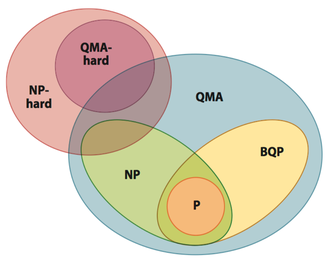
Quantum Computing for Science and Engineering
Programming, Architecture, and Applications

Quantum Computing Paradigms

Quantum Computing (QC) leverages quantum physics to solve problem more efficiently, quickly, and accurately. It redefines feasibility for scientific discovery.

Advantages: Algorithmic Speedups

The power of QC is captured by the BQP complexity class, which contains P but only overlaps NP.

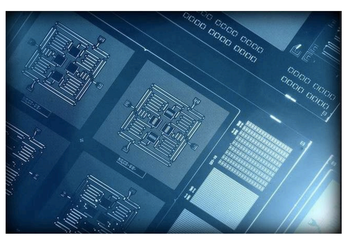


BQP-Complete Problems

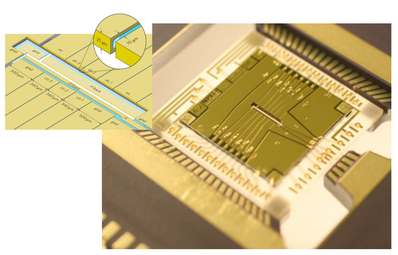
- Quantum Simulation
- Order Finding
- Approximate Jones Polynomial
- Hidden Subgroups
- Potts Model
- Hamiltonian Eigenvalues Sampling
- Phase Estimation Sampling

Challenges: Technological Precision and Scale

Individual atoms, electrons, and photons are the basis for QC technology. System engineering requires precise control and fabrication at the atomic level.



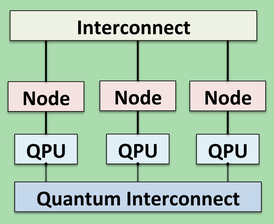
4-qubit superconducting chip
Credit IBM (USA)



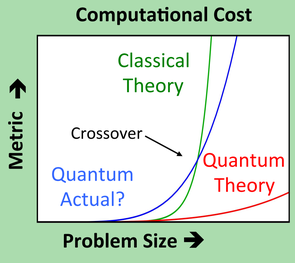
Monolithic 3D trapped ion qubits
Credit National Physical Laboratory (UK)

Quantum Programming Models

Quantum-HPC hybrid systems require programming principles akin to current accelerator models. But how will performance compare to predictions? Performance depends on programming models as well as quantum technology.



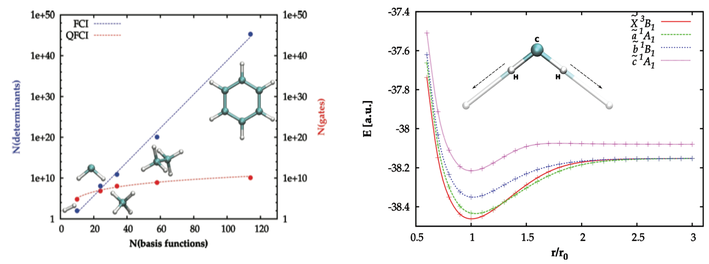
Quality	Absolute	Relative	Quantum
Performance	Time to solution	FLOPS	QOP per sec
Efficiency	Power	FLOP / Watt	QOP / Watt
Cost	Budget	FLOP / Dollar	Qubit / Dollar
Scaling	Size/Time	T1/(N*TN)	Control bottleneck
Portability	Adoption	Lines of code	Lines of code



Scientific Applications

Computational Chemistry and Biology

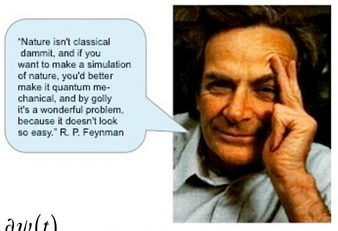
QC exponentially speed-ups ab initio electronic structure calculations and supports studies of molecular reactions, biological interactions, and heavy atoms.



Result using quantum full configuration interaction algorithm (QFCI) for computing electronic structure of CH_2 stretching modes (Veis, 2010).

Modeling and Simulation

QC is a natural venue for the simulation of quantum system, as well as other linear systems, for which there is an exponential speed up relative to classical algorithms.

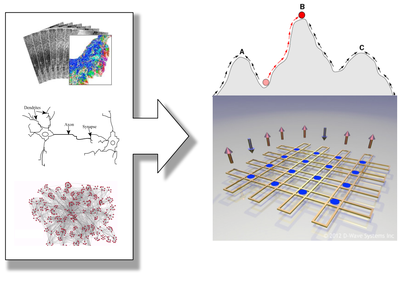


$$i\hbar\frac{\partial\psi(t)}{\partial t} = H(t)\psi(t)$$

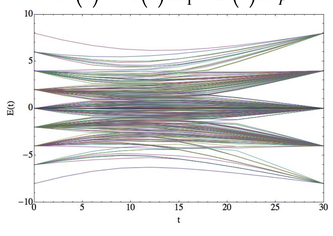
$$\frac{\partial\phi(\mathbf{r},t)}{\partial t} = D\nabla^2\phi(\mathbf{r},t) \qquad L\frac{d^2Q(t)}{dt^2} + R\frac{dQ(t)}{dt} + \frac{Q(t)}{C} = E(t) \qquad \nabla\times\mathbf{H} = \mathbf{J} + \varepsilon\frac{\partial\mathbf{E}}{\partial t}$$

Data Mining and Machine Learning

QC accelerates search and optimization, which are the computational bottlenecks for many applications.



$$H(t) = A(t)H_1 + B(t)H_P$$



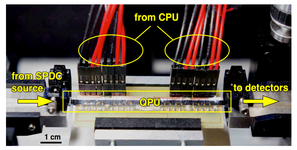
Additional Applications

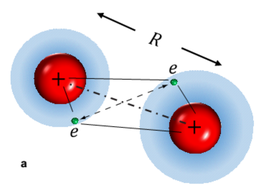
Network Flows, Quantum Field Theories, Graph Theoretic Analysis, Partition Functions, Reaction Rates, Curve Fitting, String Rewriting, Matrix Powers, Graph Collisions, Riemann Zeta Functions, Hidden Legendre Symbols, Pell's Equation, and many many more.

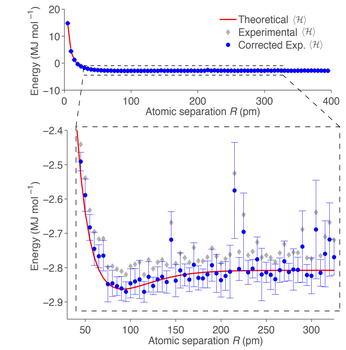
Recent Results

Quantum Chemistry Calculations

A quantum calculation of the He^+-H potential surface carried out in 2013 had chemical accuracy. The hybrid algorithm takes the results of a quantum chip as input to a classical variational eigensolver (Peruzzo et al. 2013). Follow up experiments using NV diamond were able to recover excited state spectrum (Wang et al., 2014)

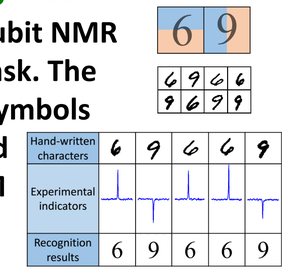






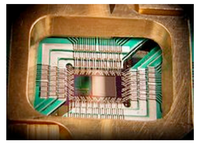
Quantum Artificial Intelligence

In 2014, USTC used a four-qubit NMR computer to solve an OCR task. The computer first learned the symbols '6' and '9' and then classified variants using quantum SVM (Li et al. 2014).



Protein Folding

Low-energy configurations of a six-unit protein were found using the Miyazawa-Jernigan potential and a quantum optimization algorithm in 2012. Calculations with a D-Wave *Rainier* recovered (Perdomo et al. 2012).



ORNL Quantum Computing Institute

QCI serves as the interaction point for CCSD resources in quantum computing. We have a broad emphasis on theory, computation, and experiment for the research and development of quantum computing systems.

Travis Humble
humblets@ornl.gov