Google AI Quantum

Quantum computation for science

Jarrod McClean
@JarrodMcClean
Senior Research Scientist

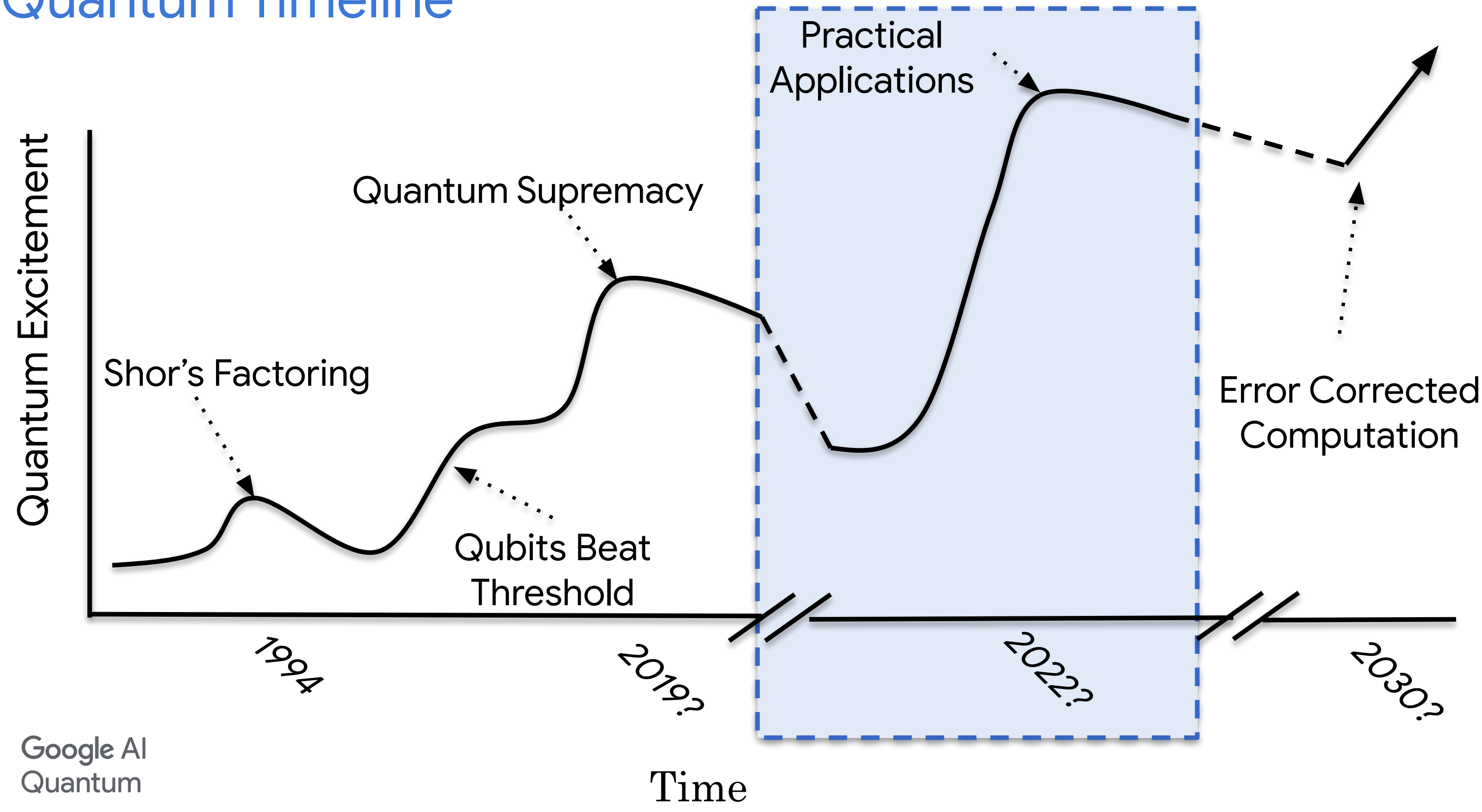
CSGF and my path...

DOE
CSGF

VE RI
TAS

BERKELEY LAB

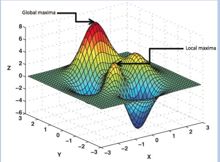
Quantum Timeline

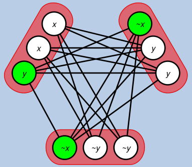


Google AI Quantum

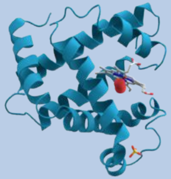
Early application areas

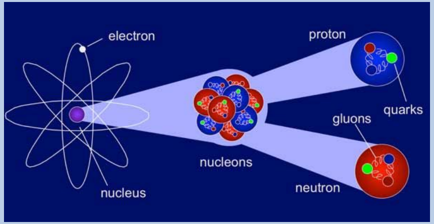
Optimization





Quantum Simulation





Quadratic Speedup

1 year → 2 weeks

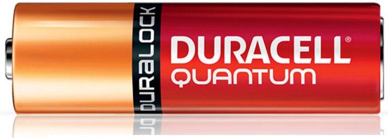
Exponential Speedup

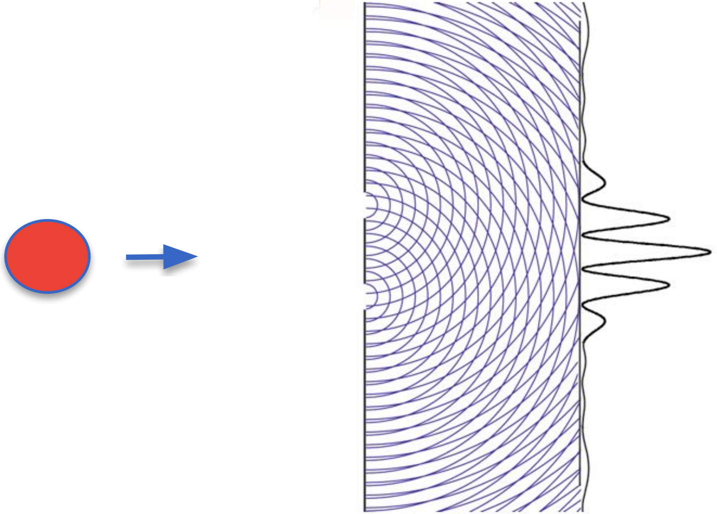
10^{82} years → 300 seconds

Age of universe ~ 14 x 10^9 years

Google AI Quantum

What is quantum?





"Classical"

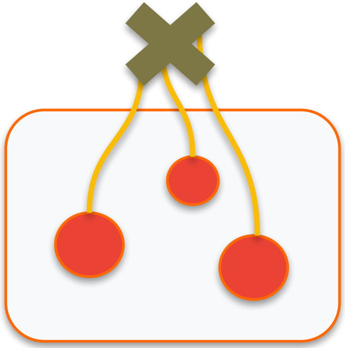
"Quantum"

Quantum System – A physical system operated in a regime where we need effects like discrete energy levels and interference are required to accurately describe it.

Simulation

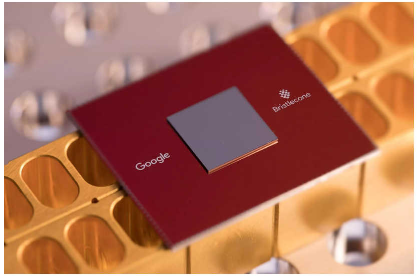
Orrery

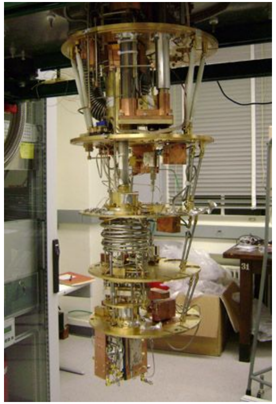
Antikythera Mechanism (125 B.C)

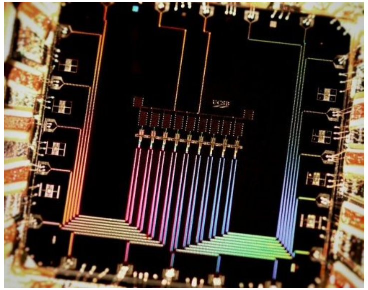


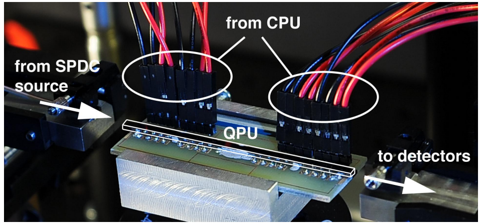
Quantum System → Quantum System

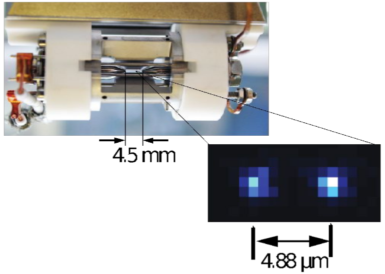
Quantum systems



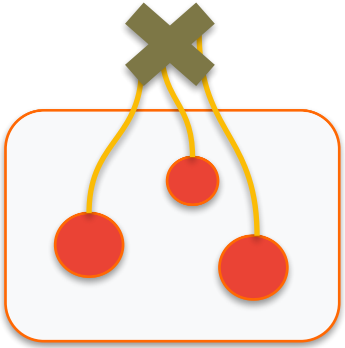


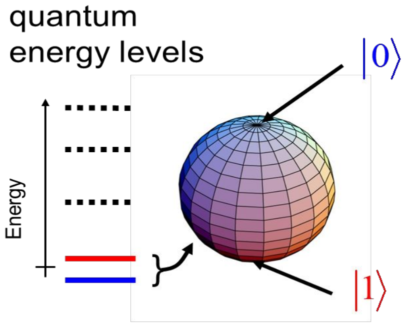






Quantum simulation - the quantum advantage





$$|\Psi\rangle = \alpha|0\rangle + \beta|1\rangle$$

Quantum Simulation

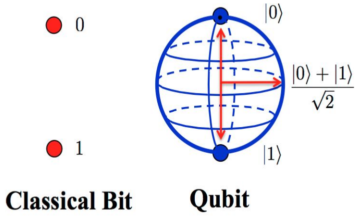
Abstraction

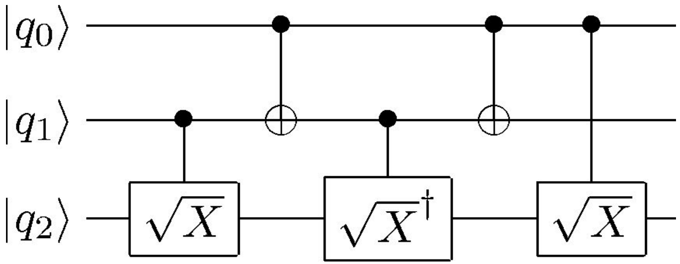
Quantum Computation

- Factoring Products of Two Large Primes
- Linear Partial Differential Equations
- Solution of Linear Equations

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

Quantum computing abstraction





$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

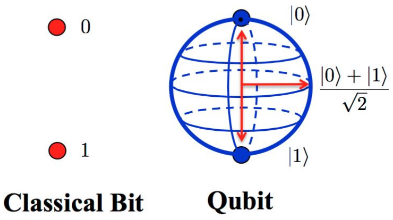
$$X = \mathrm{NOT} = \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$X\,|0\rangle = |1\rangle$$

$$X\,|1\rangle = |0\rangle$$

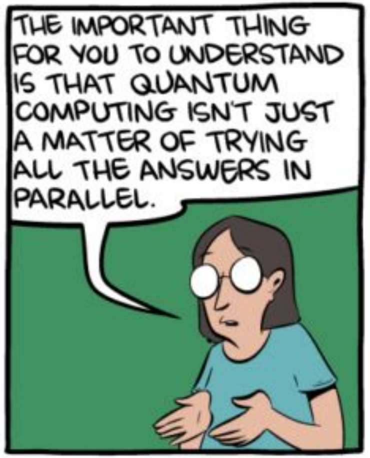
Debunking quantum myths

MYTH 1: Faster/better because it can use an exponential number of states



MYTH 2: Faster/better because bits can be 0 and 1 at the same time.

MYTH 3: Work by computing all the answers in parallel



Google AI Quantum

*https://www.smbc-comics.com/comic/the-talk-3

Challenges in quantum computation

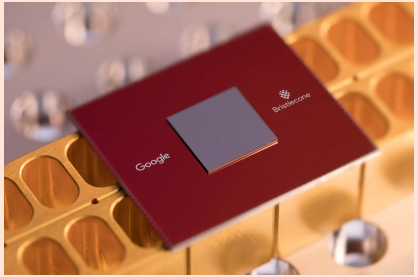
Prep $|\psi\rangle$ → Evolution → Measurement → $\{|\Psi_i\rangle, E_i\}$

Number of Qubits
+Scalable manufacture
+(N-1) qubit problem

Coherence Time & Fidelity
+Robust control & stable qubits
+Algorithm timescale problem

Information Extraction
+New input/output spec
+Full readout loses advantage

Better Hardware



Co-Design Better Algorithms

Previous: Coherence time flexible

Future:

- Improved coherence time flexibility, novel property extraction, and demonstration
- Qubit number flexible algorithms and larger demonstrations

Thinking differently for speedups

Classical:

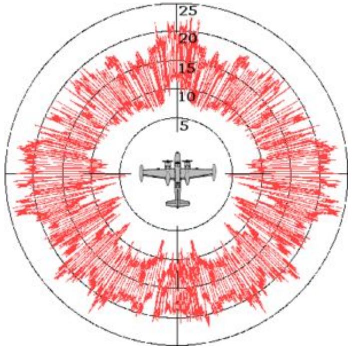
$$Ax = b$$

Solution translates to writing down the entries of x

Quantum*:

$$A|x\rangle = |b\rangle$$

Solution translates to preparing state x from which one can sample



Solving the problem, not reproducing the classical algorithm!

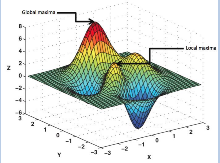
Google AI Quantum

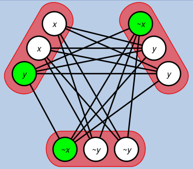
*A. Harrow, A. Hassidim, S. Lloyd, Phys. Rev. Lett. **103**, 150502 (2009)

**B. D. Clader, B. C. Jacobs, and C. R. Sprouse Phys. Rev. Lett. 110, 250504 (2013)

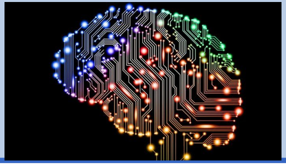
Early application areas

Optimization

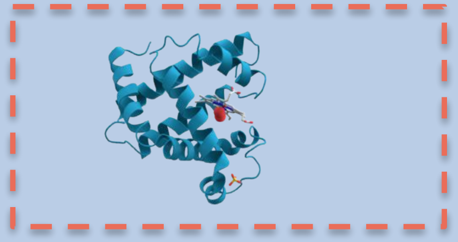


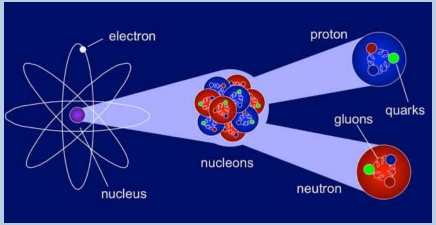


Relation Representation



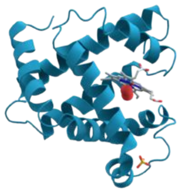
Quantum Simulation



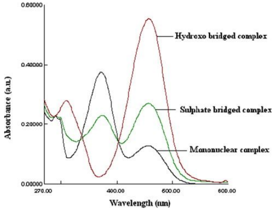


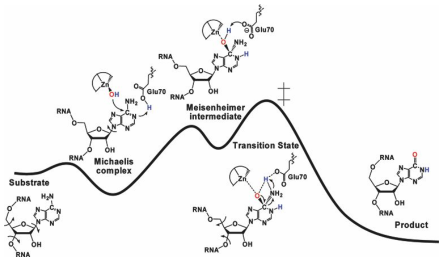
Google AI
Quantum

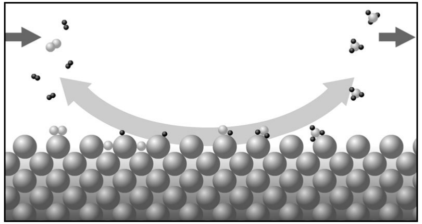
Simulating Chemistry



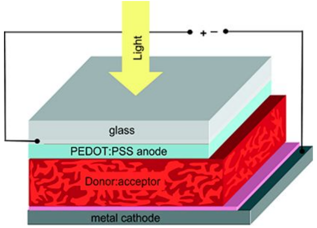
Understanding

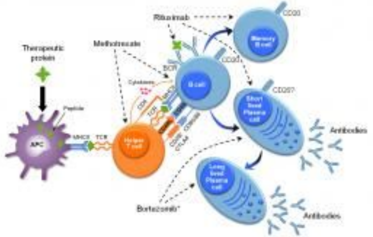






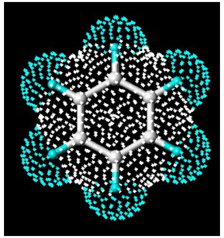
Control





Google AI Quantum

Electronic structure

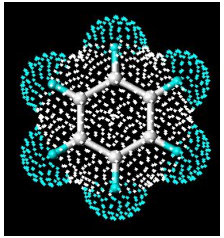


$$\mathcal{H} |\psi\rangle = E |\psi\rangle$$

"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

How big might the speedup be?

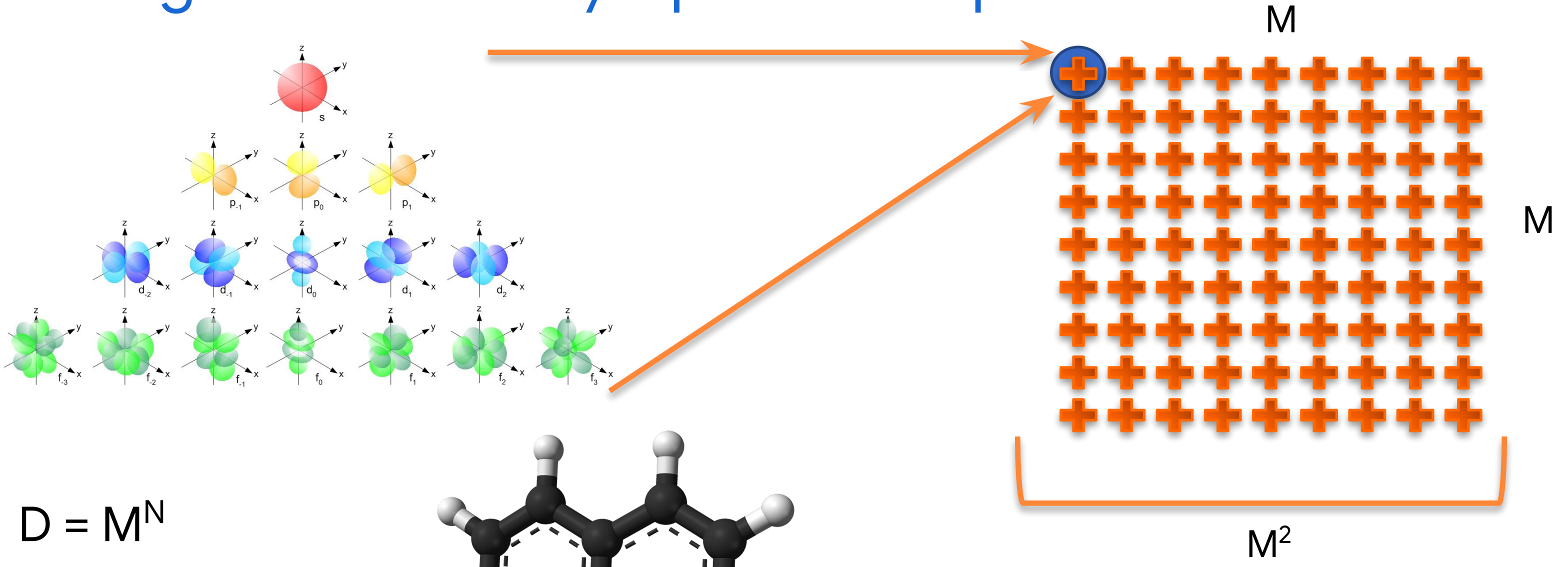


$$\mathcal{H}\left|\psi\right\rangle = E\left|\psi\right\rangle$$

Exponential Speedup: 10^{82} Years $\longrightarrow$ 300 Seconds
(Age of the Universe ~ 10^{10} Years)

Google AI Quantum

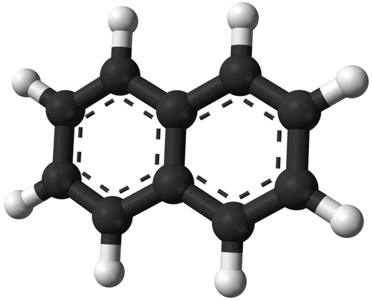
Challenge of chemistry - power of quantum



$D = M^N$

$M = 100$

$N = 80$

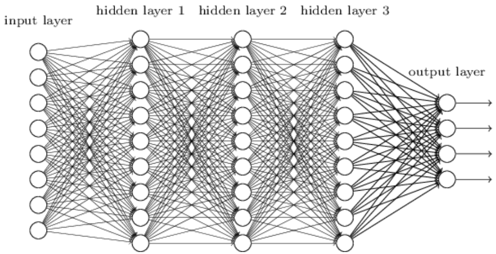


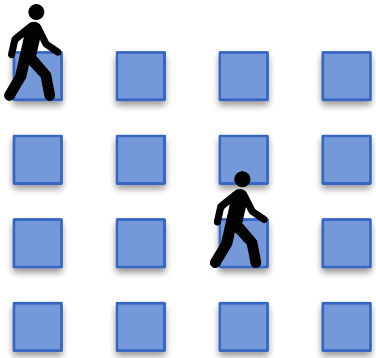
Particles in universe

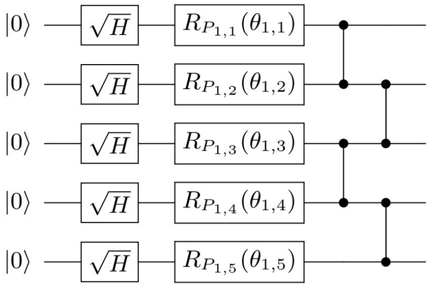
10^{80}

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

But classical probability distributions...?







$$P_1(\text{Store}_i) \qquad P_2(\text{Store}_j)$$

$$P_{12}(\text{Store}_i, \text{Store}_j) \neq P_1(\text{Store}_i)P_2(\text{Store}_j)$$

$$O(N^P)$$

Google AI Quantum

Key caveat: Our distributions may be complex valued

Towards an important problem

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

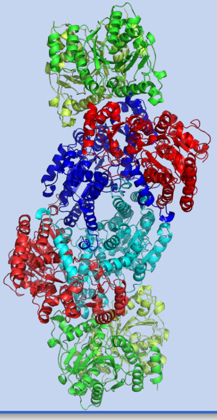
Humans: Haber Process

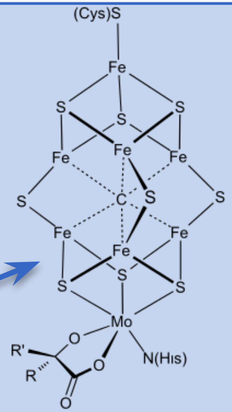
400°C & 200 atm

1-2% of ALL energy on earth, used on Haber process

Nature: Nitrogenase

25° C & 1 atm





FeMoco

Beyond current classical methods

Both electronic structure and substrate attachment almost totally unknown

Classically – No clear path to accurate solution
Quantum Mechanically – 150-200 logical qubits for solution

Google AI Quantum

Using a post-supremacy device for simulation

Goal: Simulation of interesting physical phenomena as close to classically intractable as possible

Not: Largest possible experiment one can squint at and see a curve through - **fidelity and accuracy** matter

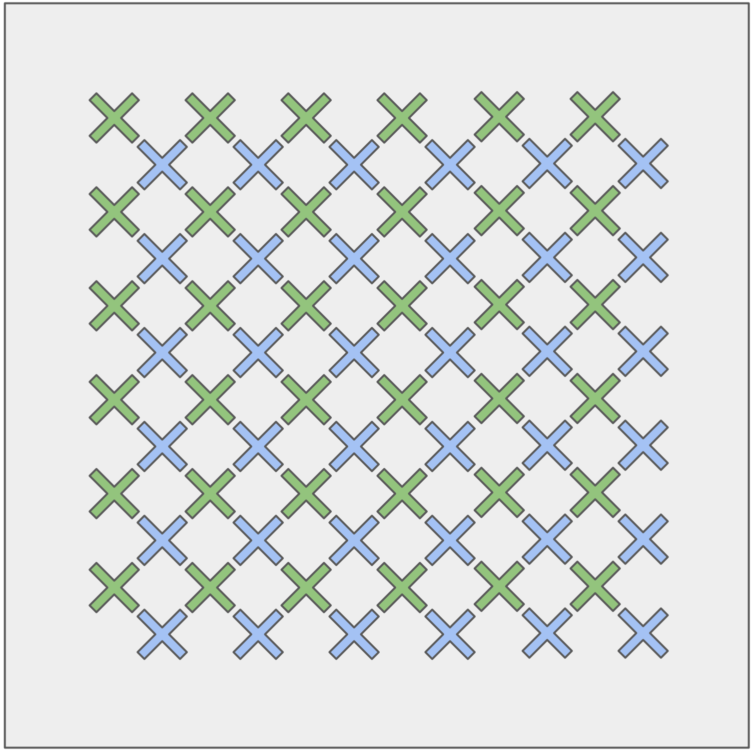
Prediction (opinion): Doing an interesting simulation beyond 20 qubits will be extremely difficult without error reduction techniques, even with great fidelities

$$f_{2q} = 0.999 \qquad F(n, L) \approx f_{2q}^{Ln/2}$$

$$\Delta_{\mathrm{H}_2} \approx 0.5 \ E_h \qquad F(20, 20) \approx 0.81$$

$$\Delta E_{\mathrm{H}_2} \geq (1 - F)\Delta_{\mathrm{H}_2} \approx 0.09 \ E_h$$

Bristlecone

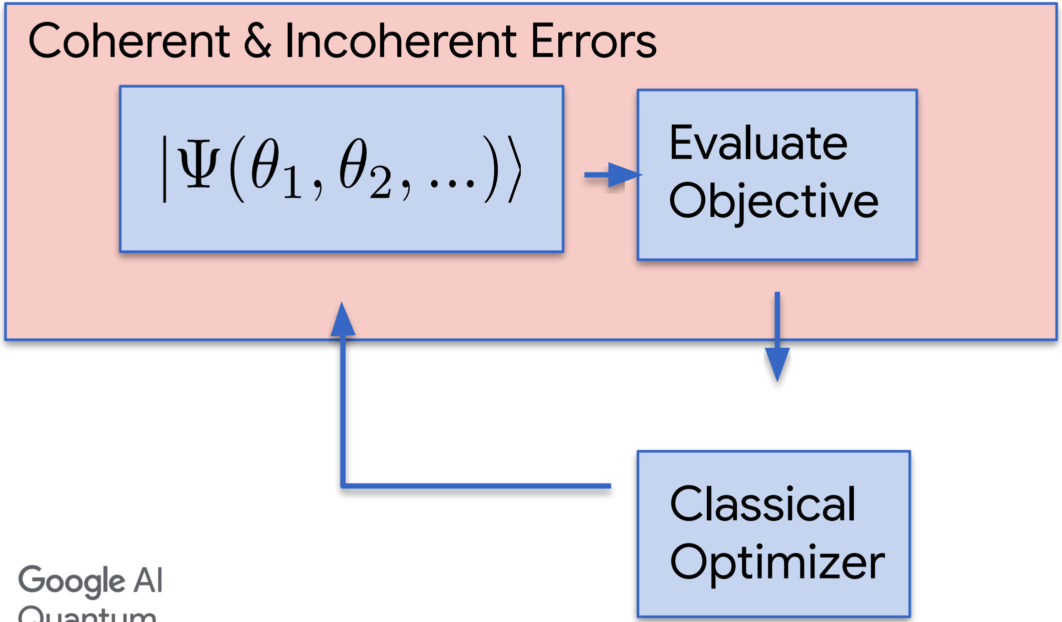


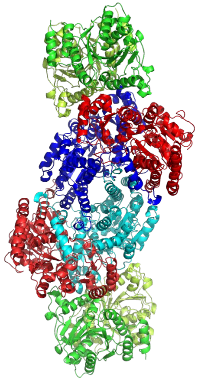
Today: Can quantum error correction theory help us on NISQ devices? And some additional challenges...

Google AI Quantum

Quantum-Classical variational algorithms in a nutshell

Solve $H|\Psi_0\rangle = E_0|\Psi_0\rangle \quad \leftrightarrow \quad \underset{|\Psi(\theta_1, \theta_2, \ldots)\rangle}{\mathrm{Min}} \langle\Psi|H|\Psi\rangle$

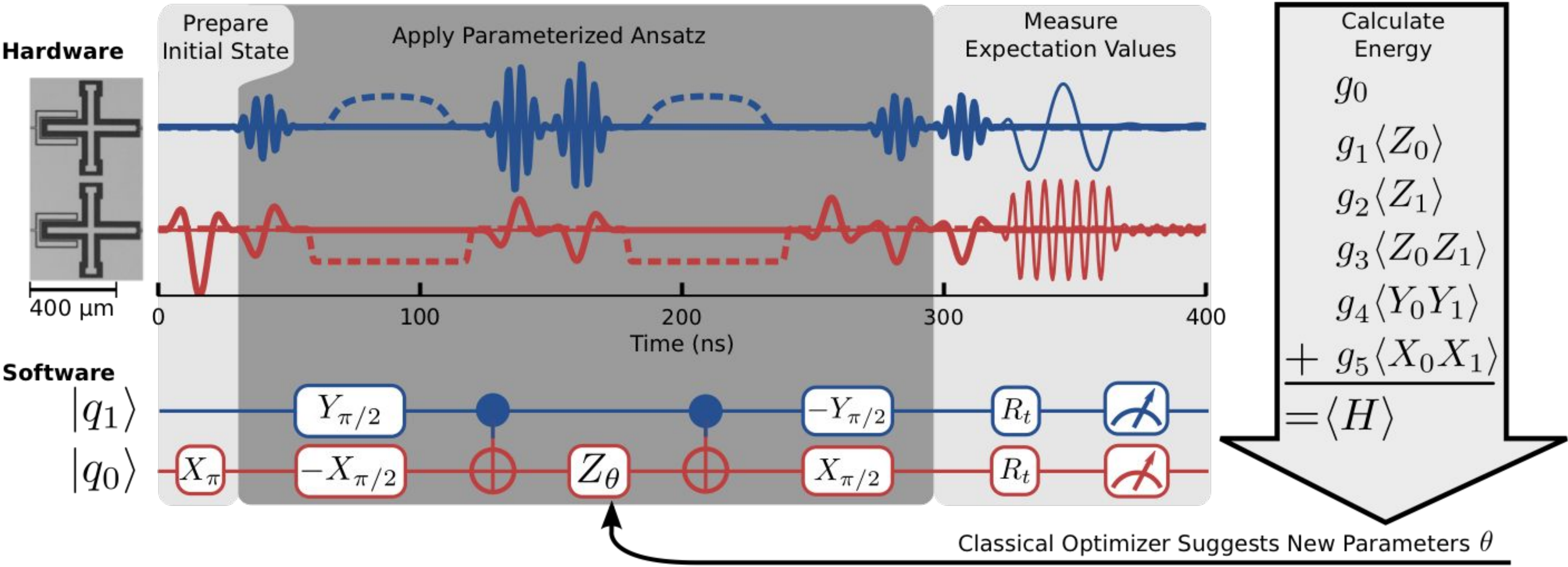




Chemistry
Nuclear Physics
Optimization (QAOA)
Machine learning
Algorithm learning
...

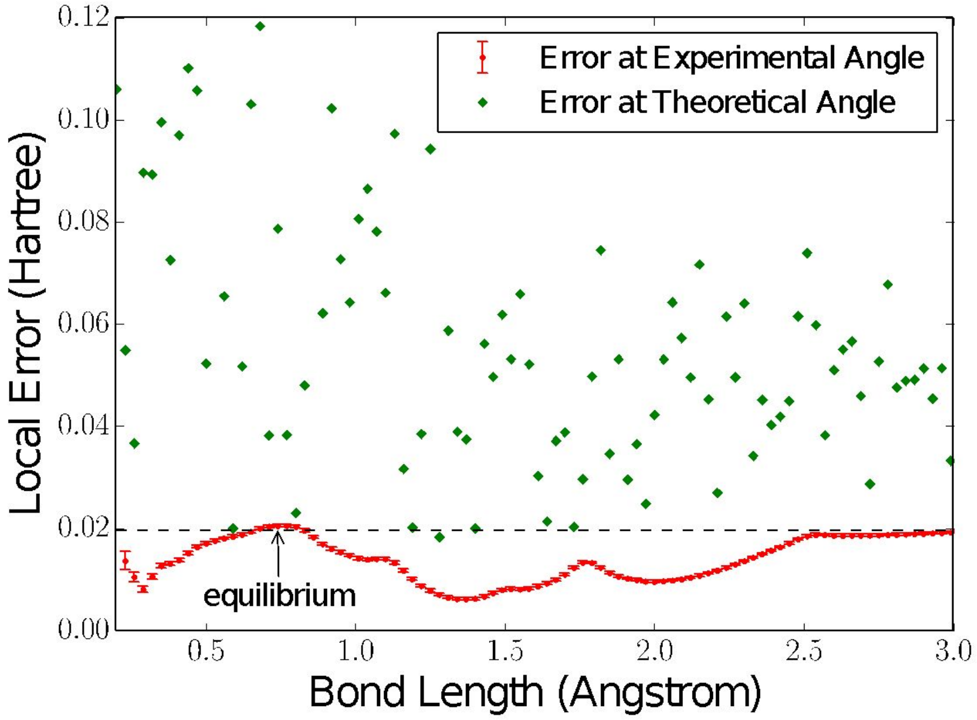
Peruzzo†, **McClean†**, Shadbolt, Yung, Zhou, Love, Aspuru-Guzik, O'Brien. *Nature Communications*, **5** (4213):1–7, 2014.
† Equal Contribution by authors

A network in hardware



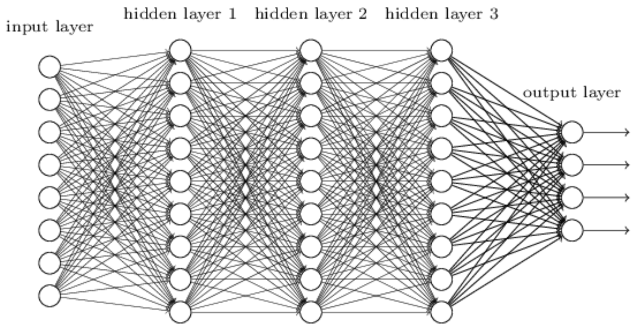
P.J.J. O'Malley, R. Babbush,..., J.R. McClean et al.
"Scalable Simulation of Molecular Energies"
Physical Review X 6 (3), 031007 (2016)

Displays natural error suppression



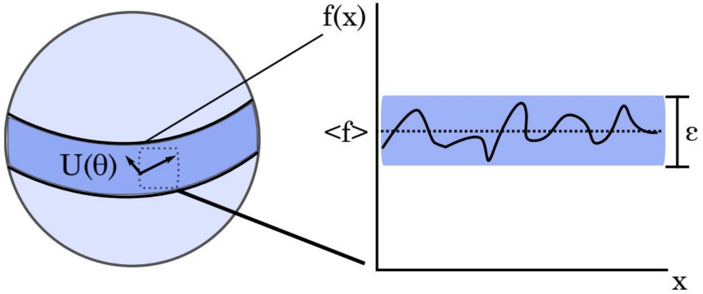
Google AI
Quantum

Learning from history - vanishing gradients



$$\delta^l = \Sigma'(z^l)(w^{l+1})^T \Sigma'(z^{l+1})(w^{l+2})^T \ldots \Sigma'(z^L)\nabla_a C$$

Loss/Objective

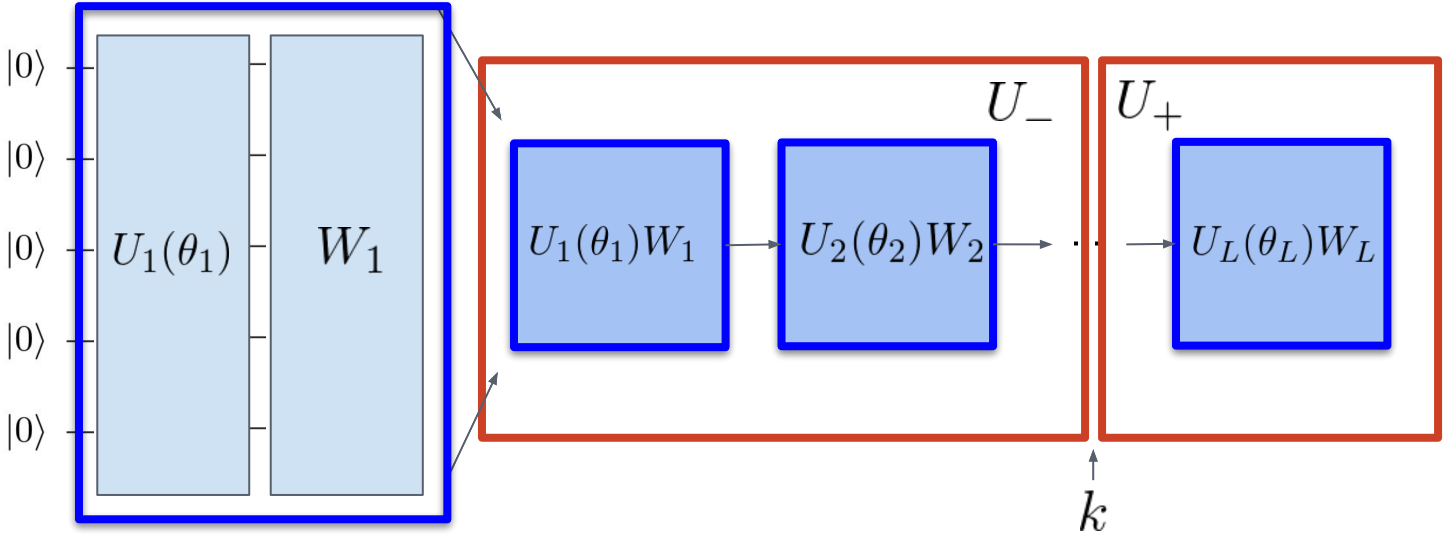


Estimation Complexity

Classical $O(\log(1/\epsilon))$

Quantum $O(1/\epsilon^{\alpha})$

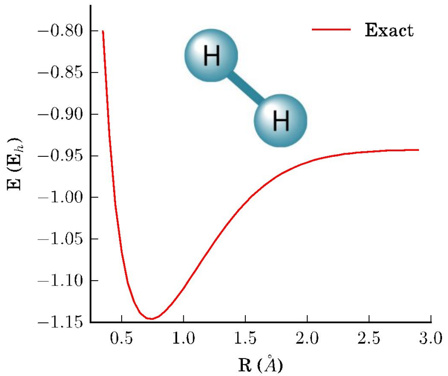
BLACK HOLES IN YOUR CIRCUITS?



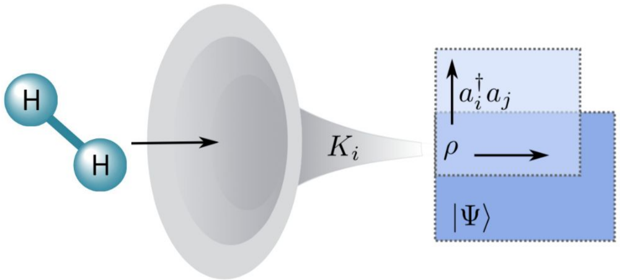
J.R. McClean, S. Boixo, V.N. Smelyanskiy, R. Babbush, H. Neven
"Barren plateaus in quantum neural network training landscapes"
Nature Communications Vol **9**, 4812 (2018)

Going beyond VQE without more qubits or gates

Quantum State on Quantum Device



Extra Quantum Measurements



Classical Generalized Eigenvalue Problem

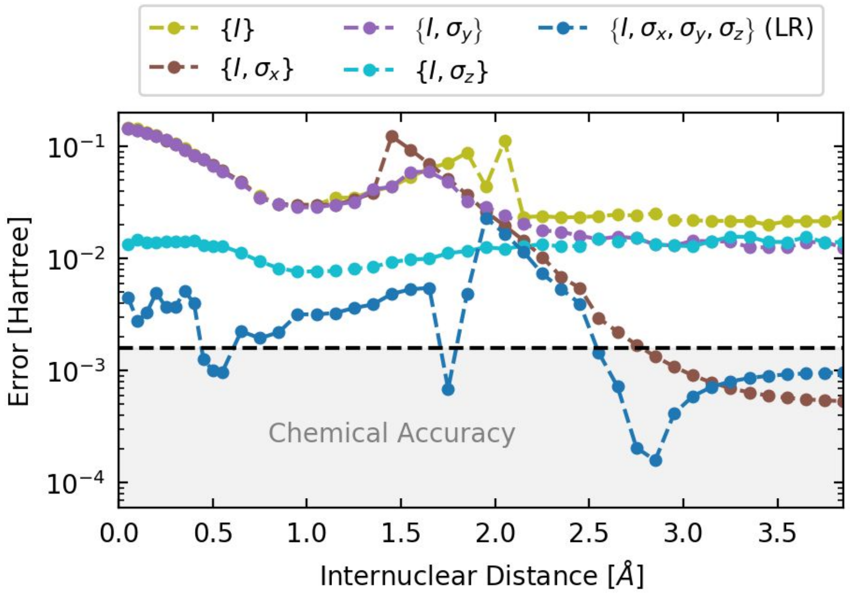
$$HC = SCE$$

A lot more than you'd think...

Google AI Quantum

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)

Surprise - Mitigates incoherent errors in experiment



"Computation of Molecular Spectra on a Quantum Processor with an Error-Resilient Algorithm"
Colless, Ramasesh, Dahlen, Blok, Kimchi-Schwartz, **McClean**, Carter, de Jong, Siddiqi
Phys. Rev. X **8**, 011021 (2018)

Google AI Quantum

Error correction at a glance

Code words / logical states

$$\bar{0} = 000 \qquad \bar{1} = 111$$

Ex. Single Bit Flip

$$\bar{0}' = 100 \xrightarrow{\text{Majority Vote}} \bar{0}$$

Ex. Two Bit Flips

$$\bar{0}'' = 101 \xrightarrow{\text{Majority Vote}} \bar{1}$$

Code words / logical states

$$|\bar{0}\rangle = |000\rangle \qquad |\bar{1}\rangle = |111\rangle$$

$$|\bar{\Psi}\rangle = \alpha|000\rangle + \beta|111\rangle$$

Ex. Single Bit Flip

$$|\bar{\Psi}'\rangle = \alpha|100\rangle + \beta|011\rangle$$

$$\{Z_1Z_2, Z_2Z_3\} \rightarrow \{s_1, s_2\}$$

$$\Big\downarrow \text{Decode error, Recover}$$

$$|\bar{\Psi}\rangle = \alpha|000\rangle + \beta|111\rangle$$

Google AI Quantum

A sketch of stabilizer codes

Choose a commuting group of Pauli operators on n qubits $\mathcal{S}$
denote this the “stabilizer group”

Define codewords to be set of +1 eigenstates of these operators

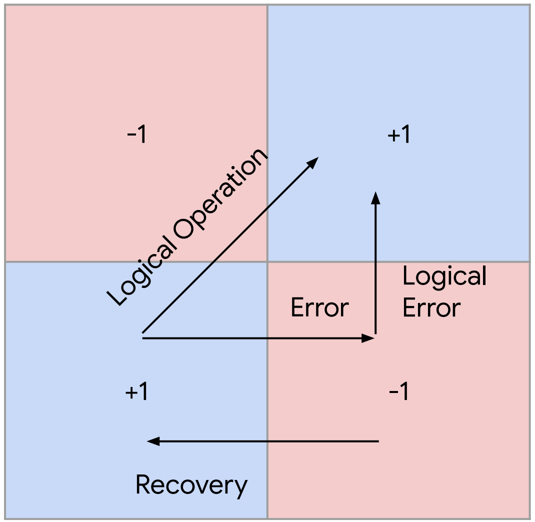
Ex. For the repetition code $\mathcal{S} = \langle Z_1 Z_2, Z_2 Z_3 \rangle$

Choose a set of commuting operators from the Pauli group $\mathcal{L}$
to denote logical operations

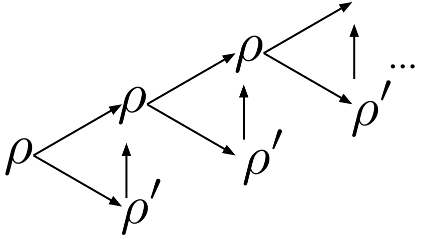
Ex. For the repetition code

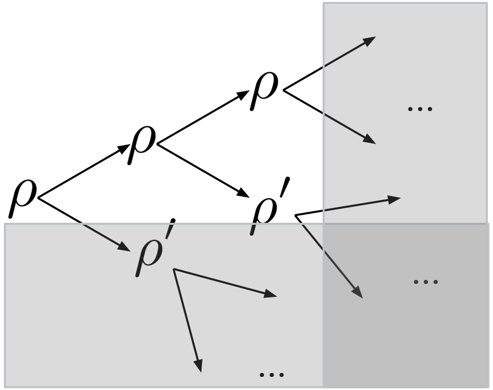
$$\mathcal{L} = \langle X_1 X_2 X_3, Z_1 Z_2 Z_3 \rangle$$

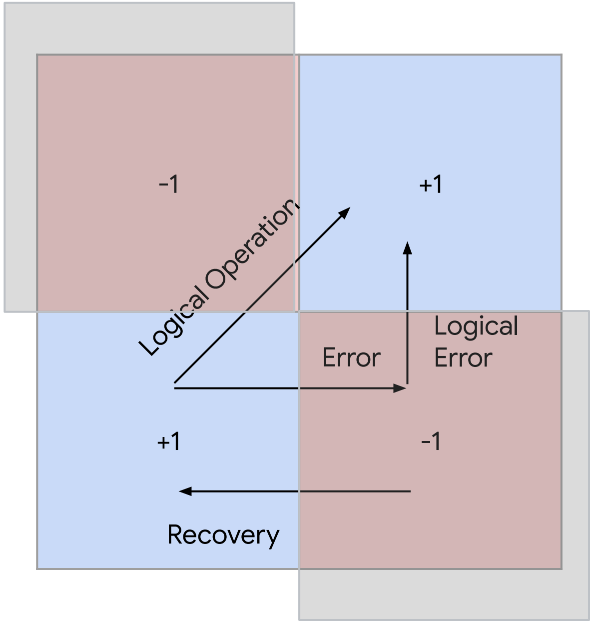
$$\bar{X}|\bar{0}\rangle = X_1 X_2 X_3 |000\rangle = |111\rangle = |\bar{1}\rangle$$



Error correction vs projection







(+) Scalable to exponential error suppression
(-) Requires explicit syndrome measurements
(-) Requires feedforward or unitary decoding

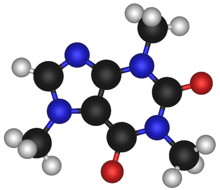
$$P_i = \frac{1}{2}(1 + S_i) \qquad \bar{P}_{\text{code}} = \prod_i P_i$$

(+) Often reduces errors considerably for small experiments
(+) Doesn't require explicit syndrome measurements or feedforward
(+) Can be used to test codes without full hardware for correction
(+) Like error detection but without explicit stabilizers and can explore some recovery channels
(-) May require many measurement repetitions
(-) Not scalable to exponential error suppression by construction

Domain knowledge matters

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	$\mathcal{O}(N)$

Typical chemistry problem workflow



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

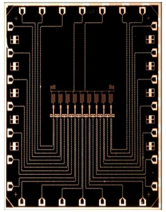
$$H = \sum_{ij} h_{ij} a_i^\dagger a_j + \frac{1}{2} \sum_{ijkl} h_{ijkl} a_i^\dagger a_j^\dagger a_k a_l$$

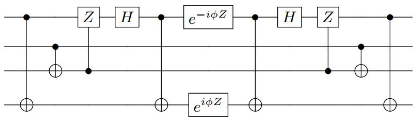
Integral Generation
- Depends on basis set, often uses external software

Starter Calculation (e.g. Hartree-Fock)
- Integral basis change
- Initial state preparation

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

Map to Qubits
- Jordan-Wigner
- Bravyi-Kitaev



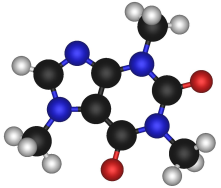


Select Problem & Algorithm
- Energies, properties etc.
- Quantum Phase Estimation
- Variational Quantum Eigensolver (& Ansatz)

Map to hardware

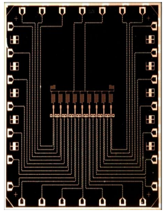
Google AI Quantum

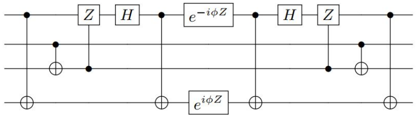
Typical chemistry problem workflow



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

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





Google AI Quantum

```
geometry = [['H', [0, 0, 0]],
            ['H', [0, 0, 0.74]]]
basis = 'sto-3g'
multiplicity = 1
charge = 0
h2_molecule = MolecularData(geometry, basis,
    multiplicity, charge)
```

```
h2_hamiltonian = (run_psi4(h2_molecule).
    get_molecular_hamiltonian())
```

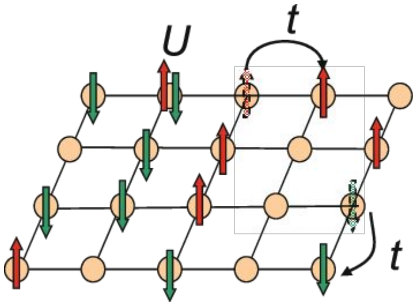
```
h2_qubit = (jordan_wigner(
    get_fermion_operator(h2_hamiltonian)))
```

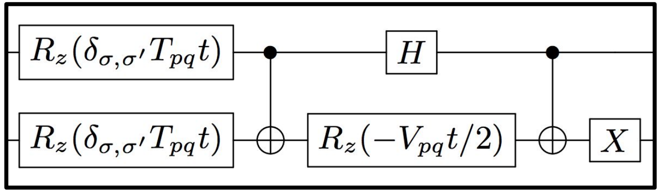
```
...
evolution_operator = (
    uccsd_singlet_evolution(test_amplitudes,
                            n_qubits,
                            n_electrons))
evolution_operator | wavefunction
...
```

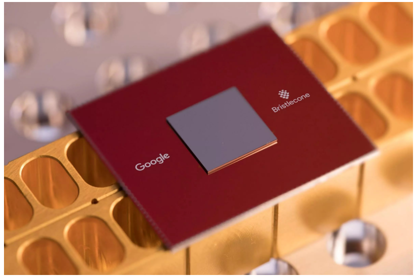
OF-Cirq

OpenFermion **is**

- An open source Python framework for quantum simulation on near term quantum hardware







Google AI
Quantum

The Electronic Structure Package for Quantum Computers

OpenFermion

www.openfermion.org/

pyscf

PSI4 OPEN-SOURCE QUANTUM CHEMISTRY

OpenFermion is an Apache 2 open source project for quantum simulation:

- Generate Hamiltonians for arbitrary molecules and materials in arbitrary basis sets
- Automatically compiles quantum algorithms to circuits for execution on hardware
- Google software engineering standards enforced; ~50K lines of code at 99.9% test coverage

OpenFermion is a community! Over two dozen contributors from over a dozen institutions

200 active (visible) forks

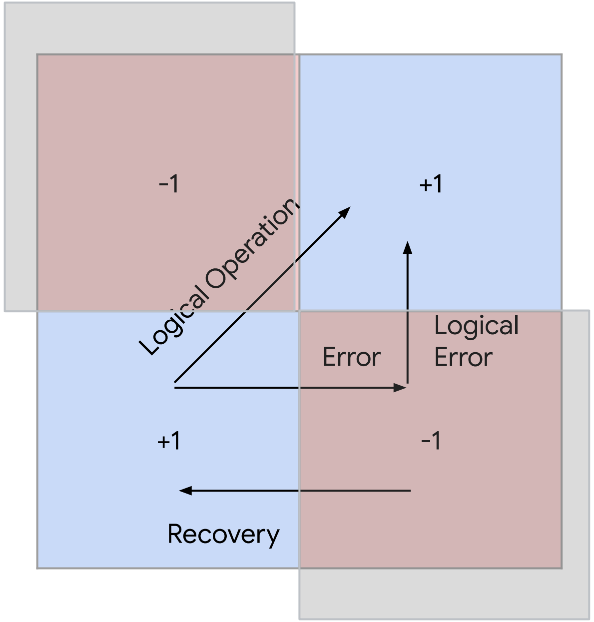
Framework and platform agnostic

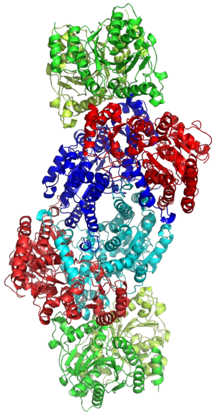
- Works with Microsoft LIQUID, IBM QISKit, Google Cirq, Xanadu Strawberry, Rigetti Forest, etc.
- Runs on Linux, Mac, and Windows with optional Docker installation

Summarizing...

Bristlecone

Progress has been rapid in hardware and algorithms
Even with a great device, will be challenging to get good simulations





OpenFermion

Google AI Quantum

Acknowledgements

DOE CSGF

Google

Google
Zhang Jiang
Ryan Babbush
Nicolas Rubin
Sergio Boixo
Vadim Smelyanskiy
Hartmut Neven

Daimler
Tyler Takeshita