Quantum computing as a platform for scientific discovery in chemical sciences

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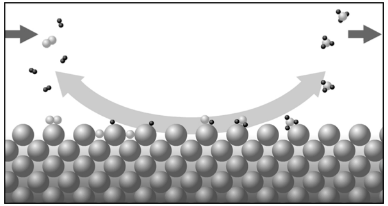
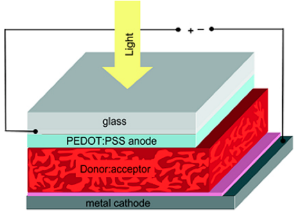
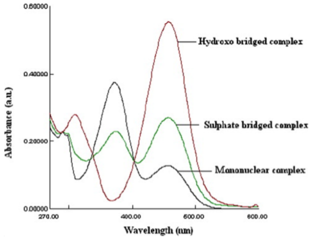
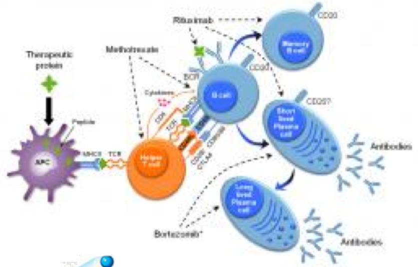
From understanding to control with quantum chemistry

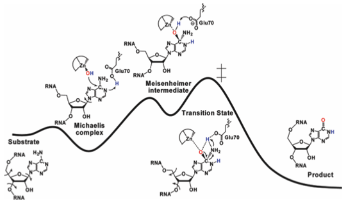




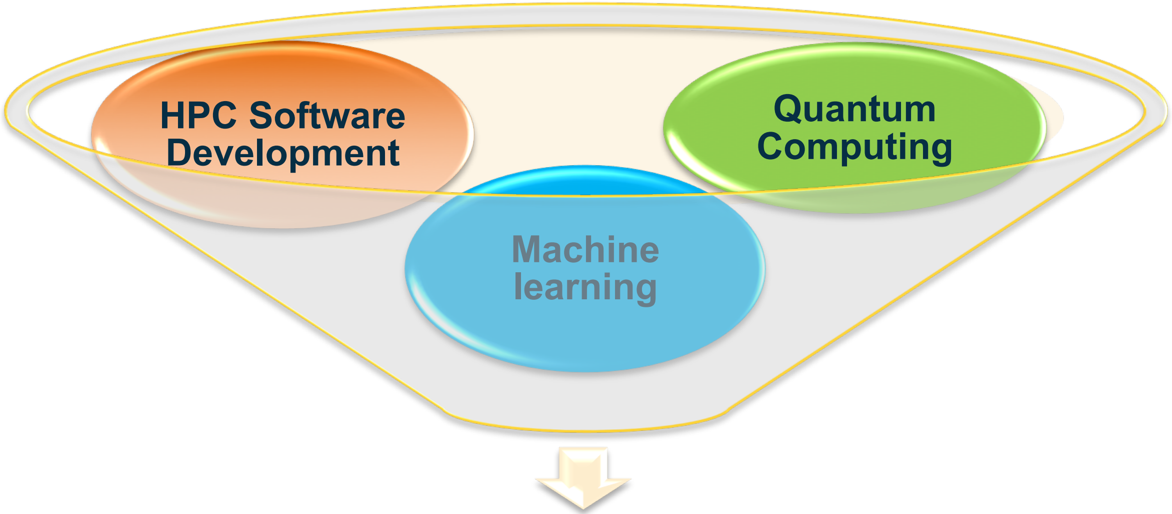


Understanding → Control





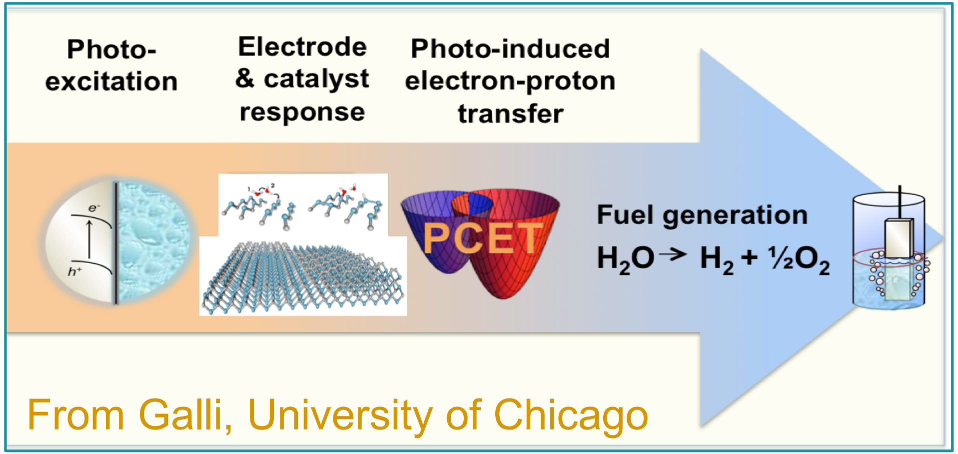
Expanding computational toolset for chemical sciences



Discovery of new materials, molecular systems and pathways

Quantum computing may help us tackle exponential complexity

Why quantum chemistry on quantum computers?



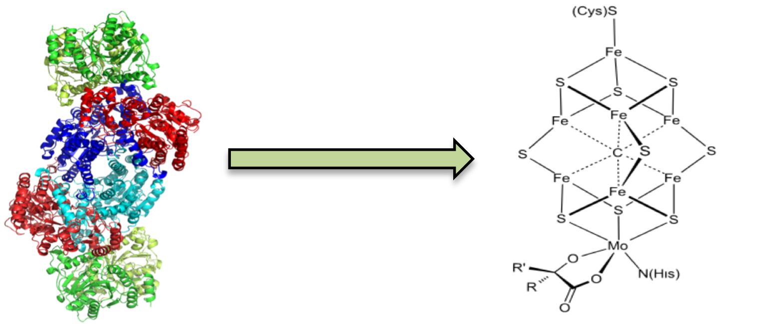
From Galli, University of Chicago

Photo-induced catalysis of water

Nitrogenase enzyme

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

"FeMoco"

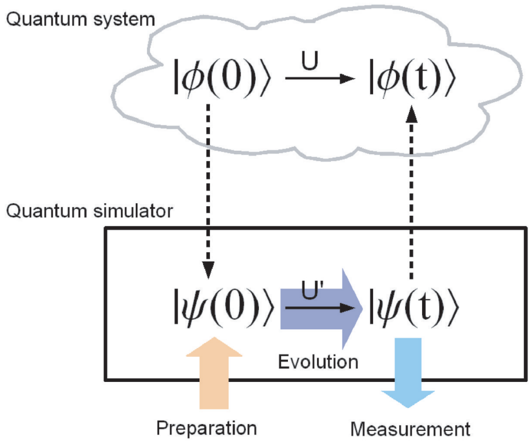


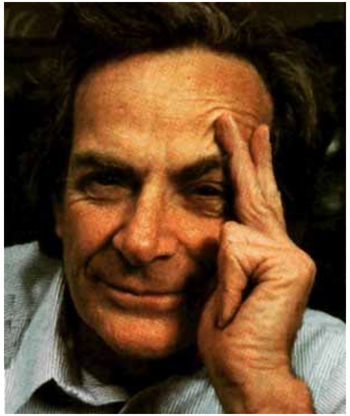
Nature's answer to Haber Process

Inaccessible, even at exascale!
Quantum computer requires ~100 ideal qubits for solution

Quantum computing and quantum chemistry a natural fit

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

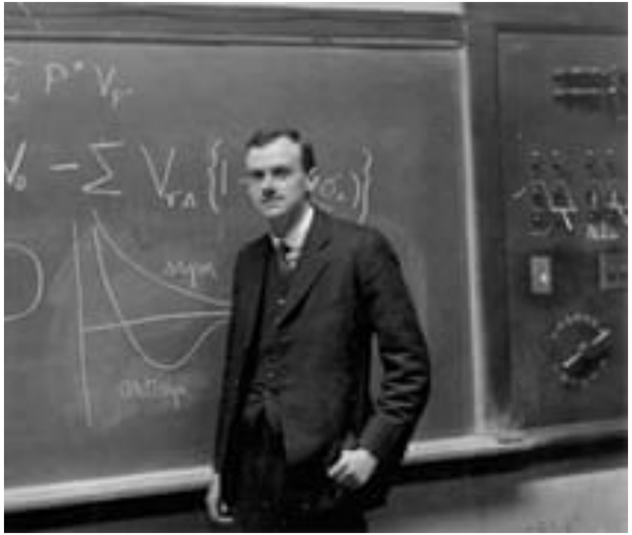




Challenge on classical computers is exponential complexity

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



Solving quantum chemistry simulations

$$H\psi = E\psi$$

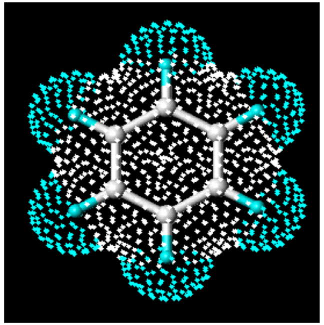
$$H = -\sum_{i} \frac{\nabla_i^2}{2} - \sum_{i,A} \frac{Z_A}{r_{iA}} + \sum_{i,j>i} \frac{1}{r_{ij}} + \sum_{A,B>A} \frac{Z_A Z_B}{R_{AB}}$$

Expanding the wave function ψ

We end up really solving:

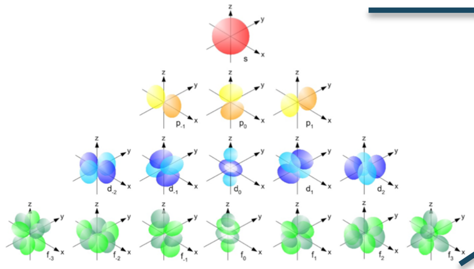
$$E = min_\theta(\langle\psi(\theta)|H|\psi(\theta)\rangle)$$

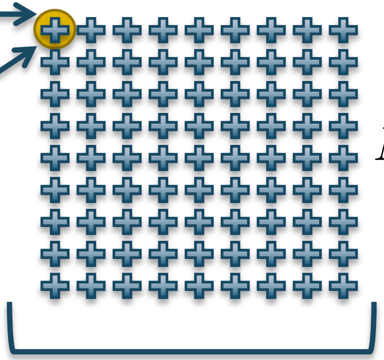
- Discretization of space for one-electron wave functions
- Many-electron wave function ψ often approximated
  - Full configuration interaction is exact solution
  - Unitary coupled cluster most widely used



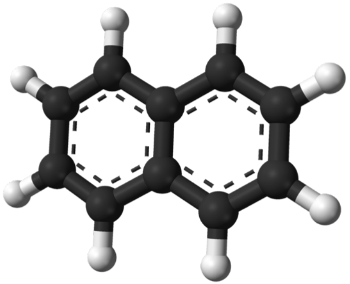
$$\left(\begin{array}{ll} \psi = e^{\hat{T}-\hat{T}^\dagger}\varphi_0 & \hat{T} = \hat{T}_1 + \hat{T}_2 + \cdots \\ \hat{T}_1 = \frac{1}{2}\sum_{pq} t_p^q\, \hat{a}_q^\dagger \hat{a}_p & \hat{T}_2 = \frac{1}{4}\sum_{pqrs} t_{pq}^{rs}\, \hat{a}_r^\dagger \hat{a}_s^\dagger \hat{a}_p \hat{a}_q \end{array}\right)$$

Accurate solutions are an exponential problem





$$D = M^N$$



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

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

Electrons:

$$D = \binom{M}{N_\alpha}\binom{M}{N_\beta}$$

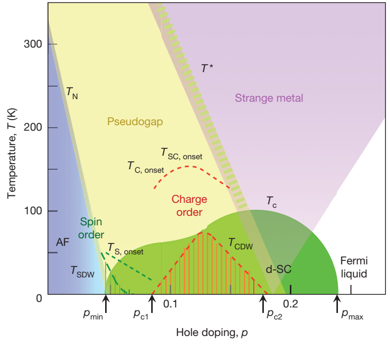
One mole

10^{23}

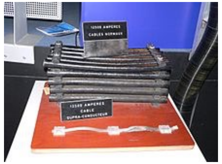
Particles in universe

10^{80}

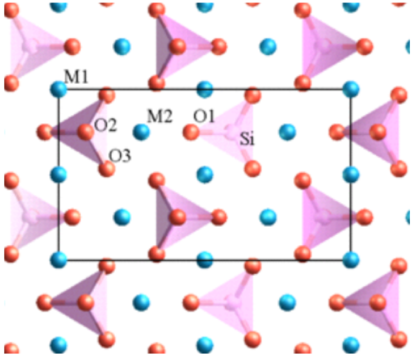
Electron correlation in materials drives many technologies



Taken from Keimer et al., Nature 2015



Superconductivity in MRI magnets and wires for current transmission



Strongly correlated materials are used in battery materials

Challenging to nearly impossible on classical computers

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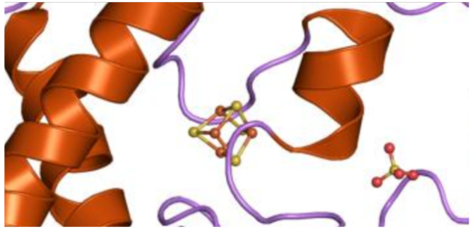
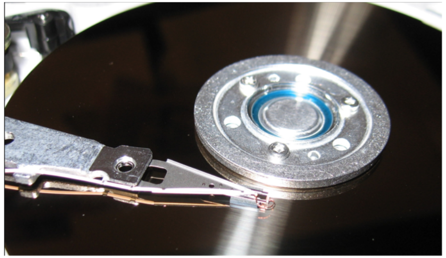
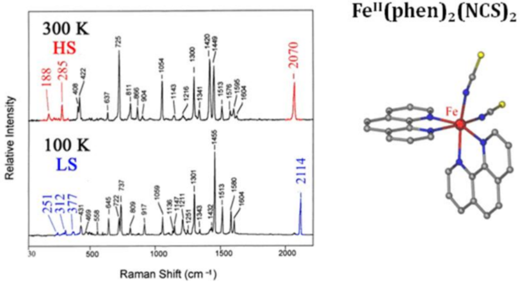
Electron correlation ubiquitous in biology and chemistry



FeS enzymatic active center



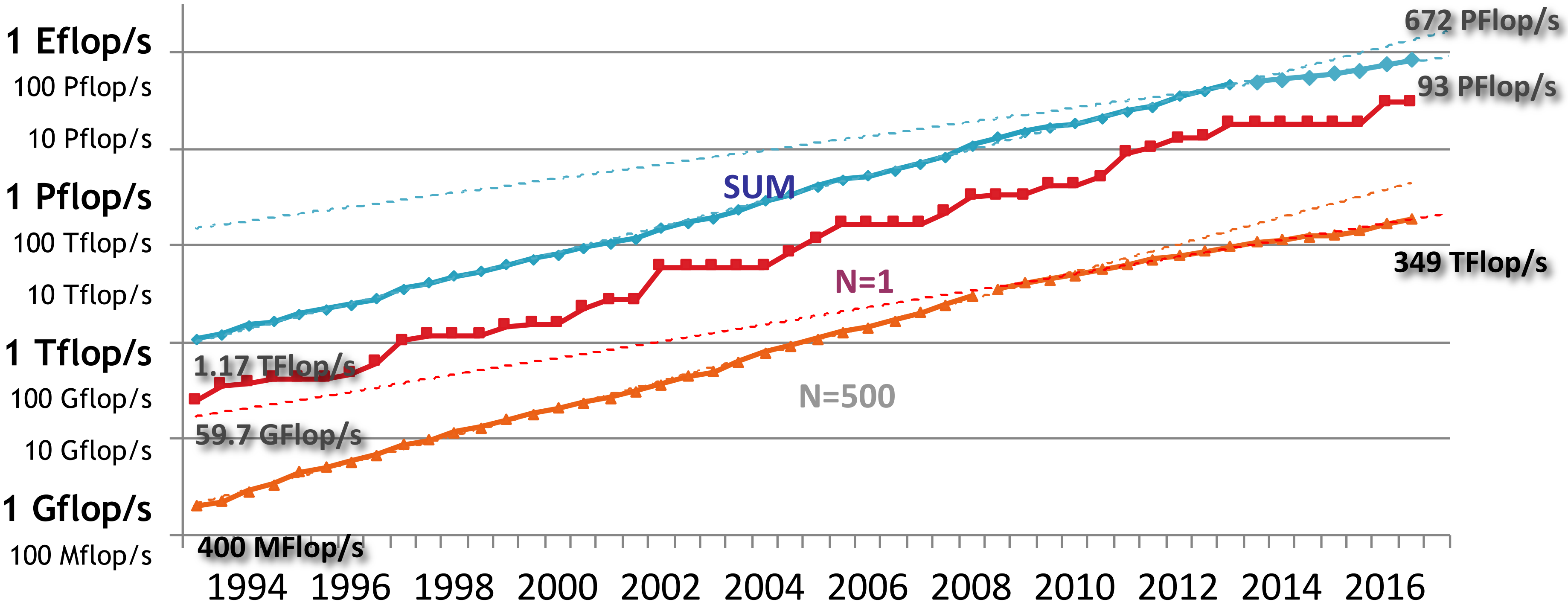
Molecular magnets used in hard drive coating



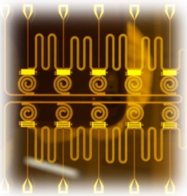
Spin-crossover and molecular switches

These are a challenge to calculate with classical computers

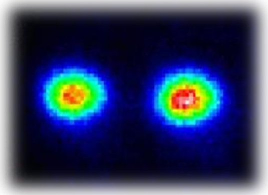
Exaflop gives us only a factor of 10x … we need a lot more



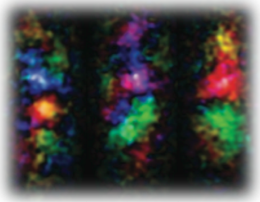
Challenges with quantum hardware



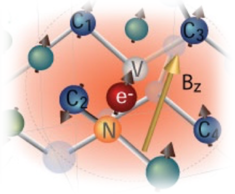
CIRCUITS



IONS



ATOMS



SOLID STATE

- # of qubits not yet enough for quantum supremacy/science
- Diverse technologies, each with its own instruction set
- Coherence (available compute time) very short (10s-100s of ops)
- Noise and errors still pretty large

HW Challenges lead to tradeoffs developing algorithms

Prep $|\psi\rangle$
(Set bits)
→ Evolution
(Operations)
→ Measurement
(Read bits)
→ $\{|\Psi_i\rangle, E_i\}$

Number of Qubits

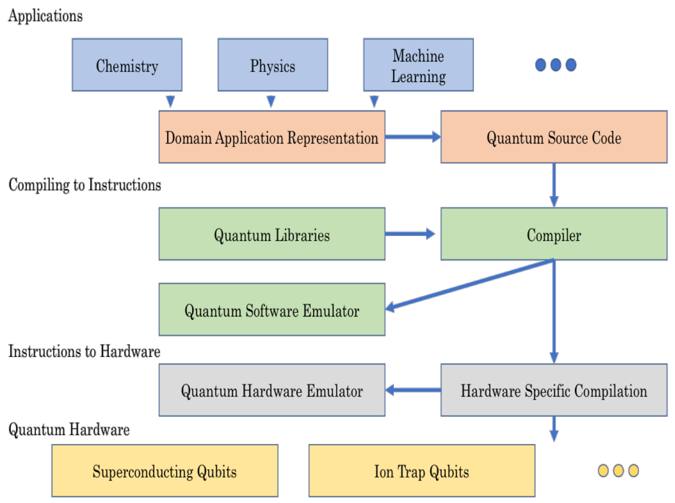
Coherence Time & Fidelity
- Robust control & stable qubits
- Algorithm timescale problem
- Accessible operations

Information Extraction
- Translate input/output
- Full readout loses advantage

Limit data in → Minimize ops → Limited data out

Challenges with algorithms and software stack

Few algorithms, and an exploding software stack



End-to-end software stack needed

Software standards needed

Towards useful quantum computing for science

Hardware technology

Scientific algorithms and software

- Increasing qubit count
- Increasing lifetimes
- Increasing fidelity and reducing errors

- Reducing qubit count
- Decreasing operation counts
- Incorporating error resiliency

Chemistry on quantum computers so far

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

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	$\mathcal{O}(N)$

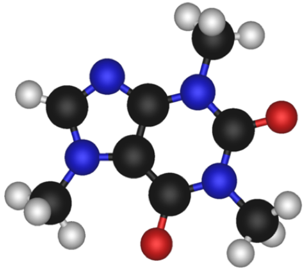
Bounding computational complexity ever more tightly, from $O(N^{11})$ in 2013 to $O(N^3)$-$O(N)$ in 2017

Source: McClean & Babbush (Google)

Converting to a language a quantum computer knows

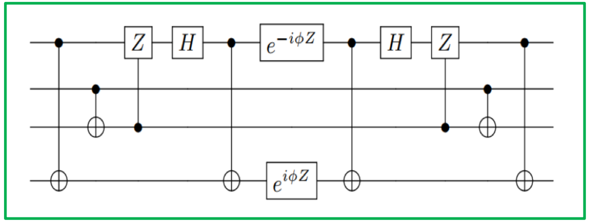
Molecule Specification:
- XYZ Coordinates
- Spin & Number of electrons
- Discretization (Basis set / grid)

Integral Generation
- Depends on basis set, uses external software
- Integral basis change
- Initial state preparation



Map to Qubits:
- Jordan-Wigner
- Bravyi-Kitaev, …

Algorithm and Trotterization of exponentials
- Quantum Phase Estimation
- Variational Quantum Eigensolver & Ansatz



Error correction, ancillas, gadgets

Map to hardware specific gates, connectivity, etc.

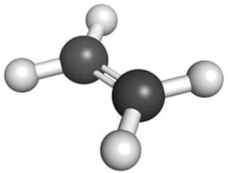
Explicit example, Hamiltonian for ethylene

$$H = \sum_{ij} h_{ij} a_i^\dagger a_j + \frac{1}{2} \sum_{ijkl} h_{ijkl} a_i^\dagger a_j^\dagger a_k a_l$$

```
-76.86638025450547 +
-0.81070034906153O7 [0^ 0] +
-0.8107003490615307 [1^ 1] +
-0.48815588090871 64 [2^ 2] +
-0.4881558809087164 [3^ 3] +
0.2194320533986508 [0^ 1^ 1 0] +
0.0452018005598162 [0^ 1^ 3 2] +
0.04520180055981617 [0^ 2^ 0 2] +
0.18143769455049882 [0^ 2^ 2 0] +
0.04520180055981617 [0^ 3^ 1 2] +
0.18143769455049882 [0^ 3^ 3 0] +
0.2194320533986508 [1^ 0^ 0 1] +
0.0452018005598162 [1^ 0^ 2 3] +
0.04520180055981617 [1^ 2^ 0 3] +
0.18143769455049882 [1^ 2^ 2 1] +
0.04520180055981617 [1^ 3^ 1 3] +
0.18143769455049882 [1^ 3^ 3 1] +
0.18143769455049896 [2^ 0^ 0 2] +
0.04520180055981622 [2^ 0^ 2 0] +
```

$$H = \sum_{i\alpha} g_i^\alpha \sigma_\alpha^i + \sum_{i\alpha j\beta} g_{ij}^{\alpha\beta} \sigma_\alpha^i \sigma_\beta^j + \ldots$$

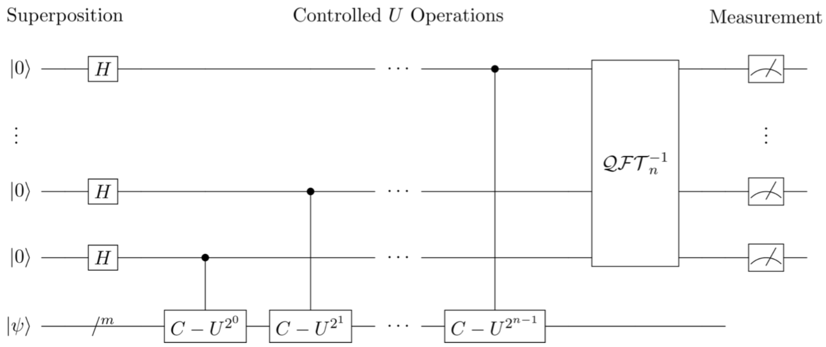
```
-77.65548161283827 <I> +
0.13679735356084918 <Z0> +
0.13679735356084918 <Z1> +
0.0028758897867 6678 <Z2> +
0.00287588978676674 <Z3> +
0.06811794699534135 <Z0 Z2> +
0.1097160266993254O <Z0 Z1> +
0.0226009002799081O <Y0 X1 X2 Y3> +
-0.0226009002799081 <Y0 Y1 X2 X3> +
-0.0226009002799081 <X0 X1 Y2 Y3> +
0.0226009002799081O <X0 Y1 Y2 X3> +
0.09071884727524945 <Z0 Z3> +
0.06811794699534135 <Z1 Z3> +
0.09071884727524945 <Z1 Z2> +
0.08236525639700065 <Z2 Z3>
```



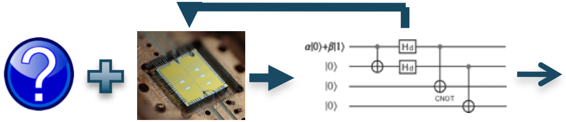
Jordan-Wigner transformation to spin-Hamiltonian

Two most common solvers for chemistry

Quantum Phase Estimation (QPE)

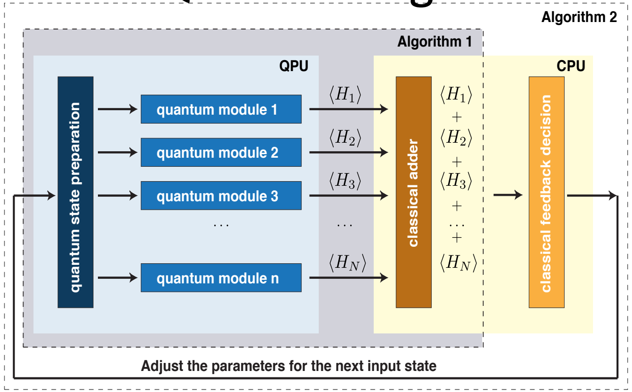


Prepare, evolve, FT and measure to find eigenvalue for eigenvector



42.02

Variational Quantum Eigensolver (VQE)



$$H = \sum_{i\alpha} g_i^{\alpha} \langle \sigma_\alpha^i \rangle + \frac{1}{2} \sum_{ij\alpha\beta} g_{ij}^{\alpha\beta} \langle \sigma_\alpha^i \sigma_\beta^j \rangle + \cdots$$

Only prepare and measure, do the rest classically

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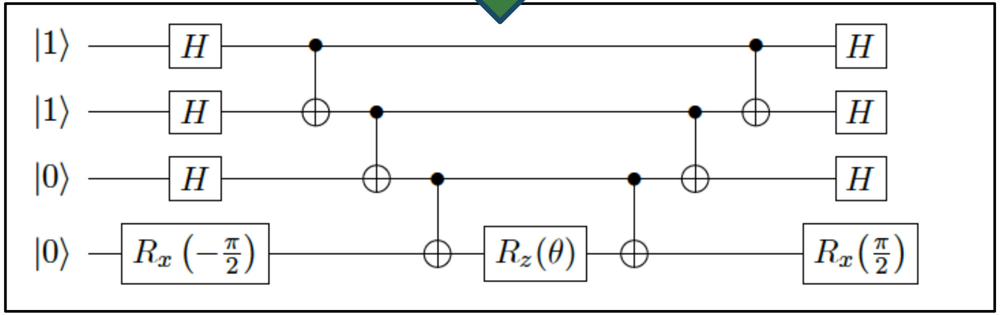
Encoding ψ and measure within VQE solve

Expansion of wave function with unitary coupled cluster

$$\psi = e^{-i\theta X_0 Y_1/2}\varphi_0 \quad \text{with} \quad \varphi_0 = |01>$$



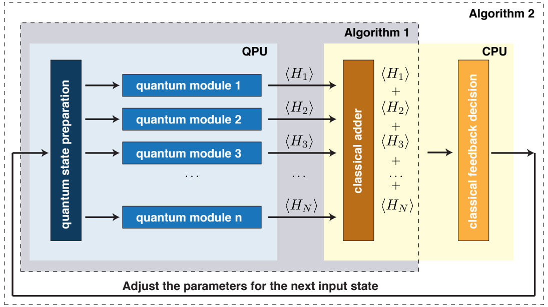
Measuring the expectation values

```
Allocate | Qureg[0]
Allocate | Qureg[1]
Allocate | Qureg[2]
Allocate | Qureg[3]
X | Qureg[0]
X | Qureg[1]
H | Qureg[0]
H | Qureg[1]
H | Qureg[2]
Rx(10.995574287564276) | Qureg[3]
CX | ( Qureg[0], Qureg[1] )
CX | ( Qureg[1], Qureg[2] )
CX | ( Qureg[2], Qureg[3] )
Rz(0.0013188585279302356) | Qureg[3]
CX | ( Qureg[2], Qureg[3] )
CX | ( Qureg[1], Qureg[2] )
CX | ( Qureg[0], Qureg[1] )
H | Qureg[0]
H | Qureg[1]
H | Qureg[2]
Rx(1.5707963267948966) | Qureg[3]
```

Follow with measurement of 14 expectation values

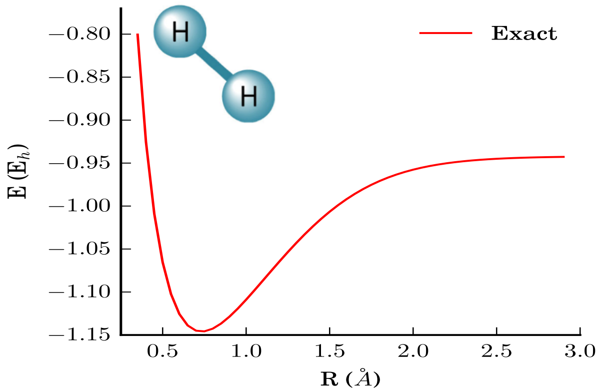
<Z0>, <Z1>, <Z2>, <Z3>, <Z0 Z2>, <Z0 Z1>,
<Y0 X1 X2 Y3>, <Y0 Y1 X2 X3>,
<X0 X1 Y2 Y3>, <X0 Y1 Y2 X3>,
<Z0 Z3>, <Z1 Z3>, <Z1 Z2>, <Z2 Z3>

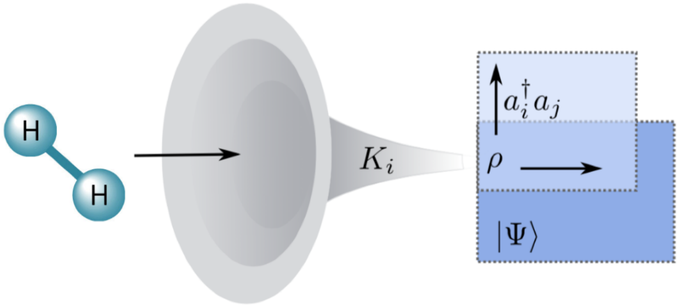
Need to be measured in z-basis



Pioneering work through LBNL LDRD:
Excited states through quantum subspace expansion (QSE)

Quantum State on Quantum Device → Expand to Linear Response (LR) Subspace
Extra Quantum Measurements



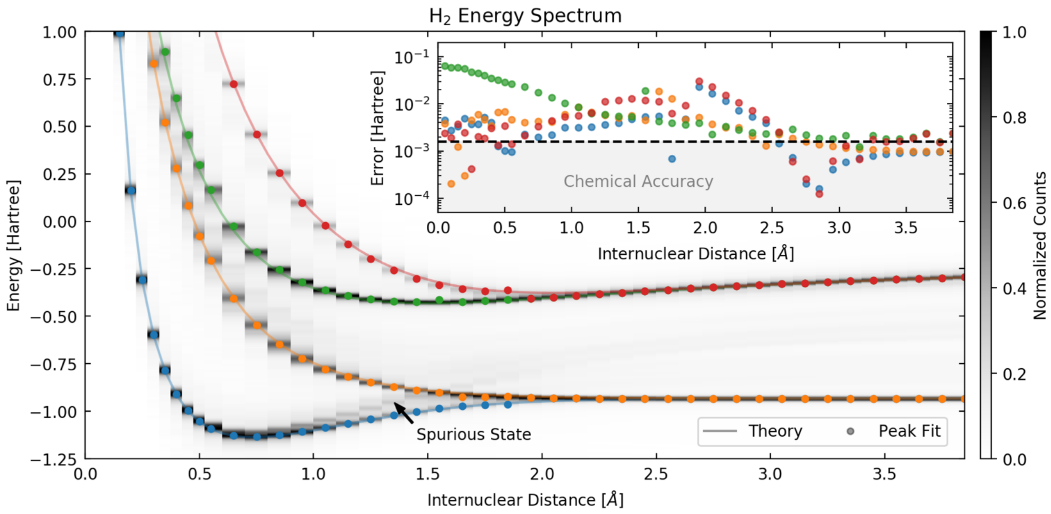


Excited State Energy and Properties ← Classical Generalized Eigenvalue Problem

$$HC = SCE$$

McClean, J.R., Schwartz, M.E, Carter, J., de Jong, W.A. - Physical Review A 95 (4), 042308 (2017)

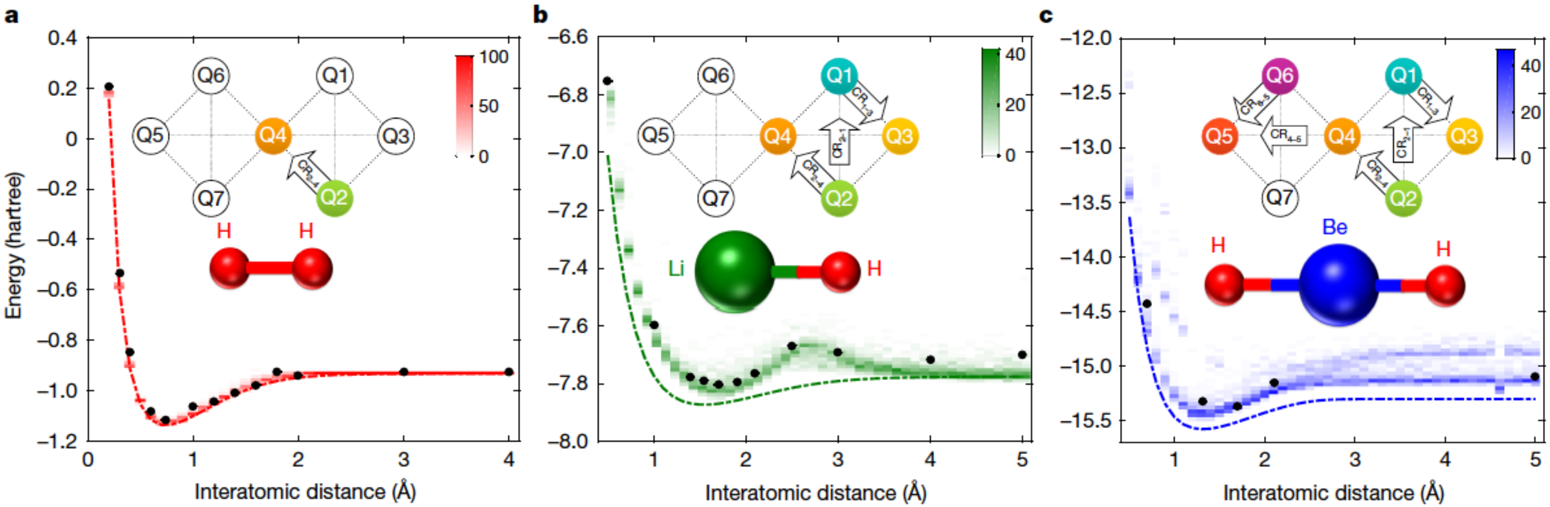
Pioneering work through LBNL LDRD: Demonstrating end-to-end simulation on Berkeley hardware



Choice of QSE measurements can lead to spurious states

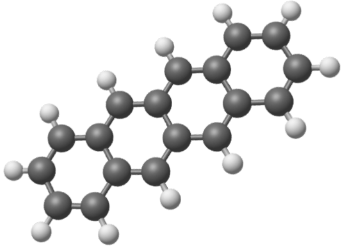
Colless, J.I., Ramasesh, V.V., Dahlen, D., Blok, M.S., McClean, J.R., Carter, J., de Jong, W.A., Siddiqi, I. - Phys. Rev. X 8, 011021 (2018)

IBM has since pushed larger chemical systems

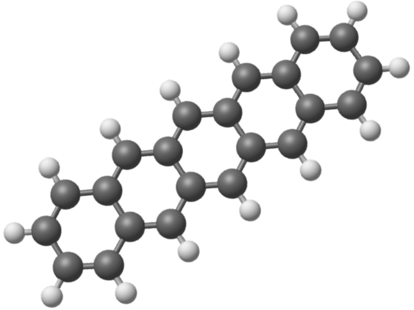


Kandala et al. Nature 549, 242 (2017)

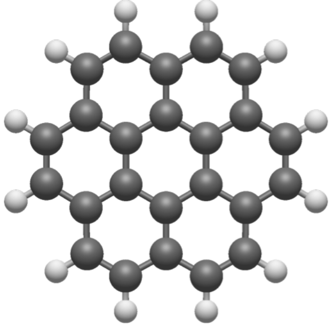
But, quantum supremacy demo far away



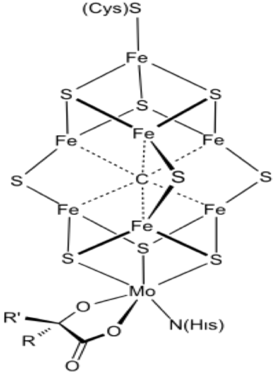
Tetracene
CAS(18,18)
300 million SD



Pentacene
CAS(22,22)
100 billion SD



Coronene
CAS(24,24)
1 trillion SD



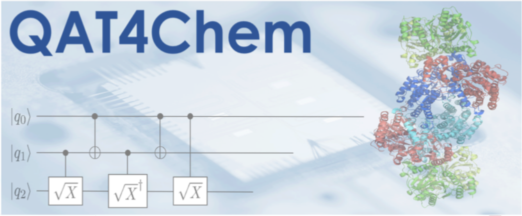
FeMoCo

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

BERKELEY LAB

LBNL’s Quantum Algorithm Team

Deliver algorithmic, computational and mathematical advances to enable scientific discovery in chemical sciences on quantum computers



BERKELEY LAB · Berkeley UNIVERSITY OF CALIFORNIA · UNIVERSITY OF TORONTO · Argonne NATIONAL LABORATORY

Multidisciplinary 

from across computing sciences

Novel Quantum Algorithms

Develop new algorithms for chemical sciences that can utilize noisy quantum computers

- Distinguishing quantum information scrambling from decoherence
- More efficient ansatzes for chemical simulations
- Efficient encoding
- Quantum autoencoders

Computer Science on Quantum Devices

Analyzing, optimizing and controlling algorithms and simulations on noisy quantum hardware

- Implemented noise injection in ProjectQ
- Algorithmic error mitigation techniques
- Generalized swap networks for low-depth parallelization of gates

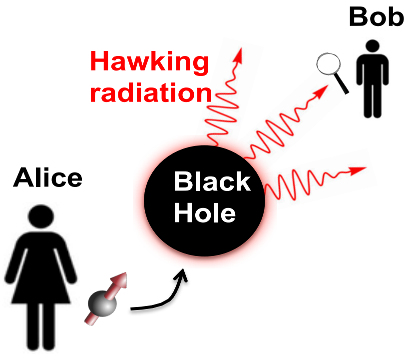
Applied Mathematics for Quantum Computing

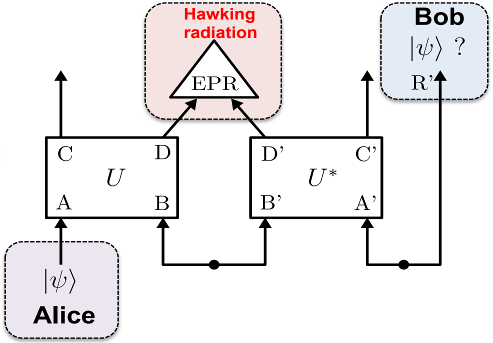
Develop better optimizers for noisy stochastic optimization problems in quantum computing

- Development of scikit-quant-opt library of optimizers
- Multistart methods for VQE and QAOA
- Exploring optimizers for hardware gate optimization

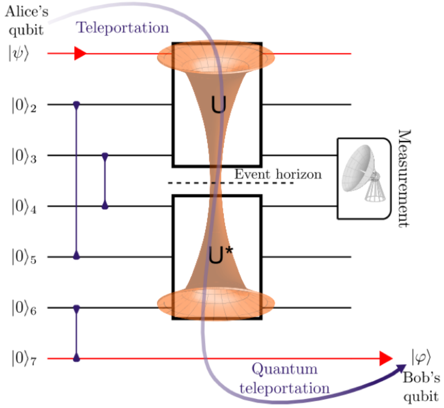
Algorithm example:
Verifiable simulation of a fast scrambling quantum circuit

First demonstration with trapped ions





AQT experiment ongoing

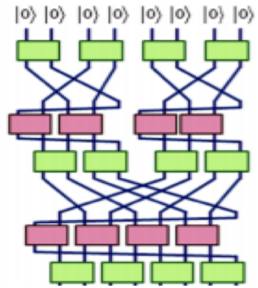


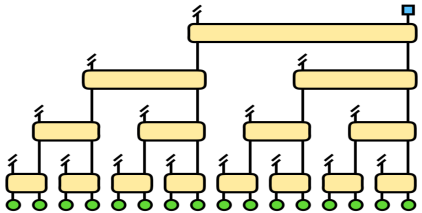
Teleportation protocol as "intrinsic" verifier of many-body quantum circuits

arXiv:1803.10772 *Yao Group UCB* arXiv:1806.02807

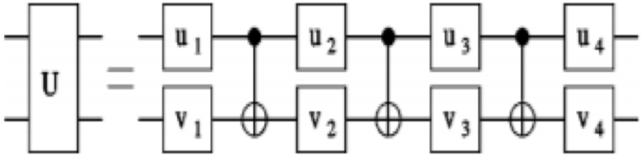
Algorithm example:
Tensor Networks for VQE and machine learning

- States prepared with tensor network ansatz (MERA)
  - Low gate complexity
  - Noise resilience





- Tensor networks for image classification
  - Easy to prepare
  - High level of noise resilience

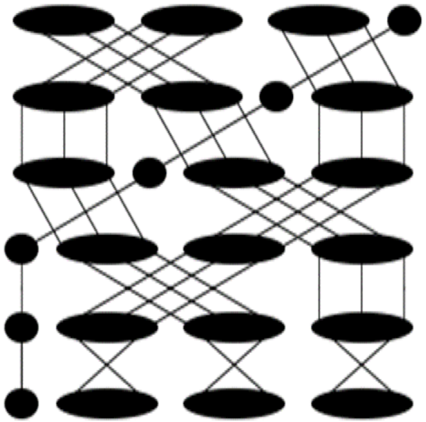


Whaley Group UCB

Computer science integral part in advancing quantum computing

Overall improvement of software stack

- Better compilers and circuit optimizers
- Towards comprehensive gcc for quantum computers
- Tackling error propagation and mitigation
- Efficient circuits for most accurate solutions
  - Accounting for error due to noise and limitations of architecture

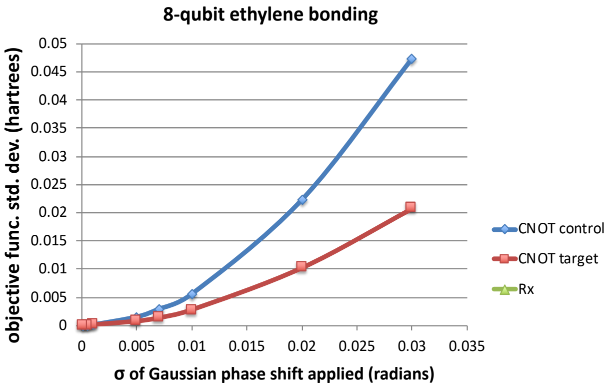


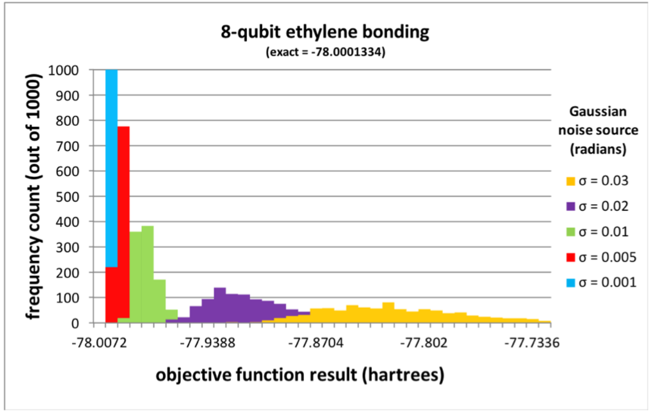
- Extensive effort in error control, modeling and understanding

We need to understand impact of gate noise

Individual gate noise affects how distributions are sampled

- Random noise shift and broadens sampling distribution
- VQE most sensitive to noise on control qubit in CNOT
- Additions to ProjectQ allow testing of different noise levels at individual gates

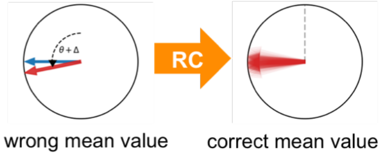




We are pursuing practical fault-tolerance

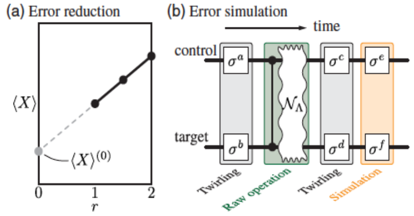
Apply different techniques to different part of the simulation

- Heralding for correct initial state
- Individual operations error corrected
- Mitigating readout errors with confusion matrix
- Machine learning to tackle decoherence



2-4 qubit circuits are under development

- Testing on simulators with error models
- Experimental validation on LBNL testbed, IBM and Rigetti



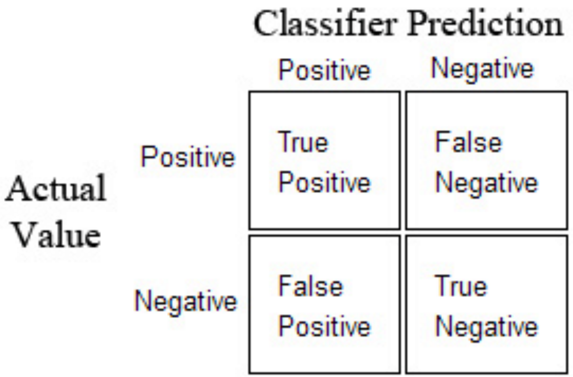
Correcting measurement errors

One qubit measurement (IBMQX4):

|0> {'00000': 7904, '00001': 197, '00010': 85, '00011': 6}
|1> {'00000': 800, '00001': 7285, '00010': 11, '00011': 96}

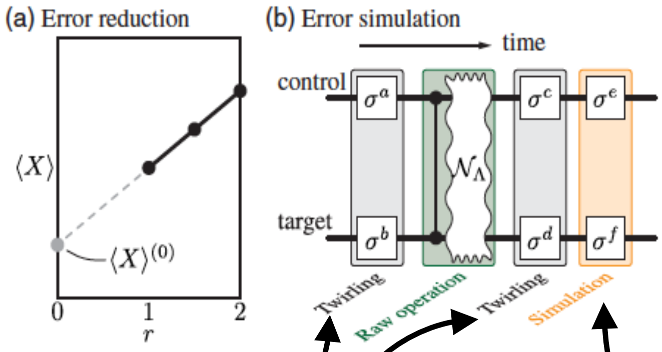
Two qubit measurement

|00> {'00000': 7909, '00001': 191, '00010': 89, '00011': 3}
|01> {'00000': 707, '00001': 7382, '00010': 8, '00011': 95}
|10> {'00000': 585, '00001': 19, '00010': 7409, '00011': 179}
|11> {'00000': 66, '00001': 507, '00010': 686, '00011': 6933}



Correction with covariance matrices, disentangling confusion

Reducing stochastic noise

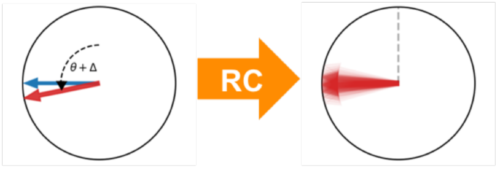


Converting non-stochastic to stochastic (randomized benchmarking)

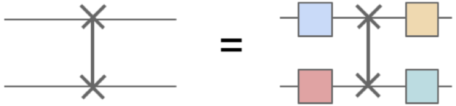
Adding error on purpose

Concept

- **Add gates that randomize signs of errors each run so *average* result is correct:**

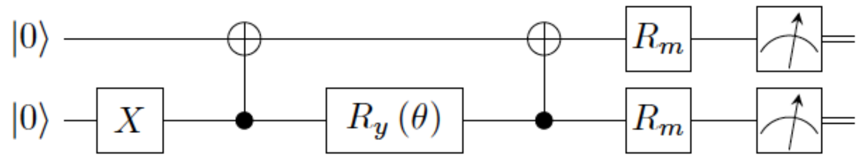


- Implementation: Sandwich “hard” gates between certain random “easy” gates



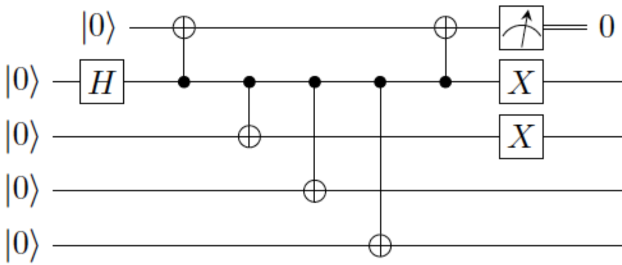
Ying Li and Simon C. Benjamin - Phys. Rev. X 7, 021050 (2017)

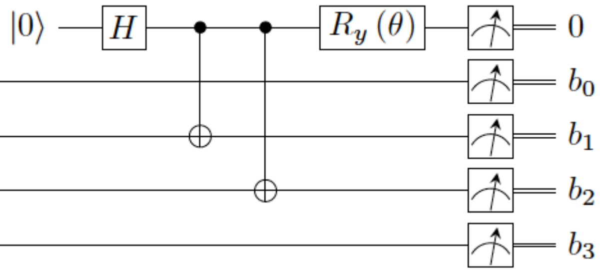
Building error correction into circuits



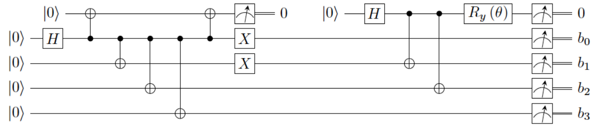
Single error detection

Magic states





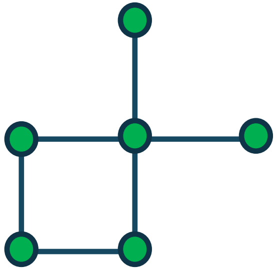
Not every qubit is equal on real hardware

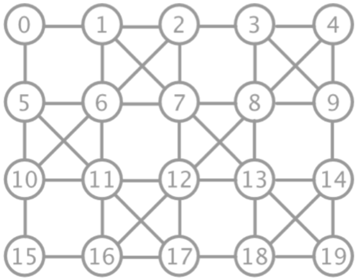


Circuit

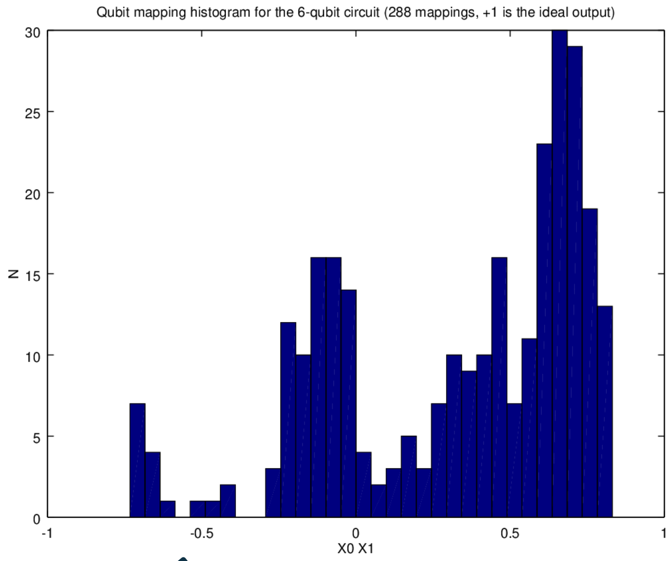
+

Topology





IBMQ Tokyo Hardware



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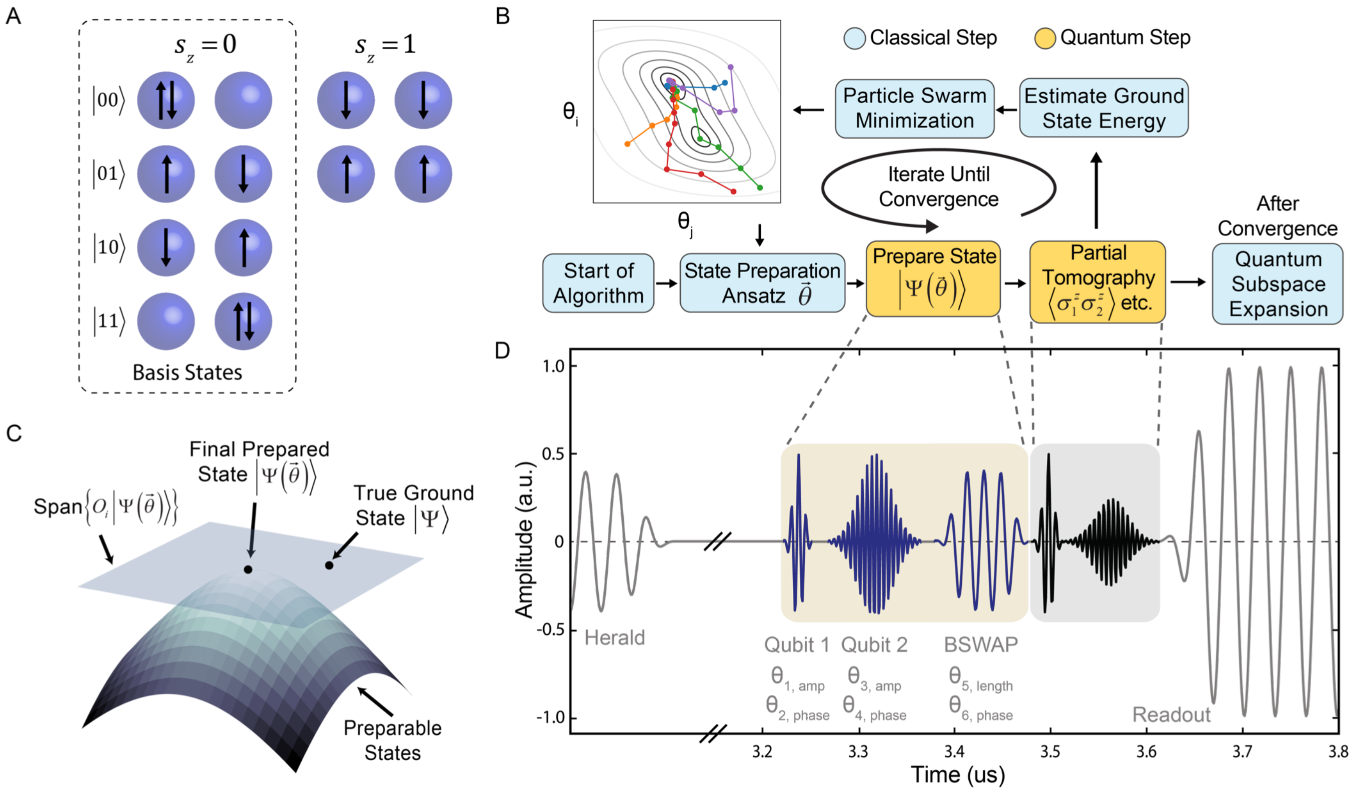
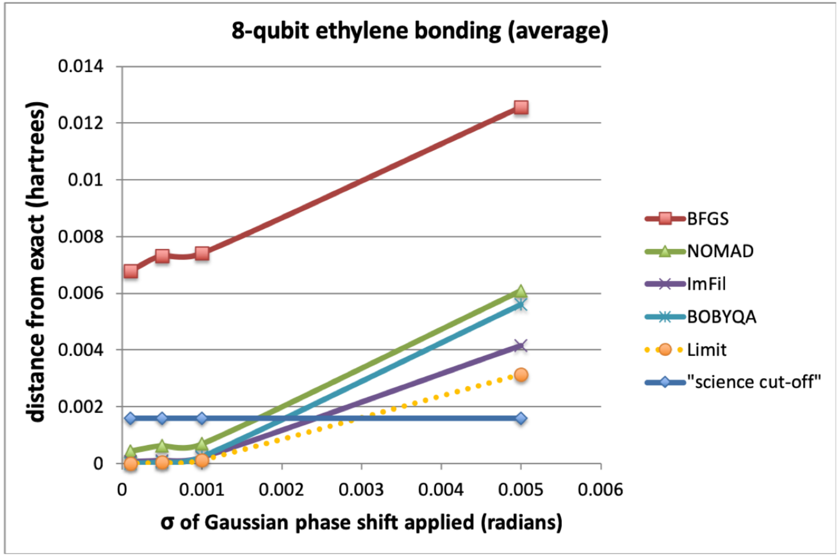
Applied math advances needed for stochastic optimization



Skquant-opt: Optimizers for noisy intermediate-scale quantum devices

Exploring ability of known stochastic optimizers to handle noise

- Some are better then others
- Building ***scikit-quant*** suite containing optimizers
- http://scikit-quant.org



Collaboration between LBNL, ANL, Google, Universities, *ORNL, Sandia*

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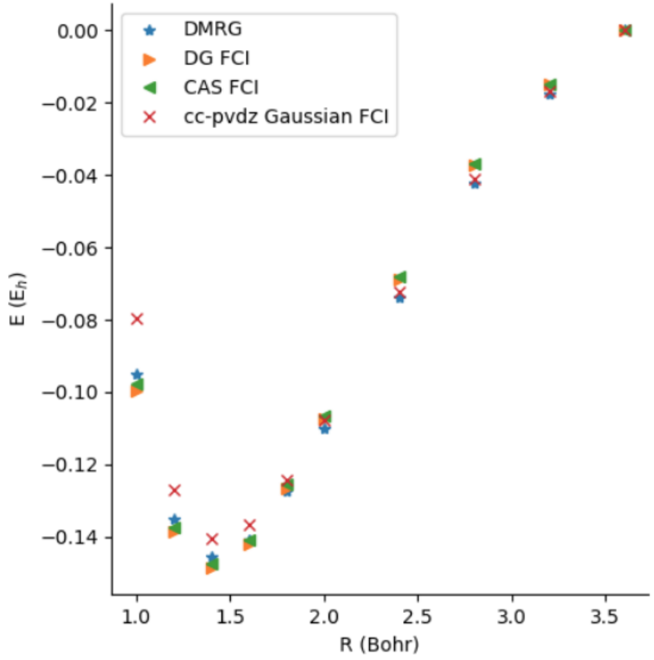
Discontinuous Galerkin as a new mathematical wave function basis

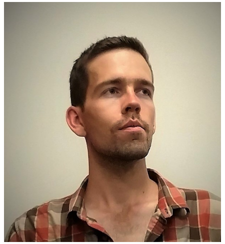
- **Diagonal basis for the Coulomb operator highly advantageous for reducing complexity**

- **Discontinuous Galerkin (DG)**
  - Block diagonal basis set
  - Preserves sparsity structure
  - Reduces the preconstant for representing the Coulomb operator

Ongoing work Lin Lin



Development of talented workforce is badly needed



Development of computer science and applied math areas essential

QAT Teams organize SC18 Tutorial, more needed

Quantum Computing for Scientific Applications at SC18 attracted 100 professionals

Planning boot camps and other information exchange possibilities, including at LBNL

Connections with industrial partners essential

bleximo

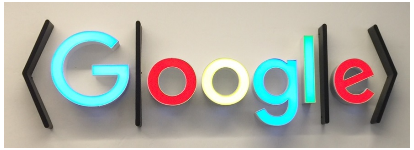
LBNL Cyclotron Road Incubator
Novel hardware architectures

IBM Q™

Hardware access
Error mitigation and software

CQC CAMBRIDGE QUANTUM COMPUTING LIMITED

Compiler development



Algorithm development
Classical optimizer development

rigetti

Hardware access
Integration of tools into Forest

Siemens supporting graduate student at UC Berkeley

Algorithm development partnerships with VW and Daimler

In summary

LBNL is driving quantum computing forward as a platform for scientific discovery

LBNL's QAT is trying to push things forward for chemistry

Acknowledgements

This work was supported by the DOE Office of Advanced Scientific Computing Research (ASCR) through the Quantum Algorithm Team and Quantum Testbed Pathfinder Program

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https://qat4chem.lbl.gov

https://berkeleyquantum.org

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