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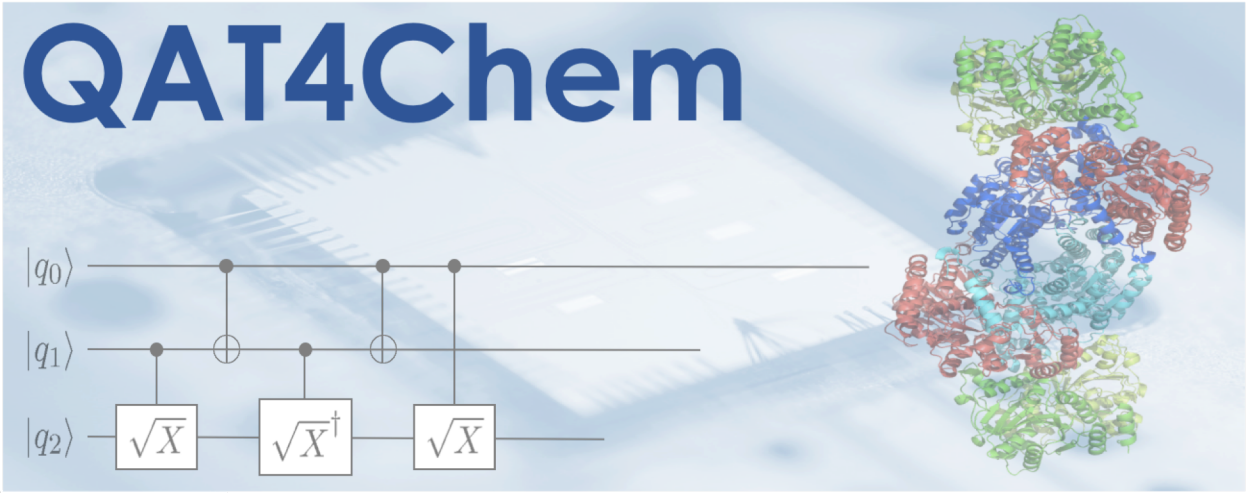
Quantum Algorithms, Mathematics and Compilation Tools for Chemical Sciences



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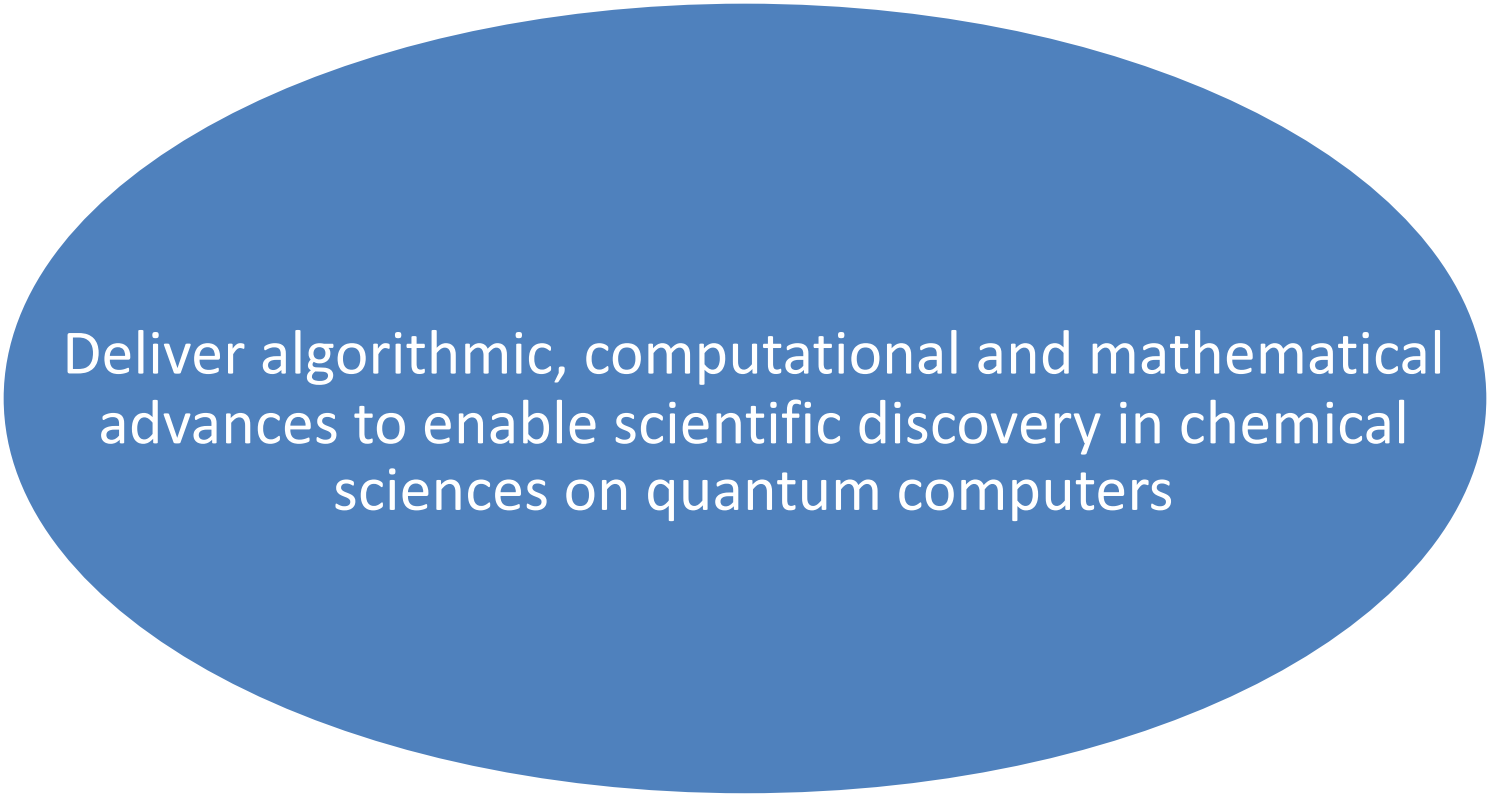
Quantum Algorithms Team for Chemical Sciences



Verified Quantum Information Scrambling Algorithm and Experiment Published in Nature

Scientific Achievement

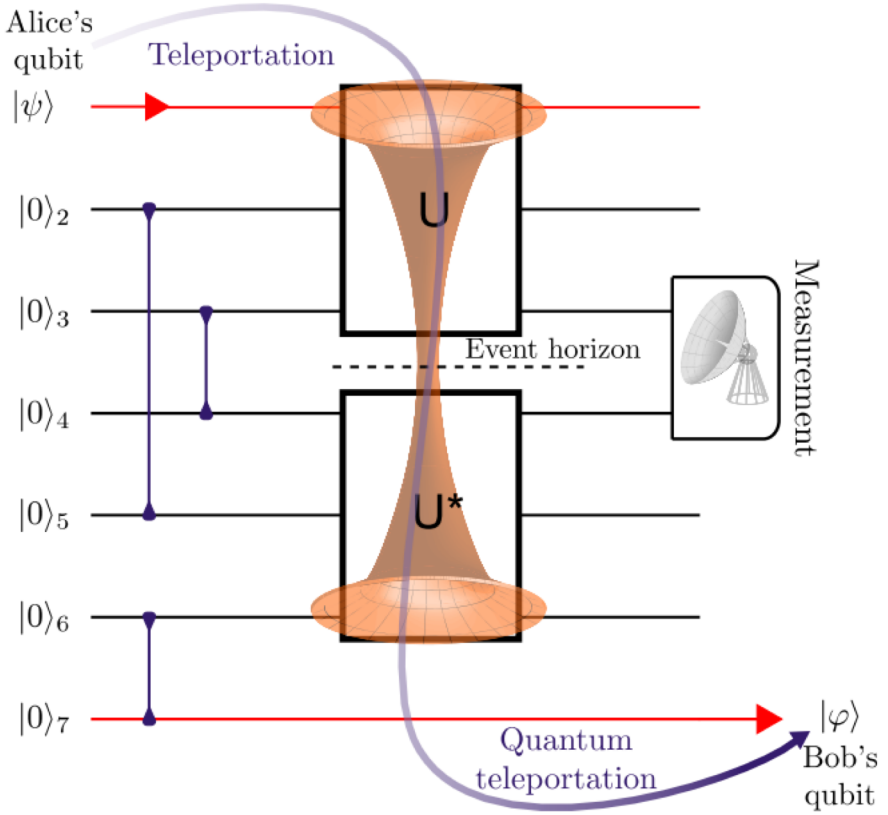
Monroe Group at UMD experimentally implemented the recent proposal from Yao and Yoshida to distinguish between decoherence and scrambling via quantum teleportation

Significance and Impact

First demonstration of verified quantum information scrambling in a quantum system
Experimental data can be used to bound the value of OTOC correlation functions

Research Details

7-qubit all-to-all connected quantum simulation of black hole scrambling. Required a gate depth > 24 to initialize EPR pairs and perform the maximally scrambling three-qubit circuit



Caption: Schematic of the 7-qubit circuit, which uses quantum teleportation to detect information scrambling. The underlay depicts an analogy between our protocol and information propagation through a traversable wormhole.

"Verified quantum information scrambling", Landsman, Figgatt, Schuster, Linke, Yoshida, **Yao**, Monroe, **Nature 567, 61 (2019)**

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Work was a collaboration between UC Berkeley (QAT4Chem PI: Norman Yao) and the Monroe group (UMD)

BERKELEY LAB

An Artificial Quantum Spiking Neuron

Scientific Achievement

- **Proposal of a building block for quantum neuromorphic networks.**
- **Demonstration of its capabilities as a Bell state classifier.**

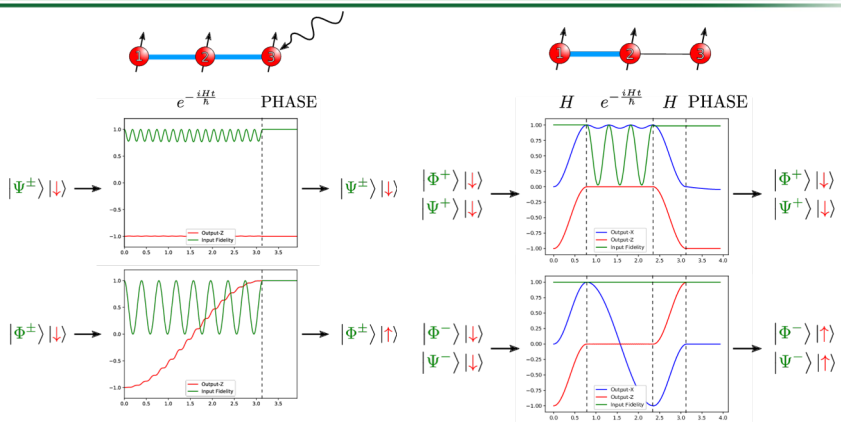
Significance and Impact

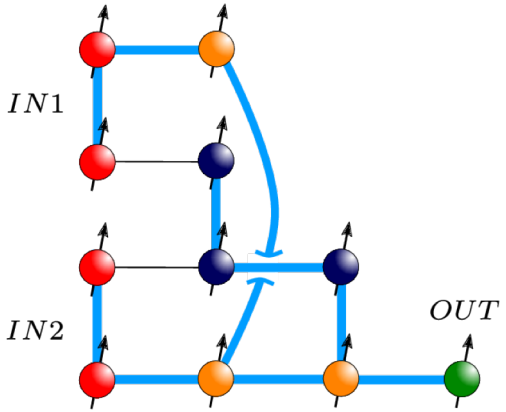
Neuromorphic learning architectures attract a lot of attention as a low power alternative to neural networks. We have combined this promsing scheme with non-classical effects through entanglement between inputs and outputs.

Research Details

– The neuron consists of two driven spin models that measure excitiations and discriminate the relative phase

– The model is not bound by a specific architecture but can be executed whenever time evolution under the simple spin Hamiltonian can be performed.





Top: Schematics of the resonant dynamics of the excitation counting and phase discrimination circuits
Bottom: Assembly of the two parts in to a Bell state comparator

Lasse Bjørn Kristensen, Matthias Degroote, Peter Wittek, Alán Aspuru-Guzik, Nikolaj T. Zinner arXiv:1907.06269

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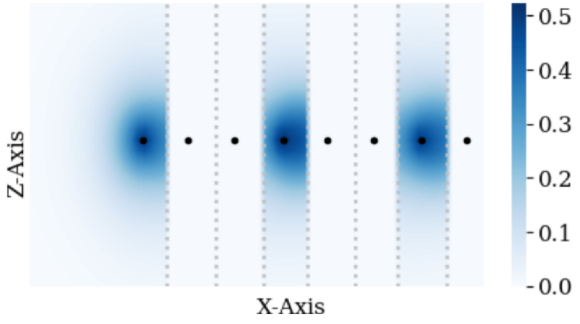
This work was a collaboration between University of Toronto (PI: Alán Aspuru-Guzik) and Aarhus University.

UNIVERSITY OF TORONTO

Discontinuous Galerkin discretization for quantum simulation of chemistry

Lin Lin (UC Berkeley Math, LBNL Math, CAMERA)



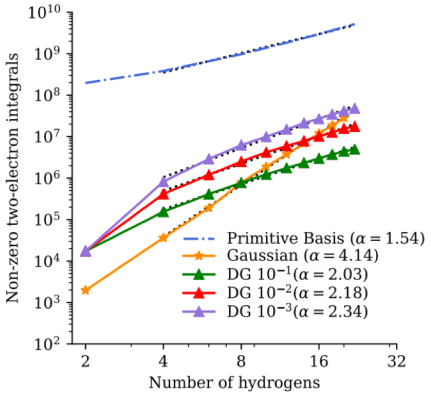


Fig. (Top) Three DG functions in the X-Z plane, represented in real space for a hydrogen chain system; (Bottom) Reduction of the number of two-electron integrals using the DG representation versus the primitive planewave representation and the Gaussian basis set

Scientific Achievement

Develop a new basis set for efficient quantum chemistry calculations on quantum computers, motivated by the discontinuous Galerkin (DG) method

Significance and Impact

Quantum chemistry simulation with a realistic basis set involves a prohibitively large number of terms in the Hamiltonian. We propose a method to significantly reduce the number of terms to be encoded in the Hamiltonian, particularly those due to the Coulomb interaction. Combined with the recently developed fermionic swap network to yield a low depth implementation, the new approach may significantly reduce the pre-constant for quantum simulation.

Research Details

–Diagonal basis for the Coulomb operator is highly advantageous for reducing the complexity of quantum computing [Babbush et al PRX 2018; Kivlichan et al PRL 2018]

–We introduce a DG based basis set, which is a block diagonal basis set that preserves sparsity structure and reduces the preconstant for representing the Coulomb operator

–New basis set is found to be efficient for both quantum computing, as well as accurate classical computing methods such as DMRG

J. R. McClean, F. M. Faulstich, Q. Zhu, B. O'Gorman, Y. Qiu, S. R. White, R. Babbush, **L. Lin**, arXiv:1909.00028

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QAT4Chem

New Algorithms for Solving Quantum Linear System Problem

Scientific Achievement

We propose two quantum algorithms for solving linear system (Ax=b) based on time-optimal adiabatic quantum computing (AQC(p)) and quantum approximate optimization algorithm (QAOA), respectively. Both algorithms achieve the optimal complexity with respect to the condition number.

Significance and Impact

AQC(p) and QAOA outperform most existing quantum algorithms for solving linear system with the optimal condition number scaling are much simpler to implement. The success of AQC(p) demonstrates the significance of time scheduling for accelerating AQC. Numerical simulations suggest QAOA is a very competitive algorithm for solving quantum linear system with the near optimal scaling with respect to the condition number and accuracy.

Research Details

- Developed AQC(p) motivated by the randomization method and the optimal time scheduling for Grover's search algorithm.
- Analyzed and rigorously proved the runtime complexity of AQC(p) based on the quantum adiabatic theorem, which implies an upper bound of the complexity of QAOA for solving quantum linear system due to the natural connection between AQC and QAOA.
- Numerically studied the scaling of the runtime of AQC(p) and QAOA as a function of the condition number and the accuracy with both Hermitian positive definite matrices and general non-Hermitian matrices.

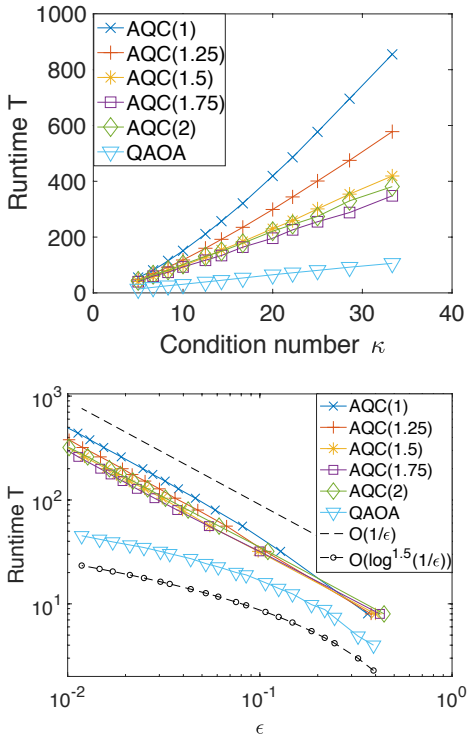


Fig. The runtime of AQC(p) and QAOA as a function of the condition number and the accuracy.

D. An, **L. Lin** (2019). arXiv:1909.05500

Low Depth Quantum Circuit Parallelization

Scientific Achievement

Generalized swap networks for low-depth parallelization of gates.

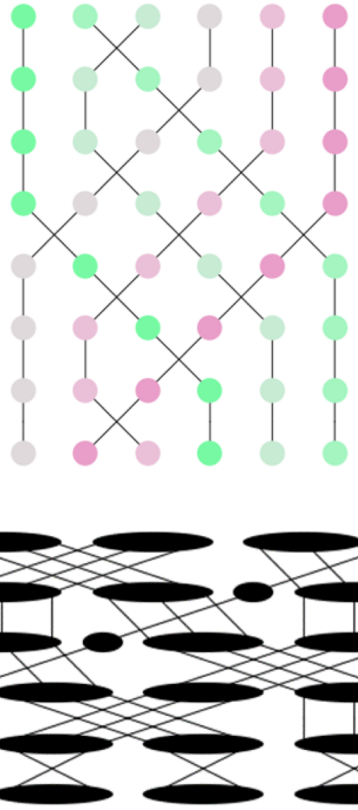
Significance and Impact

The state of available superconducting quantum computers is rapidly advancing, but in the near term such devices will have limited coherence and connectivity. In particular, there is great interest in implementing circuits related to quantum chemistry and classical optimization. In both cases, parallelization allows for minimal depth; in circuits originating from fermionic Hamiltonians, there is also a need to address the locality of the gates.

Research Details

- We develop methods based on generalized swap networks for several families of circuits.
- We show that a Trotter step (or related VQE circuit) can be done in $O(n^3)$ depth, compared to previous $O(n^4)$.
- We show that QAOA for k-CSP can be done in $O(n^{k-1})$ depth.

https://arxiv.org/abs/1905.05118



Top: Circuit for a "3-SWAP" gate in which two sets of 3 qubits each are swapped.
Bottom: Generalized swap network in which sets of up to 3 qubits each are moved around so that each pair of sets is adjacent at least once.

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Work was a collaboration between UC Berkeley (PI: Birgitta Whaley) and NASA Ames.

BERKELEY LAB

Quantum error detection improves accuracy of chemical calculations on a quantum computer

Scientific Achievement

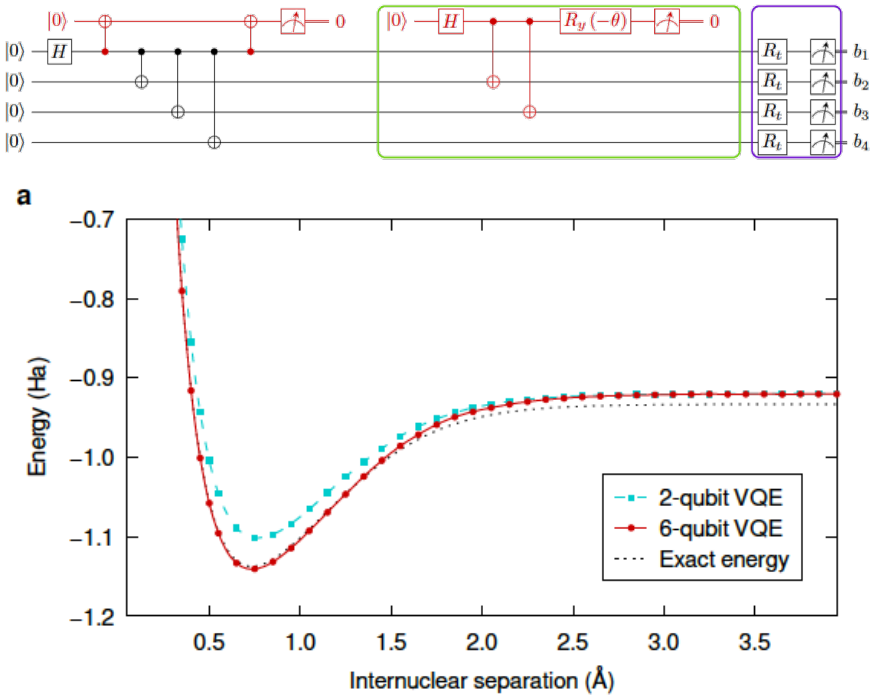
For the first time we demonstrate experimentally that the [[4, 2, 2]] quantum error detecting code can be used to improve the accuracy of an end-to-end chemical simulation of the hydrogen molecule on a quantum computer.

Significance and Impact

Quantum computing's major challenge is errors due to noisy hardware. For the first time it is shown that error detection codes can enable scientific discovery on NISQ quantum computers.

Research Details

- The [[4, 2, 2]] error correction code was used where two logical qubits were encoded into four qubits.
- Variational Quantum Eigensolver and high-energy physics 'unfolding' for readout correction were used.
- Circuit was applied to H_2, though could be used for any 2 orbital – 2 electron system.



6-qubit error detection circuit is shown to get much closer to the exact energy curve than the standard 2-qubit circuit.

Collaboration with QuantISED

Urbanek, Nachman, de Jong

http://arxiv.org/abs/1910.00129

Unfolding Quantum Computer Readout Noise

Scientific Achievement

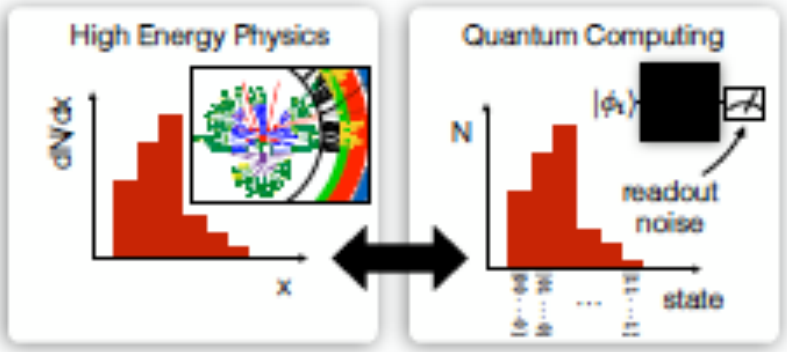
Iterative Bayesian unfolding, widely used in high-energy physics, is shown to avoid pathologies from commonly used matrix inversion and least squares methods correcting readout errors in quantum computing.

Significance and Impact

One of quantum computing's major challenges is bias errors reading out the qubits. Solid correction methods derived from the world of high-energy physics better correct these errors and advance quantum computing for scientific discovery.

Research Details

- Various unfolding methods from high-energy physics were studied and compared to those currently used on the quantum computing community.
- 'Unfolding' method from high-energy physics performs significantly better than (constraint) matrix inversion.



A schematic diagram illustrating the connection between binned differential cross section measurements in high energy physics (left) and interpreting the output of repeated measurements from quantum computers (right).

Collaboration with QuantISED for High Energy Physics

Nachman, Bauer, de Jong, Urbanek

https://arxiv.org/abs/1910.01969

Efficient and Noise Resilient Measurements for NISQ Quantum Chemistry

Scientific Achievement

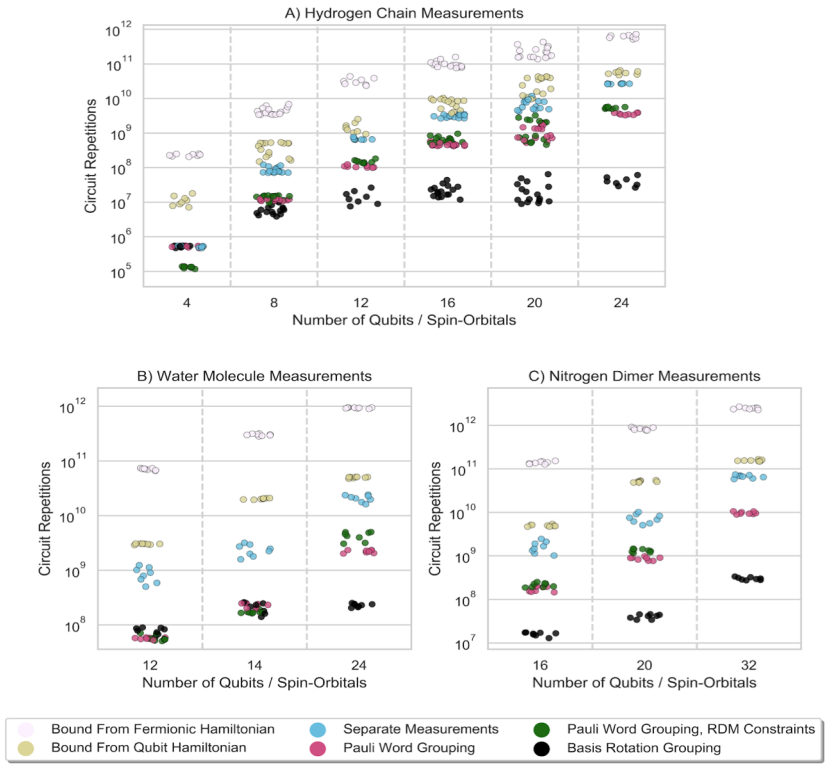
Developed measurement protocol with lower variance and natural ability to perform symmetry verification.

Significance and Impact

Our approach reduces the required time by an order of magnitude for a variety of systems when compared to state-of-the-art approaches and more than four orders of magnitude compared to commonly cited bounds.

Research Details

- We propose a scheme for measuring expectation value of the quantum chemical Hamiltonian using a tensor factorization of the two-electron integral tensor.
- We show how our approach naturally enables error mitigation by post selection.

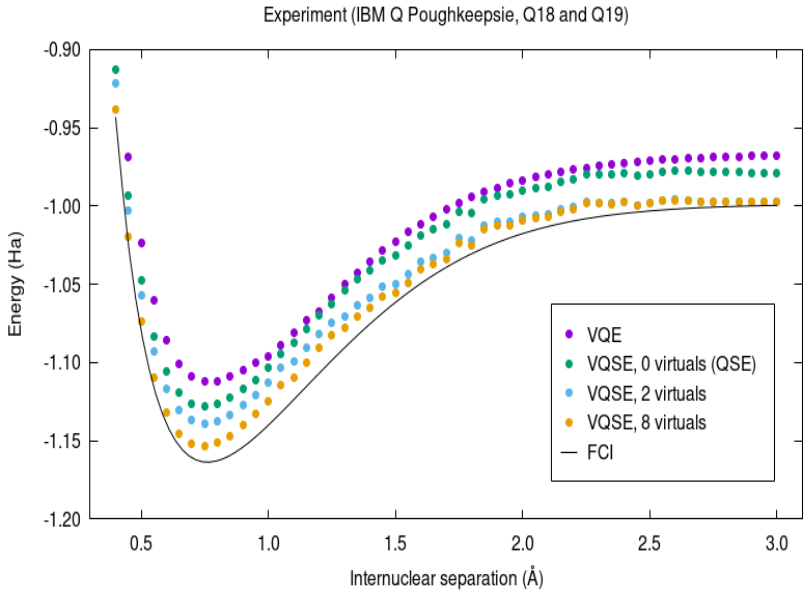


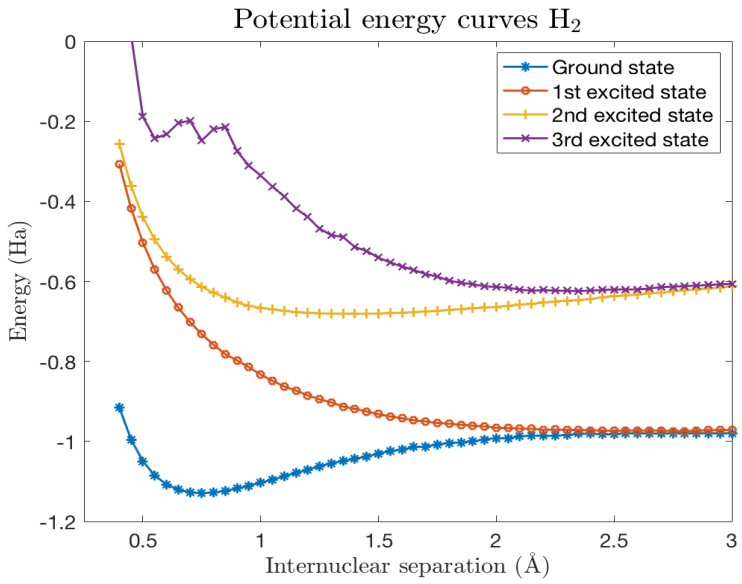
A comparison of circuit repetitions required by a variety of different methods for three model systems. Our results are referred to as "Basis Rotation Grouping."

Work was performed as a collaboration between Google and UC Berkeley (Berkeley PI:: Birgitta Whaley). arXiv:*1907.13117*
W. Huggins, J. McClean, N. Rubin, Z. Jiang, N. Wiebe, K. B. Whaley, R. Babbush

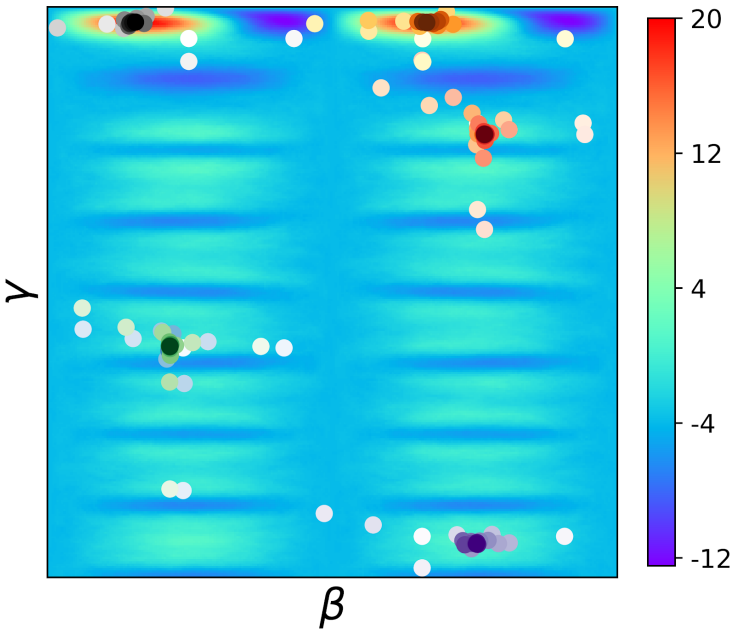
Virtual quantum subspace expansion (VQSE)

- **Better basis sets without more quantum resources**
  - Builds on quantum subspace expansion
  - Based on https://arxiv.org/pdf/1902.10679.pdf
  - Collaboration with Takashita (Daimler)
  - Opens door to a lot more chemistry





Identifying Variational Parameters for the Quantum Approximate Optimization Algorithm (QAOA)



Objective landscape for a single-gate ansatz parameterized by angles γ and β is multimodal. Dots show points evaluated by our multistart optimizer, which is better suited for finding good maxima for this problem.

Scientific Achievement

Using classical numerical optimization routines to drive IBM Q simulations of Hamiltonians from QAOA to solve community-detection problems

Significance and Impact

Performance of QAOA depends heavily on being able to identify variational parameters corresponding to the Hamiltonian ground state modeling the original problem

Research Details

- Traditional algorithms used to identify variational parameters are highly sensitive to initial conditions and can get stuck in local optima
- Currently extending studies to higher dimensions and integrating robust local optimization algorithms within the multistart APOSMM optimizer

QAT4Chem

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R. Shaydulin, I. Safro, and J. Larson.
Multistart methods for quantum approximate optimization.
https://arxiv.org/abs/1905.08768

SKQuant-Opt: Optimizers for Noisy Intermediate-Scale Quantum Devices

Scientific Achievement

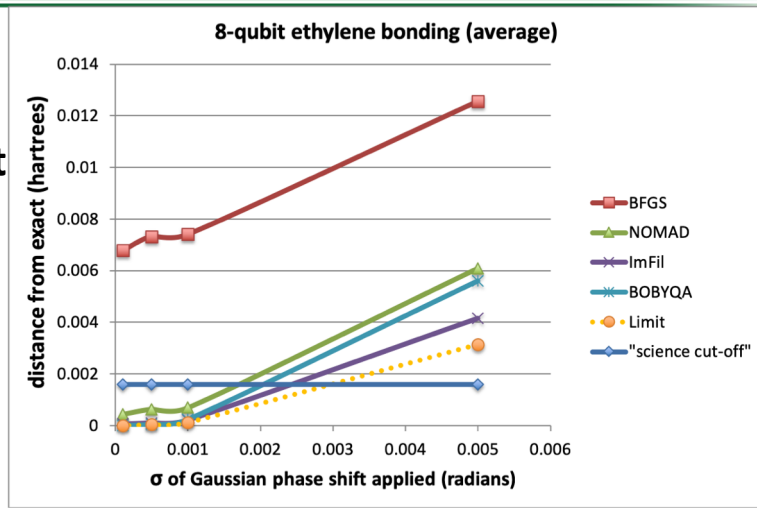
First demonstration that classical minimizers can handle the noisy behavior of NISQ devices within the full context of the Variational Quantum Eigensolver (VQE) algorithm applied to quantum chemistry problems.

Significance and Impact

Variational algorithms are considered the path to early science results on NISQ hardware. These algorithms employ a hybrid iterative approach, combining a quantum circuit with a classical minimization step. The latter was the weak link: most results to date therefore skip it in favor of full space exploration, which is clearly not scalable. We have demonstrated, by adapting noise-aware minimizers and developing algorithm tuning methodology, that the classical step no longer limits the VQE as a feasible path to successful science on NISQ.

Research Details

- We assembled and tuned a suite of optimizers (mesh and trust region methods) for VQE domain science usage
- Software release Dec 2018 - **github.com/scikit-quant**
- We present the co-tuning of quantum circuit and optimizer
- We present the performance aspects of optimizer choice



(Hybrid) Mesh methods

- Implicit Filtering (ImFil) – Prof. Kelley, NCSU
- Nonlinear Optimization by Mesh Adaptive Direct Search (NOMAD) – Sébastien Le Digabel, GERAD, Canada
- Stable Noisy Optimization by Branch and Fit (SnobFit) – Prof. Neumaier, Uni. Wien, Austria

Trust region methods

- Optimization by radial basis function interpolation in trust-regions (ORBIT) – Stefan Wild, ANL
- Bound Optimization BY Quadratic Approximation (bobyqa) – Lindon Roberts, Oxford, UK

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Wim Lavrijsen (LBL), Ana Tudor (UCB), Costin Iancu (LBL), Wibe de Jong (LBL)

BERKELEY LAB
Lawrence Berkeley National Laboratory

QAT Teams Join Forces with Industry to Organize SC18 Tutorial

Scientific Achievement

QAT Teams organize and run the "Quantum Computing for Scientific Applications" tutorial at SC18 in Dallas, TX.

Significance and Impact

Led by LBNL, the three QAT teams from LBNL, ONRL and Sandia together with industry speakers from Google and IBM provided an introduction to quantum computing and hands-on experience with Cirq and QISKit software stacks.

Research Details

- Lead organizer was Costin Iancu from LBNL's QAT Team
- All day tutorial had attendance of approximately 100 people, many computer scientists and applied mathematicians
- Many active discussions and Q&A on challenges and possibilities in quantum computing

Find more information

QAT4Chem.lbl.gov