QC WARE

Q2B

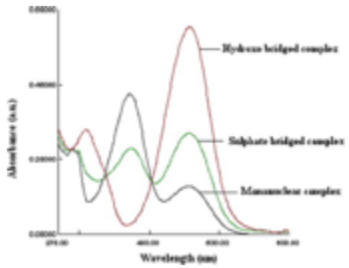
2017

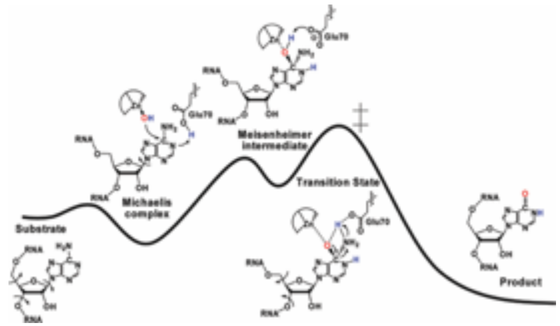
BERKELEY LAB
Bringing Science Solutions to the World

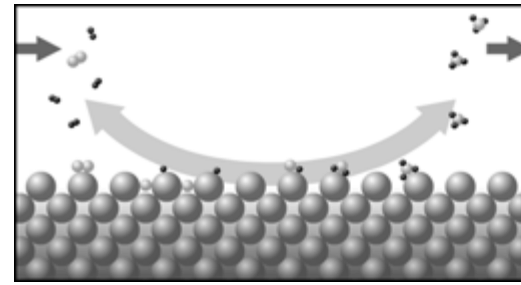
Enabling Scientific Discovery in Chemical Sciences on Quantum Computers

Bert de Jong wadejong@lbl.gov

Why quantum chemistry on quantum computers?

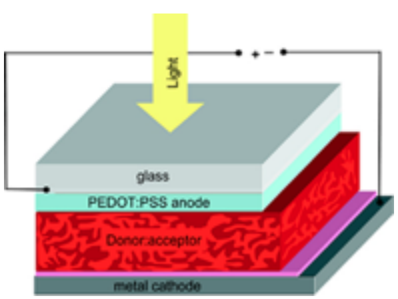


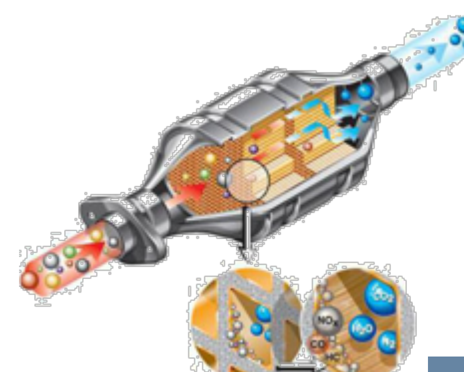




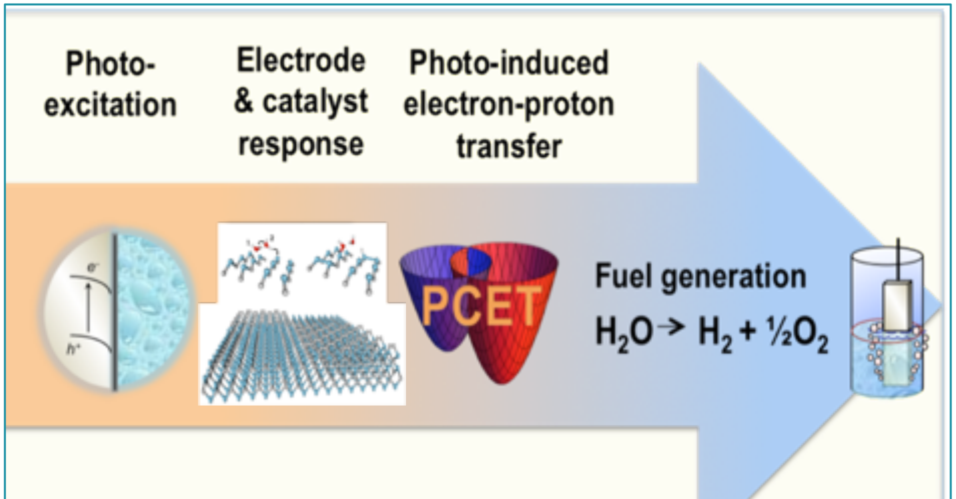
Understanding

Control





Quantum simulation to discover guiding principles for catalytic activity



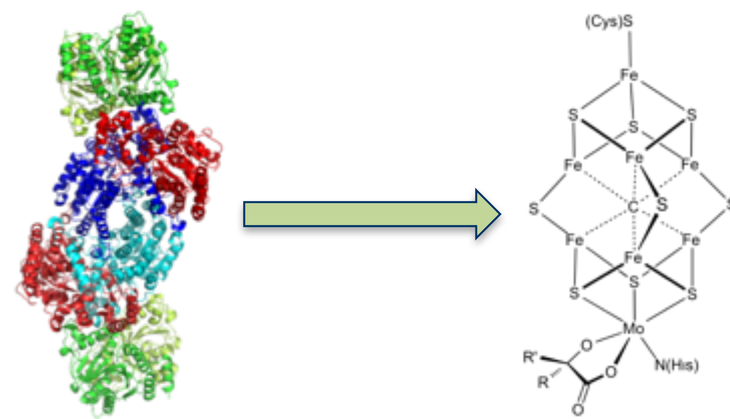
From Galli, University of Chicago

Photo-induced catalysis of water

Nitrogenase enzyme

$$N_2 + 3\ H_2 \rightarrow 2\ NH_3$$

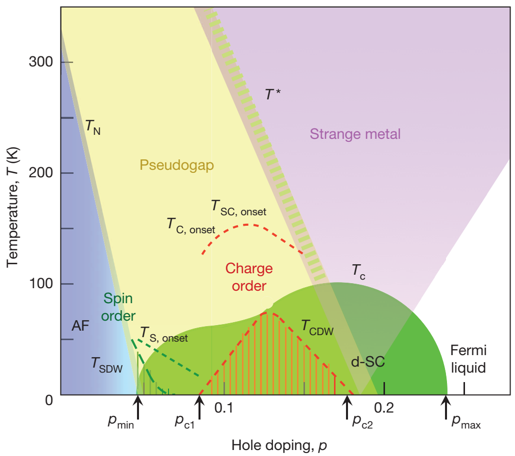
“FeMoco”



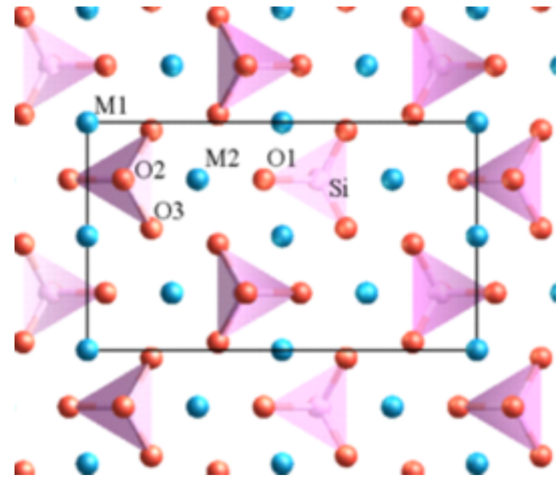
Nature’s answer to Haber Process

Quantum Mechanically: ~100 ideal qubits for solution

Electron correlation in materials drives many technologies



Taken from Keimer et al., Nature 2015

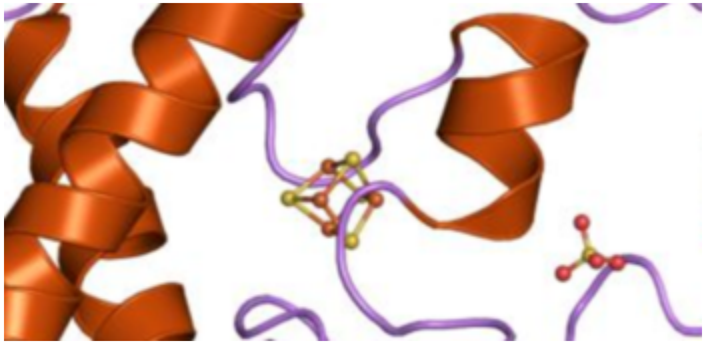


Superconductivity in MRI magnets and wires for current transmission

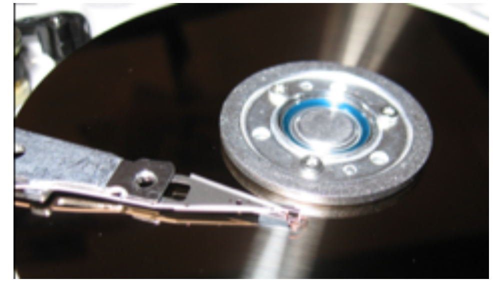
Strongly correlated materials are used in battery materials

These solids are very difficult to calculate with classical computers

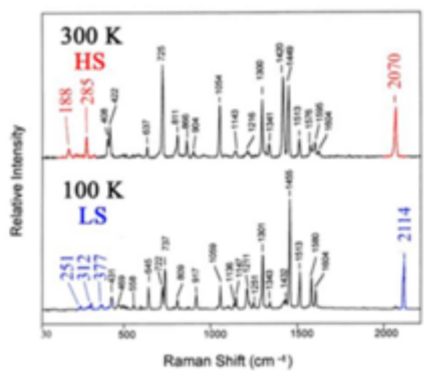
Electron correlation ubiquitous in biology and chemistry



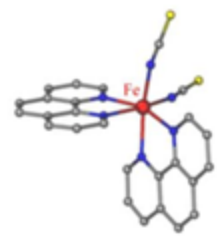
FeS enzymatic active center



Molecular magnets used in hard drive coating



$Fe^{II}(phen)_2(NCS)_2$



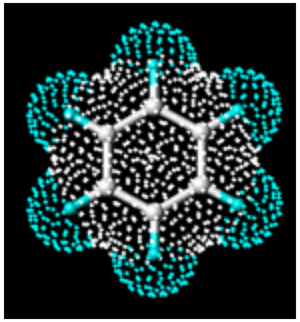
Spin-crossover and molecular switches

These molecules are a challenge to calculate with classical computers

Electron correlation problem in quantum chemistry

The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble.

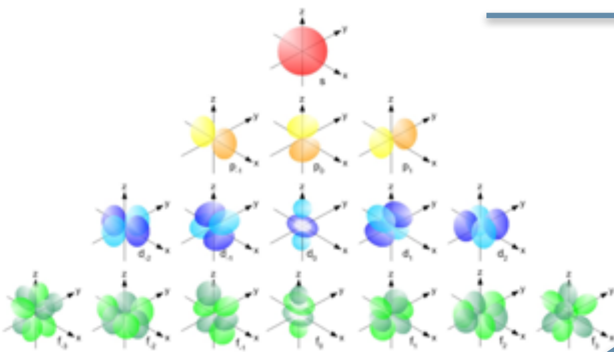
-Paul Dirac



↔

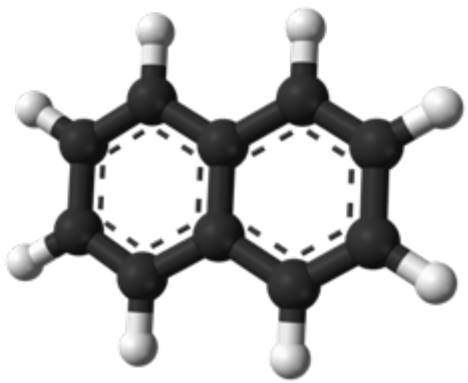
$$\mathcal{H} \left|\psi\right\rangle = E \left|\psi\right\rangle$$

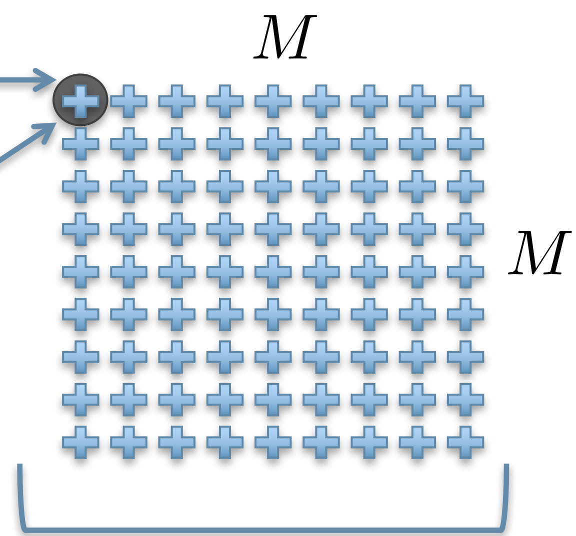
Solving quantum chemistry: An exponential problem



$$D = M^N$$

$$M = 100$$
$$N = 80$$





$$D = 100^{80} = 10^{160}$$

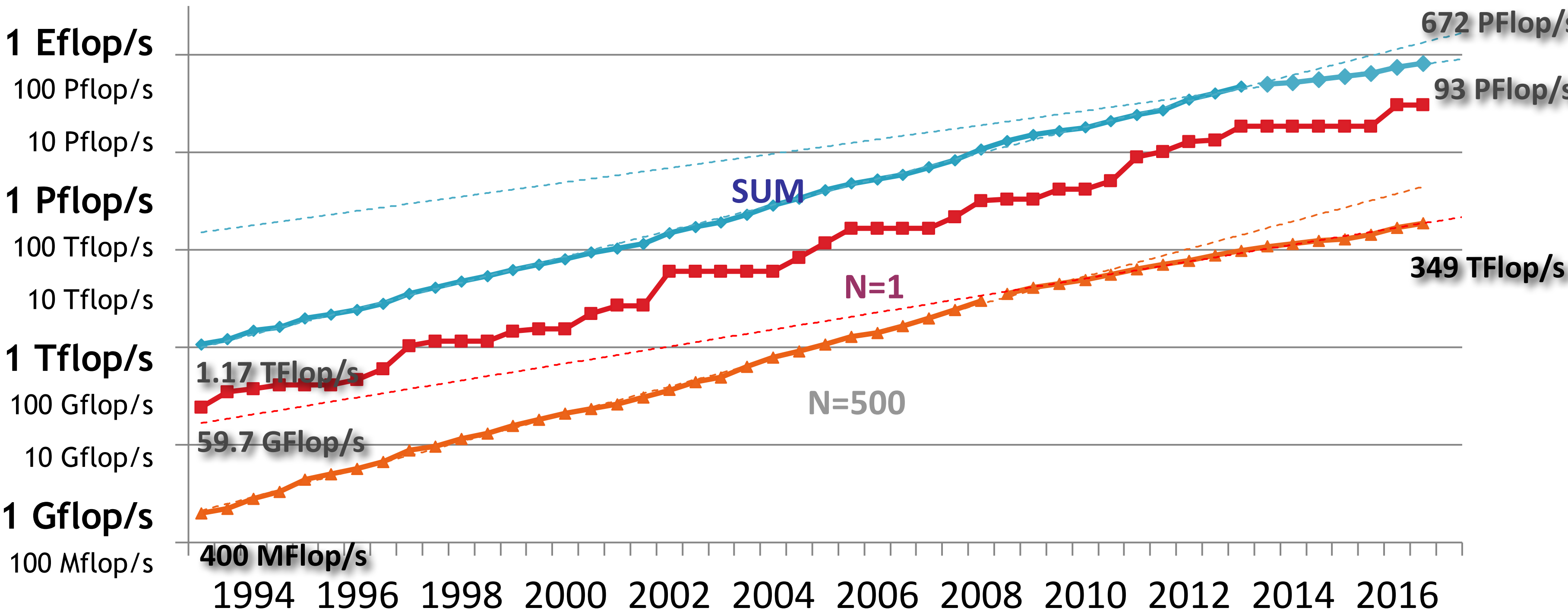
Electrons:

$$D = \begin{pmatrix} M \\ N_\alpha \end{pmatrix} \begin{pmatrix} M \\ N_\beta \end{pmatrix}$$

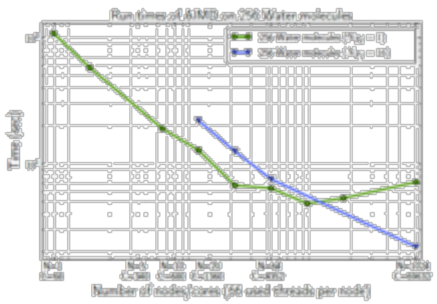
One mole
10^{23}

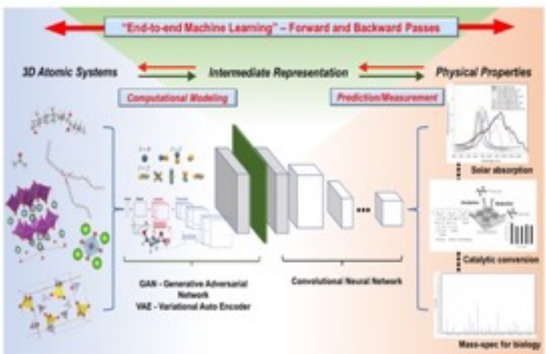
Particles in universe
10^{80}

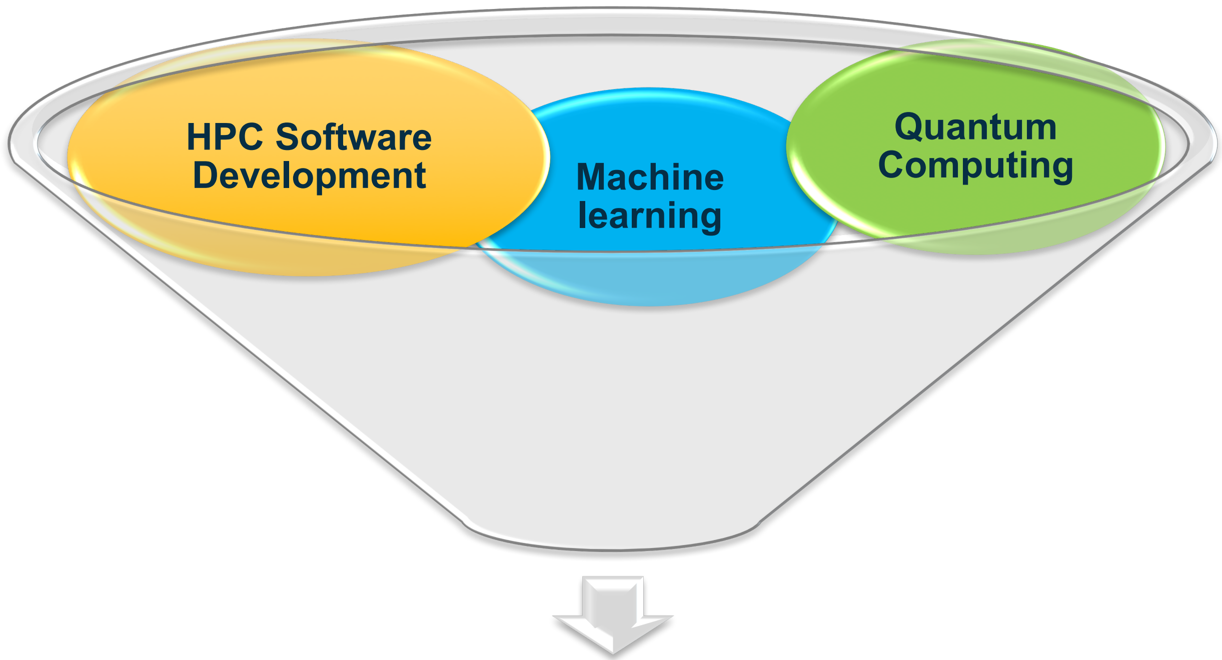
An exaflop in 2021 gives us only a factor of 10 performance…



Expanding toolset for chemical sciences







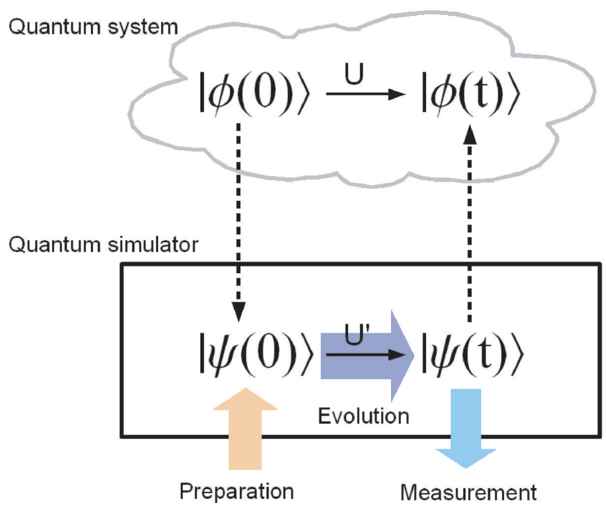
Discovery of new materials, molecular systems and pathways

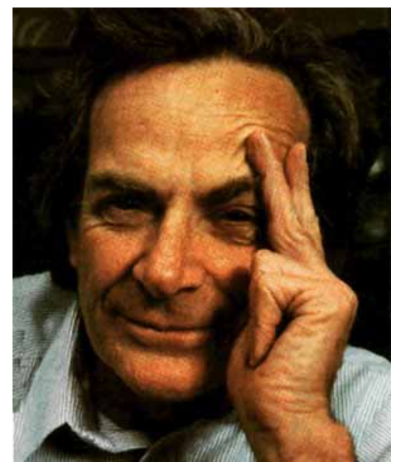
Machine learning in chemistry and materials for discovery

Quantum computing to tackle exponential complexity

Quantum chemistry on quantum computers

Simulating evolution of a quantum system on a classical computer in an efficient way is impossible (Feynman, 1982)





Feynman proposed idea of universal quantum simulators

Quantum chemistry and quantum computers are a great match

Quantum simulations on quantum computers can revolutionize the field of computational chemistry

- Theory and algorithmic work since 2000
- First demonstration in 2010

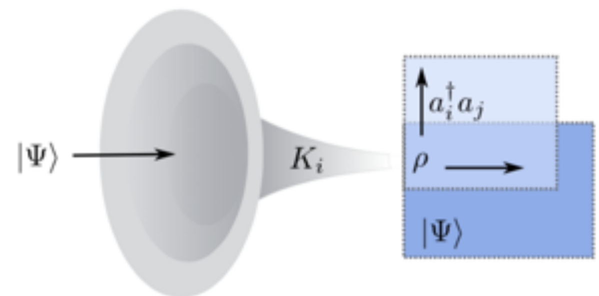
Classical: Exponential cost vs Quantum: Polynomial cost

Aspuru-Guzik, Dutoi, Love, Head-Gordon, *Science* 309, 1704–1707 (2005).

Algorithms for chemistry evolving rapidly

Benefits of interdisciplinary collaboration

Year	Reference	Representation	Algorithm	Time Step Depth	Coherent Repetitions	Total Depth
2005	Aspuru-Guzik et al. [1]	JW Gaussians	Trotter	$\mathcal{O}(\text{poly}(N))$	$\mathcal{O}(\text{poly}(N))$	$\mathcal{O}(\text{poly}(N))$
2010	Whitfield et al. [2]	JW Gaussians	Trotter	$\mathcal{O}(N^5)$	$\mathcal{O}(\text{poly}(N))$	$\mathcal{O}(\text{poly}(N))$
2012	Seeley et al. [3]	BK Gaussians	Trotter	$\widetilde{\mathcal{O}}(N^4)$	$\mathcal{O}(\text{poly}(N))$	$\mathcal{O}(\text{poly}(N))$
2013	Perruzzo et al. [4]	JW Gaussians	UCC	Variational	Variational	$\mathcal{O}(\text{poly}(N))$
2013	Toloui et al. [5]	CI Gaussians	Trotter	$\mathcal{O}(\eta^2 N^2)$	$\mathcal{O}(\text{poly}(N))$	$\mathcal{O}(\text{poly}(N))$
2013	Wecker et al. [6]	JW Gaussians	Trotter	$\mathcal{O}(N^5)$	$\mathcal{O}(N^6)$	$\mathcal{O}(N^{11})$
2014	Hastings et al. [7]	JW Gaussians	Trotter	$\mathcal{O}(N^4)$	$\mathcal{O}(N^4)$	$\mathcal{O}(N^8)$
2014	Poulin et al. [8]	JW Gaussians	Trotter	$\mathcal{O}(N^4)$	$\sim N^2$	$\sim N^6$
2014	McClean et al. [9]	JW Gaussians	Trotter	$\sim N^2$	$\mathcal{O}(N^4)$	$\sim N^6$
2014	Babbush et al. [10]	JW Gaussians	Trotter	$\mathcal{O}(N^4)$	$\sim N$	$\sim N^5$
2015	Babbush et al. [11]	JW Gaussians	Taylor	$\widetilde{\mathcal{O}}(N)$	$\widetilde{\mathcal{O}}(N^4)$	$\widetilde{\mathcal{O}}(N^5)$
2015	Babbush et al. [12]	CI Gaussians	Taylor	$\widetilde{\mathcal{O}}(N)$	$\widetilde{\mathcal{O}}(\eta^2 N^2)$	$\widetilde{\mathcal{O}}(\eta^2 N^3)$
2015	Wecker et al. [13]	JW Gaussians	UCC	Variational	Variational	$\mathcal{O}(N^4)$
2016	McClean et al. [14]	BK Gaussians	UCC	Variational	Variational	$\mathcal{O}(\eta^2 N^2)$
2017	Babbush et al. [15]	JW Plane Waves	Trotter	$\mathcal{O}(N)$	$\mathcal{O}(\eta^{1.83} N^{0.67})$	$\mathcal{O}(\eta^{1.83} N^{1.67})$
2017	Babbush et al. [15]	JW Plane Waves	Taylor	$\widetilde{\mathcal{O}}(1)$	$\widetilde{\mathcal{O}}(N^{2.67})$	$\widetilde{\mathcal{O}}(N^{2.67})$
2017	Babbush et al. [15]	JW Plane Waves	TASP	Variational	Variational	$\mathcal{O}(N)$



Quantum Subspace expansion to allow for simulation of excited state and error mitigation

Bounding computational complexity ever more tightly, from O(N^{11}) in 2013 to O(N^3)-O(N) in 2017
Source: McClean & Babbush (Google)

Adapting algorithms to achieve useful accuracy with imperfect qubits

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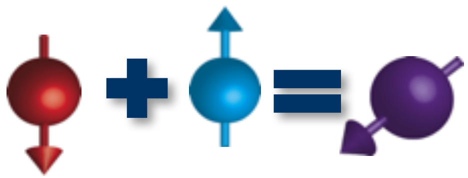
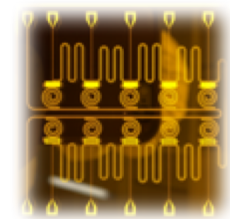
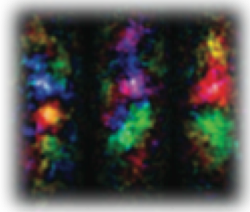
Diverse qubits and quantum hardware available



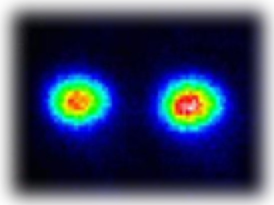
ELECTRONS
SPIN UP + SPIN DOWN



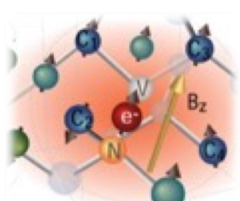
CIRCUITS



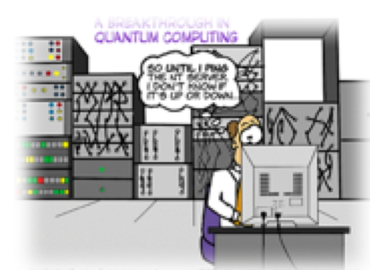
ATOMS



IONS



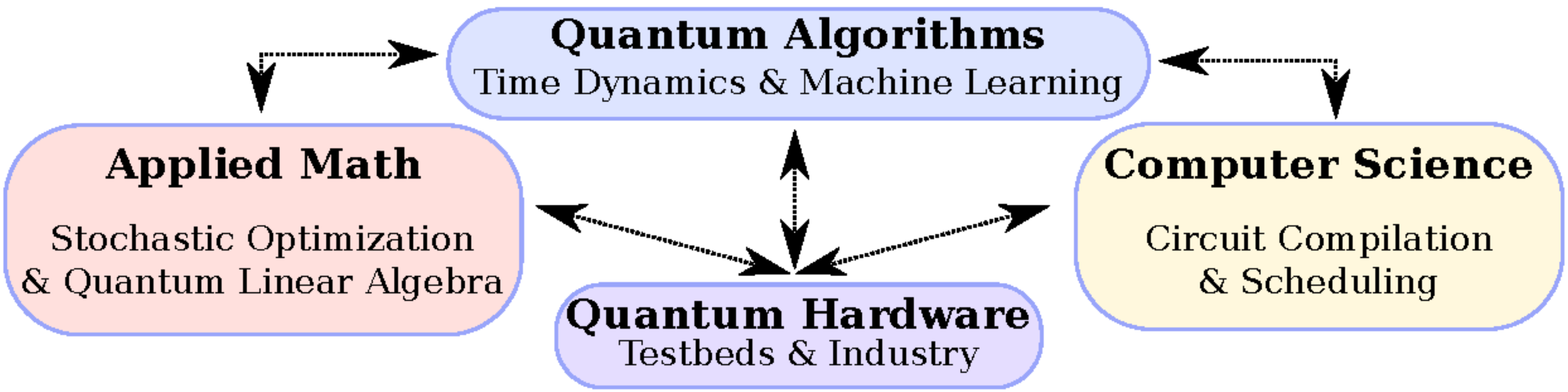
SOLID STATE



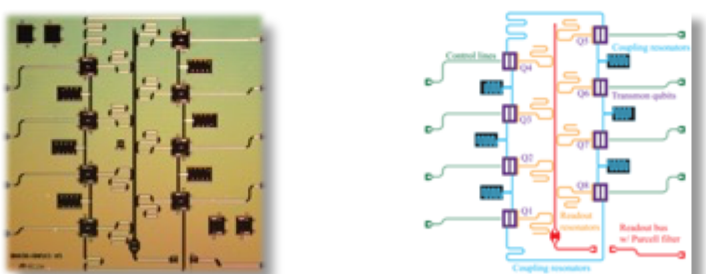
D-Wave The Quantum Computing Company
IBM
Google
rigetti
IONQ

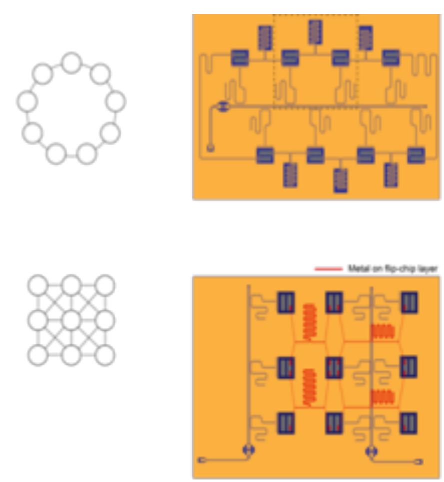
Quantum computing at Berkeley Laboratory

Entanglement between disciplines



QAT – de Jong





- 8-Qubit ring topology with nearest-neighbor coupling
- Independent control and simultaneous readout
- Measured lifetimes (T_2) consistently > 60 ms

AQuES Testbed – Carter

Collaboration with Quantum Nanoelectronics Lab at UC Berkeley

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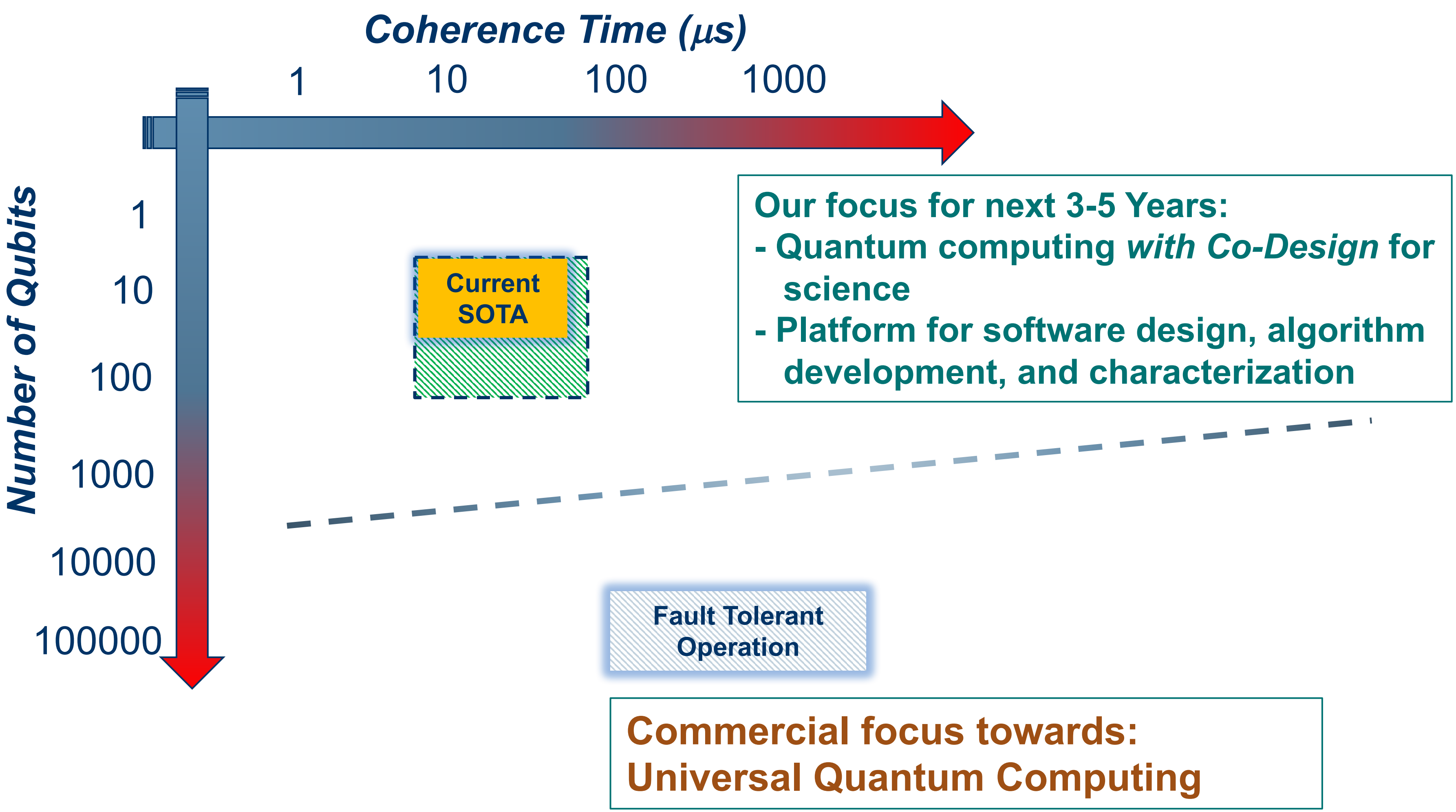
Berkeley Laboratory testbed roadmap



Tradeoffs in quantum computation for scientific discovery

Prep $|\psi\rangle$ → Evolution → Measurement → $\{|\Psi_i\rangle\,,E_i\}$

Coherence Time & Fidelity

- Robust control & stable qubits
- Algorithm timescale problem

Number of Qubits

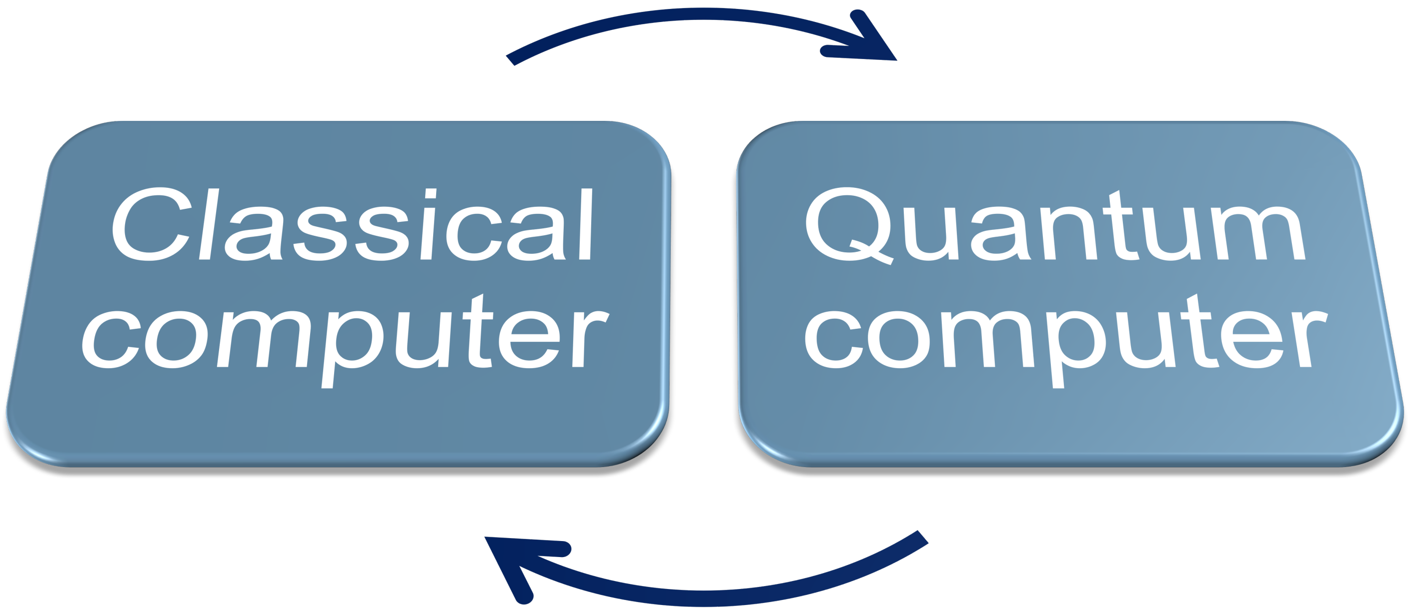
Information Extraction

- Translate input/output
- Full readout loses advantage

Tradeoffs in generality, coherence time, operation speed

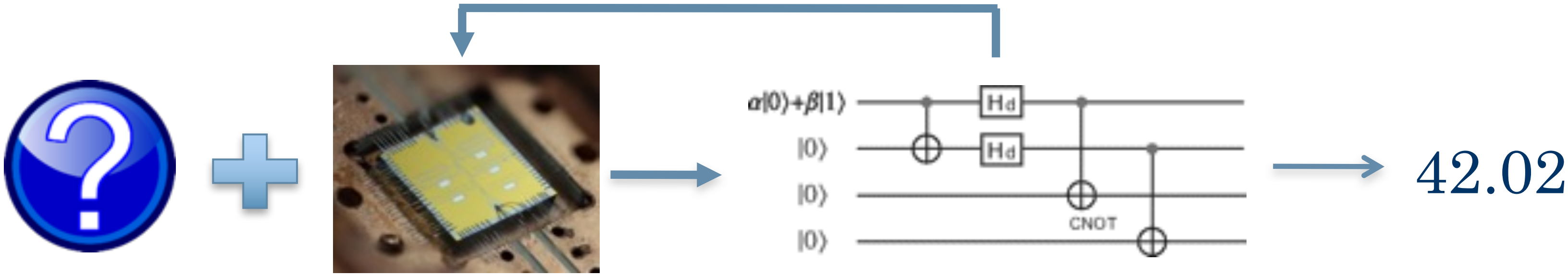
Physical Qubit errors > 10^{-4}
Classical Bit errors < 10^{-10}

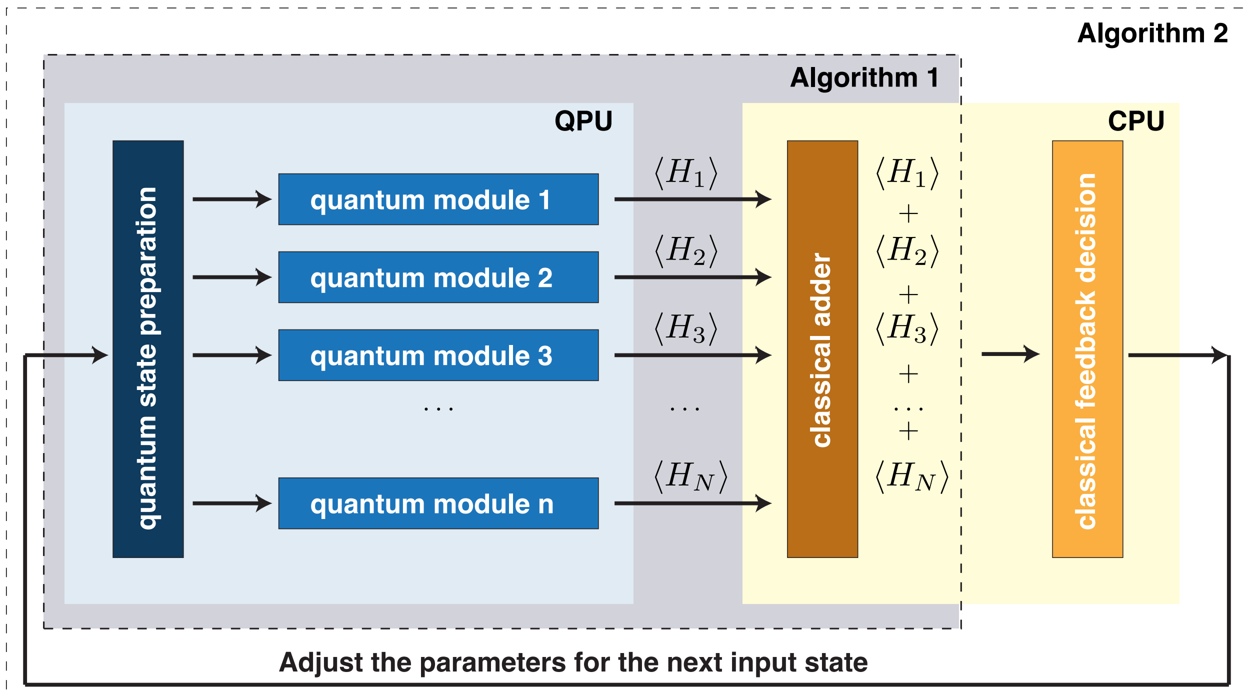
Hybrid approaches to use strength of all available tools



Can circumvent coherence time and compute errors

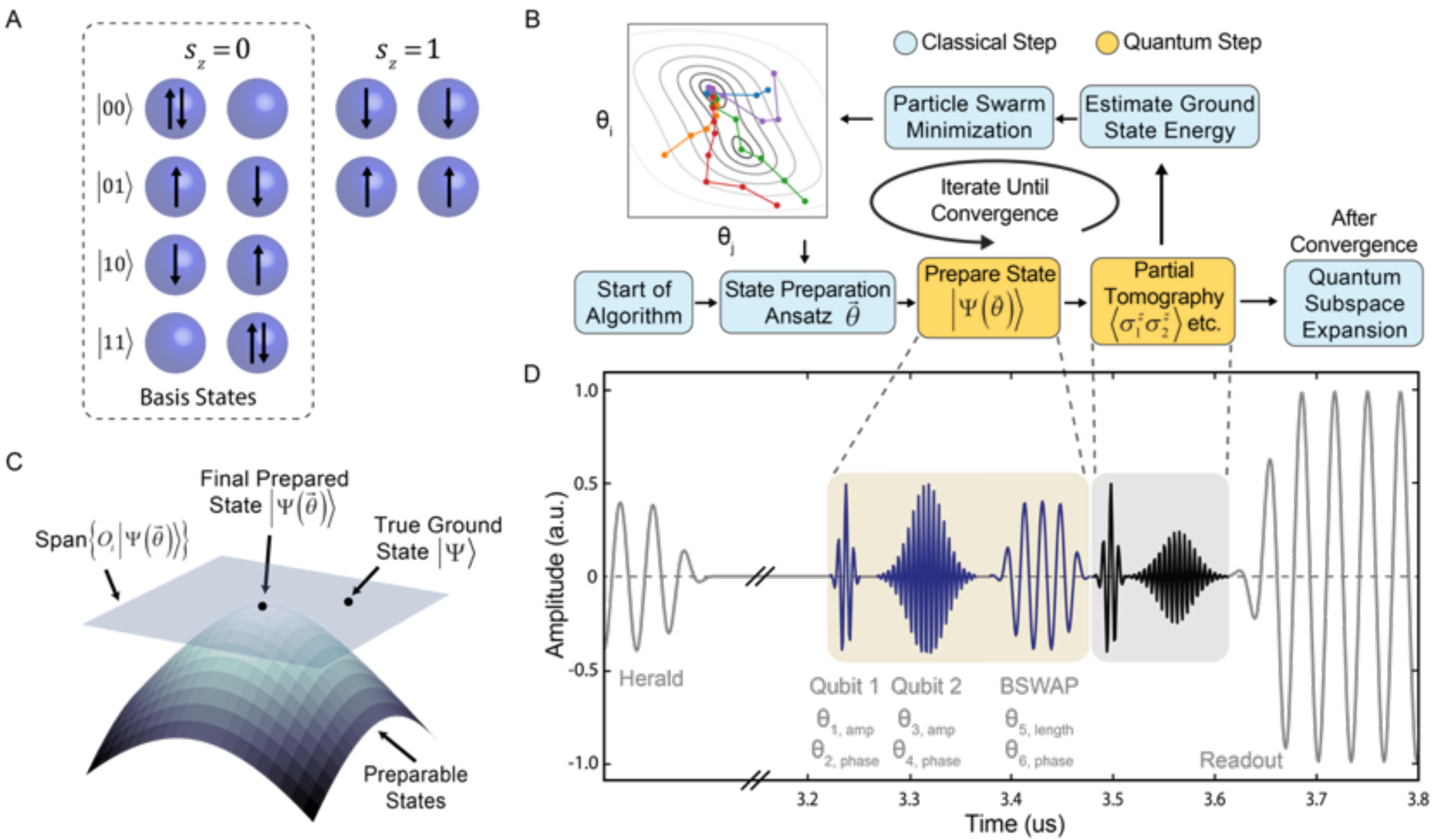
Variational Quantum Eigensolver (VQE)





A Variational Eigenvalue Solver On A Photonic Quantum Processor
Peruzzo†, **McClean†**, Shadbolt, Yung, Zhou, Love, Aspuru-Guzik, O'Brien († Equal Contribution by authors)
Nature Communications (2014)

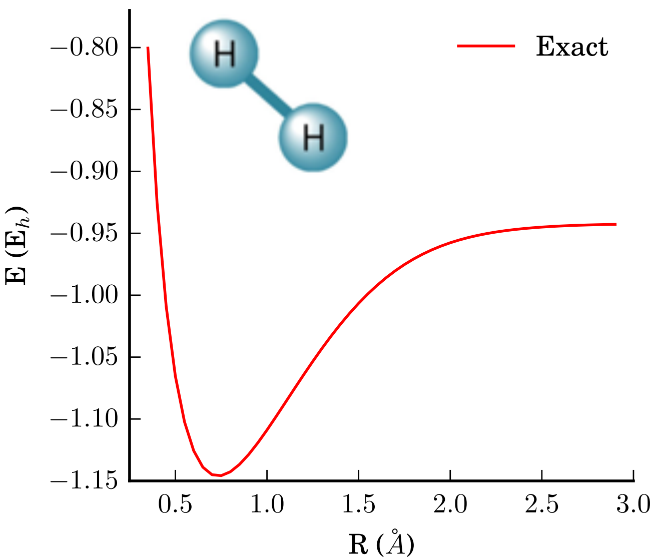
VQE Challenge: Stochastic optimization



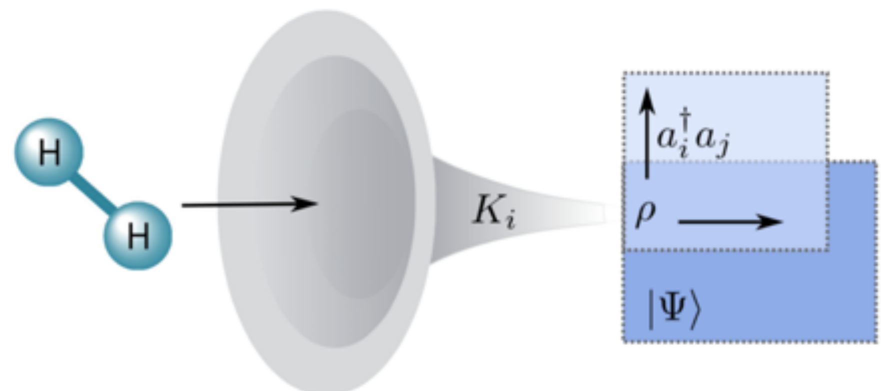
Quantum Subspace Expansion (QSE)

Expand to Linear Response (LR) Subspace

Quantum State on Quantum Device



Extra Quantum Measurements



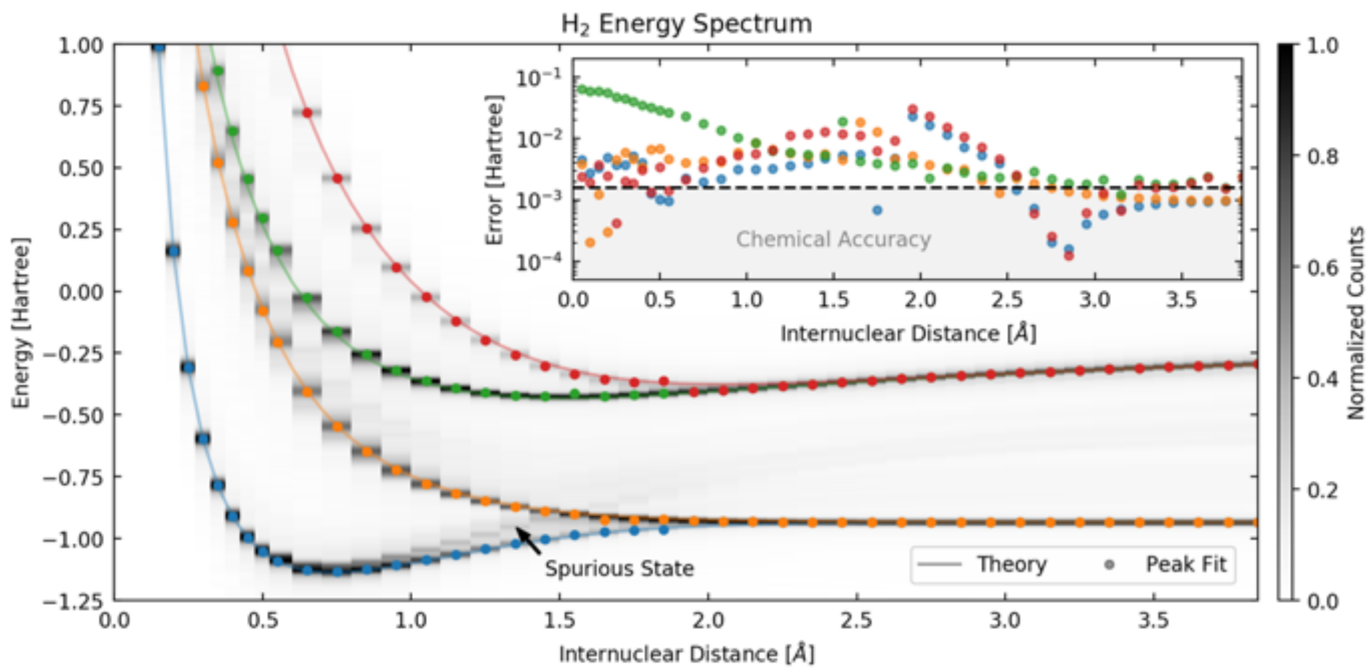
Classical Generalized Eigenvalue Problem

$$HC = SCE$$

Excited State Energy and Properties

Hybrid Quantum-Classical Hierarchy for Mitigation of Decoherence and Determination of Excited States
McClean, J.R., Schwartz, M.E, Carter, J., de Jong, W.A.
Physical Review A 95 (4), 042308 (2017)

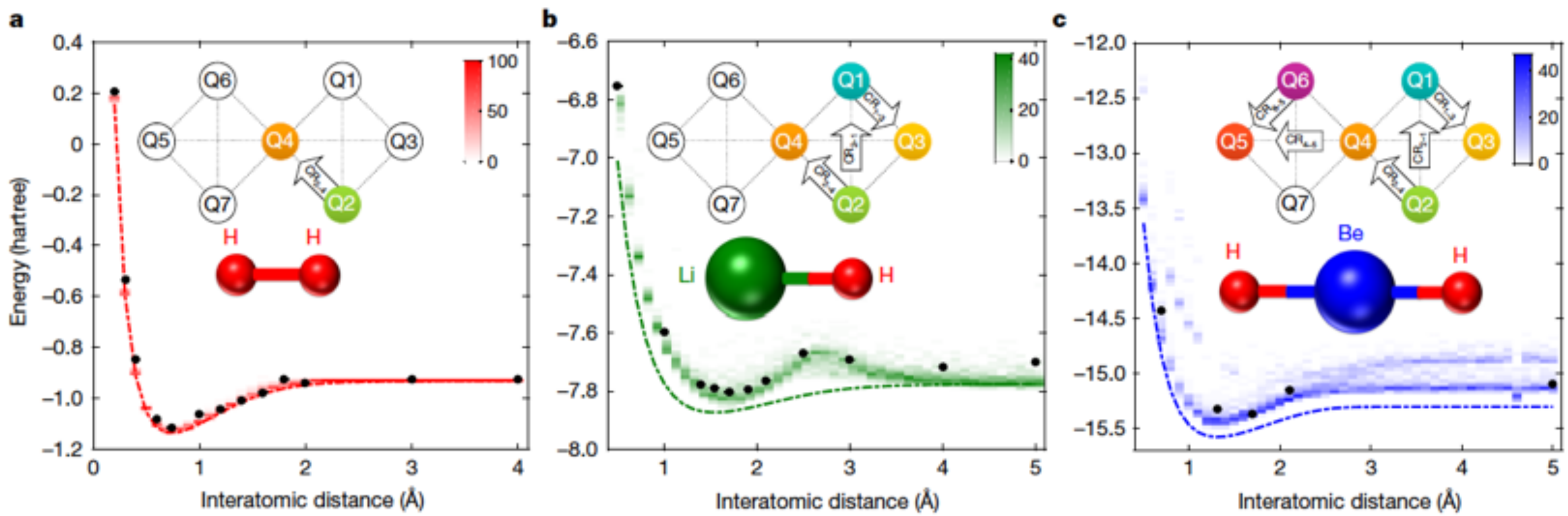
Accurate H_2 with excited states



Work with LBNL testbed / UC Berkeley
Imperfect gates and qubits do introduce small errors

James I. Colless, Vinay V. Ramasesh, Dar Dahlen, Machiel S. Blok, Jarrod R. McClean, Jonathan Carter, Wibe A. de Jong, Irfan Siddiqi, arXiv:1707.06408v1

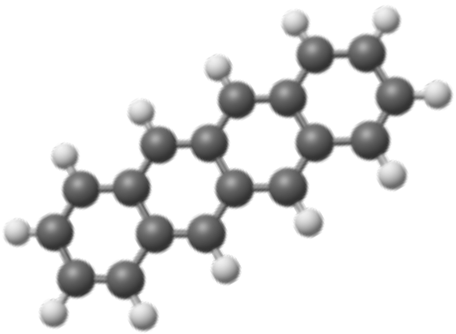
IBM has since pushed larger chemical systems



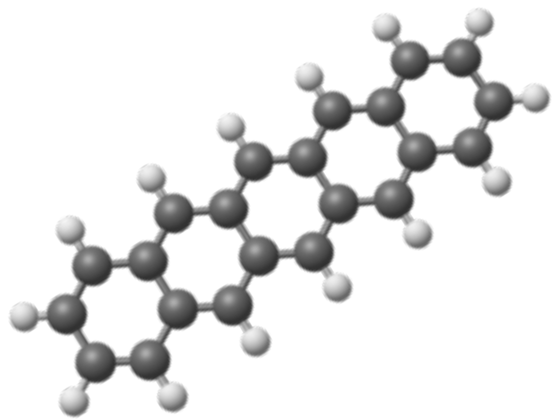
Kandala et al. Nature 549, 242 (2017)

Where can quantum chemistry go next?

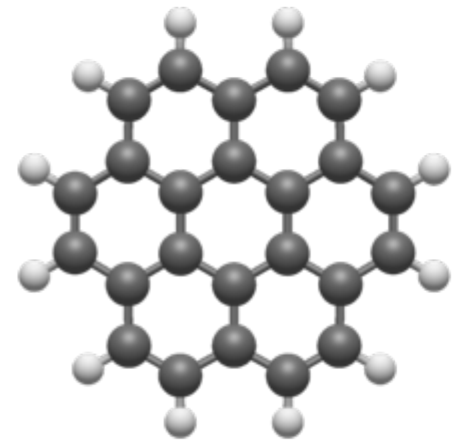
Quantum computers reaching sizes of 50 qubits



Tetracene
CAS(18,18)
300 million SD



Pentacene
CAS(22,22)
100 billion SD



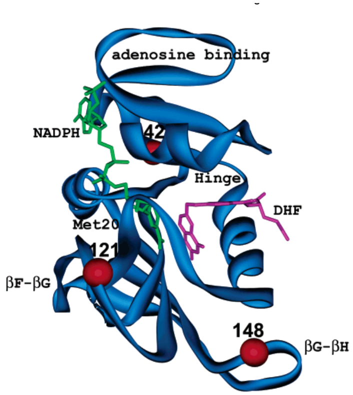
Coronene
CAS(24,24)
1 trillion SD

π-conjugated systems present in photochemistry and photobiology and as building blocks of functional nanodevices

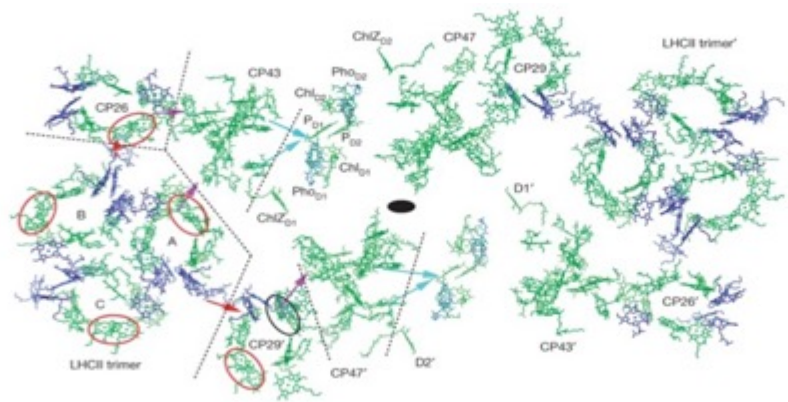
Quantum algorithm development at Berkeley

- Dynamics of chemical systems
  - Non-equilibrium behavior
  - Electron transport, response to external perturbations or driving forces
  - Exploring first and second quantization
- Quantum machine learning (led out of Harvard)
- Improving software stack with better compilers and optimizers
- Advancing stochastic optimizers and linear algebra

Tackling dynamics and electron transport



Proton-shuttle due to protein motion in enzyme reactions



Energy transfer pathways from antenna to reaction center in photosystem II.

Requires coupling between quantum nuclei and quantum electrons

Qubits → Log_2 (# Important Electronic States); # Cavity Modes → (# Nuclear DOF)

Dimension: $2^{N_{qubits}} \times (d)^{N_{modes}}$

$$D = 2^{10} \times 10^{10} \approx 10^{13} \approx 9 \text{ Peta-Bytes}$$

Exascale Supercomputer Capacity (Year 2021)

BERKELEY LAB

Berkeley Lab works extensively with industry

Berkeley lab science focus areas

Biosciences

Energy Technologies

Energy Sciences

Physical Sciences

Computing Sciences

Earth & Environmental Sciences

Berkeley Lab hosts five National User Facilities…

FY2016

The Advanced Light Source

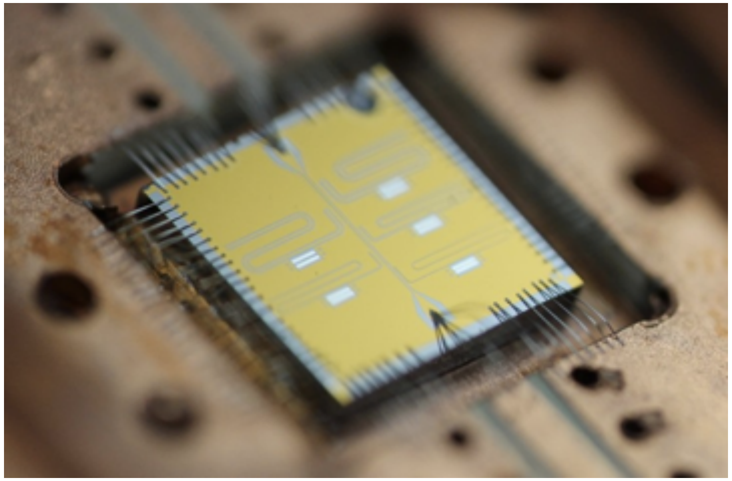
The Joint Genome Institute

NERSC

Energy Sciences Network

The Molecular Foundry

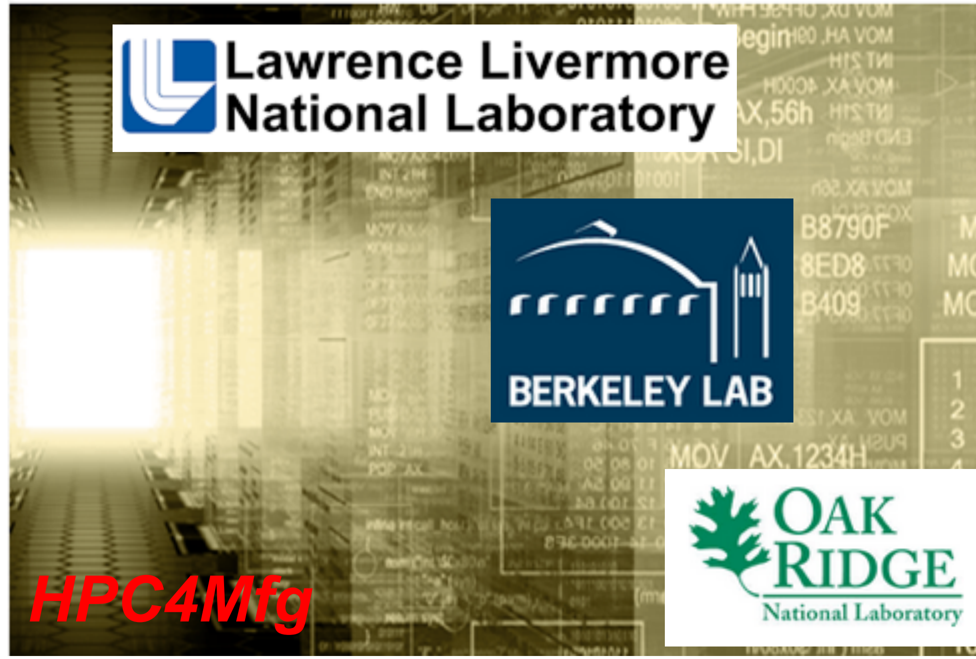
and Berkeley Lab will soon be hosting a quantum testbed



Details, talk to Jonathan Carter - jtcarter@lbl.gov

Berkeley Lab participates in HPC4Mfg program

- Accelerate innovation
- Lower energy costs
- Reduce testing cycles
- Reduce waste
- Optimize design
- Shorten the time to market



Apply High Performance Computing (HPC) capabilities and expertise at the national labs to increase US Manufacturing innovation and energy efficiency and de-risk the adoption of HPC by US industries

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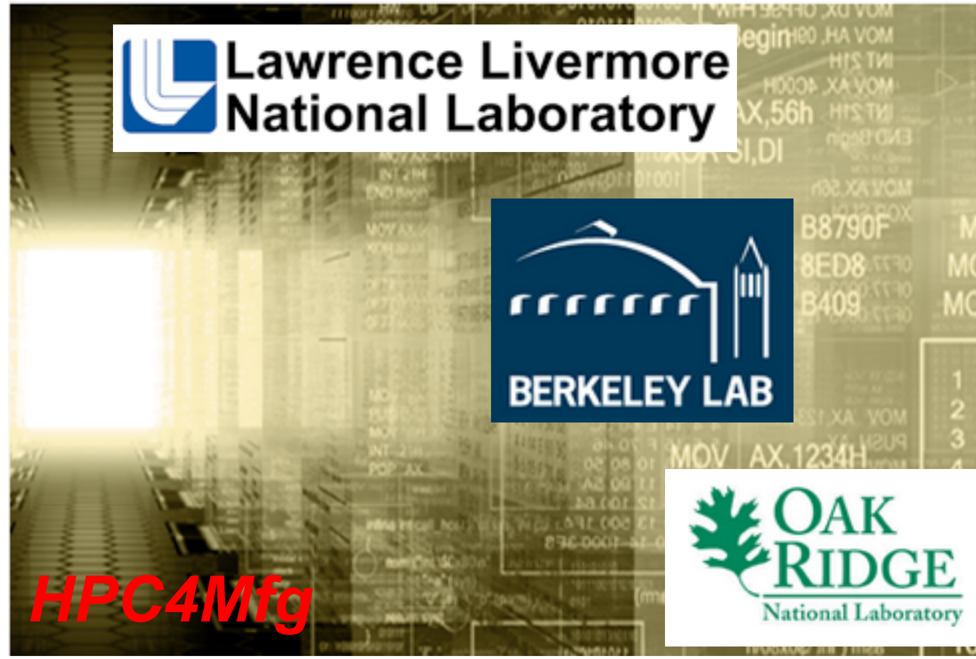

AND

Quantum computing

Apply High Performance Computing (HPC) capabilities and expertise at the national labs to increase US Manufacturing innovation and energy efficiency and de-risk the adoption of HPC by US industries

New ACT: Agreement for Commercializing Technology

More flexibility regarding Intellectual Property Rights

Better alignment with industry regarding payments and indemnification

Multi-party research and development partnerships now possible

QC WARE

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