Vamos a comenzar en breve, a las 1 CDT / 2 EDT

Cómputo Cuántico para Química

El cómputo cuántico es una de las áreas de expansión prometedora para la química teórica. Las computadoras cuánticas usan efectos cuánticos para realizar procesos de cómputo. Este nuevo tipo de computadora puede simular a los átomos y a las moléculas, así como a los materiales de manera exacta.

En esta presentación, el Dr. Alán Aspuru-Guzik Profesor de Química y de Ciencias de Computación en la Universidad de Toronto describirá qué es el cómputo cuántico, cuál es el estado actual del campo y algoritmos y experimentos que recientemente se han realizado en estas computadoras.

Lo Que El Público Aprenderá

- Qué son las computadoras cuánticas
- Por qué las computadoras cuánticas prometen ser una herramienta valiosa para las ciencias químicas
- El estado actual del cómputo cuántico para la química

Ponente y Moderadora

Alán Aspuru-Guzik
Universidad de Toronto

Ingrid Montes
Universidad de Puerto Rico, Recinto de Río

El Vigésimo Webinar en Español auspiciado por ACS y SQM

http://bit.ly/ComputoCuantico

1

¿Tiene preguntas para el ponente?

"¿Por qué he sido "silenciado"?

No se preocupe. Todo el mundo ha sido silenciado, excepto el ponente y la moderadora. Gracias, y disfruten de la presentación.

Escriba y someta sus preguntas durante la presentación

2

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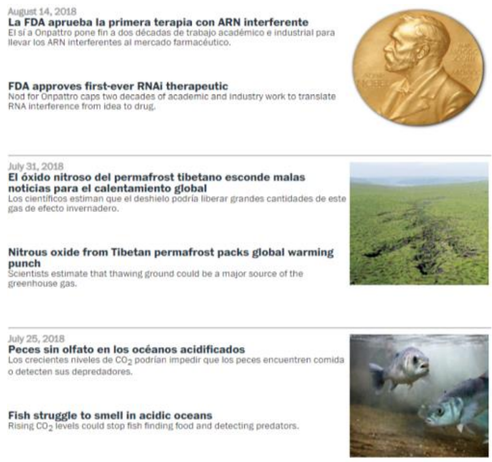
C&EN pone a su disposición traducciones al español de sus artículos más populares.


August 14, 2018
La FDA aprueba la primera terapia con ARN interferente
El sí a Onpattro pone fin a dos décadas de trabajo académico e industrial para llevar los ARN interferentes al mercado farmacéutico.

FDA approves first-ever RNAi therapeutic
Nod for Onpattro caps two decades of academic and industry work to translate RNA interference from idea to drug.

July 31, 2018
El óxido nitroso del permafrost tibetano esconde malas noticias para el calentamiento global
Los científicos estiman que el deshielo podría liberar grandes cantidades de este gas de efecto invernadero.

Nitrous oxide from Tibetan permafrost packs global warming punch
Scientists estimate that thawing ground could be a major source of the greenhouse gas.

July 25, 2018
Peces sin olfato en los océanos acidificados
Los crecientes niveles de CO_2 podrían impedir que los peces encuentren comida o detecten sus depredadores.

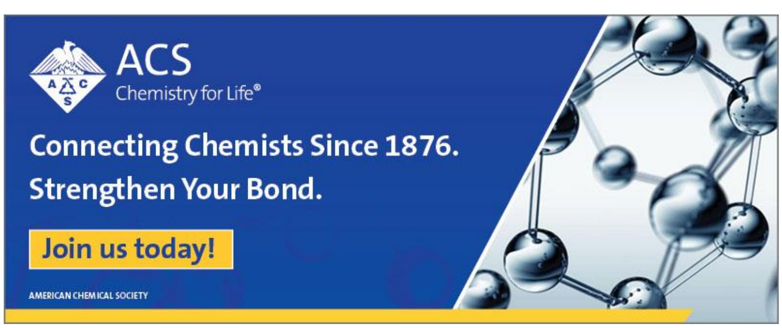
Fish struggle to smell in acidic oceans
Rising CO_2 levels could stop fish finding food and detecting predators.

Gracias a una colaboración con la organización española Divúlgame.org, C&EN ahora es capaz de ofrecer traducciones al español de algunos de nuestros mejores contenidos. Queremos hacer de la ciencia de vanguardia más accesible a la comunidad química de habla española, y esta es nuestra contribución. Le da a los nacidos en España, América Latina, o los EE.UU., pero cuyo primer idioma es el español la oportunidad de leer este contenido en su lengua materna. Esperamos que les guste y sea de su utilidad.

Dr. Bibiana Campos Seijo
Editora en Jefe, *C&EN*

http://bit.ly/CENespanol

Únase a una comunidad global de más de 150,000 profesionales de la química



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Desde sus comienzos de la Sociedad Química de México, se buscaba un emblema sencillo, no demostrar partidarismo alguno y significar al gremio, debería representar un símbolo no sólo para los químicos, sino también para ingenieros, farmacéuticos, metalurgistas, en fin que englobe e identifique por igual a los científicos en todas sus áreas de las ciencia química.

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Alberto Nuñez Sellés,
Universidad Nacional Evangélica

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SOCIEDAD QUÍMICA DE MÉXICO, A.C.
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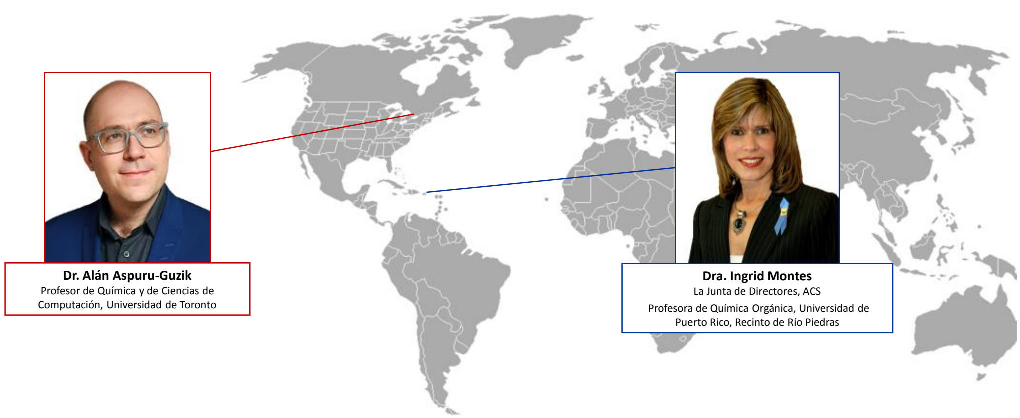
"Cómputo Cuántico para Química"



Las imágenes de la presentación están disponibles para descargar ahora desde el panel de GoToWebinar

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El Webinar de hoy esta auspiciado por la Sociedad Química de México y the American Chemical Society

10

The Age of Variational Quantum Algorithms

Alán Aspuru-Guzik

Professor of Chemistry
Professor of Computer Science
University of Toronto
Vector Institute for Artificial Intelligence

Chief Scientific Officer
Zapata Computing

Chief Vision Officer
Kebotix

12

Early classical mechanical simulators

Antykythera Mechanism

circa 200 BC

Digital Computer Simulation

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)

Simulating Matter

Flow batteries

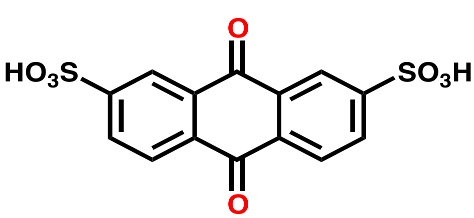
e.g. Huskinson, et al., Nature 505 195 2014

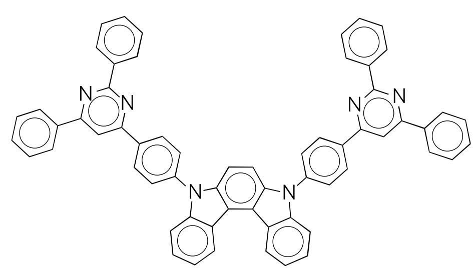
Organic light-emitting diode displays

e.g. R. Gomez-Bombarelli, Nature Materials 15, 1120 2016

15

Simulating Matter





L1

Flow batteries

e.g. Huskinson, et al., Nature 505 195 2014

Organic light-emitting diode displays

e.g. R. Gomez-Bombarelli, Nature Materials 15, 1120 2016

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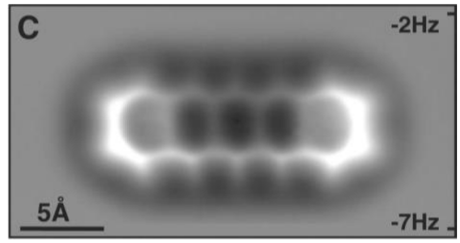
Simulating Matter

Flow batteries

e.g. Huskinson, et al., Nature 505 195 2014

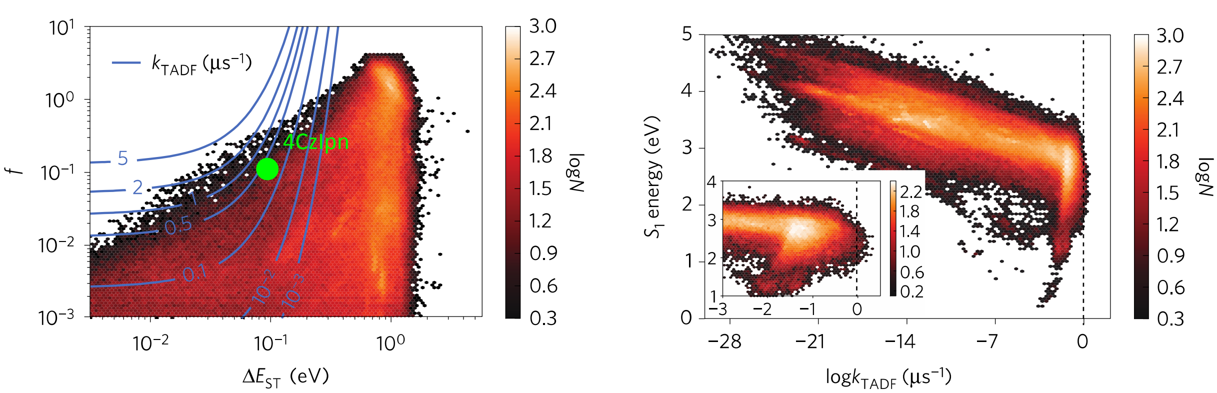


Pentacene on a surface

Gross et. al., Science 325 1110 2009

17

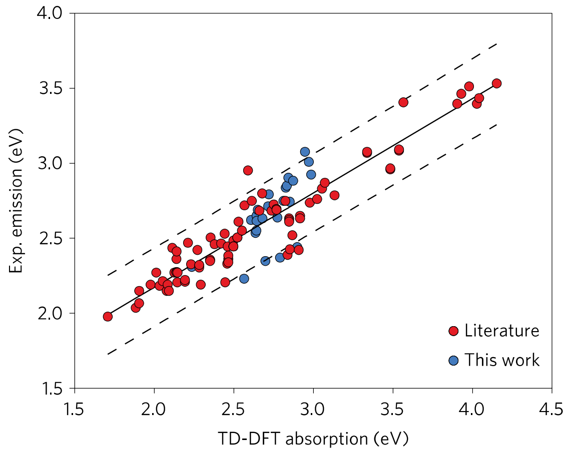
Data Mining 500,000 Quantum Calculations



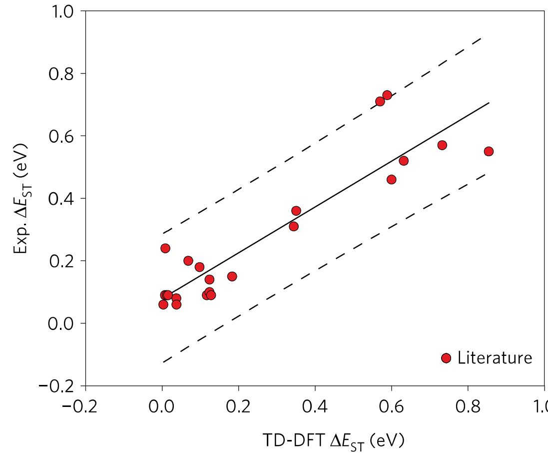
R. Gomez-Bombarelli, et al. Nature Materials 15, 1120 2016

18

Calibration of TDDFT with Experiment

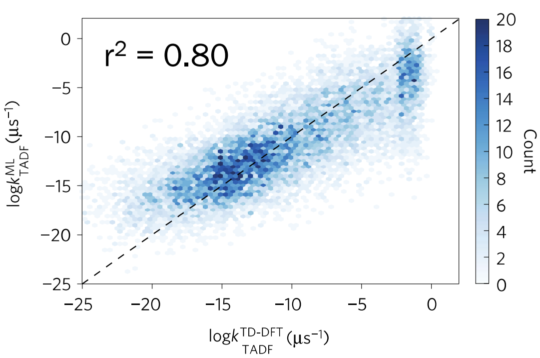


TD-DFT/B3LYP/6-31G(d) vertical absorption against PL emission maximum in **toluene**



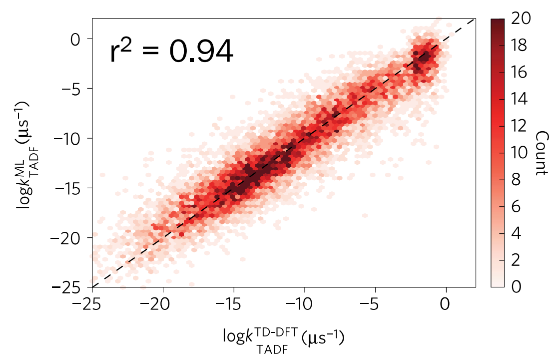
TD-DFT/B3LYP/6-31G(d) ST-Gap vs thermal activation in frozen **toluene**

Machine Learning

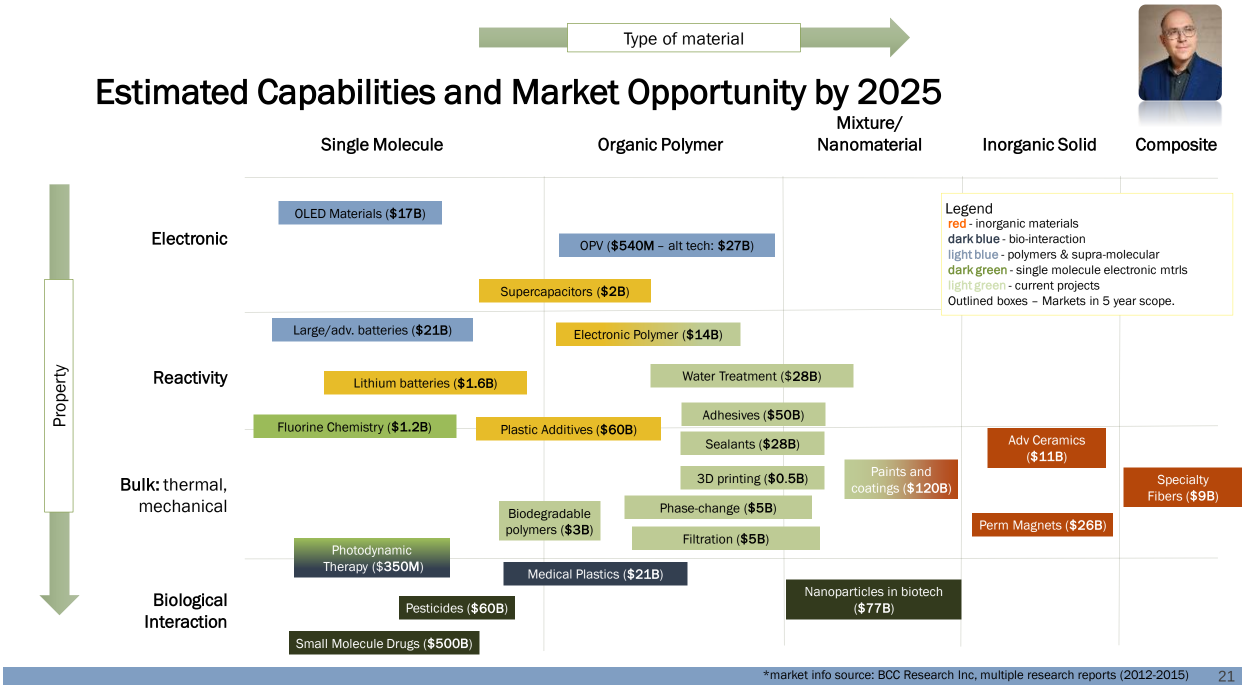


Linear regression model (c.f. QSAR)

vs

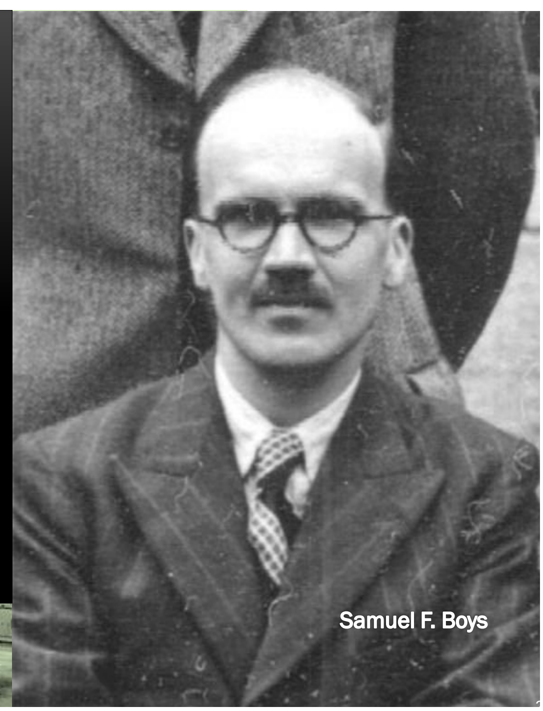


Convolutional neural network (modern machine learning)

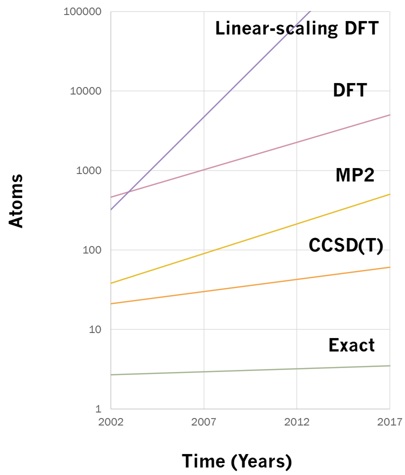


"[H]e produced a paper tape of his whole computer program and unrolled it along the length of the chemical lecture bench. There, in one roll, was something, of which one could ask a chemical question at one end and it would produce an answer at the other! . . . most of the audience probably thought the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

Handy, Pople, Shavitt, JPCA (1996)



Classical Computer Algorithms



Density functional theory

Errors of ~ kT for molecular properties

Full Configuration Interaction

Exact within a basis

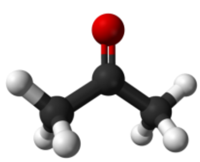
Method	Formal Scaling[1,2]
Hartree-Fock	$O(N^4)$
MP2	$O(N^5)$
CCSD(T)	$O(N^7)$
DMRG	$O(N^3M^3)$

Figure adapted from M. Head-Gordon, M. Artacho, *Physics Today* 4 (2008)

23

The Current Paradigm

quantum system



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

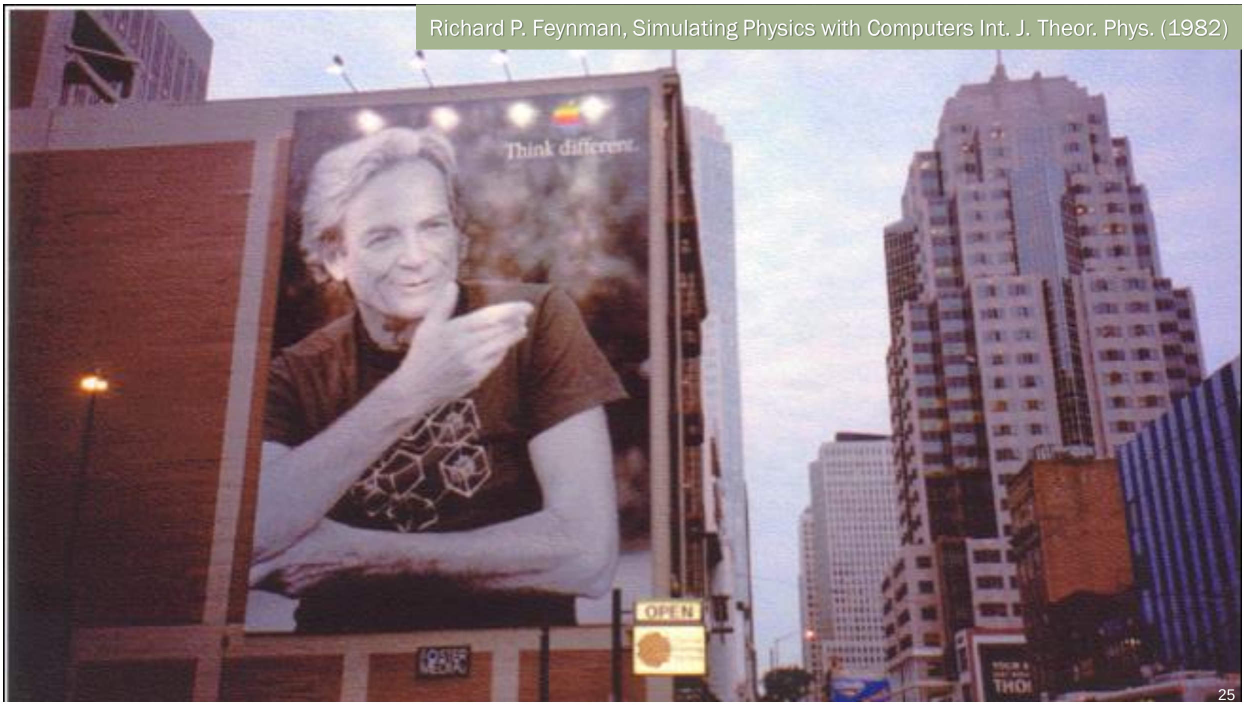
quantum model (quantum information)

classical information processor

classical information

E= -192.0492 Hartree

24



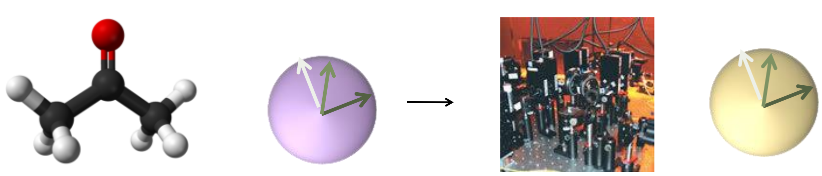
Richard P. Feynman, Simulating Physics with Computers Int. J. Theor. Phys. (1982)

25

Quantum Computer Simulation

$$|\Psi^{mol}\rangle \quad \rightarrow \quad |\Psi^{QC}\rangle$$

$$\hat{U}^{mol}(t) = e^{-i\hat{H}^{mol}t} \quad \rightarrow \quad \hat{U}^{QC}(t) = e^{-i\hat{H}^{QC}t}$$



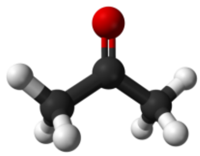
quantum system

quantum system
(quantum information)

26

The Quantum Simulation Way

quantum system

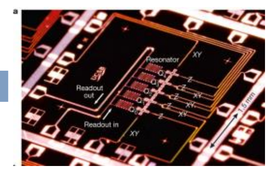


$$\hat{H}|\Psi\rangle = E|\Psi\rangle$$

quantum model
(quantum information)

classical
information

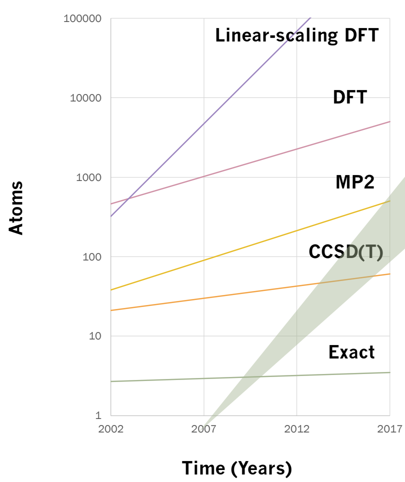
E= -192.0492
Hartree



Quantum information
processor

27

Disruption and Quantum Supremacy



Exact simulation via quantum computers

Predictive rather than explanatory simulation of matter

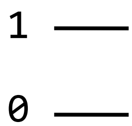
Quantum supremacy

"Quantum information word of the year 2015"
When a quantum computer outperforms a classical computer

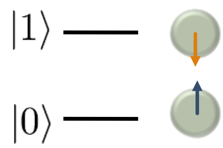
Figure adapted from M. Head-Gordon, M. Artacho, *Physics Today* 4 (2008)

28

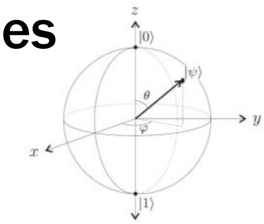
Quantum Computers in 3 slides



classical bit



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

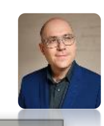
quantum computer

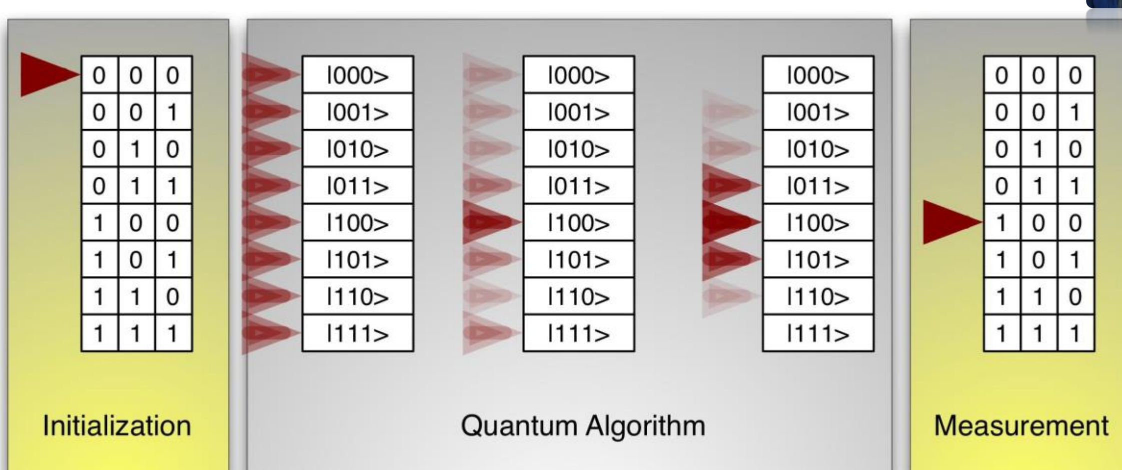
Collection of controllable qubits

Subject to decoherence

Ability for quantum error correction

Quantum Computation





Quantum Gates and Circuits

Single qubit gates

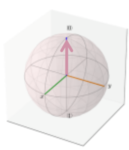
Rotations

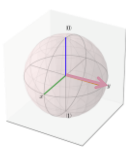
$$-\boxed{R_{\hat{n}}}- = \exp[-i(\vec{\sigma}.\hat{n})\theta/2]$$

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

Hadamard gate

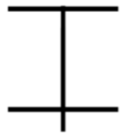
$$-\boxed{\mathrm{H}}- = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$





Two qubit gates

Controlled-not (CNOT) gate

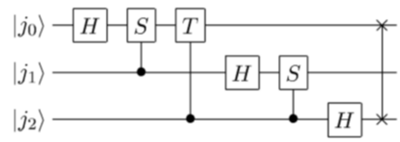


$$= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

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

Subroutines

Quantum Fourier Transform



The Power of Quantum Computers

Myth — Quantum algorithms are always faster and more efficient than classical ones

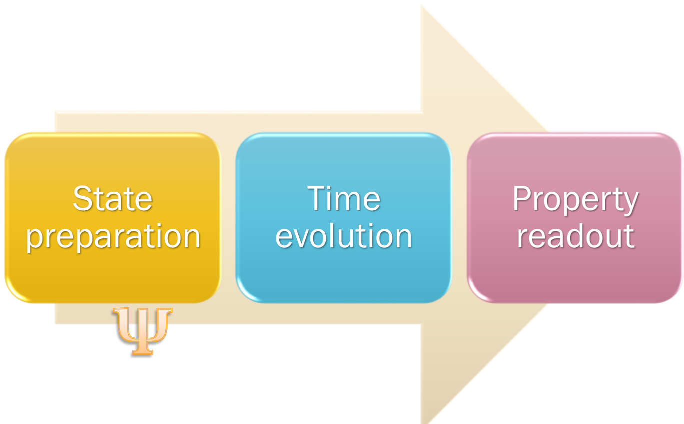
Quantum algorithm hall of fame

Search	quadratic speedup
Factoring	exponential speedup
Quantum simulation	exponential speedup*

* Restrictions may apply. Read your owner's manual.

Quantum Computer Simulation

Merlin



Arthur

33

Complexity Classes

- Quantum Merlin Arthur
  (**Complete:** two-body Hamiltonian problem)

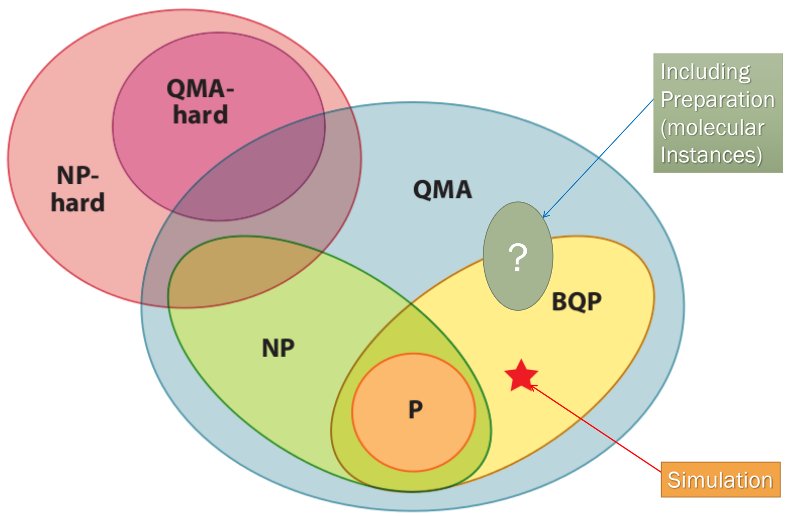
> Decision problems that have a proof that can be verified by a quantum computer

- Bounded Quantum Polynomial (BQP)

> The class of decision problems **solvable in polynomial time** by a quantum computer

34

Quantum Complexity of Chemical Simulation



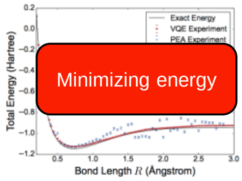
http://www.youtube.com/watch?v=6ybd5rbQ5rU

35

36

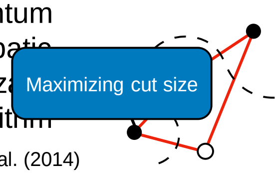
The age of variational quantum algorithms
... training quantum circuits.

Variational quantum eigensolver

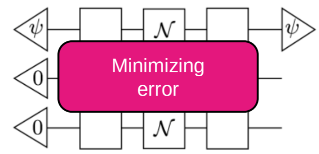


Peruzzo et al. (2014)

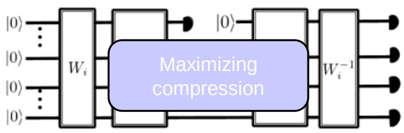
Quantum adiabatic optimization algorithm



Farhi et al. (2014)

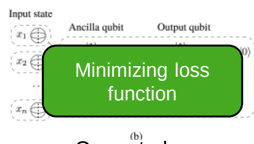


Quantum Variational error corrector (QVECTOR)
arXiv:1711.02249



Quantum autoencoder

Romero, et al.
Quantum Sci. Technol. 2 (2017): 045001



Cao, et al.
arXiV:1711.11240

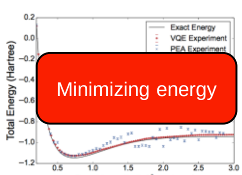
Quantum neuron

... and many other algorithms, e.g. Machine Learning

37

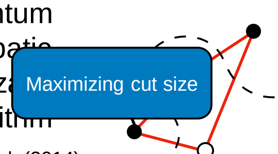
The age of variational quantum algorithms
… training quantum circuits.

Variational quantum eigensolver

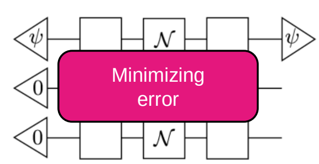


Peruzzo et al. (2014)

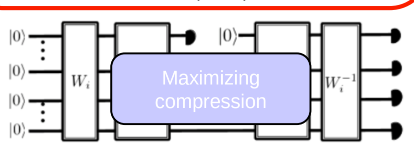
Quantum adiabatic optimization algorithm



Farhi et al. (2014)

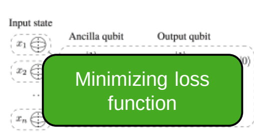


Quantum Variational error corrector (QVECTOR)



Quantum autoencoder

Romero, et al.
Quantum Sci. Technol. 2 (2017): 045001

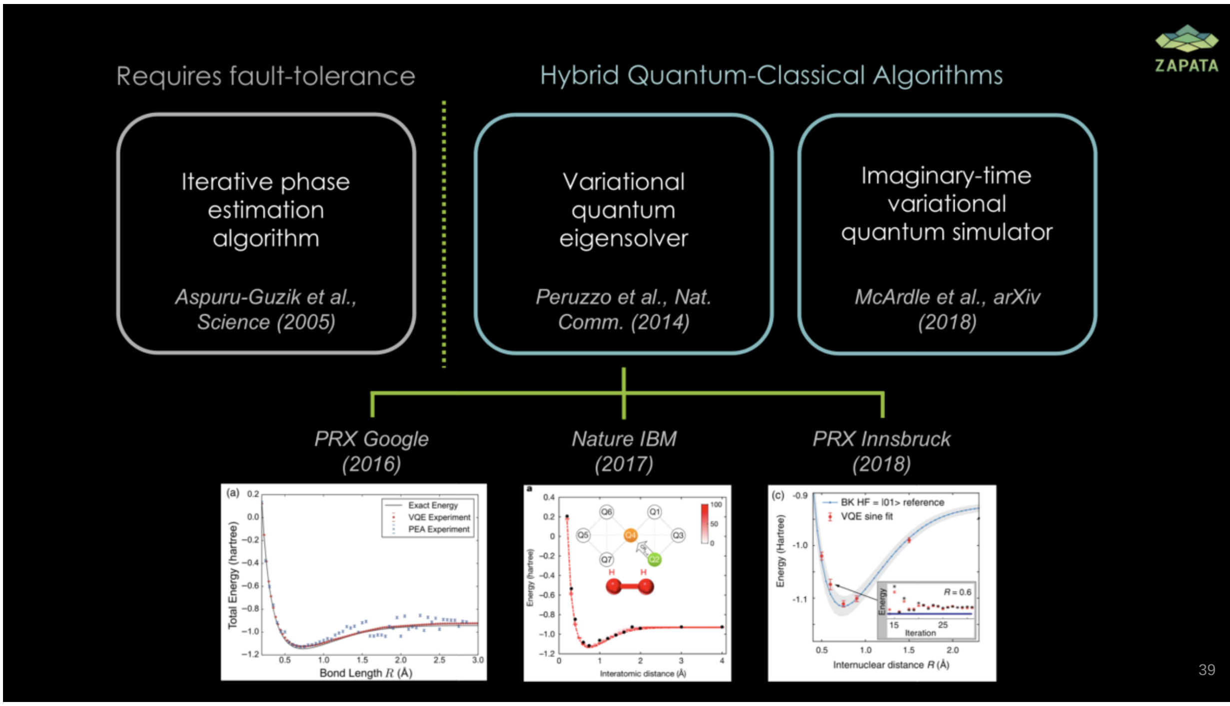


Cao, et al.
arXiV:1711.11240

Quantum neuron

... and many other algorithms, e.g. Machine Learning

38



The Variational Quantum Eigensolver (VQE)

Guess a trial wave function → Prepare trial wave function → Evaluate its energy

Variational energy minimization

Peruzzo, McClean, Shadbolt, Yung, Zhou, Love, Aspuru-Guzik, O'Brien. Nature Communications 5 4213 2014

Romero, et al arXiV:1701.02691. Quantum Science and Technology (2018) In Press

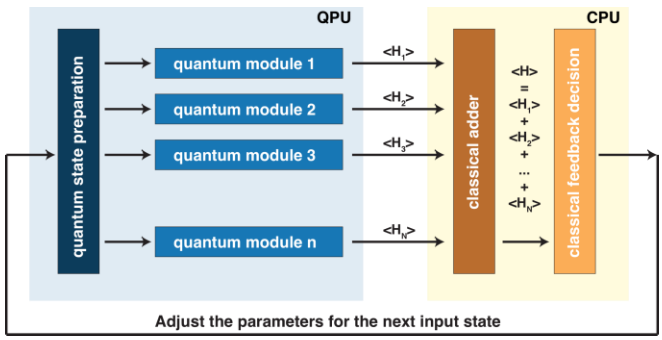
40

The Variational Quantum Eigensolver (VQE)

Minimize energy: $\underset{|\psi\rangle}{\operatorname{argmin}} \frac{\langle\psi|\,\mathcal{H}\,|\psi\rangle}{\langle\psi|\psi\rangle}.$

$$\mathcal{H} = h^i_\alpha \sigma^i_\alpha + h^{ij}_{\alpha\beta}\sigma^i_\alpha\sigma^j_\beta + h^{ijk}_{\alpha\beta\gamma}\sigma^i_\alpha\sigma^j_\beta\sigma^k_\gamma + \ldots$$

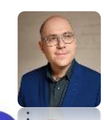
$$\langle\psi|\,\mathcal{H}\,|\psi\rangle \equiv \langle\mathcal{H}\rangle = \mathcal{H} = h^i_\alpha\,\langle\sigma^i_\alpha\rangle + h^{ij}_{\alpha\beta}\,\langle\sigma^i_\alpha\sigma^j_\beta\rangle + h^{ijk}_{\alpha\beta\gamma}\,\langle\sigma^i_\alpha\sigma^j_\beta\sigma^k_\gamma\rangle + \ldots$$

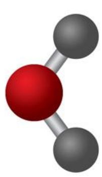


Peruzzo, McClean, Shadbolt, Yung, Zhou, Love, Aspuru-Guzik, O'Brien. Nature Communications 5 4213 2014

41

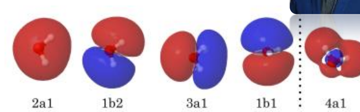
Quantum Chemistry in 1 Slide





Self-consistent solution in local basis

Molecular orbitals and "integrals"



Molecular Hamiltonian

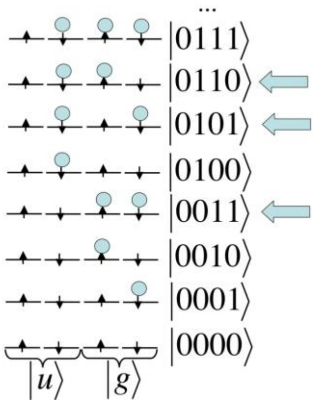
$$\hat H = \sum_X \hat h_X = \sum_{p,q}\langle p|\hat T + \hat V_N|q\rangle \hat a_p^\dagger \hat a_q \pm \frac{1}{2}\sum_{p,q,r,s}\langle p|\langle q|\,\hat V_e|r\rangle|s\rangle \hat a_p^\dagger \hat a_q^\dagger \hat a_r \hat a_s$$

One electron integrals

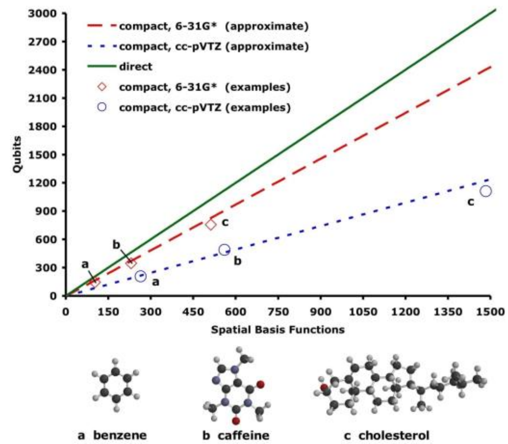
Two-electron integrals

42

Mapping and Baseline Resource Requirements



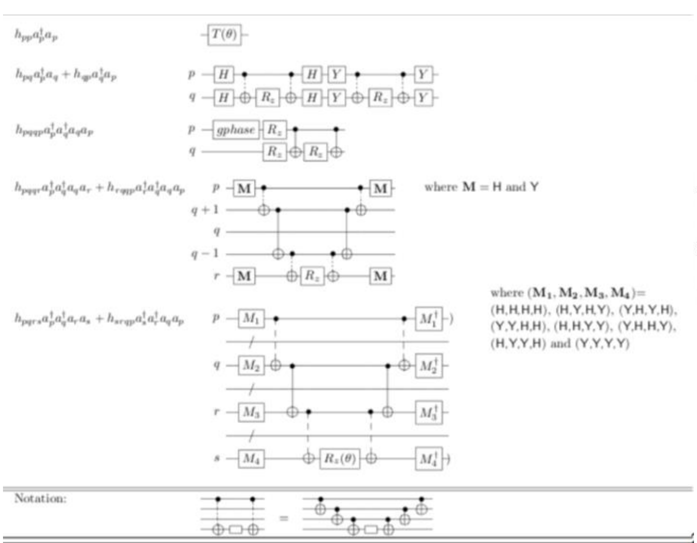
Direct mapping

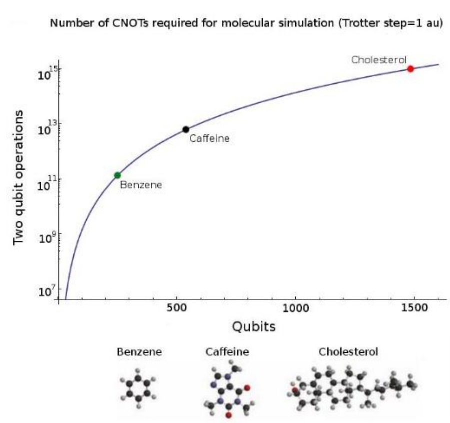


A. Aspuru-Guzik, A. D. Dutoi, P. J. Love, M. Head-Gordon, Science (2005) **Full quantum circuit:** J. D. Whitfield, et. al., Mol. Phys. (2011) **Error correction:** N. Cody Jones, J. D. Whitfield, et al. New. J. Phys.(2012)

43

Steep Scaling for Baseline Algorithm



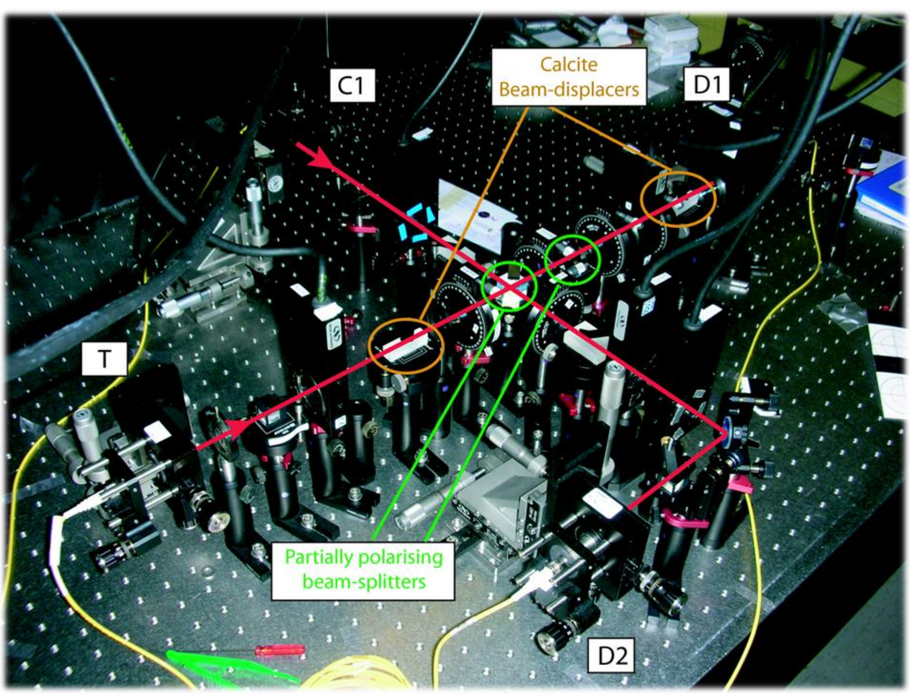


44

Experimental Implementations

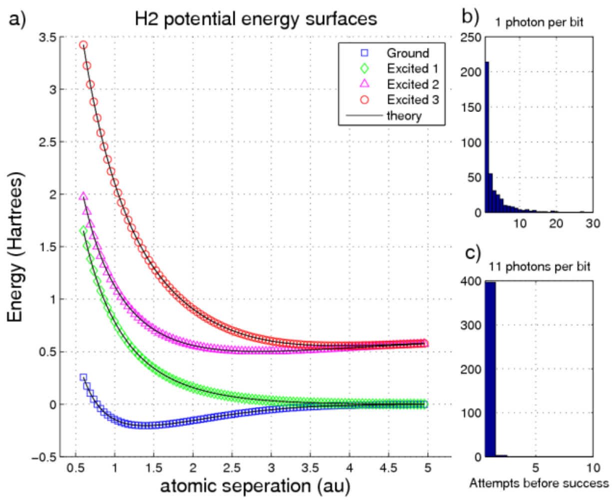
Quantum optics				
Hydrogen molecule	2 qubits	Lanyon, et al.,	Nat Chem 2 106	2010
HeH^+	2 qubits	Peruzzo, et al.,	Nat Comms 5 4213	2014
Nuclear Magnetic Resonance				
Hydrogen molecule	2 qubits	Du, et al,	Phys Rev Lett 104 030502	2010
Nitrogen vacancy centers				
HeH^+	2 qubits	Wang, et al.,	ACS Nano 9 7769	2015
Superconducting qubits				
Hydrogen molecule	3 qubits	O'Malley, et al,	Phys Rev X 6 031007	2016
BeH_2	6 qubits	Kandala, et al.	Nature 548 242	2017
Ion traps				
HeH+	3 qubits	Shen, et al,	arXiV:1506.00443	2015
LiH	3 qubits	Hempel, et al.	To be submitted	2016

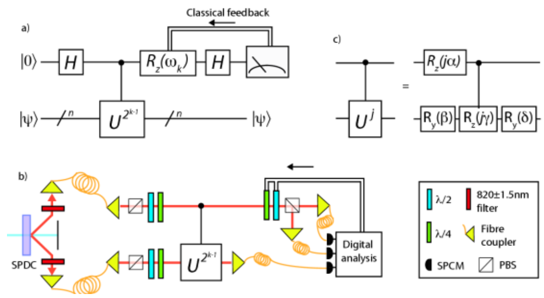
45



46

First Quantum Simulation of Hydrogen Molecule Potential Energy Surface



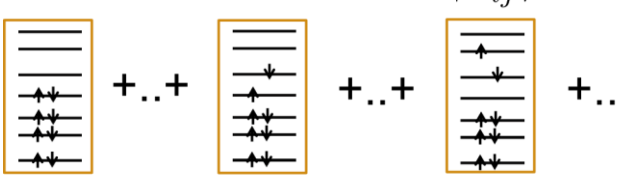


Lanyon, et al., Nat Chem 2 106 2010

Hierarchy of Post-HF Methods

We can recover the **electron correlation** by expanding the wavefunction in the configurational space.

$|\Phi_0\rangle$ $|\Phi_i^a\rangle$ $|\Phi_{ij}^{ab}\rangle$



$$\Phi_i^a = a_a^\dagger a_i |\Phi_0\rangle$$

$$\Phi_{ij}^{ab} = a_a^\dagger a_b^\dagger a_i a_j |\Phi_0\rangle$$

$$\binom{N}{\eta} \; determinants$$

$$|FCI\rangle = \left(c_0 + \sum_{i,a} c_i^a a_a^\dagger a_i + \sum_{i>j,a>b} c_{ij}^{ab} a_a^\dagger a_i + \dots \right) |\Phi_0\rangle$$

Configuration interaction (CI)

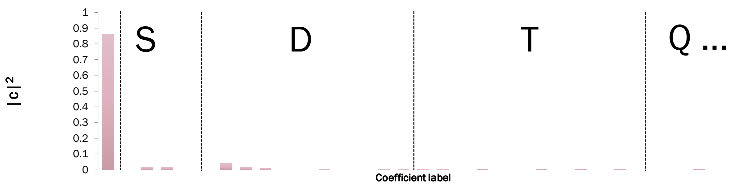
$$|CC\rangle = exp\left(\sum_{i,a} t_i^a a_a^\dagger a_i + \sum_{i>j,a>b} t_{ij}^{ab} a_a^\dagger a_b^\dagger a_i a_j + \dots \right) |\Phi_0\rangle$$

Coupled cluster (CC)

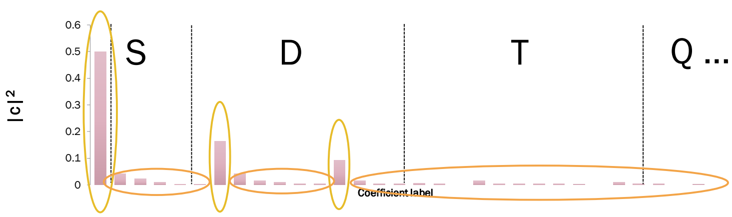
Helgaker, T., Jorgensen, P. and Olsen, J., 2014. Molecular electronic-structure theory.

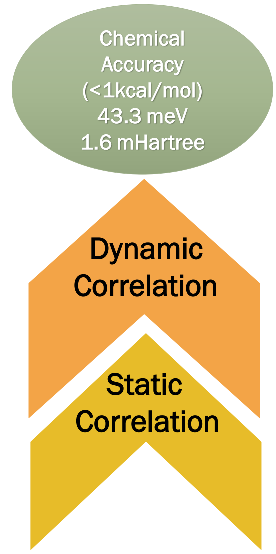
Dynamic and Static Correlation

Single reference

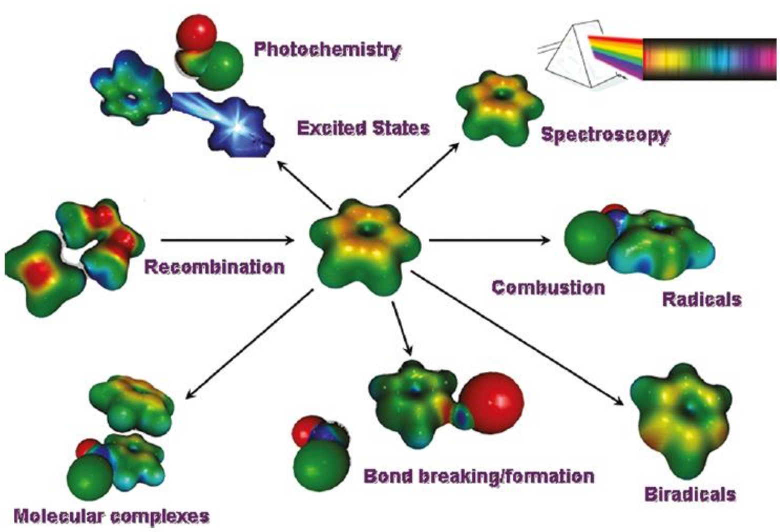


Strongly correlated = "Multireference"





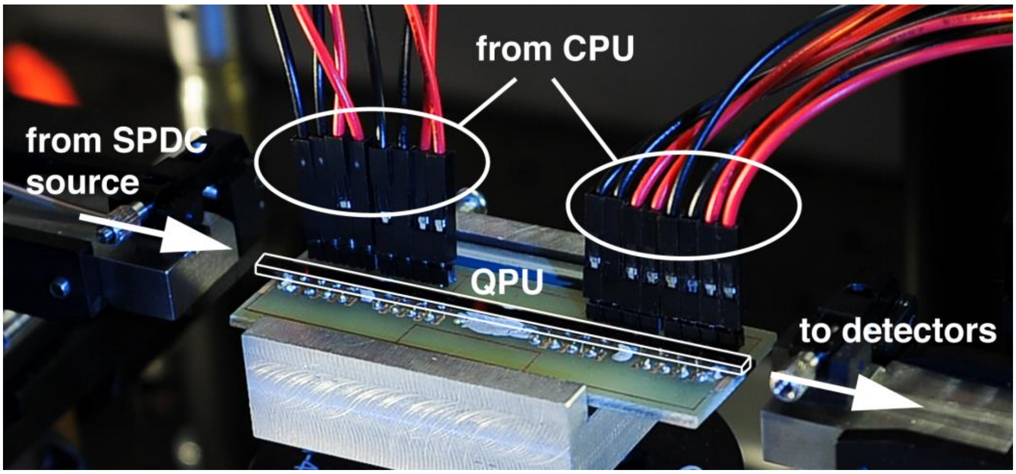
"Multireference" World of Chemistry



From: Lyakh et al. *Chem. Rev.* **102**, 182, (2012).

The accurate modeling of multireference phenomena is perhaps the biggest challenge for quantum chemistry.

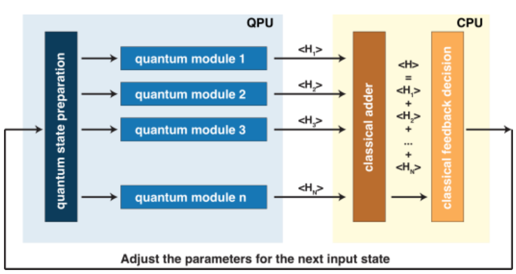
The Variational Quantum Eigensolver (VQE)



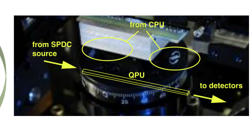
Peruzzo, McClean, Shadbolt, Yung, Zhou, Love, Aspuru-Guzik, O'Brien. Nature Communications 5 4213 2014

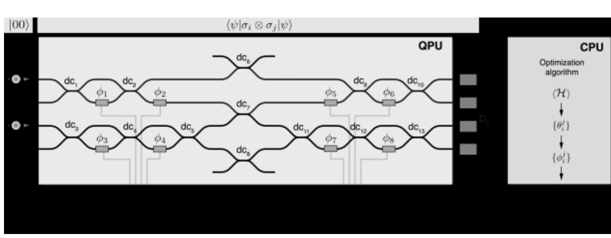
51

Physical Implementation



Integrated Quantum Photonic Technology

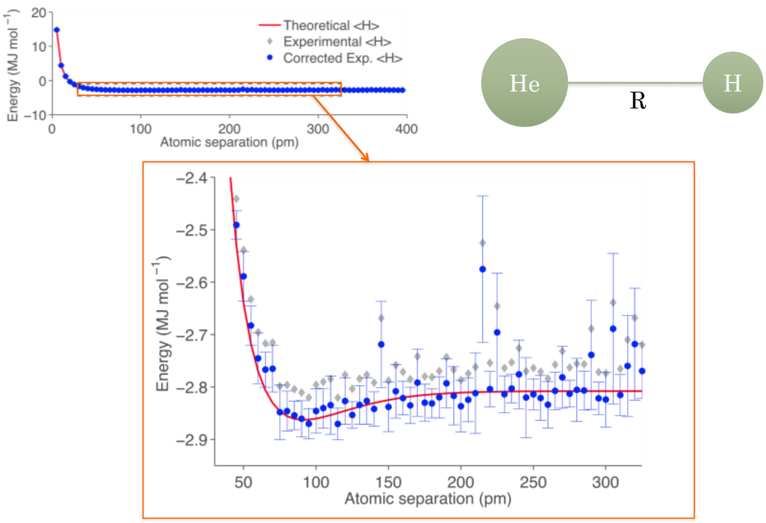




Features:
•Single 2-Qubit entangling gate
•Reconfigurable 1-qubit gates
•Produces arbitrary 2-qubit pure state with fidelity F > 99%

52

Experimental Electronic Curve for HeH^+



53

Unitary Coupled Cluster Ansatz

$$U(\vec{t}) = exp\left[-i(T - T^{\dagger})\right] = exp\left[-i\sum_a t_a(\tau_a - \tau_a^{\dagger})\right]$$

τ_a : *excitation operator*

In a quantum computer we can implement an approximated unitary:

$$U\left(\vec{t}\right) \approx U_{Trot}\left(\vec{t}\right) = \left(\prod_i e^{\frac{t_i}{\rho}(\tau_i - \tau_i^{\dagger})}\right)^{\rho}$$

Parameter scaling
$O(n_e^2 N^2)$

The BCH expansion for UCC is **infinite.** [1]

1. Taube, A.G. and Bartlett, R.J., 2006. Int. J. Quantum Chem. **106**(15), pp.3393-3401.

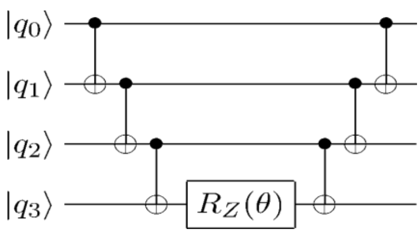
54

Romero, et al arXiV:1701.02691

VQE for UCC: How it all fits together

1 Second-quantized excitation operator —Jordan-Wigner transformation or Bravyi-Kitaev transformation→ 2 Pauli operators

3 Exponentiation

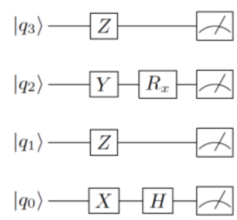


... for all terms ...

This circuit implements $e^{-i\frac{\theta}{2}\sigma_3^Z\sigma_2^Z\sigma_1^Z\sigma_0^Z}$

H and R_x are used to changed from Z to X and Y basis.

4 Measurement



... for all terms ...

Measuring the term

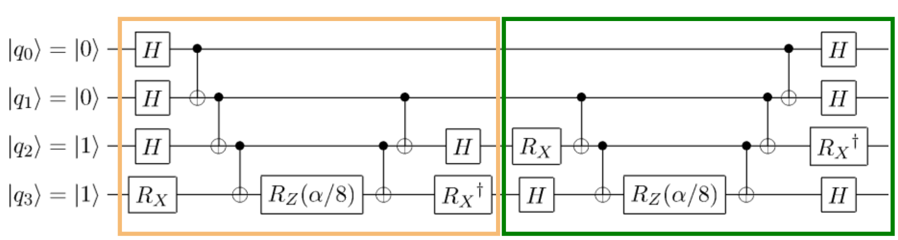
$$\sigma_z^3\sigma_y^2\sigma_z^1\sigma_x^0$$

55

Example: Minimal-basis H_2 Jordan-Wigner

$$\hat{H}_{JW} = f_1\mathbf{1} + f_2(\sigma_0^z + \sigma_1^z) + f_3(\sigma_2^z + \sigma_3^z) + f_4\sigma_3^z\sigma_2^z$$
$$+ f_5\sigma_1^z\sigma_0^z + f_6(\sigma_2^z\sigma_0^z + \sigma_3^z\sigma_1^z) + f_7(\sigma_2^z\sigma_1^z + \sigma_3^z\sigma_0^z)$$
$$+ f_8(\sigma_3^x\sigma_2^y\sigma_1^y\sigma_0^z - \sigma_3^x\sigma_2^x\sigma_1^y\sigma_0^y + \sigma_3^y\sigma_2^x\sigma_1^x\sigma_0^y - \sigma_3^y\sigma_2^y\sigma_1^x\sigma_0^x)$$

$$\hat{U}(\alpha) = exp[i\alpha/8(-\sigma_3^y\sigma_2^x\sigma_1^x\sigma_0^x + \sigma_3^x\sigma_2^y\sigma_1^x\sigma_0^x + \sigma_3^x\sigma_2^x\sigma_1^y\sigma_0^x + \sigma_3^x\sigma_2^x\sigma_1^x\sigma_0^y +$$
$$\sigma_3^x\sigma_2^y\sigma_1^y\sigma_0^y + \sigma_3^y\sigma_2^x\sigma_1^y\sigma_0^y - \sigma_3^y\sigma_2^y\sigma_1^x\sigma_0^y - \sigma_3^y\sigma_2^y\sigma_1^y\sigma_0^x)]$$

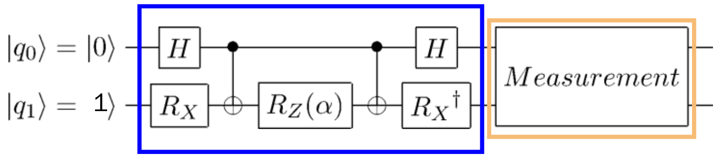


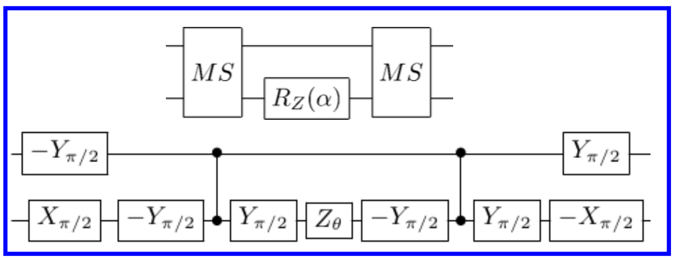
$$|0011\rangle \to (1-c)|0011\rangle + c|1100\rangle$$

56

Example: Minimal-basis H_2 Bravyi-Kitaev

$$H_2^{BK} = c_0\mathbf{1} + c_1\sigma_0^z + c_2\sigma_1^z + c_3\sigma_0^z\sigma_1^z + c_4\sigma_0^x\sigma_1^x + c_5\sigma_0^y\sigma_1^y$$





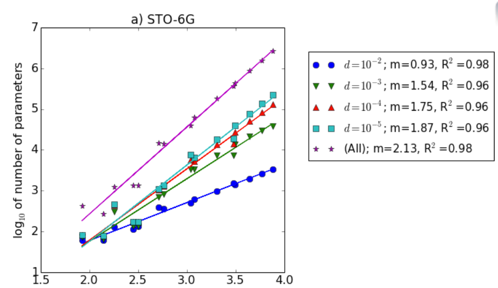
Ion trap implementation

Superconducting implementation

Romero, et al arXiV:1701.02691

Optimization of the Cost of UCC

Use classical approximations of the amplitudes to reduce circuit size

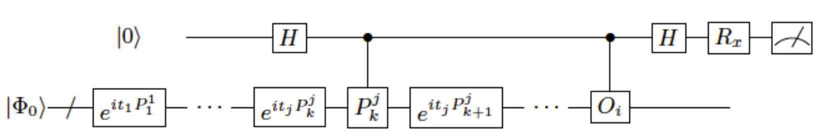


Select terms using MP2

$$t_i^a = 0; \quad t_{ia}^{ab} = \frac{h_{ijba} - h_{ijab}}{\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b}$$

Gradients for UCC

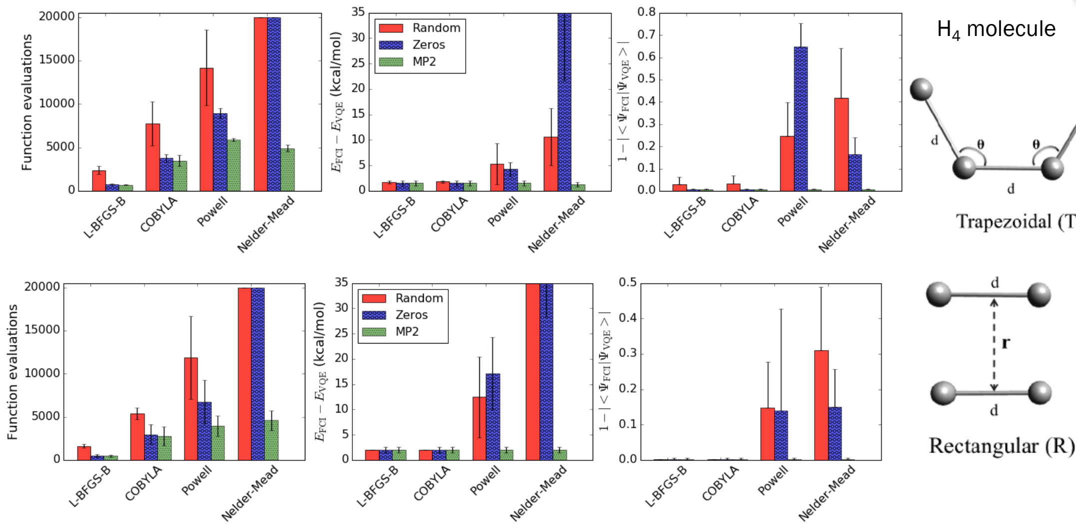
$$\frac{\partial E(\vec{t})}{\partial t_j} = 2\sum_i^M \sum_k^{N_S^j} h_i \,\mathrm{Im}(\langle \Phi_0 | V_k^{j\dagger}(\vec{t}) O_i U(\vec{t}) | \Phi_0 \rangle)$$



Romero et al. *arXiv: 1701.02691* (2017).

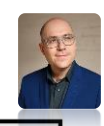
Romero, et al arXiV:1701.02691

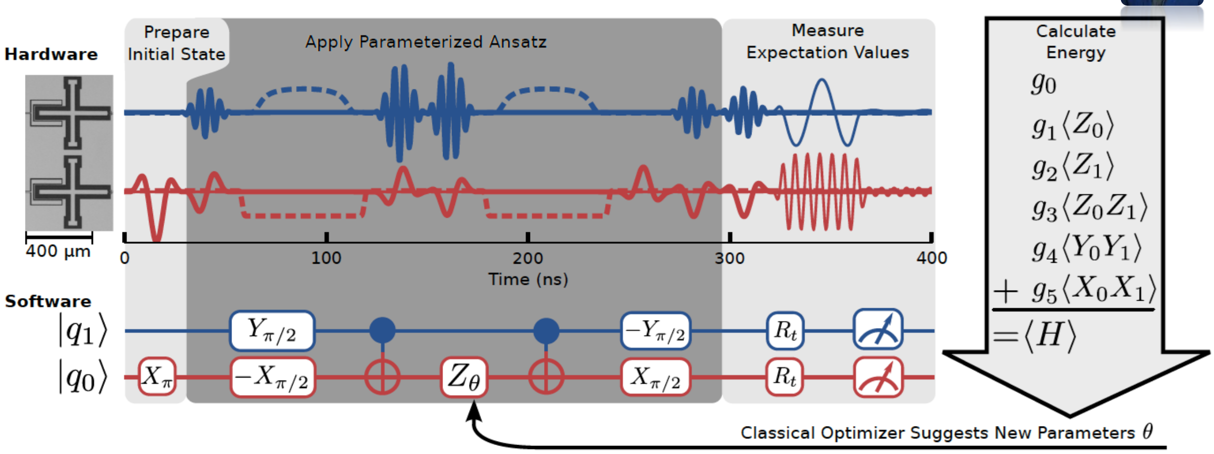
Strategies for UCC Calculations



Romero et al. *arXiv: 1701.02691* (2017).

Superconducting VQE for H_2

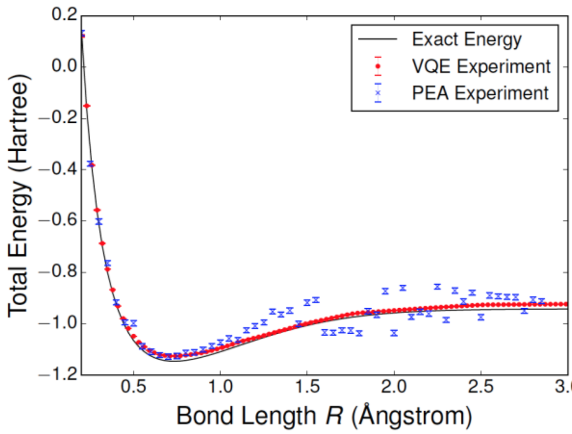




Used Xmon qubits to compute energy surface of molecular hydrogen
Started in Hartree-Fock state, used unitary coupled cluster, got chemical accuracy

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

Superconducting VQE vs Phase Estimation



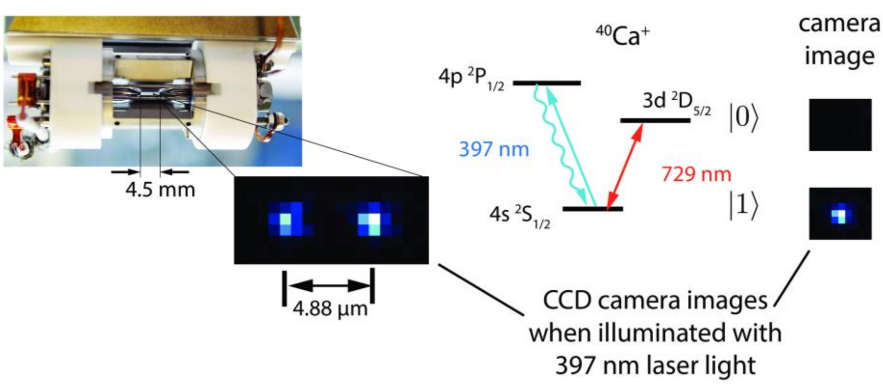
Predicted dissociation energy without exponentially costly compilation for first time
Substantial robustness to systematic errors seen

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

61

Ion Trap Implementation

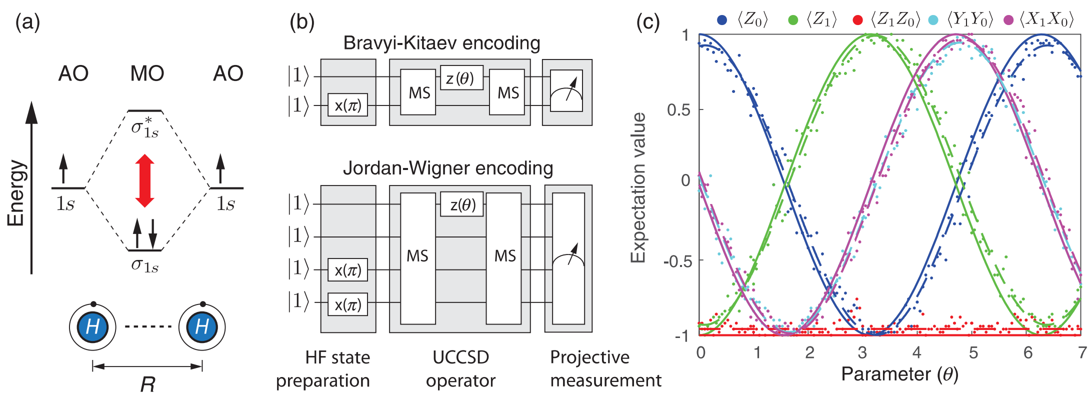
Collaboration with Rainer Blatt (Innsbruck)



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

62

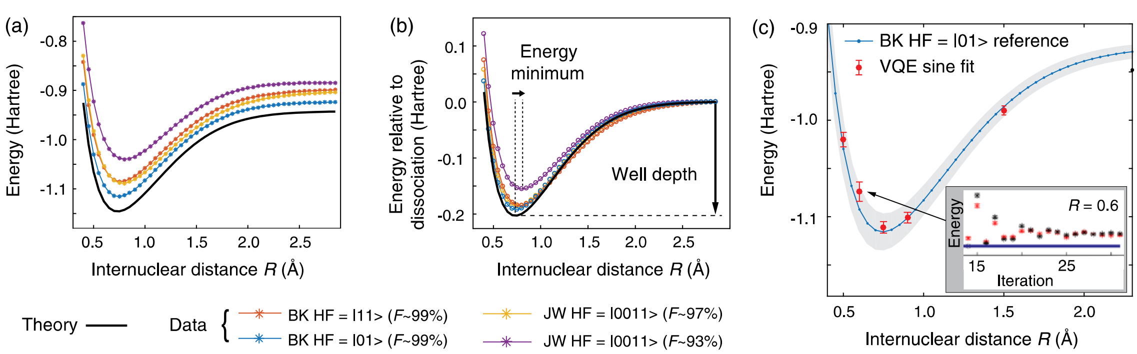
Ion Trap Implementation (H_2)



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

63

Ion Trap Implementation (H_2)



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Phys. Rev. X **8**, 031022

64

Ion Trap Implementation (H_2)

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Phys. Rev. X **8**, 031022

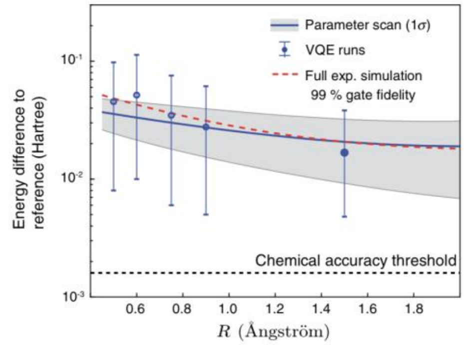
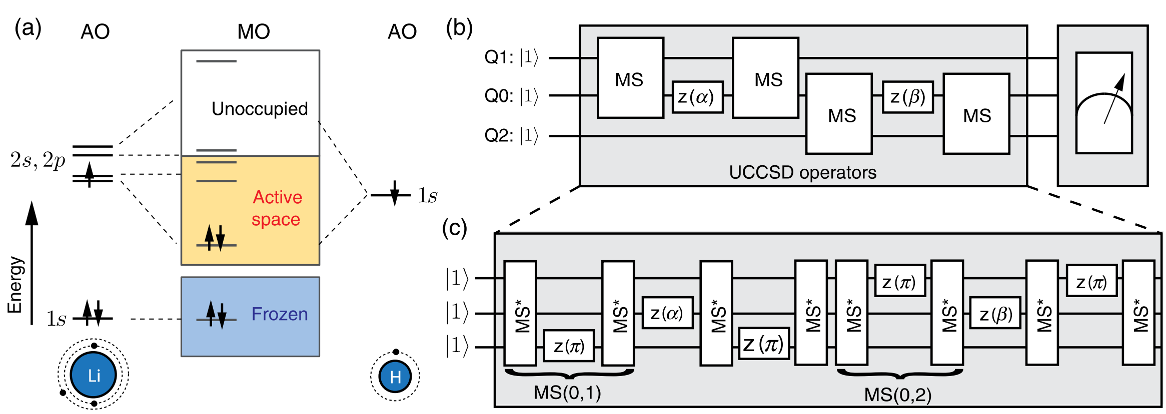


FIG. 7. Energy errors of the reconstructed H_2 potential energy surface and the influence of decoherence. Differences are given with respect to the full configuration interaction (FCI) calculation performed in the chosen molecular basis. The red line corresponds to a full simulation of the quantum circuit, including multiple decoherence channels and the experimentally determined gate fidelity (see Appendix B 6 for details).

65

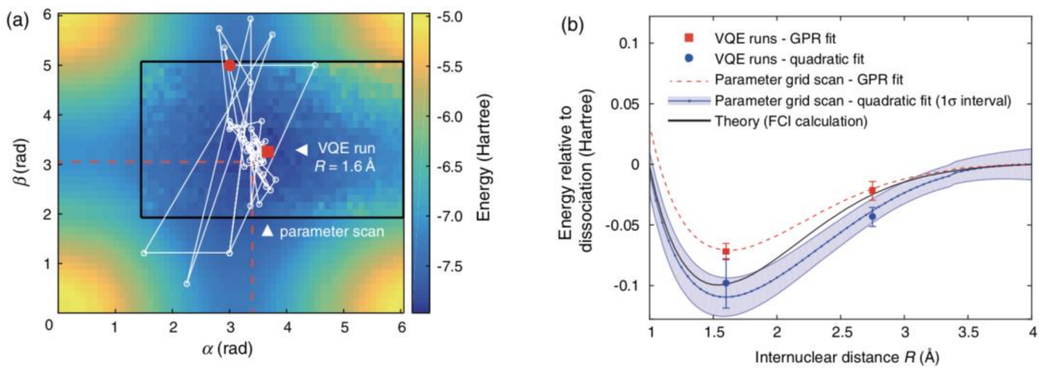
Ion Trap Implementation (LiH)



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

66

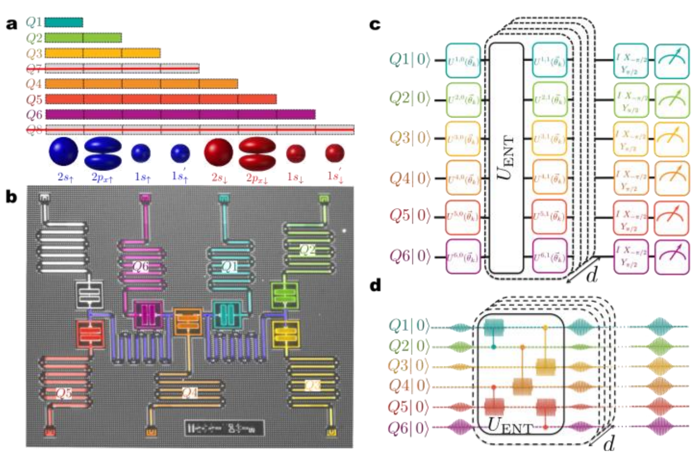
Ion Trap Implementation (LiH)

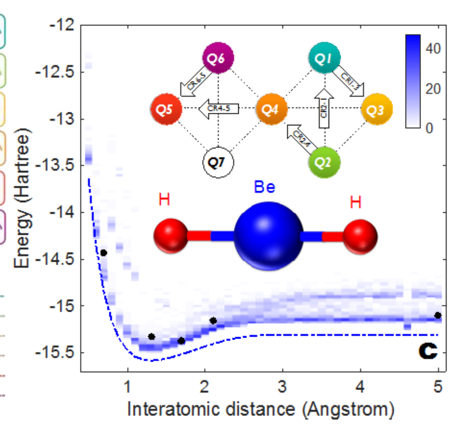


Cornelius Hempel, Christine Maier, Jonathan Romero, Jarrod McClean, Thomas Monz, Heng Shen, Petar Jurcevic, Ben P. Lanyon, Peter Love, Ryan Babbush, Alán Aspuru-Guzik, Rainer Blatt, and Christian F. Roos
Phys. Rev. X **8**, 031022

67

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)

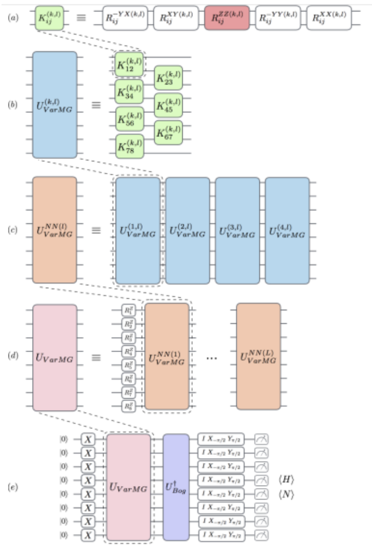
H-Be-H, 6 qubit simulations.

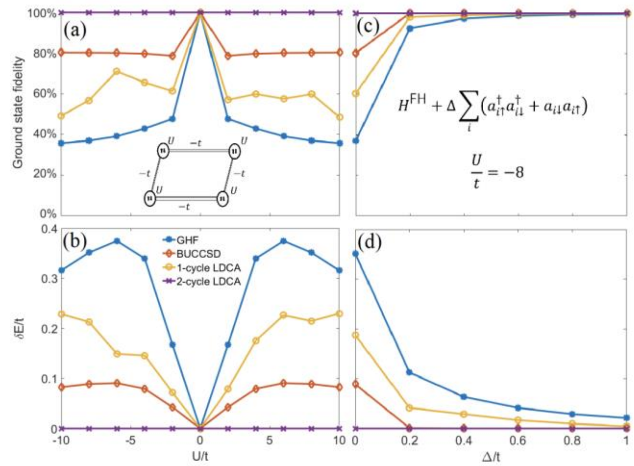
Kandala, et al Nature 549 242 (2017)

68

Low-depth Correlated Ansatz (LDCA)

Approach motivated by Bogoliubov coupled cluster theory





Dallaire-De Mers, J. Romero, L. Veis, S. Sim, A. Aspuru-Guzik arXiV:1801.01053 (2018)

69

VQE Pipeline

Hamiltonian mapping
- Jordan-Wigner
- Bravyi-Kitaev
- Bravyi-Kitaev superfast
- Particle/hole picture
- Planewave basis
- Orbital freezing
- ⋮

Circuit ansatz
- Unitary coupled cluster
- Hardware efficient ansatz
- **LDCA**
- ⋮

Compilation
- Quipper
- ProjectQ compiler
- Google cirq compiler
- Rigetti pyquil compiler
- ***Zapata compiler***
- ⋮

Classical optimization
- Nelder-Mead
- SPSA
- Adiabatic assist
- **PHOENICS Bayesian Optimization**
- ⋮

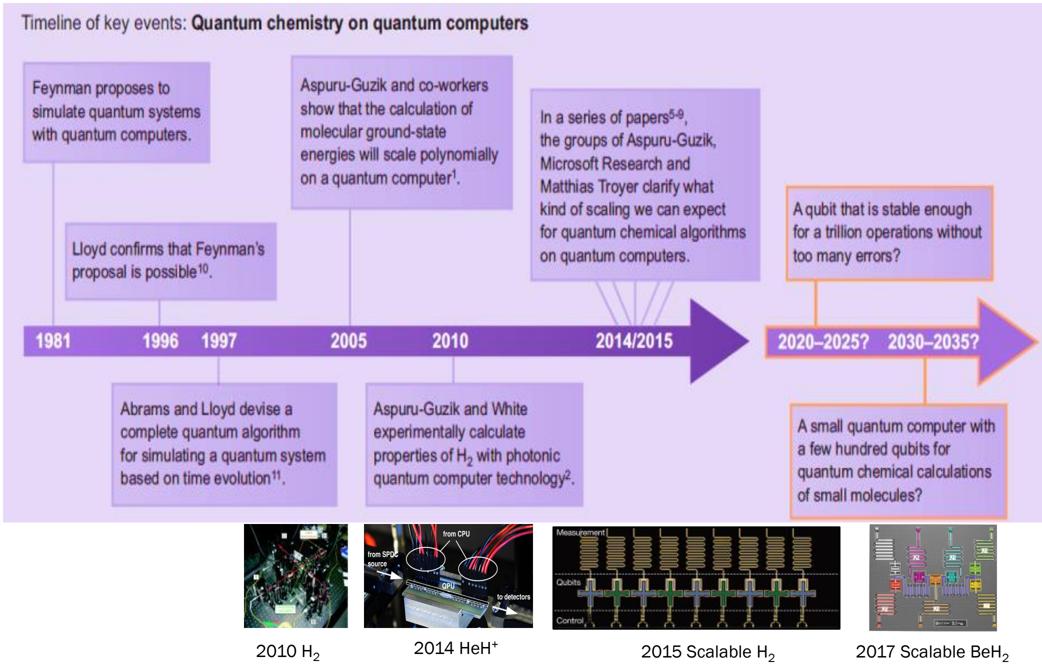
Post-processing
- Pauli-term grouping
- Error-mitigation
- Quantum subspace expansion
- Marginal projection technique
- Symmetry error detection
- ***Zapata post-processing routine***
- ⋮

Software for implementation
- pyQuil
- Cirq
- Qiskit
- ⋮

ZAPATA

70

Quantum Chemical Advantage?



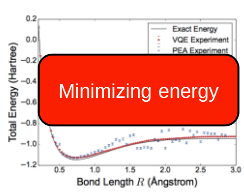
2010 H_2 2014 HeH^+ 2015 Scalable H_2 2017 Scalable BeH_2

Leonie Mueck. Nature Chemistry 7 361 2015

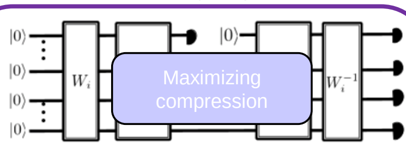
71

The age of variational quantum algorithms
… training quantum circuits.

Variational quantum eigensolver



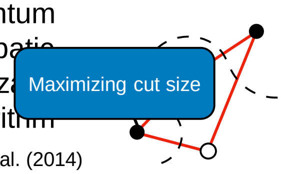
Peruzzo et al. (2014)



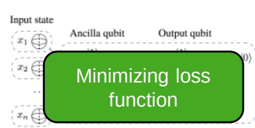
Quantum autoencoder

Romero, et al.
Quantum Sci. Technol. 2 (2017): 045001

Quantum adiabatic optimization algorithm

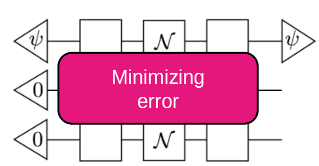


Farhi et al. (2014)



Cao, et al.
arXiV:1711.11240

Quantum neuron



Quantum Variational error corrector (QVECTOR)

… and many other algorithms, e.g. Machine Learning

72

Machine Learning

The goal of *machine learning* is to design algorithms that can learn from and make predictions on data.

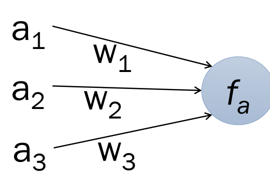
"A computer program is said to learn from experience E with respect to a class of tasks T and performance measure P, if its performance at tasks T, as measured by P, improves with experience E"

-Tom Mitchell (CMU)

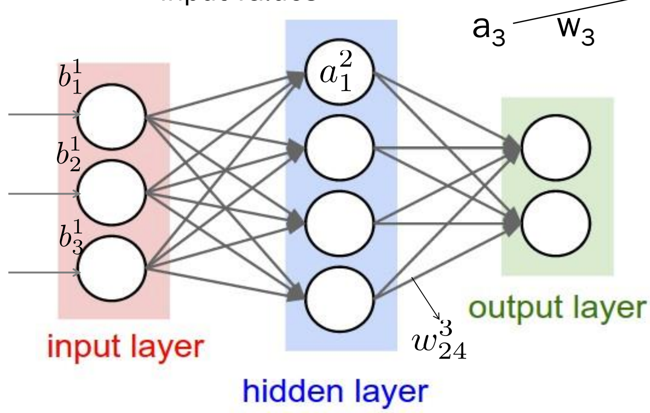
73

Feedforward Neural Networks

Neuron:
Non-linear weighted sum of input values



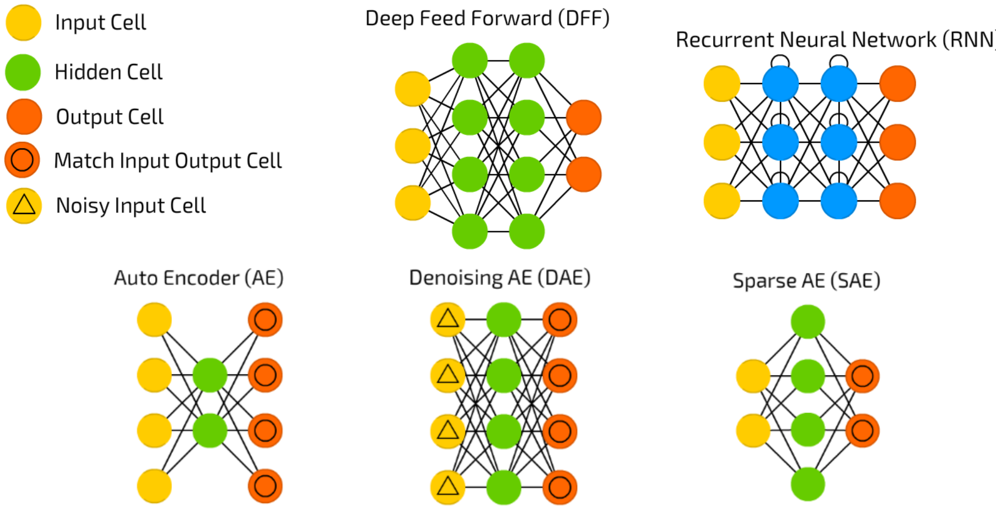
$$f_a\left(\sum_k w_k a_k + b\right)$$



Michael A. Nielsen "Neural networks and deep learning", Determination press. 2015.

74

Diversity of Neural Networks

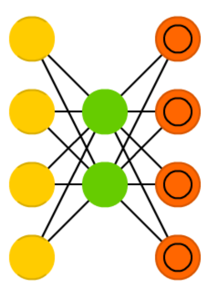


Reproduced from: http://www.coolinfographics.com/blog/2016/9/20/the-mostly-complete-chart-of-neural-networks.html. May28 th, 2017.

75

Autoencoders

Image



Image

Input Cell

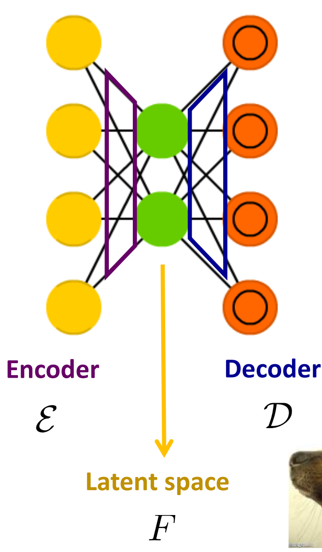
Hidden Cell

Match Input Output Cell

Input Hidden layers Output

Image: asimovinstitute.org

Autoencoders

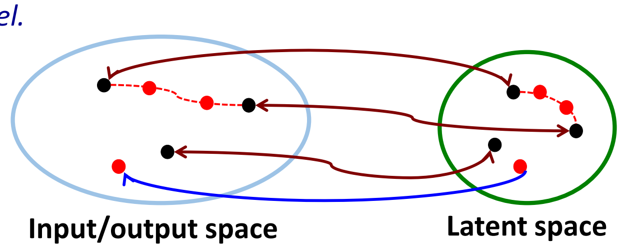


$$\mathcal{E} : X \to F \qquad \underset{\mathcal{E},\mathcal{D}}{argmin} \quad ||X - (\mathcal{D} \circ \mathcal{E})X||^2$$

$$\mathcal{D} : F \to X'$$

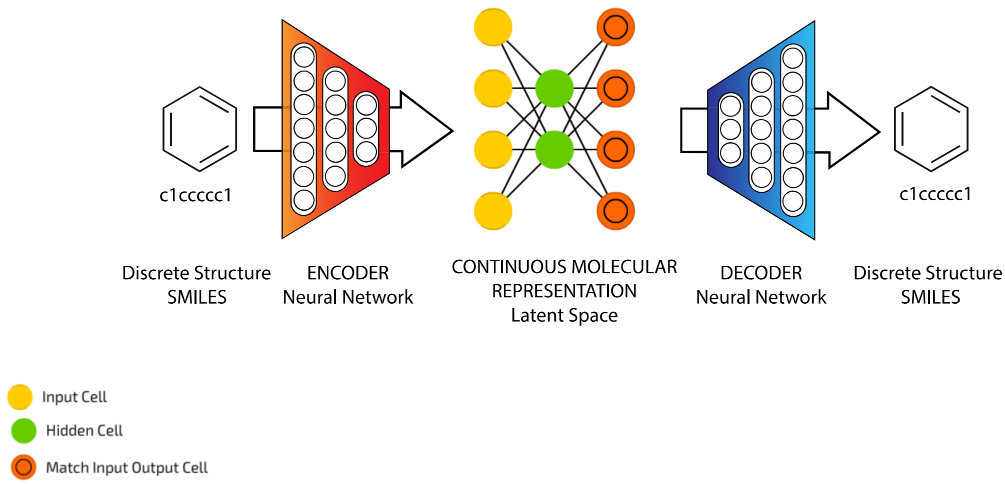
The encoding network can be used for dimensionality reduction and feature extraction

The decoding network can be used as a *generative model.*



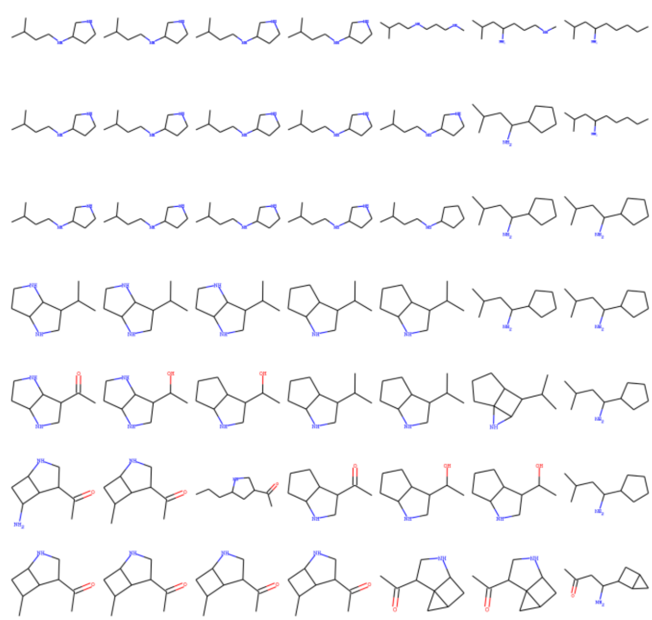
78

Autoencoders for Chemical Space



R. Gomez-Bombarelli, et al ACS Central Science 10.1021/acscentsci.7b00572 (2018)

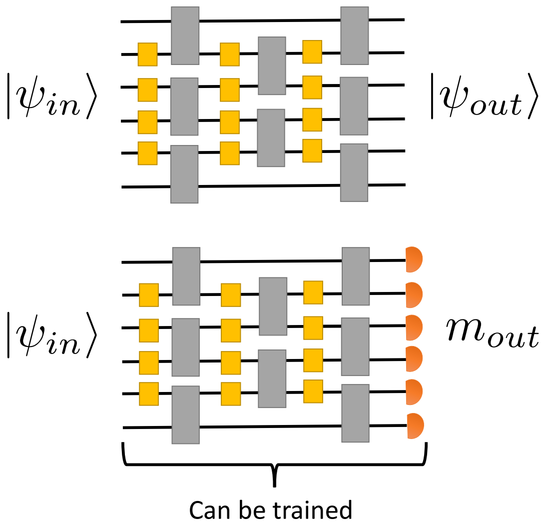
Exploring latent space



80

Training Quantum Circuits

An analogy to machine learning



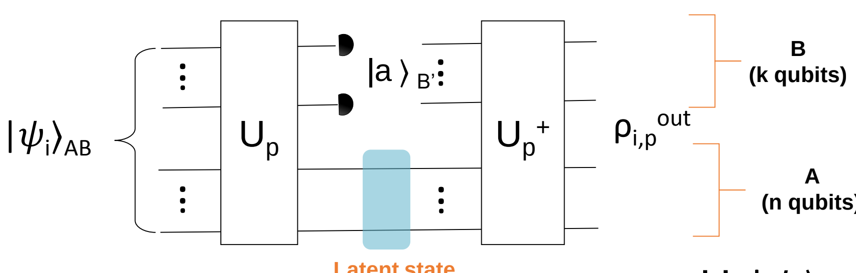
Define suitable cost functions as expectation values of observables

Optimize them to train quantum circuits for performing quantum tasks

Near-term quantum computers, without error correction and short-depth, are excellent candidates for these *task-driven* applications.

81

Quantum Autoencoder Model



$$U_p|\psi_i\rangle_{AB}=|\psi^c_i\rangle_A|a\rangle_B$$

Given:

- An ensemble of pure states $\{q_i, |\psi_i\rangle_{AB}\}$ and a pure reference state $|a\rangle_{B'}$ on k qubits.
- A family of unitary operators $\{U^p\}$ acting on n+k qubits, parameterized according to a parameter vector **p** = (p_1, p_2,…).

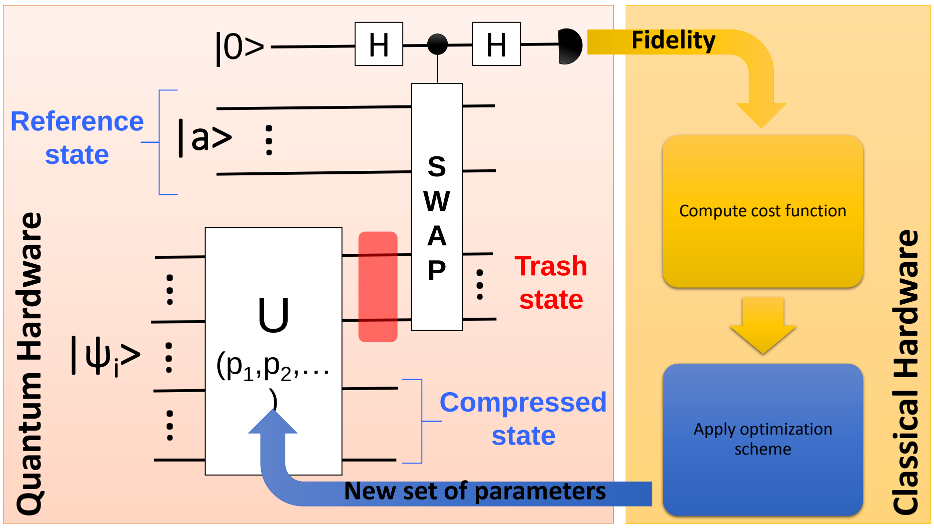
Task:

- Find the unitary U^p which maximizes: $C(p) = \sum_i q_i F(|\psi_i\rangle_{AB}, \rho_{i,p}^{out})$

Romero, J., Olson, J. and Aspuru-Guzik, A., . Quantum autoencoders for efficient compression of quantum data. *Quantum Sci. Technol.* 2 (2017): 045001.

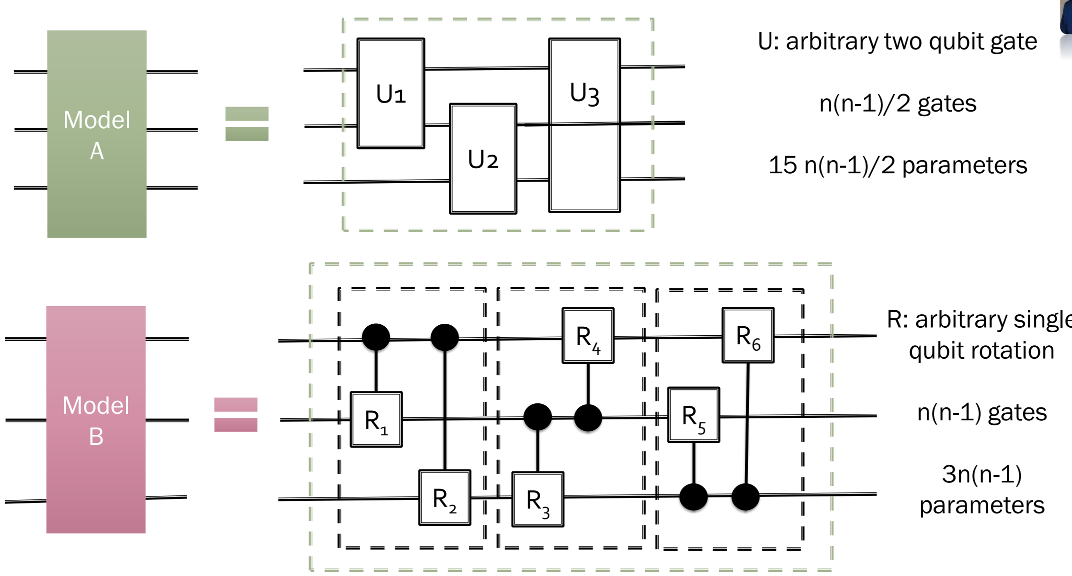
82

Hybrid Approach for Circuit Training



Romero, J., Olson, J. and Aspuru-Guzik, A., 2016. Quantum autoencoders for efficient compression of quantum data. *Quant Sci Tech* 2 045011 (2017)

Heuristics for Autoencoder Unitaries



Romero, J., Olson, J. and Aspuru-Guzik, A., 2016. Quantum autoencoders for efficient compression of quantum data. *Quant Sci Tech* 2 045011 (2017)

Application: Wave Function Compression

Romero, et al *Quant Sci Tech* 2 045011 (2017)

For many Hamiltonians, eigenstates are generally sparse and obey certain symmetries.

Example: In many body systems there are

Restriction in the number of particles: with m particles within a second quantized representation, wavefunctions are spanned by a subspace of size $\binom{N}{m}$, compared to 2^N.

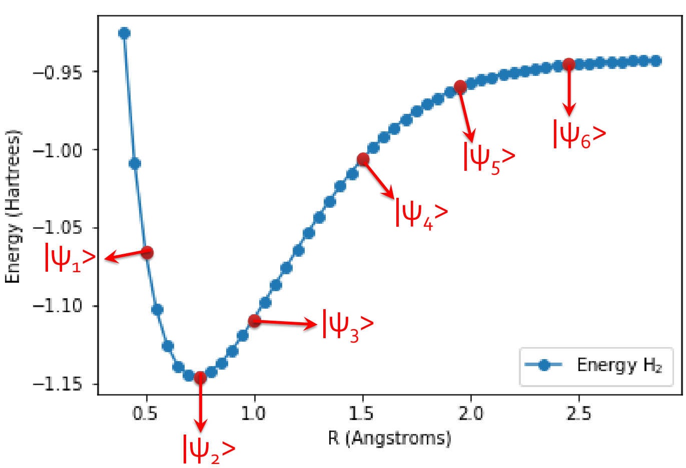
Restriction in spin projection: The total wavefunction is spanned by determinants with the correct spin projection:

$$S_z|k\rangle = M|k\rangle; \quad M = \frac{n_\alpha - n_\beta}{2}$$

85

Example: H_2 molecule (4-2-4 autoencoder)

Romero, et al *Quant Sci Tech* 2 045011 (2017)



- We selected some points in the PES for which we have the wavefunction (Use VQE as oracle).
- Use these states as training set for the autoencoder. (6)
- Use other points in the PES as test set. (44)

86

H_2 Results

Romero, et al arXiV:1612.02806

Circuit	Final size (# qubits)	Set	$-\log_{10}(1-\mathcal{F})$ MAE	-$\log_{10}$ Energy MAE (Hartrees)
Model A	2	Training	6.96(6.82-7.17)	6.64(6.27-7.06)
	2	Testing	6.99(6.81-7.21)	6.76(6.18-7.10)
	1	Training	6.92(6.80-7.07)	6.60(6.23-7.05)
	1	Testing	6.96(6.77-7.08)	6.72(6.15-7.05)
Model B	2	Training	6.11(5.94-6.21)	6.00(5.78-6.21)
	2	Testing	6.07(5.91-6.21)	6.03(5.70-6.21)
	1	Training	3.95(3.53-5.24)	3.74(3.38-4.57)
	1	Testing	3.81(3.50-5.38)	3.62(3.35-4.65)

* MAE: Mean Absolute Error. Log chemical accuracy in Hartrees ≈-2.80

Average error in the fidelity after one cycle of compression and decompression using the quantum autoencoder trained from ground states of the Hydrogen molecule

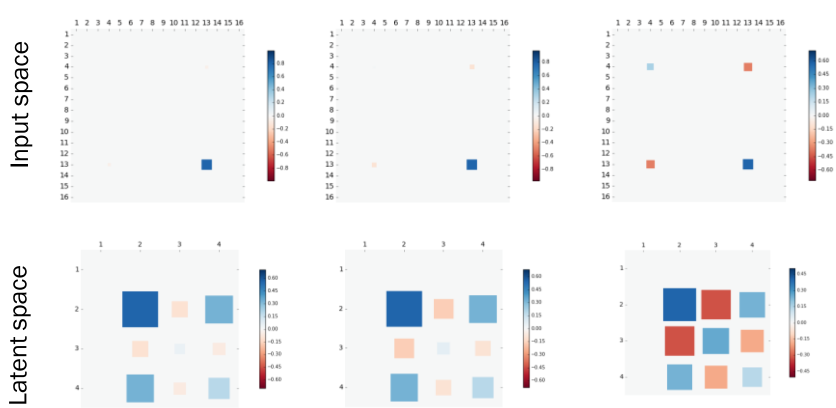
87

Compressed H_2

Romero, et al *Quant Sci Tech* 2 045011 (2017)

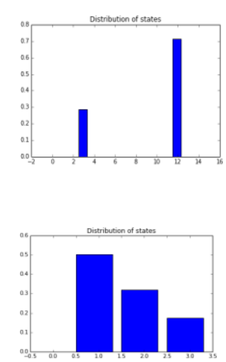
- Average fidelity in training set: 0.9895 - Average fidelity in testing set: 0.9873

R=0.5Å R=1.0Å R=2.0Å



Density matrices of the input and latent spaces at different distances

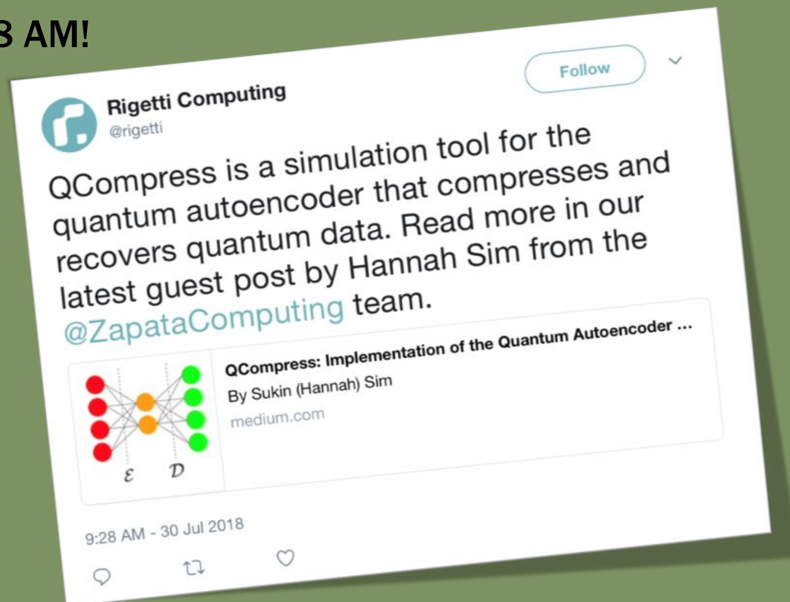
R=2.0Å



Distribution of states at R=2.0Å

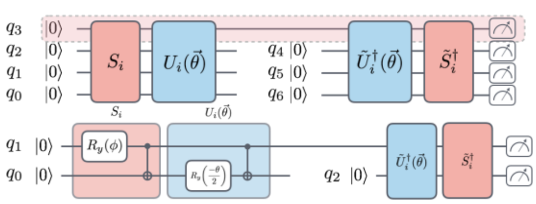
88

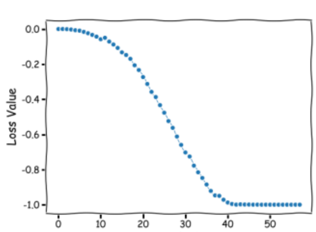
Twitter alert at 9:28 AM!



https://medium.com/rigetti/qcompress-implementation-of-the-quantum-autoencoder-using-forest-and-openfermion-7f99f7e45ff8

Experiment!: H_2 molecule (4-1-4, 2-1-2 autoencoder)





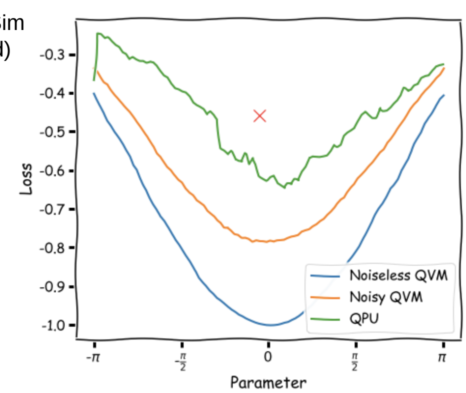
Run in Noiseless QVM

Hannah Sim (Harvard)

Rigetti Computing Follow
On a mission to build the world's most powerful computer.
Jul 30 · 5 min read

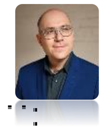
QCompress: Implementation of the Quantum Autoencoder using Forest and OpenFermion

By Sukin (Hannah) Sim

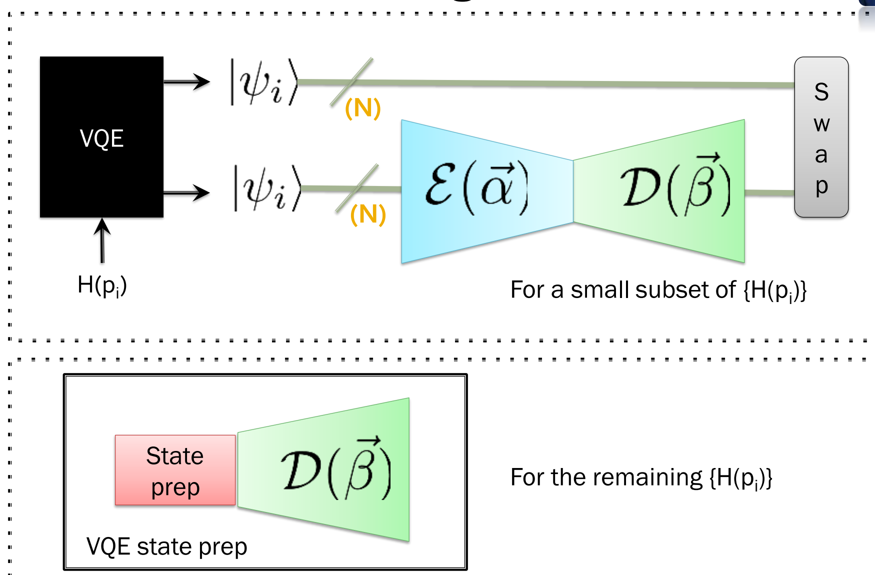


https://medium.com/rigetti/qcompress-implementation-of-the-quantum-autoencoder-using-forest-and-openfermion-7f99f7e45ff8

CUSP (Zapata Computing + Google) Autoencoder + Variational eigensolver

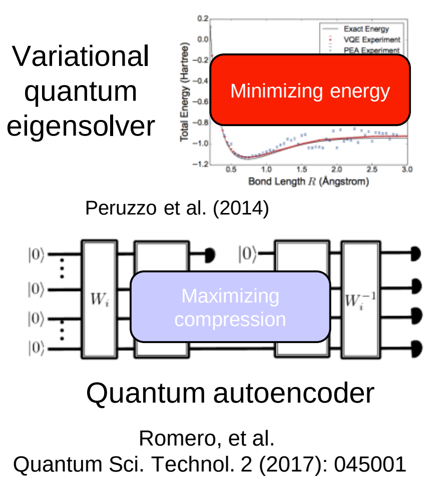


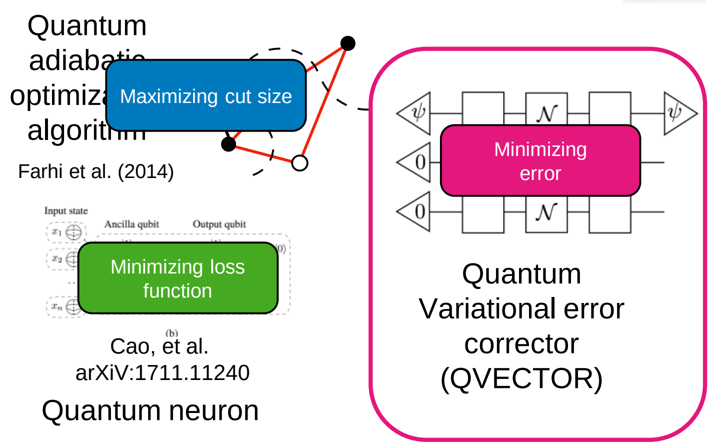
For a family of Hamiltonians {H(p_i)} i=1, ...,M



The purpose is to reduce the number of parameters for the state preparation

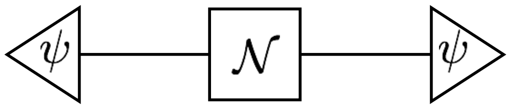
The age of variational quantum algorithms
… training quantum circuits.





… and many other algorithms, e.g. Machine Learning

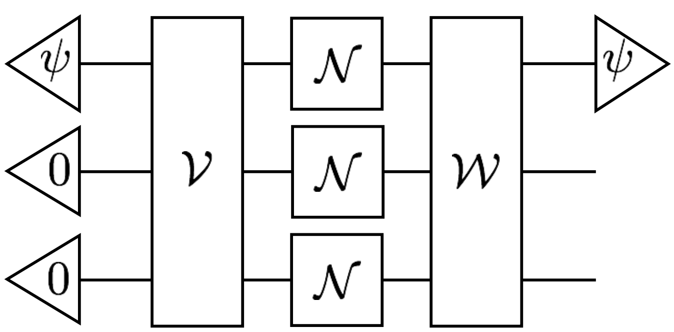
Quantum Error Correction in a Nutshell



$$\mathcal{F}_{\text{avg}} = \int d\psi \sum_i \langle\psi|N_i|\psi\rangle\langle\psi|N_i^\dagger|\psi\rangle$$

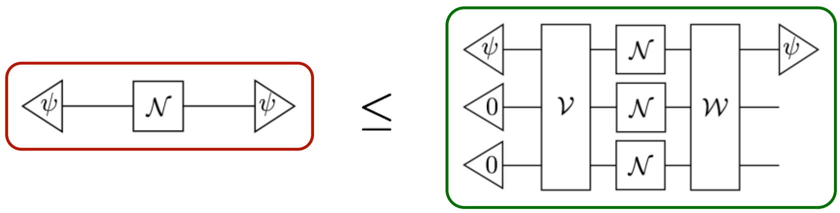
93

Quantum Error Correction in a Nutshell



94

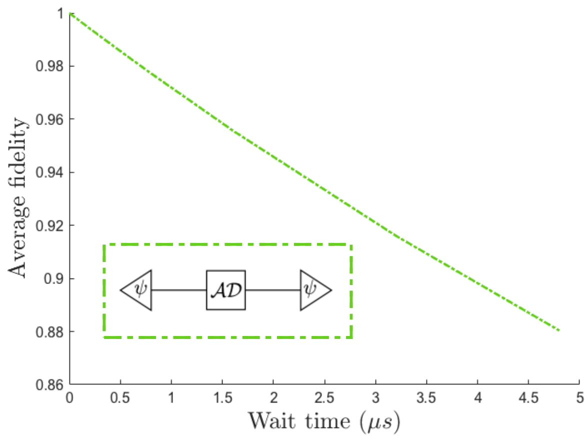
Quantum Error Correction in a Nutshell



Quantum Error Correction in a Nutshell

What is the quality of error correction for this process?

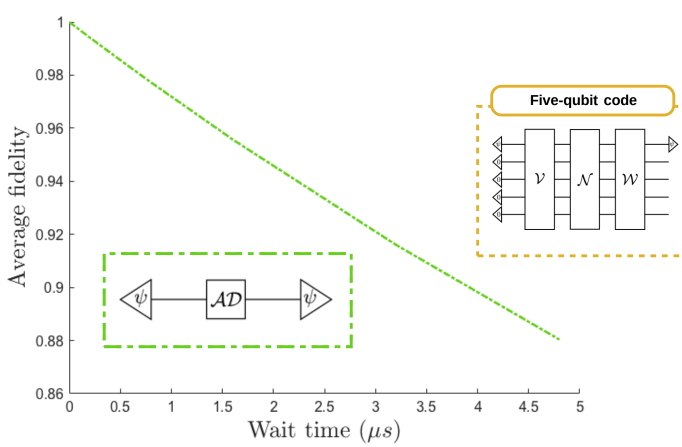
Single Qubit Decoherence



$$T_2 = 60\mu s = T_1/3$$

97

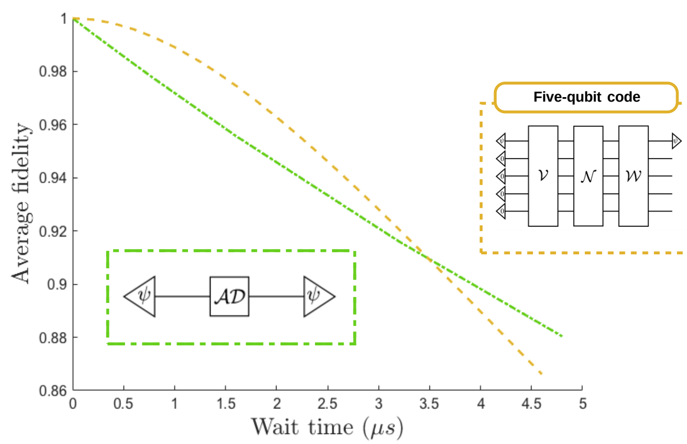
Single Qubit Decoherence



$$T_2 = 60\mu s = T_1/3$$

98

Encode-Wait-Decode for 5-Qubit Stabilizer Code

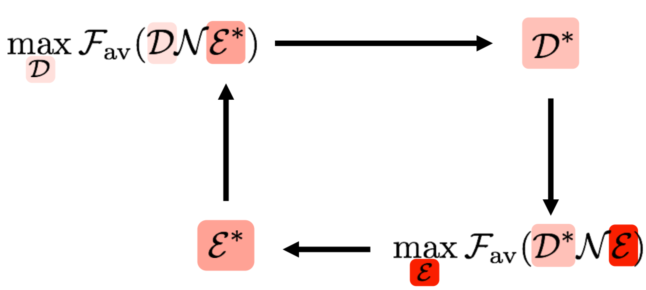


$$T_2 = 60\mu s = T_1/3$$

99

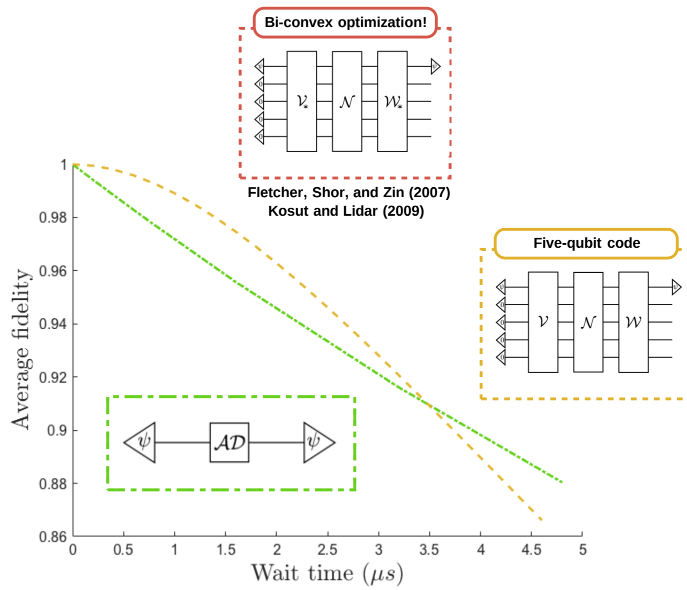
Bi-convex Optimization of Average Fidelity

1) Solve SDP for optimal decoding
2) Plug in optimized decoding
3) Solve SDP for optimal encoding
4) Plug in optimized encoding
5) Repeat 1-4 until sufficient convergence of average fidelity



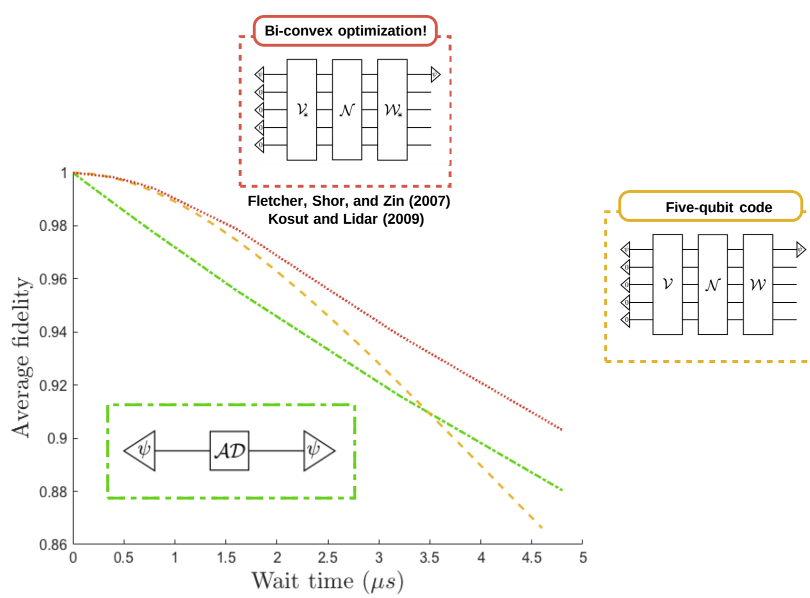
Fletcher, Shor, and Zin (2007)   Kosut and Lidar (2009)

100



$$T_2 = 60\mu s = T_1/3$$

101



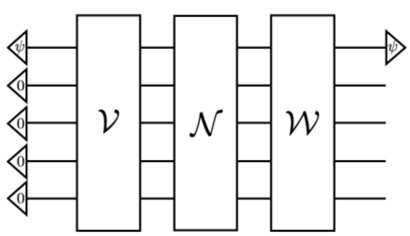
$$T_2 = 60\mu s = T_1/3$$

102

Previous Approaches	**Our Algorithm (QVECTOR)**
1. Require noise model	Model Free
2. Optimization unscalable	Efficient Evaluation
3. Gate compilation needed	Built-in Gate Decomposition

103

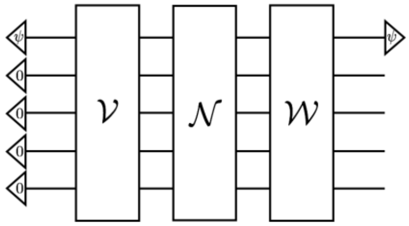
Quantum Variational Error CorrecTOR



Variational quantum optimization algorithm for designing quantum error correcting schemes…

104

QVECTOR

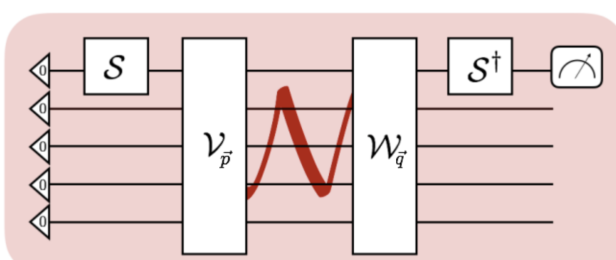


Variational quantum optimization algorithm for designing quantum error correcting schemes…

Objective: maximize average fidelity

105

Model Free

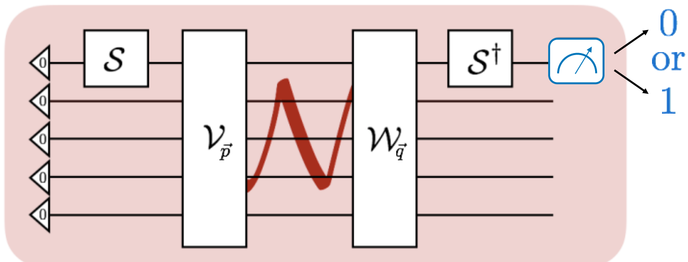


In situ optimization…

… noise "perfectly" simulates itself.

106

Efficient Evaluation



N random samples $\mathcal{S}$ (from 2-design)

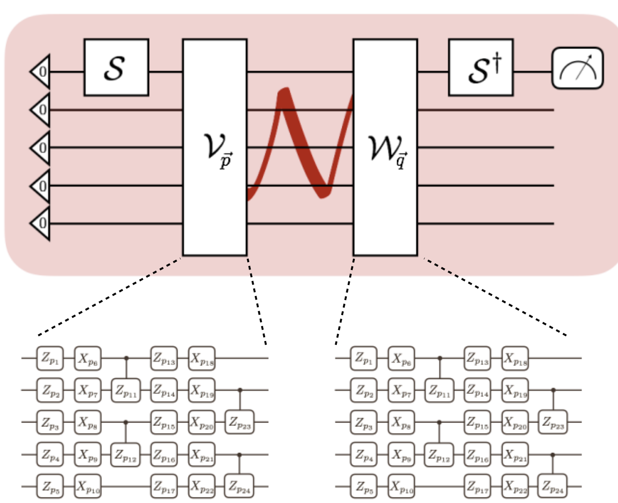
Fraction of 0-outcomes estimates average fidelity to $\mathcal{O}(1/\sqrt{N})$.

2-design samples from Clifford group instead of Haar-random unitaries

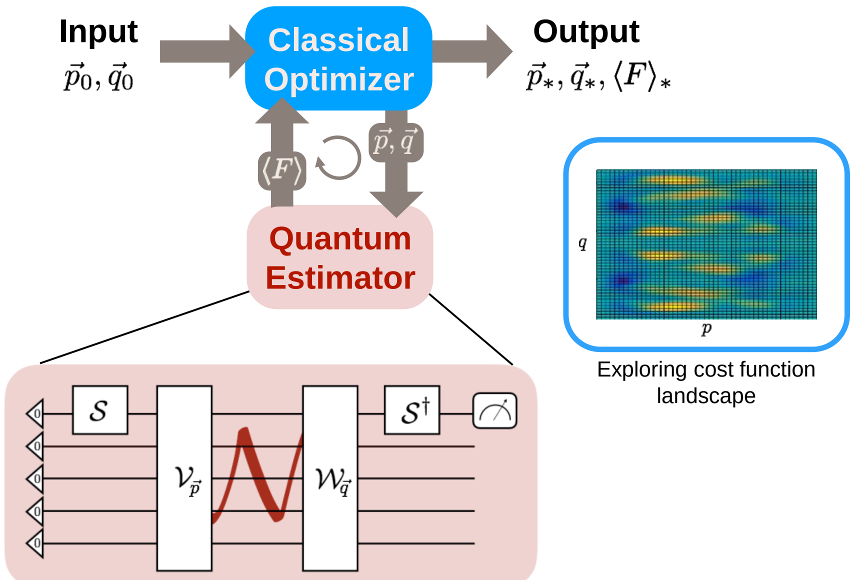
Dankert et al. (2009)

107

Built-in gate decomposition



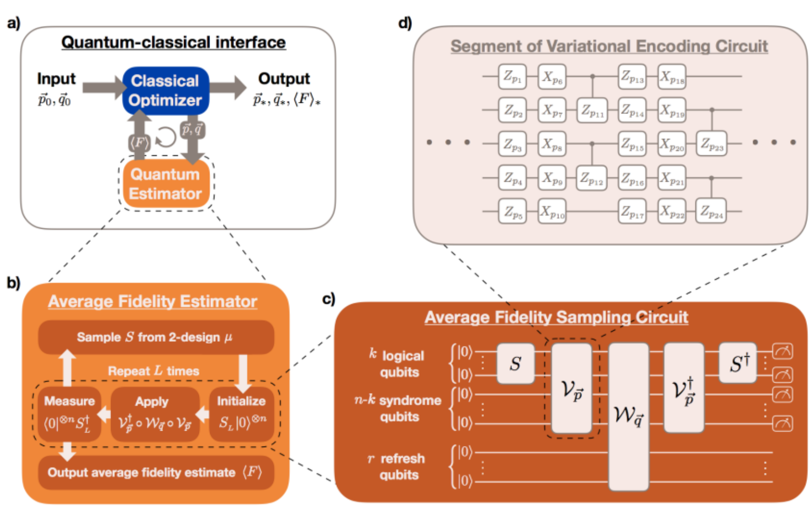
108



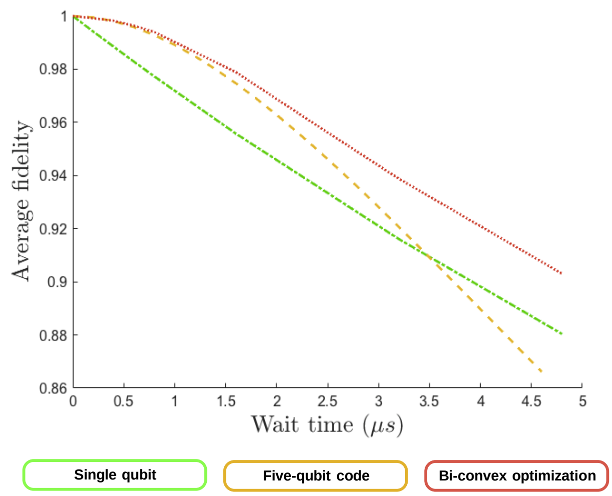
Exploring cost function landscape

109

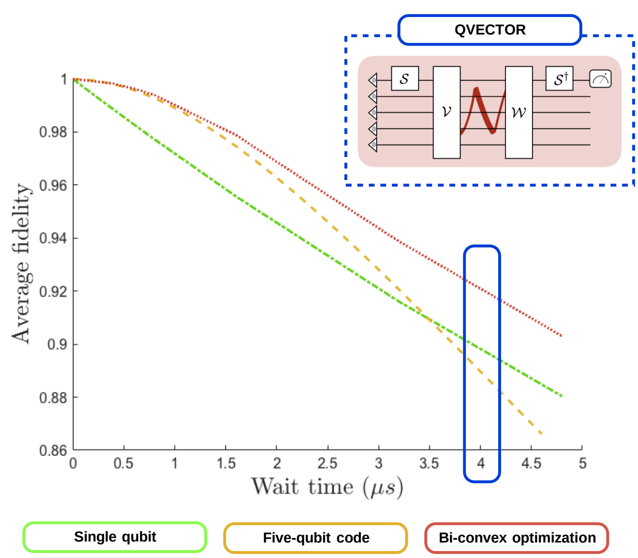
QVECTOR Schematic



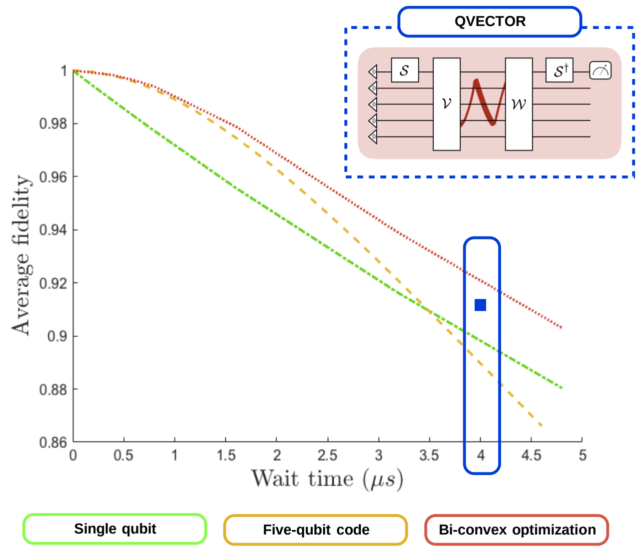
110


Average fidelity
1
0.98
0.96
0.94
0.92
0.9
0.88
0.86
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
Wait time (μs)
Single qubit
Five-qubit code
Bi-convex optimization

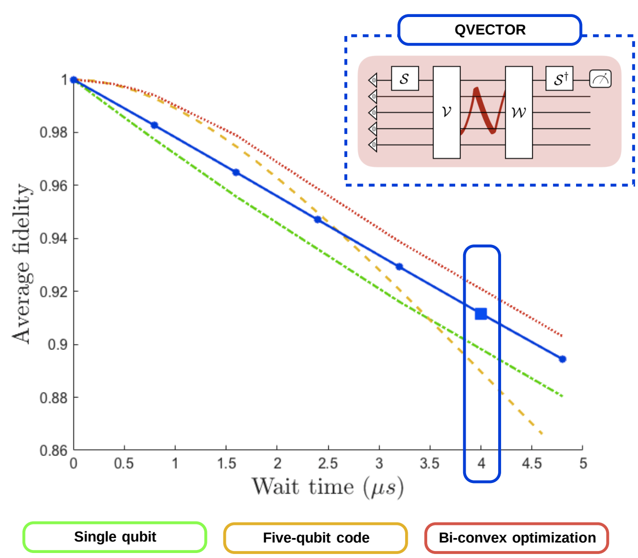
111


QVECTOR
$\mathcal{S}$
$\mathcal{V}$
$\mathcal{W}$
$\mathcal{S}^\dagger$
Average fidelity
1
0.98
0.96
0.94
0.92
0.9
0.88
0.86
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
Wait time (μs)
Single qubit
Five-qubit code
Bi-convex optimization

112

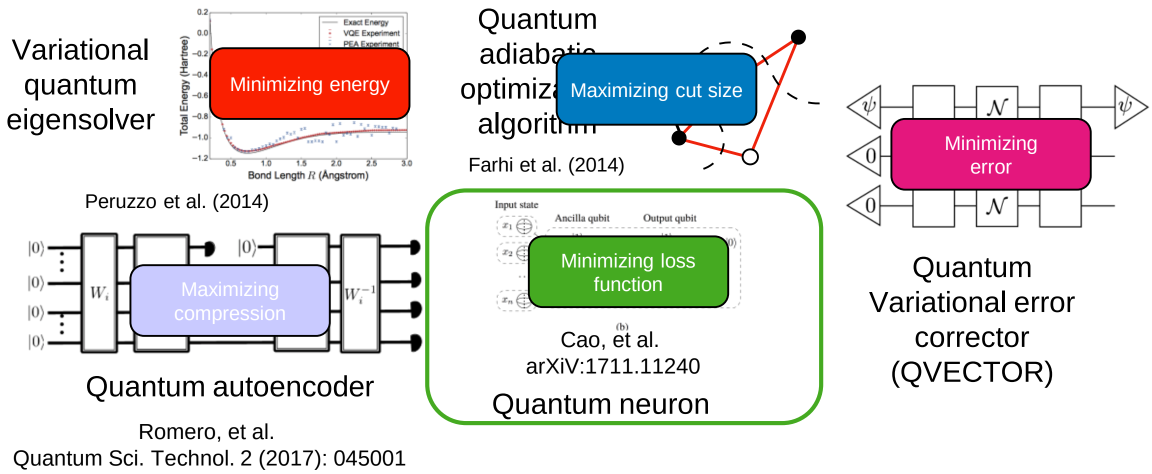

QVECTOR
Average fidelity
Wait time (μs)
Single qubit
Five-qubit code
Bi-convex optimization

113


QVECTOR
Average fidelity
Wait time (μs)
Single qubit
Five-qubit code
Bi-convex optimization

114

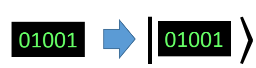
The age of variational quantum algorithms
… training quantum circuits.



… and many other algorithms, e.g. Machine Learning

Basic requirements for quantum NN

1. Initial state encodes any *N*-bit binary string



2. Reflects one or more basic neural computing mechanisms

e.g. attractor dynamics, synaptic connections, integrate & fire, training rules, structure of a NN

3. The evolution is based on quantum effects

Superposition and entanglement

Schuld, M., Sinayskiy, I. & Petruccione, F. *Quantum Inf Process* (2014) 13: 2567

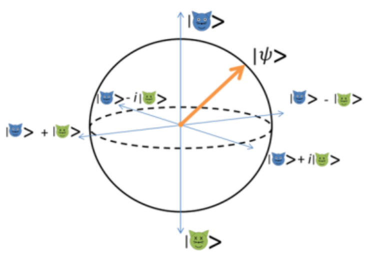
QM + NN: an unlikely match ?

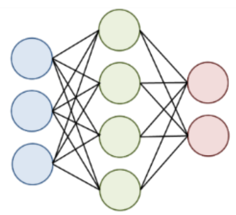
Quantum Mechanics (QM)

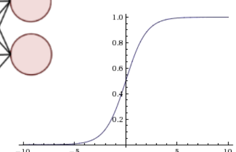
- Unitary evolution
- Rotation in Hilbert space

Neural Networks (NN)

- Lossy transformations
- Clustering, classification, compression etc

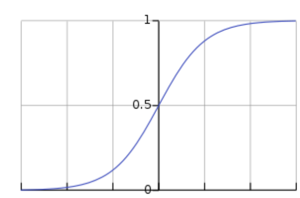






117

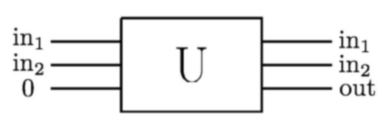
Challenges



- Sigmoid / step function activation

  How to realize on quantum computers, whose dynamics is **linear**?

Reversible circuits
Dissipative dynamics



Cost scaling?

- Measurement? Open system?

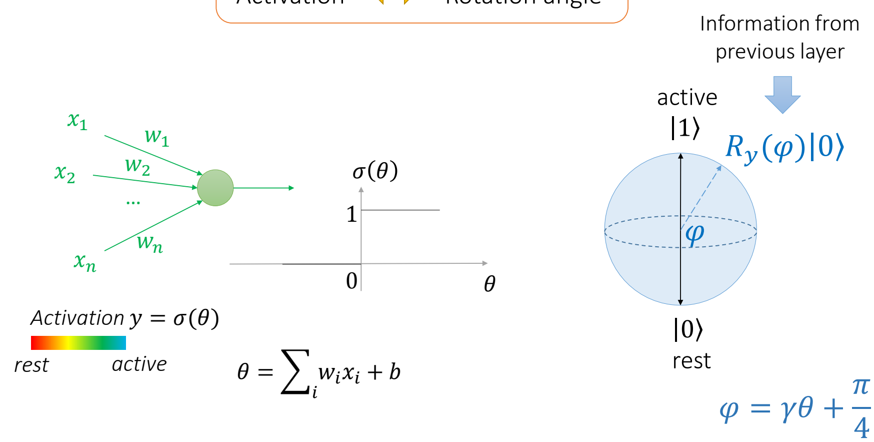
  May collapse the state / reduce to classical probabilistic algorithms

  Story of quantum error correction

118

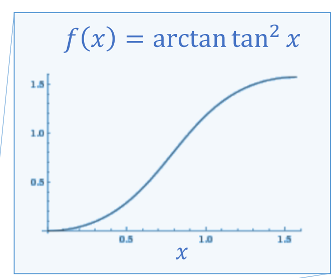
Our Proposal

Neuron	⇔	Qubit
Activation	⇔	Rotation angle



119

Introduce Nonlinearity

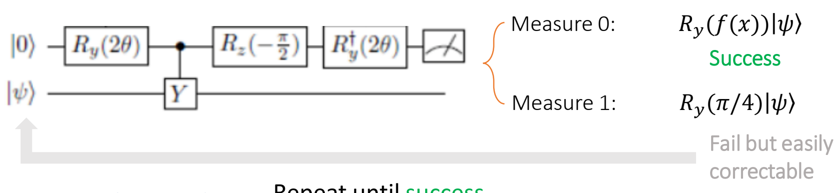


Repeat-until-success (RUS) circuits:

Given ability to realize $R_y(2x)$

One could use RUS to realize $R_y(2f(x))$

Nonlinear!

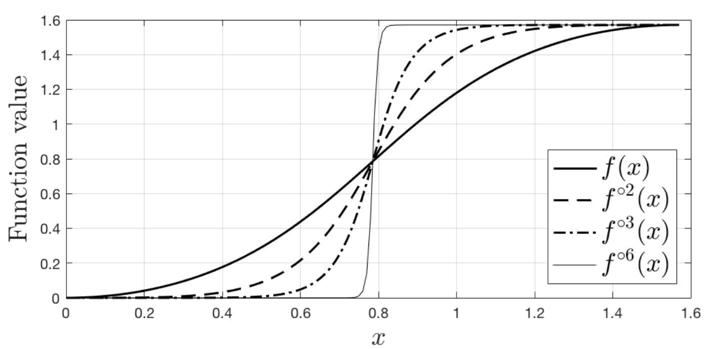


$$R_y(\theta) = \begin{pmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix}$$

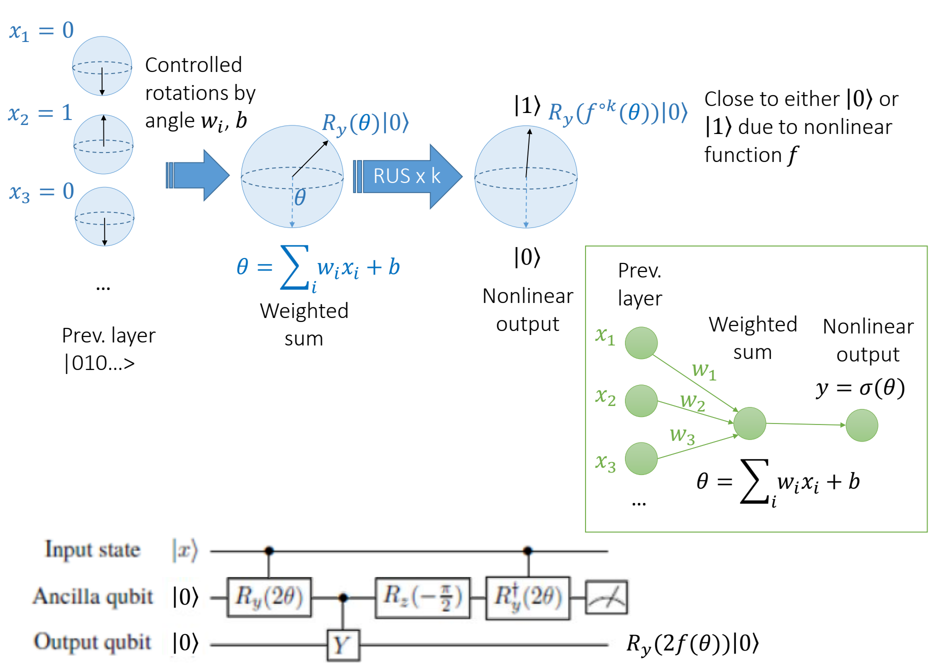
120

$$R_y(x) \Rightarrow R_y(f(x)) \Rightarrow \dots \dots \Rightarrow R_y\left(f^{\circ k}(x)\right)$$

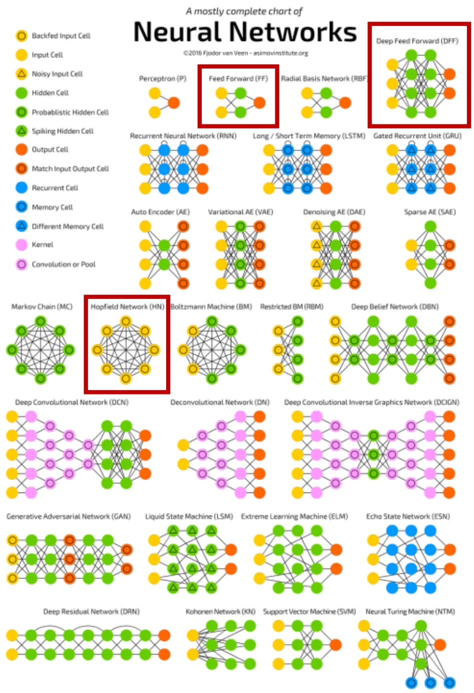
$$\underbrace{f\left(f(\dots f(x)\dots)\right)}_{k \text{ times}} = f^{\circ k}(x)$$



121



122



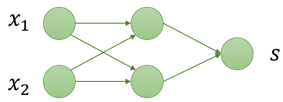
- Size
- Neuron type
- Connectivity
- Activation function
- Weight/bias setting
- Training method
- ...

123

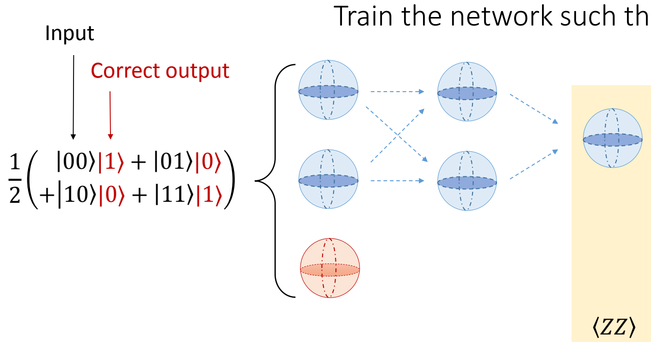
124

XOR Network

x_1	x_1	s
0	0	1
0	1	0
1	0	0
1	1	1

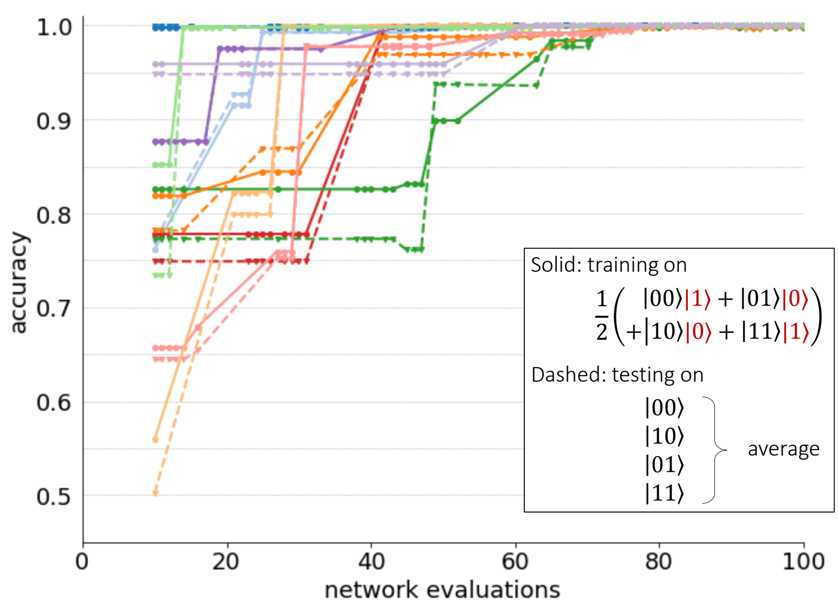


Train the network such that $s = x_1 \oplus x_2$



Accuracy: $\frac{1+\langle ZZ \rangle}{2}$

125



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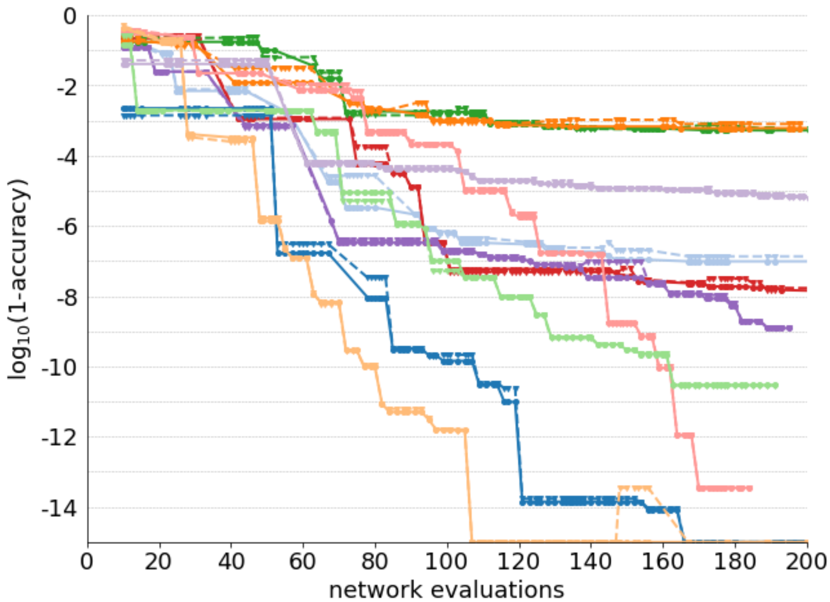


127

Summary

- Building block for quantum neural network satisfying
  - Initial state encoding *n*-bit strings
    Neuron <-> Qubit
  - One or more neural computing mechanisms
    Sigmoid/step function, attractor
  - Evolution based on quantum effects
    Train with superposition of examples
- Application and extensions
  - Superposition of weights (networks) ?
  - Different forms of networks
  - Different activation functions

128

Enter the quantum *software* era.

How about a *platform neutral*, near-term focused quantum software startup?

Look no further!

Z is the new Q

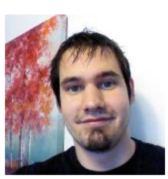
ZapataComputing

Email: info@zapatacomputing.com

129

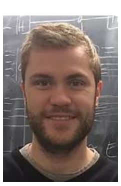
Collaborators

Jonathan Romero



Jonathan Olson

Hanna Sim



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Mattias DeGroote
Jonny Olson
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130

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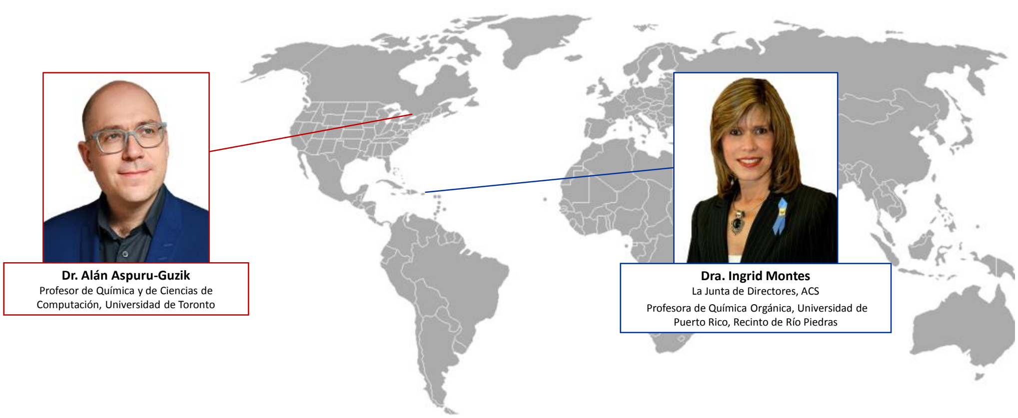

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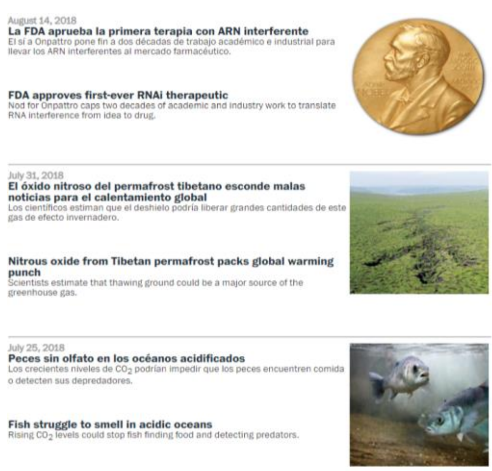

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La FDA aprueba la primera terapia con ARN interferente
El sí a Onpattro pone fin a dos décadas de trabajo académico e industrial para llevar los ARN interferentes al mercado farmacéutico.

FDA approves first-ever RNAi therapeutic
Nod for Onpattro caps two decades of academic and industry work to translate RNA interference from idea to drug.

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Scientists estimate that thawing ground could be a major source of the greenhouse gas.

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Dr. Bibiana Campos Seijo
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136