts of scheduling results of a job-shop scheduling problem with eight jobs and machines obtained using a) MILP solver Gurobi and b) Hybrid QC-MILP decomposition method.

Quantum Computing User Program Projects

Physical Sciences

- Cloud quantum computing of an atomic nucleus
- E. F. Dumitrescu et al., Phys. Rev. Lett. 120, 210501 (2018)
- Used the IBM and Rigetti systems to demonstrate parallel quantum computing while calculating the deuteron nuclear binding energy



Identical calculations for the expectations values of the QX5 (IBM) and 19Q (Rigetti)

Data Sciences

- 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

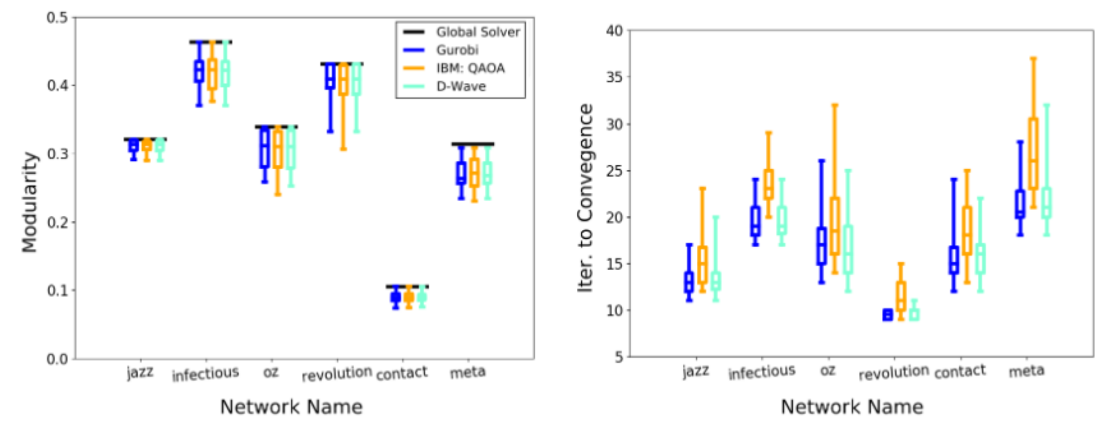
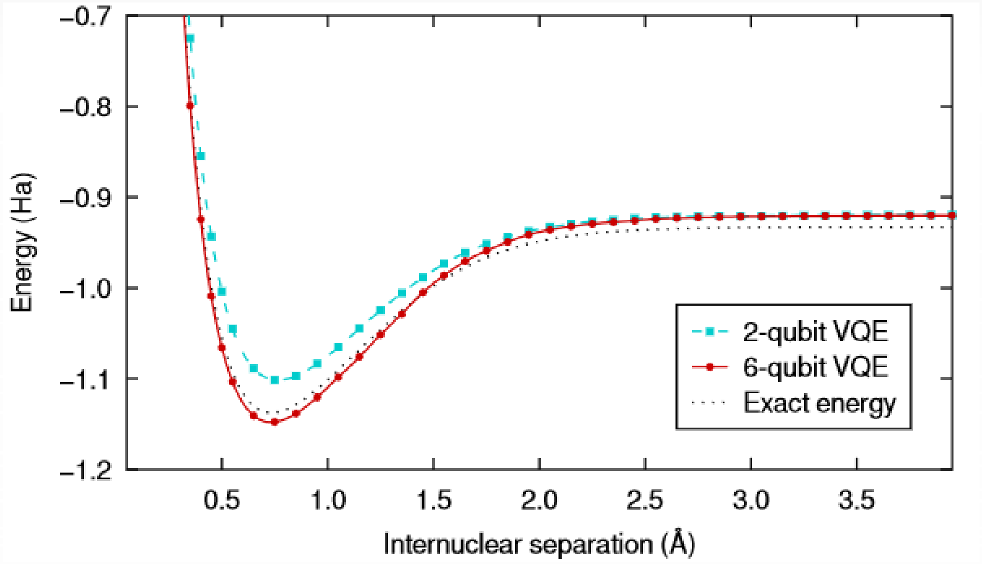


Fig 1. Box-plots showing the range of modularity scores for 2-community detection (left, greater is better) and number of solver calls (right, less is better) respectively for the three different subproblem solvers. The results show that the proposed approach is capable of achieving results close to the state-or-the-art (Global Solver)

Quantum Computing User Program Projects

Physical Sciences

- Quantum error detection improves accuracy of chemical calculations on a quantum computer
- M. Urbanek et al., arXiv:1910.00129 (2019)
- Used an IBM system to test improvements in accuracy from error detection techniques



Improvements in chemical energy calculation using the demonstrated error detection technique

Physical Sciences

- Quantum computing for neutrino-nucleus scattering
- A. Roggero et al., arXiv:1911.06368 (2019)
- Used an IBM system to test calculations of the nuclei ground (triton) using variational algorithms

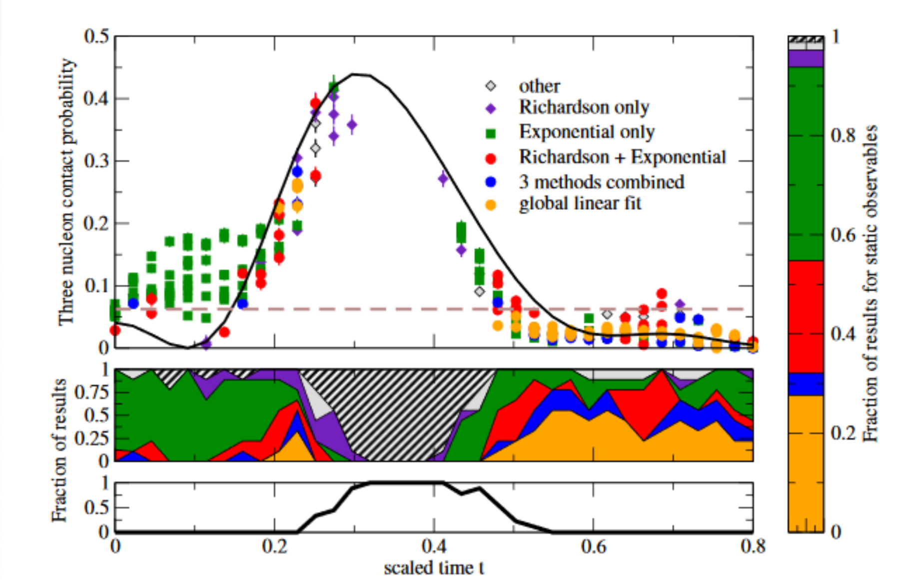


FIG. 8. Extrapolation procedures used to mitigate errors in the results for the 3 nucleon contact density $C_3(t)$ shown in Fig. 7. See main text for a description of the different panels.

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Quantum Computing User Program Priorities

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 computing ecosystems by engaging with users, developers, vendors, providers, and stakeholders

Quantum Computing User Forum

Brings together users to discuss common practices in the development of applications and software for quantum computing systems.

DATE

April 21-23 2020

TIME *ET*

08:00 AM - 05:00 PM

LOCATION

Building 8600, Room A103
Oak Ridge National Laboratory, Oak Ridge, TN 37831

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

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