OLCF User Meeting

Scientific Computing with Quantum Computers

Travis Humble

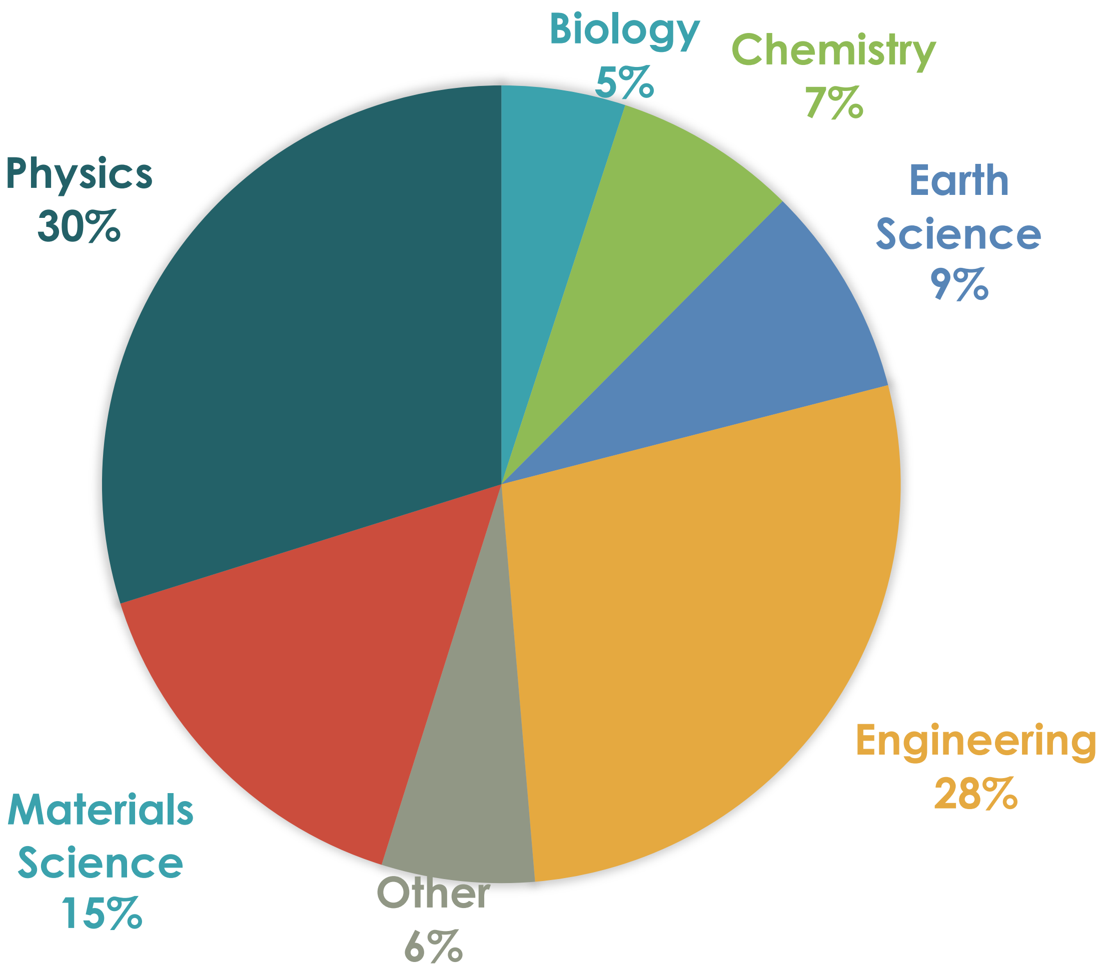
Quantum Computing Institute

Oak Ridge National Laboratory

Oak Ridge National Laboratory


19

Large-Scale Scientific Computing

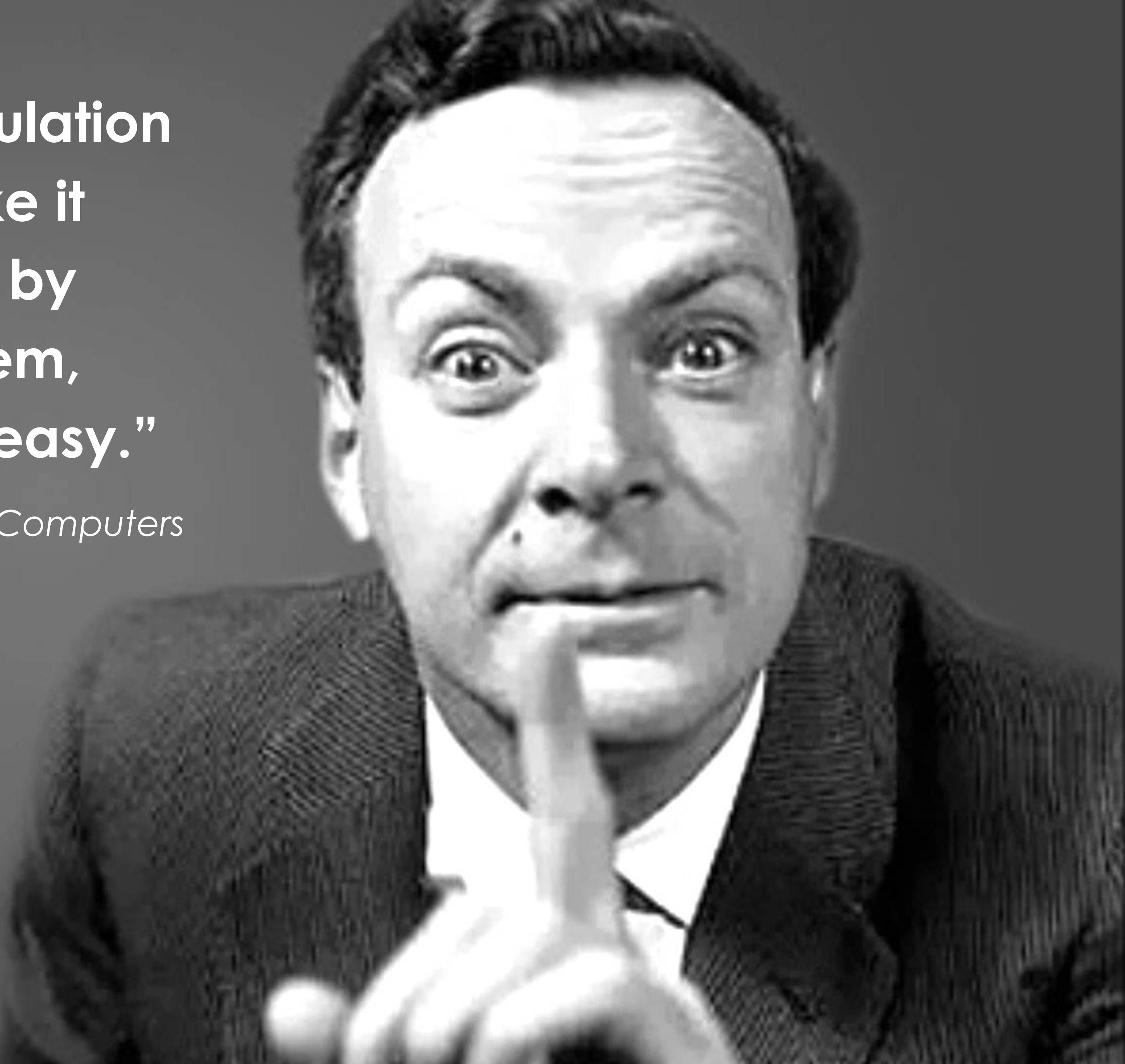


2019 INCITE Allocations by Category

“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*

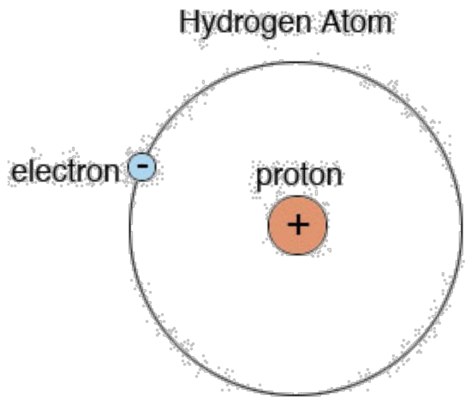
(1982)

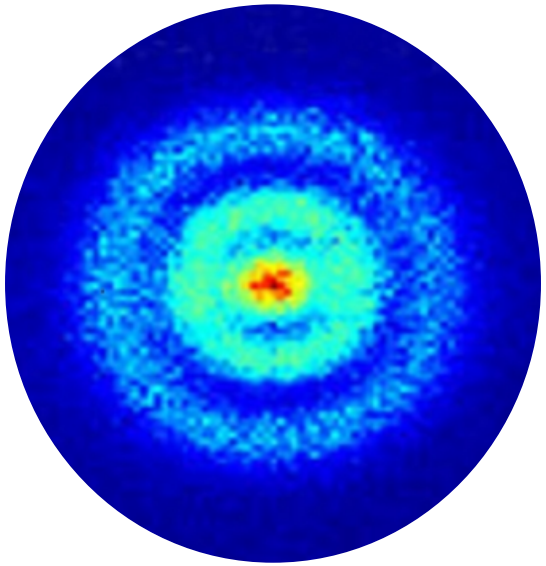


What is Quantum Computing?

- 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

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





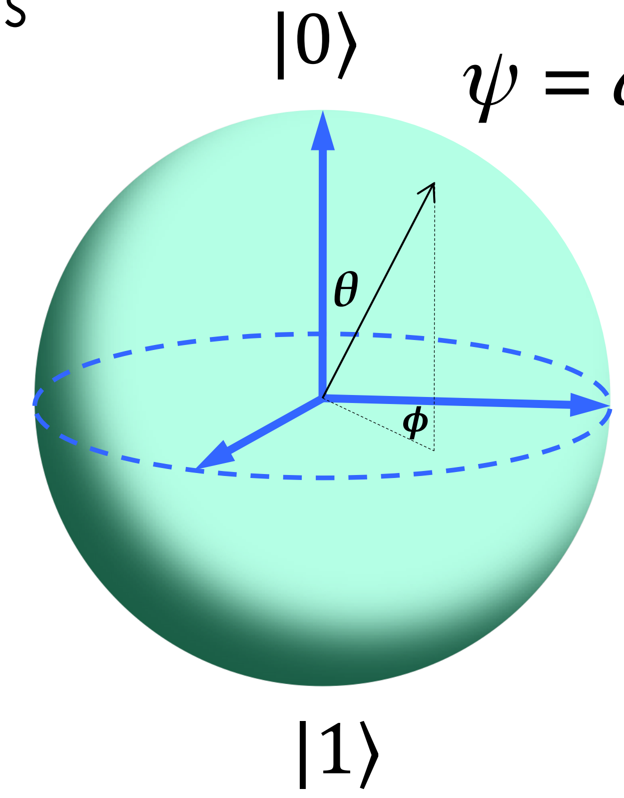
Stodolna et al. PRL 110, 213001 (2013)

Basic Requirements of a Quantum Computer

D. DiVincenzo, “The Physical Implementation of Quantum Computation,” (2000)

- A scalable system of well-characterized qubits
- The ability to initialize qubits in well-defined fiducial states
- A universal set of quantum gates
- Decoherence times much longer than gate operation times
- A qubit-specific measurement capability
- The ability to swap qubit locations
- The ability to move qubits

Qubit



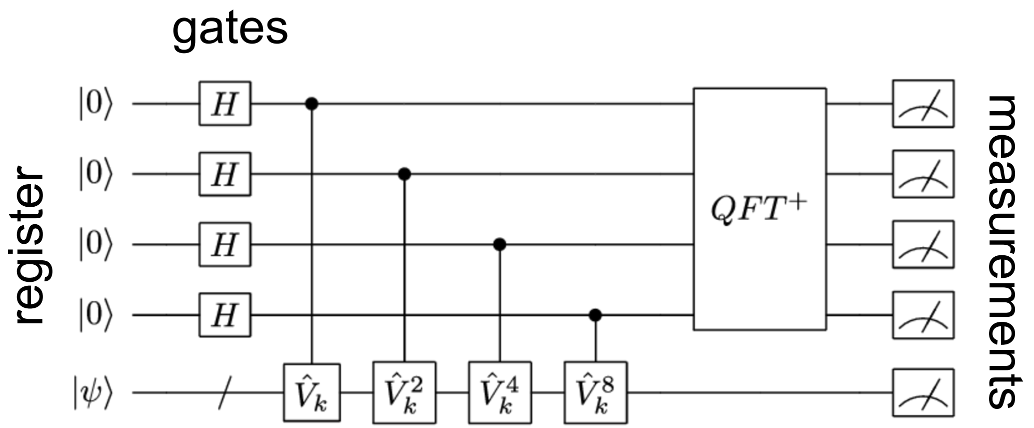
$$\psi = a|0\rangle + b|1\rangle$$

$$a = \cos\theta/2$$

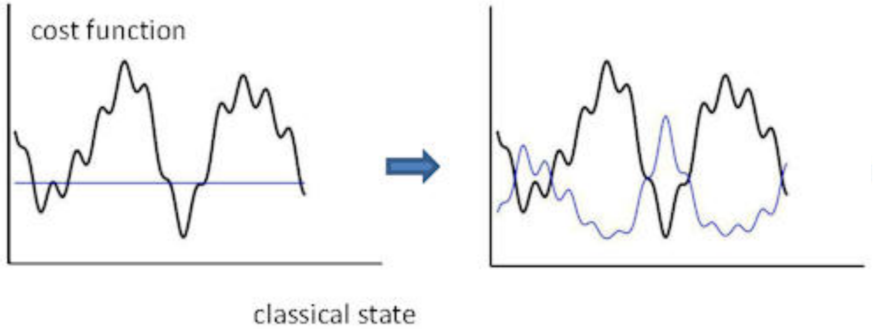
$$b = e^{i\phi}\sin\theta/2$$

Principles of Operation for Quantum Computers

- Prepare a register of qubits in a well-defined initial state
- Apply a sequence of unitary operators, gates, to the register elements
- Measure the register elements and decode the resulting information
- Measurement feedback may guide the next gate choice, required by algorithm
- Operations may be realized using several different computational models
  - Circuit/Gate vs Adiabatic



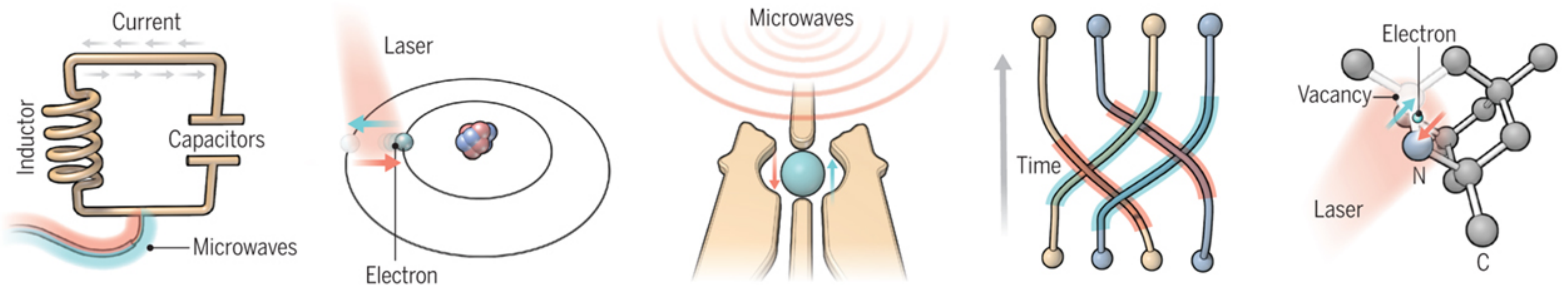
Gate model operations represent discrete sequences of gates acting on a register.



Adiabatic model operations represent continuous-time dynamics applied to a register.

Oak Ridge National Laboratory

A Race for Quantum Technology



Superconducting loops
A resistance-free current oscillates back and forth around a circuit loop. An injected microwave signal excites the current into super-position states.

Trapped ions
Electrically charged atoms, or ions, have quantum energies that depend on the location of electrons. Tuned lasers cool and trap the ions, and put them in superposition states.

Silicon quantum dots
These "artificial atoms" are made by adding an electron to a small piece of pure silicon. Microwaves control the electron's quantum state.

Topological qubits
Quasiparticles can be seen in the behavior of electrons channeled through semi-conductor structures.Their braided paths can encode quantum information.

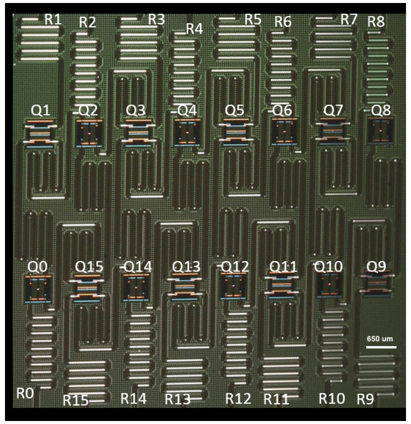
Diamond vacancies
A nitrogen atom and a vacancy add an electron to a diamond lattice. Its quantum spin state, along with those of nearby carbon nuclei, can be controlled with light.

	Superconducting loops	Trapped ions	Silicon quantum dots	Topological qubits	Diamond vacancies
Longevity (seconds)	0.00005	>1000	0.03	N/A	10
Logic success rate	99.4%	99.9%	~99%	N/A	99.2%
Number entangled	20	22	2	N/A	6

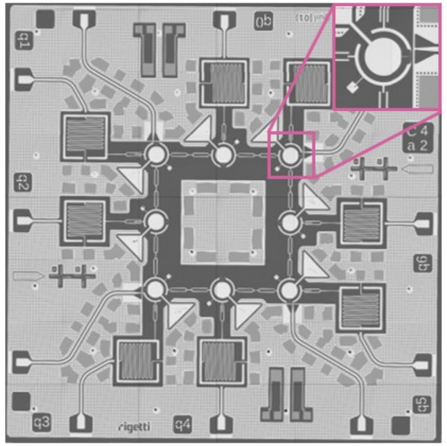
updated

CREDITS: (GRAPHIC) C. BICKEL/*SCIENCE*; (DATA) GABRIEL POPKIN (2016)

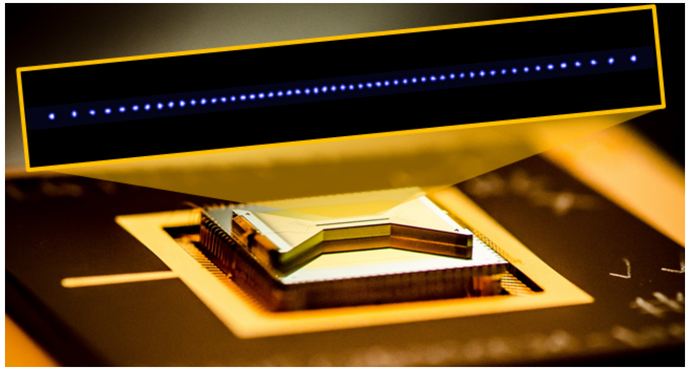
Quantum Processing Units



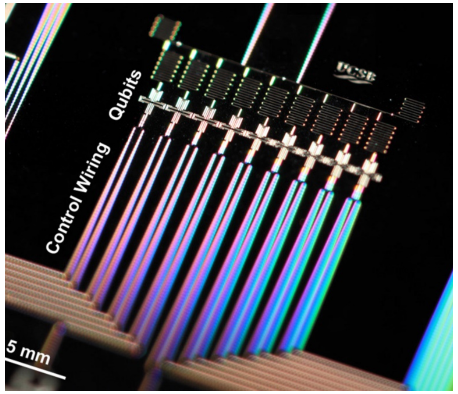
Superconducting chip from IBM



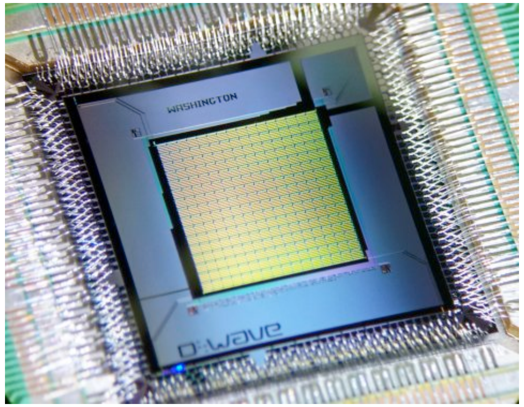
Superconducting chip from Rigetti



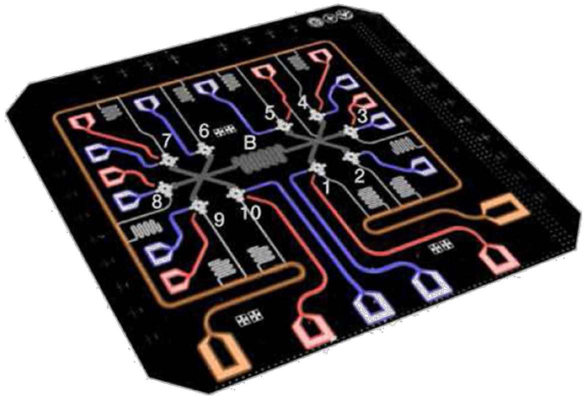
Ion trap chip from ionQ



Superconducting chip from Google



Superconducting chip from D-Wave Systems

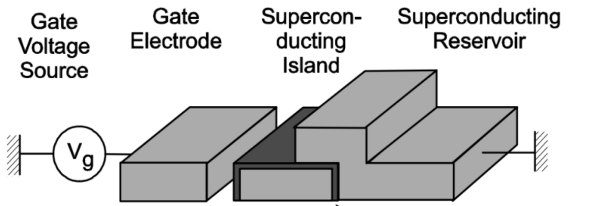


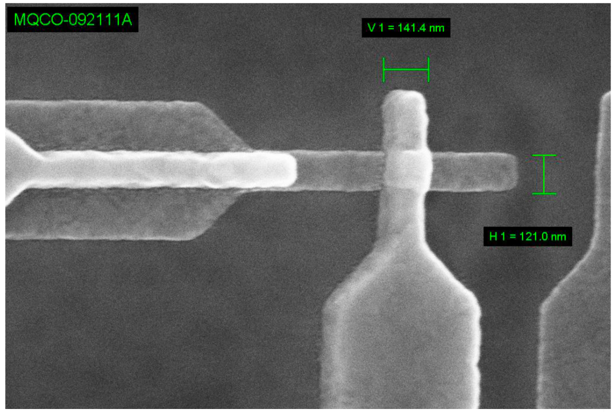
Superconducting chip from USTC

Example: IBM Q System

Materials

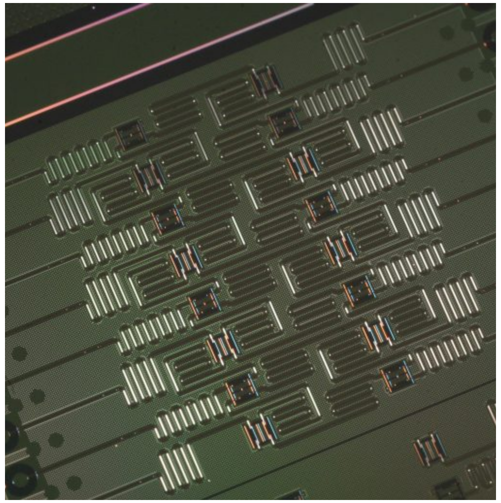
- Transmon qubits encode information in charge states
- Cooper pair electrons coupled by circuit QED resonators





Devices

- Integrated circuit with 20-transmon register
- Coherence, ~100 μs
- Gate pulses ~100 ns
- Gate errors ~1%, measure errors ~5%



Computing

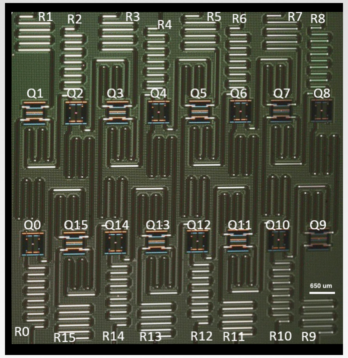
- Cryogenically cooled to ~13mK, isolated
- Signal power ~1 nW

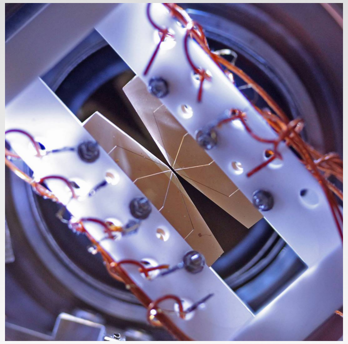
Applications

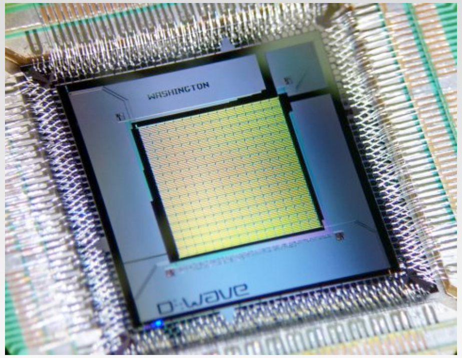
- Cloud-based access

```
import xacc

# Initialize the framework
xacc.Initialize()

# Get the desired QPU and
# allocate some qubits
qpu =
xacc.getAccelerator('ibm')

qubits =
qpu.createBuffer('q',3)

# Define the XACC Kernel
@xacc.qpu(accelerator=qpu)
def teleport(buffer):
  X(0)
  H(1)
  CNOT(1,2)
  CNOT(0,1)
  CNOT(1,2)
  CNOT(2,0)
  Measure(2, 0)

# Use the kernel
teleport(qubits)

# Display the results
print(qubits)

# Finalize the framework
xacc.Finalize()
```

Measuring Quantum Computer Capabilities



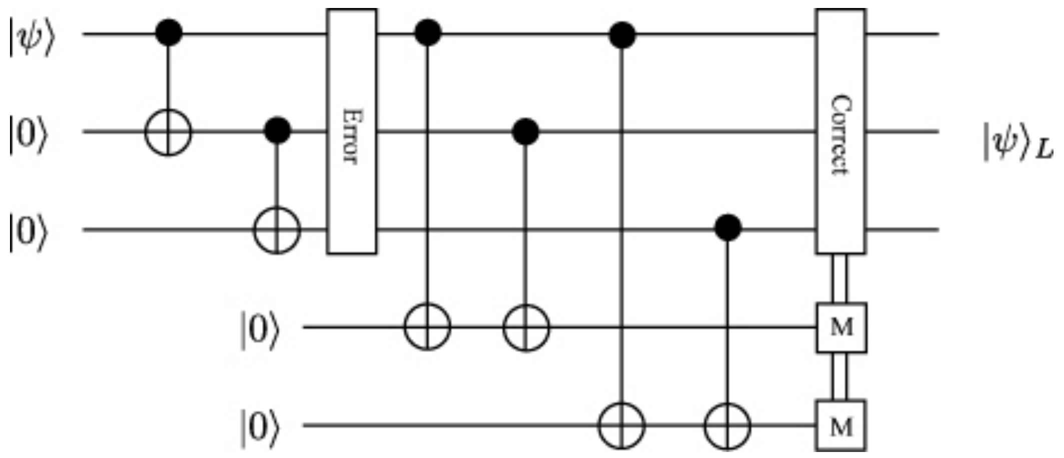


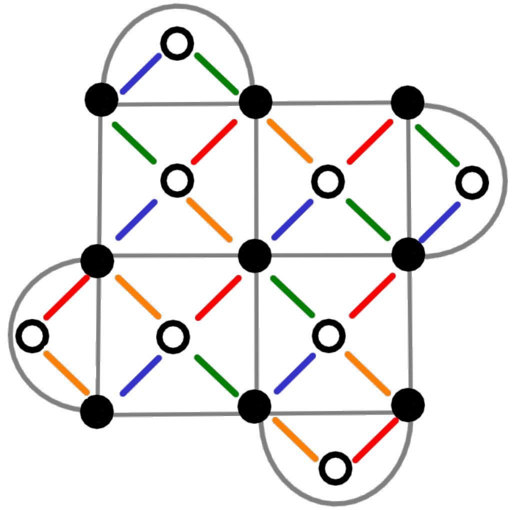


Metrics	IBM	IonQ	D-Wave
Scale of qubits	5-50	5-79	2048
Initialization fidelity	95%	95%	99.9%
Gate set fidelity	99-95%	99-97%	N/A
Duty cycle	400	2,000	10^(-1)
Measurement fidelity	95%	95%	99.9%
Swap fidelity	98%	97%	N/A
Transport fidelity	N/A	N/A	N/A

Fault-tolerant Operation of a Quantum Computer

- The redundant encoding of information can mitigate errors
  - Familiar strategy for classical information
  - Modified for quantum information due to no-cloning theorem
- Fault-tolerant device operation can be established provided:
  - Code is sufficiently large
  - Error rates are sufficiently small
- Current estimates
  - Code size ~100-1000 physical qubits per logical qubit
  - Error rates 10-100x improvements in gates, 100x improvement in coherence time

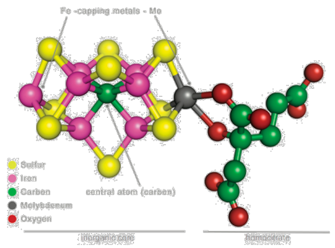


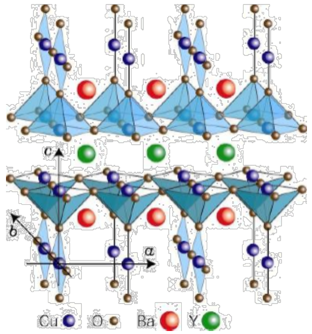


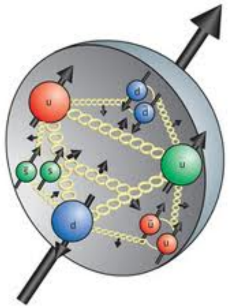
OAK RIDGE National Laboratory

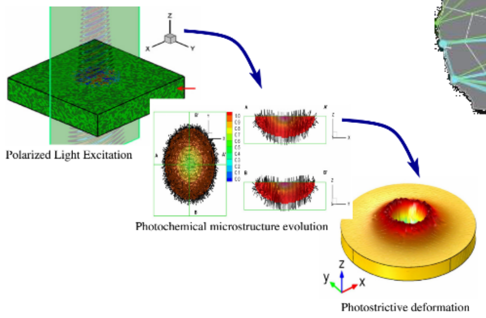
Scientific Applications of Quantum Computing

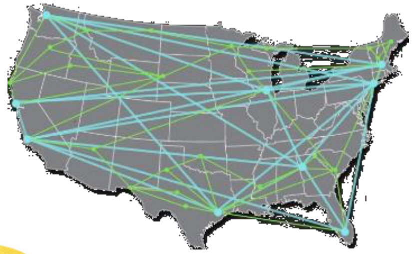
- Algorithms in the quantum computing model have been found to take fewer steps to solve problems
    - Quantum Simulation
    - Partition Functions
    - Discrete Optimization
    - Machine Learning
    - Factoring
    - Unstructured Search
    - Eigensystems
    - Linear Systems
- Several physical 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







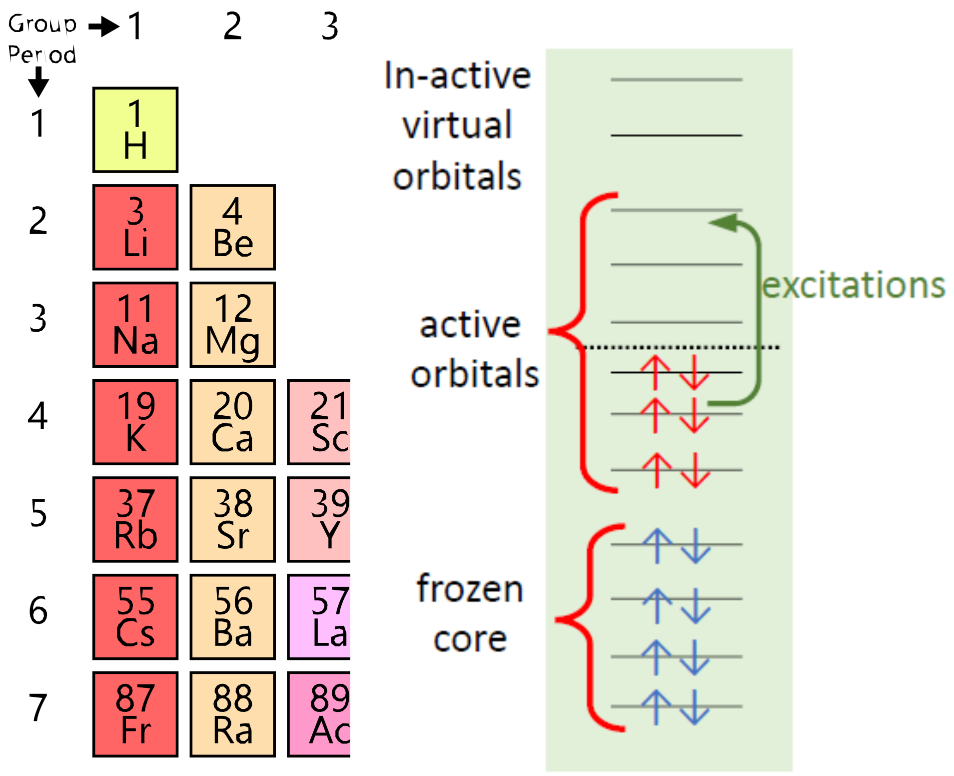




Computational Chemistry with Quantum Computing

A. McCaskey et al. “Quantum Chemistry as a Benchmark for Near-Term Quantum Computers” (2019)

- Quantum mechanics offers a natural representation of chemistry problems
- Electronic structure calculations offer a well-studied series of test cases
- We have created an automated benchmarks suite for metal hydrides
- Tradeoffs in algorithm design and compiler options dominate behavior



Computational Chemistry with Quantum Computers

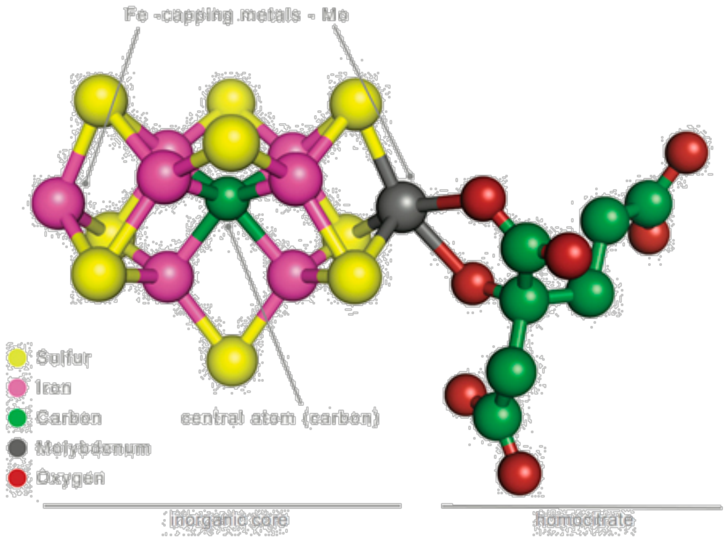
- Unitary evolution of a quantum register under a synthetic Hamiltonian can be decomposed into a sequence of gates using Trotterization.

$$|\Psi(t)\rangle = U(t,t_0)|\Psi(t_0)\rangle \cong \prod_i U_i(t_i,t_{i-1})|\Psi(t_i)\rangle$$

- Phase estimation can probe the eigenenergy, but this is sensitive to noise and approximation errors.

$$QFT^\dagger\, U_c(t,t_0)H^{\otimes n}|\Psi(t_0)\rangle|0\rangle^{\otimes n} \rightarrow \sum_i c_i|\phi_i\rangle|E_i\rangle$$

- Protection against noise is possible but at the expense of significant overhead from fault-tolerant operations using quantum error correction codes.



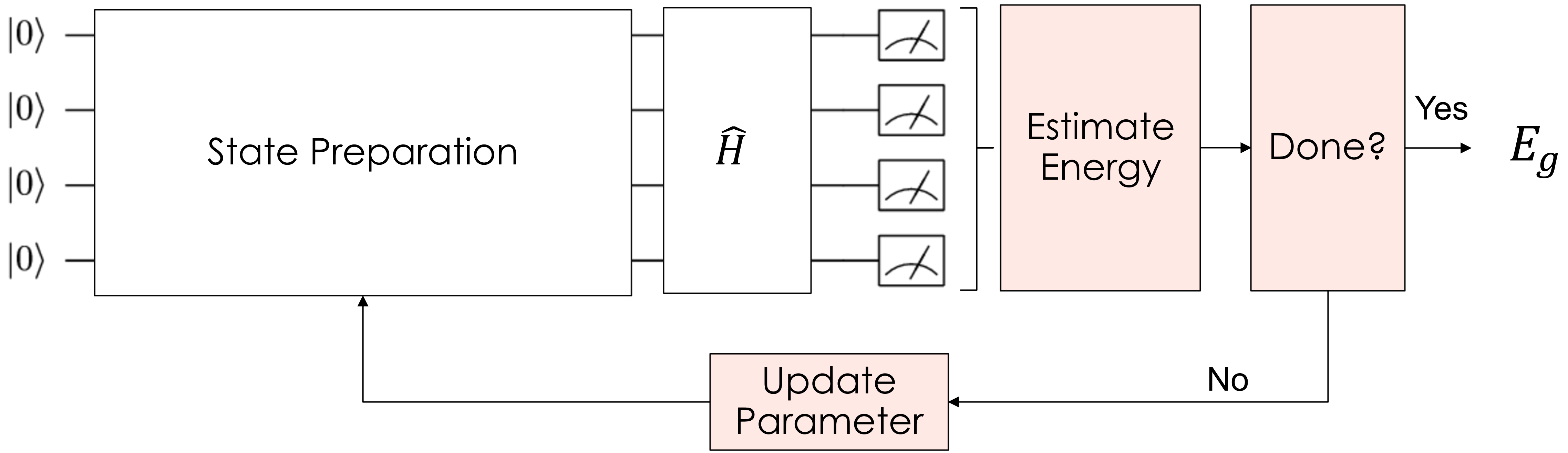
Quantitatively accurate simulation (0.1 mHa)				
Struct. **1**	T-Gates	Clifford Gates	Time	Log. Qubits
Serial	1.1×10^{15}	1.7×10^{15}	130 days	111
Nesting	3.5×10^{15}	5.7×10^{15}	15 days	135
PAR	3.1×10^{16}	3.1×10^{16}	110 hours	1982

M. Reiher et al. “Elucidating reaction mechanisms on quantum computers“ (2017)

Computational Chemistry with Quantum Computers

- A more economical algorithm uses the variational principle, which searches for the quantum state that minimizes the energy defined by the Hamiltonian.

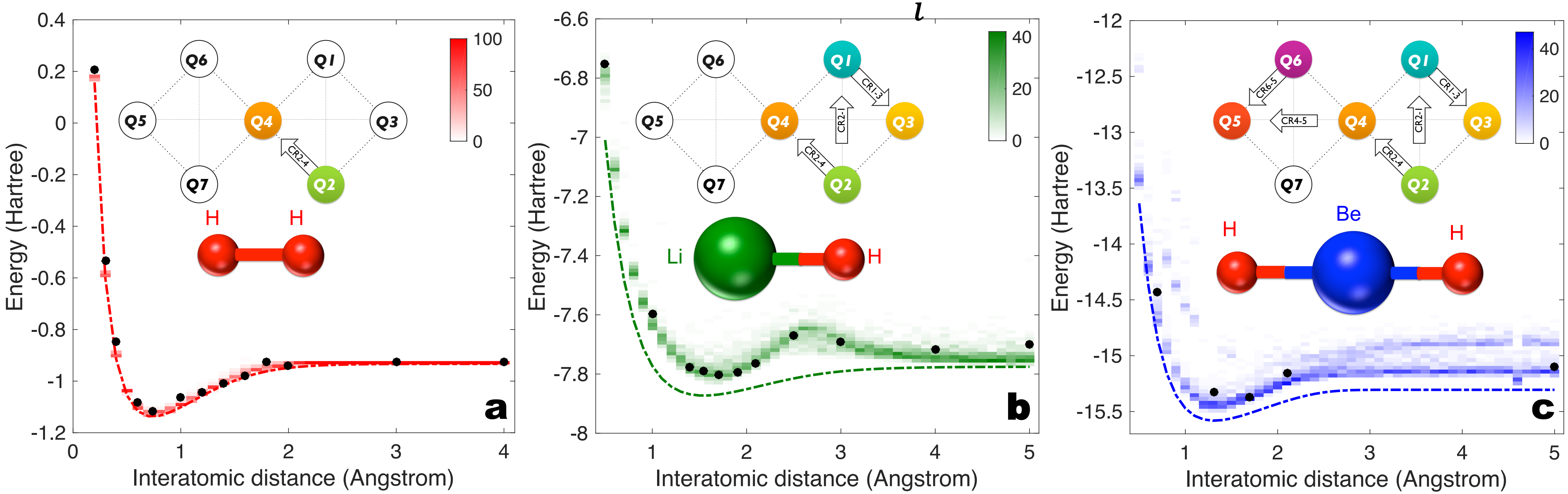
$$\min_{\theta} \langle \Psi(t;\theta) | \hat{H} | \Psi(t;\theta) \rangle \qquad |\Psi(t;\theta_k)\rangle = \prod_i U_i(t_i, t_{i-1}; \theta_k) |\Psi(t_i;\theta_k)\rangle$$



Computational Chemistry with Quantum Computers

- A more economical algorithm uses the variational principle, which searches for the quantum state that minimizes the energy defined by the Hamiltonian.

$$\min_{\theta}\langle \Psi(t;\theta)|\hat{H}|\Psi(t;\theta)\rangle \qquad |\Psi(t;\theta_k)\rangle = \prod_i U_i(t_i, t_{i-1};\theta_k)|\Psi(t_i;\theta_k)\rangle$$

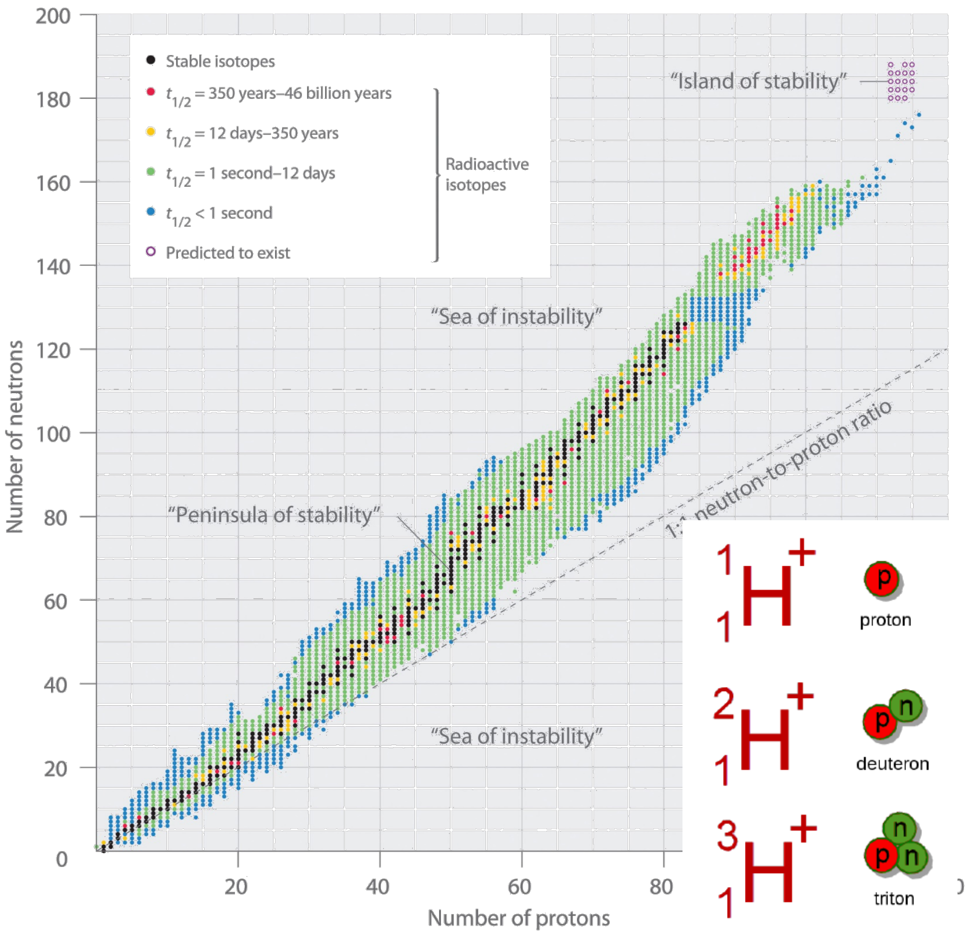


Experimental results (black circles), exact energy surfaces (dotted lines) and density plots of outcomes from numerical simulations, Credit Kandala et al., Nature 549, 242 (2017).

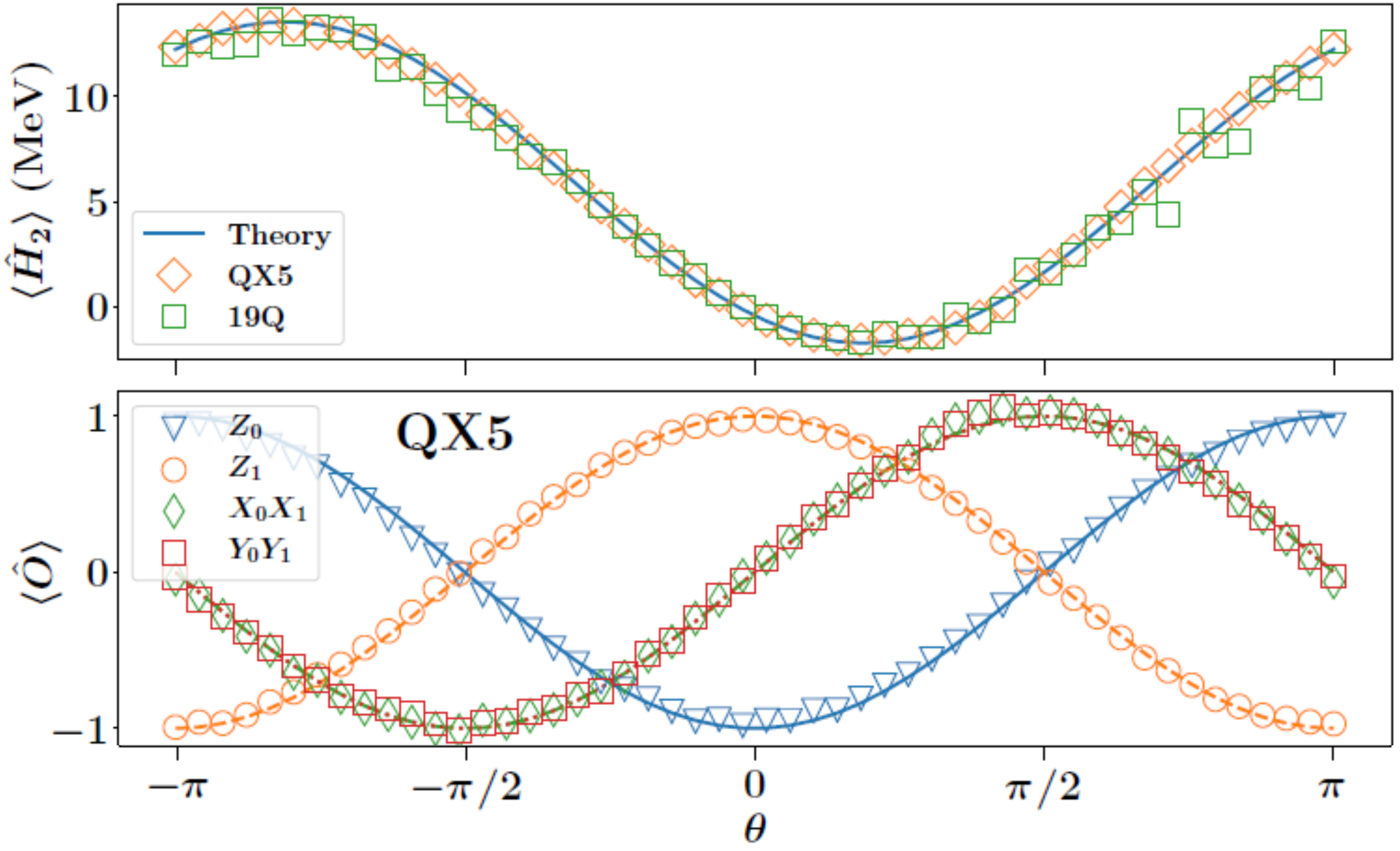
Nuclear Physics with Quantum Computing

E. Dumitrescu et al. “Cloud Quantum Computing of an Atomic Nucleus” (2018)

- Nuclear binding energy determines the stability of nuclear isotopes
- Predicting heavy isotope stability is a quantum many-body problem
- We calculation the binding energy of deuteron, the simplest example with a proton-neutron bound state.



The Binding Energy of Deuteron



Top Panel

- This is the energy estimate of the theta-parameterized state
- Data were taken on two processors, IBM and Rigetti

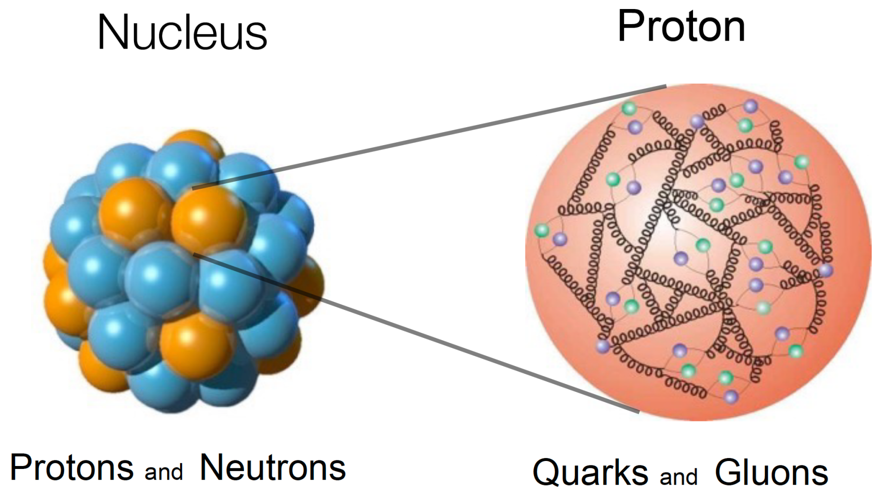
Bottom Panel

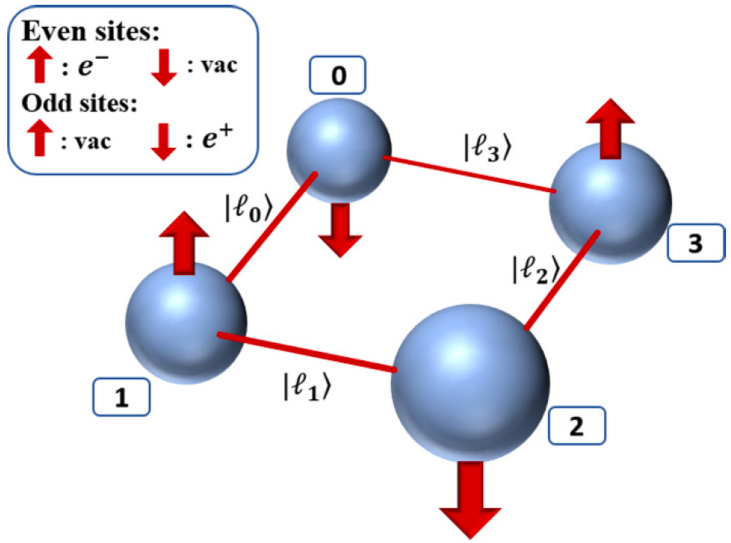
- The weighted sum of these terms gives the energy estimate
- These results yield a binding energy of 2.18 MeV based on fits of Luscher’s formula

High-energy Physics with Quantum Computing

N. Klco et al. “Quantum-classical computation of Schwinger model dynamics using quantum computers” (2018)

- Quantum chromodynamics is a quantum field theory to describe the strong force
- Calculations of low-energy processes are dominated by symmetry breaking dynamics
- We use a simple lattice QCD model to simulate the dynamics of the quantum fields.

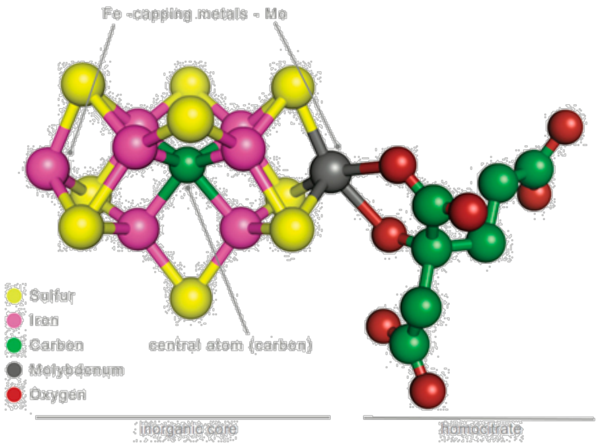




Quantum Computing Use Cases for Scientific Computing

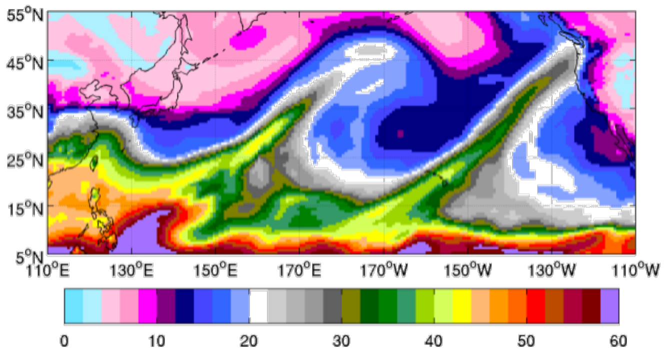
Physical Sciences

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



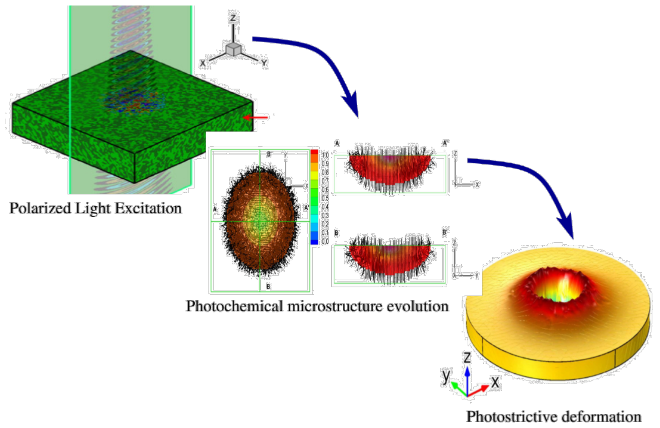
Data Sciences

- Artificial Intelligence, Machine Learning, Inference and Mining



Applied Sciences

- Engineering, Verification and Validation, Energy Sciences



0-3 Years 3-5 Years +10 Years

OAK RIDGE National Laboratory

Quantum Computing User Forum

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

DATE **SPRING 2020**

~~Apr 24 2019 - Apr 25 2019~~

TIME *ET*

08:00 AM - 05:00 PM

LOCATION

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

quantum@ornl.gov

Thank You!

Travis Humble, humblets@ornl.gov