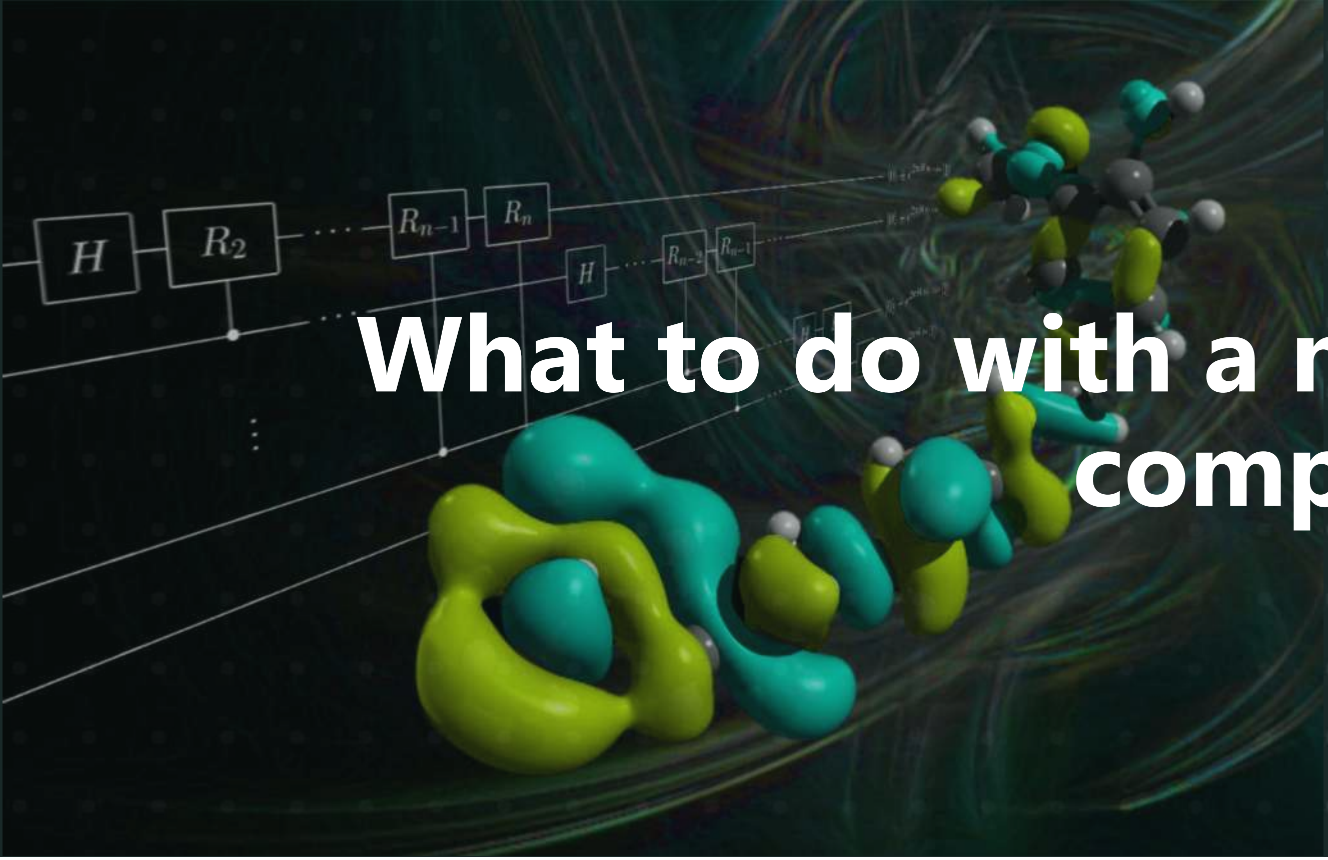



# What to do with a near-term quantum computer

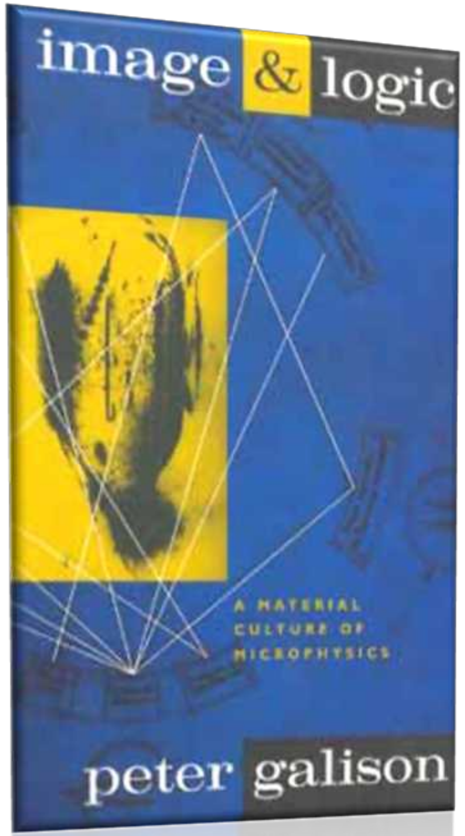
**Alán Aspuru-Guzik**
Professor of Chemistry and Computer Science
University of Toronto
Vector Institute for Artificial Intelligence

# Early classical mechanical simulators

Antykythera Mechanism

circa 200 BC

# Digital computer simulators




Without the computer-based simulation, the material culture of late-twentieth-century microphysics is not merely inconvenienced – It does not exist. […] Machines […] are inseparable from their virtual counterparts – all are bound to simulations.

–Peter Galison

From *Image and Logic: A material culture of microphysics* (1997)

“[H]e produced a paper tape of his whole computer program and unrolled it along the length of the chemical lecture bench. There, in one roll, was something, of which one could ask a chemical question at one end and it would produce an answer at the other! . . . most of the audience probably thought the demonstration bizarre. But it was prescient”

Handy, Pople, Shavitt, JPCA (1996)

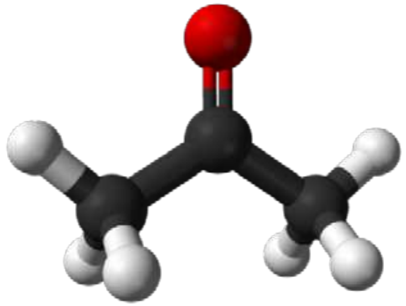
Samuel F. Boys


Richard P. Feynman,
Simulating Physics with Computers
Int. J. Theor. Phys. (1982)


What happens on your iPhone, stays on your iPhone.
apple.com/privacy
SPRINGHILL SUITES
Marriott
Elite

# The quantum simulation way

quantum system

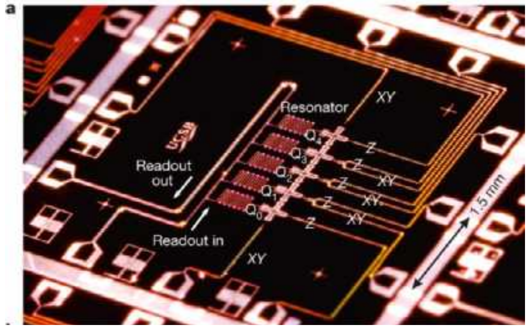


$$\hat{H}|\Psi\rangle = E|\Psi\rangle$$

quantum model
(quantum information)

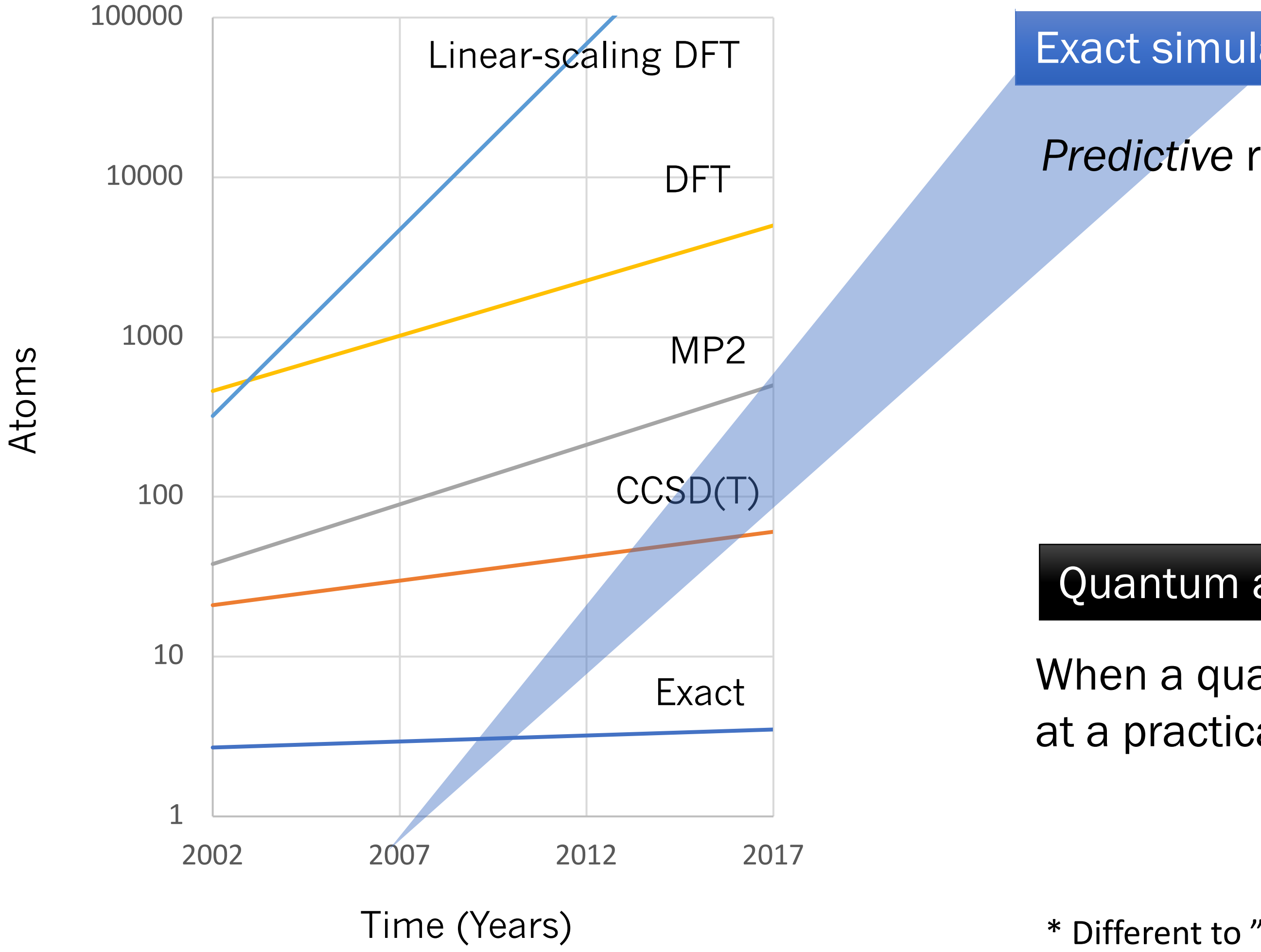
classical information

E= -192.0492
Hartree




Quantum information processor

# Disruption and quantum simulation




**Exact simulation via quantum computers**

*Predictive* rather than explanatory simulation of matter

**Quantum advantage***

When a quantum computer outperforms a classical computer at a practical stask

* Different to ”quantum supremacy”

# Quantum computers intro

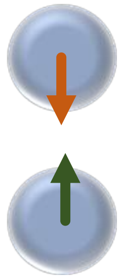
1 ——

0 ——

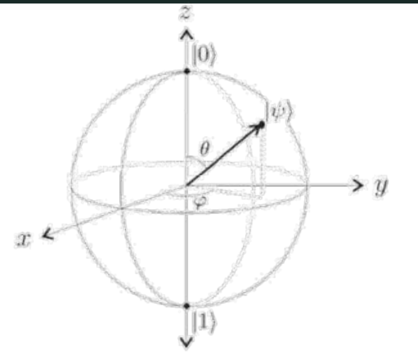
classical bit

$|1\rangle$ ——

$|0\rangle$ ——



quantum bit




$$|\psi\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\phi}\sin\frac{\theta}{2}|1\rangle$$

Bloch sphere

**quantum bit**

Superposition

Entanglement

Collapse upon measurement

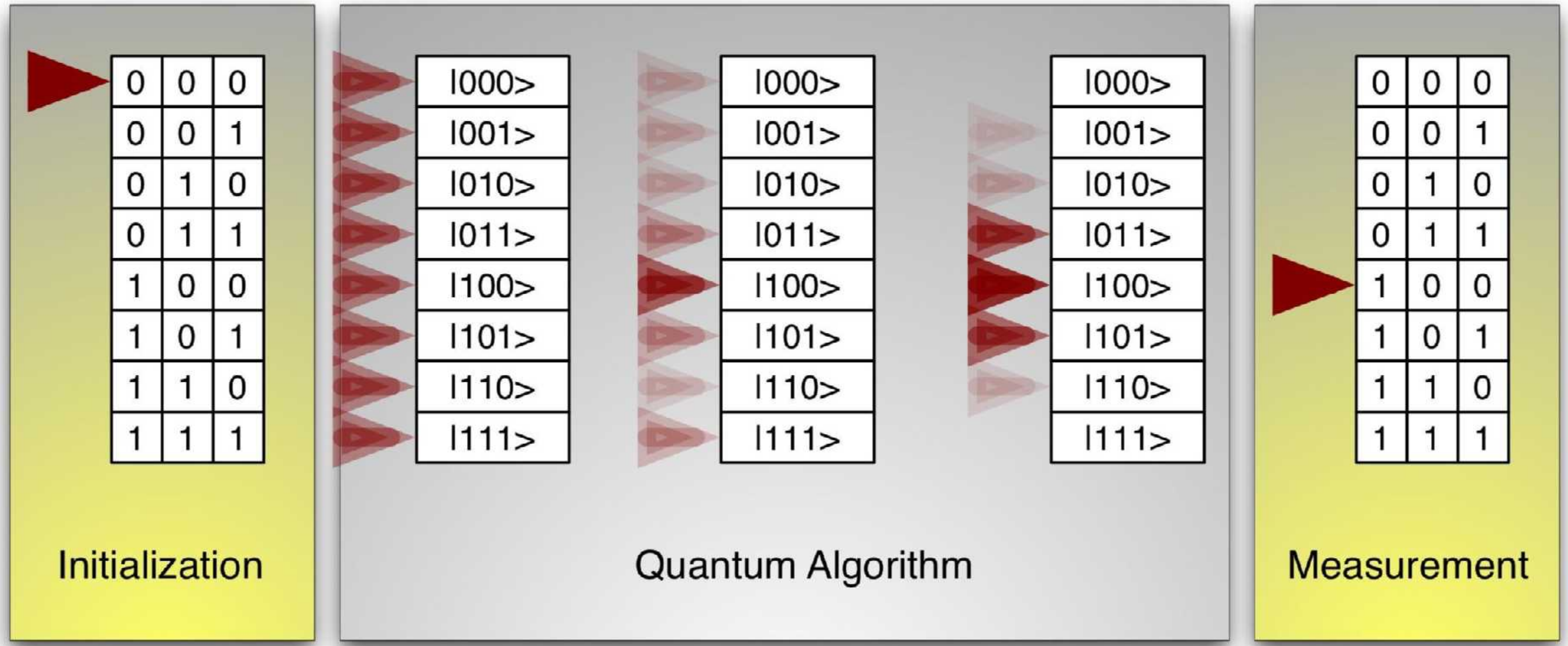
**quantum computer**

Collection of controllable qubits

Subject to decoherence

Ability for quantum error correction

# Quantum computation



# Quantum gates and circuits

## Single qubit gates

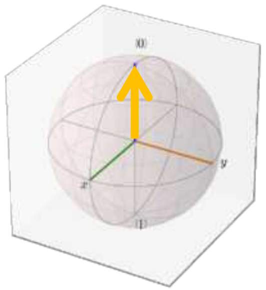
### Rotations

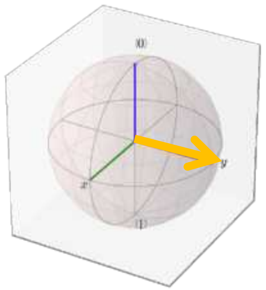
$$-\boxed{R_{\hat{n}}}- = \exp[-i(\vec{\sigma}.\hat{n})\theta/2]$$

$$\vec{\sigma} \equiv [\sigma_x, \sigma_y, \sigma_z]$$

### Hadamard gate

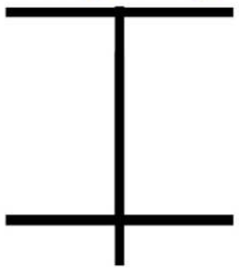
$$-\boxed{H}- = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$





## Two qubit gates

### Controlled-not (CNOT) gate

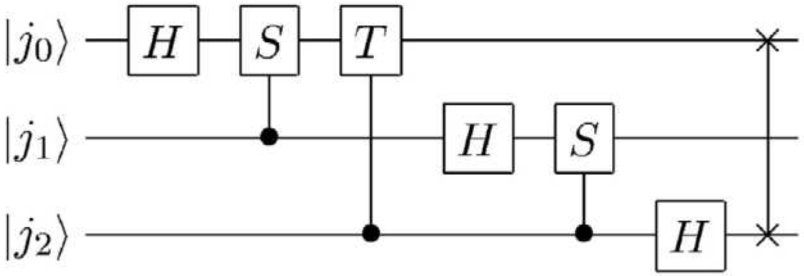


$$= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

$$\begin{array}{ccc} |00\rangle & \rightarrow & |00\rangle \\ |01\rangle & \rightarrow & |01\rangle \\ |10\rangle & \rightarrow & |11\rangle \\ |11\rangle & \rightarrow & |10\rangle \end{array}$$

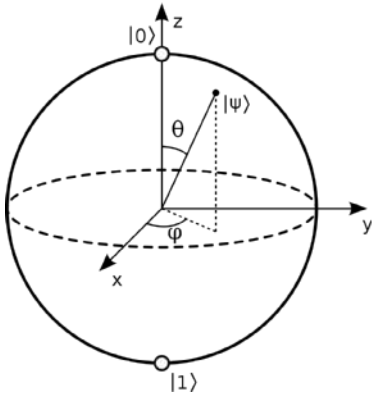
## Subroutines

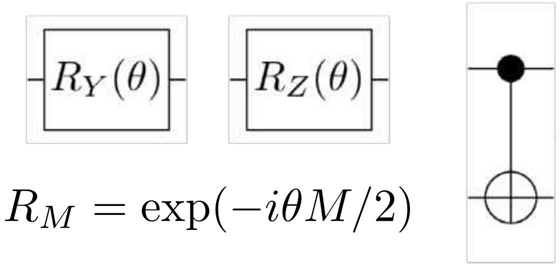
### Quantum Fourier Transform



# Quantum computing with quantum circuits in one slide

Information is stored on qubit registers



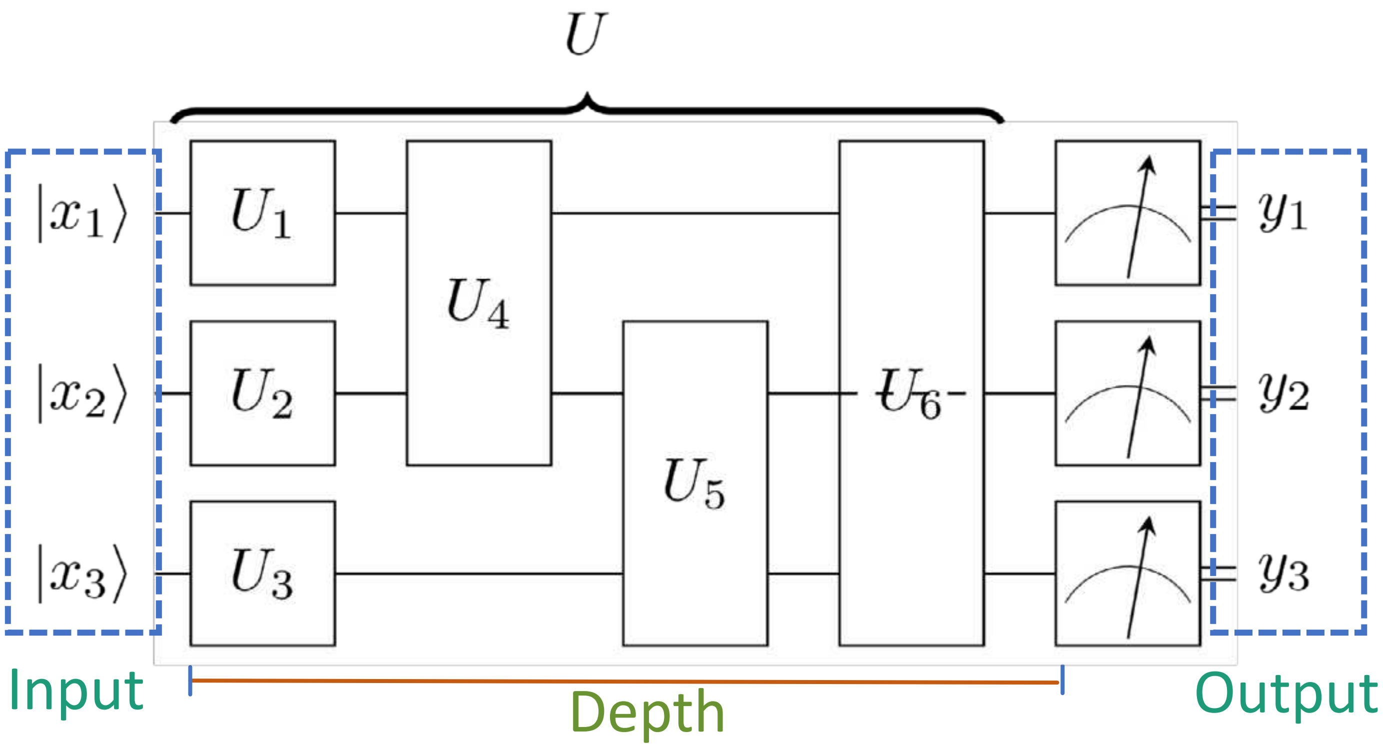




$$R_M = \exp(-i\theta M/2)$$

$$= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

$$X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}; \quad Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}; \quad Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

Example of a universal gate set

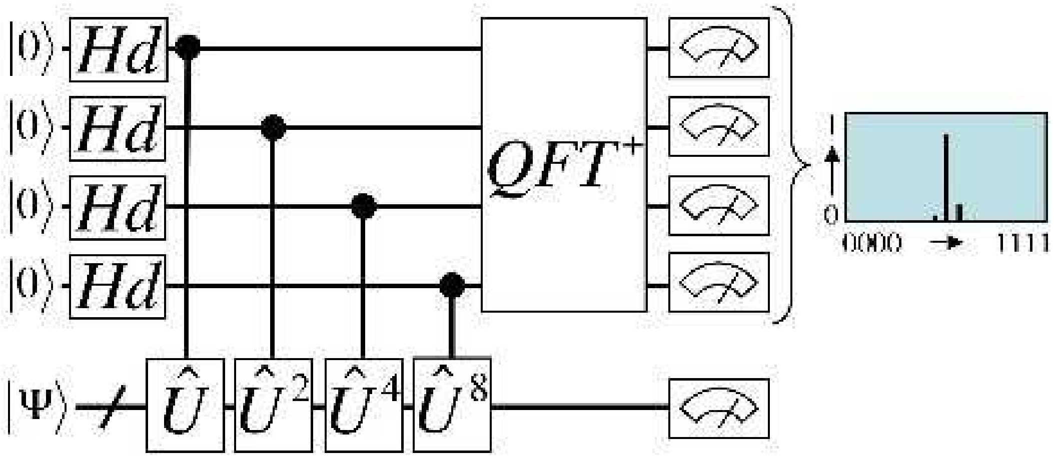



$$U\,|x_1,\ldots,x_n,0,\ldots,0\rangle = \sum_{y_1,\ldots,y_m} c_{y_1,\ldots,y_m}\,|y_1,\ldots,y_m\rangle$$

$$F:\{0,1\}^n \to \{0,1\}^m \quad if \quad |c_{F(x_1,\ldots,x_m)}|^2 = 1-\epsilon$$

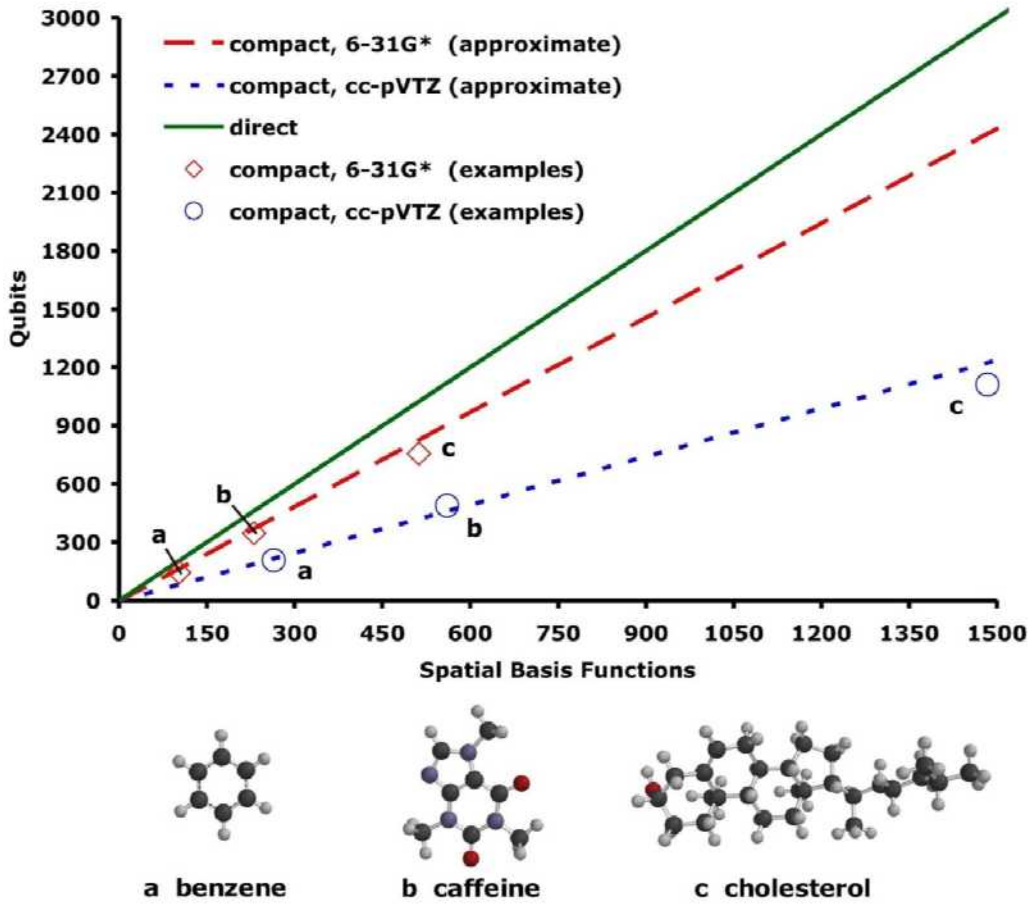
# Quantum compujting for Chemistry circa 2005

Quantum phase estimation algorithm



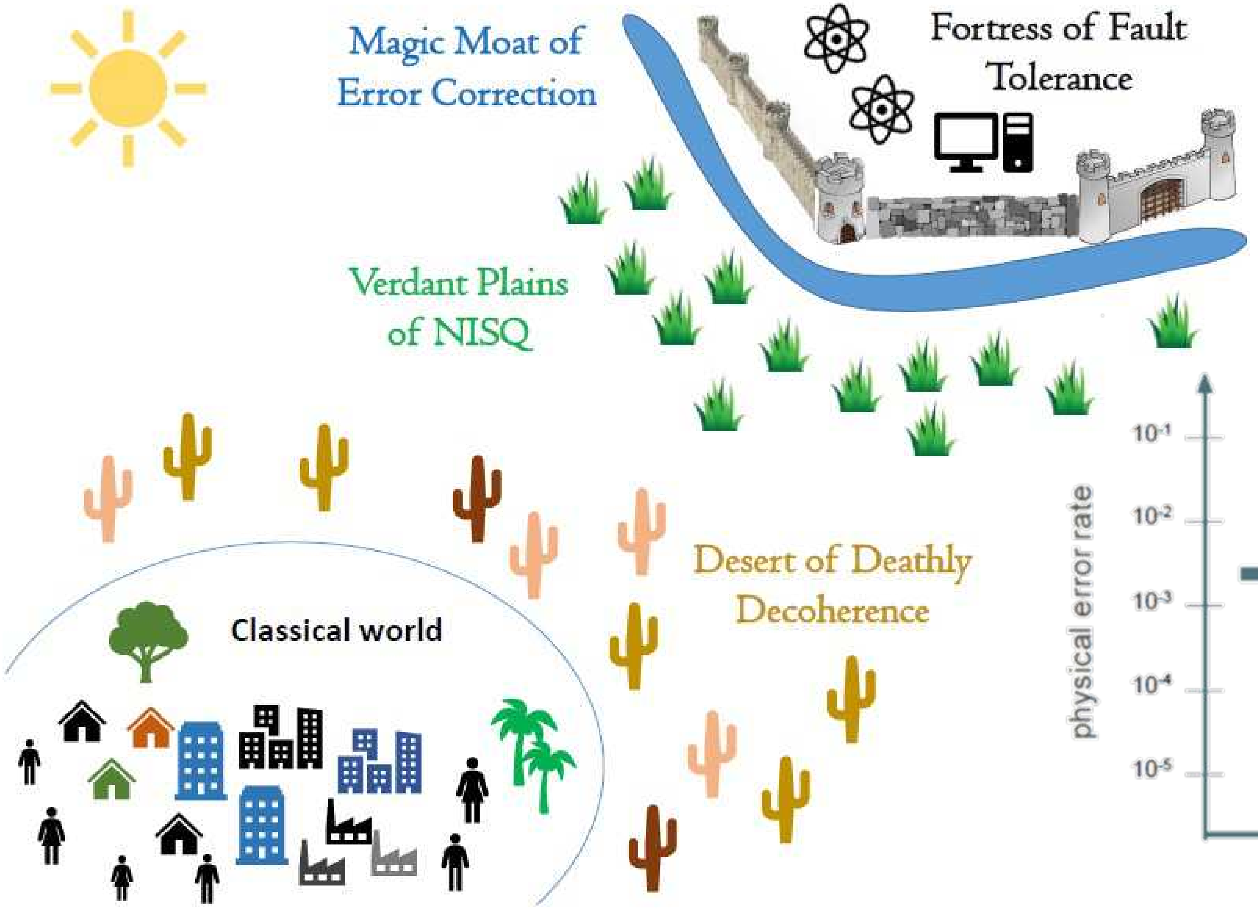

Choose $t$; $Et = -2\pi\phi$

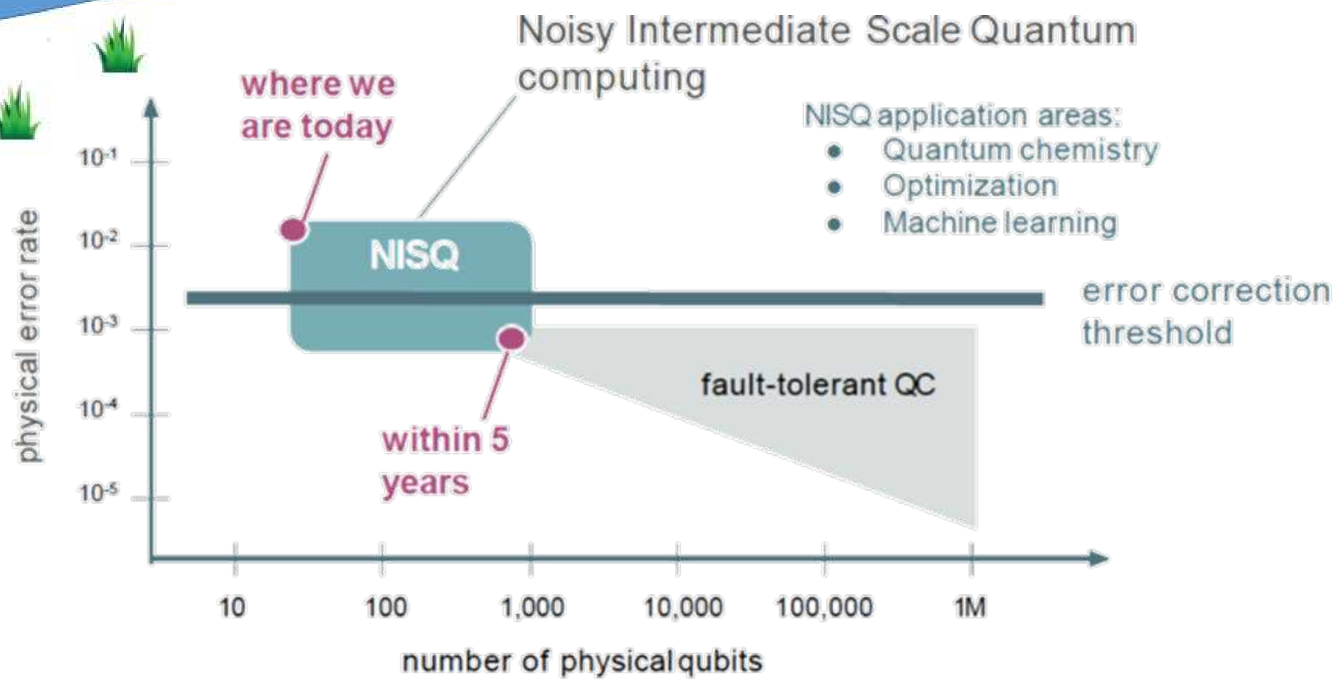
$$\hat{U}(t)|\Psi\rangle = e^{-i\hat{H}t}|\Psi\rangle = e^{-iEt}|\Psi\rangle$$




A. Aspuru-Guzik, A. D. Dutoi, P. J. Love, M. Head-Gordon, Science (2005) **Full quantum circuit**: J. D. Whitfield, et. al., Mol. Phys. (2011) **Error correction**: N. Cody Jones, J. D. Whitfield, et al. New. J. Phys.(2012)

# Noisy intermediate  scale quantum (NISQ) computers




"Quantum computing in the NISQ era and beyond" Preskill, 2018 https://arxiv.org/abs/1801.00862

Left figure: Daniel Gottesman

Preskill, 2018 arXiV:180100862

# Noisy intermediate  scale quantum (NISQ) algorithms

**Noisy intermediate-scale quantum (NISQ) algorithms**

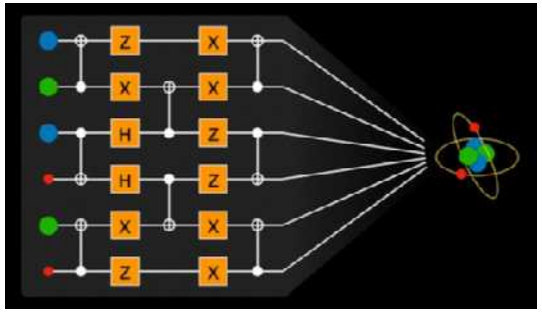
Kishor Bharti,[1,*] Alba Cervera-Lierta,[2,3,*] Thi Ha Kyaw,[2,3,*] Tobias Haug,[4] Sumner Alperin-Lea,[3] Abhinav Anand,[3] Matthias Degroote,[2,3,5] Hermanni Heimonen,[1] Jakob S. Kottmann,[2,3] Tim Menke,[6,7,8] Wai-Keong Mok,[1] Sukin Sim,[9] Leong-Chuan Kwek,[1,10,11,†] and Alán Aspuru-Guzik[2,3,12,13,‡]

arXiv:2101.08448v1

**Quantum Chemistry in the Age of Quantum Computing**

Yudong Cao, Jonathan Romero, Jonathan P. Olson, Matthias Degroote, Peter D. Johnson, Mária Kieferová, Ian D. Kivlichan, Tim Menke, Borja Peropadre, Nicolas P. D. Sawaya, Sukin Sim, Libor Veis, and Alán Aspuru-Guzik*

Cite this: *Chem. Rev.* 2019, 119, 19, 10856–10915

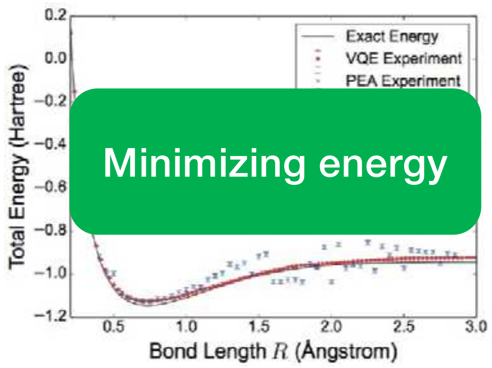

Quantum computational chemistry

Sam McArdle, Suguru Endo, Alán Aspuru-Guzik, Simon C. Benjamin, and Xiao Yuan
Rev. Mod. Phys. **92**, 015003 – Published 30 March 2020

# Variational quantum algorithms

Variational quantum eigensolver

Peruzzo et al.
Nat Comm (2014)




Quantum adiabatic optimization algorithm

Farhi et al. (2014)


Quantum autoencoders

Romero, et al.
Quantum Sci. Technol. (2017)


Variational Quantum Generators

Romero, et al.
arXiv:1901.00848 (2019)

# NISQ algorithms: many body physics

| Algorithm/Application | Proposed implementations |
|---|---|
| Variational quantum eigensolver (VQE) and related solvers | |
| VQE | (McClean *et al.*, 2016; Peruzzo *et al.*, 2014; Wecker *et al.*, 2015) |
| Adaptive VQE | (Grimsley *et al.*, 2019b; Ryabinkin *et al.*, 2018b; Sim *et al.*, 2020) |
| IQAE | (Bharti, 2020; Bharti and Haug, 2020a) |
| Krylov approaches | (Huggins *et al.*, 2020; Jouzdani and Bringuier, 2020; Stair *et al.*, 2020) |
| Imaginary time evolution | (Bharti and Haug, 2020b; McArdle *et al.*, 2019a; Motta *et al.*, 2020; Sun *et al.*, 2020c) |
| VQE for excited states | |
| Folded spectrum | (Peruzzo *et al.*, 2014; Ryabinkin *et al.*, 2018a) |
| Orthogonally constrained VQE | (Higgott *et al.*, 2019; Kottmann *et al.*, 2020b; Lee *et al.*, 2018) |
| Subspace expansion and linear-response based | (McClean *et al.*, 2017; Ollitrault *et al.*, 2020; Takeshita *et al.*, 2020) |
| Subspace-search VQE | (Nakanishi *et al.*, 2019) |
| Multistate contracted VQE | (Parrish *et al.*, 2019a) |
| Fourier transform of evolutions | (Aleiner *et al.*, 2020; Roushan *et al.*, 2017) |
| WAVES | (Santagati *et al.*, 2018) |
| Adiabatically-Assisted | (Garcia-Saez and Latorre, 2018; McClean *et al.*, 2016) |
| Hamiltonian simulation | |
| Variational quantum simulator | (Endo *et al.*, 2020c; Kubo *et al.*, 2020; Li and Benjamin, 2017; McArdle *et al.*, 2019a; Yuan *et al.*, 2019) |
| Subspace variational quantum simulator | (Heya *et al.*, 2019) |
| Variational fast forwarding | (Cirstoiu *et al.*, 2020; Commeau *et al.*, 2020) |
| Quantum assisted simulator | (Bharti and Haug, 2020b) |
| Quantum information scrambling and thermalization | |
| Scrambling | (Holmes *et al.*, 2020; Joshi *et al.*, 2020; Landsman *et al.*, 2019) |
| Thermal state | (Verdon *et al.*, 2019b) |
| Open quantum systems | |
| Generalized variational quantum simulator | (Endo *et al.*, 2020c; Liu *et al.*, 2020b; Yuan *et al.*, 2019) |
| Generalized quantum assisted simulator | (Haug and Bharti, 2020) |
| Trotter simulation | (Hu *et al.*, 2020; Koppenhöfer *et al.*, 2020) |
| | |
| State preparation | |
| Non-equilibrium steady state | (Yoshioka *et al.*, 2020)(Endo *et al.*, 2020b; Jaderberg *et al.*, 2020; Kreula *et al.*, 2016) |
| Gibbs-state | (Chowdhury *et al.*, 2020; Endo *et al.*, 2020c; Haug and Bharti, 2020) |
| Many-body ground state | (Ho and Hsieh, 2019; Ho *et al.*, 2019; Wauters *et al.*, 2020a) |
| Quantum autoencoder | |
| Quantum autoencoder | (Bondarenko and Feldmann, 2020; Bravo-Prieto, 2020; Huang *et al.*, 2020a,b; Pepper *et al.*, 2019; Romero *et al.*, 2017) |
| Quantum computer-aided design | |
| Optical setups | (Kottmann *et al.*, 2020c) |
| Superconducting circuits | (Kyaw *et al.*, 2020b) |

Table I NISQ algorithms for Many-body physics and chemistry applications from Sec. V.A.

# NISQ algorithms: machine learning and optimization

| Algorithm/Application | Proposed implementations |
|---|---|
| | Supervised learning |
| Quantum kernel methods | (Havlíček *et al.*, 2019; Kusumoto *et al.*, 2019; Schuld *et al.*, 2020b; Schuld and Killoran, 2019) |
| Variational quantum classifiers (VQC) | (Farhi and Neven, 2018; Lloyd *et al.*, 2020; Mitarai *et al.*, 2018; Pérez-Salinas *et al.*, 2020a; Schuld *et al.*, 2020a,c; Vidal and Theis, 2019) |
| Encoding strategies in VQA | (Cervera-Lierta *et al.*, 2020; Mitarai *et al.*, 2019) |
| Quantum reservoir computing | (Chien and Whitfield, 2020; Fujii and Nakajima, 2017; Ghosh *et al.*, 2019; Mitarai *et al.*, 2018; Nakajima *et al.*, 2019; Negoro *et al.*, 2018; Nokkala *et al.*, 2020) |
| Supervised QUBO classifier | (Li *et al.*, 2018) |
| | Unsupervised learning |
| Quantum Boltzmann machines (QBM) | (Amin *et al.*, 2018; Kieferová and Wiebe, 2017; Zoufal *et al.*, 2020) |
| Quantum circuit Born machines (QCBM) | (Alcazar *et al.*, 2020; Benedetti *et al.*, 2019a; Coyle *et al.*, 2020a; Hamilton *et al.*, 2019; Leyton-Ortega *et al.*, 2019; Liu and Wang, 2018; Rudolph *et al.*, 2020) |
| Quantum generative adversarial networks (QGAN) | (Dallaire-Demers and Killoran, 2018; Hu *et al.*, 2019; Lloyd and Weedbrook, 2018; Romero and Aspuru-Guzik, 2019; Situ *et al.*, 2020; Zeng *et al.*, 2019) |
| | Reinforcement learning |
| Reinforcement learning | (Albarrán-Arriagada *et al.*, 2020; Cárdenas-López *et al.*, 2018; Chen *et al.*, 2020; Crawford *et al.*, 2016; Jerbi *et al.*, 2019; Lamata, 2017; Lockwood and Si, 2020a,b; Yu *et al.*, 2019) |

Table II NISQ algorithms for machine learning applications from Sec. V.B.

| Algorithm/Application | Proposed implementations |
|---|---|
| Max cut | (Bravyi *et al.*, 2019; Farhi *et al.*, 2014; Hastings, 2019; Headley *et al.*, 2020; Otterbach *et al.*, 2017) |
| Max clique | (Arrazola and Bromley, 2018; Banchi *et al.*, 2020a) |
| Maximum independent set | (Choi *et al.*, 2020; Saleem, 2020; Utkarsh *et al.*, 2020) |
| Max hafnian | (Arrazola *et al.*, 2018) |
| Vertex cover | (Cook *et al.*, 2019) |
| Exact cover | (Bengtsson *et al.*, 2020; Garcia-Saez and Latorre, 2018; Vikstål *et al.*, 2020) |
| Knapsack | (de la Grand'rive and Hullo, 2019) |
| Graph multi-coloring | (Oh *et al.*, 2019) |

Table III NISQ algorithms for combinatorial optimization from Sec. V.C.

# NISQ algorithms: numerical solvers, finance

| Algorithm/Application | Proposed implementations |
|---|---|
| Factoring | (Anschuetz *et al.*, 2019; Karamlou *et al.*, 2020) |
| SVD | (Bravo-Prieto *et al.*, 2020; Wang *et al.*, 2020c) |
| Linear systems | (Bravo-Prieto *et al.*, 2019; Huang *et al.*, 2019; Xu *et al.*, 2019b) |
| Non-linear differential equations | (Gaitan, 2020; Haug and Bharti, 2020; Kyriienko *et al.*, 2020; Lubasch *et al.*, 2020) |

Table IV NISQ algorithms for numerical solvers applications from Sec. V.D.

| Algorithm/Application | Proposed implementations |
|---|---|
| Portfolio optimization | (Bouland *et al.*, 2020; Cohen *et al.*, 2020; Egger *et al.*, 2020a; Marzec, 2016; Rosenberg *et al.*, 2016; Venturelli and Kondratyev, 2019) |
| Fraud detection | (Egger *et al.*, 2020a,b; Zoufal *et al.*, 2020) |
| Option pricing | (Kubo *et al.*, 2020) |

Table V NISQ algorithms for finance applications from Sec. V.E

# NISQ algorithms: other applications

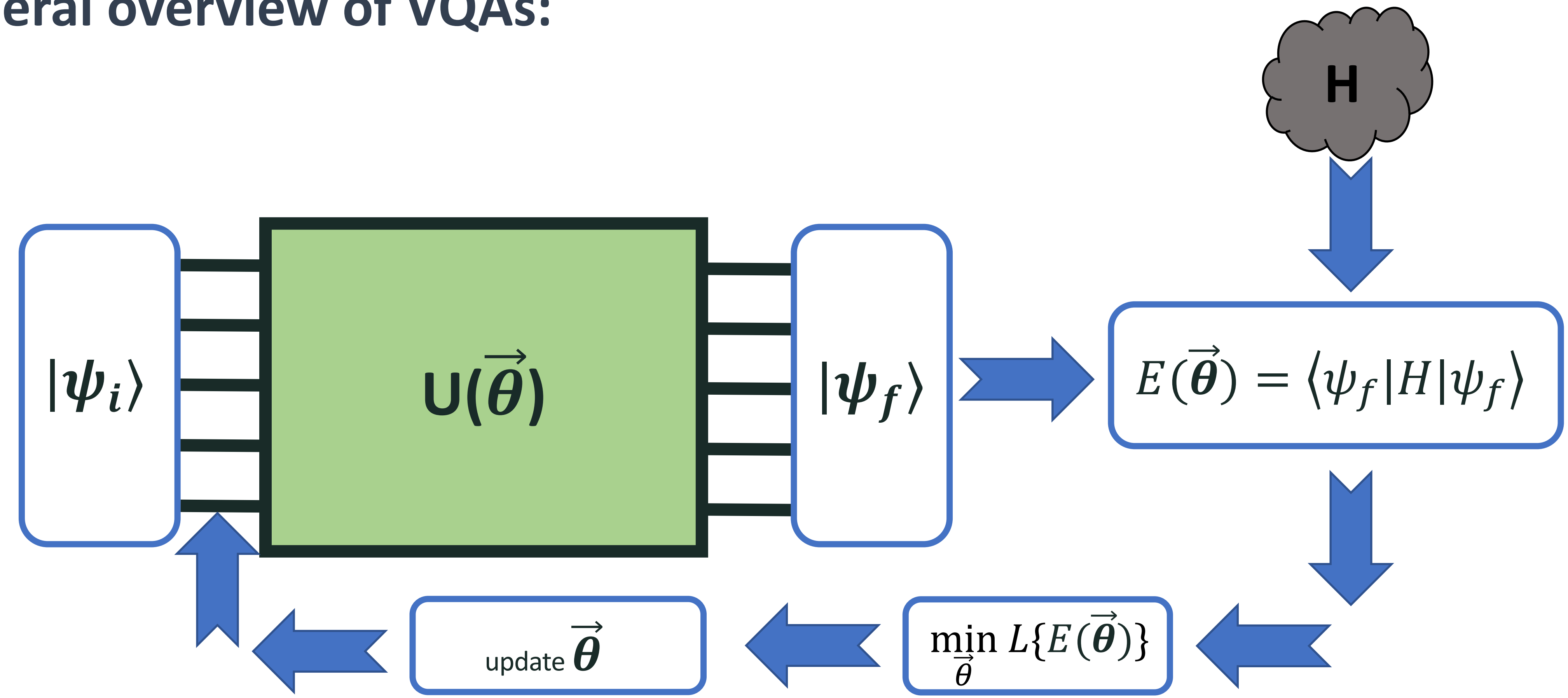
| Algorithm/Application | Proposed implementations |
|---|---|
| Quantum foundations | |
| Bell inequalities | (Alsina and Latorre, 2016) |
| Contextuality | (Kirby and Love, 2019; Kirby *et al.*, 2020) |
| Variational consistent history (VCH) | (Arrasmith *et al.*, 2019) |
| Quantum optimal control | |
| Quantum optimal control | (Dive *et al.*, 2018; Li *et al.*, 2017a; Lu *et al.*, 2017; Magann *et al.*, 2021; Policharla and Vinjanampathy, 2020) |
| Quantum metrology | |
| Quantum metrology | (Beckey *et al.*, 2020; Kaubruegger *et al.*, 2019; Koczor *et al.*, 2020; Ma *et al.*, 2020; Meyer *et al.*, 2020) |
| Fidelity estimation | |
| Fidelity estimation | (Cerezo *et al.*, 2020a) |
| Quantum error correction (QEC) | |
| Quantum variational error corrector (QVECTOR) | (Johnson *et al.*, 2017) |
| Variational circuit compiler for QEC | (Xu *et al.*, 2019a) |
| Nuclear physics | |
| Nuclear physics | (Avkhadiev *et al.*, 2020; Dumitrescu *et al.*, 2018; Hauke *et al.*, 2013; Klco *et al.*, 2018; Kokail *et al.*, 2019; Liu and Xin, 2020; Martinez *et al.*, 2016; Roggero *et al.*, 2020) |
| Entanglement properties | |
| Schmidt decomposition | (Bravo-Prieto *et al.*, 2019; Wang *et al.*, 2020a) |
| Multipartite entanglement | (Pérez-Salinas *et al.*, 2020b) |
| Entanglement spectrum | (Cerezo *et al.*, 2020b; LaRose *et al.*, 2019) |

Table VI NISQ algorithm for other applications listed in Sec. V.F.

Bharti et al, arXiV:2101.08448 (2021)

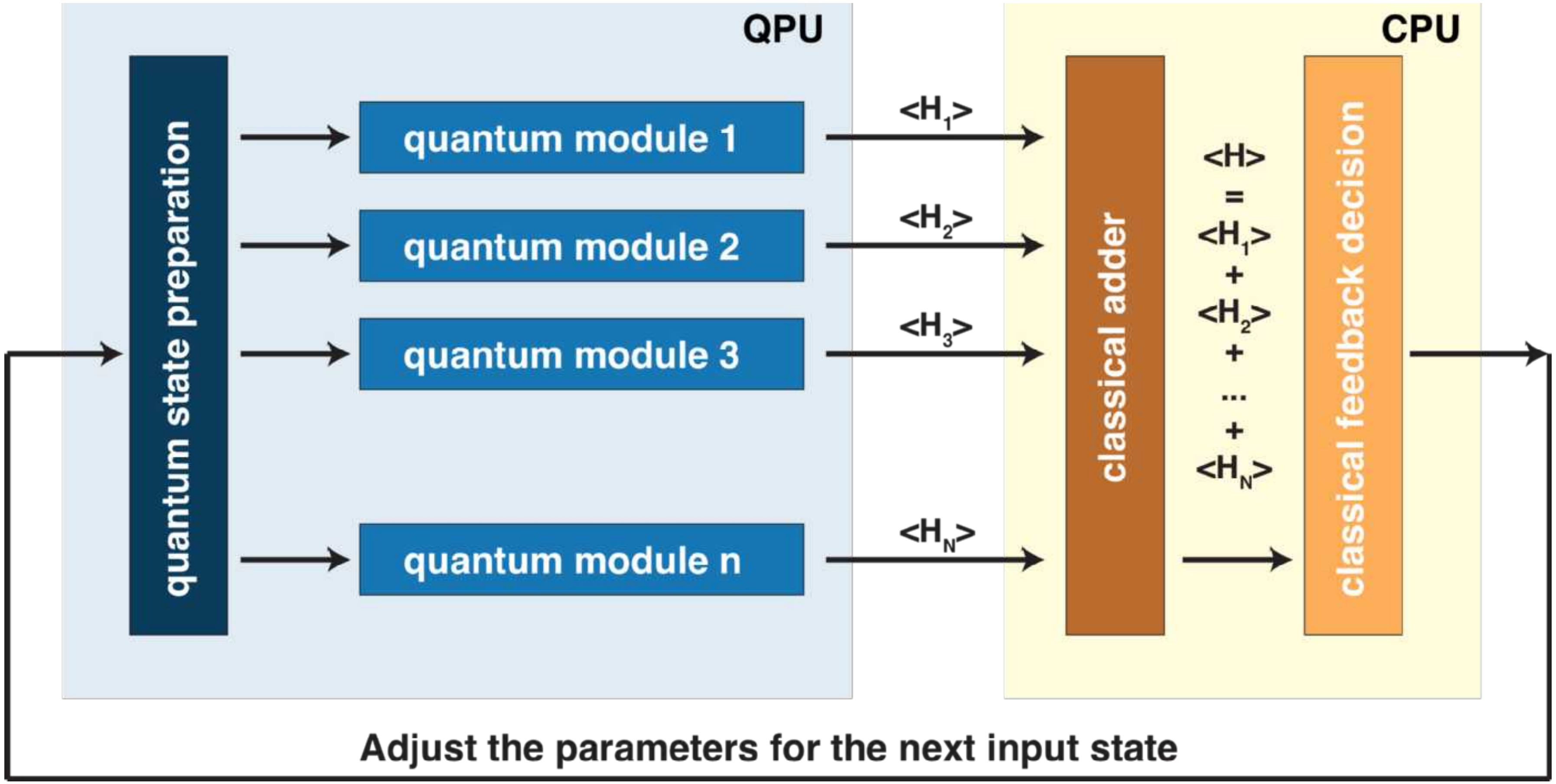
# Variational Quantum Algorithms (VQAs)

## A general overview of VQAs:

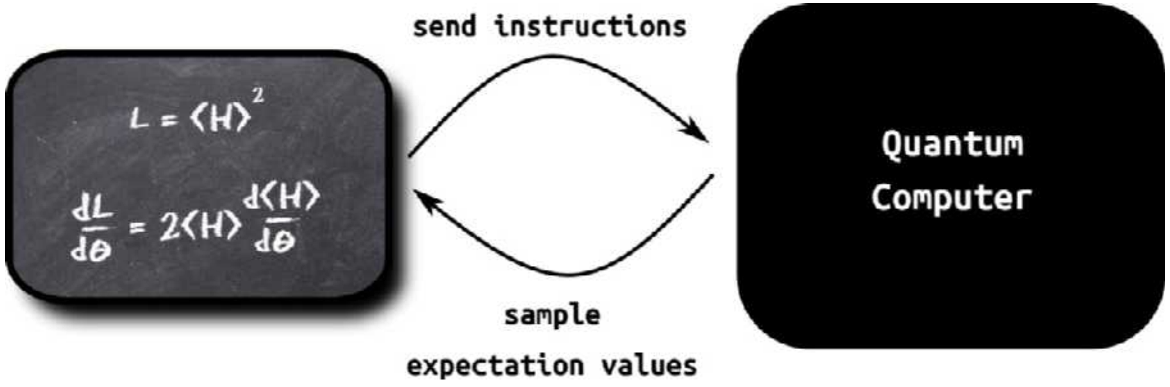


# The Variational Quantum Eigensolver

# Variational Quantum Eigensolver



# How are things done under the hood in a VQE?




Generators: Hermitian Operators

$$G_{abkl} = i(a_a^\dagger a_i a_b^\dagger a_j - h.c.)$$

Circuits from unitaries

$$U(\theta) = e^{-i\frac{\theta}{2}G}$$

Fermionic operators are mapped to Pauli strings

$$a_k^\dagger = 1^{\otimes k-1} \sigma_k^- \sigma_Z^{\otimes n-k}$$

Variational optimization

$$\min_\theta \left(\langle H \rangle_{U_\theta}\right) \equiv \min_\theta \left(\langle 0| U^\dagger(\theta) H U(\theta) |0\rangle\right)$$

# The fast-moving VQE algorithm development landscape.

Excited-state methods

Adaptive methods

Measurement reduction

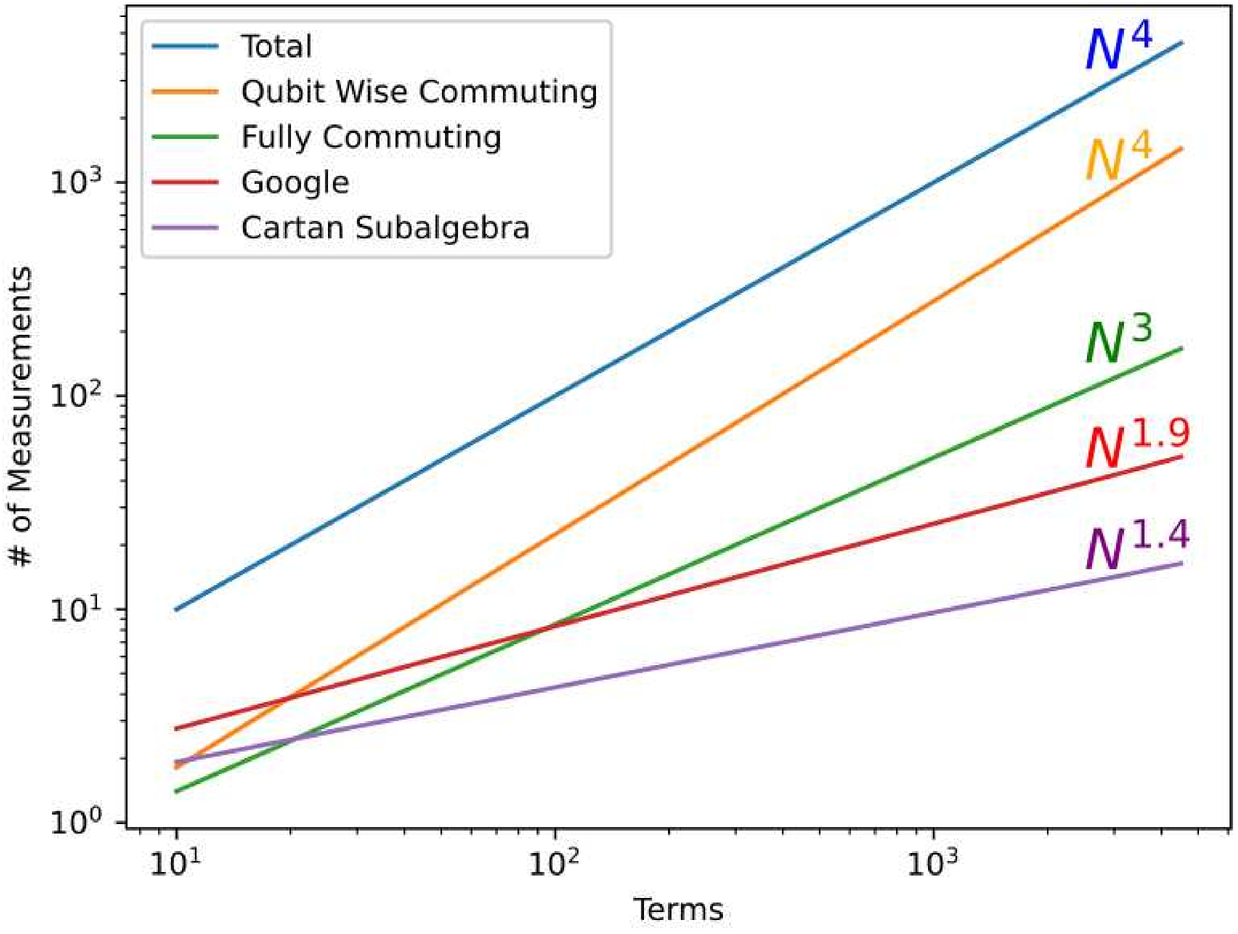
New UCC methods

Circuit ansatze

Optimization methods

| | |
|---|---|
| **Academic groups** | Artur Izmaylov, Nick Mayhall, Keisuke Fuji, Simon Benjamin, … |
| **Industry** | Zapata Computing, Google, IBM, OTI Lumionics, … |

# Example: The Measurement reduction race




Measurement reduction

**Total:** Pauli strings in a Hamiltonian
**Qubit-wise commuting:** Izmaylov, et al. JCP (2020).
**Fully commuting:** Izmaylov, et al. JCTC (2020).
**Google+Berkeley:** Huggins, et al. arXiv (2019).
**Cartan subalgebra:** T.C. Yen, A.F. Izmaylov, arXiv (2020).

Plot : TC Yen and Artrur Izmaylov (UofT)

# The Tequila Package

https://github.com/aspuru-guzik-group/tequila

Quantum Science and Technology

ACCEPTED MANUSCRIPT

## TEQUILA: A platform for rapid development of quantum algorithms.

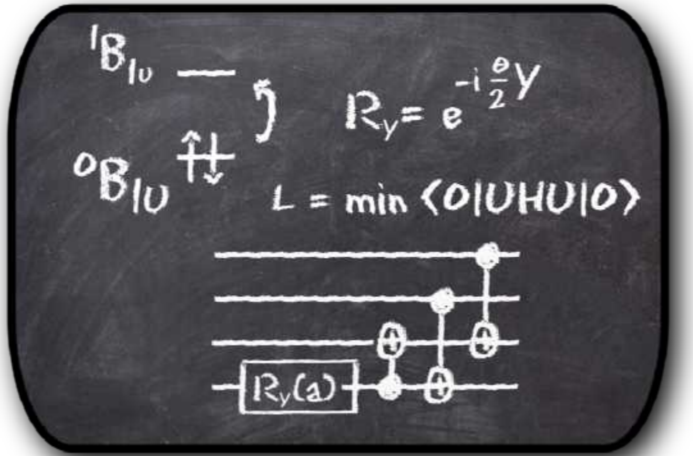
Jakob Kottmann[1], Sumner Alperin-Lea[2], Teresa Tamayo-Mendoza[3], Alba Cervera-Lierta[4], Cyrille Lavigne[5], Tzu-Ching Yen[6], Vladyslav Verteletskyi[7], Philipp Schleich[8], Abhinav Anand[9], Matthias Degroote[4] + Show full author list

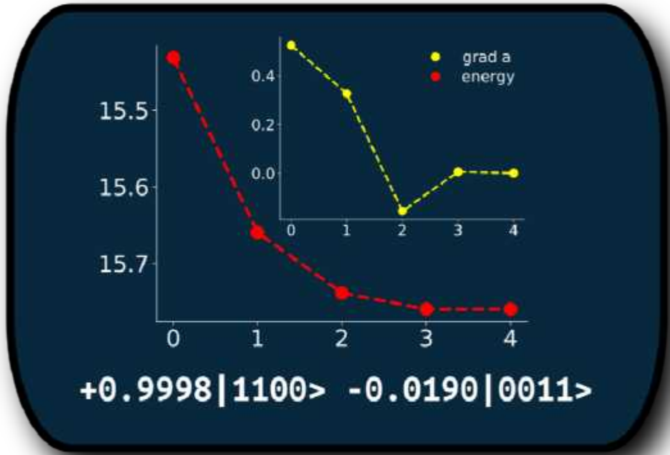
Accepted Manuscript online 11 February 2021 • © 2021 IOP Publishing Ltd

What is an Accepted Manuscript?

Kottmann, et al. Quantum Science and Technology (2021) In Press

# The Tequila Package: Hello world



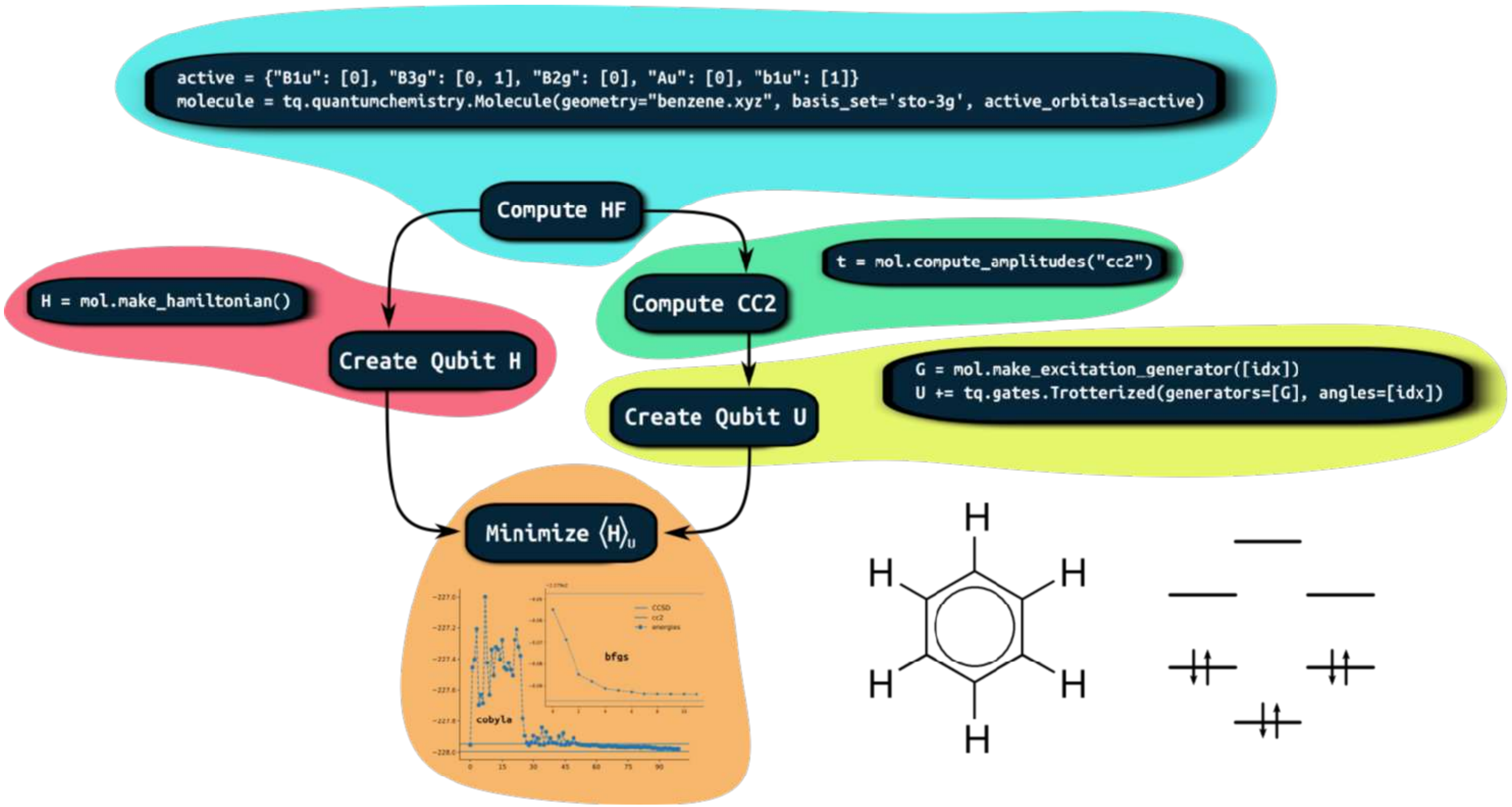




```
active = {"b1u": [0, 1]}
mol = tq.chemistry.Molecule("beh2.xyz", "6-31g", active)
H = mol.make_hamiltonian()
U = tq.gates.Ry("a", 0)
U += tq.gates.CNOT(0, 1) + tq.gates.CNOT(0, 2)
U += tq.gates.CNOT(1, 3) + tq.gates.X([2, 3])
expv = tq.ExpectationValue(U, H)
result = tq.optimizer_scipy.minimize(expv, "bfgs")
wfn = tq.simulate(U, variables=result.angles)
```

https://github.com/aspuru-guzik-group/tequila

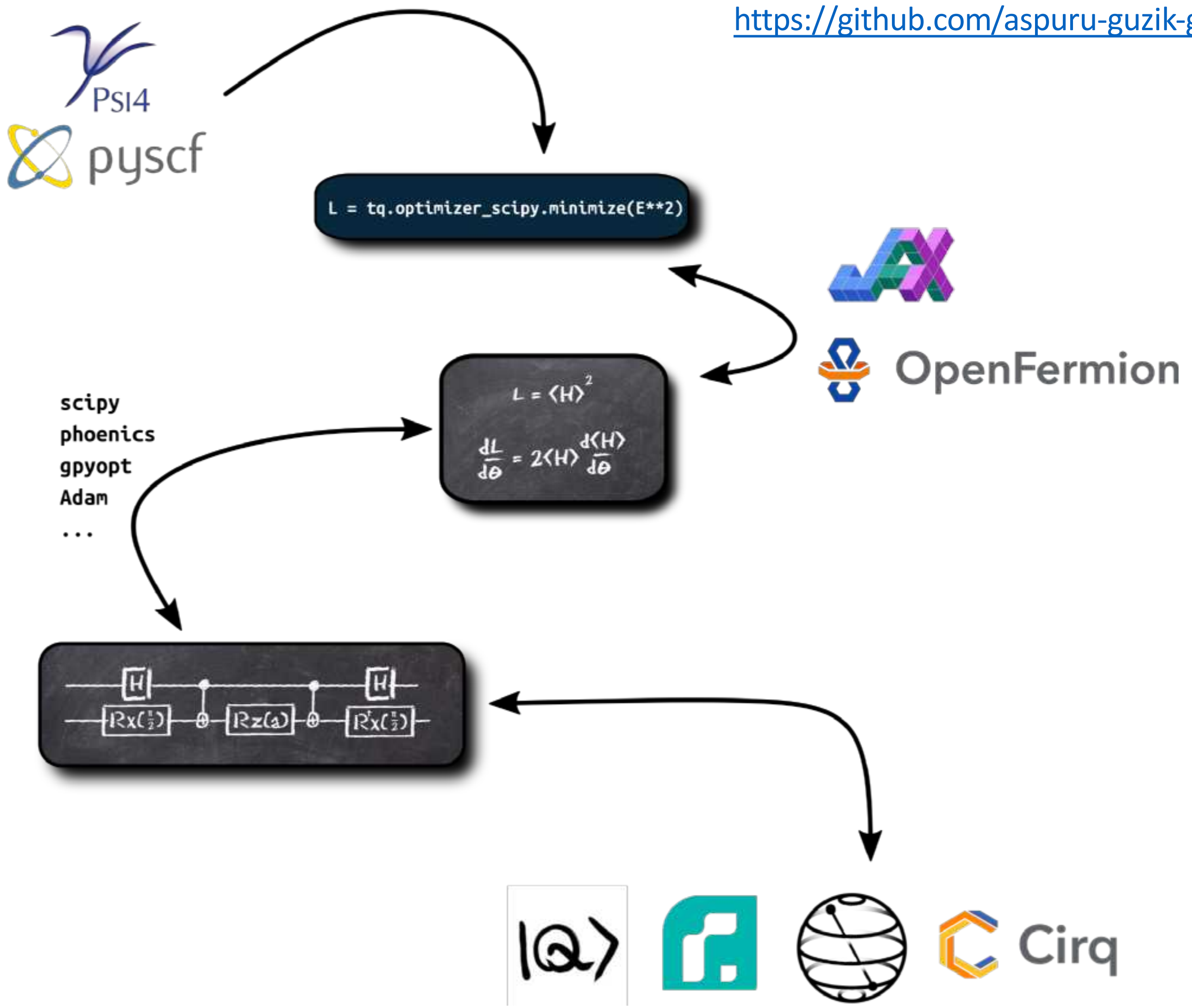
# The Tequila Package: Benzene example

https://github.com/aspuru-guzik-group/tequila



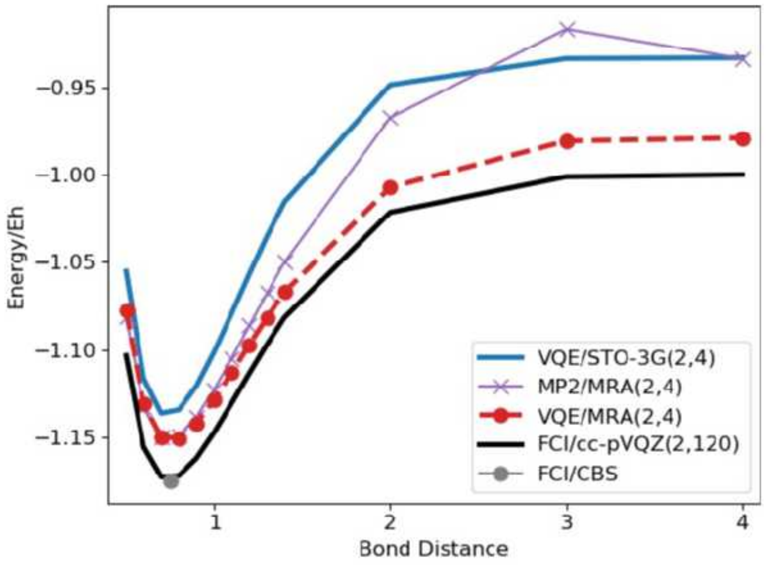
# The Tequila Package: How it works

https://github.com/aspuru-guzik-group/tequila



# Multi-resolution analysis Variational Quantum Eigensolver

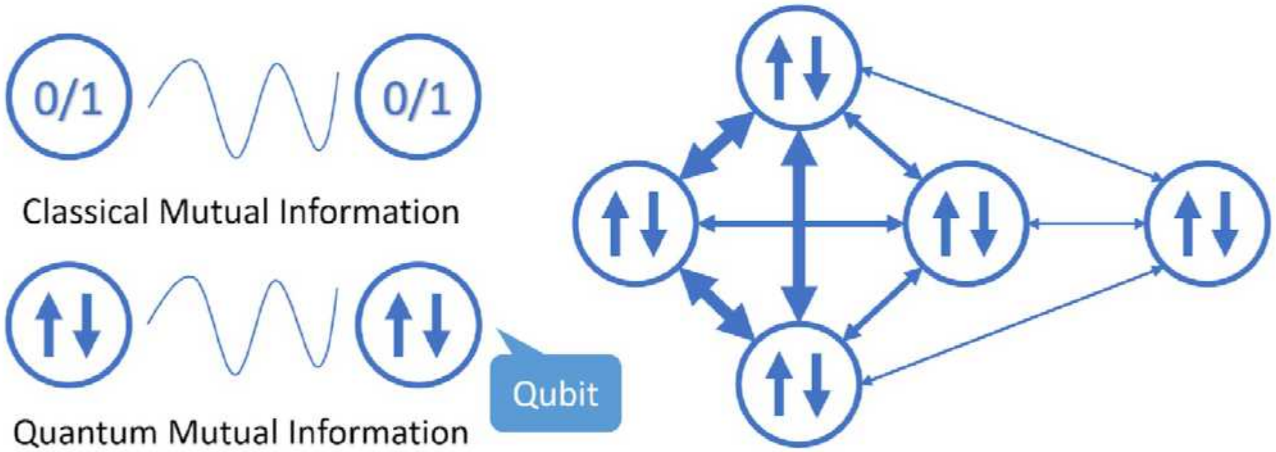
# Multi-resolution analysis Variational Quantum Eigensolver




Hydrogen molecule VQE/MRA

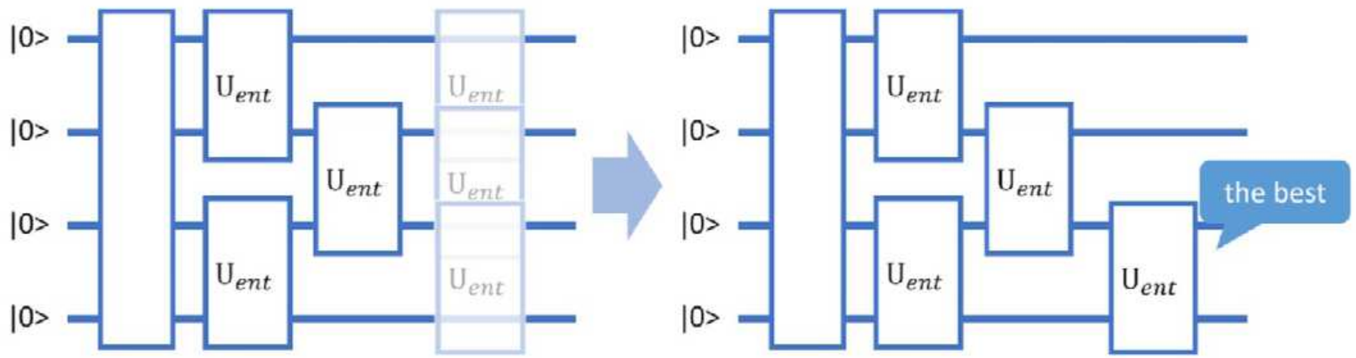
| System | Metric | Qubits/MRA | Qubits/GBS | More |
|---|---|---|---|---|
| He | MAX | **4** | 4-10 | Fig. 3 |
| Be | MAX | **10** | 10-18 | Fig. 3 |
| $H_2$ | NPE | **4** | 20-56 | Figs. 5, 4 |
| $H_2$ | NPE | **8** | 20-56 | Figs. 5, 4 |
| $H_2$ | NPE | **20** | 56-120 | Figs. 5, 4 |
| $H_2$ | MAX | **4** | 8 | Figs. 5, 4 |
| $H_2$ | MAX | **8** | 20-56 | Figs. 5, 4 |
| $H_2$ | MAX | **20** | 56 | Figs. 5, 4 |
| LiH | NPE | **12** | 20-38 | Figs. 5, 4 |
| LiH | NPE | **20** | 38 | Figs. 5, 4 |
| LiH | MAX | **12** | 20-38 | Figs. 5, 4 |
| LiH | MAX | **20** | 170-288 | Figs. 5, 4 |
| BH | NPE | **12-20** | 38-88 | Figs. 5, 4 |
| BH | MAX | **12-20** | 38-88 | Figs. 5, 4 |
| $NH_3$ | $\Delta E$ | **12-18** | 58-100 | Fig. 2 |

# Mutual-Information Adaptive Unitary Coupled Cluster



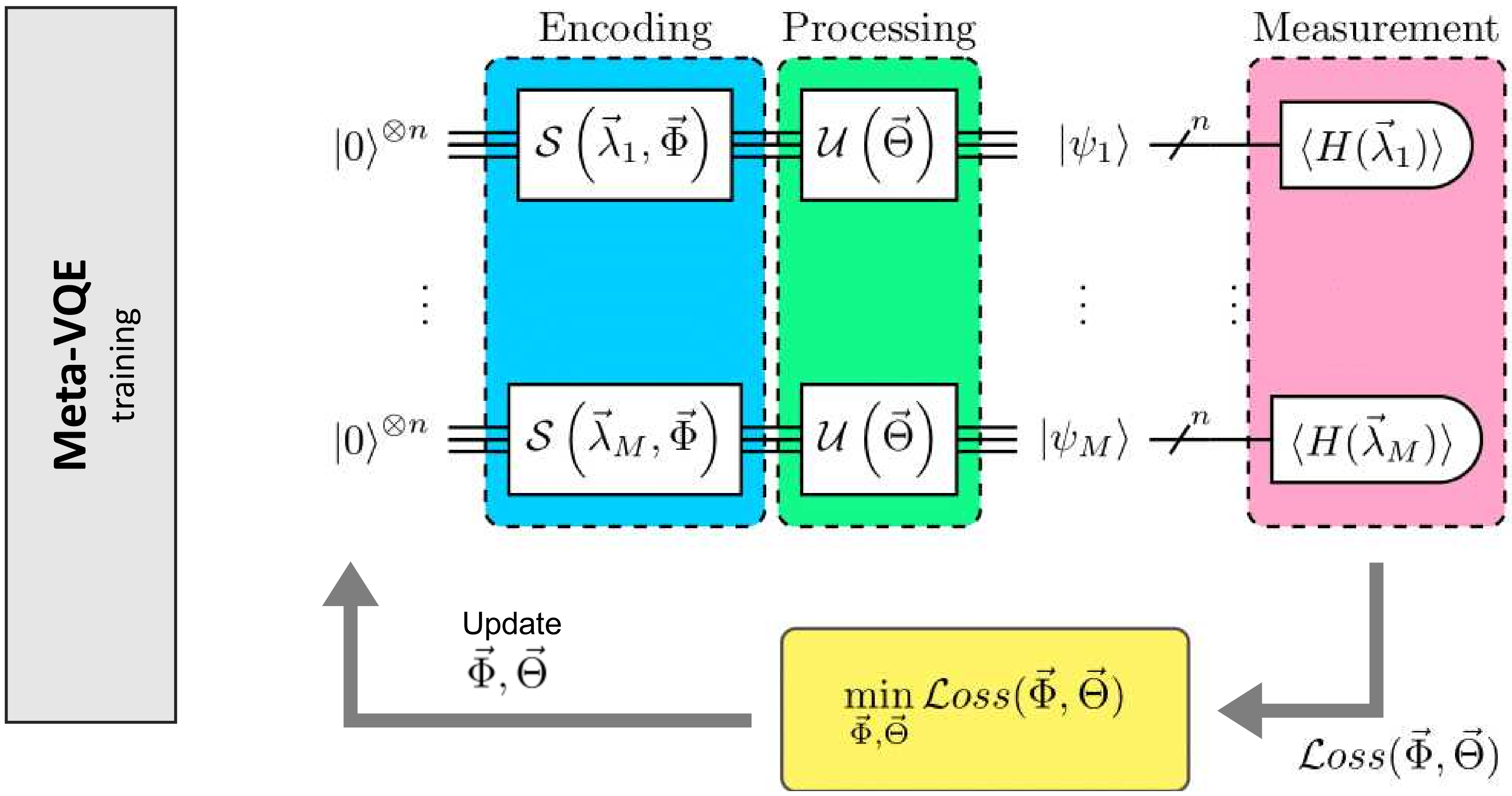

**Strategy:**

Leverage classical-computing DMRG mutual information to iteratively construct compact entangler circuits.




Also: Qubit-Coupled Cluster by Izmaylov, and co-workers, Adapt-VQE by Mayhall and co-workers

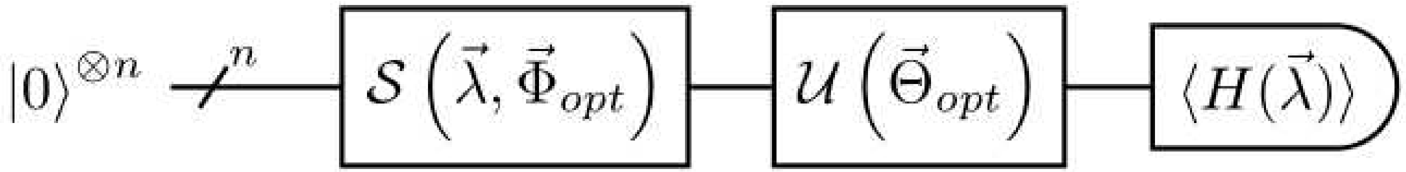
# The Meta Variational Quantum Eigensolver




**Strategy:** Add encoding layer to learn parameterized Hamiltonians: **QML + VQE** hybrid.
See also: Mitarai, et al. PR Applied 11 044087 (2019)

# The Meta Variational Quantum Eigensolver

**Meta-VQE**

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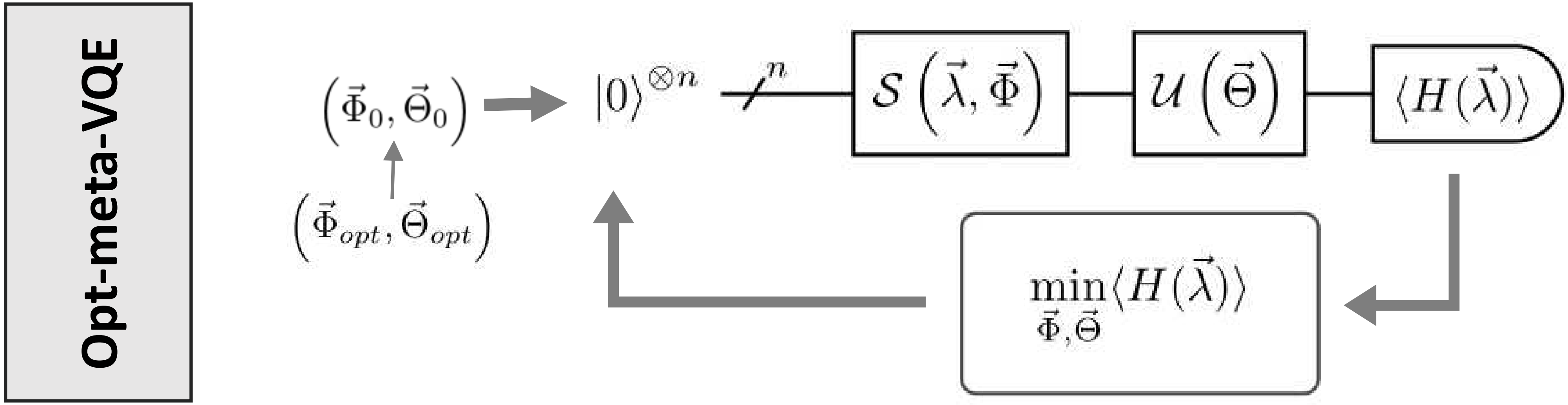
# The Meta Variational Quantum Eigensolver

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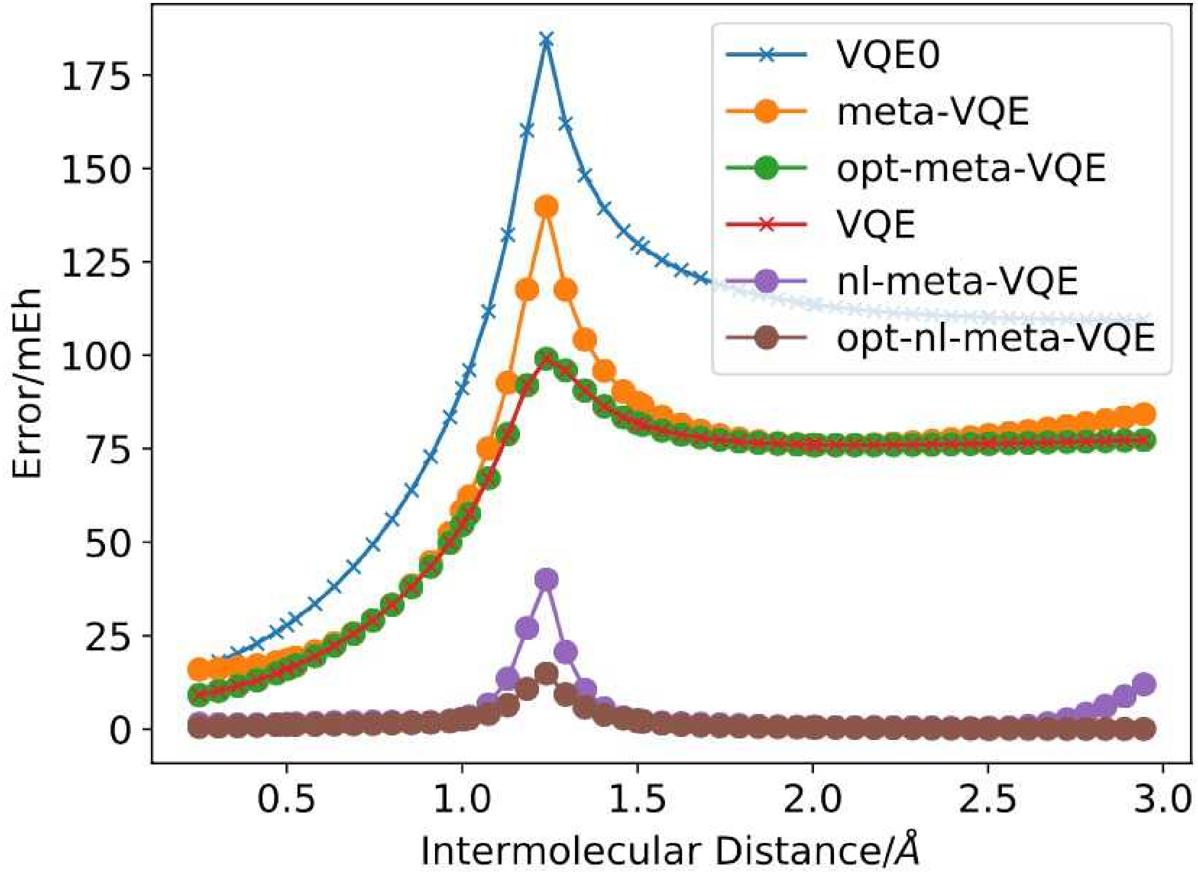
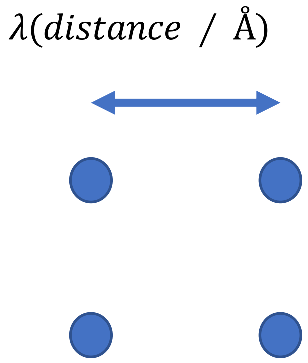
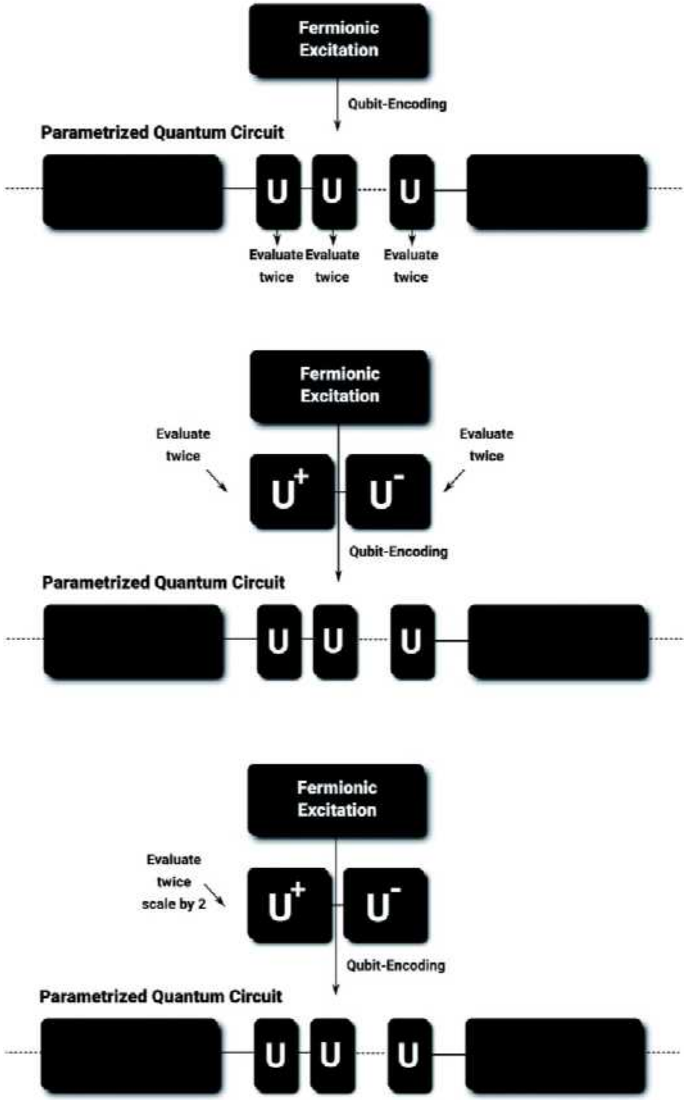
# The Meta Variational Quantum Eigensolver



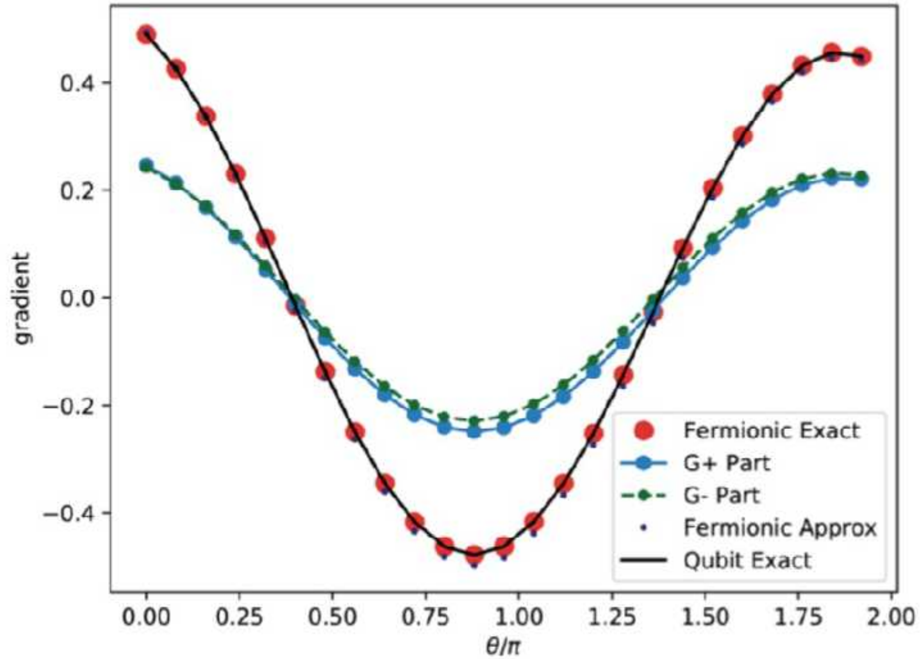




**Example:** $H_4$ molecule as the atomic square is deformed into a rectangle

# A feasible approach for derivatives for UCC




| Generator form | Gradient cost | Strategy |
|---|---|---|
| $G_{pq} = \sum_i c_i \sigma_i$ | $\mathcal{O}(2^{2n})$ | Shift-rule (6) |
| $G_{pq} = \frac{1}{2}(G_+ + G_-)$ | 4 | Fermionic-shift (16) |
| Real wavefunctions | | |
| $G_{pq} = \frac{1}{2}(G_+ + G_-)$ | 2 | Fermionic-shift (19) |
| Generator approximation | | |
| $G_{pq} \approx G_\pm$ | 2 | Shift-rule (6) |




$H_2$ minimal basis
4 orbital example

Kottman, Anand, Aspuru-Guzik Chemical Science (2021) In Press. Hot Article https://doi.org/10.1039/D0SC06627C

# Quantum Computer-Aided Design (QCAD)

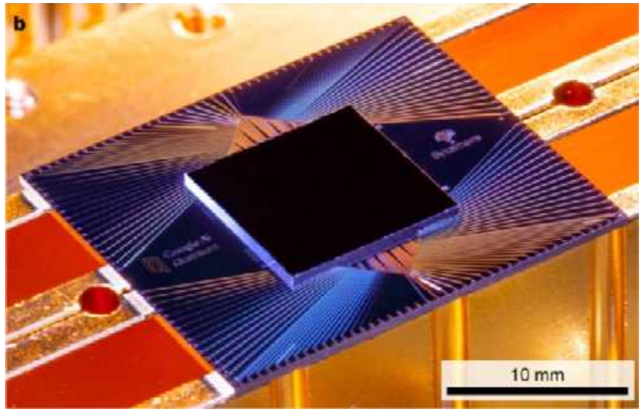
Kyaw, Menke, Sim, Sawaya, Oliver, Guerreschi, Aspuru-Guzik, arXiV:2006.03070 (2020)

Kottman, Krenn, Kyaw, Alperin-Lea, Aspuru-Guzik arXiv:2006.03075 (2020)

Kottman, Krenn, Tischler, Aspuru-Guzik, arXiV:2005.06443 (2020)

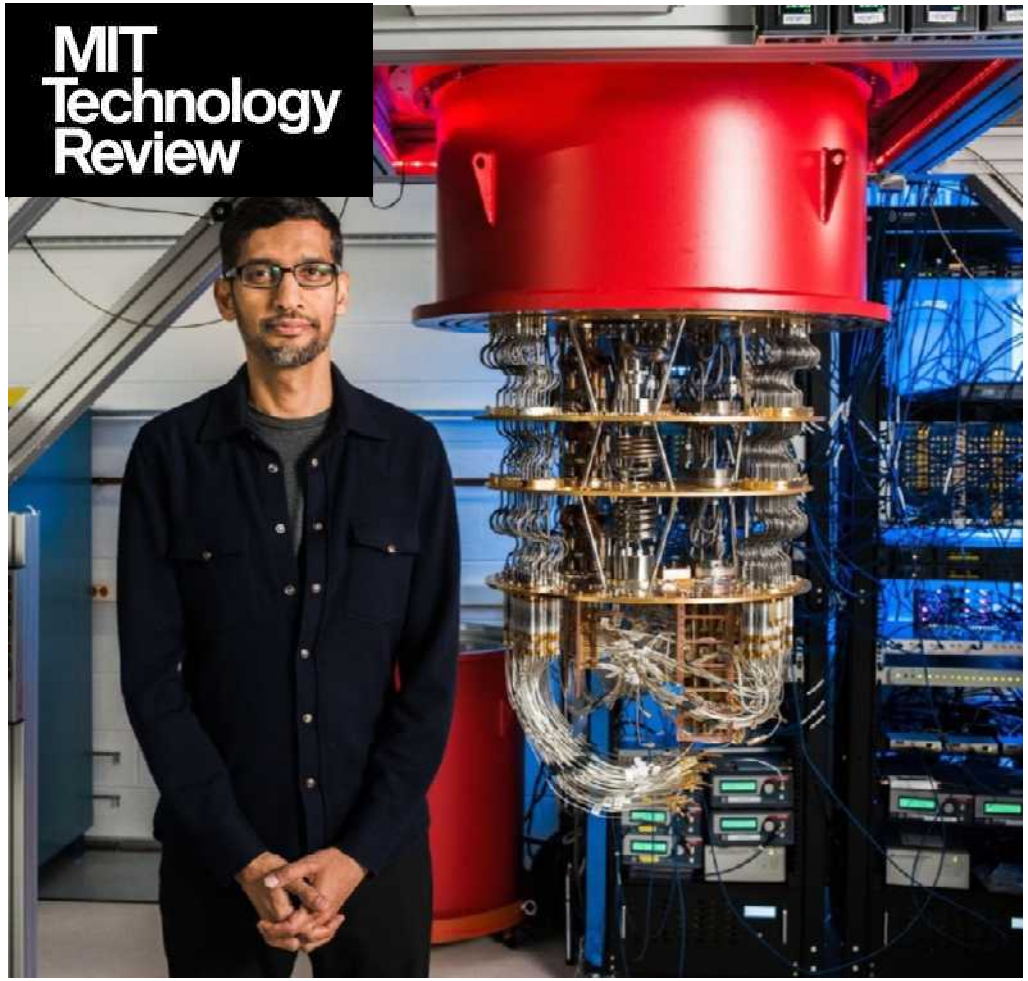
Sawaya, Menke, Kyaw, Johri, Aspuru-Guzik, Guerresci, npJ Quantum Information 6, 1 (2020)

# Enter Sycamore




Courtesy: Google Quantum

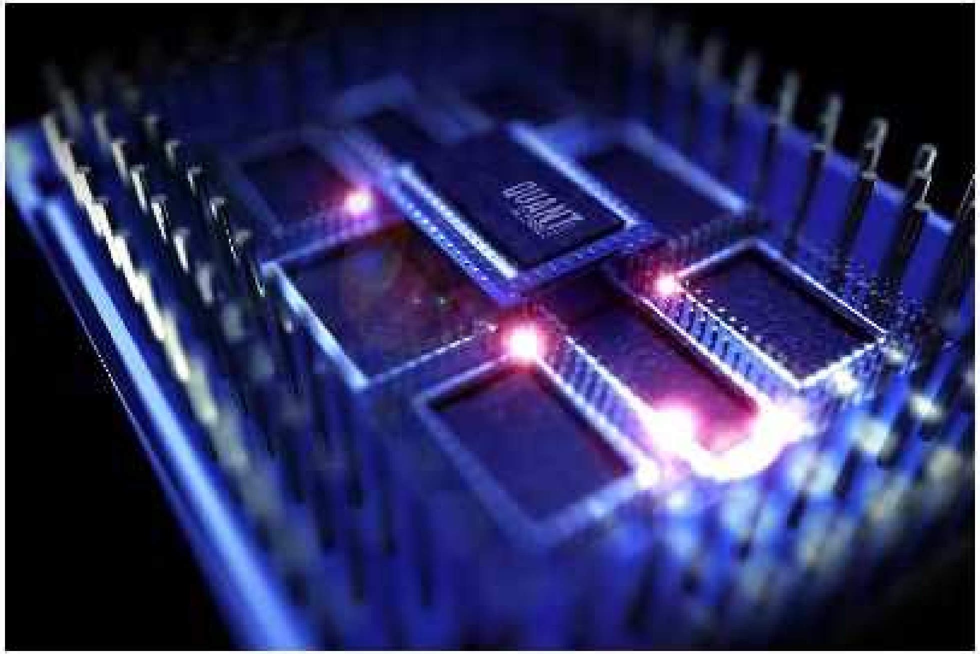
“Google researchers claim to have attained **“quantum supremacy”** for the first time. Their 53-bit quantum computer, named Sycamore, took 200 seconds to perform a calculation that, according to Google, would have taken the world’s fastest supercomputer 10,000 years.”




Dated 23 Oct. 2019

# … and unconfirmed Gaussian Boson Sampling machine!

South China Morning Post



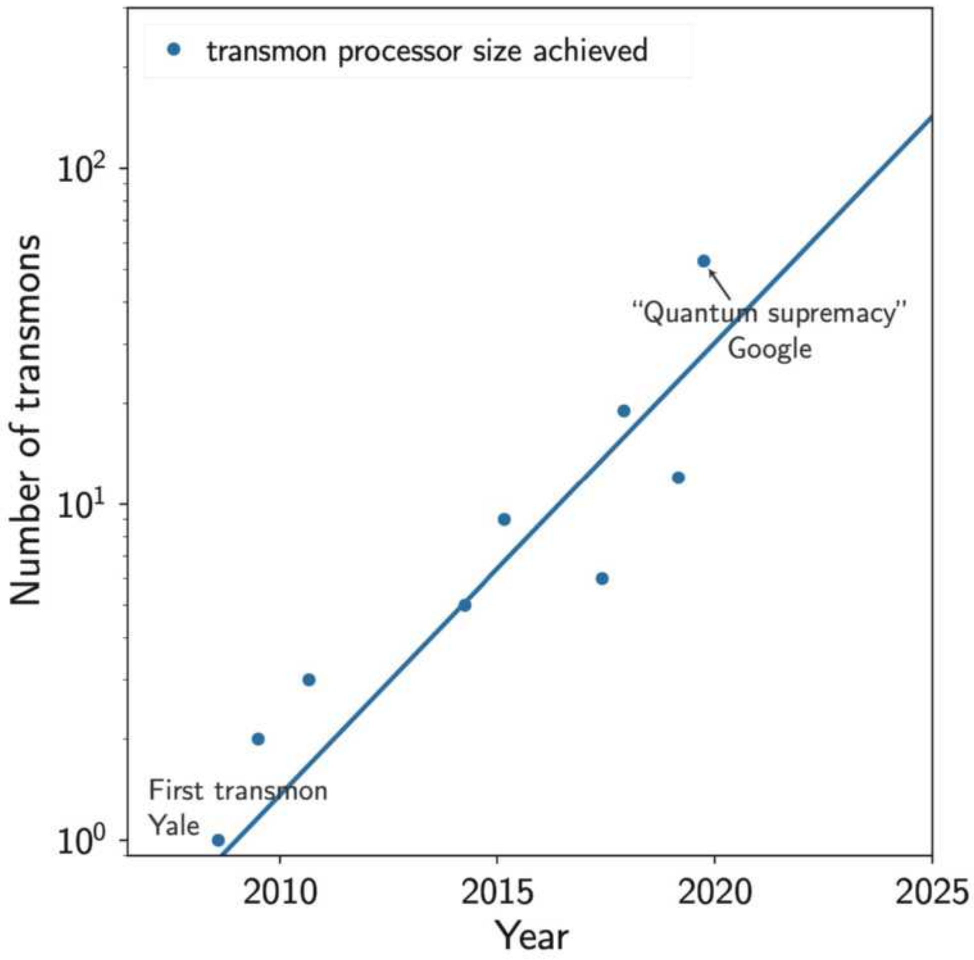
## Chinese quantum computer declared a million times greater than Sycamore

- Physicist Pan Jianwei says his team achieved quantum supremacy but ‘further verification’ is necessary
- Pan’s team has received generous and consistent financial support from the Chinese government

12 Sep 2020 - 1:07AM

32

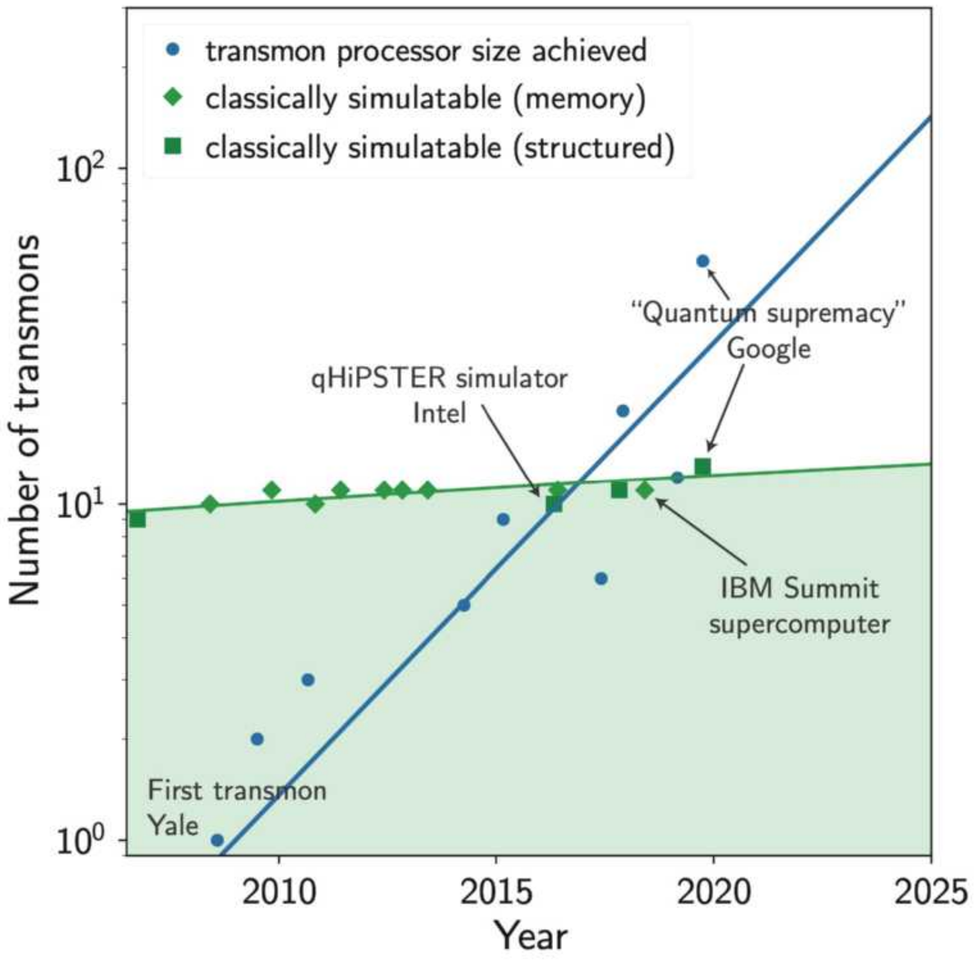
# How will we simulate large-scale quantum computers?




- Number of transmons in a processor is growing exponentially

**Case study:** Transmons.

# How will we simulate large-scale quantum computers?

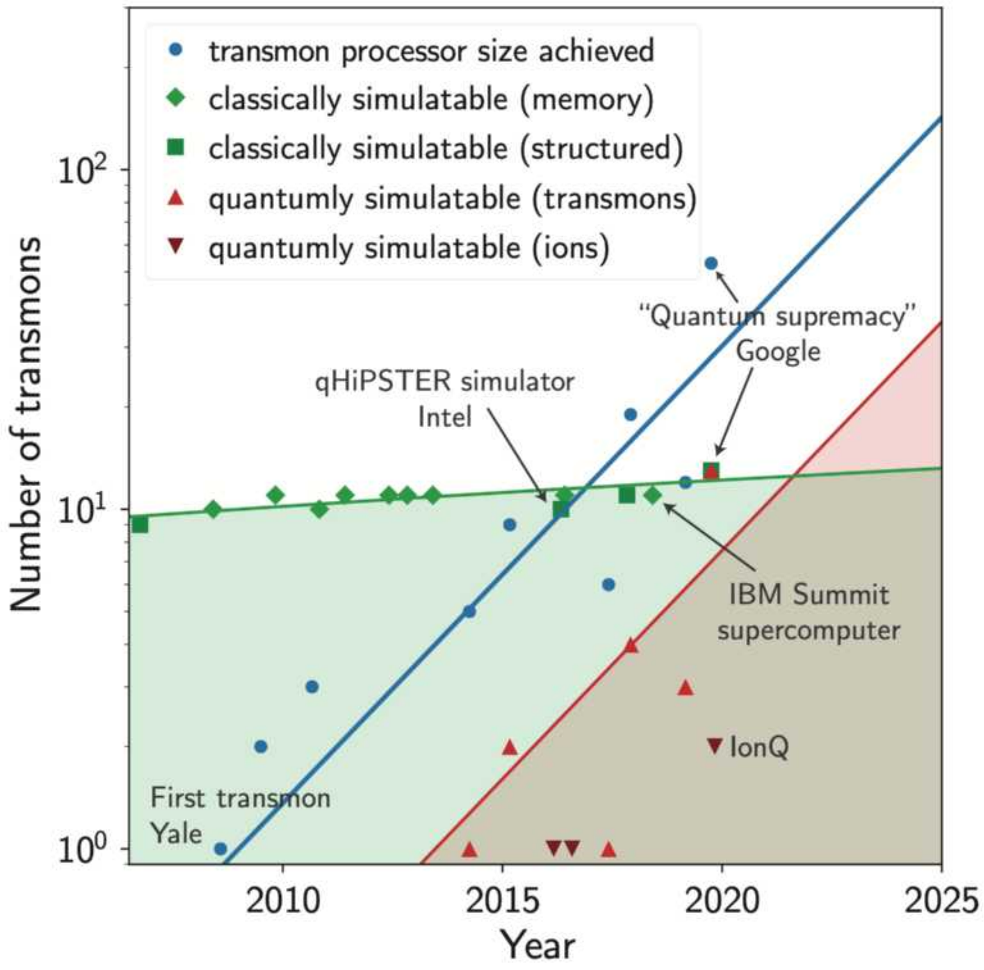



- Number of transmons in a processor is growing exponentially
- Classical hardware simulation capacity hits roadblock just above ten transmons

**Case study:** Transmons.

Kyaw, Menke, Sim, Sawaya, Oliver, Guerreschi, Aspuru-Guzik, arXiV:2006.03070 (2020)

# How will we simulate large-scale quantum computers?




- Number of transmons in a processor is growing exponentially
- Classical hardware simulation capacity hits roadblock just above ten transmons
- Quantum computers can simulate one *physical* transmon per $\log_2(16) = 4$ *data* qubits in the computer
- Quantum simulation capabilities will soon surpass classical capacity

Future quantum computers need to be designed with the aid of existing quantum computers

**Case study:** Transmons.

Kyaw, Menke, Sim, Sawaya, Oliver, Guerreschi, Aspuru-Guzik, arXiV:2006.03070 (2020)

# Digital Simulation of Transmon quantum processors

**Methods for simulating transmon hardware on digital quantum computers**

- Encoding of the transmon Hamiltonian into Pauli strings
- Energy spectrum from variational simulations
- Gate operation from Suzuki-Trotter simulations
- Quantum simulation of large quantum computer modules

# Efficient encoding of d-level Hamiltonians into Pauli Strings

Example

$$|3\rangle\langle 4| + |4\rangle\langle 3|$$

$$\begin{bmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \star & \cdot \\ \cdot & \cdot & \cdot & \star & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix}$$

Conversion rules

$$|0\rangle\langle 1| = \frac{1}{2}(X + iY)[= \sigma^-]$$

$$|1\rangle\langle 0| = \frac{1}{2}(X - iY)[= \sigma^+]$$

$$|0\rangle\langle 0| = \frac{1}{2}(\mathbb{1} + Z)$$

$$|1\rangle\langle 1| = \frac{1}{2}(\mathbb{1} - Z)$$

Standard binary

$3 = 011$

$4 = 100$

$$\boxed{\frac{1}{4}(\hat{\sigma}_x^{(2)}\hat{\sigma}_x^{(1)}\hat{\sigma}_x^{(0)} + \hat{\sigma}_y^{(2)}\hat{\sigma}_y^{(1)}\hat{\sigma}_x^{(0)} + \hat{\sigma}_y^{(2)}\hat{\sigma}_x^{(1)}\hat{\sigma}_y^{(0)} - \hat{\sigma}_x^{(2)}\hat{\sigma}_y^{(1)}\hat{\sigma}_y^{(0)})}$$

Hamming distance = 3

Gray code

$3 = 010$

$4 = 110$

$$\boxed{\frac{1}{4}(-\hat{\sigma}_x^{(2)}\hat{\sigma}_z^{(1)}\hat{\sigma}_z^{(0)} + \hat{\sigma}_x^{(2)}\hat{\sigma}_z^{(0)} - \hat{\sigma}_x^{(2)}\hat{\sigma}_z^{(1)} + \hat{\sigma}_x^{(2)})}$$

Gray encoding is simpler and more efficient.

Hamming distance = 1

# Efficient encoding of d-level Hamiltonians into Pauli Strings

$$\hat{H}_{\mathrm{transmon}} = 4E_{\mathrm{C}}\hat{N}^2 - 2E_{\mathrm{J}}|\cos(2\pi\Phi_{\mathrm{ext}}/\Phi_0)|\,\underline{\cos\left(2\pi\hat{\phi}/\Phi_0\right)}$$

$$\underline{\cos\left(2\pi\hat{\phi}/\Phi_0\right)} \approx \begin{pmatrix}
0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
1&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&1&0&1&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&1&0&1&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&1&0&1&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&1&0&1&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&1&0&1&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&1&0&1&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&1&0&1&0&0&0&0&0&0\\
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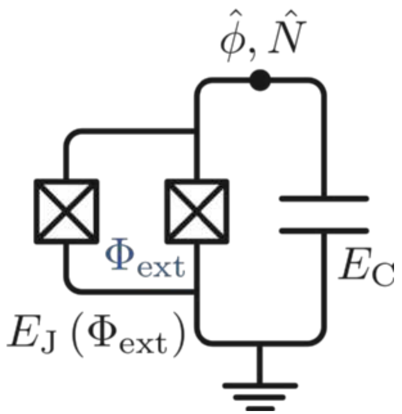
0&0&0&0&0&0&0&0&0&0&0&1&0&1&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&1&0&1&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&1\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0
\end{pmatrix}$$

$$\begin{aligned}
&= 0.5X_0 + 0.25X_1 - 0.25Z_0X_1\\
&+0.125X_2 - 0.125Z_1X_2\\
&+0.125Z_0X_2 - 0.125Z_0Z_1X_2\\
&+0.0625X_3 - 0.0625Z_2X_3\\
&+0.0625Z_1X_3 - 0.0625Z_1Z_2X_3\\
&+0.0625Z_0X_3 - 0.0625Z_0Z_2X_3\\
&+0.0625Z_0Z_1X_3 - 0.0625Z_0Z_1Z_2X_3
\end{aligned}$$

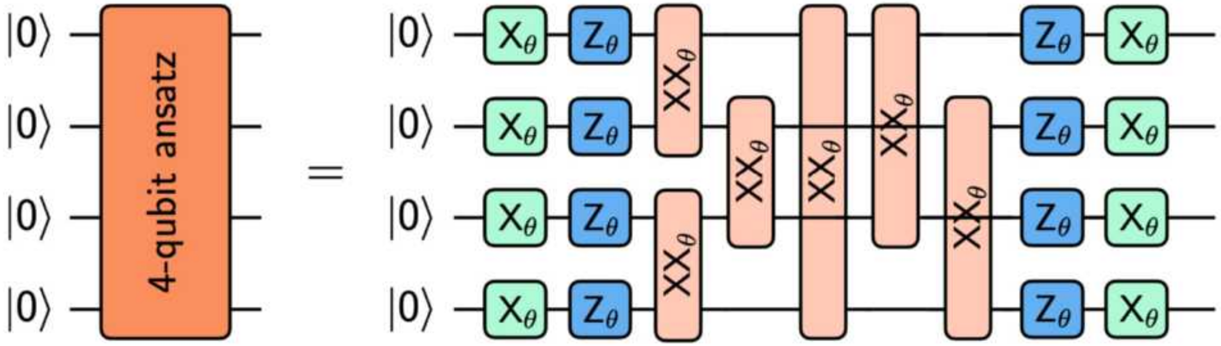
Mapped Hamiltonian can be simulated on any type of digital quantum computer
(superconducting, ion traps, quantum optics, cold atoms, etc.)

Kyaw, Menke, Sim, Sawaya, Oliver, Guerreschi, Aspuru-Guzik, arXiV:2006.03070 (2020)

# QCAD Example: Qubit Energy Levels




**physical** qubit

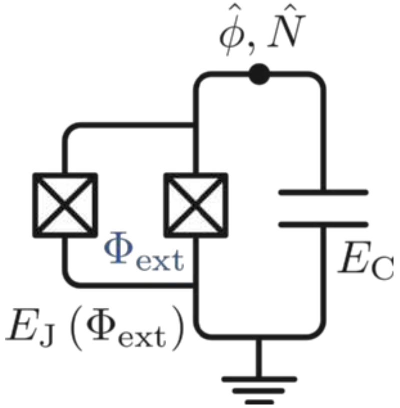



**data** qubits used for simulation of physical qubit

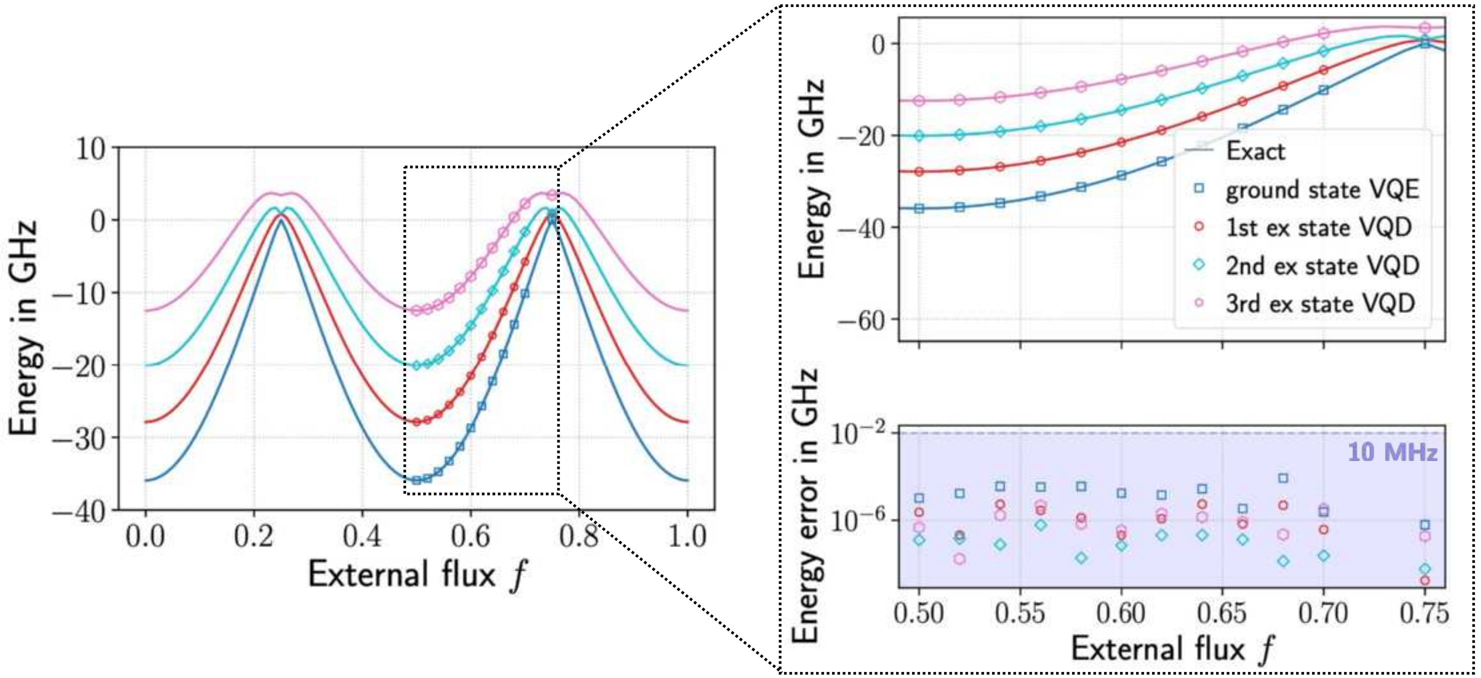
Ansatz gates: Fully-connected ion-trap qubits

Find ground-state by VQE, Determine Excited States by Variational Quantum Deflation (VQD)

# QCAD Example: Qubit Energy Levels



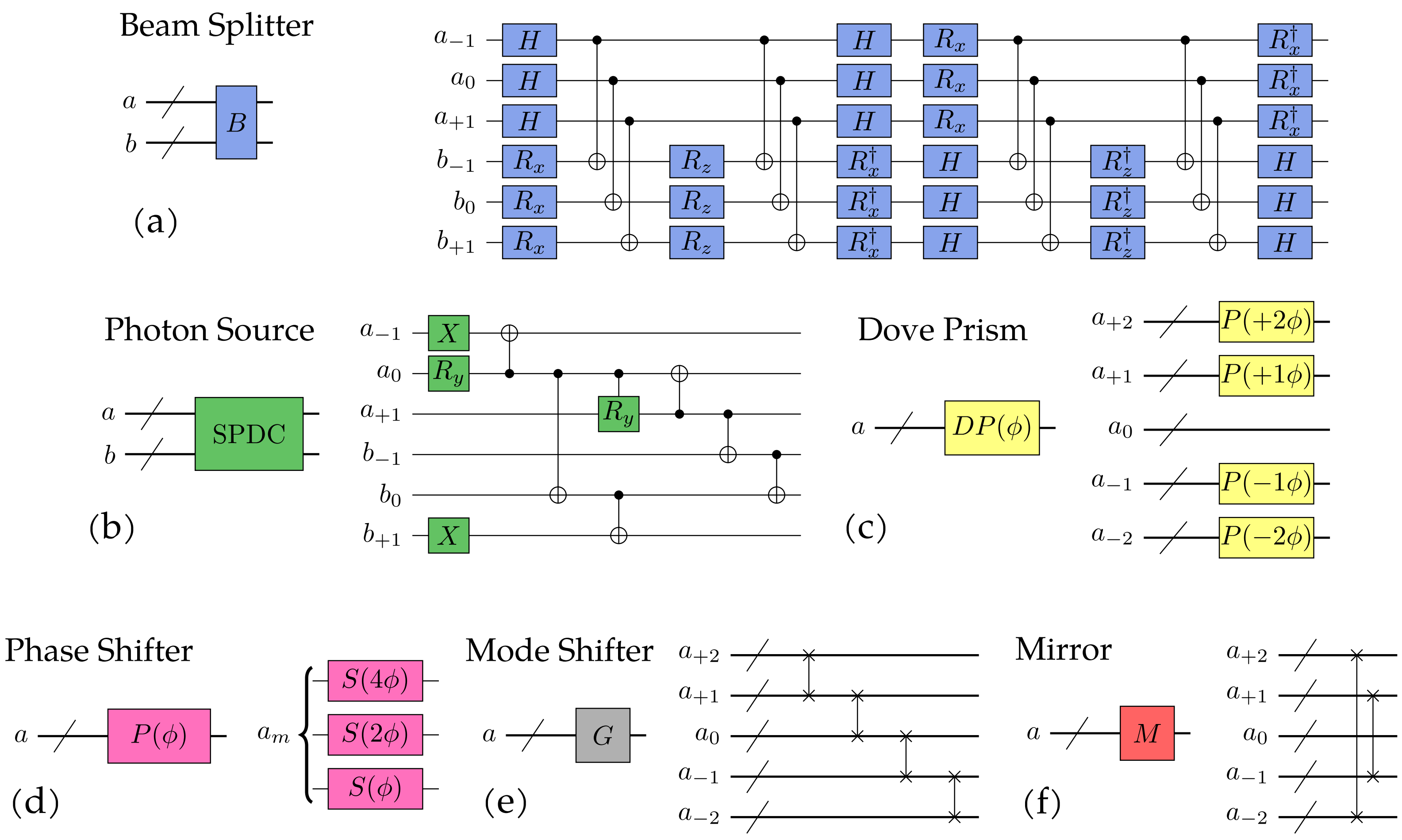

VQD result




- VQD algorithm finds transmon energy levels to experimentally relevant accuracy
- Spectrum informs frequency range, noise sensitivity estimates, and gate operation

Kyaw, Menke, Sim, Sawaya, Oliver, Guerreschi, Aspuru-Guzik, arXiV:2006.03070 (2020)

# QCAD for quantum optical experiments



# QCAD for quantum optical experiments

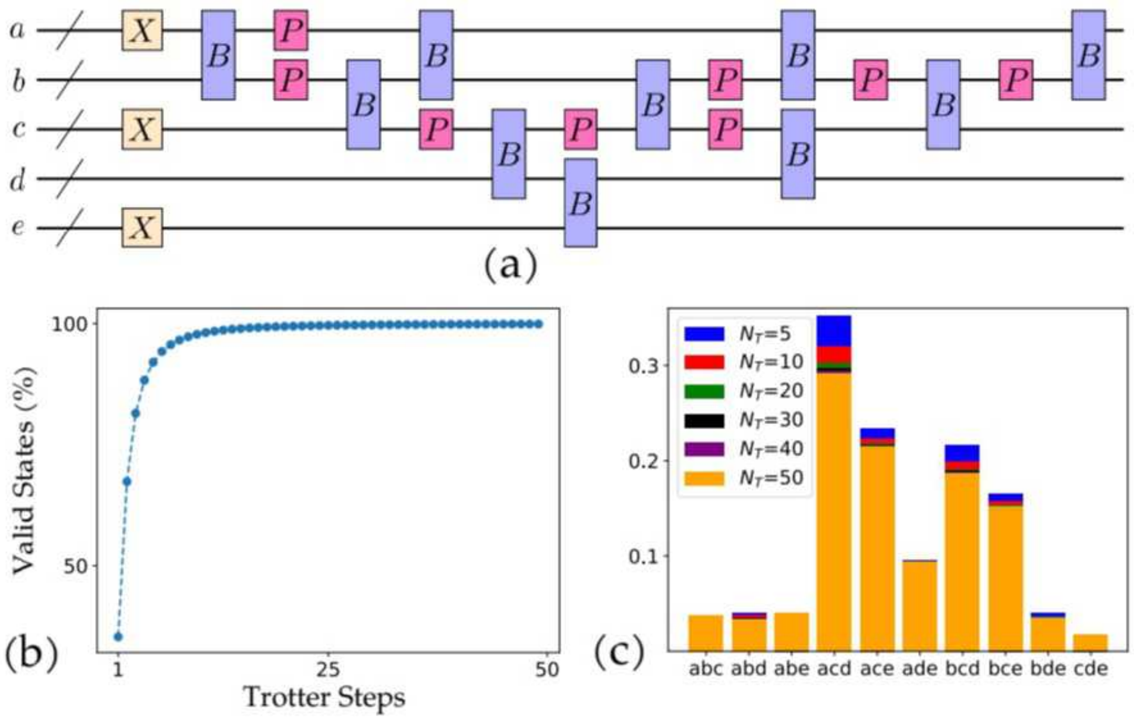


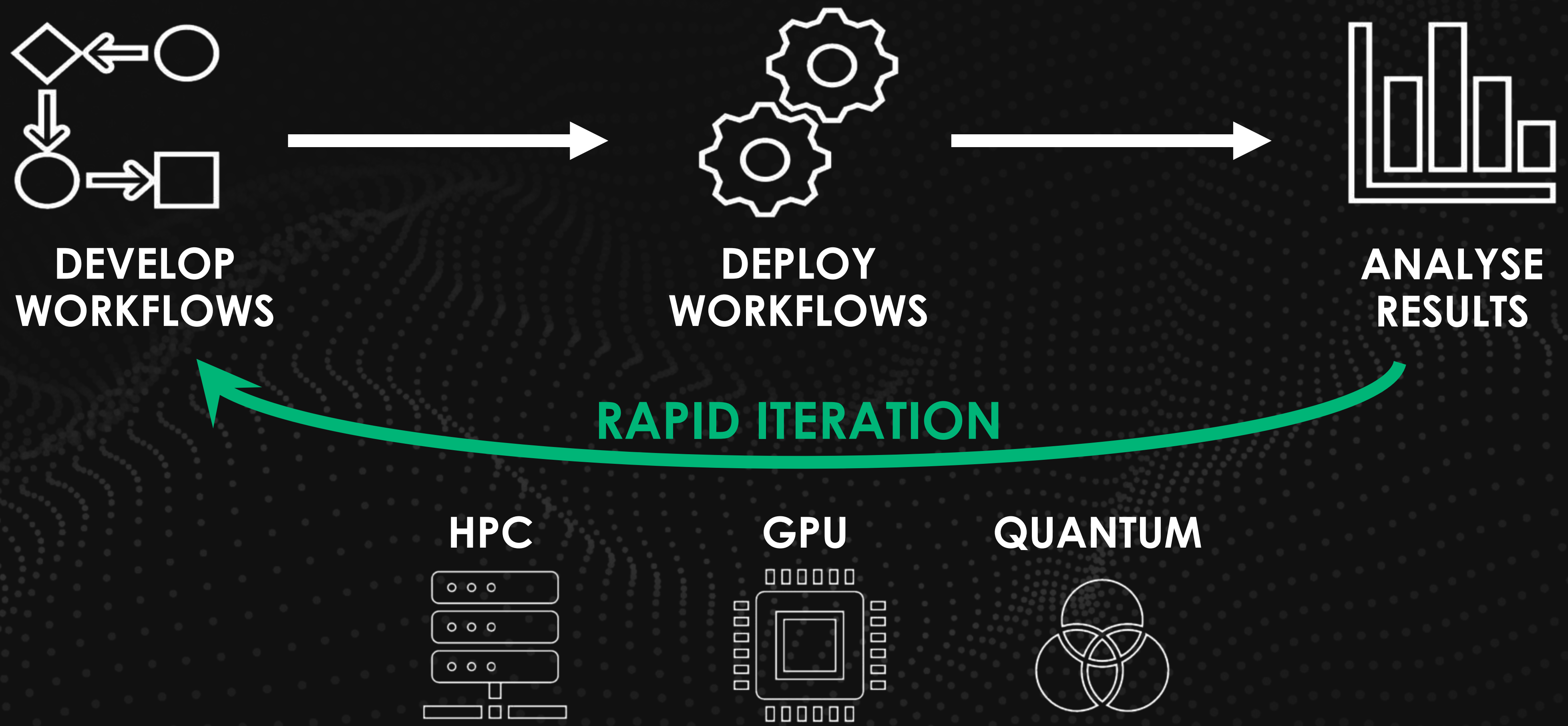

FIG. 2. **Digital simulation of a Boson sampling experiment [31].** (a) In the abstract representation of the setup each path is represented by two qubits (allowing to represent 0-3 photons in each path). The setup consists of beam-splitters (B) and phase shifters (P) and is initialized with three photons in paths $a$, $c$ and $d$ ($|1_a 0_b 1_c 0_d 1_e\rangle$). (b) Percentage of physically valid states (obeying photon number conservation) as an indicator of the error introduced by the Trotter expansion. (c) Simulated distribution of three photon states with each photon in a separate path. At 10 Trotter steps the error with respect to the exact quantum optical setup is about 2 percent, and consistent with the experimental results presented in [31].

# Orquestra

# Orquestra

The Unified Quantum Operating Environment

# WE CAN SOLVE THESE CHALLENGES WITH WORKFLOW MANAGEMENT TOOLS

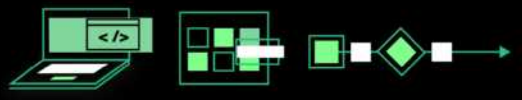


## COMPOSE

Build *quantum-enabled workflows*™ from Zapata tasks, your own tasks, and open-source libraries.

### DEVELOPMENT ENVIRONMENT

**Orquestra Workflow Composer**




Task Builder — Task Library — Workflow Composer

### OPEN SOURCE TOOLS

**QUANTUM**
- Cirq
- Qiskit
- OpenFermion
- PennyLane*
- PyQuil
- Q#*

**MACHINE LEARNING**
- Scikit-learn
- TensorFlow*

**CHEMISTRY**
- Psi4
- NWChem
- GAMESS

**FINANCE**
- Quantlib

**DISCRETE OPTIMIZATION**
- Qbsolv

*Coming Soon 2020

**WORKFLOW LIFECYCLE MANAGEMENT**

Local Infrastructure

## CONDUCT

Smart backend deploys workflows, orchestrating across quantum and classical hardware.

### COMMAND LINE INTERFACE

**Orquestra Quantum Engine**

### HARDWARE

**GATE MODEL DEVICES**
- Superconducting qubits
- Photonic qubits*
- Ion traps

**QUANTUM ANNEALERS***

**DEDICATED CLASSICAL HARDWARE***

**QUANTUM CIRCUIT SIMULATORS**

*Coming Soon 2020

**CONTAINERIZED EXECUTION**

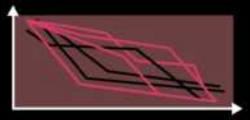
Zapata Cloud/Customer Environment Infrastructure (eg. Azure, AWS)

## RECORD

Analyze intermediate and final data, iterate and reproduce at scale.

### COMMAND LINE INTERFACE

**Orquestra Data Management Services**



### DATA ANALYSIS & VIZ

**WORKFLOW**
- Aggregation Service
- Correlation Service

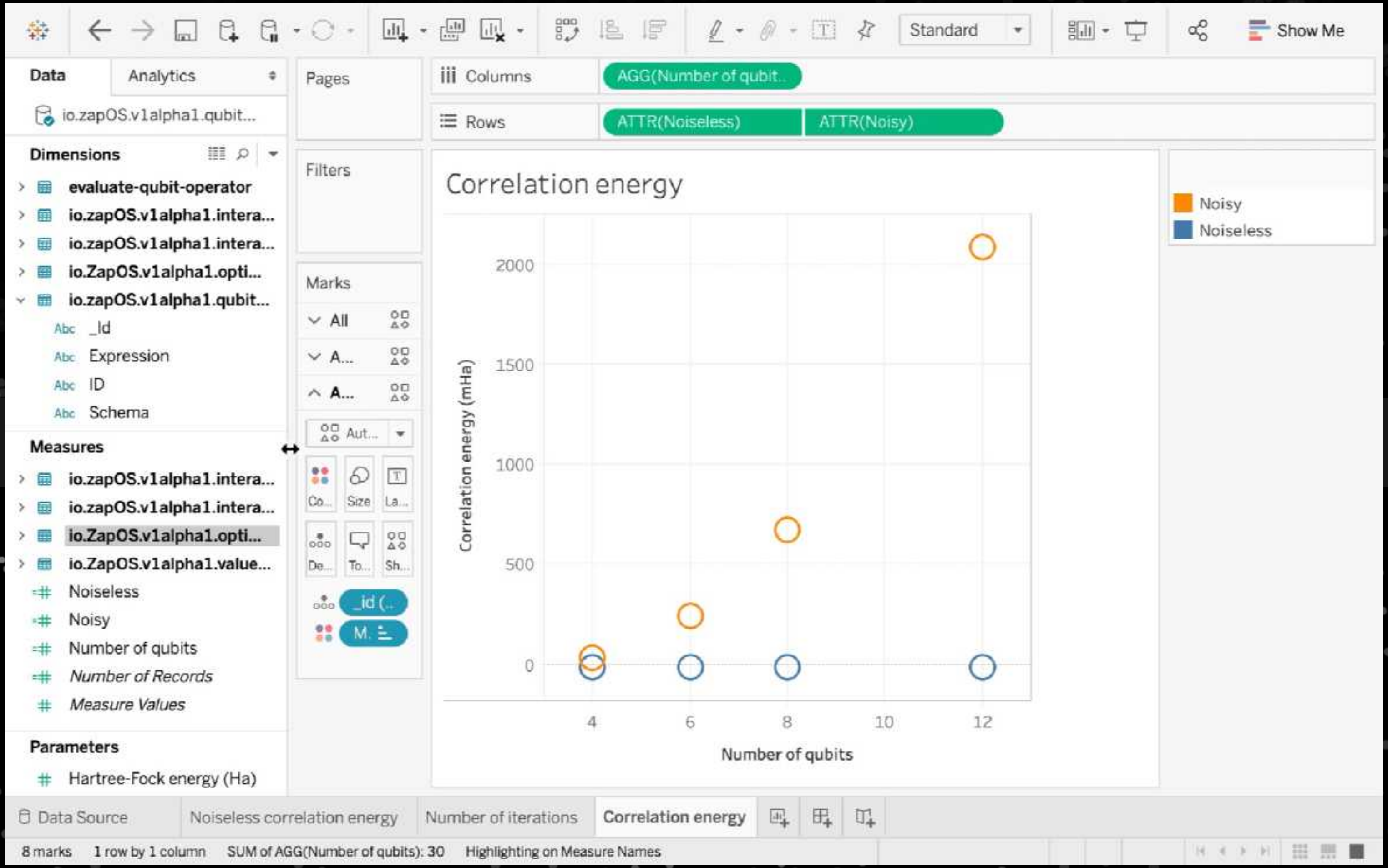
**ANALYSIS**
- Jupyter
- Pandas

**PLOTTING**
- Matplotlib
- Tableau
- Excel

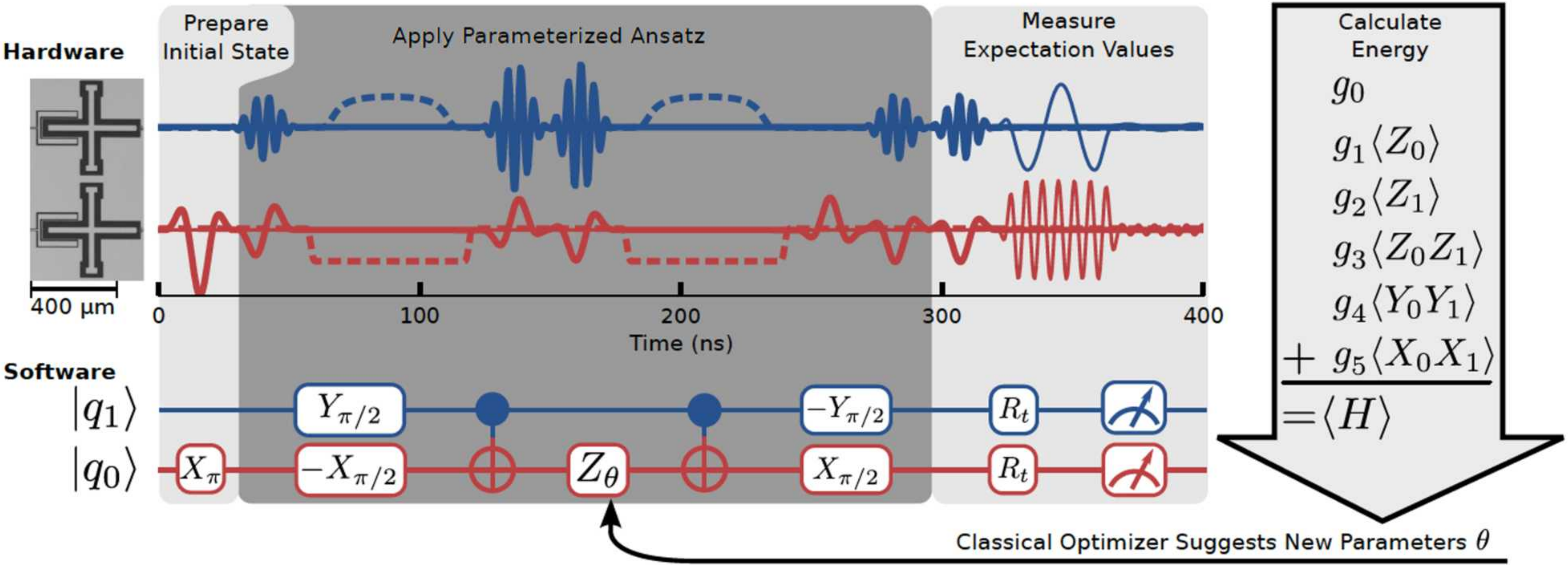
**SCALABLE DATA MANAGEMENT**

Zapata Cloud/Customer Environment Infrastructure(eg. Azure, AWS)

# Using Tableau + Orquestra Data Correlation Service (ODCS) to visualize results.



# Superconducting VQE for $H_2$

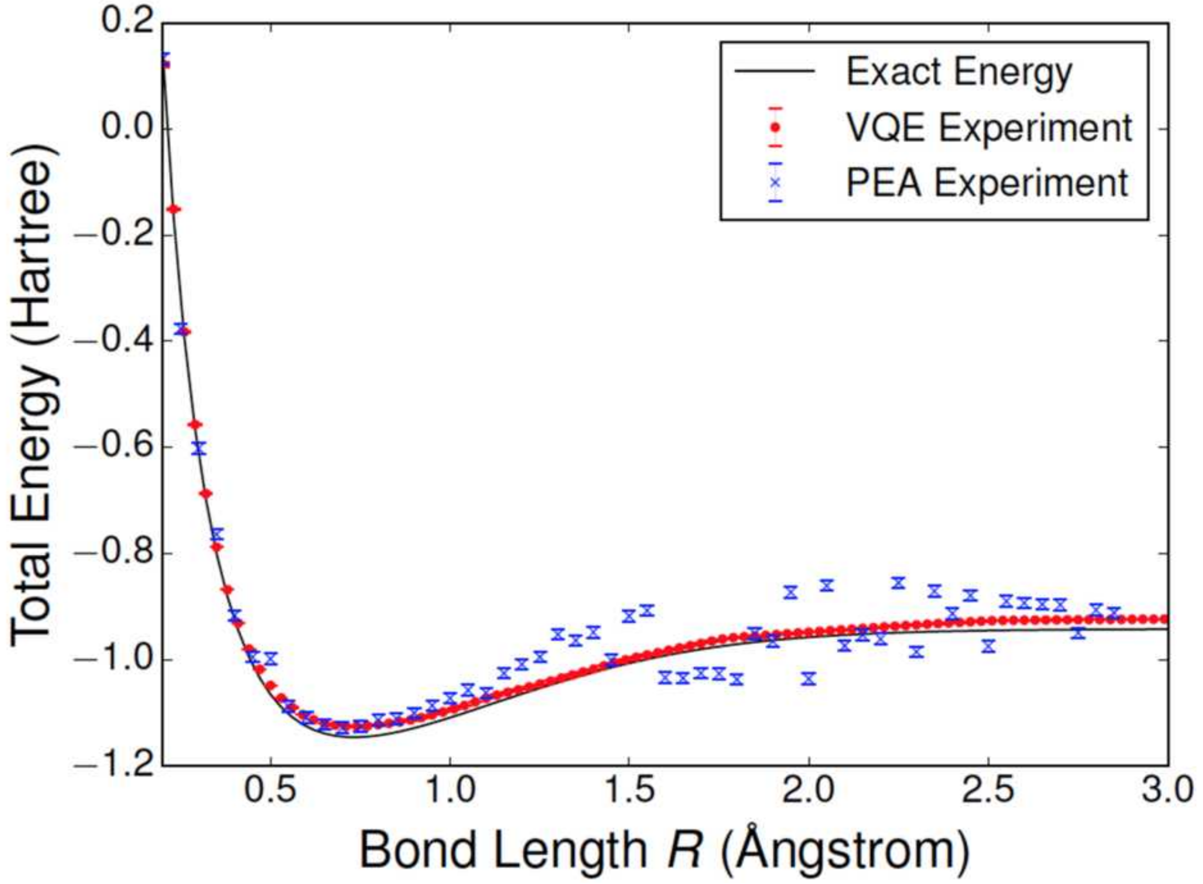



Used Xmon qubits to compute energy surface of molecular hydrogen

Started in Hartree-Fock state, used unitary coupled cluster, got chemical accuracy

P. O'Malley, et al. Physical Review X 6 031007 2016

# Superconducting VQE vs Phase Estimation

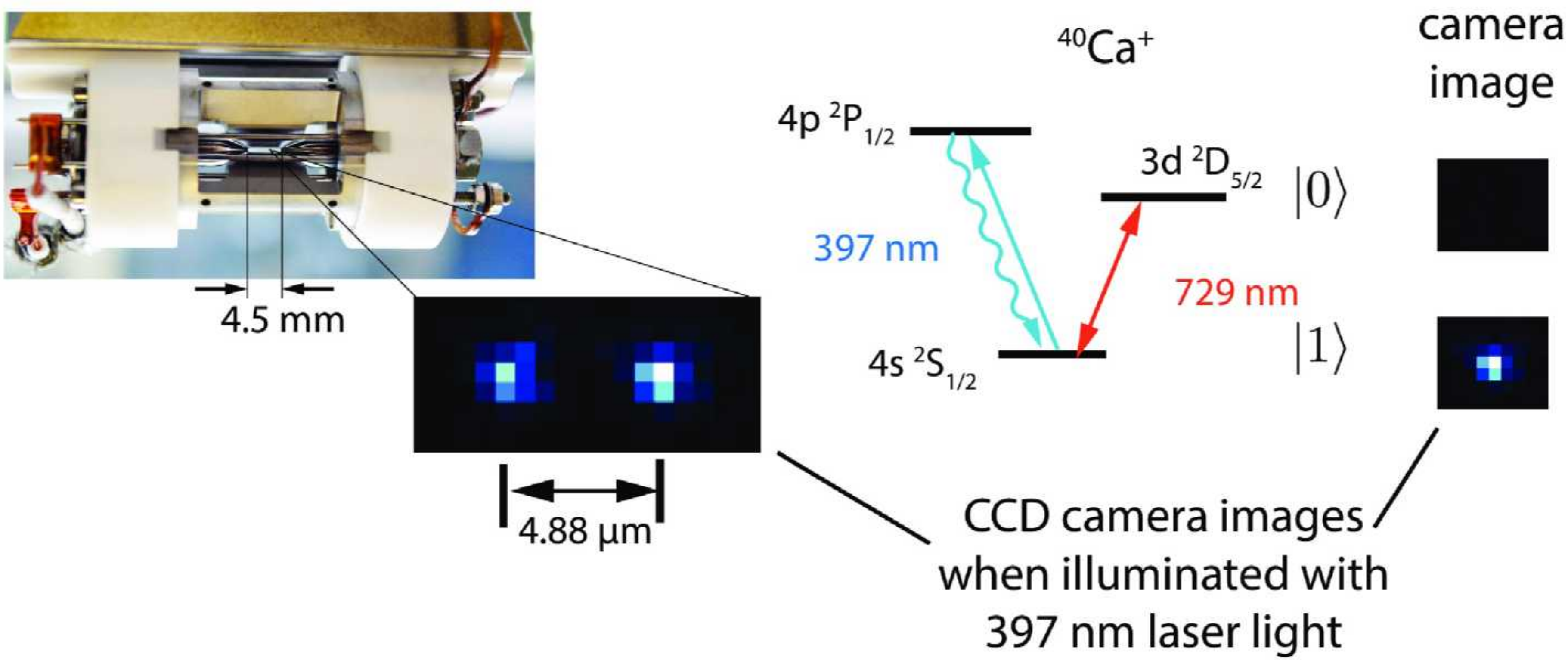



Predicted dissociation energy without exponentially costly compilation for first time
Substantial robustness to systematic errors seen

P. O'Malley, et al. Physical Review X 6 031007 2016

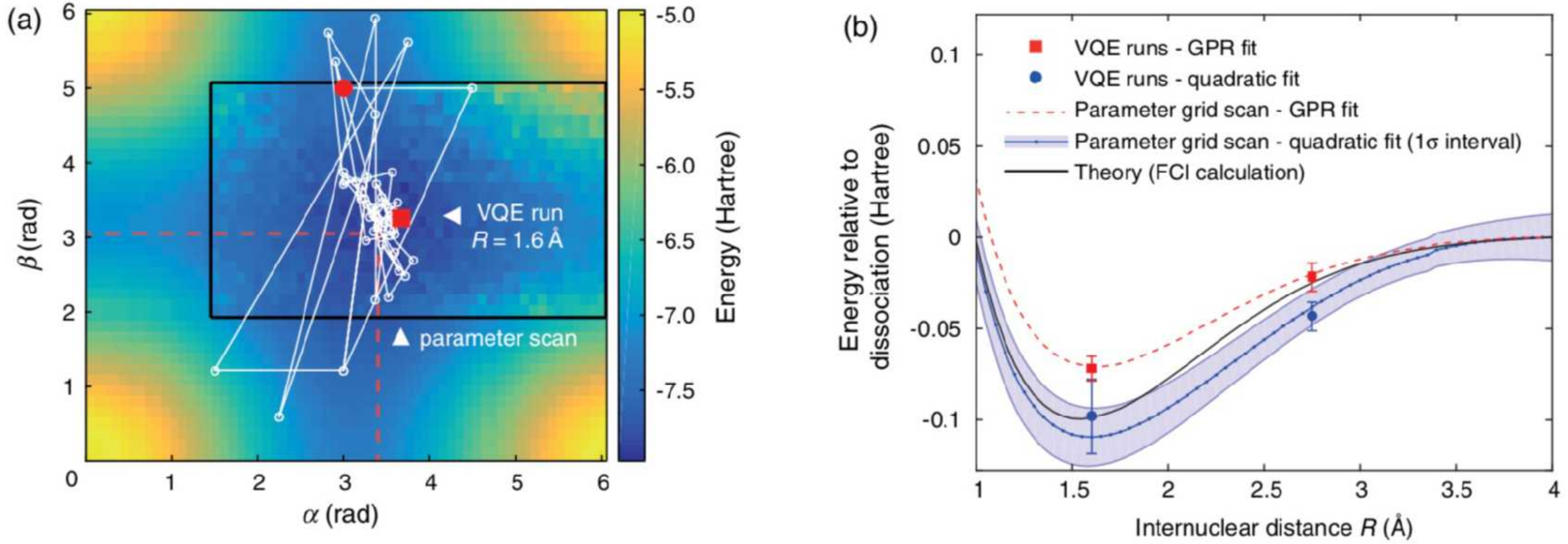
# Ion trap implementation

Collaboration with Rainer Blatt (Innsbruck)



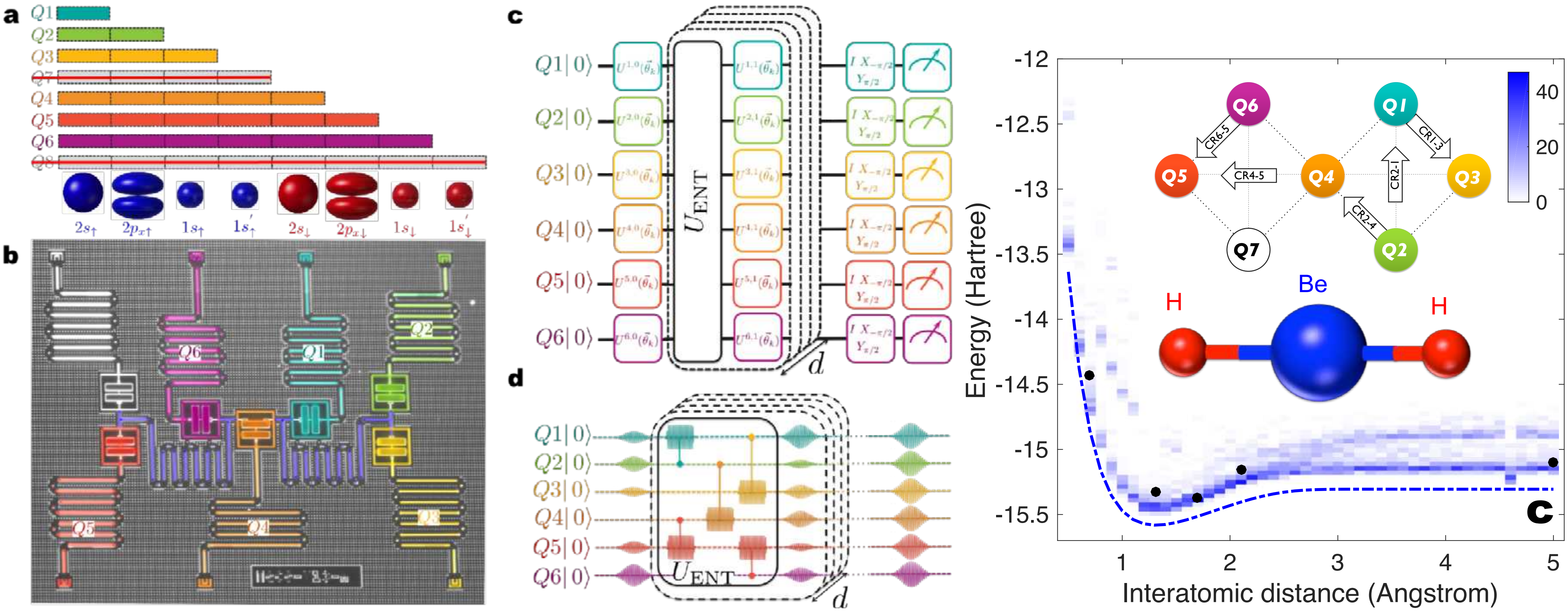

Cornelius Hempel, Christine Maier, Jonathan Romero, Jarrod McClean, Thomas Monz, Heng Shen, Petar Jurcevic, Ben P. Lanyon, Peter Love, Ryan Babbush, Alán Aspuru-Guzik, Rainer Blatt, and Christian F. Roos
Phys. Rev. X **8**, 031022

# Ion trap implementation (LiH)




Cornelius Hempel, Christine Maier, Jonathan Romero, Jarrod McClean, Thomas Monz, Heng Shen,
Petar Jurcevic, Ben P. Lanyon, Peter Love, Ryan Babbush, Alán Aspuru-Guzik, Rainer Blatt, and Christian F. Roos
Phys. Rev. X **8**, 031022

# Variational Eigensolver by IBM team!




**Hardware-efficient Quantum Optimizer for Small Molecules and Quantum Magnets**


Abhinav Kandala,* Antonio Mezzacapo,* Kristan Temme, Maika Takita, Jerry M. Chow, and Jay M. Gambetta
*IBM T.J. Watson Research Center, Yorktown Heights, NY 10598, USA*


(Dated: April 18, 2017)

H-Be-H, 6 qubit simulations.

Kandala, et al Nature 549 242 (2017)

# Water in Ion traps

## Ground-state energy estimation of the water molecule on a trapped ion quantum computer

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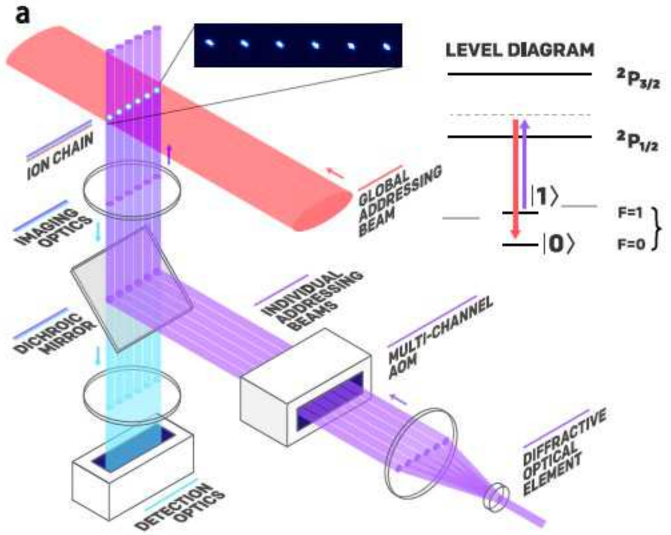
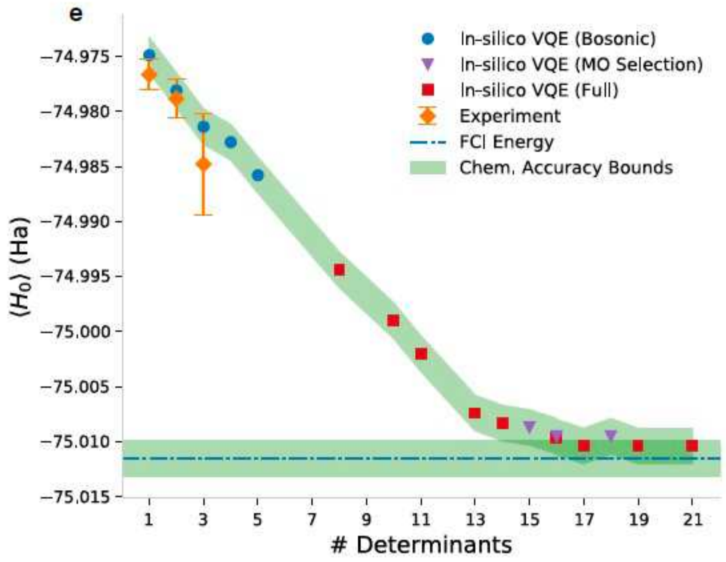
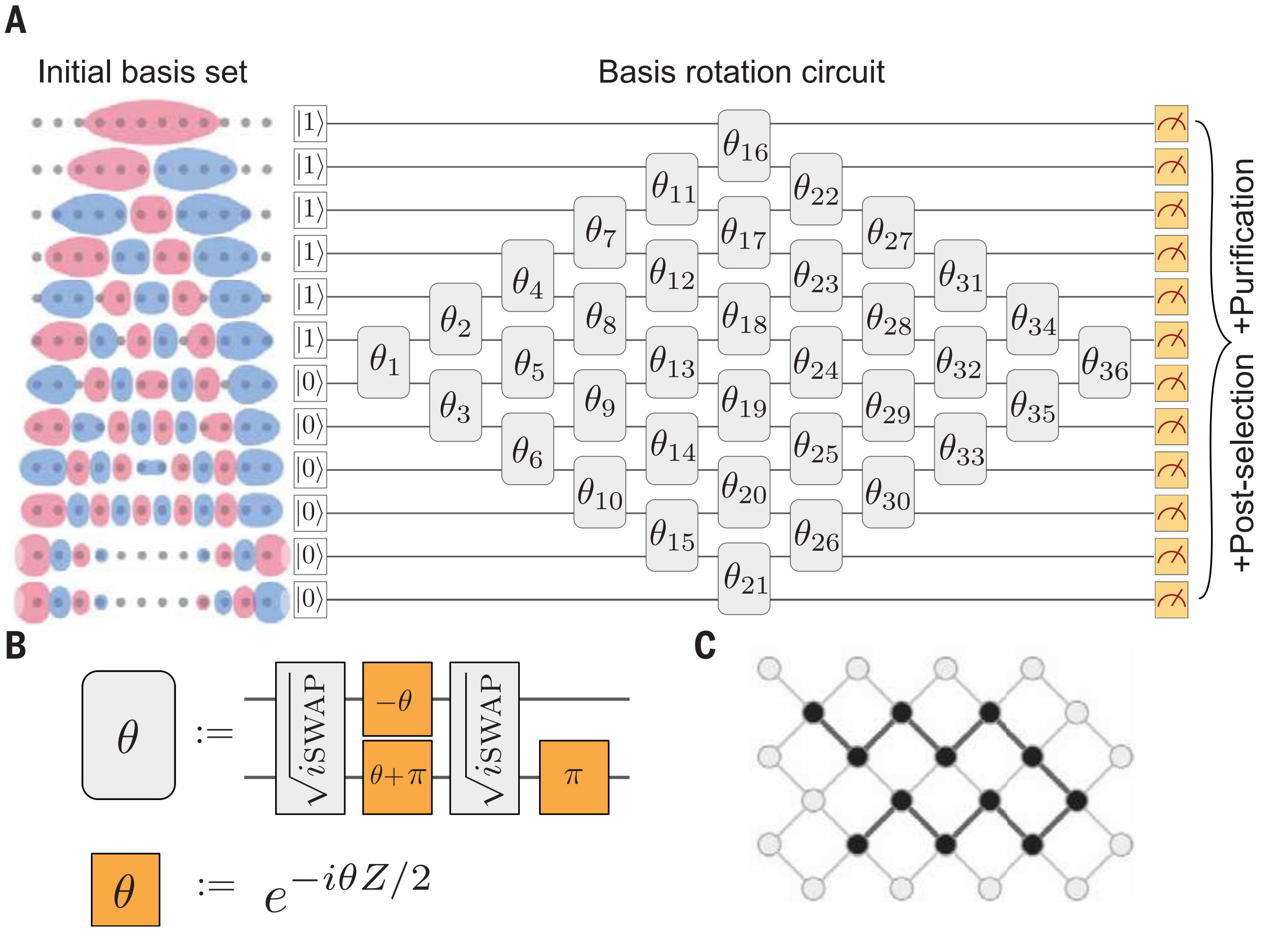
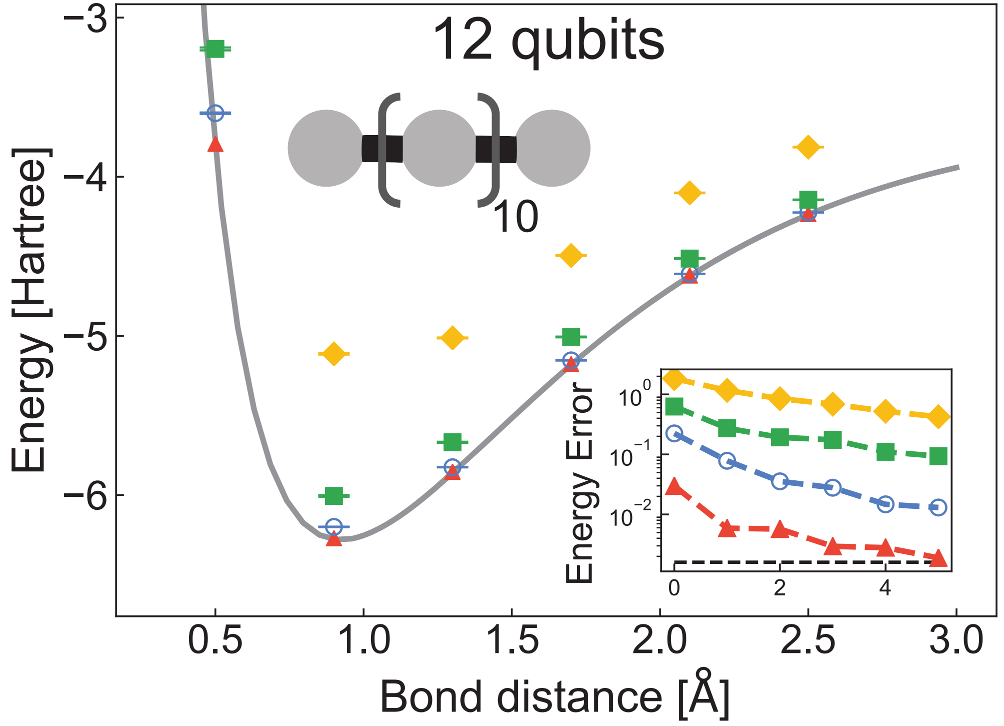



Y. Nam, et al. Arxiv:1902.10171 (2019)

# Largest simulation to date:
# Hartree Fock,  12 qubits. Hydrogen chains.




QUANTUM COMPUTING

## Hartree-Fock on a superconducting qubit quantum computer


Google AI Quantum and Collaborators*†

# VQE Realistic estimations and work needed

**Identifying challenges towards practical quantum advantage through resource estimation: the measurement roadblock in the variational quantum eigensolver**

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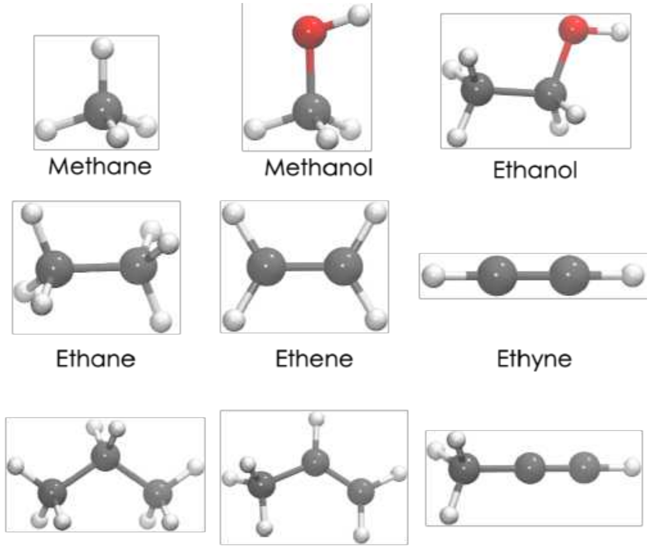
(Dated: December 9, 2020)

arXiV:2012.04001 (2020)




| Molecule | $H_2O$ | $CO_2$ | $CH_4$ | $CH_4O$ | $C_2H_6$ | $C_2H_4$ | $C_2H_2$ | $C_2H_6O$ | $C_3H_8$ | $C_3H_6$ | $C_3H_4$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| $N_{el}$ | 8 | 16 | 8 | 14 | 14 | 12 | 10 | 20 | 20 | 18 | 16 |
| $N_q$ | 104 | 208 | 104 | 182 | 182 | 156 | 130 | 260 | 260 | 234 | 208 |
| $K \cdot 10^{-3}$ | 1.9 | 16 | 1.6 | 8.4 | 8.5 | 6.6 | 3.1 | 24 | 16 | 23 | 18 |
| $M \cdot 10^{-9}$ | 3.9 | 32 | 3.2 | 17 | 17 | 13 | 6.2 | 48 | 31 | 46 | 36 |
| $t$ (days) | 2.3 | 39 | 1.9 | 18 | 18 | 12 | 4.6 | 71 | 47 | 62 | 44 |

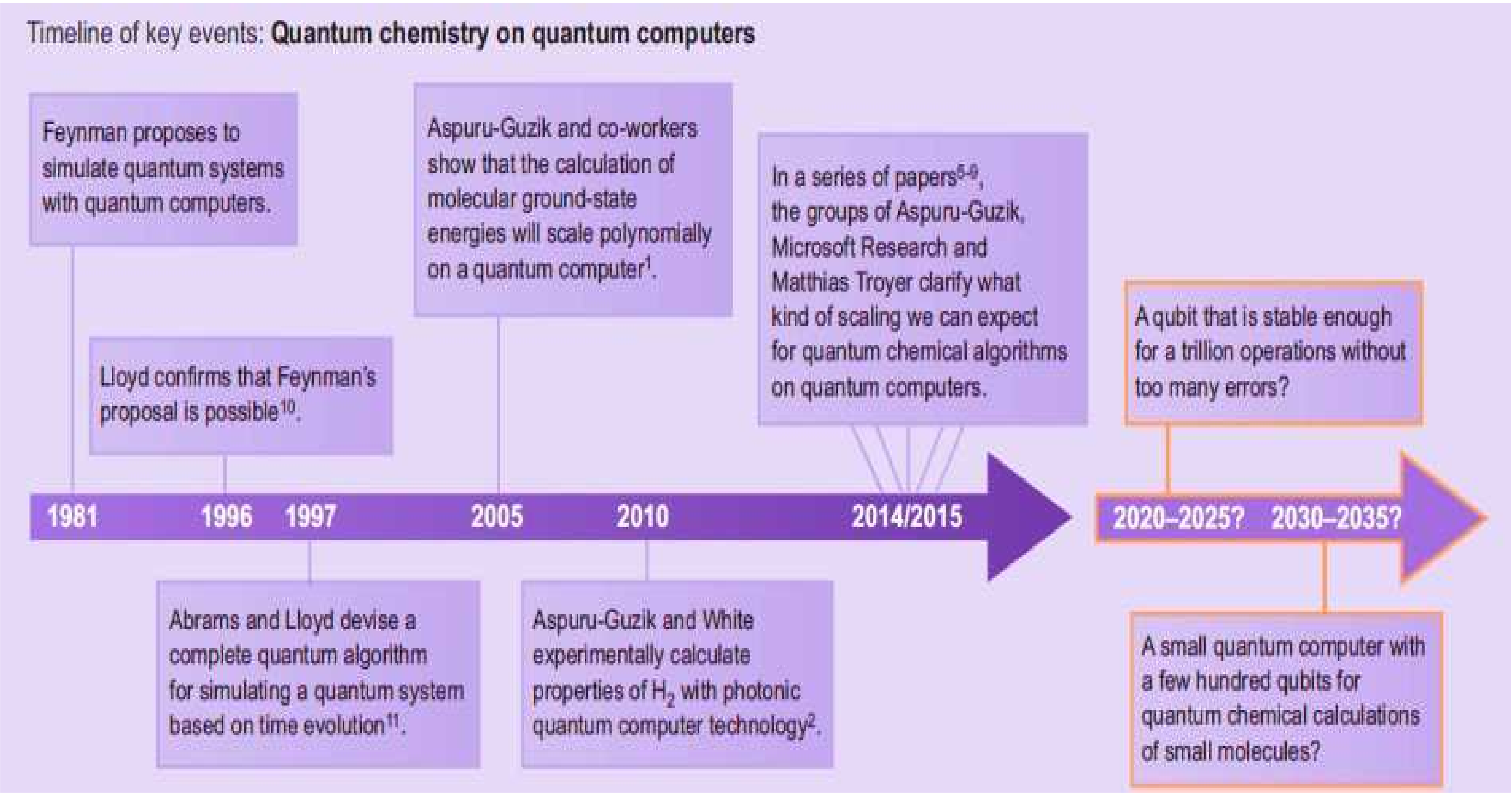
TABLE IV. Estimated runtimes $t$ in days for a single energy evaluation using the number of measurements $M$ from extrapolated values of $K$ (Equation 17 and Table III), with $\epsilon = 0.5$ mHa and the effect of RDM constraints included by a factor of 1/2 (see Equation 18). The number of qubits $N_q$ is computed from the number of active electrons $N_{el}$ and our empirical estimations of active space size (Equation 16).

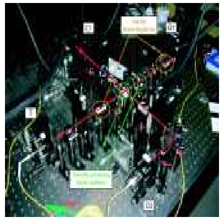
To conclude, our estimation for the number of qubits $N_q$ necessary to obtain accurate dynamical correlation energies is at least

$$N_q \approx 13 N_{el} \qquad (16)$$

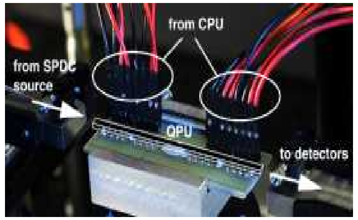
where $N_{el}$ is the number of active electrons in the system.

# Quantum chemical advantage?

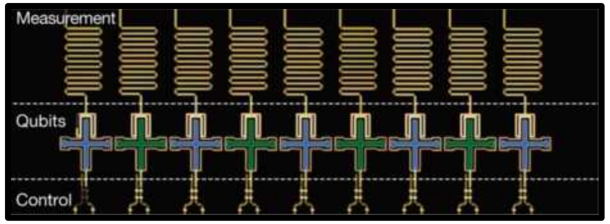


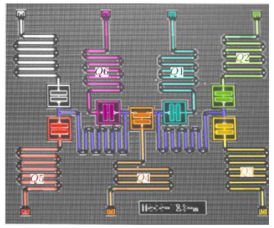
2010 $H_2$



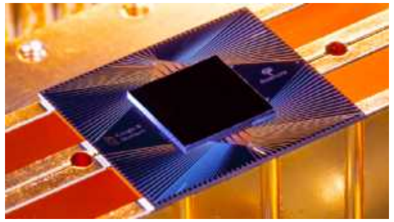

2014 $HeH^+$




2015 Scalable $H_2$



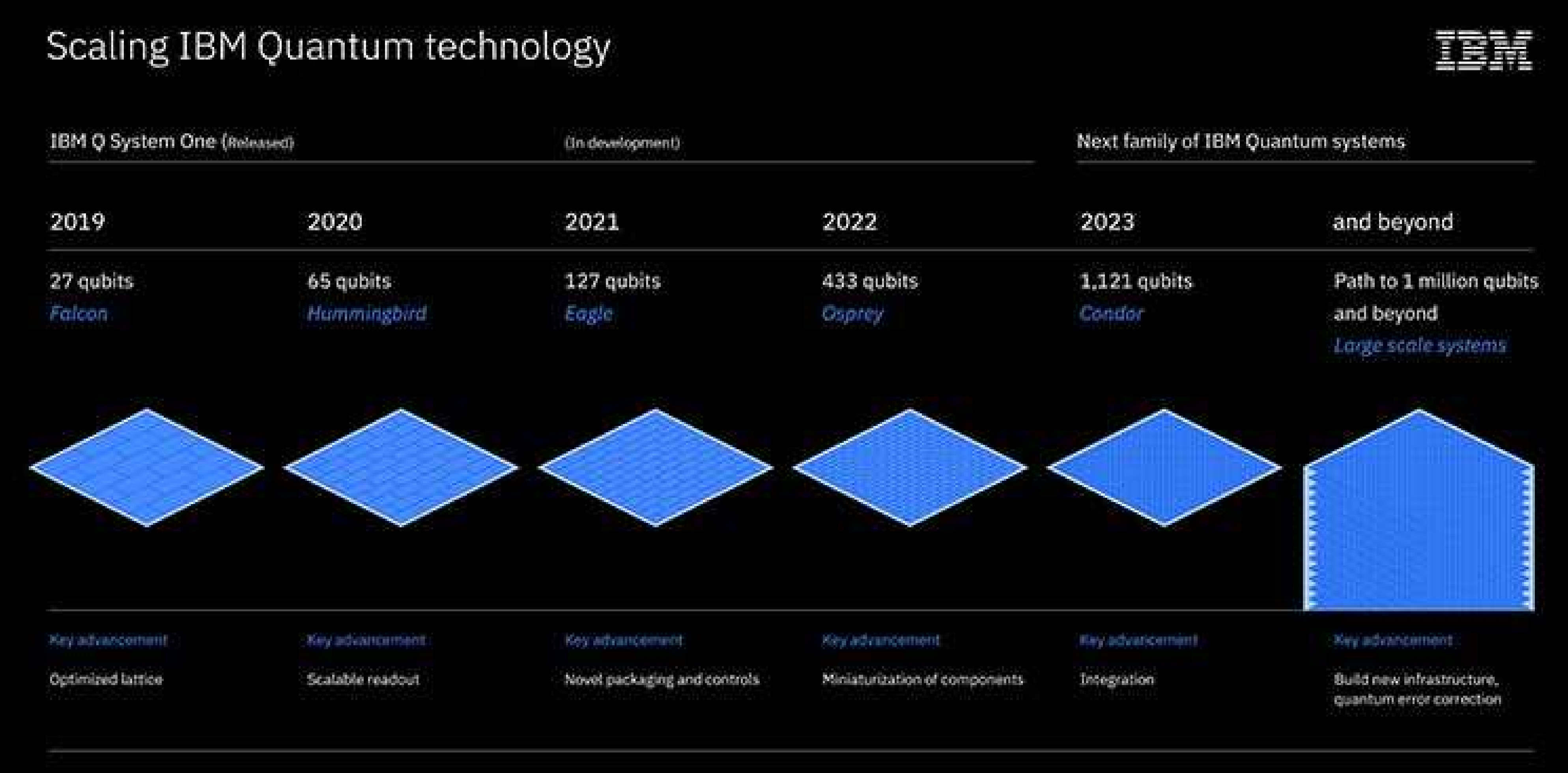
2017 Scalable $BeH_2$



2020 Hydrogen chains (HF)

Leonie Mueck. Nature Chemistry 7 361 20

# IBM Roadmap




https://www.ibm.com/blogs/research/2020/09/ibm-quantum-roadmap/

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