

# Oak Ridge Leadership Computing Facility Quantum Computing User Program

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

# Oak Ridge National Laboratory



## TITAN



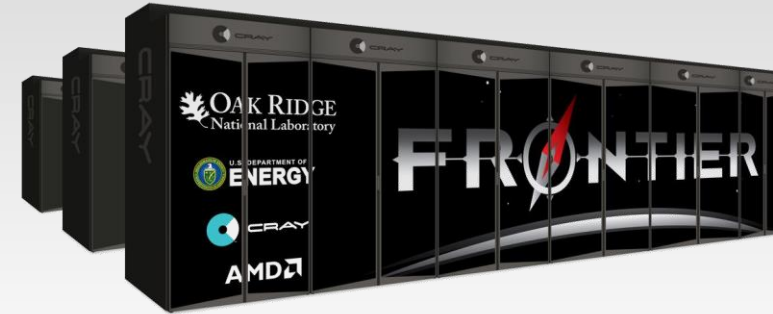
Cray XK7, 18,688 Nodes  
16-core AMD Interlagos + K20X  
17 PFLOPS, 8.2 MW,  
#1 TOP500 (2012)

## SUMMIT



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

## FRONTIER



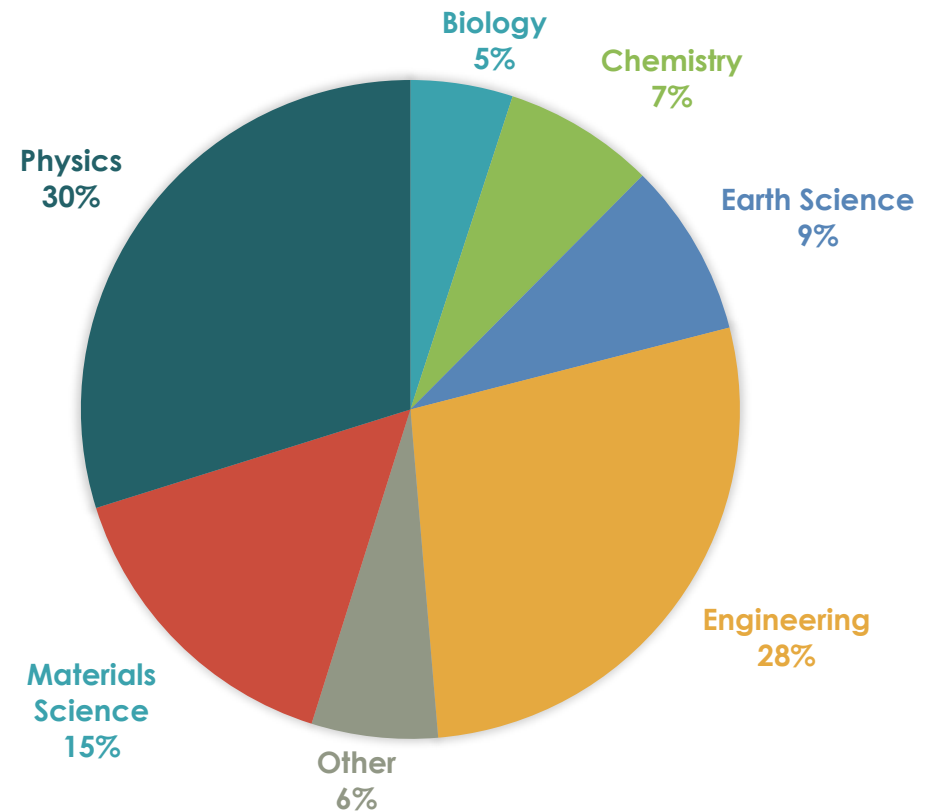
CRAY, 100 Cabinets  
1:4 AMD EPYC : Radeon Instinct  
1.5 EXAFLOPS  
Expected 2021

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

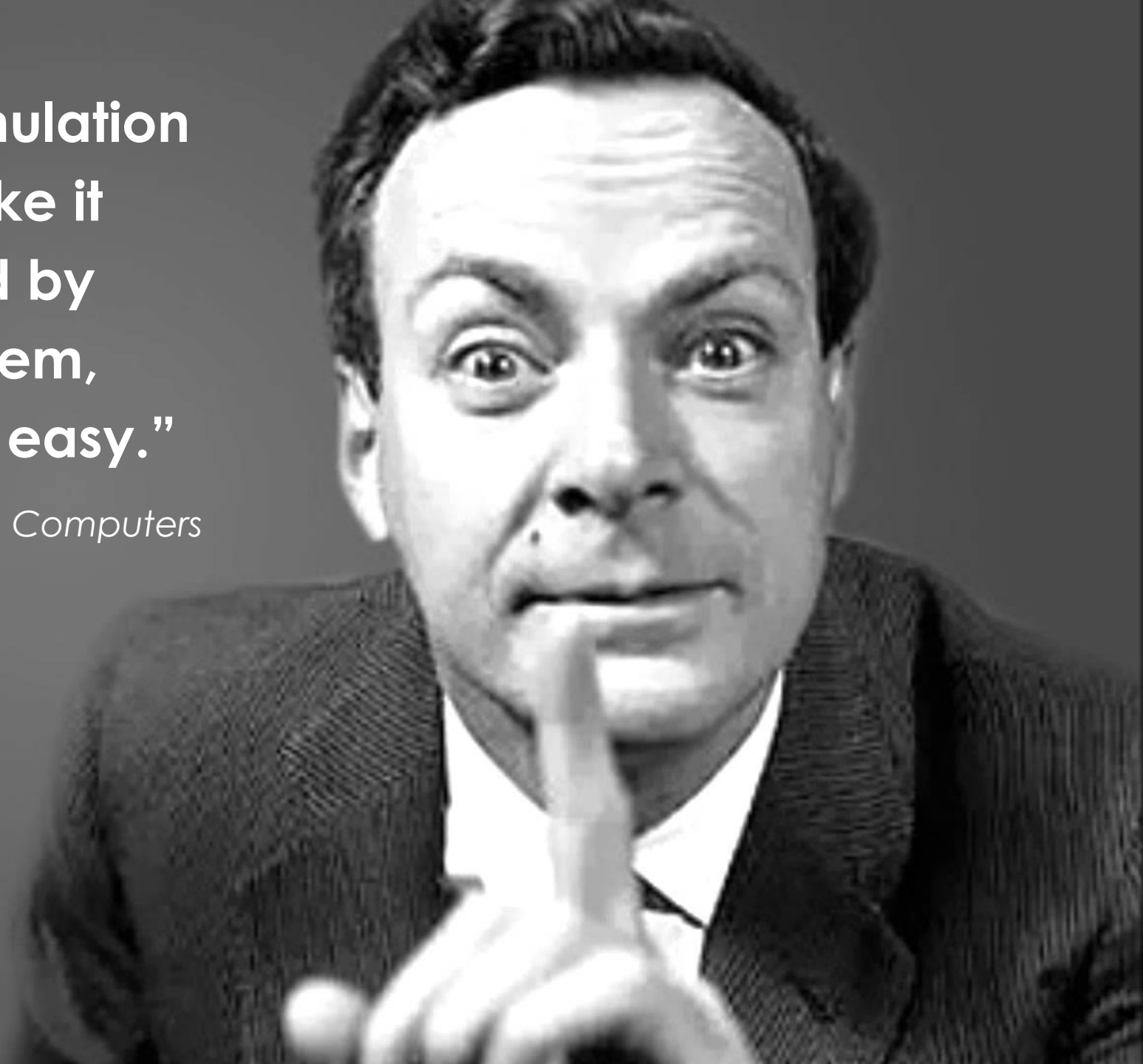
2019 INCITE Allocations by Category



**“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*

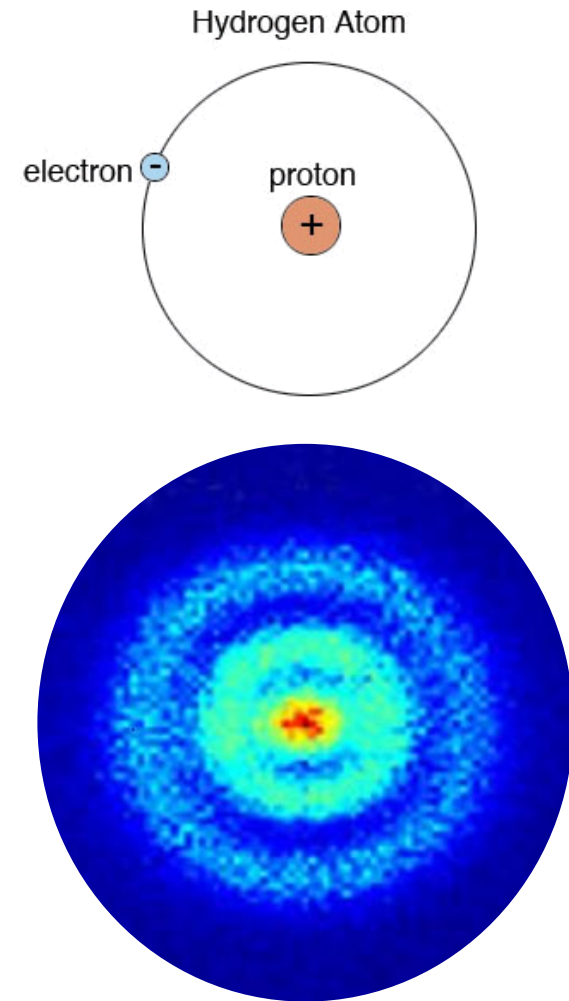
(1982)



# What is Quantum Computing?

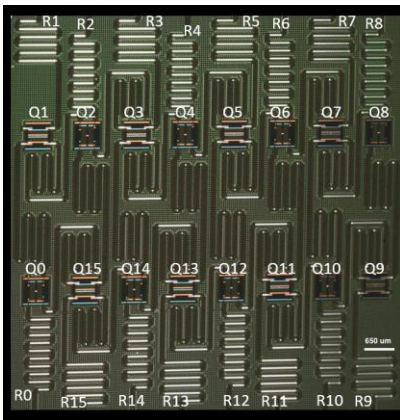
- Quantum mechanical computation
  - In quantum mechanics, the *wave function* describes all knowledge about the system
- Quantum computing manipulates the wave function to perform calculations
  - Quantum dynamical control of the Hamiltonian corresponds to computation

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

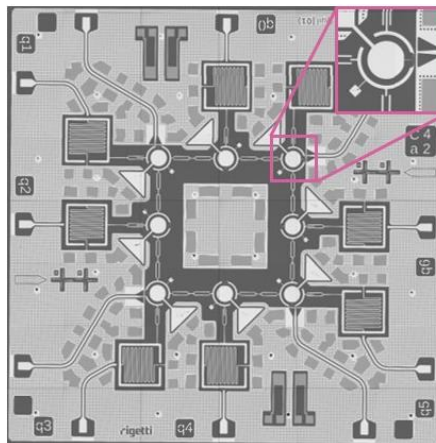


Stodolna et al. PRL 110, 213001 (2013)

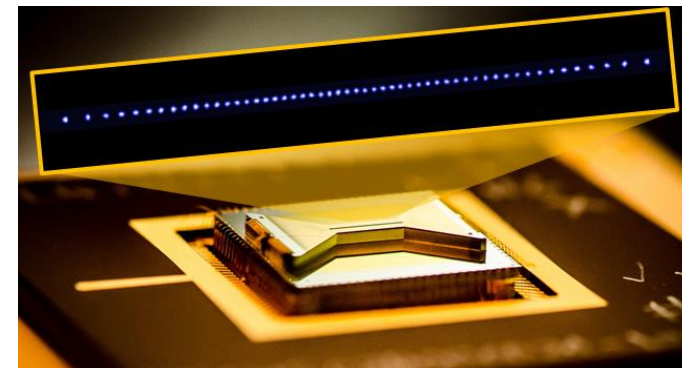
# Quantum Processing Units



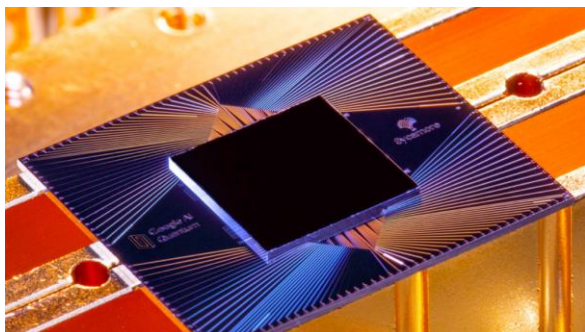
*Superconducting chip from IBM*



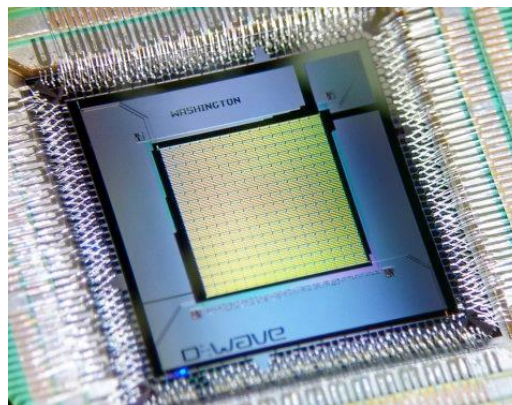
*Superconducting chip from Rigetti*



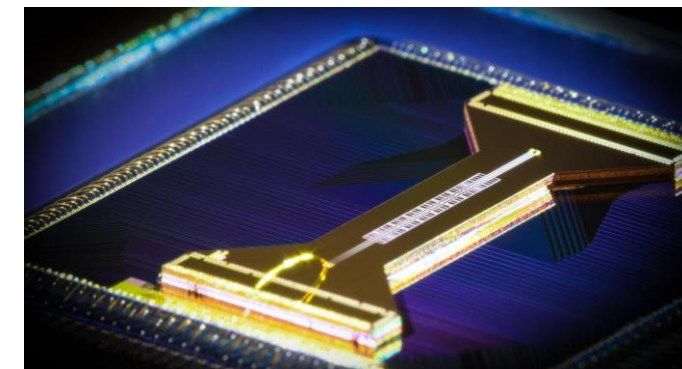
*Ion trap chip from ionQ*



*Superconducting chip from Google*



*Superconducting chip from D-Wave Systems*

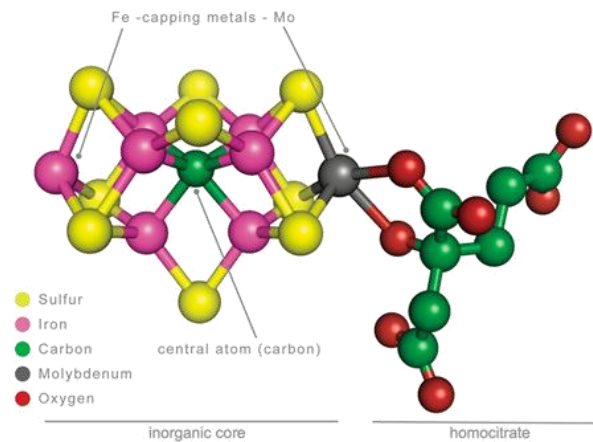


*Ion trap chip from Honeywell Quantum Solutions*

# Use Cases for Scientific Quantum Computing

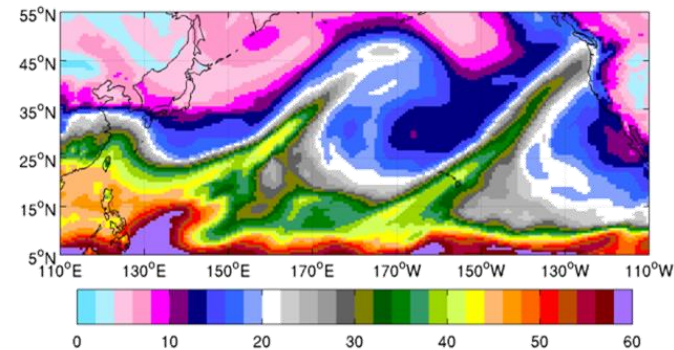
## Physical Sciences

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



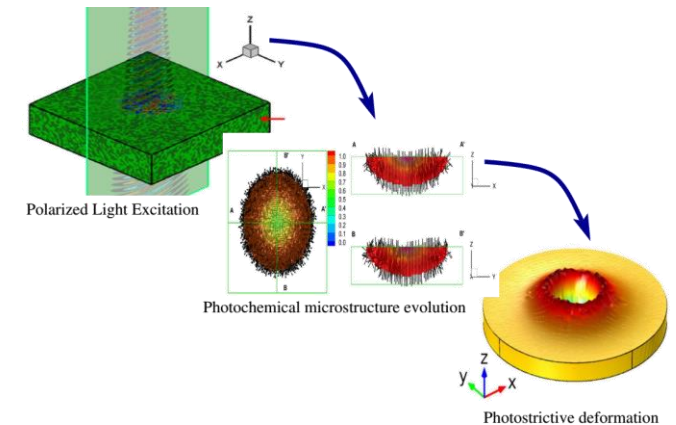
## Data Sciences

- Artificial Intelligence, Machine Learning, Inference and Mining



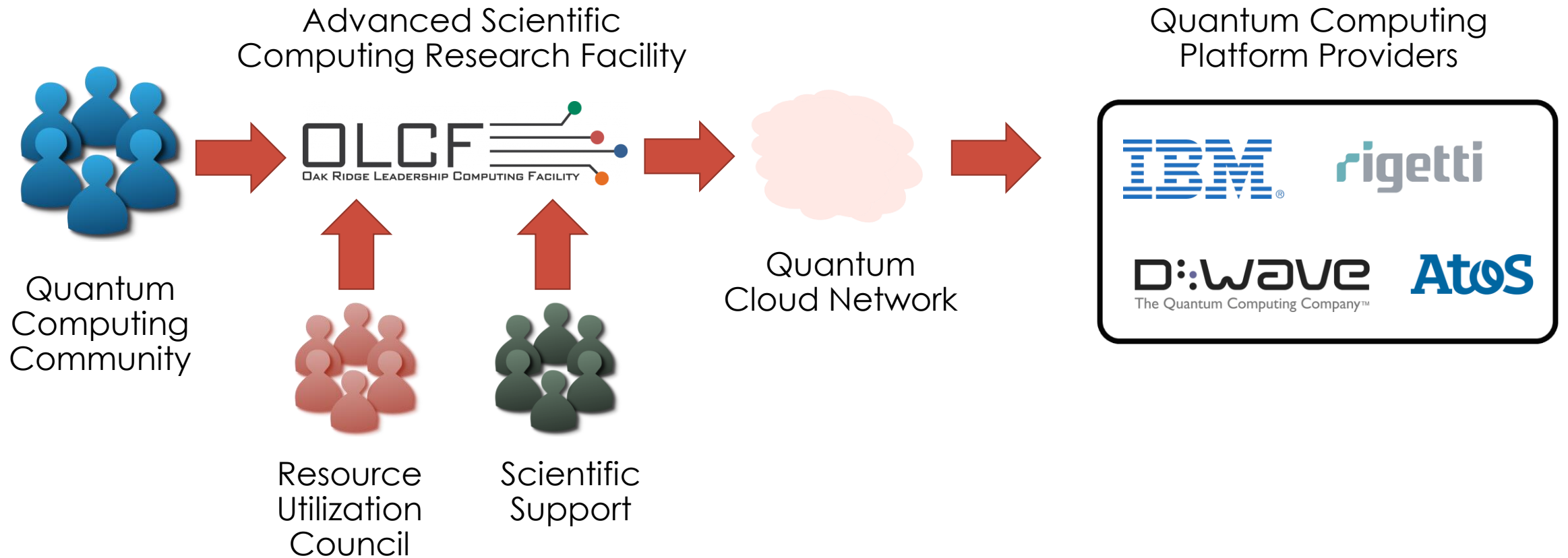
## Applied Sciences

- Optimization, Engineering, Verification and Validation, Energy Sciences



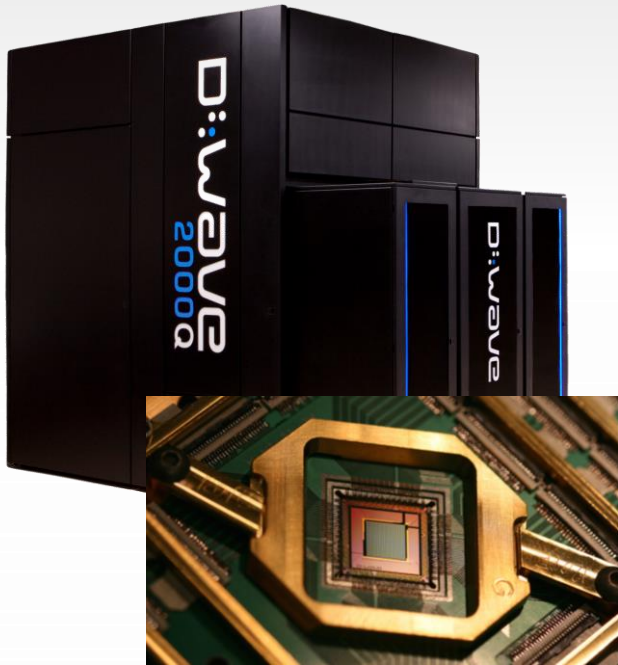


# OLCF Quantum Computing User Program Model



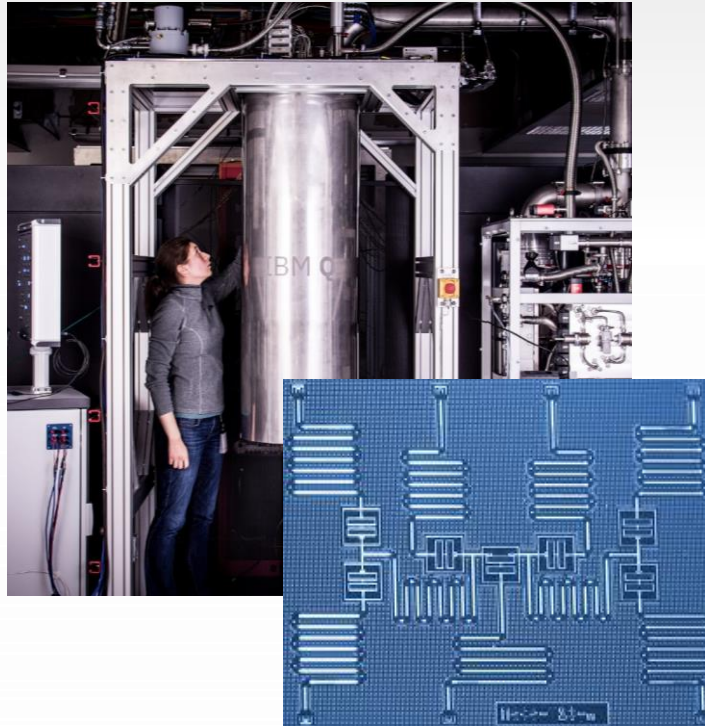
## D-Wave

- DW special-purpose annealing systems provides 2048 qubits



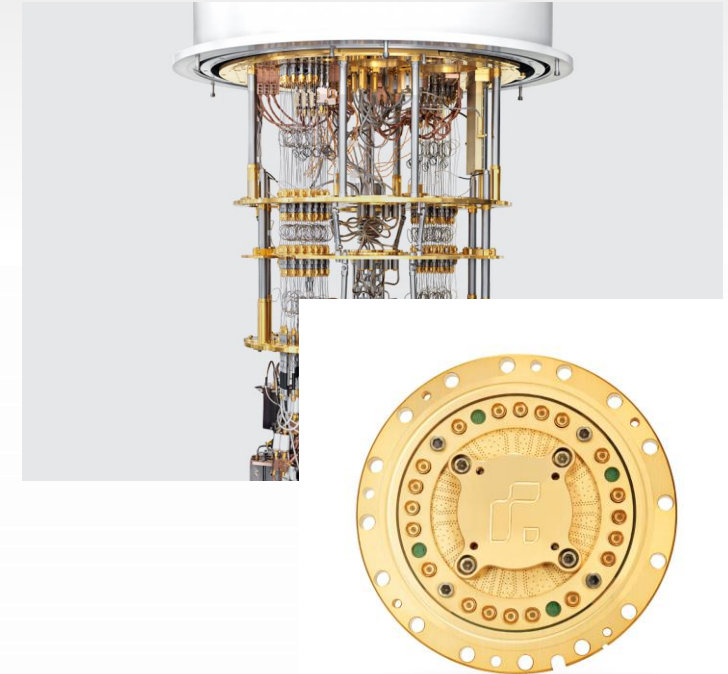
## IBM

- IBM general-purpose gate system provides 53 qubits



## Rigetti

- Rigetti general-purpose gate system provides 31 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.

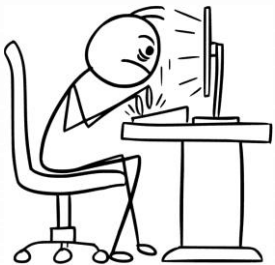
## Evaluate Scientific Quantum Computing Use Cases

- 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

# What are the steps to program access?

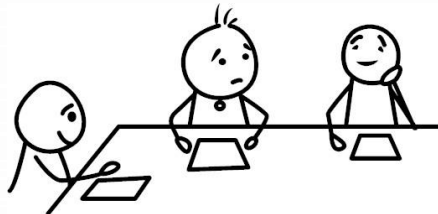
## Project Request

- 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](http://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.



# 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

# 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 21-24 2020**



**TIME** *ET*

08:00 AM - 05:00 PM



**LOCATION**

**ONLINE ONLY**

[www.olcf.ornl.gov/calendar/quantum-computing-user-forum-2020](http://www.olcf.ornl.gov/calendar/quantum-computing-user-forum-2020)

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