

Breaking the exponential wall for many-body problems: ML for quantum computing and electronic structure

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Theoretical Chemistry PhD
Miller group, Caltech





About me



2012-2016 University of Wisconsin-Madison

- BS in Chemistry, Biochemistry, Molecular biology, Math
- Research interest: Biophysics

2022.7-2023.4: Tencent Quantum Lab

- Senior research scientist
- Research interest: Quantum science & applications

2017-2022.6 California Institute of Technology

- PhD in Theoretical chemistry
- Research interest: AI for electronic structure

Experimental Biology



AI4Chemistry



AI4Physics



AI4Chemistry

Est 2023.7: Microsoft Research

Back to AI for chemistry





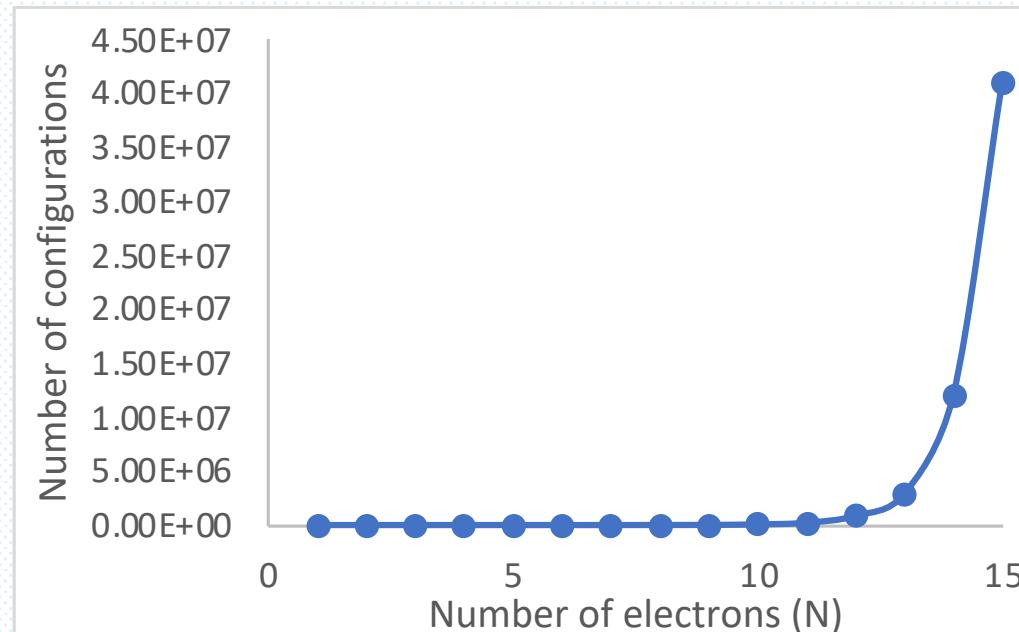
Exponential wall for many-body problems



Solving the many-body Schrodinger equation is NP-hard

Traditional multiparticle wave-function methods when applied to systems of *many particles* encounter what I call an **exponential wall** when the number of atoms N exceeds a critical value which currently is in the neighborhood of $N_0 \sim 10$ (to within a factor of about 2) for a system without symmetries.

--- W. Kohn, Nobel Prize Winner, 1999 in Noble lecture



My research is on how to break this exponential wall with different tools

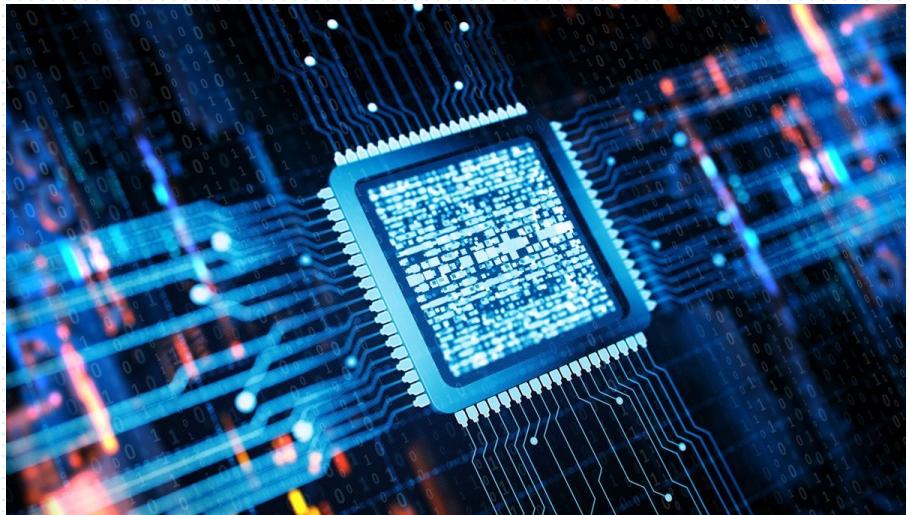


Approaches to break the exponential wall



Solving the many-body Schrodinger equation is NP-hard

Quantum computing



Machine Learning

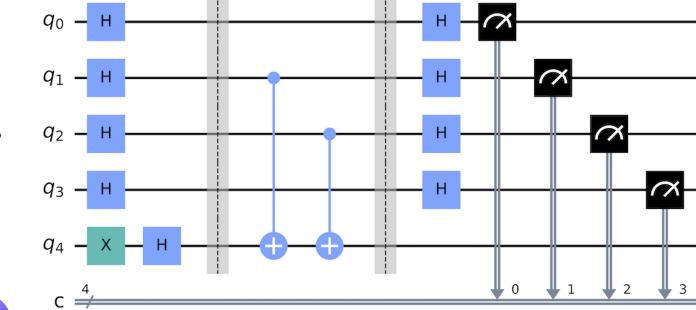
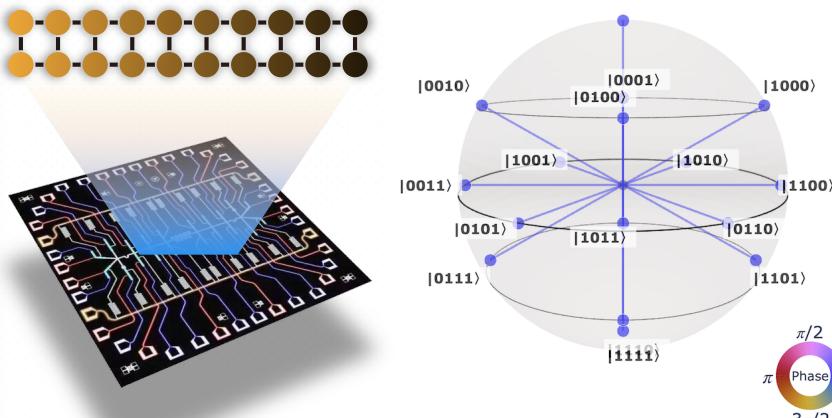
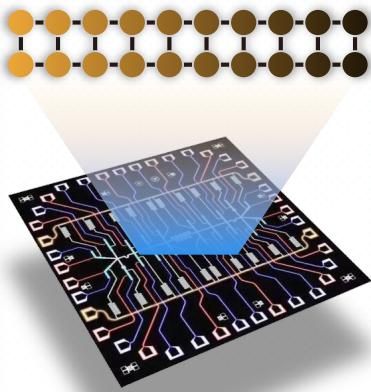


Representative work (today): BO for VQAs + QC for QC (quantum computing for quantum chemistry)

My research is on how to break this exponential wall with different tools

Representative work: Molecular-orbital-based machine learning (MOB-ML)

AI4Quantum Computing



1

Introduction

2

ML-assisted
Quantum algorithms

3

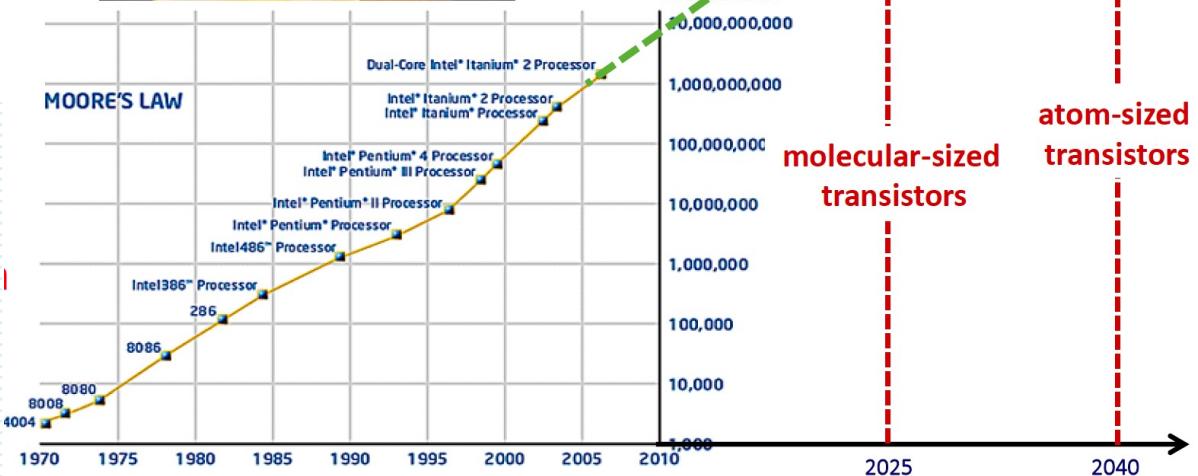
Applications & future
developments

Will not go into the physics details but focus on what ML can contribute





Moore's law & quantum computer

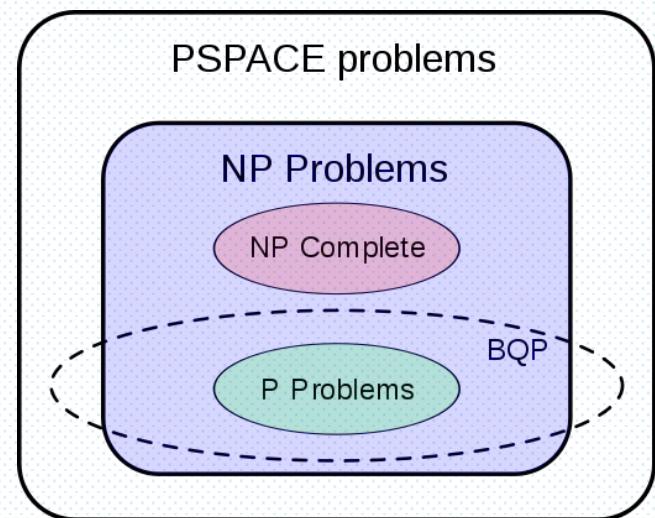


Why quantum computer: (1) More efficient algorithms (2) Quantum Parallelism (3) Cryptography (4) Simulating quantum systems

Moore's law: the observation that the number of transistors in a dense integrated circuit doubles about every two years.

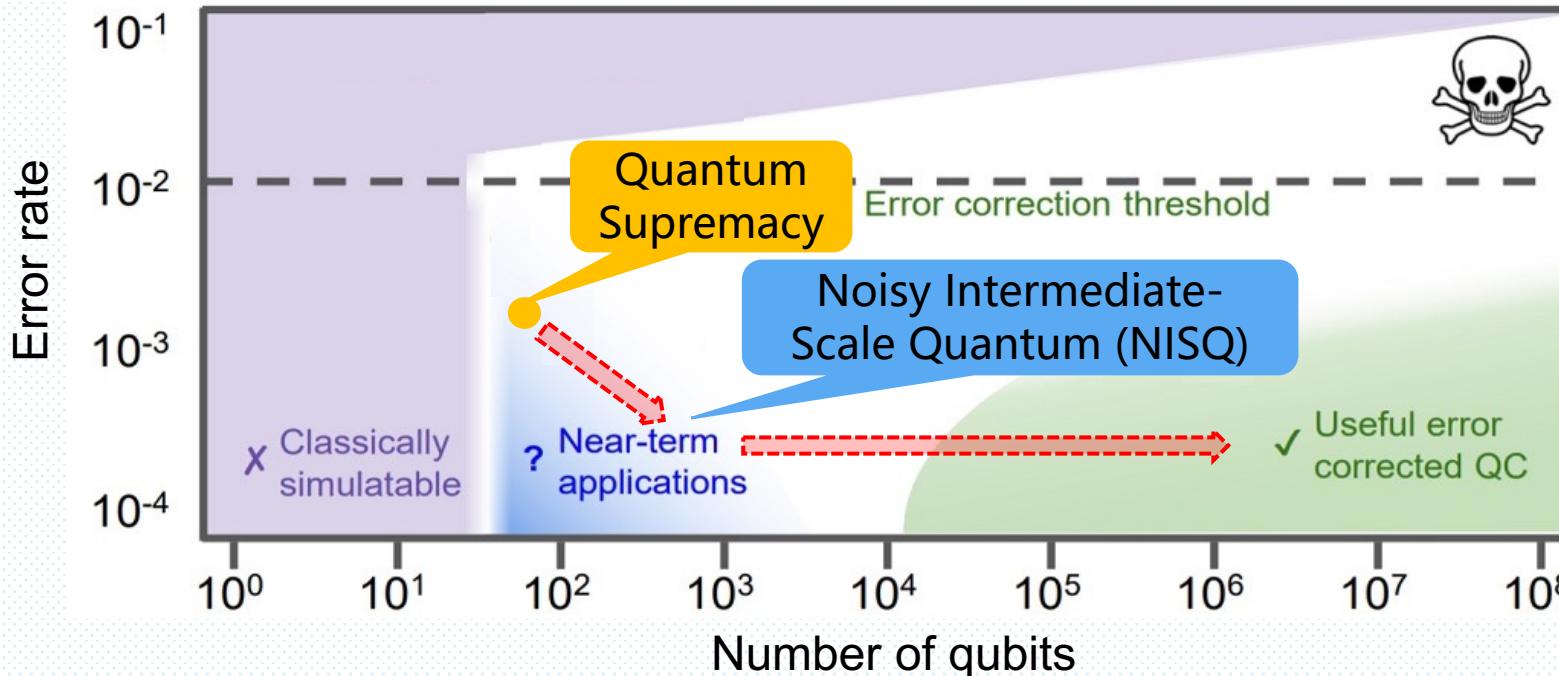
Atomic size is a fundamentally limit to the size of possible transistors.

Quantum computer: uses laws of quantum mechanics to perform massively parallel computing through superposition, entanglement, & decoherence.





Developments of quantum algorithms



John Preskill @
Caltech

Preskill 2012
Preskill 2018

NISQ development paths

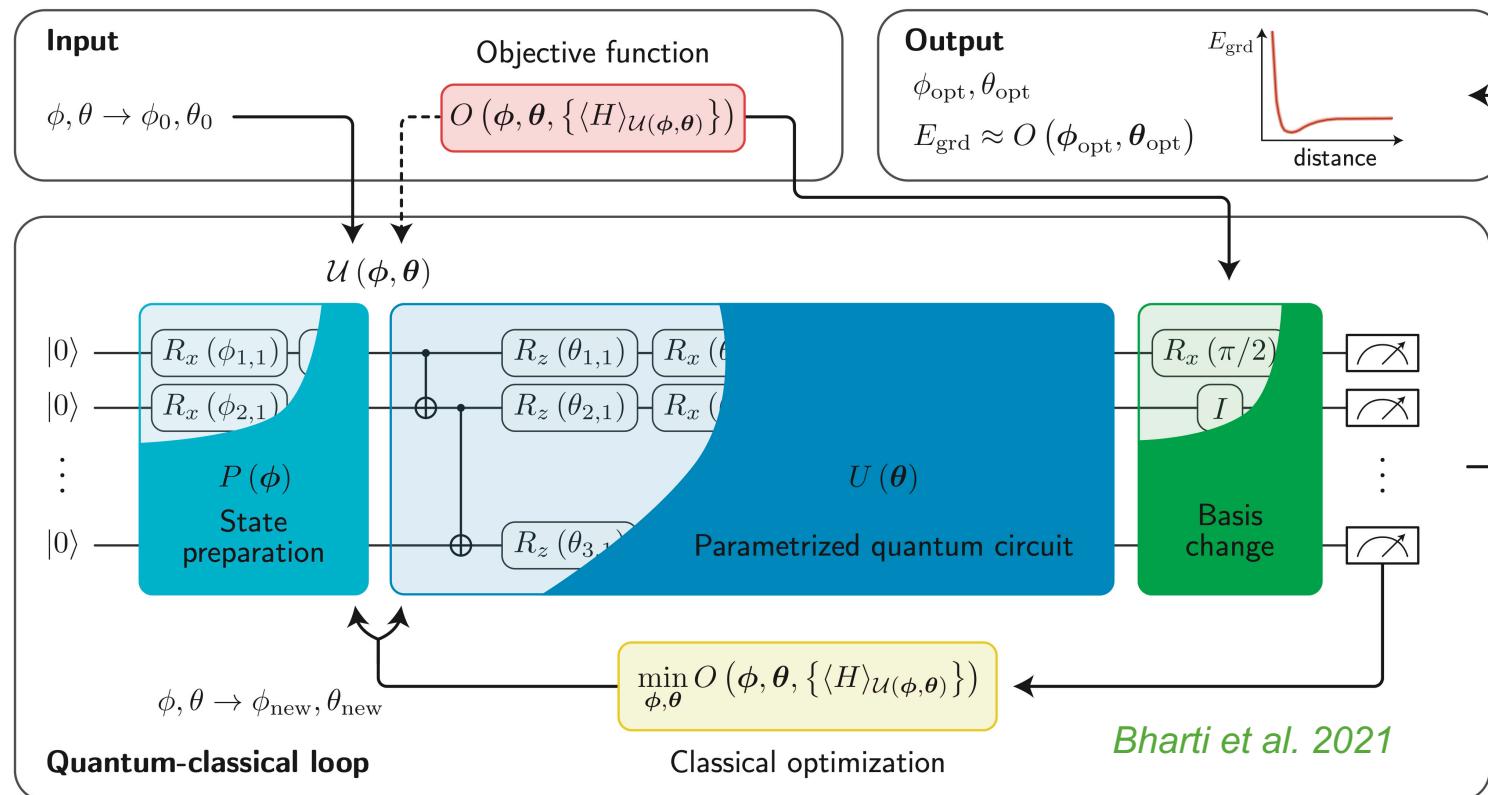
- Quantum qubit: Quality \rightarrow Quantity
- Research: Academia \rightarrow Industry + academia
- Computing style: CPU \rightarrow QPU & heterogeneous computing
- Algorithm: Theoretical design/proof \rightarrow Variational algorithms
- Noises: Quantum error correction \rightarrow Noise resilience



Variational quantum algorithms (VQA) I



VQA framework



Hybrid quantum-classical algorithms

- Parameterized quantum circuits
- **Quantum** gates with tunable parameters optimized by **Classical** optimization
- Benefit from ideas in **Deep learning**
- Wide applications w/ various challenges
- E.g. Variational Quantum Eigensolver (VQE) for ground state energy

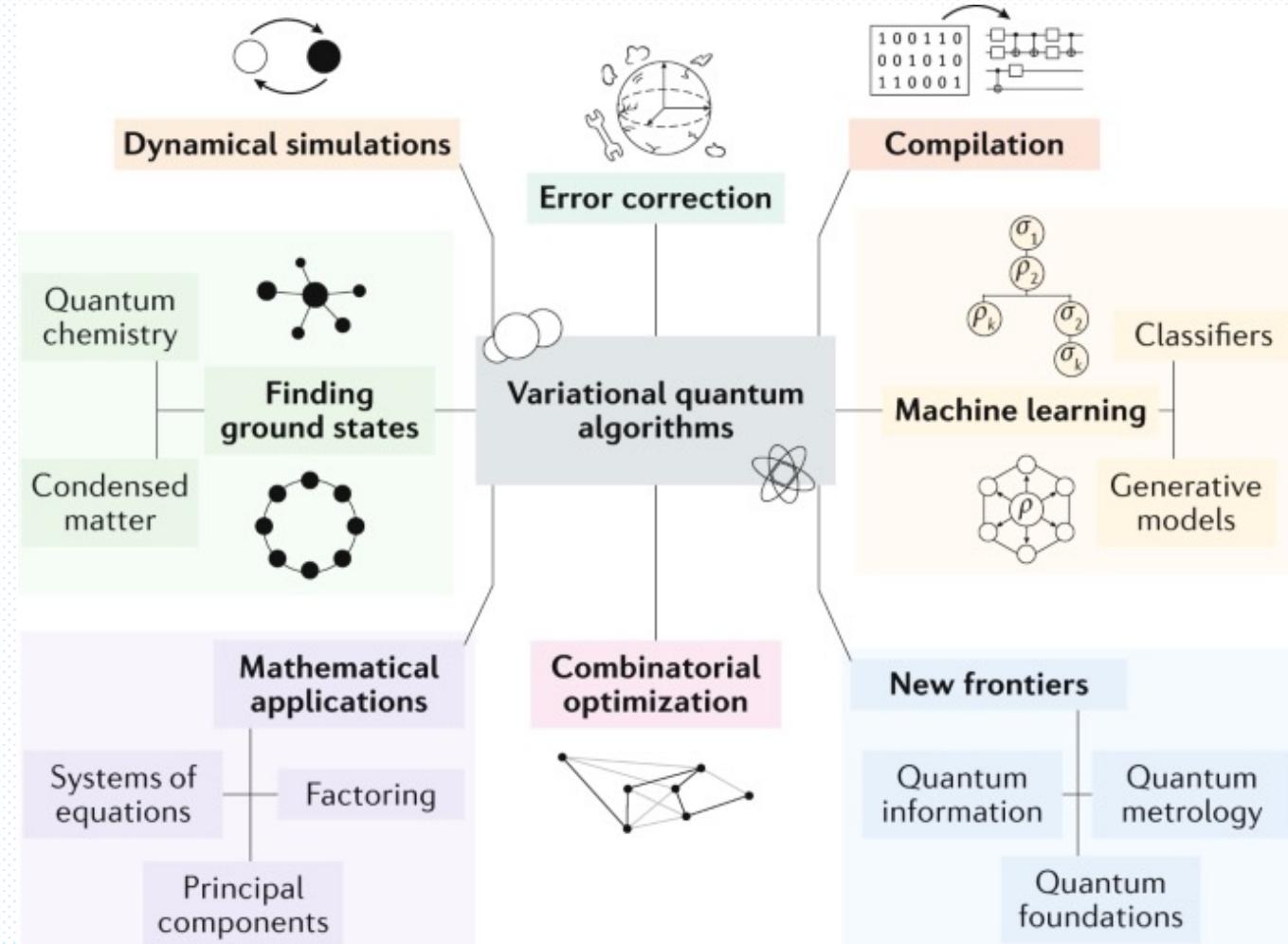
Bharti et al. 2021



Famous algorithms

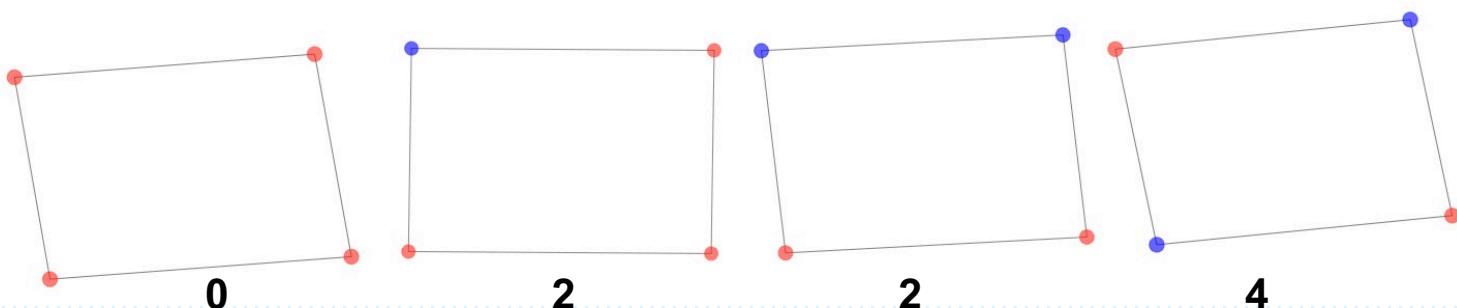
- Variational Quantum Eigensolver (VQE)
 - **Hardware-efficient ansatz (HEA)**
 - Unitary coupled clustered ansatz (UCC): lower complexity than the classical CC (Alt solution for efficient electronic structure)
- **Quantum Approximate Optimization Algorithm (QAOA)**: Approx. solutions for combinatorial optimization problems
- **Quantum Learning Algorithms (QML)**
 - Quantum SVM
 - Quantum PCA
 - Quantum NN...

Key applications of VQAs



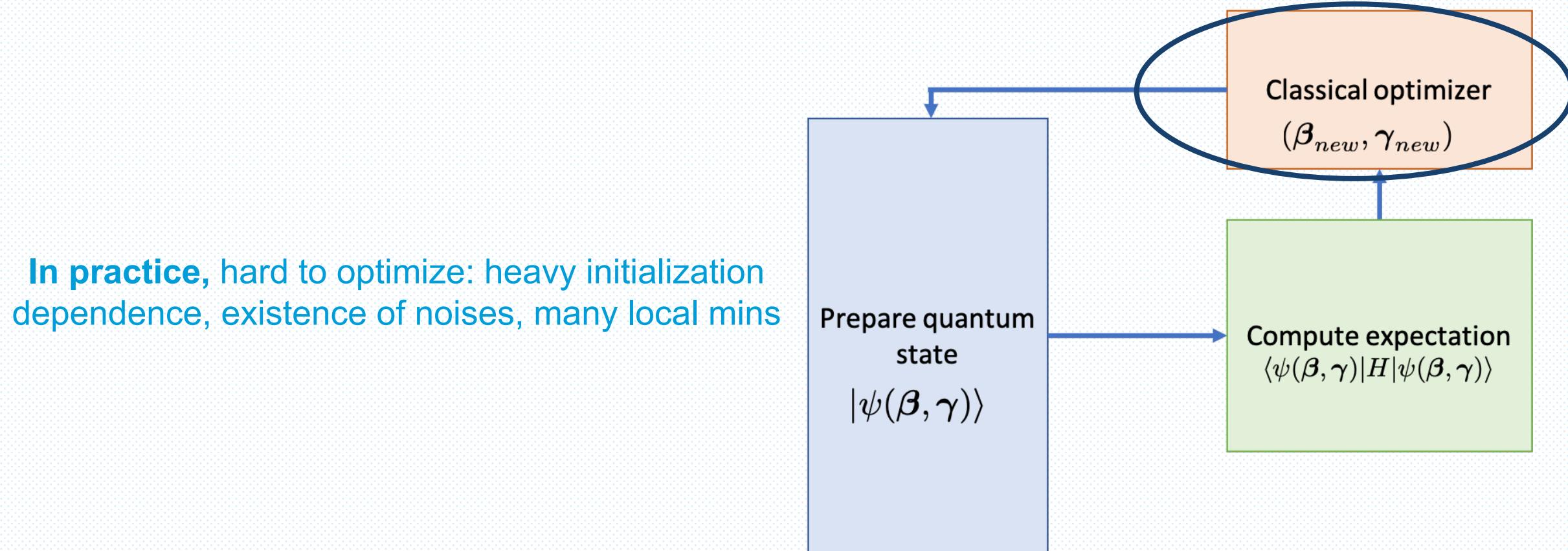


- Quantum Approximate Optimization Algorithm (QAOA)
 - Farhi et al. in 2014 (arXiv:1411.4028) $e^{i \sum_i \beta X_i} e^{i \gamma \sum_{ij \in E} Z_i Z_j} |+\rangle^{\otimes n}$
 - Only known quantum approximation algorithm framework
 - Generic framework for discrete optimization problems , suitable for near-term device
- Max-cut: partitioning nodes of a graph into 2 sets, max # of edges b/w sets
 - Example: how to partition a 4-node unweighted graph (red 0 or blue 1)
 - Convert to string lists: 0000, 1000, ... $2^n = 16$ combinations, exp increase w/ nodes n
 - Objective $C(\mathbf{z}) = \sum_{ij} w_{ij} z_i z_j$, Binary-valued variables \mathbf{z}



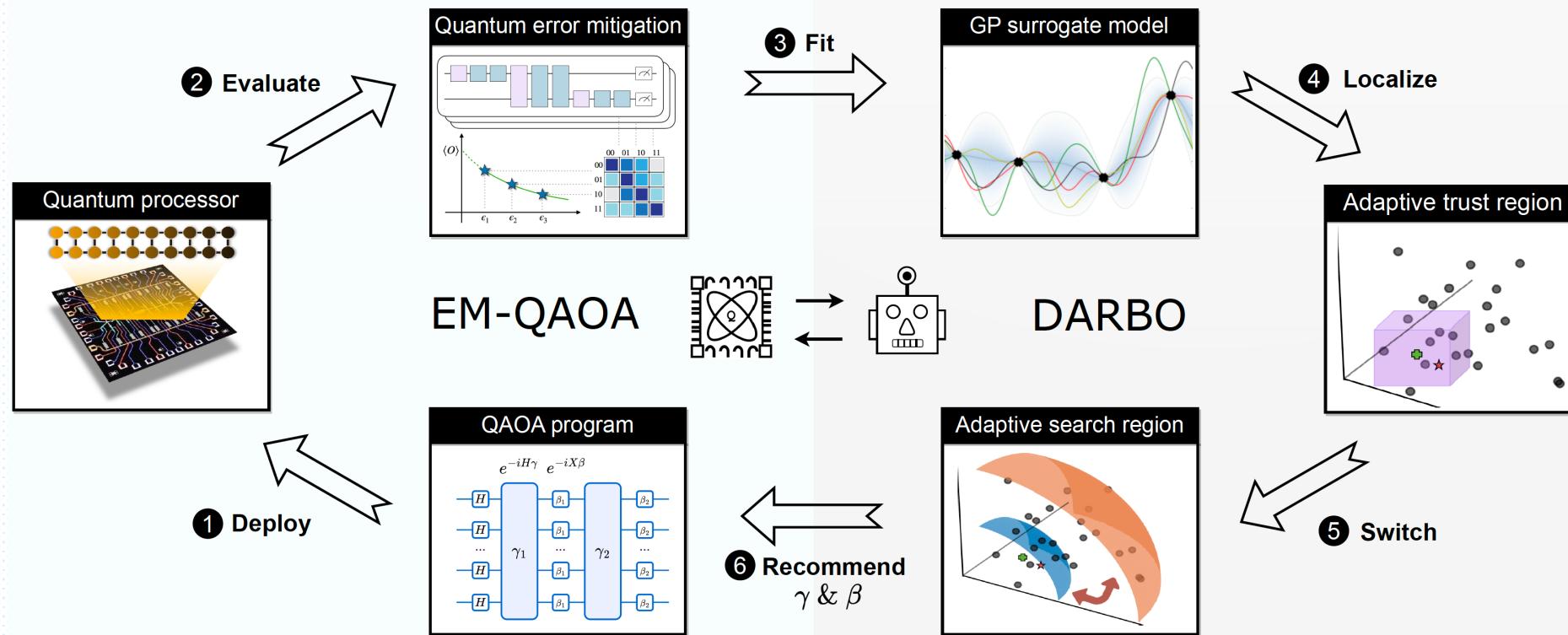


Usually Adam, COBLYA, SPSA



In practice, hard to optimize: heavy initialization dependence, existence of noises, many local mins

Targeting the optimization step: ML to replace classical optimizers



- EM (or QEM): Quantum error mitigation. Helps to reduce the effects of the gate noises in the measurements & get more accurate readouts
- DARBO: Double adaptive-region Bayesian optimization, inspired by TuRBO by Eriksson et al

L. Cheng*, Y.Q. Chen*, S.X. Zhang, S. Zhang. Error-mitigated Quantum Approximate Optimization via Learning-based Adaptive Optimization, arXiv: 2303.14877. Submitted to Nature Physics



- Overview of TuRBO

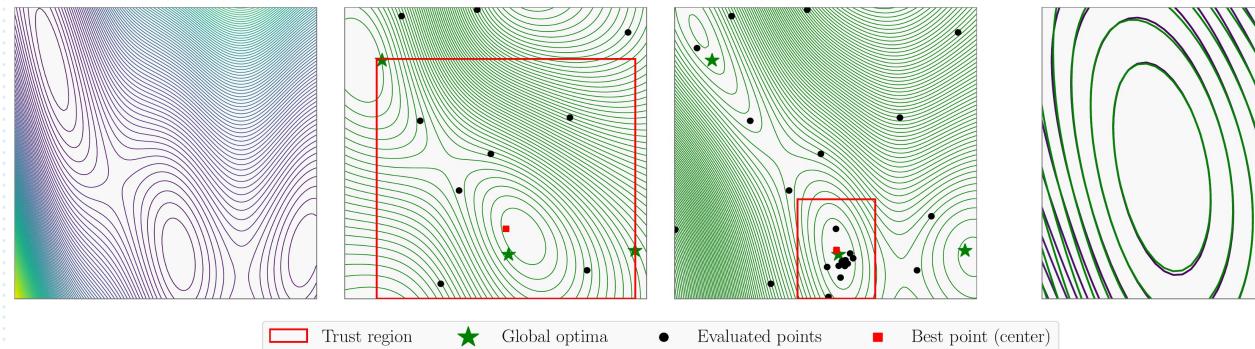


Fig from Eriksson et al, 2018

Trust region (TR) & update TR

- TR: sphere/polytope centered at current best solution
- TR is updated as the BO goes

Benefit of local modeling

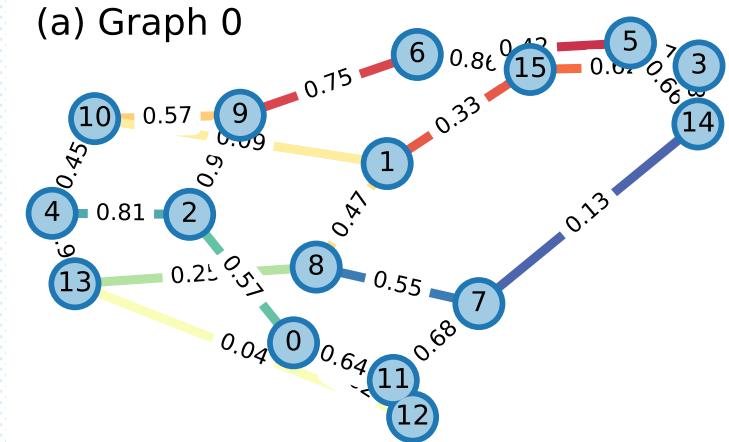
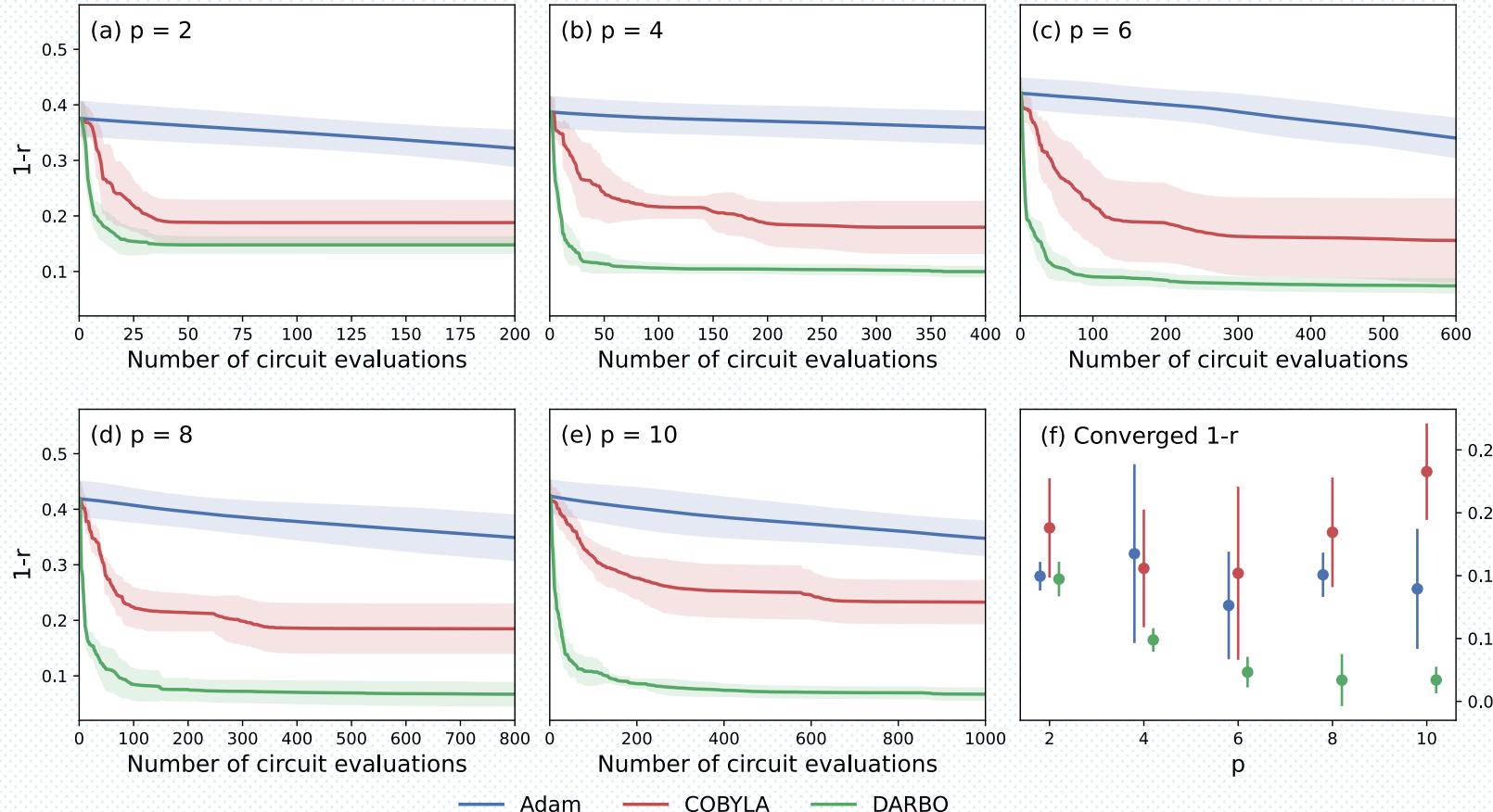
- Local GP is more accurate for heterogeneous functions
- Only suggest points within TR where GP is accurate

Our modified approach--DARBO: Inspired by heuristics on QAOA (Zhou et al, PRX, 2020) & multi-TR idea

- Optimized parameters $\beta_i \in \left[-\frac{\pi}{4}, \frac{\pi}{4}\right], \gamma_i \in [-\pi, \pi]$ for wdR graphs according to symmetries.
- Adaptive trust region: provides a more precise surrogate model around the best solution
- Adaptive searching region: constrains the candidate parameter sets temporarily by switching b/w the restricted search space and the full search space.



Optimization results on different graphs



Test on 5 randomly generated regular-3 graphs with 16 nodes (qubits) & 24 edges

$F_p(\gamma, \beta)$: The loss function QAOA has (we are optimizing)

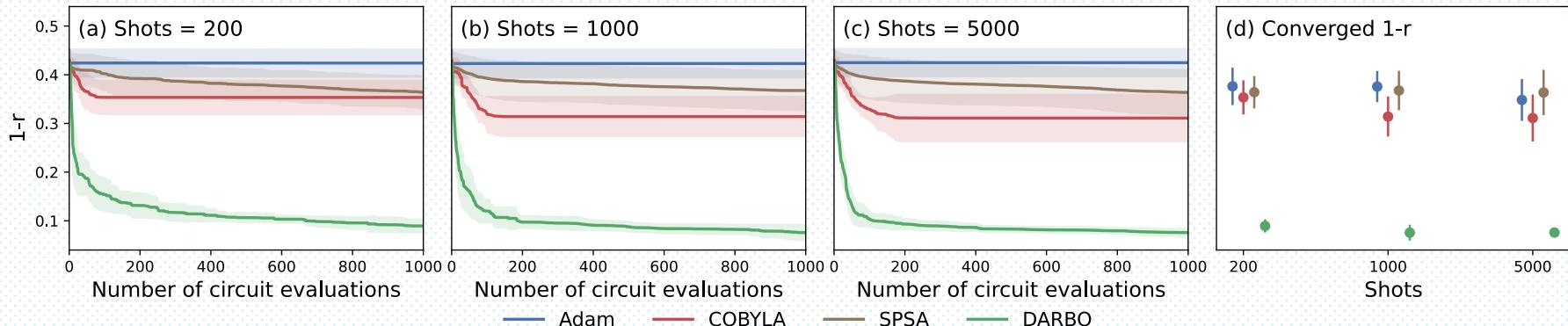
$$\text{Approximation ratio } r = \frac{F_p(\gamma^*, \beta^*)}{C_{\max}} (\gamma^*, \beta^*) = \operatorname{argmax} F_p(\gamma, \beta)$$

Evaluations: Gradient based method requires to use numerical gradients as quantum resource costs (though we use auto-differentiation in simulator)

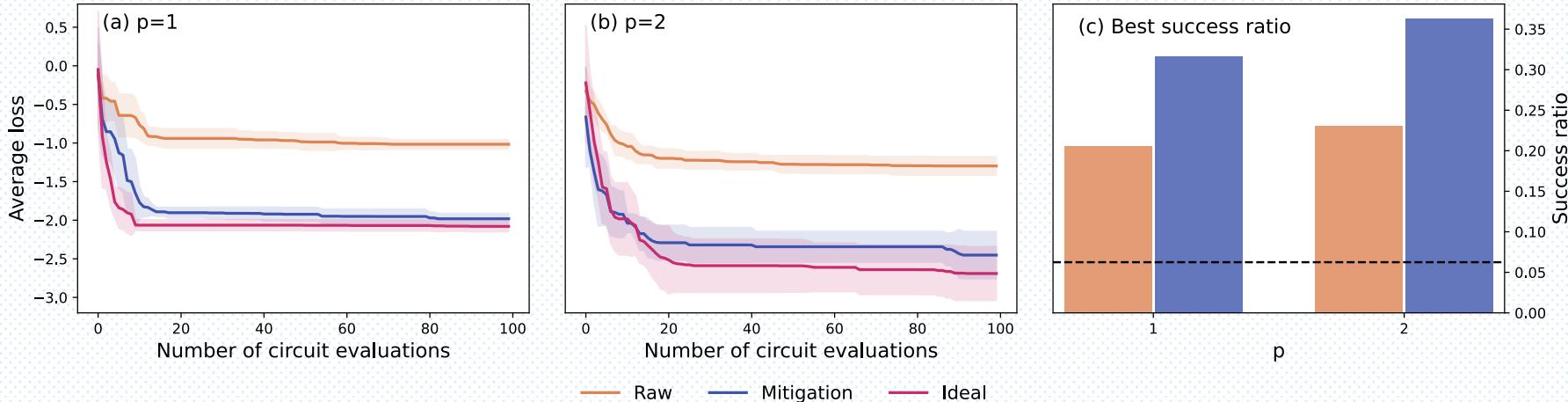


Optimization with noisy data

Shot noises (from simulator)



Gate + shot noises (from superconducting quantum device)



- ✓ Gradient free: more friendly to quantum computer (no autograds in reality)
- ✓ Less dependence of initialization: Initialization parameters affect the QAOA final answer a lot
- ✓ Fewer evaluations/faster convergence than Gradient decent (eg Adam)
- ✓ Nearly no hyperparameter tuning vs many tricks in learning rate schedule design for Adam
- ✓ Great performances with the presence of noises



Applications of Quantum Computing



Disruptive applications across major sectors



Chemicals

Molecular modelling of chemical process (for example, nitrogenase) using quantum simulations

Impact: low-cost and low-energy industrial production



Pharma

Simulation of complex organic molecules

Impact: accelerated drug development and approval through expanded use of simulation



Finance

Solve hard combinatorial optimization problems

Impact: improved efficiency in portfolio optimization and risk management



Aerospace

Real-time optimization of commercial aircraft speed and fuel consumption

Impact: step-change in the industry's sustainability performance



Automotive

Live traffic-routing system, accurate to the millisecond

Impact: more efficient traffic flow



Climate

More accurate climate models that better mimic real-world conditions

Impact: revolution in carbon capture technology
development of novel materials (for example, energy-efficient "exciton condensate")



Materials

Materials' property and behavior predictions with quantum-mechanical simulations



ICT

Optimization of machine learning algorithms through quantum-enhanced deep learning

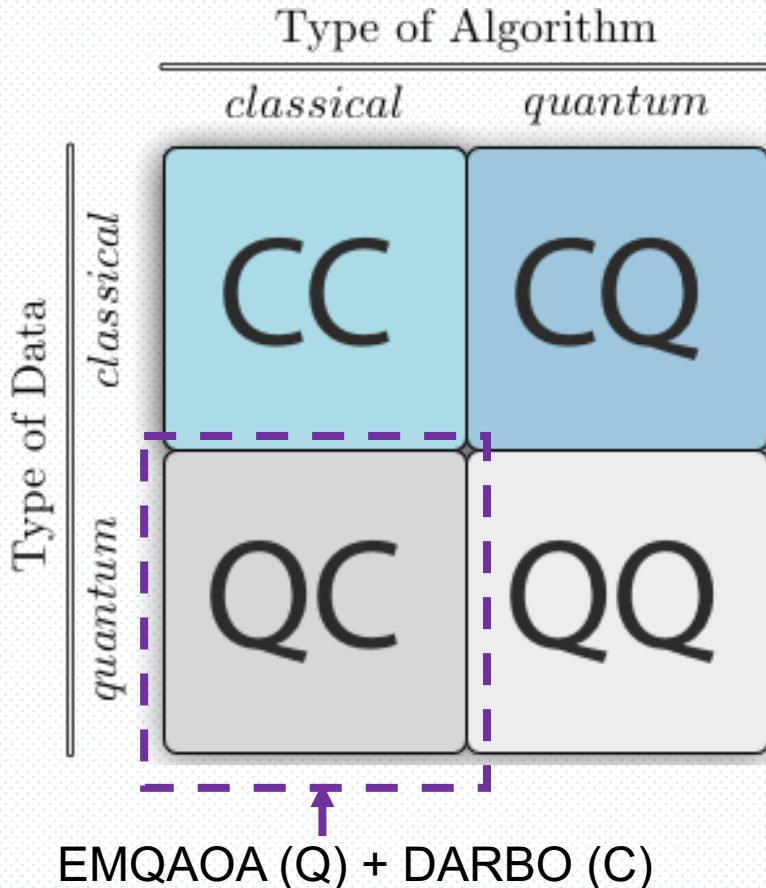
Impact: expanded applicability of neural networks



Quantum Machine Learning (QML)



Quantum machine learning: integration of quantum algorithms within ML programs



CC: Traditional ML

CQ: Generic QML, e.g. Q-SVM, Q-NN, ...

QC: Also known as ML of quantum systems

QQ: Pretty challenging, given CQ & QC are still not well-studied

Quantum data:

- Noisy data from real quantum measurements
- Simulated data (e.g. quantum properties of molecules and materials)
 - MOB-ML
 - PauliNet
 - ...

My role: Bridge physicists & computer scientists + Discover new directions for AI4Sci

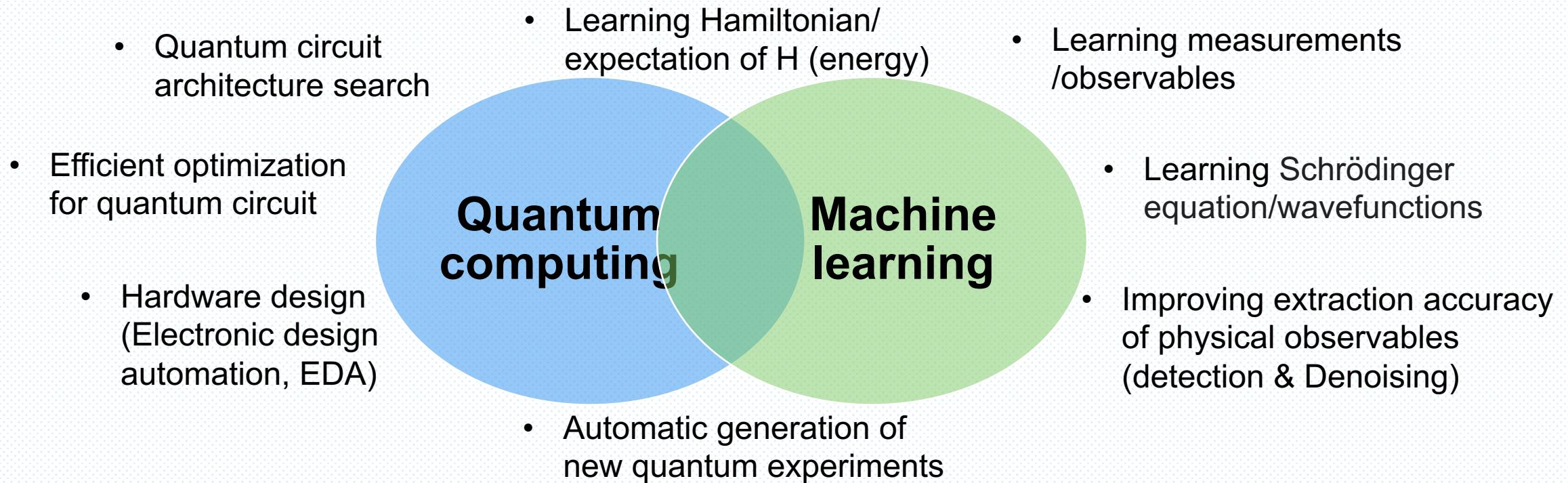
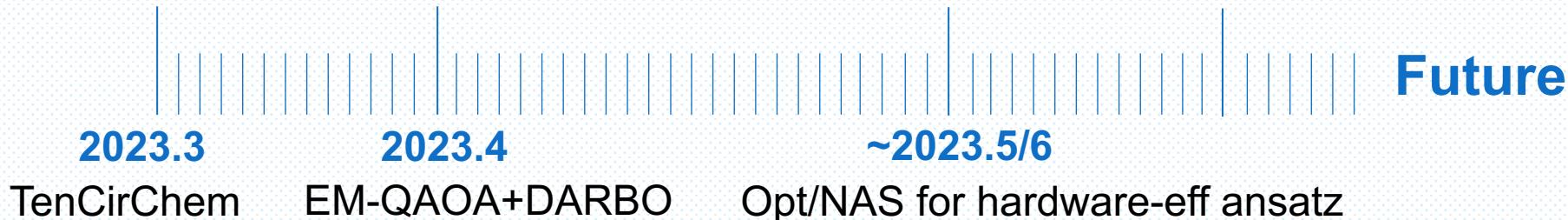
Current focus: QC type QML (ML in physics)



Future research directions on QML



Many things to be explored



AI4Sci Edu & QC software



1

AI4Sci education organization

2

Quantum computing +
quantum chemistry software:
TenCirChem





Education of AI for science



- Several nice studies on how AI can contribute to science education
- No systematic studies/guidelines on how we could cultivate next generation researchers in AI4Sci (No awesome-xxx on github). Huge number of publications to read.
- Hard to educate AI4Sci—Mind gaps are huge: my 2-yr high-school edu exp as an example

AI4Sci education initiative: Open, collaborative & supportive organization to provide more systematic study guidelines & most recent info on AI4Sci

Seeking collaborators. Please join us & contribute!

 **AI4Sci Education for Next Generation**

Goal: 1. Break the knowledge barriers for scientists from different fields 2. Share study guides on AI4Sci for better next generation education

21 followers <https://ai4sciedu.github.io/> sherryliuxuecheng@gmail.com

Unfollow

Overview Repositories 2 Discussions 2 Projects 2 Packages 2 Teams 2 People 4 Settings

README.md

Hello world 🌟

We are AI4Science Education Org. We hope to provide a platform to boost the outreach and training for next generation AI4Science researchers and fans. Please join us for better sciences and education!

Contribution guidelines: We will have complete contribution guidelines soon! (2023.4 version)

Useful resources: More resources will come soon! Plan to include suggested readings, learning paths, nice repos, and awesome previous papers/studies. Please stay tuned!

Communities in AI4Sci field: Microsoft AI4Science Lab, AI4Sci community, Machine Learning for Science, AI4Sci talks, AI4Sci Lab-Amsterdam, AI4Science101...

please feel free to add more!

View as: Public ▾ You are viewing the README and pinned repositories as a public user.
You can pin repositories visible to anyone.
You can hide the tasks we've suggested on this page and bring them back later.

Top discussions this past month

Discussions are for sharing announcements, creating conversation in your community, answering questions, and more.

Start a new discussion

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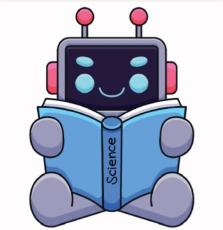
AI4Sci Education Organization

AI4Science Education organization, aiming to facilitate better education for AI4Sci

This is the home page for [AI4Science Education GitHub organization](#). We are welcome any new members and contributors to join this organization!

The goal is to share study materials, learning experiences, & useful information to facilitate better education in AI4Sci & break the knowledge barrier in AI4Sci community, i.e., Science knowledge for Computer Scientists and CS knowledge for scientists.

If you have interests, please join us at [Slack](#) and [GitHub](#) (send github user name to [Dr. Sherry Liuxue Cheng](#) or contact via [Sherry's email](#))



news

Apr 18, 2023 AI4Science Education Organization is found! Welcome! ✨ 😊





First repo: Awesome AI for chemistry



AI4Sci education initiative: Open, collaborative & supportive organization to provide more systematic study guidelines & most recent info on AI4Sci



Join & Contribute

<https://github.com/AI4SciEdu>

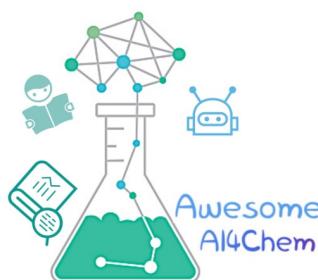


Slack

<https://github.com/sherrylixuecheng/awesome-ai4chem>

Awesome AI for Chemistry

AI4Sci Edu related repo. Still under construction🚧👩‍💻



A list of awesome AI for chemistry papers. Inspired by the "Awesome" branded repositories in Computer Science. Please feel free to contribute and help to improve the quality of this page.

Reviews

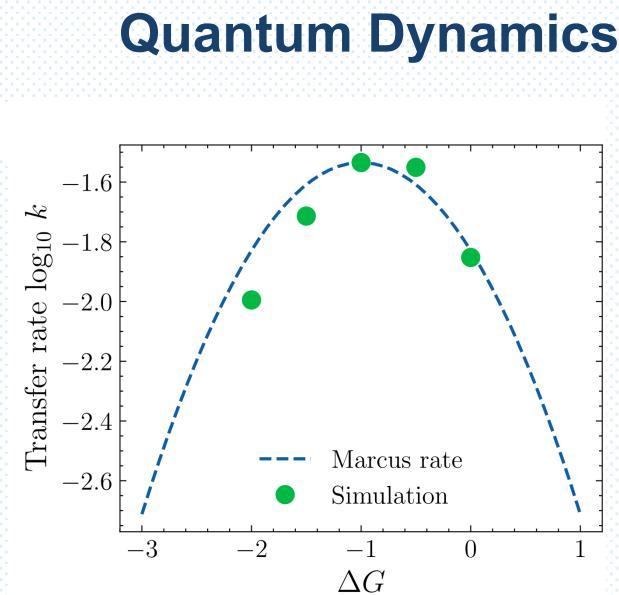
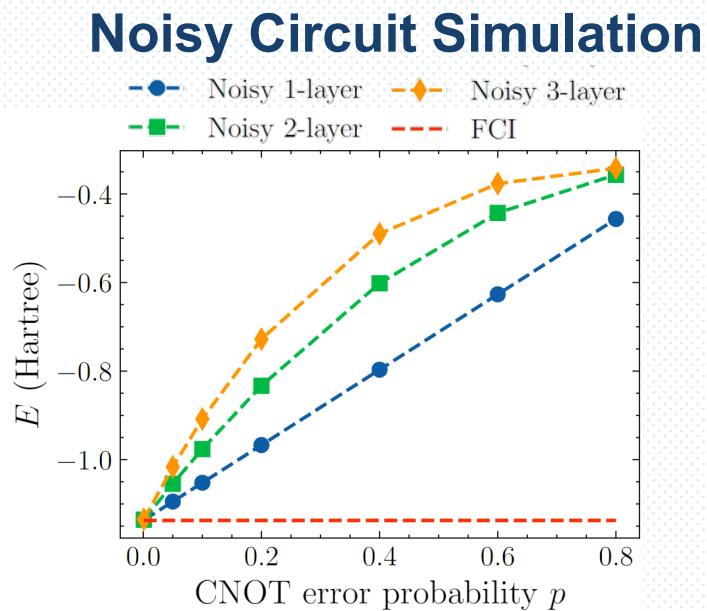
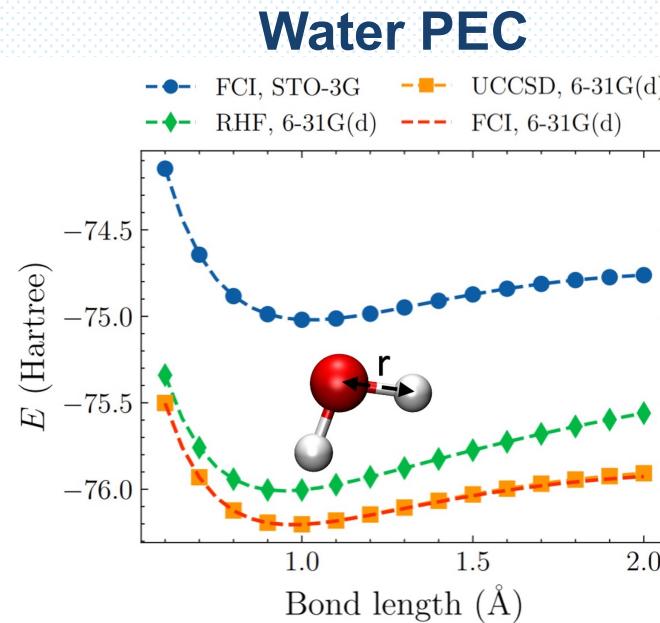
Note: We will try to provide both the most influential/comprehensive reviews and the most recent/updated reviews. The list will be updated timely manner.

1. [Roadmap on Machine learning in electronic structure](#). H. J. Kulik, T. Hammerschmidt, J. Schmidt, S. Botti, M. A. L. Marques, M. Boley, M. Scheffler, M. Todorović, P. Rinke, C. Oses, A. Smolyanyuk, S. Curtarolo, A. Tkatchenko, A. P. Bartók, S. Manzhos, M. Ihara, T. Carrington, J. Behler, O. Isayev, M. Veit, A. Grisafi, J. Nigam, M. Ceriotti, K. T. Schütt, J. Westermayr, M. Gastegger, R. J. Maurer, B. Kalita, K. Burke, R. Nagai, R. Akashi, O. Sugino, J. Hermann, F. Noé, S. Pilati, C. Draxl, M. Kuban, S. Rigamonti, M. Scheidgen, M. Esters, D. Hicks, C. Toher, P. V. Balachandran, I. Tamblyn, S. Whitelam, C. Bellinger, & L. M. Ghiringhelli, *Electronic Structure* **4**, 023004 (2022)
2. [Machine learning for molecular and materials science](#). K. T. Butler, D. W. Davies, H. Cartwright, O. Isayev, & A. Walsh, *Nature* **559**, 547–555 (2018)
3. [Four generations of high-dimensional neural network potentials](#) J. Behler, *Chemical Reviews* **121**(16), 10037–10072 (2021)
4. [Inverse molecular design using machine learning: Generative models for matter engineering](#). B. Sanchez-Lengeling, & A. Aspuru-Guzik, *Science* **361**(6400), 360–365 (2018)



Next-gen quantum chemistry software: TCC TenCirChem

- TenCirChem: Native hardware acceleration, auto-differentiation and just-in-time compilation
- Rich features: UCC and HEA ansatz, noisy circuit simulation and variational quantum dynamics
- Highly optimized UCC code enables UCCSD calculation of H₁₆ in one day on a single GPU card.



- Based on UCCSD/6-31G(d), with only the 1s of O frozen, corresponding to 34 qubits.
- Equilibrium bond length error as small as 0.01 Å.

- Based on the R_y ansatz with 2 qubits for the energy of H₂ in STO-3G basis set.
- The optimized energy increases with circuit depth because of the gate noise.

- Based on the Marcus model and variational quantum dynamics for the charge transfer rate.
- The rate increases then decreases with the driving force ΔG , consistent with the Marcus theory.



UCCSD ansatz performances



System & Circuit	Example Molecule	TenCirChem	Qiskit	PennyLane	Tequil a	HiQ
H ₄ (8 qubits) circuit depth: 78 parameters: 11	LiH	0.1 s	34 s	433 s	28 s	1.2 s
H ₆ (12 qubits) circuit depth: 462 parameters: 39	H ₂ O	0.4 s	943 s	9,954 s	2,141 s	15 s
H ₈ (16 qubits), circuit depth: 1,834 parameters: 108	N ₂	1.9 s	💀 Out of memory	💀 Out of memory	73,978 s (~1 day)	1,970 s
H ₁₀ (20 qubits), circuit depth: 5,586 parameters: 246	C ₂ H ₂	14 s	-	-	💀 Out of memory	121,836 s(~2 days)
H ₁₂ , (24 qubits), circuit depth: 13,917 parameters: 495	CO ₂	51 s	-	-	-	💀 > 1 month (est.)
H ₁₄ , (28 qubits), circuit depth: 30,428 parameters: 899	C ₂ H ₆	2,093 s	-	-	-	-
H ₁₆ , (32 qubits), circuit depth: 59,634 parameters: 1,520	CH ₃ CHO	50,909 s	-	-	-	-



Supporting functions in TCC



Functions	<u>TCC</u>	Qiskit	PennyLane	Tequila	MindQuantum	Q ² Chemistry
超大规模精确UCC						
高效能量梯度						
自动微分						
多种内置拟设						
计算约化密度矩阵						
活性空间近似						
激发态计算						
周期性体系计算						
MPS后端						
GPU支持						
带噪声模拟						
玻色子映射						
动力学模拟						

Full support

Partial support

No support



Acknowledgement



QML & software collaborators

Dr. Shengyu Zhang



Dr. Shi-Xin Zhang



Dr. Yu-Qin Chen



Dr. Weitang Li



MOB-ML collaborators

Prof. Thomas F. Miller III



Dr. Matt Welborn



Dr. Tamara Husch



Jiace Sun



Dr. Sebastian Lee



Dr. J. Emiliano Deustua

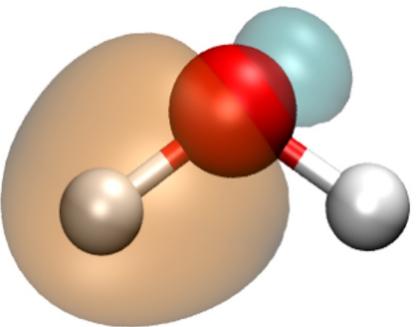


Caltech

Collaborators in NN+MOB-ML for DMC: Prof. Anne McCoy & McCoy group (U-Washington)

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- U.S. Department of Energy
- Caltech DeLogi Fund
- Camille and Henry Dreyfus Foundation
- NERSC



Thanks for your listening

Q & A

Any collaborations & Discussions are welcome