Development of QAOA and VQE Algorithms

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Areas of research

- Development of QAOA approach: new applications, scaling up size of instances, finding optimal parameters, compact ansatz design
- Development of VQE algorithm: compact ansatz design, new applications, resource estimation
- Development of quantum simulator QTensor to support research done for QAOA, VQE, QML, and quantum supremacy/advantage
- Other areas: modeling quantum devices i.e. developing accurate noise models, quantum machine learning, resource estimation, distributed quantum computing

QAOA

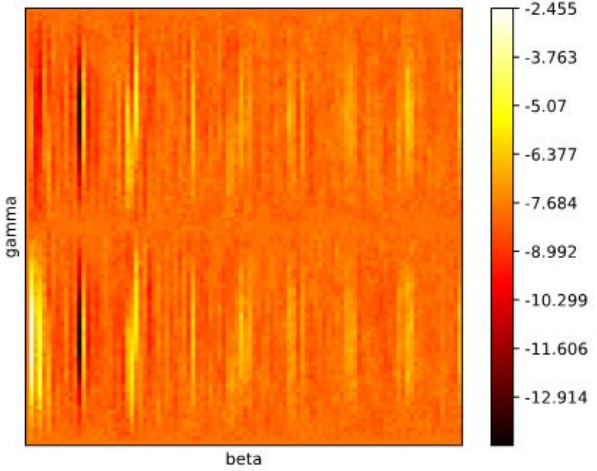
- Shaydulin, Ruslan, Hayato Ushijima-Mwesigwa, Christian FA Negre, Ilya Safro, Susan M. Mniszewski, and Yuri Alexeev. "A hybrid approach for solving optimization problems on small quantum computers." Computer 52, no. 6 (2019): 18-26.
- Shaydulin, Ruslan, Hayato Ushijima-Mwesigwa, Ilya Safro, Susan Mniszewski, and Yuri Alexeev. "Network community detection on small quantum computers." Advanced Quantum Technologies 2, no. 9 (2019): 1900029.
- Shaydulin, Ruslan, and Yuri Alexeev. "Evaluating quantum approximate optimization algorithm: A case study." In 2019 tenth international green and sustainable computing conference (IGSC), pp. 1-6. IEEE, 2019.

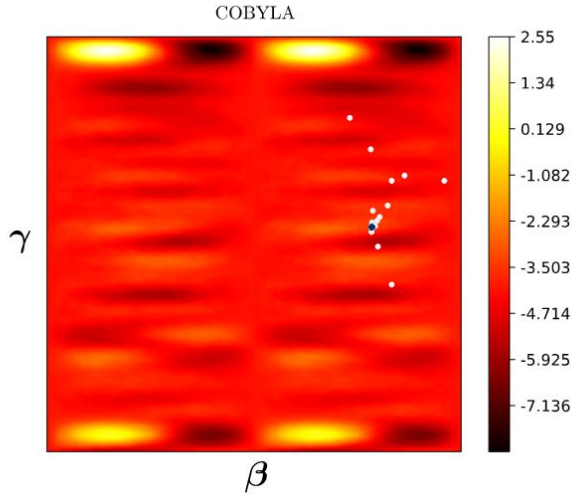
QAOA

- Khairy, Sami, Ruslan Shaydulin, Lukasz Cincio, Yuri Alexeev, and Prasanna Balaprakash. "Learning to optimize variational quantum circuits to solve combinatorial problems." In Proceedings of the AAAI Conference on Artificial Intelligence, vol. 34, no. 03, pp. 2367-2375. 2020.
- Ushijima-Mwesigwa, Hayato, Ruslan Shaydulin, Christian FA Negre, Susan M. Mniszewski, Yuri Alexeev, and Ilya Safro. "Multilevel combinatorial optimization across quantum architectures." ACM Transactions on Quantum Computing 2, no. 1 (2021): 1-29.
- Galda, Alexey, Xiaoyuan Liu, Danylo Lykov, Yuri Alexeev, and Ilya Safro. "Transferability of optimal QAOA parameters between random graphs." arXiv preprint arXiv:2106.07531 (2021). Proceedings of IEEE Quantum Week 2021

QAOA

- The parameter space is highly nonconvex and contains many low-quality, nondegenerate local optima
- Local optimizers get stuck in local optima





VQE

- Liu, Xiaoyuan, Anthony Angone, Ruslan Shaydulin, Ilya Safro, Yuri Alexeev, and Lukasz Cincio. "Layer VQE: A Variational Approach for Combinatorial Optimization on Noisy Quantum Computers." arXiv preprint arXiv:2102.05566 (2021).
- Fedorov, Dmitry A., Matthew J. Otten, Stephen K. Gray, and Yuri Alexeev. "Ab initio molecular dynamics on quantum computers." The Journal of Chemical Physics 154, no. 16 (2021): 164103.
- Fedorov, Dmitry A., Yuri Alexeev, Stephen K. Gray, and Matthew Otten. "Unitary Selective Coupled-Cluster Method." arXiv preprint arXiv:2109.12652 (2021).
- Otten, Matthew, Matthew Hermes, Riddhish Pandharkar, Yuri Alexeev, Stephen Gray, and Laura Gagliardi. "Localized Quantum Chemistry on Quantum Computers." (2021).

Molecular Dynamics Simulation on a Quantum Computer

Scientific Achievement

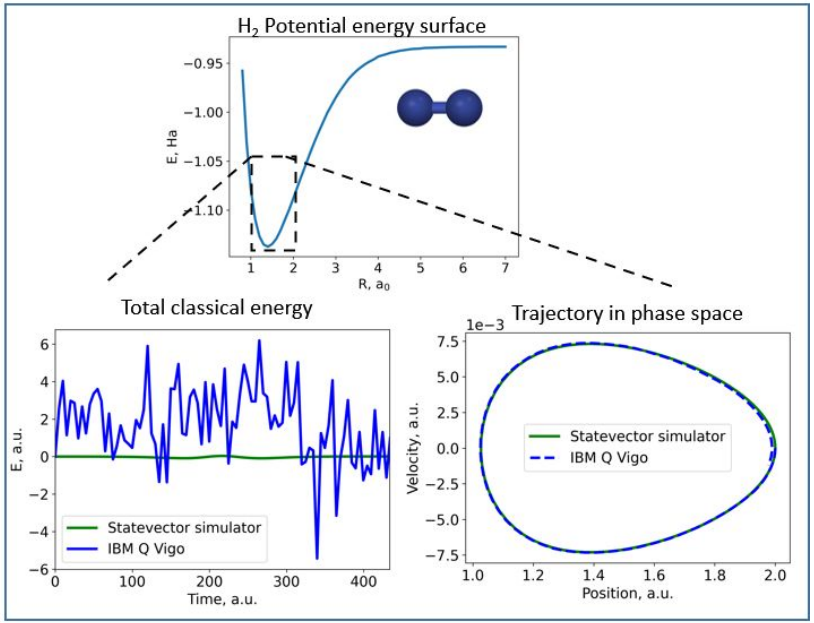
First ab initio MD simulation for a real chemical system was performed on a quantum computer

Significance and Impact

This proof of concept study shows that future generations of quantum hardware can be used to accelerate ab initio MD simulations for larger molecular systems.

Research Details

- The propagation of the nuclei was performed on a classical computer, and electronic energies and gradients were computed on IBM quantum hardware using VQE method.
- We used Hellmann-Feynman theorem and correlated sampling to compute numerical gradients, which reduced the number of quantum measurements by 3-4 orders of magnitude compared to brute force approach.



H_2 MD trajectory computed at UCCSD/STO-3G level of theory: Fluctuations in total energy due to the noise from quantum hardware. Overall shape of trajectory is reproduced well.

D. A. Fedorov, M. J. Otten, S. K. Gray, and Y. Alexeev, J. Chem. Phys. 154, 164103 (2021).

Unitary Selective Coupled Cluster Ansatz (USCC)

Scientific Achievement

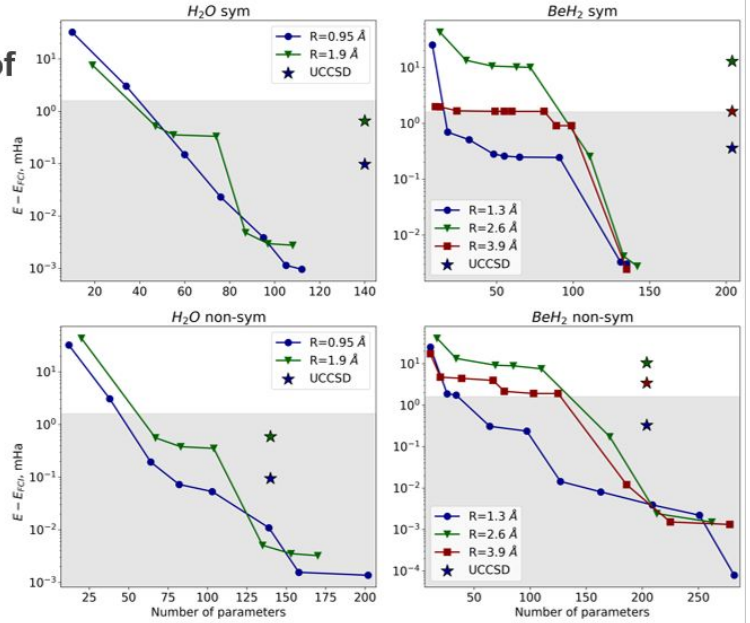
We have proposed an efficient method to reduce the number of operators in unitary coupled cluster ansatz.

Significance and Impact

Our approach allows to reduce the required circuit depth in unitary coupled cluster ansatz, which often contains many redundant and insignificant elements.

Research Details

- Circuit depth reduced through screen-out of single and double excitation operators without accuracy loss.
- Our approach uses the values of electronic Hamiltonian matrix elements for screen-out, which reduces the number of parameters by up to a factor of 5 at no extra cost.
- Higher order excitations required for some systems can be added using our iterative (USCC) algorithm.



Energy errors computed for symmetric and non-symmetric configurations of H_2O and BeH_2 molecules using USCCSDTQ method. It allows to reduce the number of parameters in unitary coupled cluster ansatz and systematically decrease the error.

D. A. Fedorov, Y. Alexeev, S. K. Gray, M. J. Otten submitted to Journal of Chemical Theory and Computation

Quantum Simulators

- Wu, Xin-Chuan, Sheng Di, Franck Cappello, Hal Finkel, Yuri Alexeev, and Frederic T. Chong. "Full State Quantum Circuit Simulation by Using Lossy Data Compression." In IEEE/ACM 29th The International Conference for High Performance computing, Networking, Storage and Analysis (SC18). 2018.
- Lykov, Danylo, Roman Schutski, Alexey Galda, Valerii Vinokur, and Yuri Alexeev. "Tensor network quantum simulator with step-dependent parallelization." arXiv preprint arXiv:2012.02430 (2020).
- Lykov, Danylo, and Yuri Alexeev. "Importance of Diagonal Gates in Tensor Network Simulations." In 2021 IEEE Computer Society Annual Symposium on VLSI (ISVLSI), pp. 447-452. IEEE, 2021.

Quantum Simulators

- Performance Evaluation and Acceleration of the QTensor Quantum Circuit Simulator on GPUs, Danylo Lykov, Angela Chen, Huaxuan Chen, Kristopher Keipert, Zheng Zhang, Tom Gibbs, and Yuri Alexeev, Proceedings for SC21 Second International Workshop on Quantum Software; full paper is accepted for IEEE digital library Xplore

Other Areas

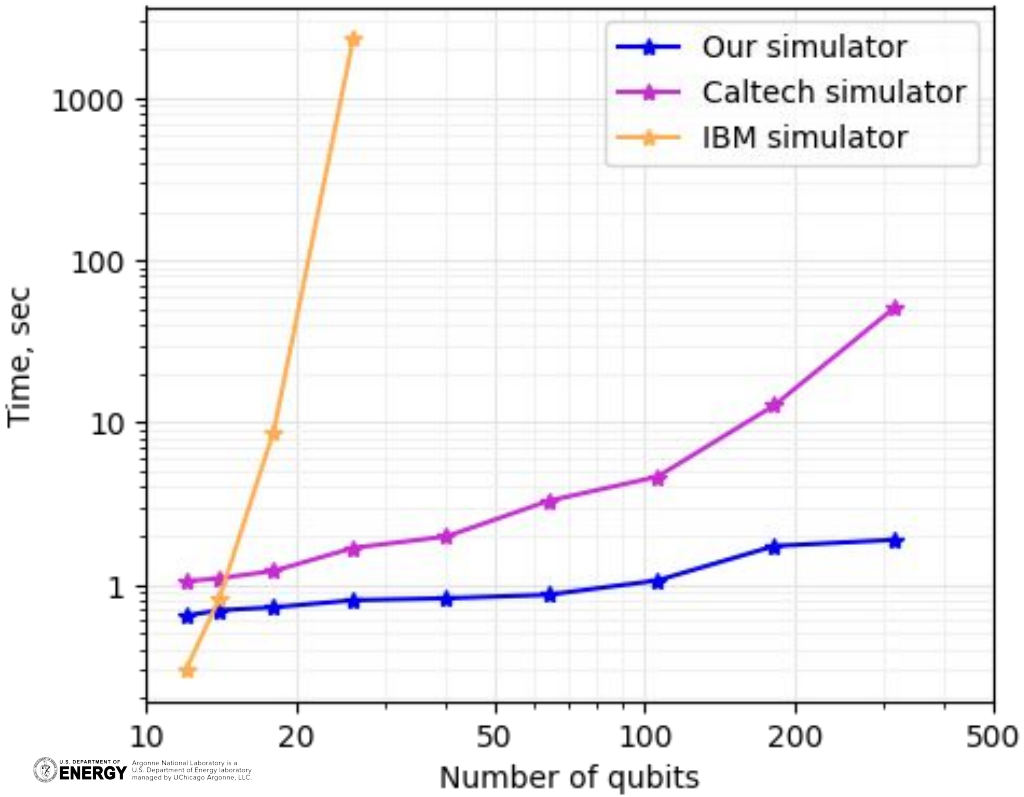
- Ayral, Thomas, François-Marie Le Régent, Zain Saleem, Yuri Alexeev, and Martin Suchara. "Quantum divide and compute: Hardware demonstrations and noisy simulations." In 2020 IEEE Computer Society Annual Symposium on VLSI (ISVLSI), pp. 138-140. IEEE, 2020.
- Ayral, Thomas, François-Marie Le Régent, Zain Saleem, Yuri Alexeev, and Martin Suchara. "Quantum divide and compute: exploring the effect of different noise sources." SN Computer Science 2, no. 3 (2021): 1-14.
- Wu, Xin-Chuan, Dripto M. Debroy, Yongshan Ding, Jonathan M. Baker, Yuri Alexeev, Kenneth R. Brown, and Frederic T. Chong. "TILT: Achieving Higher Fidelity on a Trapped-Ion Linear-Tape Quantum Computing Architecture." In 2021 IEEE International Symposium on High-Performance Computer Architecture (HPCA), pp. 153-166. IEEE, 2021.

Other Areas

- Otten, Matthew, Keshav Kapoor, A. Barış Özgüler, Eric T. Holland, James B. Kowalkowski, Yuri Alexeev, and Adam L. Lyon. "Impacts of noise and structure on quantum information encoded in a quantum memory." Physical Review A 104, no. 1 (2021): 012605.
- Exploration of Quantum Machine Learning and AI Accelerators for Fusion Science, Minzhao Liu, Ge Dong, Kyle Gerard Felker, Matthew Otten, Prasanna Balaprakash,William Tang, and Yuri Alexeev. ANL Technical report 2021

QTensor: Energy Calculations

Time for a quantum circuit simulation



The problem to solve is MaxCut with QAOA for p=3 and d=3 on 56 Intel Xeon CPUs

Parallel Simulations

The code is parallelized using both OpenMP and MPI

We calculated the QAOA expectation value for a 1,000,000 qubit circuit with depth p=6 in 1 hour and 20 minutes. The simulations were performed on the Theta supercomputer with 512 nodes.

QTensor: Energy Calculations

	$d = 3$	$d = 4$	$d = 5$
$p = 1$	1.04	1.65	2.16
$p = 2$	1.46	2.3	4.36
$p = 3$	2.42	10.2	$45.1^{\dagger}$
$p = 4$	6.83		
$p = 5$	58.0^{*}		

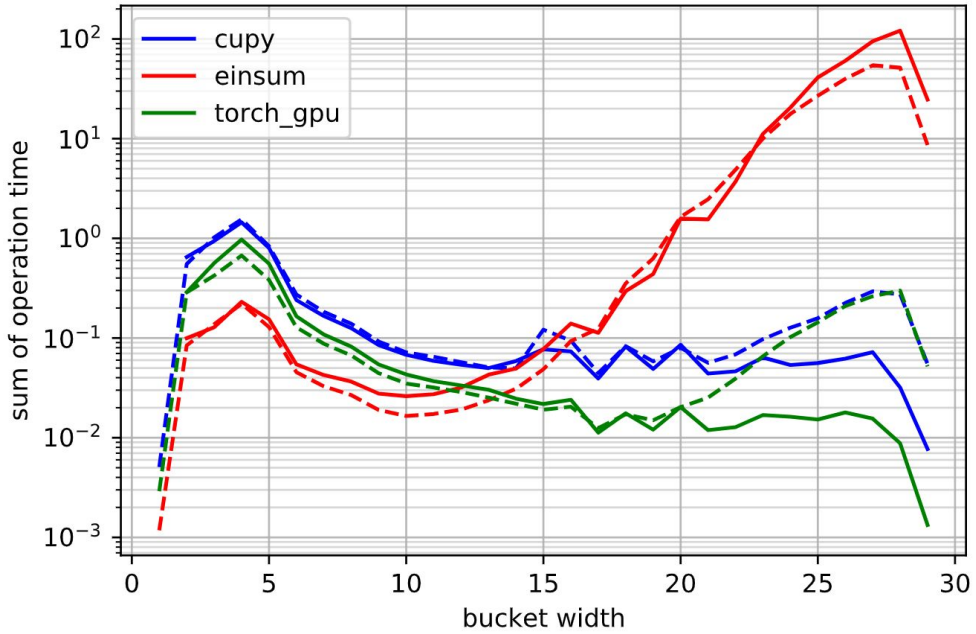
Table 1: QAOA Energy simulation time in seconds for 1000 node regular graphs. All calculations were done using QTensor simulator using NumPy backend on a single Intel Xeon Platinum 8180M CPU @ 2.50GHz with 56 physical cores.

QTensor: GPU contractions

Merged indices backend

Backend Name	Device	Time (seconds)	Speedup
NumPy_Merged	CPU	383	0.64×
NumPy (baseline)	CPU	246	1.00×
CuPy	GPU	6.7	36.7×
CuPy_Merged	GPU	5.6	43.9×
NumPy + CuPy	Mixed	2.1	117×
NumPy_Merged + CuPy_Merged	Mixed	1.4	**176**×

TABLE II: Time for full QAOA expectation value simulation using different Merged backends, as described in Section II-C. The expectation value is MaxCut on a 3-regular graph of size 30 and QAOA depth $p = 4$. **Speedup** shows the overall runtime improvement compared with the baseline CPU backend "NumPy".



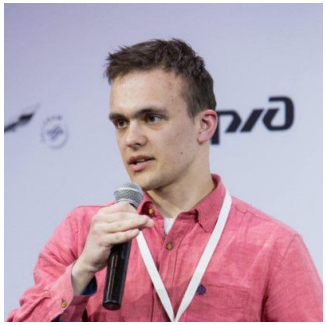
QTensor Features

- Qiskit integration (Qiskit circuit as input)
- Efficient simulation of probability amplitudes
- Simulation of batches of amplitudes for the same cost
- Efficient simulation of expectation values
- Parallelization support, both on CPUs and GPUs
- Automatic differentiation with respect to gate parameters

Team

Dmitry Fedorov

Sahil Gulania



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