Classical Support and Error Mitigation for Variational Quantum Algorithms

Gokul Subramanian Ravi

Postdoc, University of Chicago

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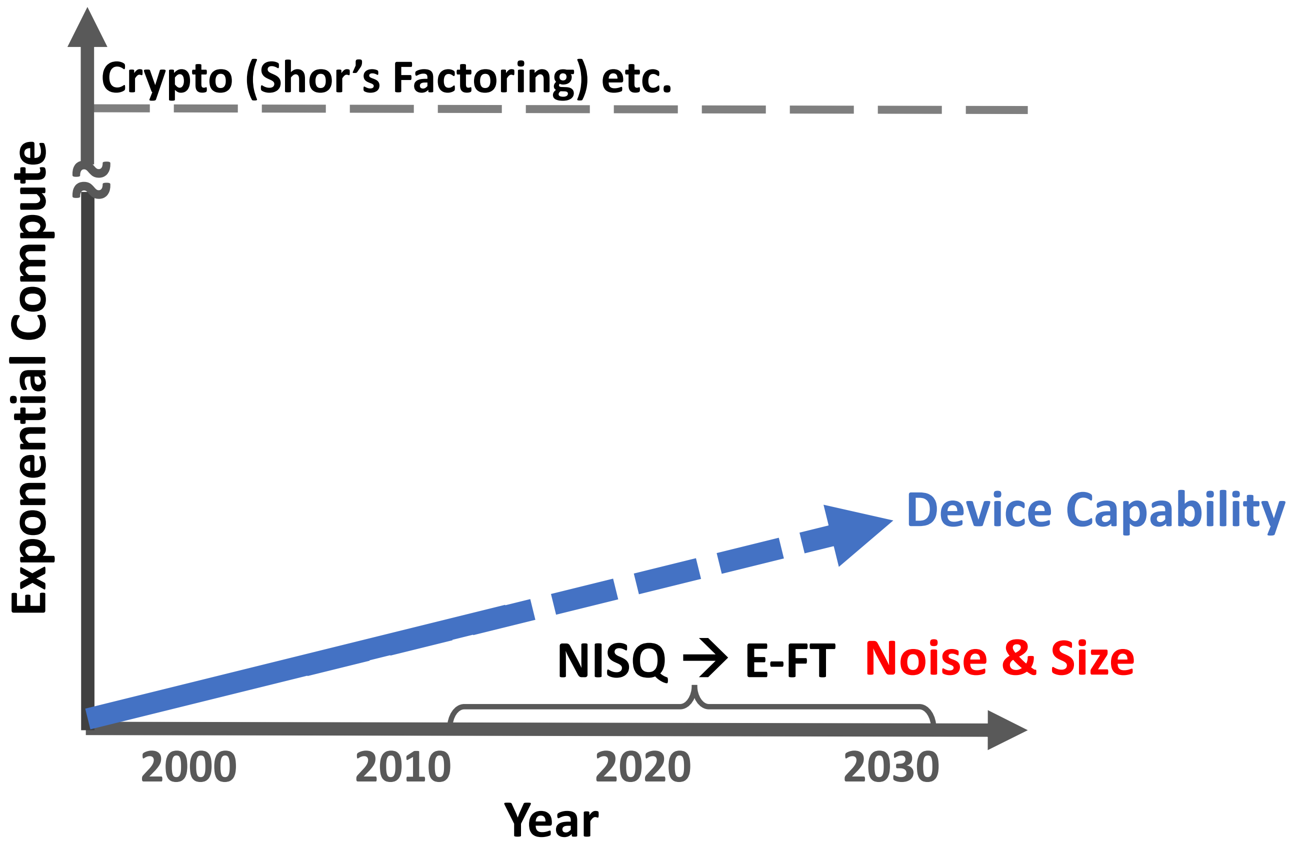
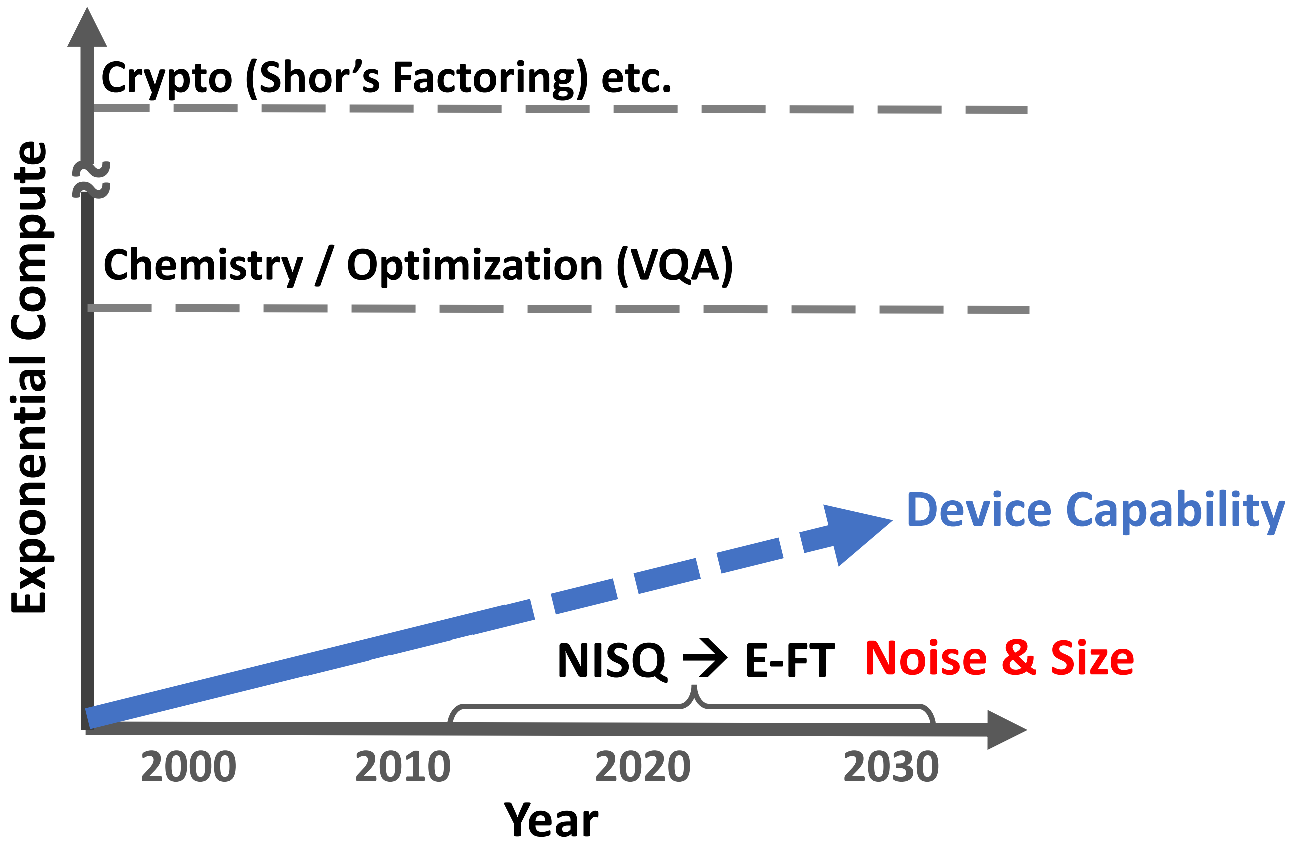
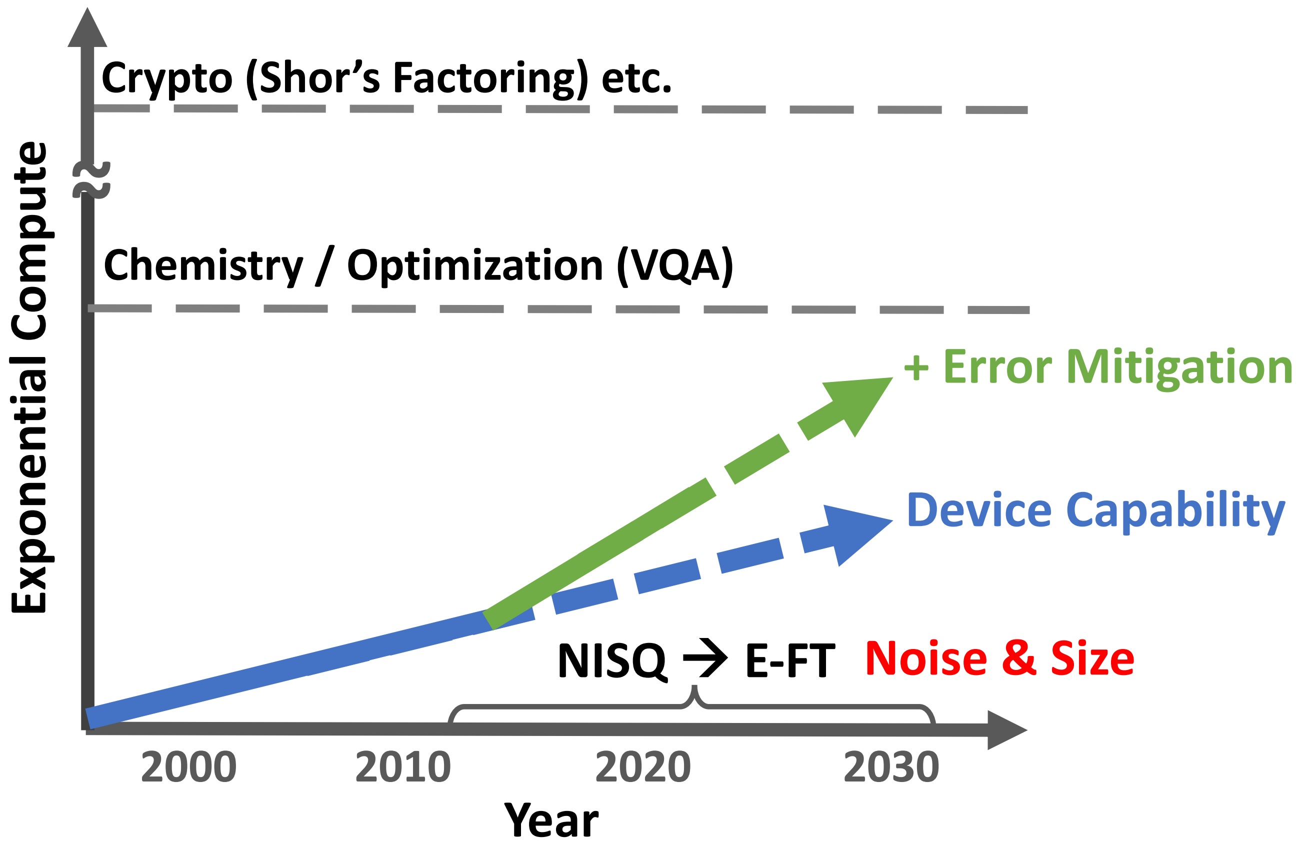
Advancing VQA Frontiers



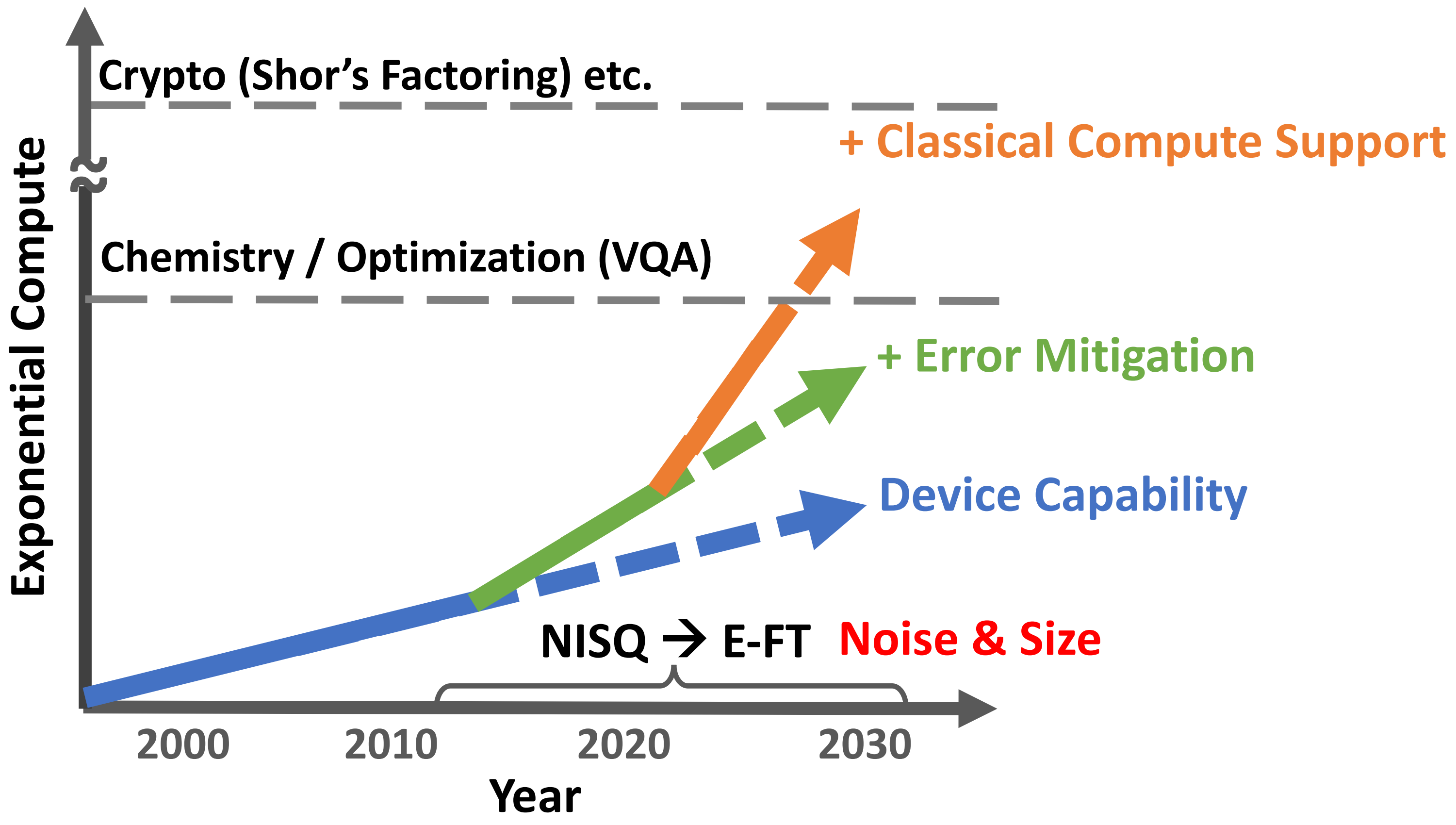
Advancing VQA Frontiers



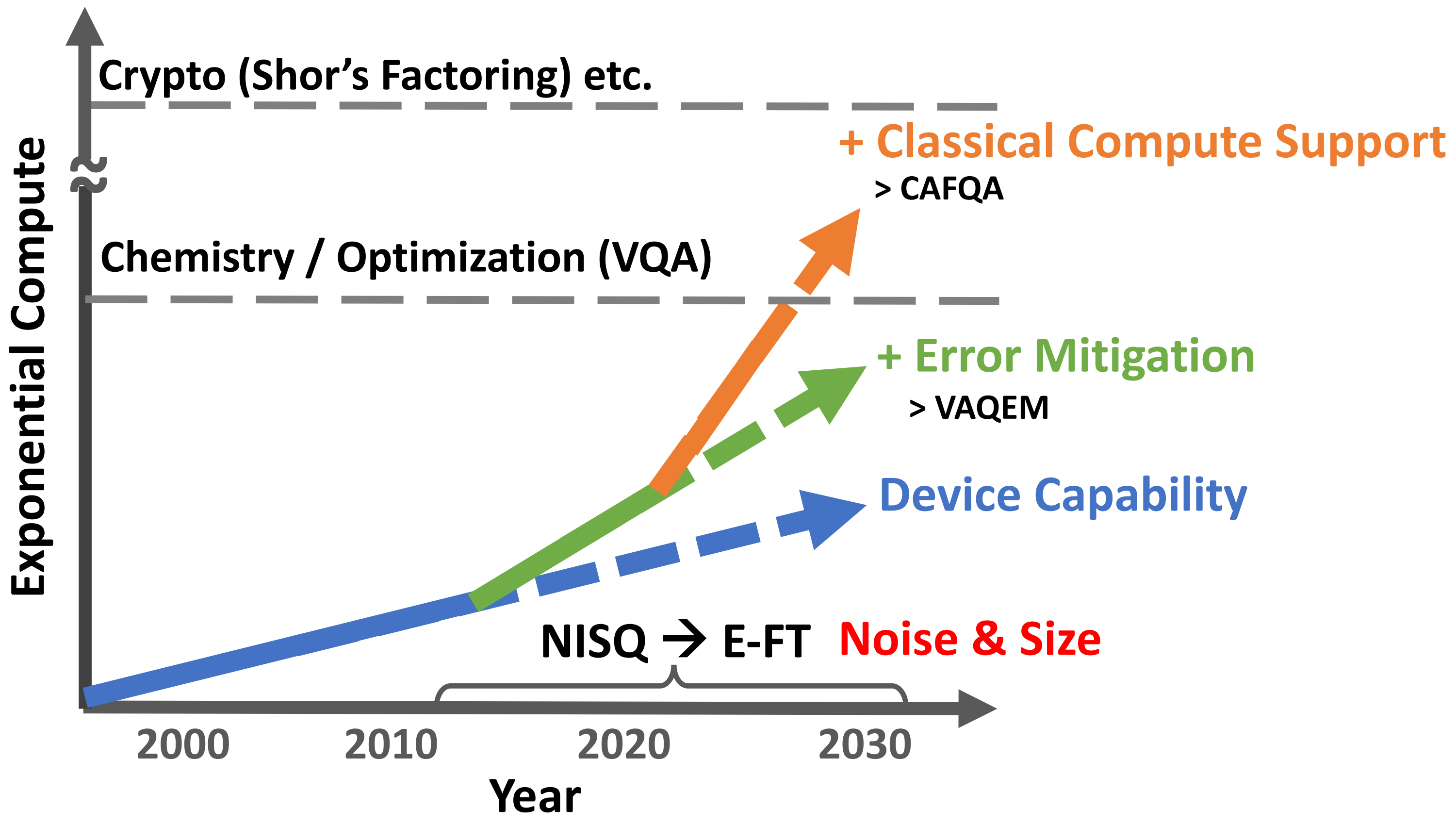
Advancing VQA Frontiers



Advancing VQA Frontiers



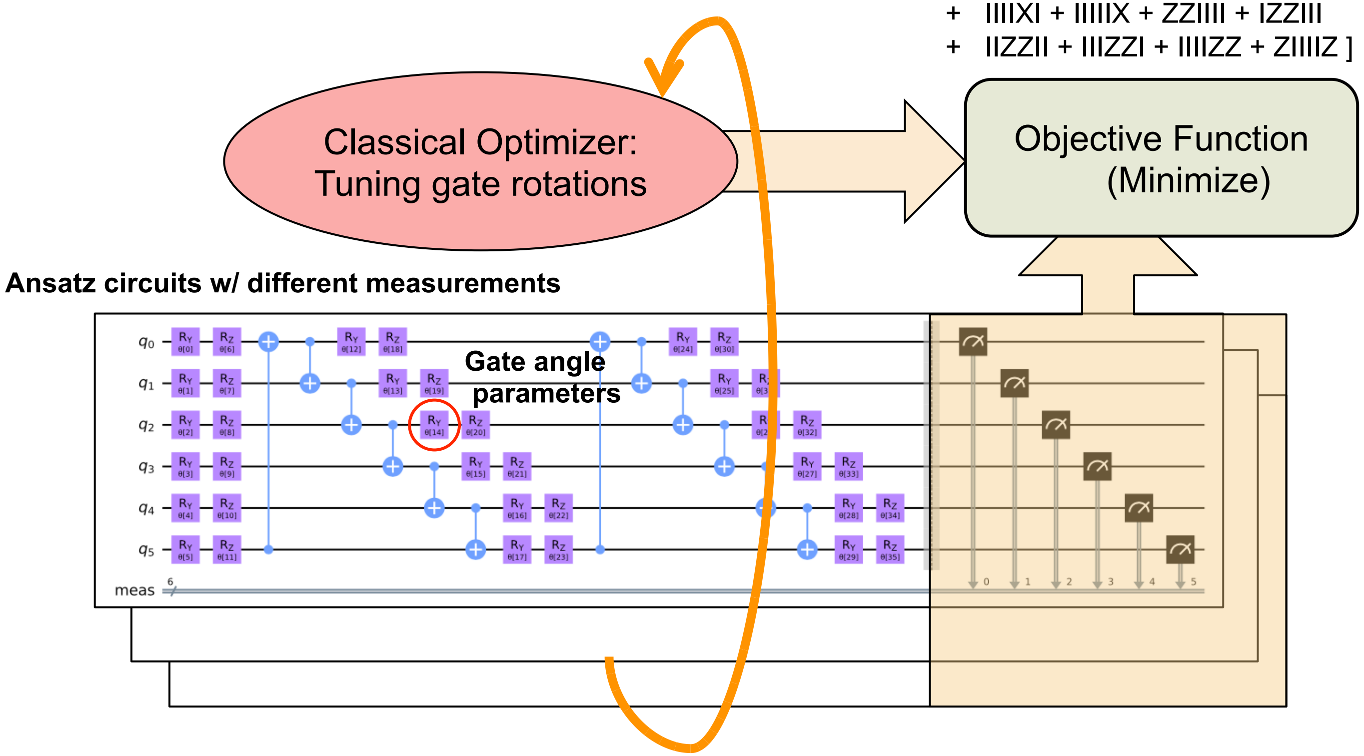
Advancing VQA Frontiers



VQA Overview

Variational Quantum Algorithms

Minimize:
H = [XIIIII + IXIIII + IIXIII + IIIXII
+ IIIIXI + IIIIIX + ZZIIII + IZZIII
+ IIZZII + IIIZZI + IIIIZZ + ZIIIIZ]

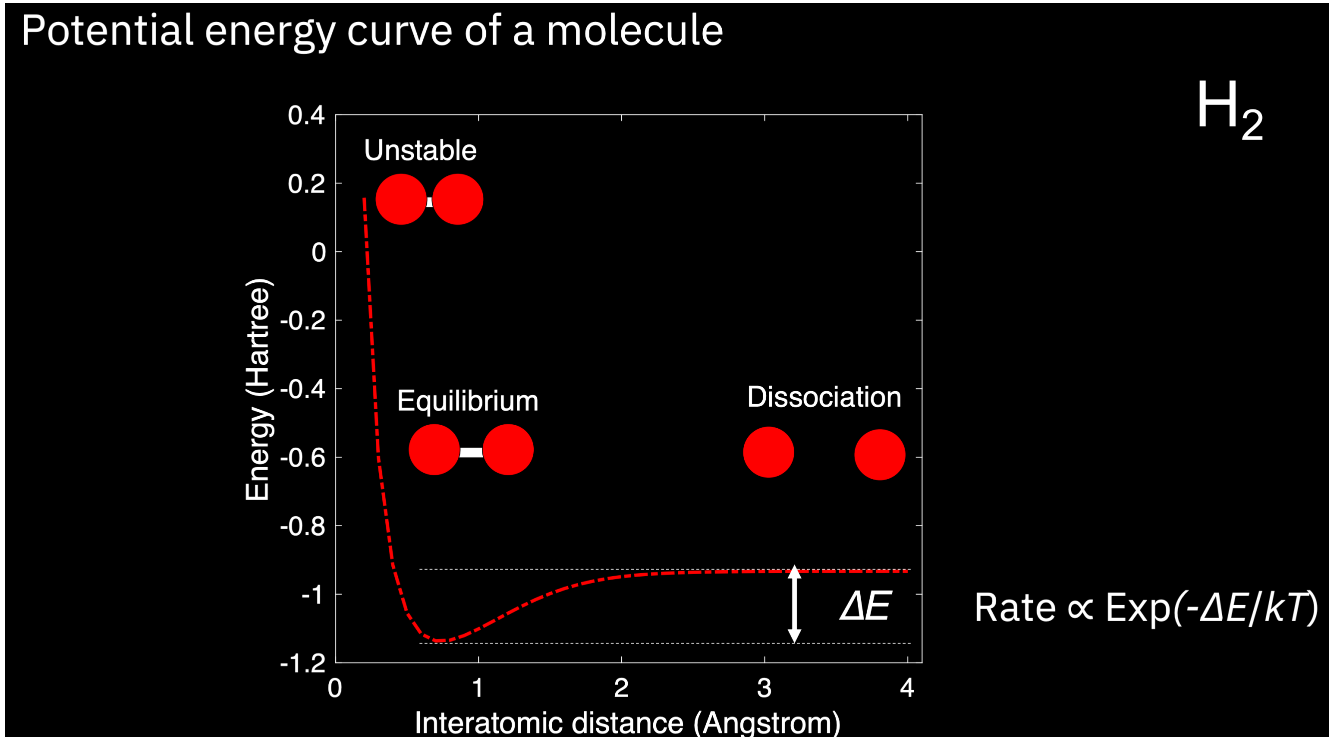


Variational principle: the energy of any trial wave-function is greater than or equal to the exact ground state energy

$$\frac{\langle \Psi(\vec{\theta}) | H | \Psi(\vec{\theta}) \rangle}{\langle \Psi(\vec{\theta}) | \Psi(\vec{\theta}) \rangle} \geq E_G$$

https://qiskit.org/learn/intro-qc-qh/

VQE for molecular chemistry



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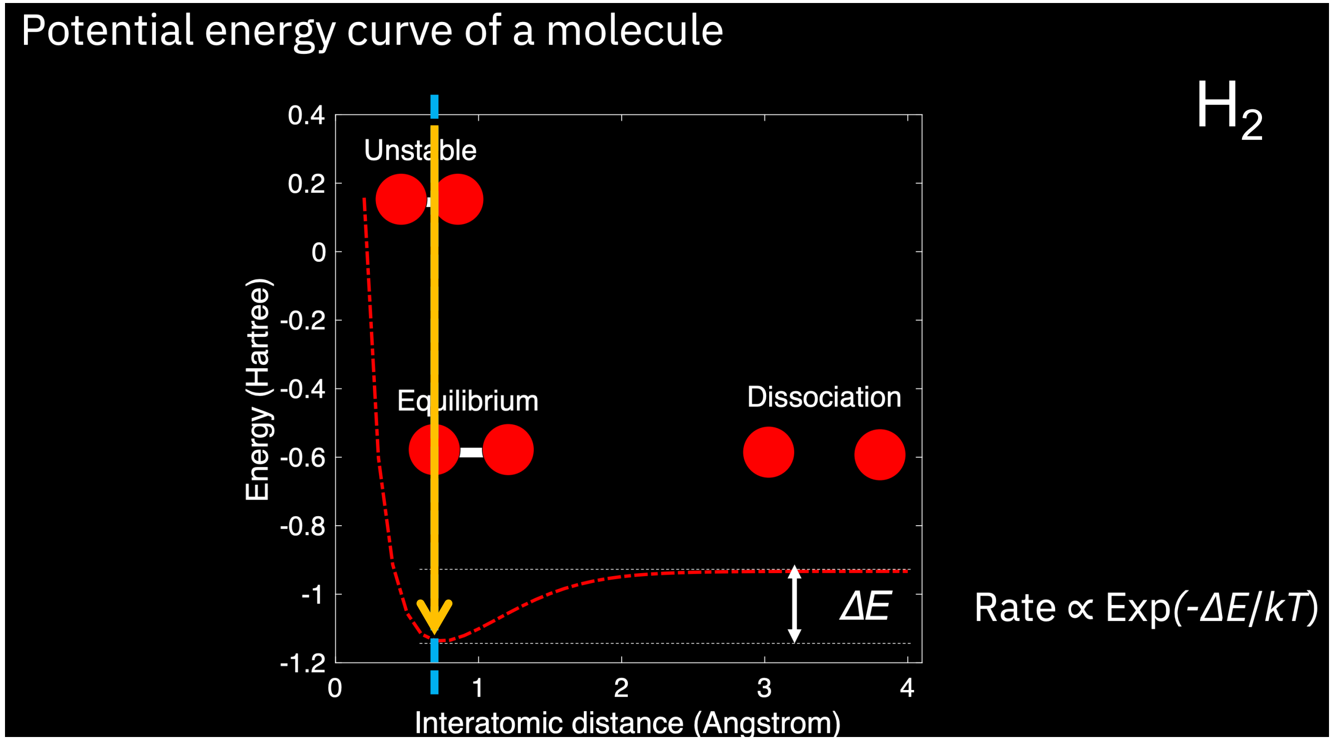
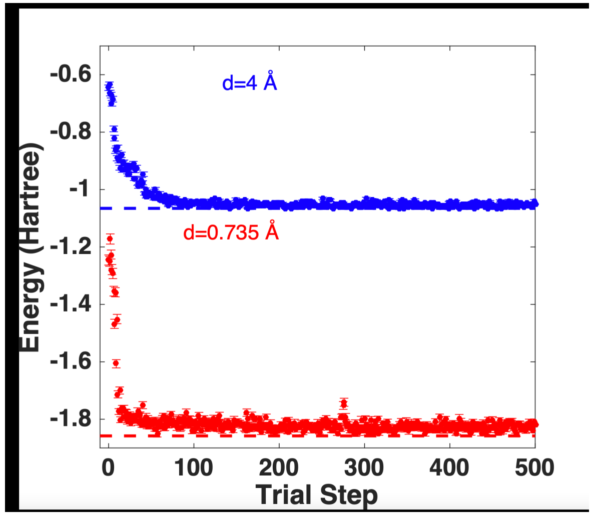
VQE for molecular chemistry





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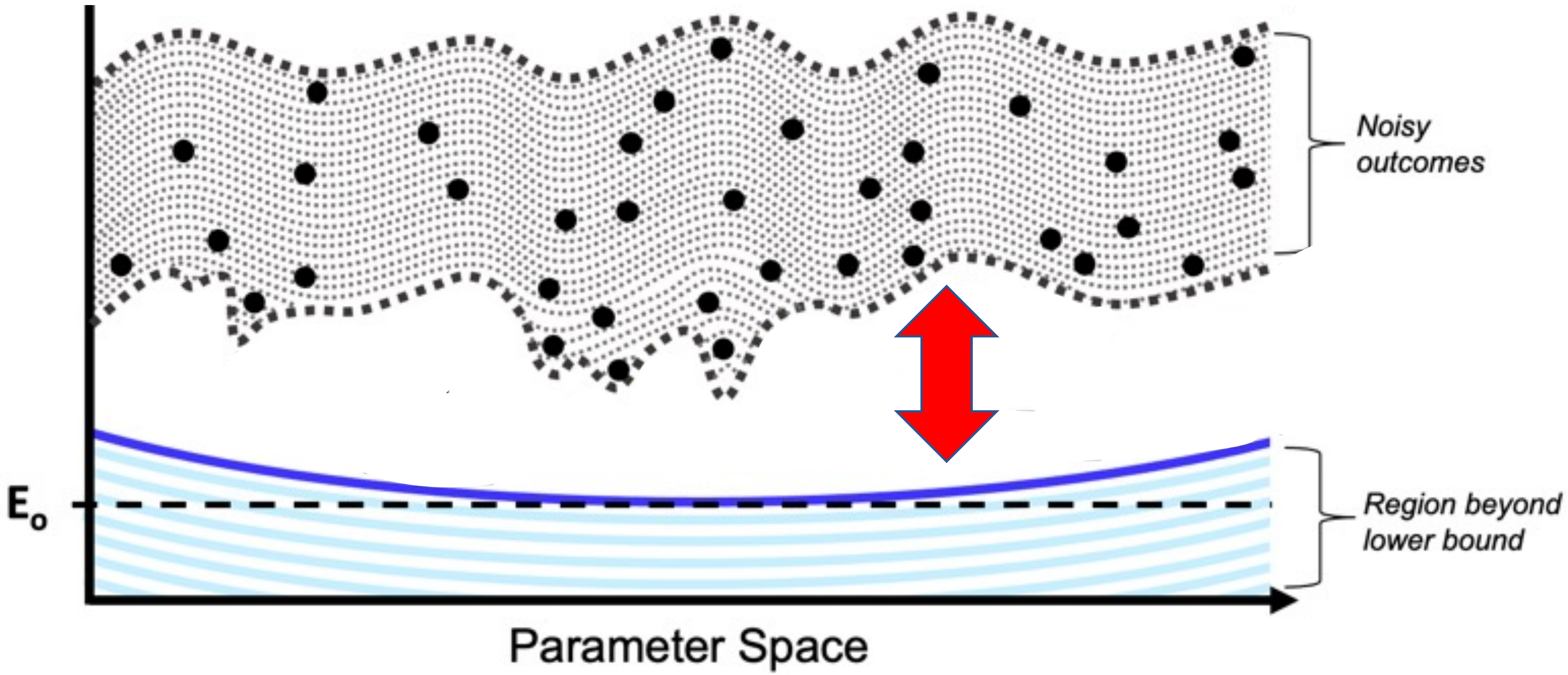
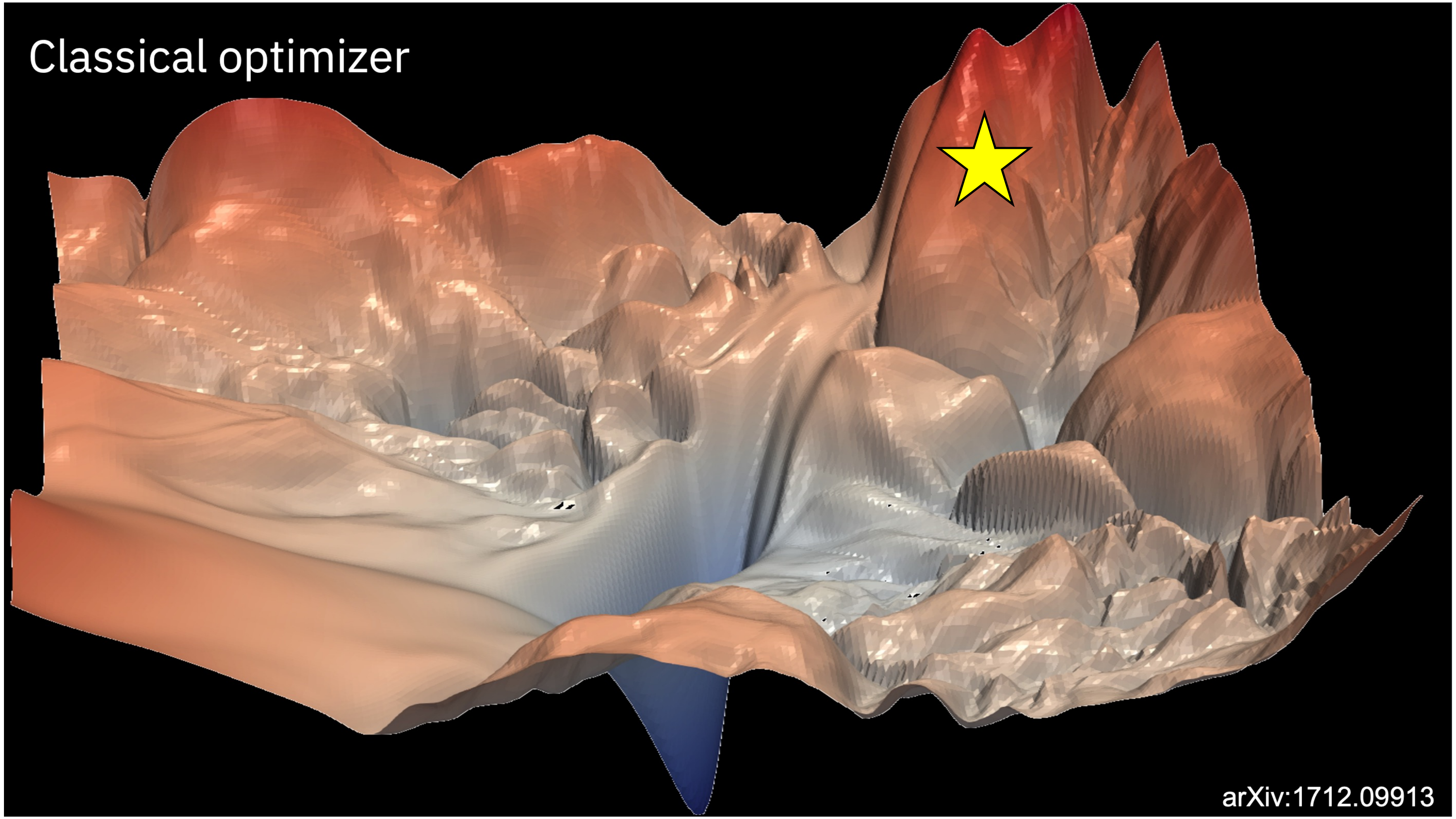
VQA Fidelity in the NISQ era



VQA tuning in the NISQ era



Some VQA NISQ Challenges / Opportunities

- (Static) Error Mitigation
- Good Initialization
- Transient errors
- Measurement Error Mitigation
- Choice of Optimizer
- Ansatz Construction

VAQEM: A Variational Approach to Quantum Error Mitigation

Gokul Subramanian Ravi[1], Kaitlin Smith*[1] ,Pranav Gokhale[2], Andrea Mari[3], Nathan Earnest-Noble[4], Ali Javadi-Abhari[4], and Fred Chong[1,2]

1: UChicago, 2: Super.tech, 3: Unitary Fund, 4: IBM

arXiv:2112.05821

* co-first authors

Summary: A variational approach to quantum error mitigation

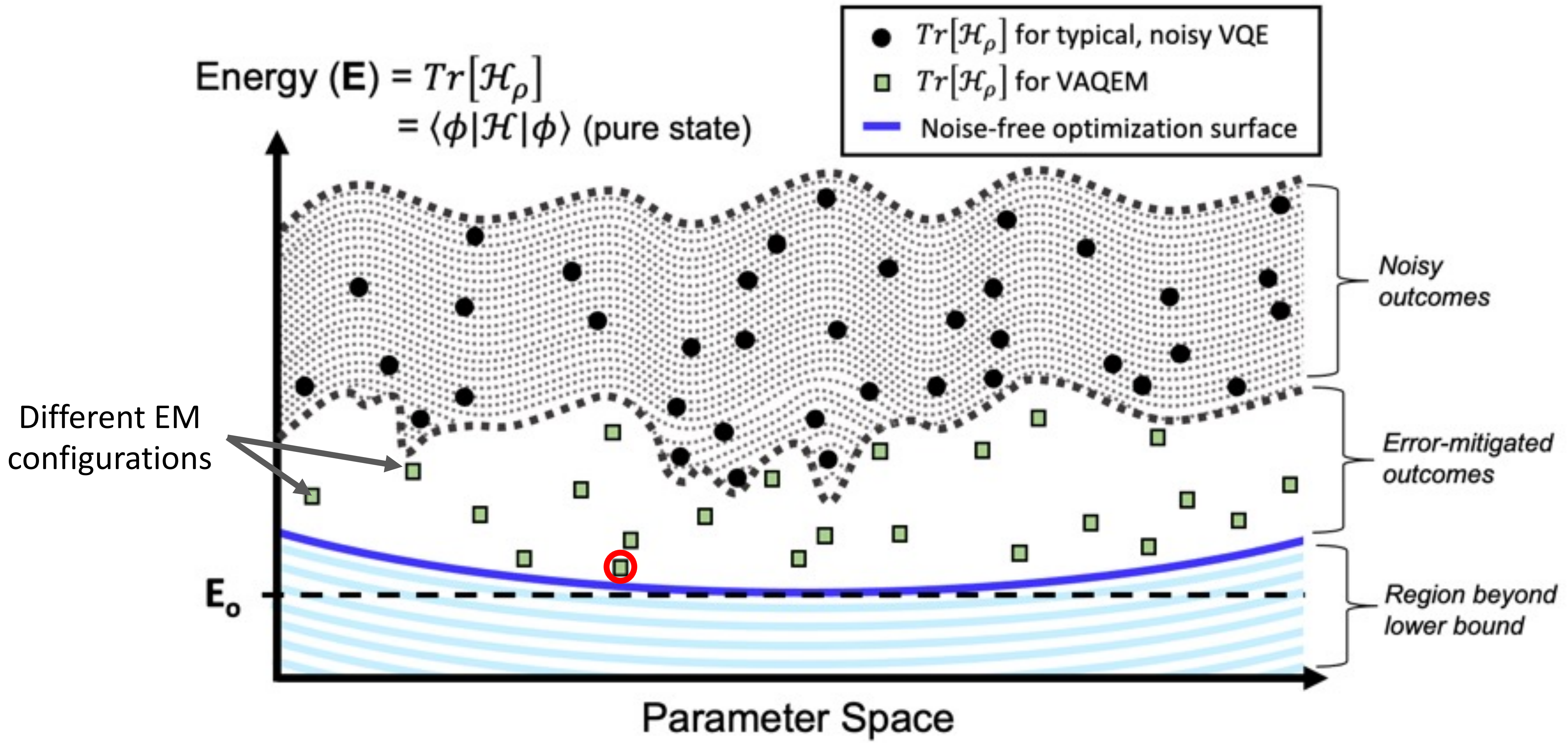
- Background: VQAs are considered suitable to the NISQ era, but machine fidelity is still too low for real world applicability.

- Goal: Apply error mitigation in an optimal manner to VQAs for max fidelity – but this is challenging as device and circuit complexity increase.

- Proposal:
  - Integrate EM techniques into VQA's framework of iterative parameter tuning: enabling a feedback-based approach towards optimal EM for the application / device.
  - Targets two idle-time EM methods: insertion of dynamical decoupling sequences and single-qubit gate scheduling.

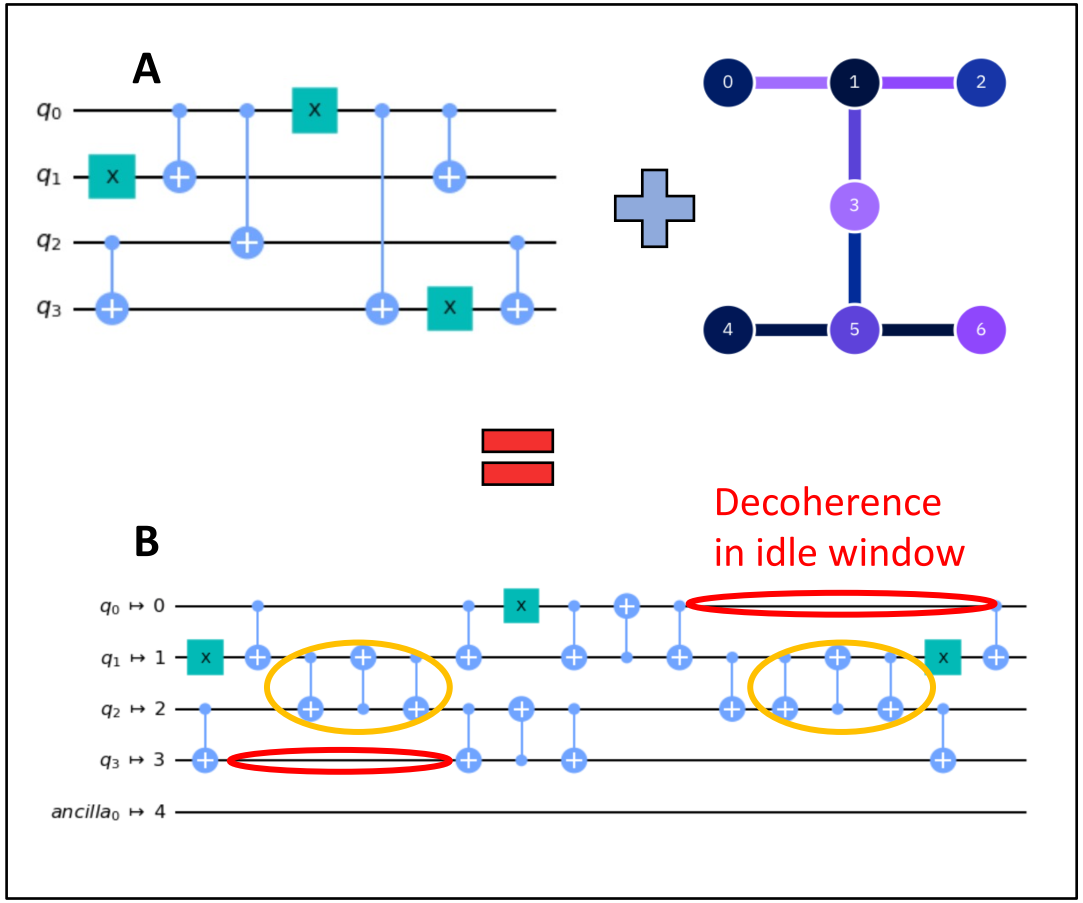
- Result: Improves the quality of the VQA measured objective by 3x on average.

Impact of Error Mitigation

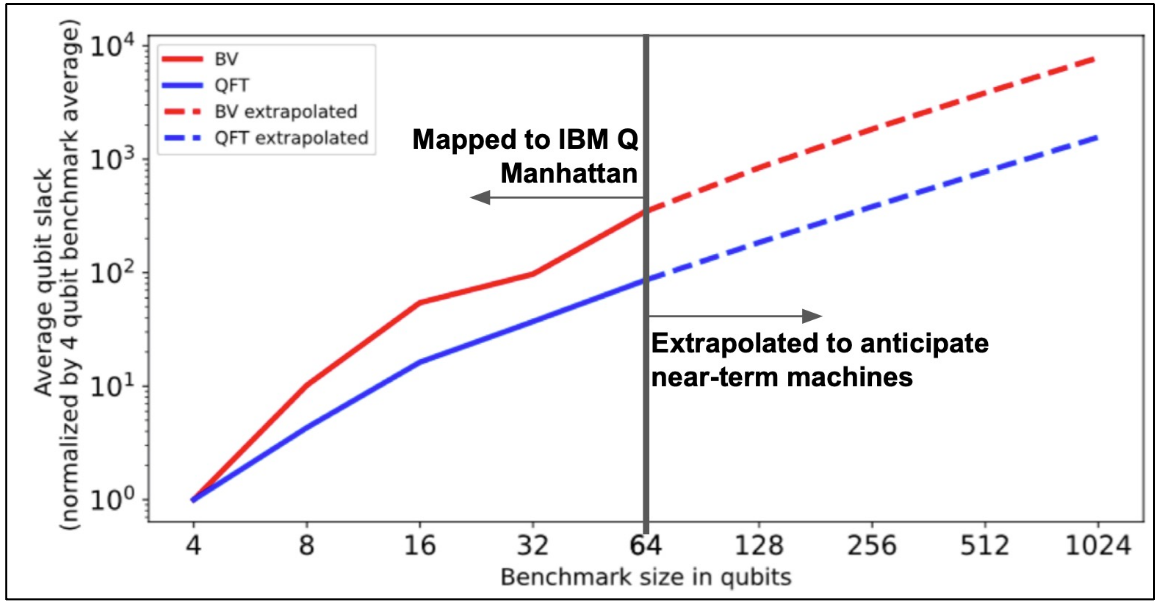


EM targeting QC Idle windows

Compiling for machines with limited connectivity leads to increased depth and long critical paths



As application sizes increases, path lengths become longer and more diverse leading to more slack

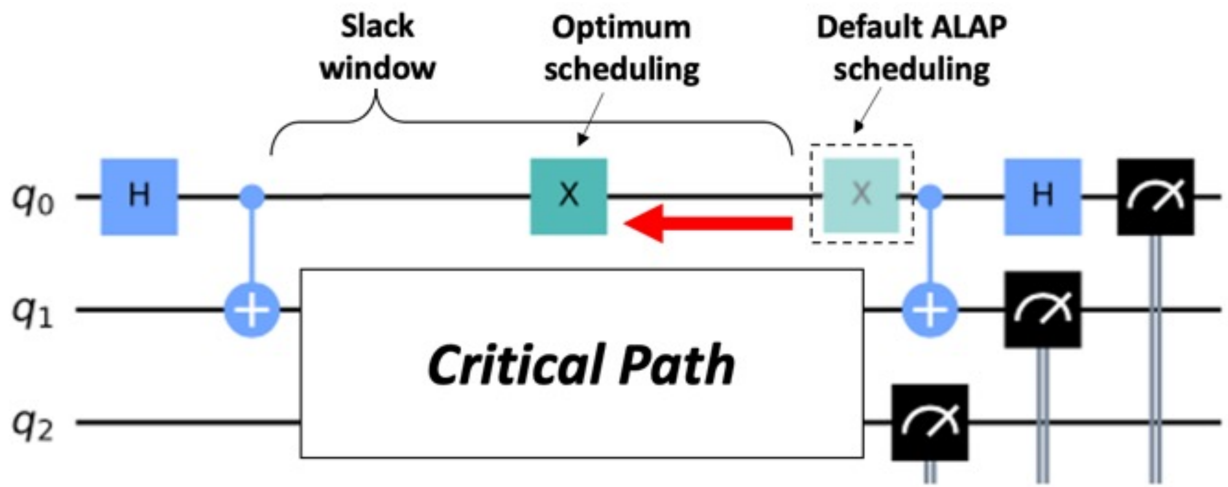


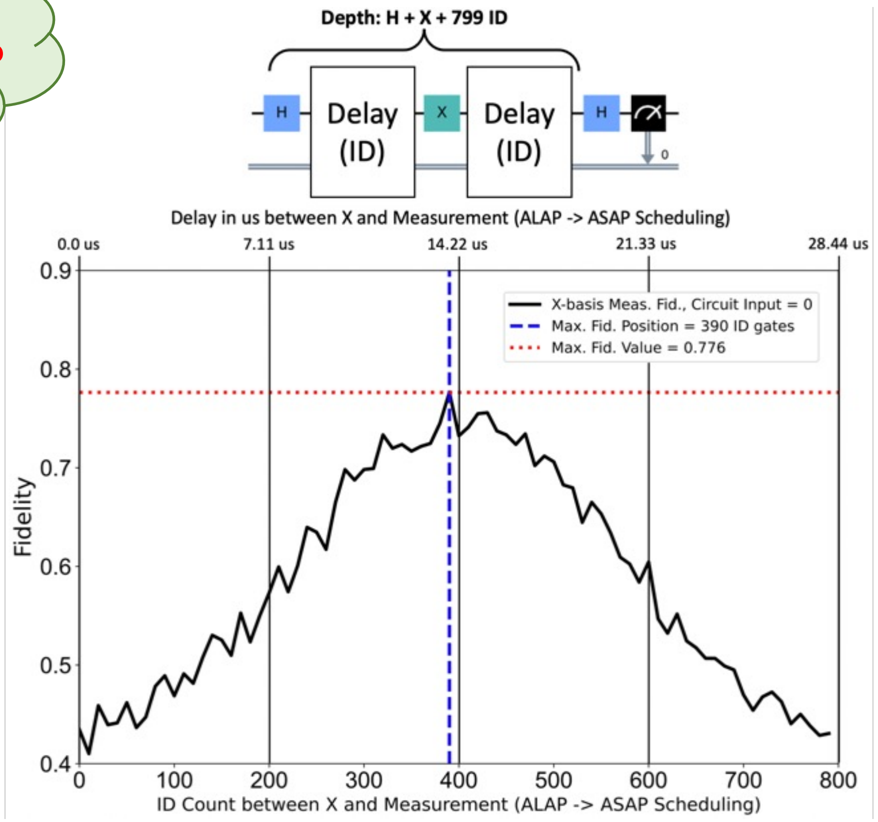
Kaitlin N. Smith , Gokul Ravi, Prakash Murali, Jonathan Baker, Nathan Earnest, Ali Javadi-Abhari, Frederic T. Chong.
TimeStitch: Error Mitigation in Quantum Computers through Instruction Scheduling. 2021

Idle Window Signal Refocusing: 1Q gate scheduling

Spin Echo Correction: Details in the paper!

optimal position?





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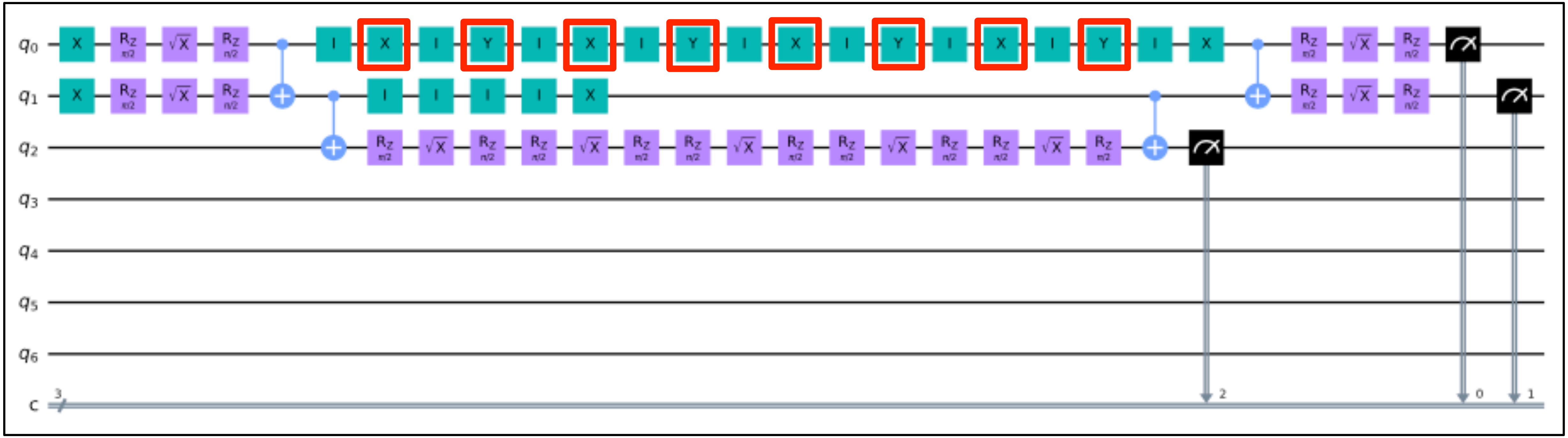
Idle Window Signal Refocusing: Dynamic decoupling

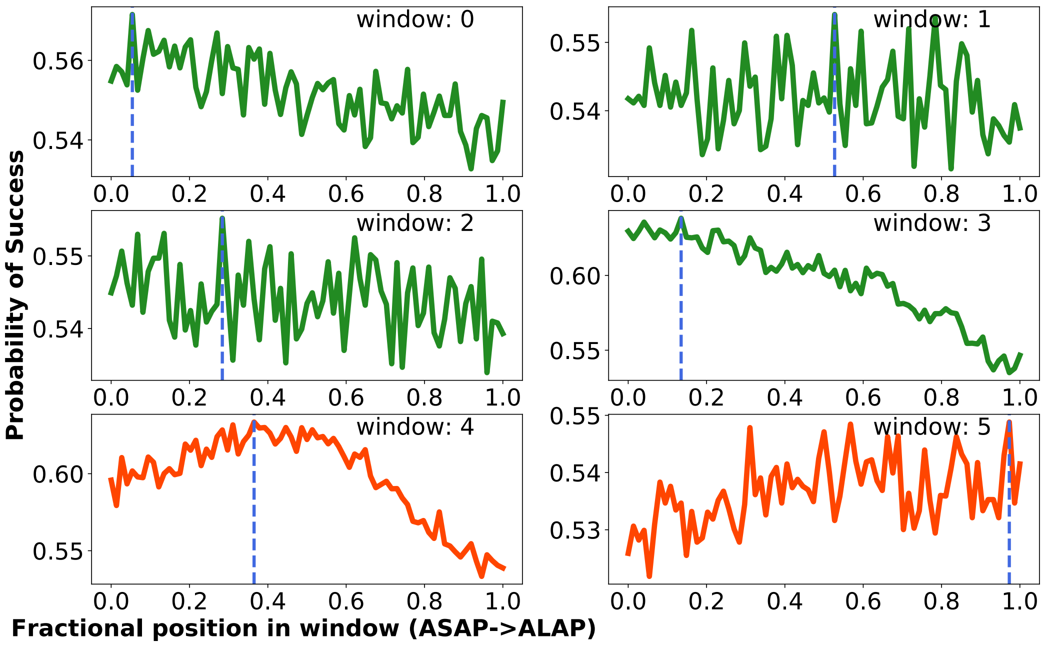
Spin Echo Correction: Details in the paper!

optimal gate types / number / spacing ?

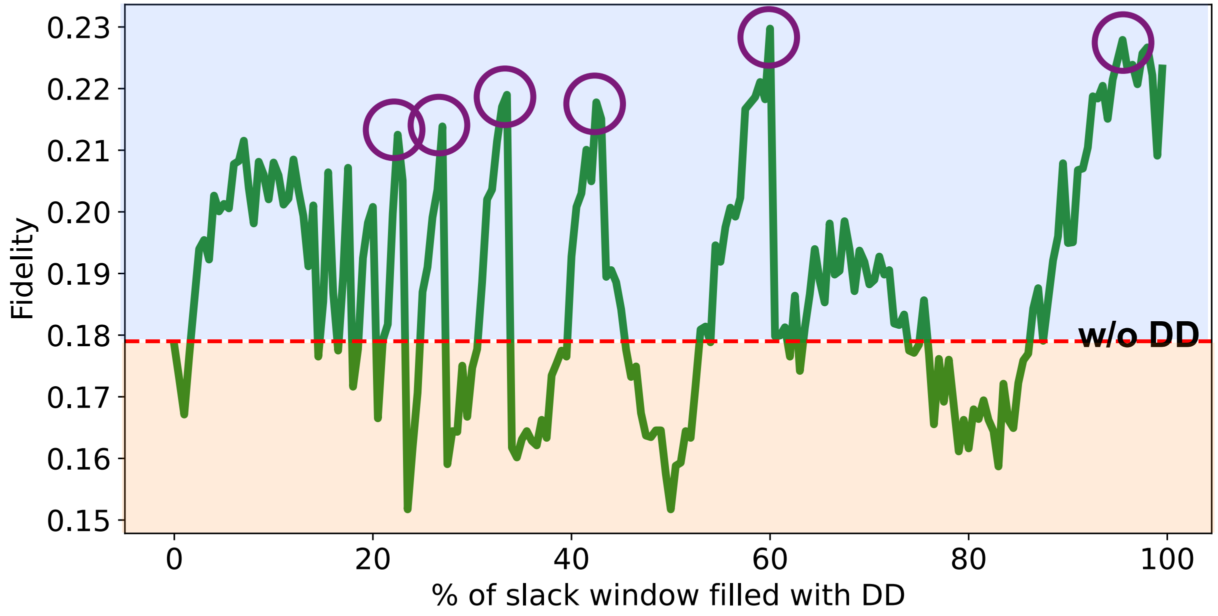


Optimizing EM: practical challenges

1) Imperfect knowledge of stimuli and their effects makes theory driven EM heuristics less effective.



1q gate scheduling



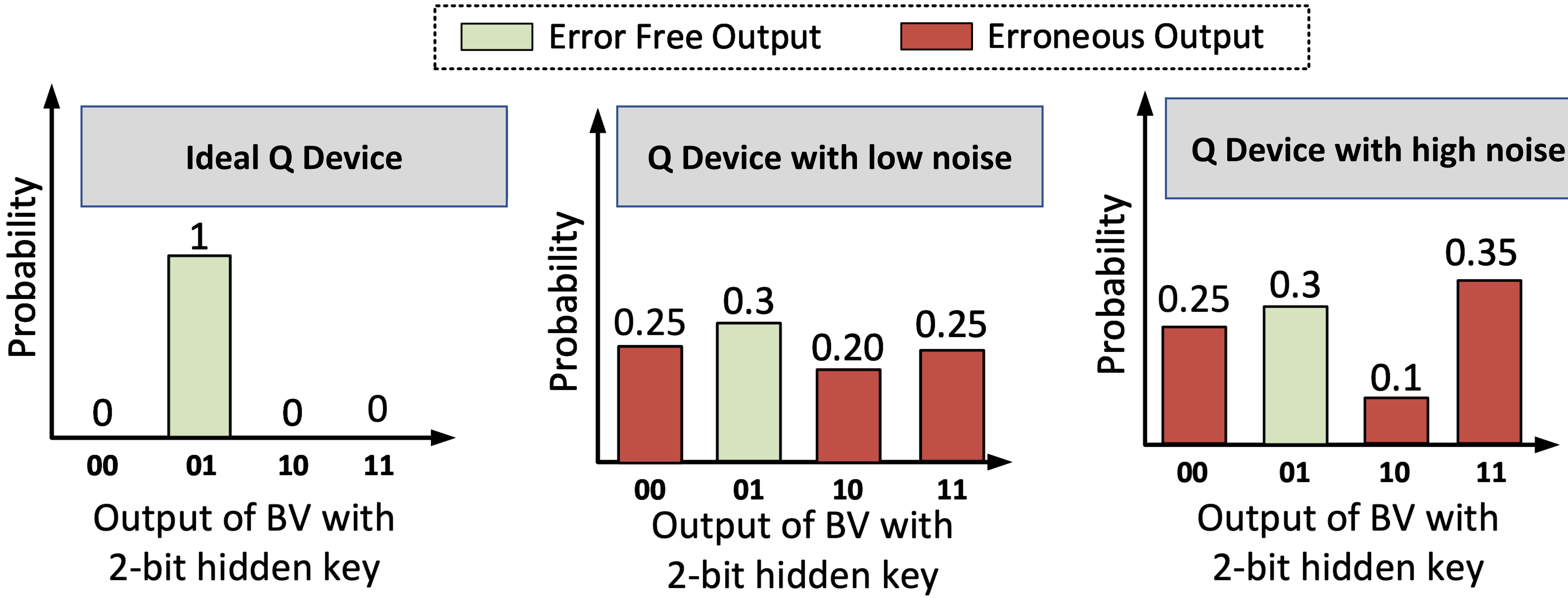
DD insertion

Optimizing EM: practical challenges

2) Micro-analyzing stimuli effects for every EM instance is not scalable.

Optimizing EM: practical challenges

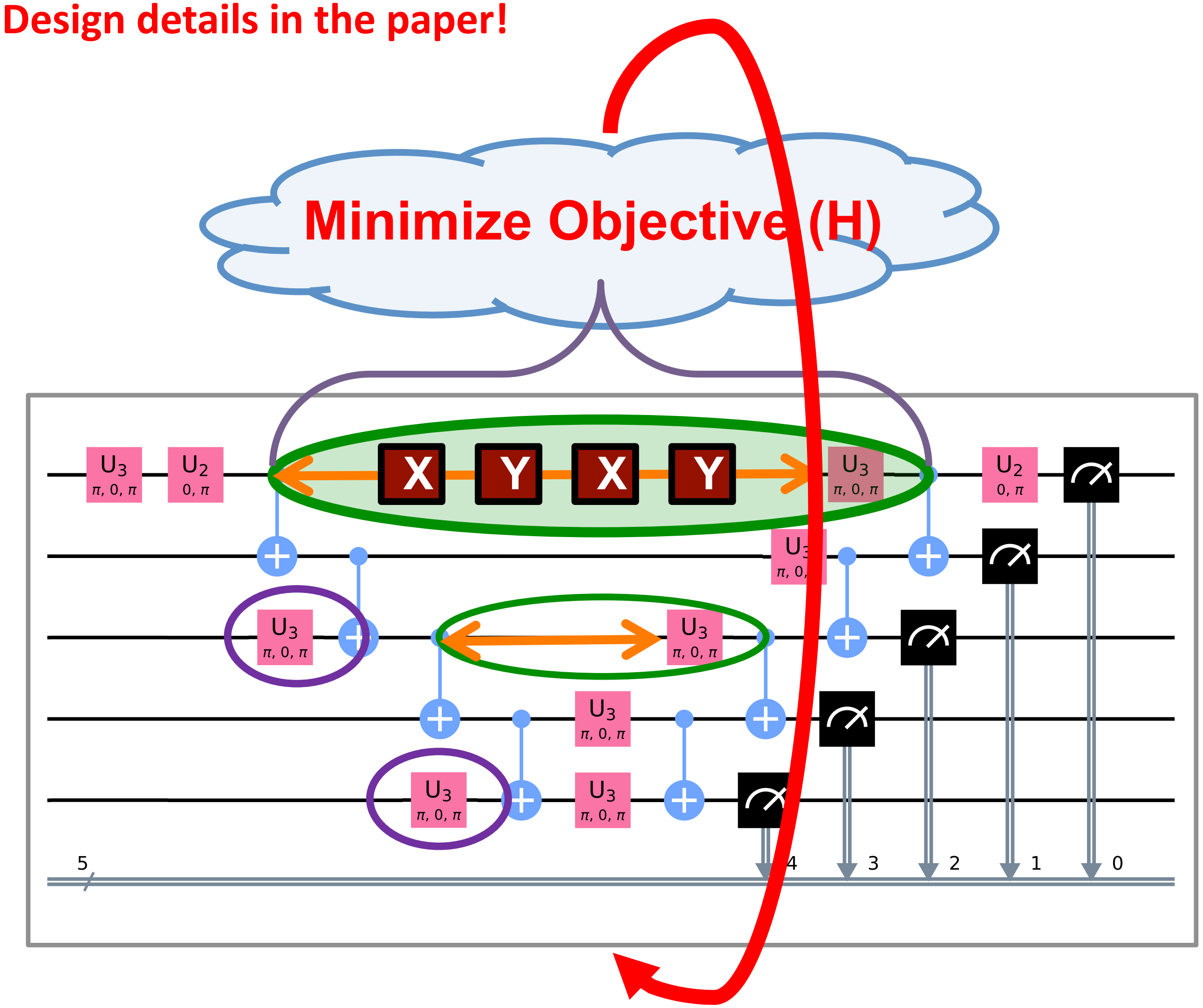
3) Stimuli-agnostic outcome driven approaches are not always possible since outcomes are often unknown and usually not of highest probability.



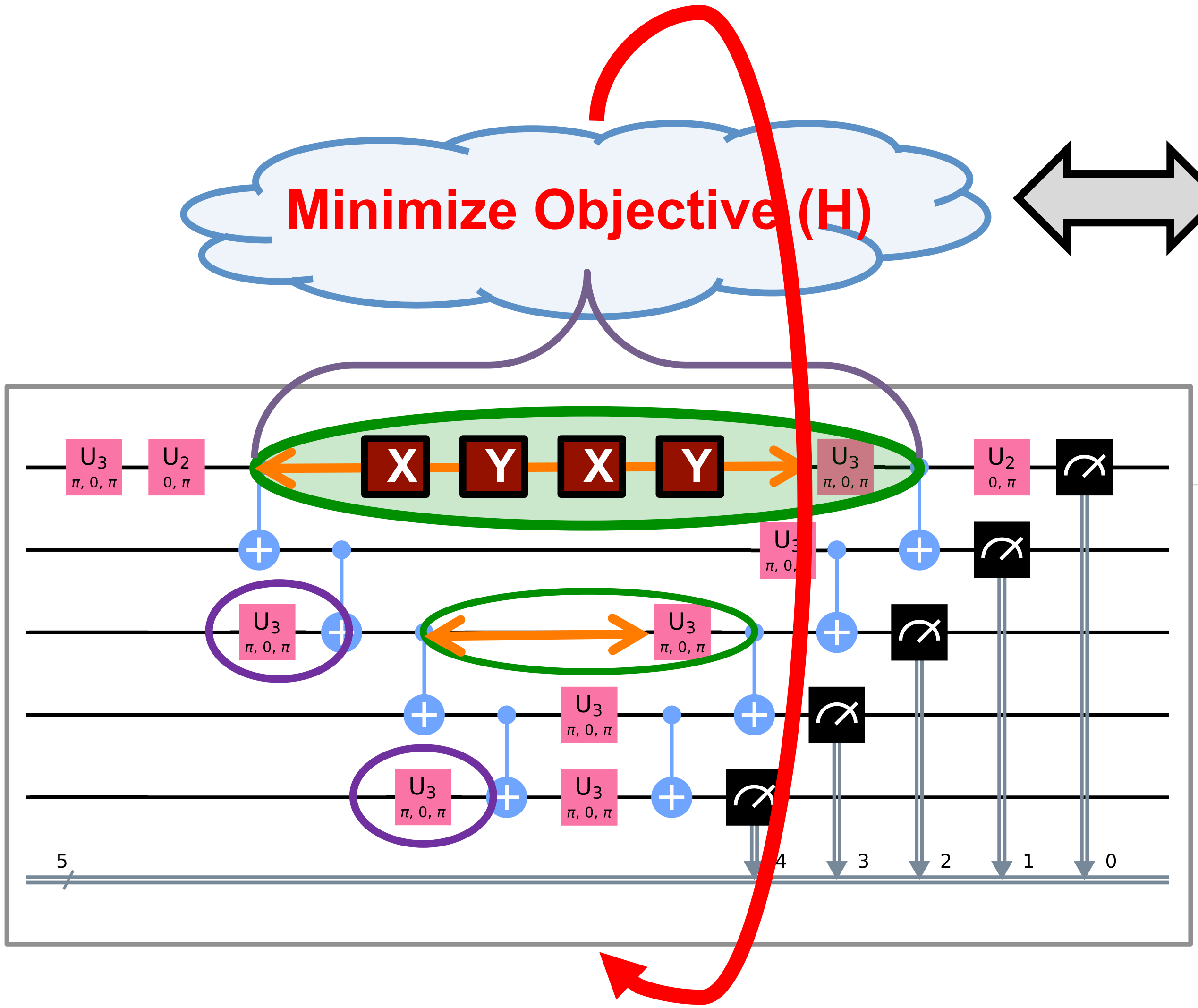
* Ensemble of Diverse Mappings MICRO2019

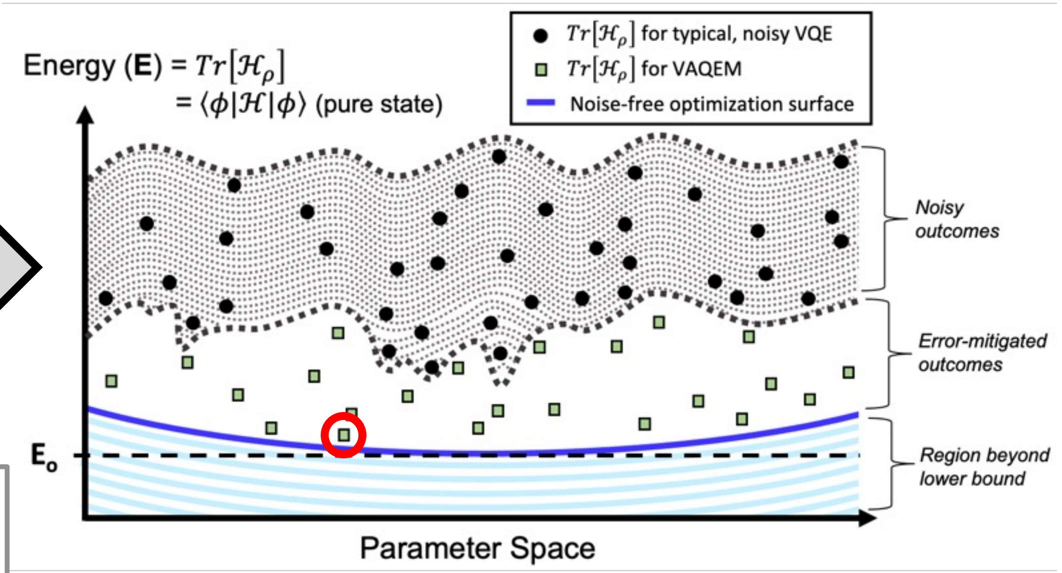
VAQEM: Tuning EM features in the VQA setting

Design details in the paper!



VAQEM: Tuning EM features in the VQA setting



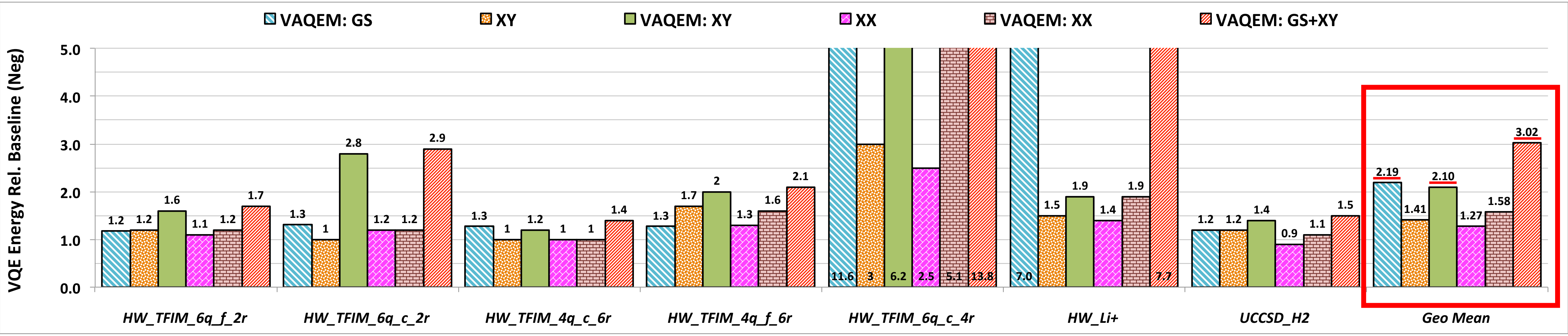


$$\frac{\langle\Psi(\vec{\theta})|H|\Psi(\vec{\theta})\rangle}{\langle\Psi(\vec{\theta})|\Psi(\vec{\theta})\rangle} \geq E_G$$

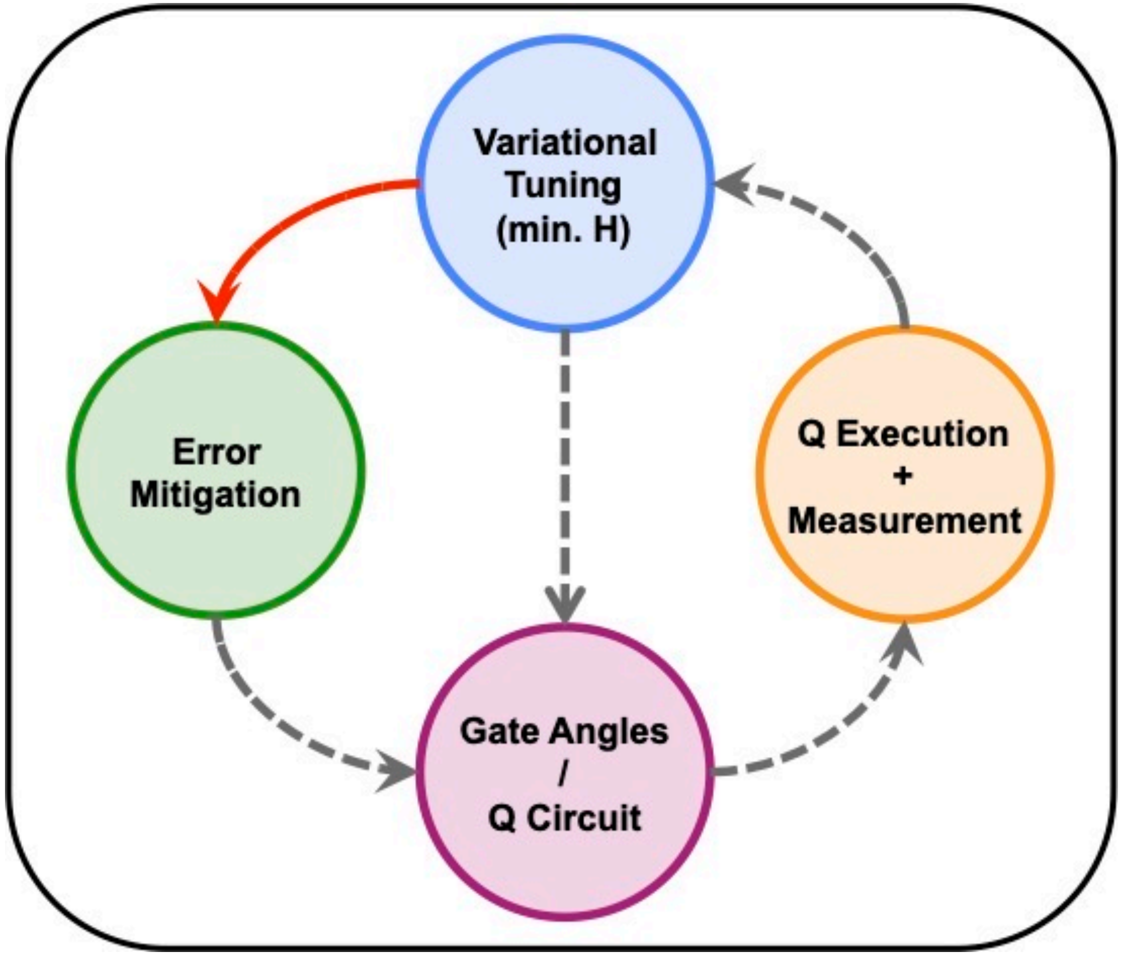
Only *quantum* EM – details in the paper!

VQE benefits from VAQEM

Bench	6q/f/2r	6q/c/2r	4q/c/6r	4q/f/6r	6q/c/4r	Li+	H2
Depth	54	31	57	101	55	90	61
# Win	42	24	22	34	30	45	26



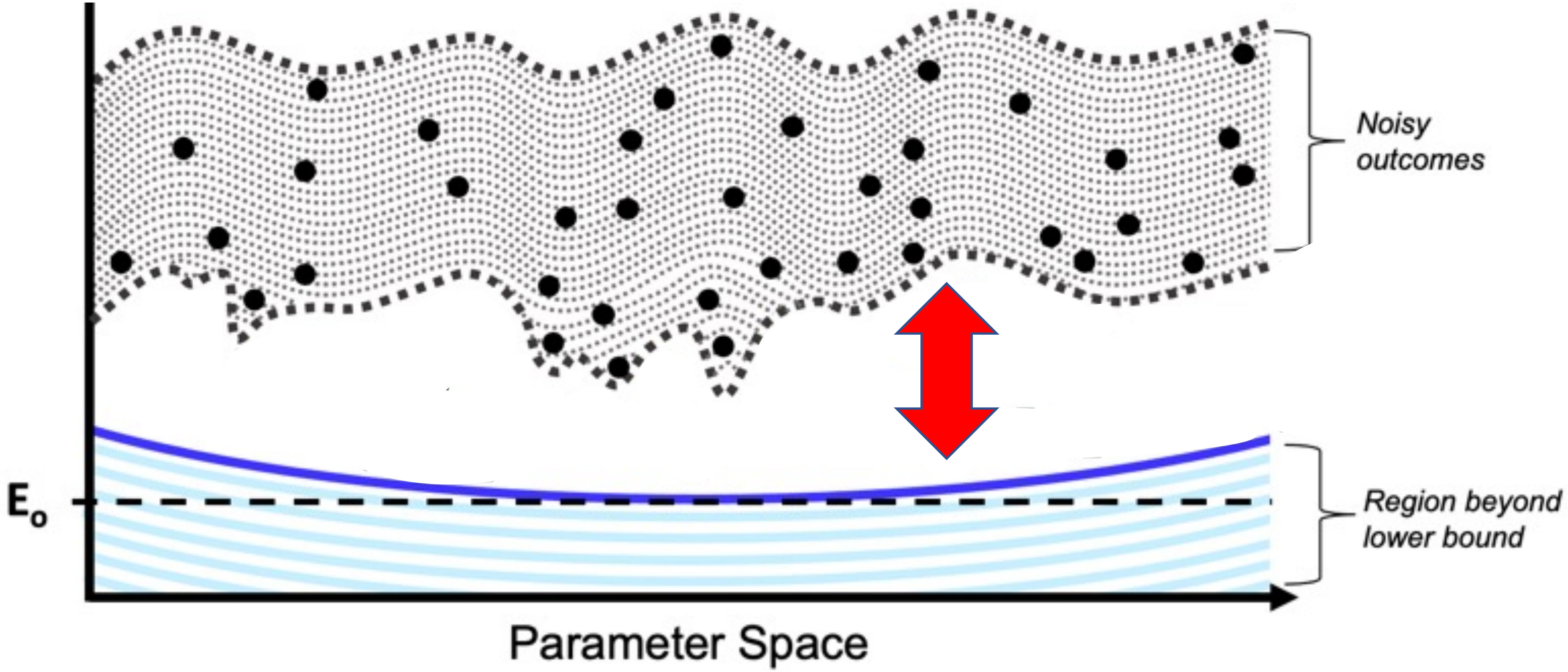
Conclusion: A variational approach to quantum error mitigation



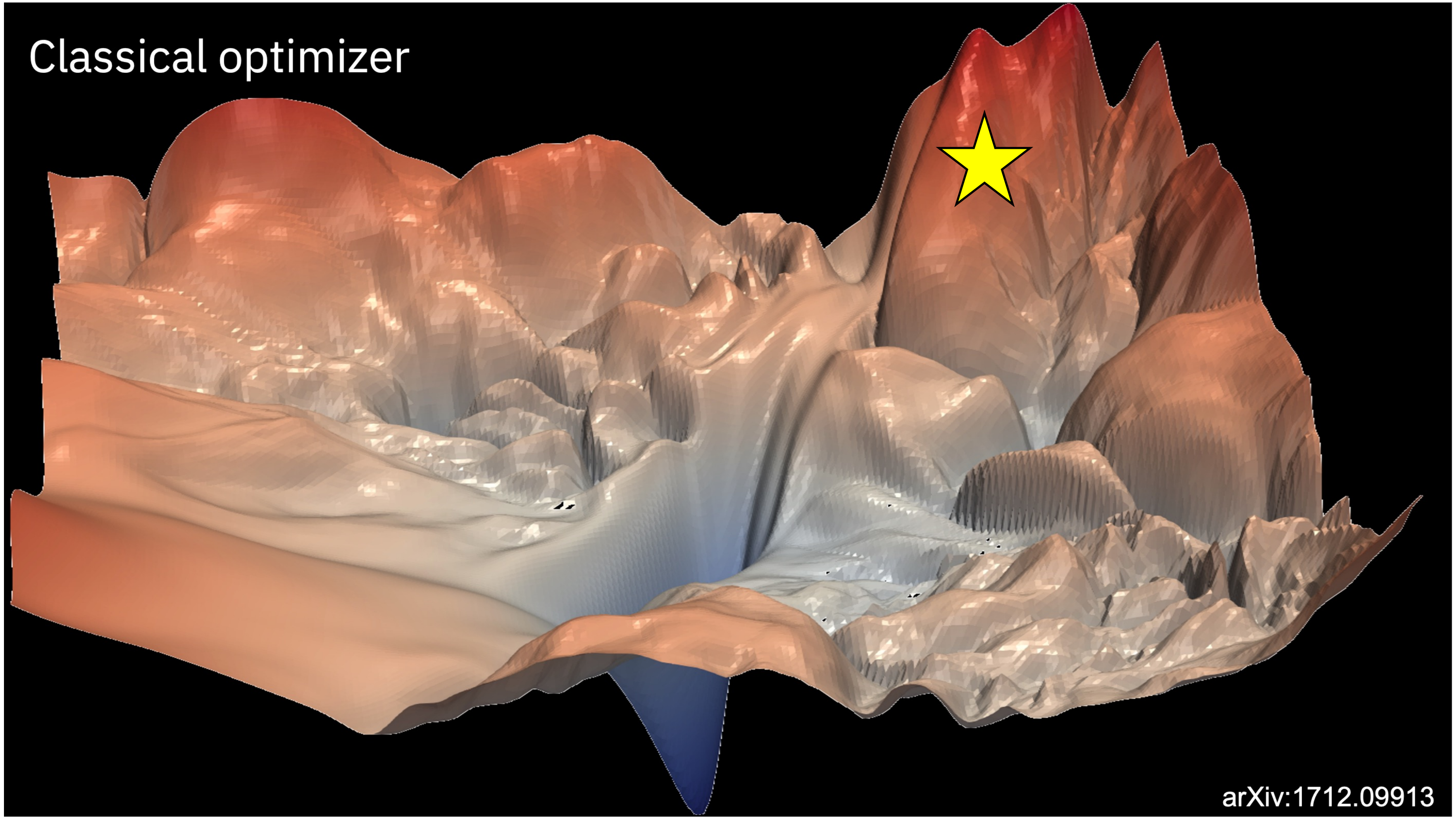
Future Directions:

- Variationally tune more features of current EM techniques
- Integrate more EM techniques into the VAQEM framework
- Explore tunable optimizations outside of error mitigation

VQA Fidelity in the NISQ era



VQA tuning in the NISQ era



CAFQA: Clifford Ansatz For Quantum Accuracy

Gokul Subramanian Ravi[1], Pranav Gokhale[2], Yi Ding[3], William Kirby[4], Kaitlin Smith[1], Jonathan Baker[1], Peter Love[4], Hank Hoffmann[1], Ken Brown[5], and Fred Chong[1,2]

1: UChicago, 2: Super.tech, 3: MIT, 4: Tufts, 5: Duke

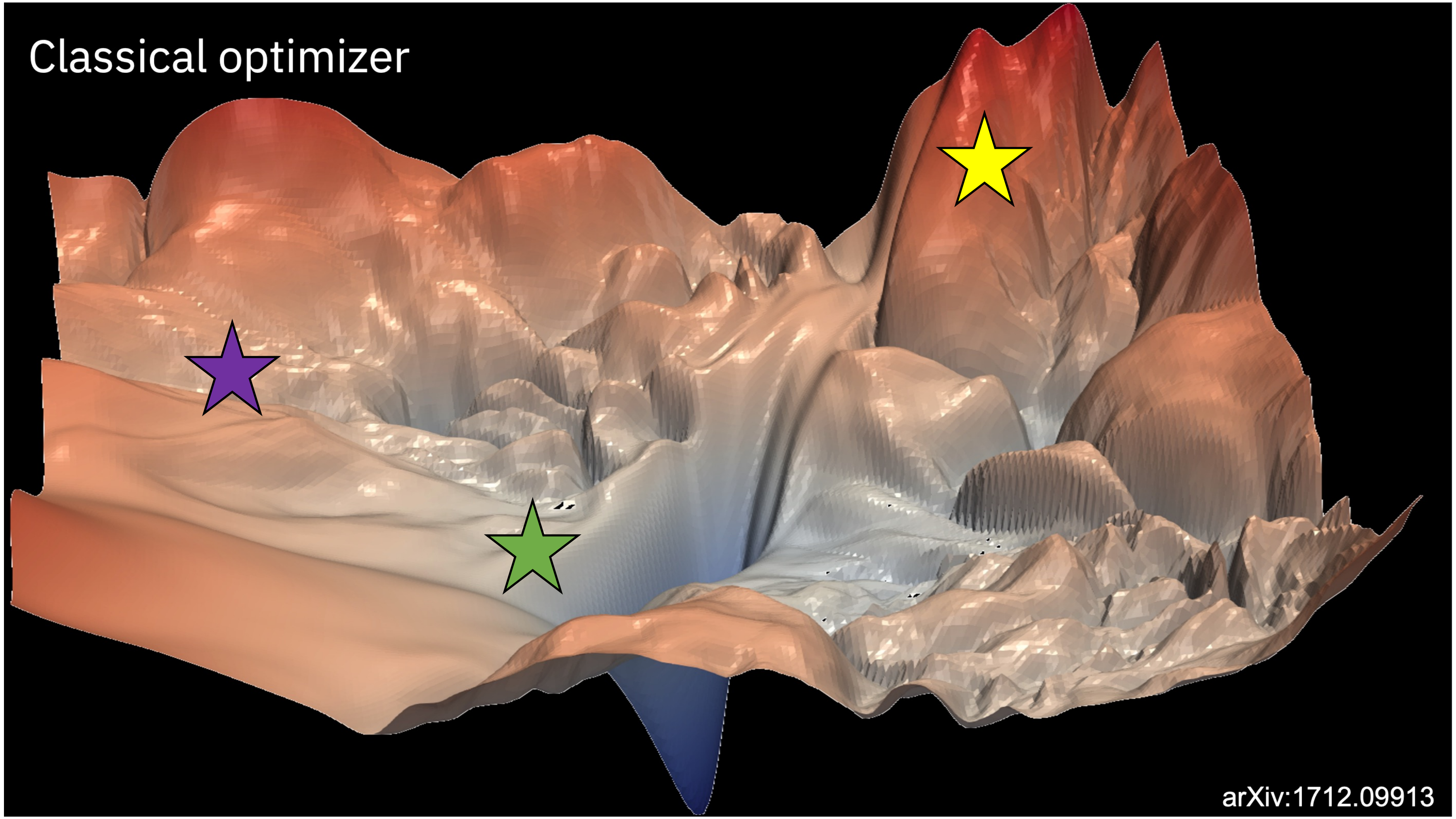
[arXiv:2202.12924](https://arxiv.org/abs/2202.12924)

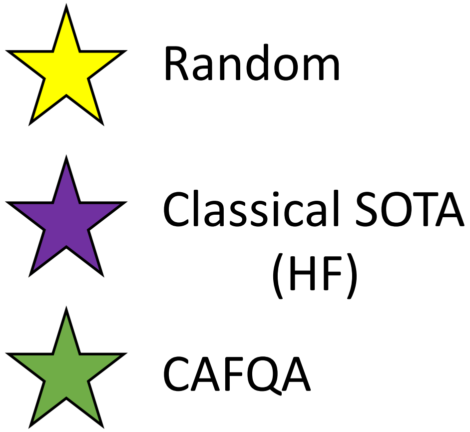
CAFQA Summary

- Motivation / Goal:
  - NISQ machines are noisy, so VQA is slow and inaccurate – unlikely to reach correct output.
  - **Explore VQA classical initialization:**
    - **Why**: Can reduce noisy exploration by the NISQ device
    - **How**: Noise-free efficient classical simulation and search in the Clifford space.
  - Can we boost NISQ machine VQA to useful results for real-world apps?

- Result:
  - ✓ Clifford search achieves 99% mean accuracy across VQE chemistry and optimization tasks.
  - ✓ Recovers up to 99.99% of the correlation energy over SOTA methods like Hartree-Fock.
  - ✓ Scalability showcased by tackling large / complex systems like Chromium Dimer.
  - ✓ 2.5x faster convergence post initialization even for small molecules.

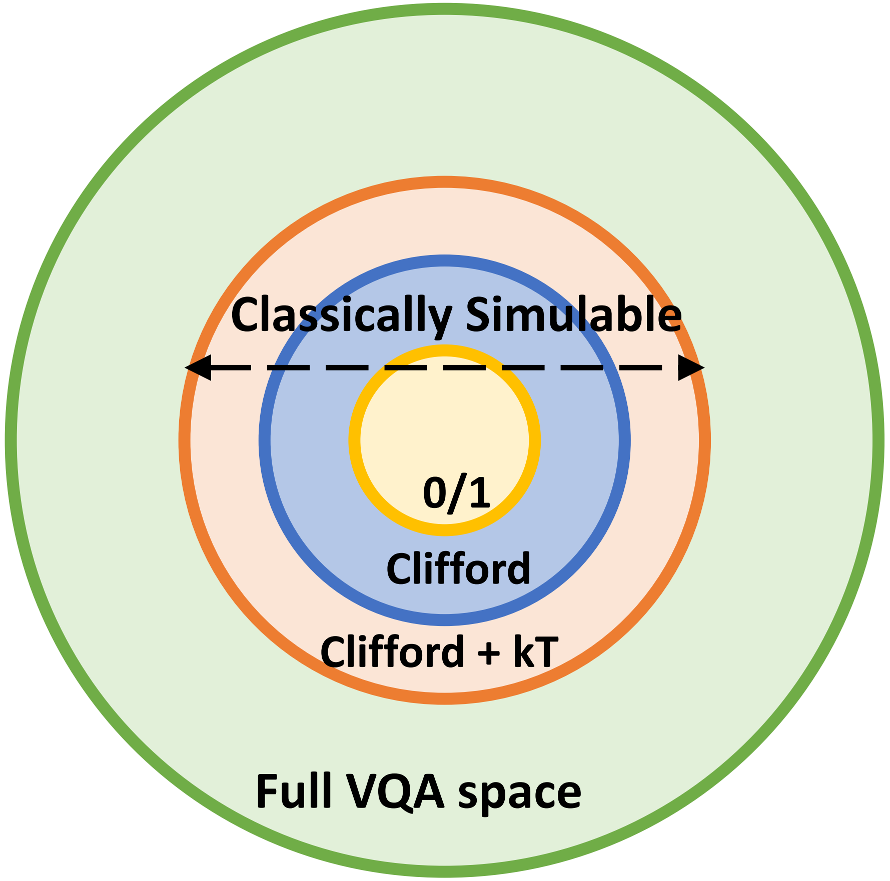
VQE in molecular chemistry





CAFQA Philosophy

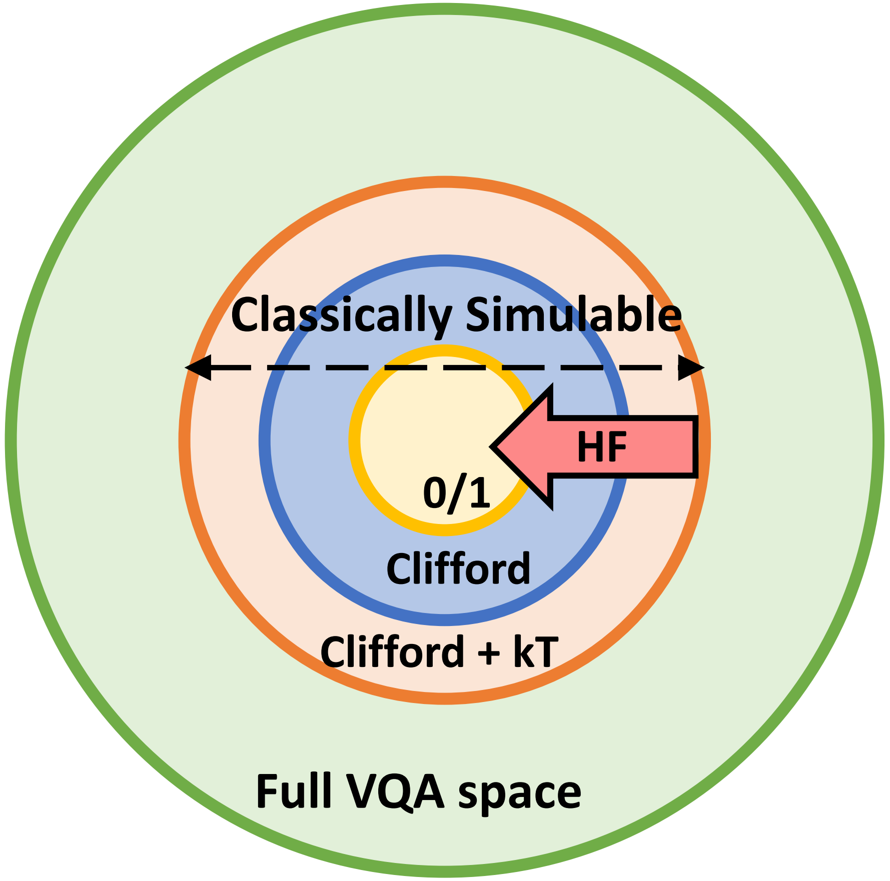
- Well chosen ansatz initialization can help VQA.
- Classical initialization can be most useful.



CAFQA Philosophy

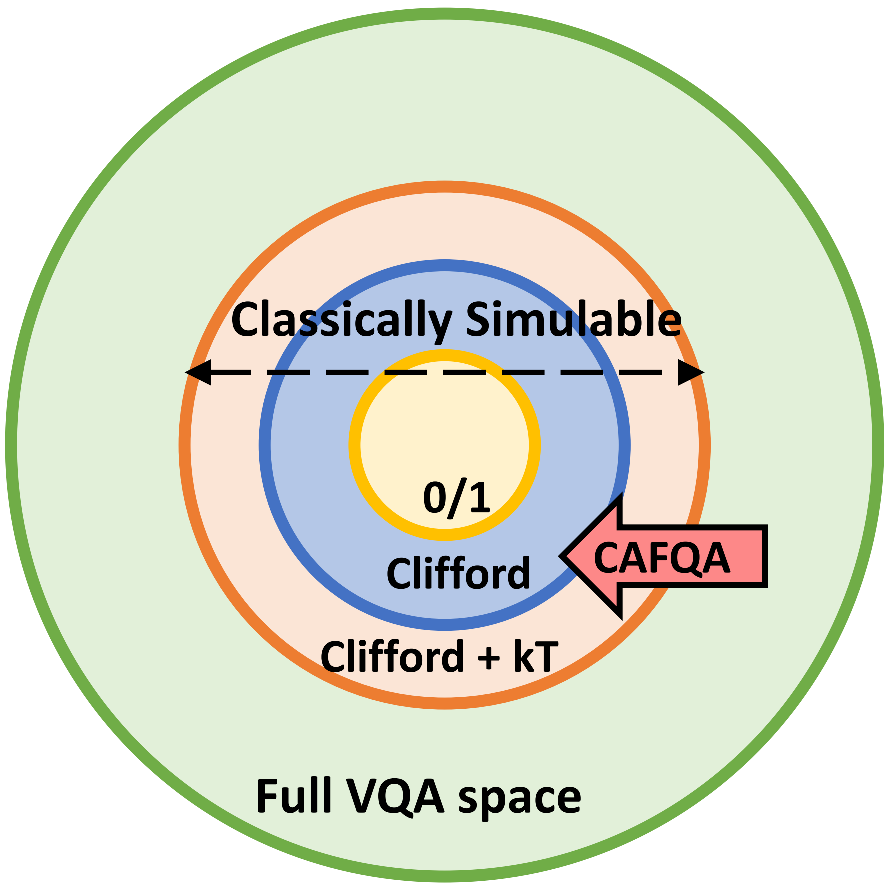
HF = A good string of 0s and 1s

- Well chosen ansatz initialization can help VQA.
- Classical initialization can be most useful.
- Prior classical initialization (HF) is limited.



CAFQA Philosophy

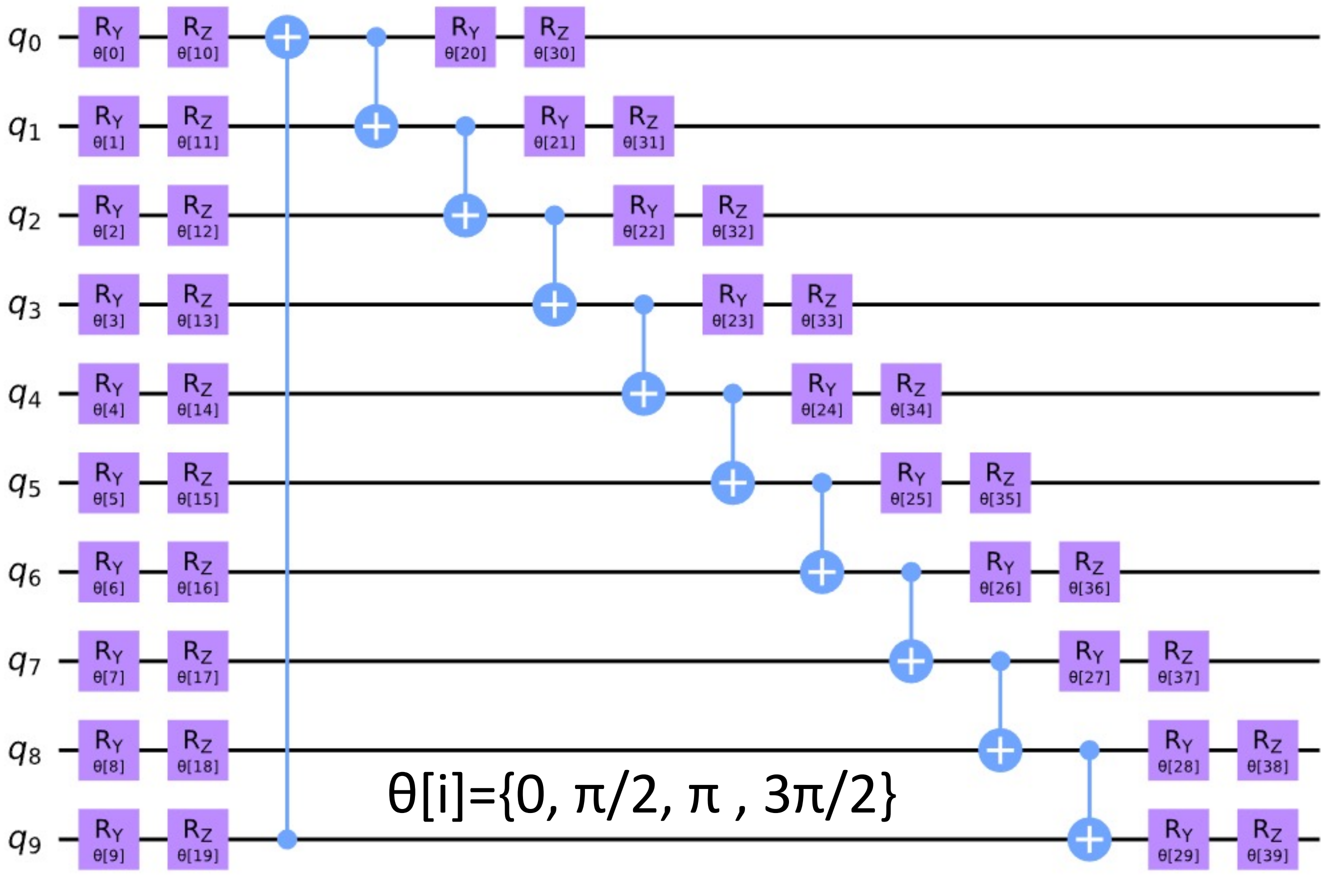
CAFQA = A good stabilizer state
(encompasses bitstrings as well)



- Well chosen ansatz initialization can help VQA.
- Classical initialization can be most useful.
- Clifford initialization is promising because its simulation is classically efficient, and it explores a larger space than HF.

Clifford Space

- Gottesman–Knill Theorem*: A quantum circuit using only the following can be classically simulated efficiently:
  - Preparation of qubits in computational basis,
  - Clifford gates (H, CNOT, *S*, etc.), and
  - Measurements in the computational basis.
- Clifford-only circuits:
  - <u>HW-efficient ansatz</u>
  - Error correction
  - Randomized benchmarking
  - Error mitigation
  - Quantum Networks
- “evolution, not of the state of the quantum computer, but instead of a set of operators that could act on the computer”



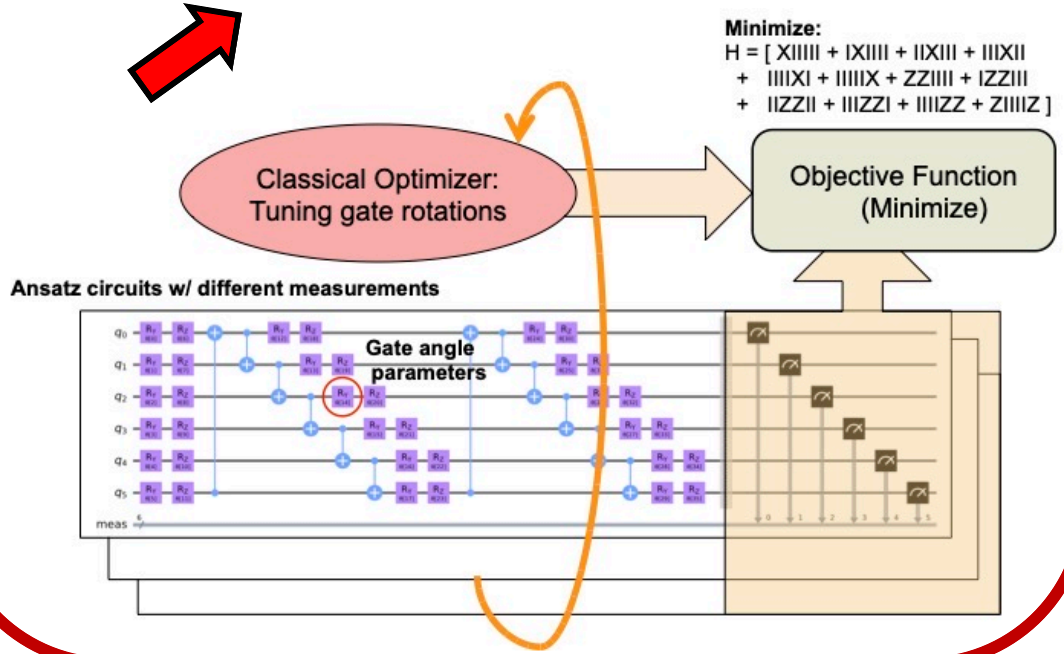
* **The Heisenberg Representation of Quantum Computers**

CAFQA Overview

Classical

Classical discrete search:

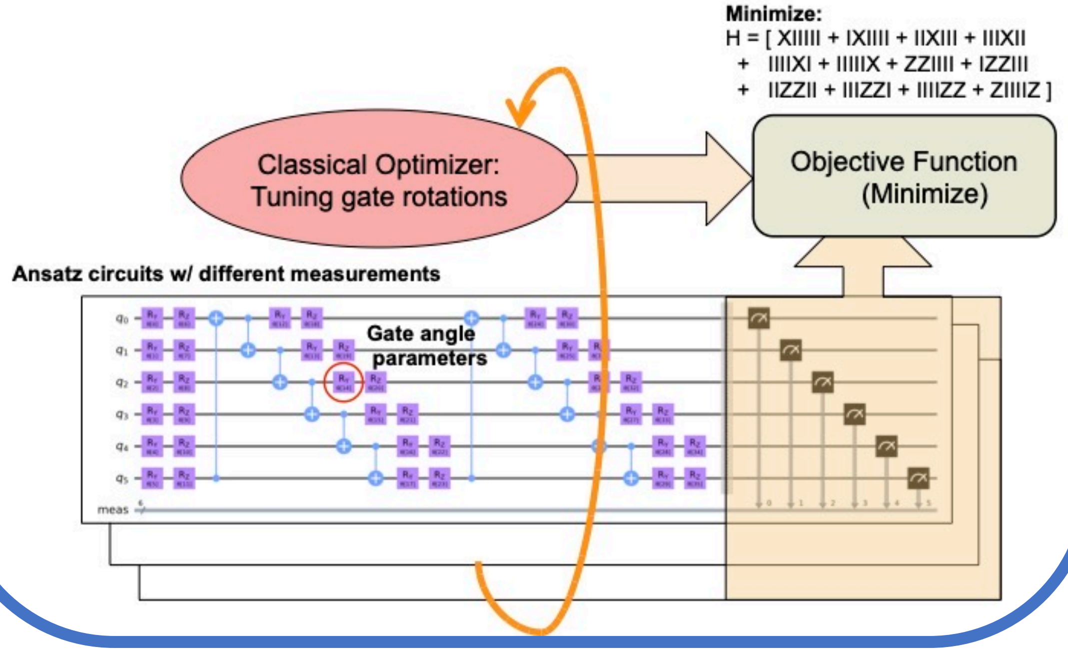
- Ideal evaluation
- Fast evaluation each iteration
- Scalable only in the Clifford space
- Efficient discrete search (Bayesian Optimization)



Quantum

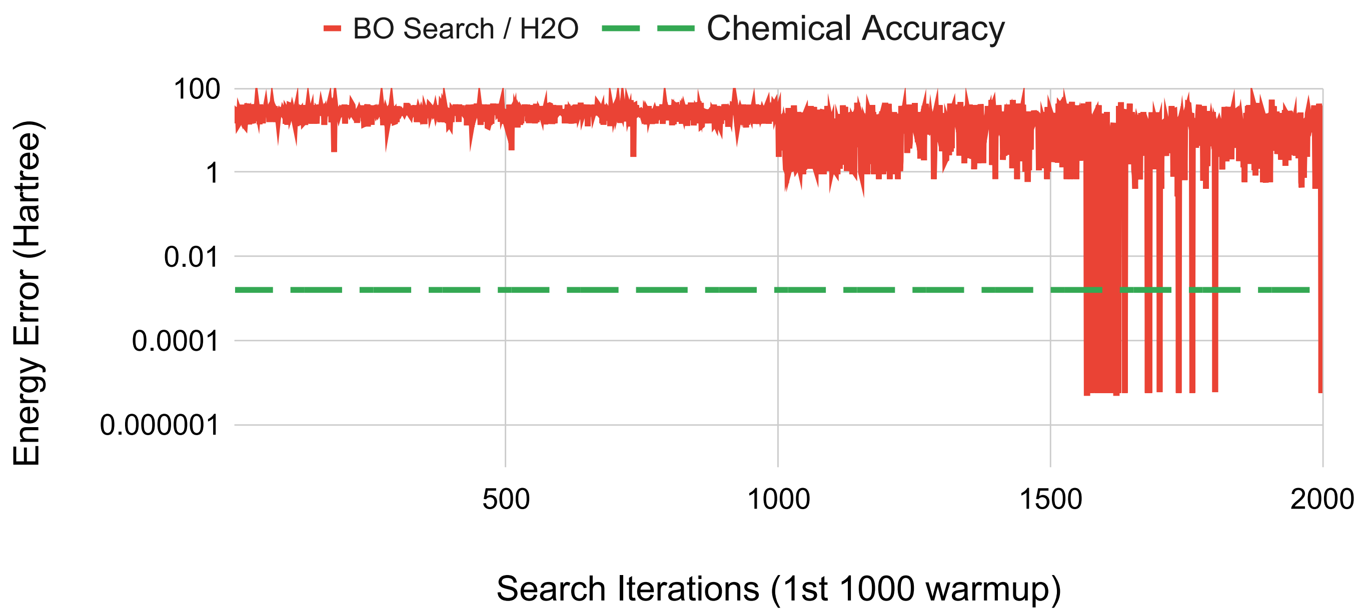
Quantum continuous search:

- Noisy evaluation
- Fast evaluation each iteration
- Scalable across the full parameter space
- Efficient continuous search (eg. SPSA, ImFil)

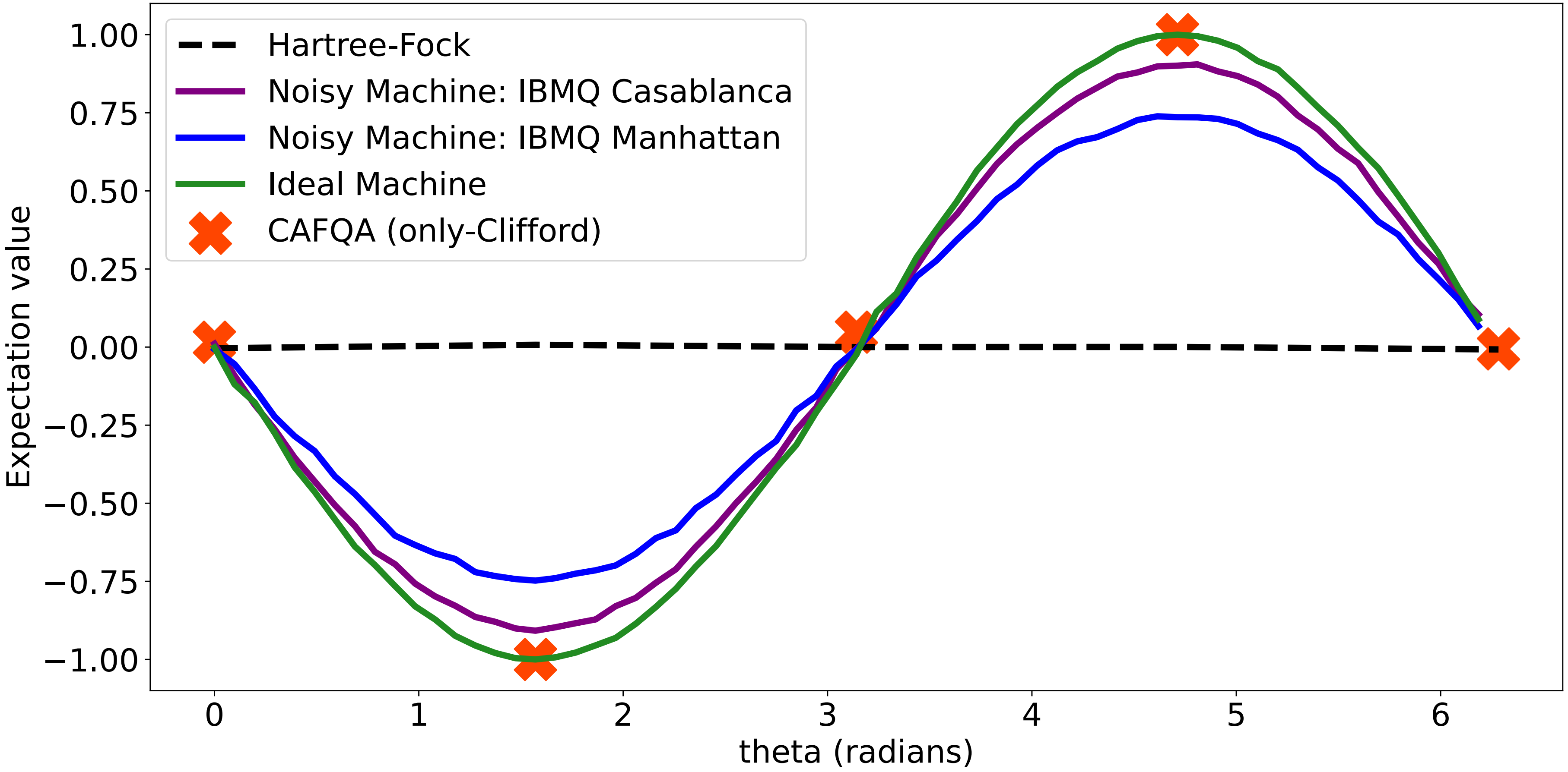


Discrete Search

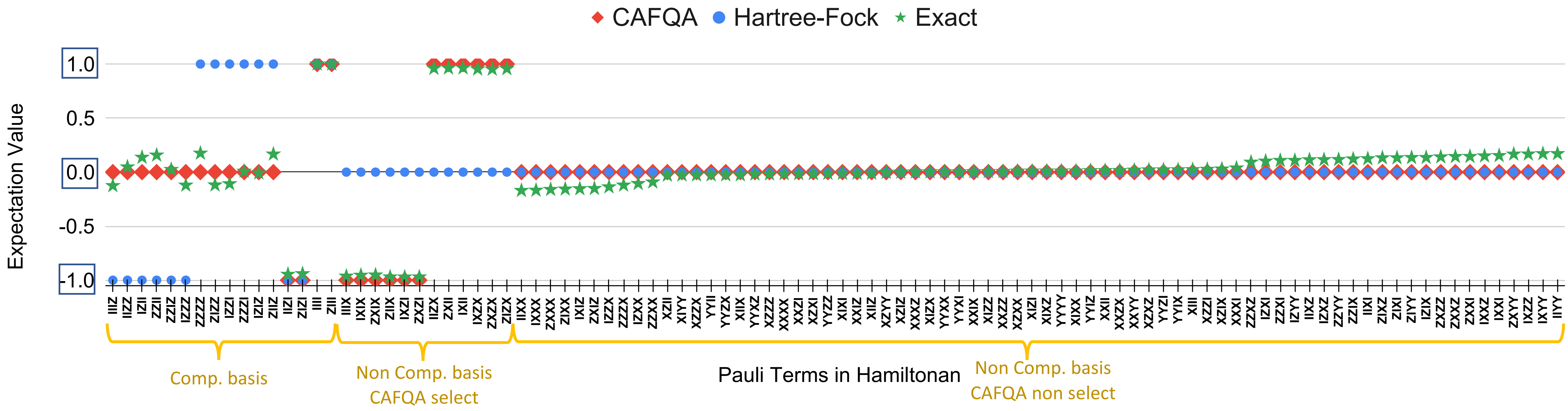
- Clifford space scales exponentially in the number of parameters (though considerably smaller than the entire quantum tuning space).
- **Bayesian Optimization** queries the most informative samples at each round.
- Surrogate model: learns the unknown function that maps the search parameters to the problem objective – *random forests*.
- Acquisition function: Search strategy to select next sample to update surrogate function – *greedy*.



Microbenchmark: XX Hamiltonian / 1 Parameter ansatz

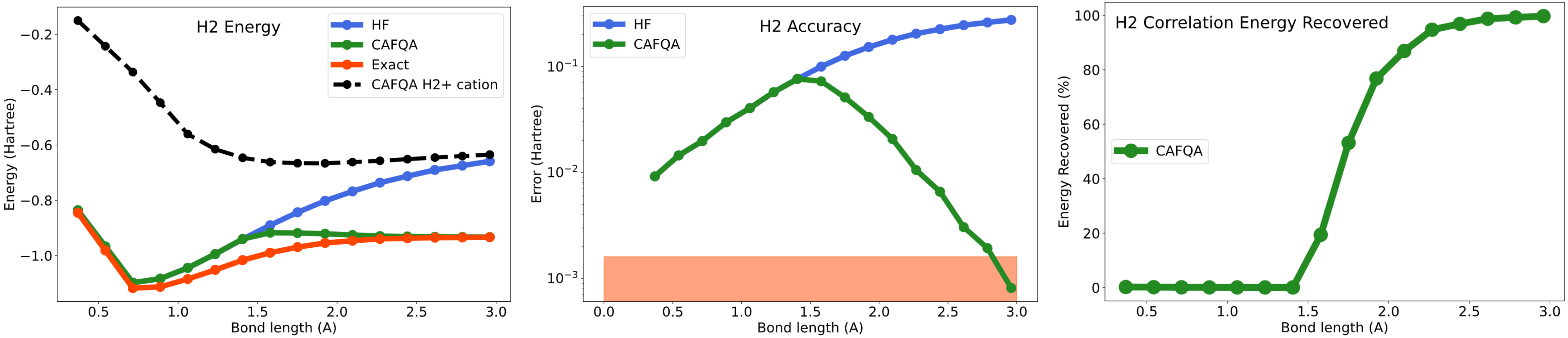


Pauli-term expectations: LiH at 4A

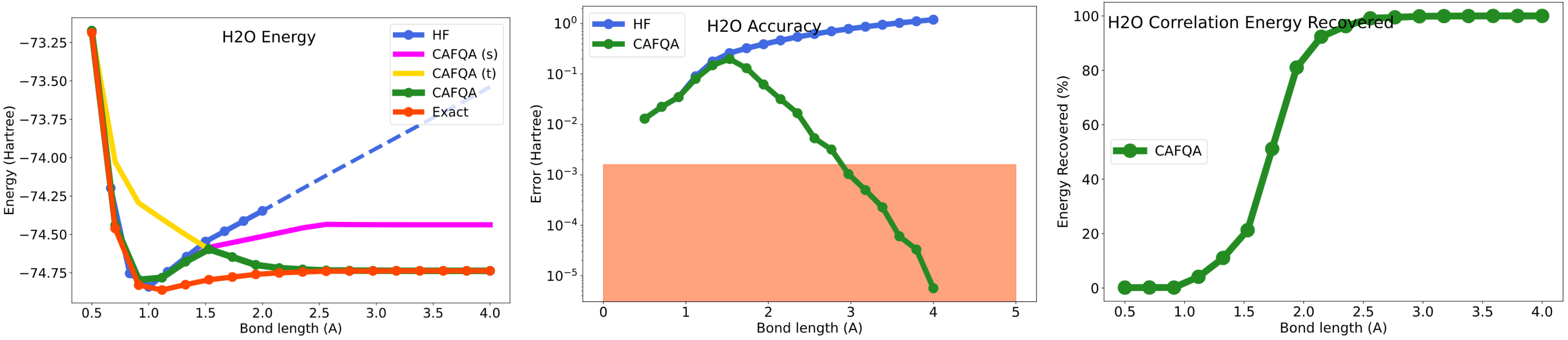


$$H = (-0.70461)II + (0.00012)ZI + (0.00012)IZ + (1.6673e\text{-}10)ZZ + (0.33438)XX$$

H_2

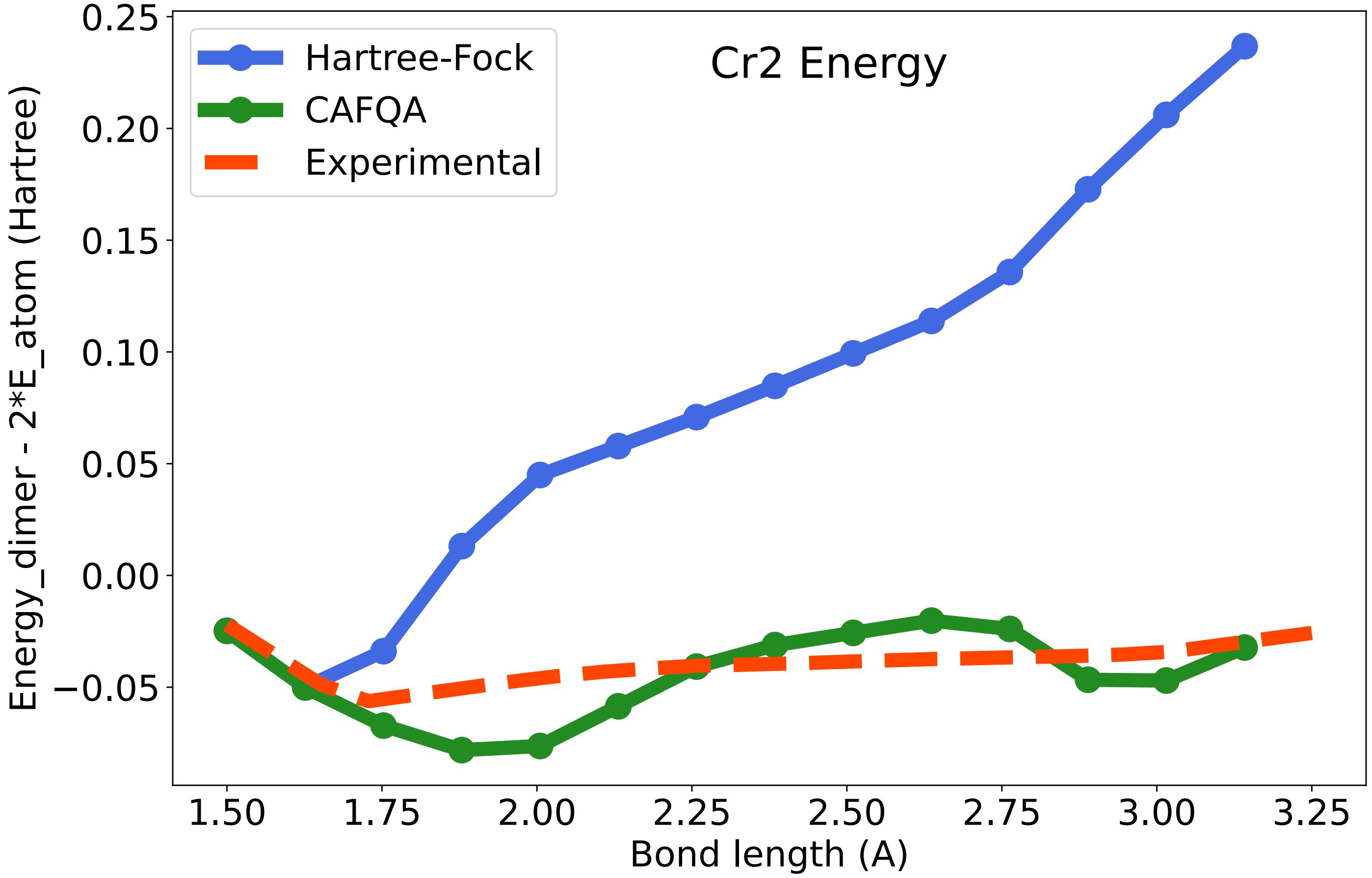

H2 Energy
HF
CAFQA
Exact
CAFQA H2+ cation
Energy (Hartree)
Bond length (A)
H2 Accuracy
Error (Hartree)
H2 Correlation Energy Recovered
Energy Recovered (%)

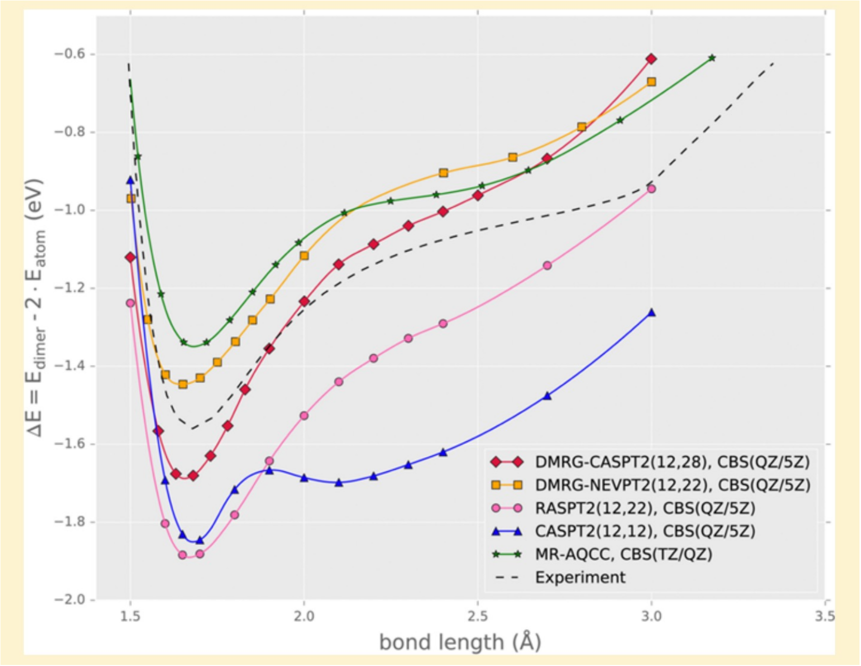
H_2O



H2O Energy
HF
CAFQA (s)
CAFQA (t)
CAFQA
Exact
Energy (Hartree)
Bond length (A)
H2O Accuracy
HF
CAFQA
Error (Hartree)
Bond length (A)
H2O Correlation Energy Recovered
CAFQA
Energy Recovered (%)
Bond length (A)

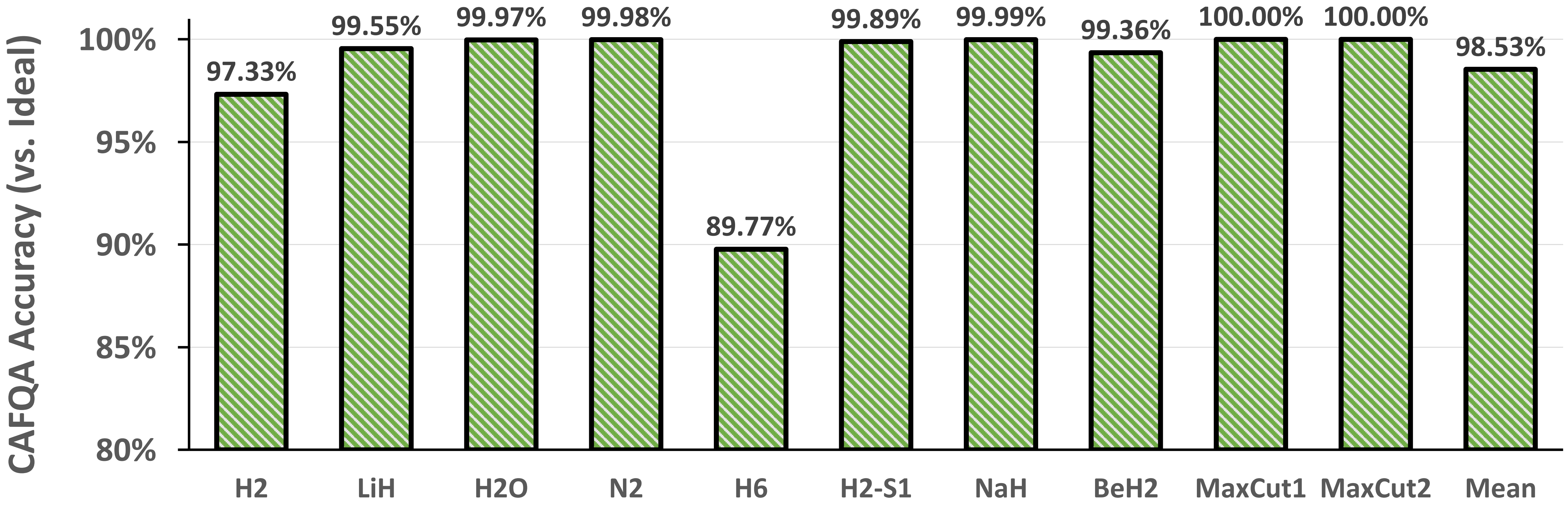
Cr_2



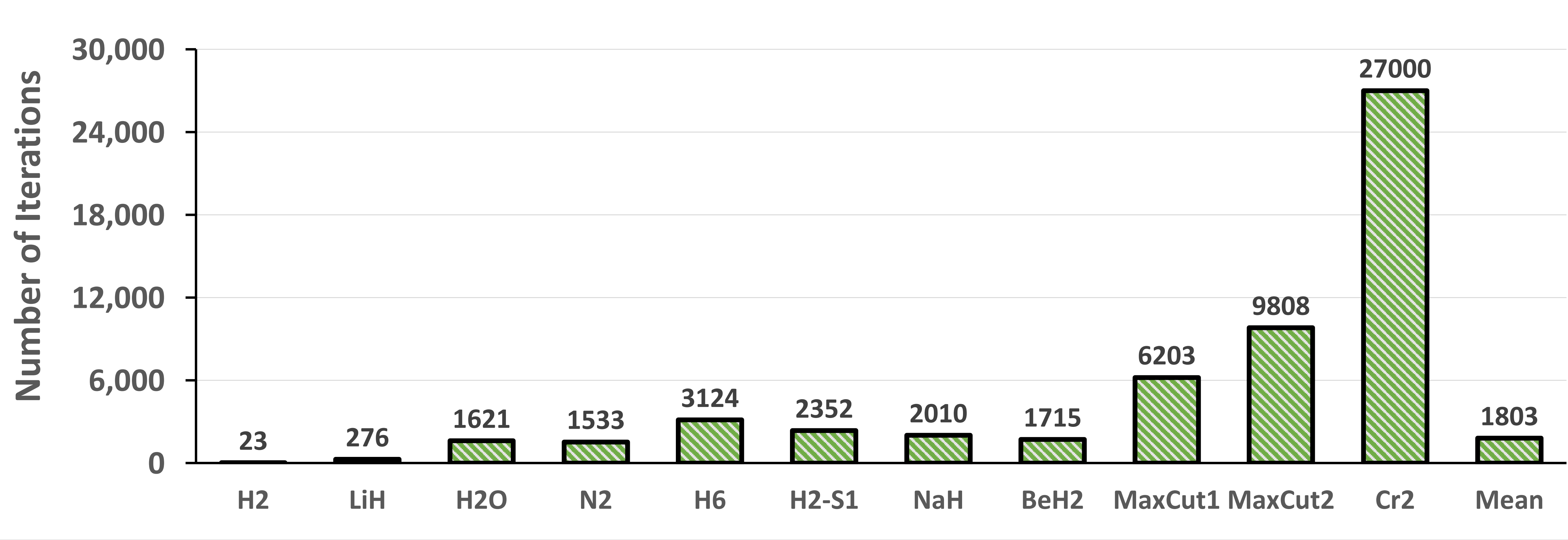


* Potential Energy Surface of the Chromium Dimer Re-re-revisited with Multiconfigurational Perturbation Theory, J. Chem. Theory Comput. 2016

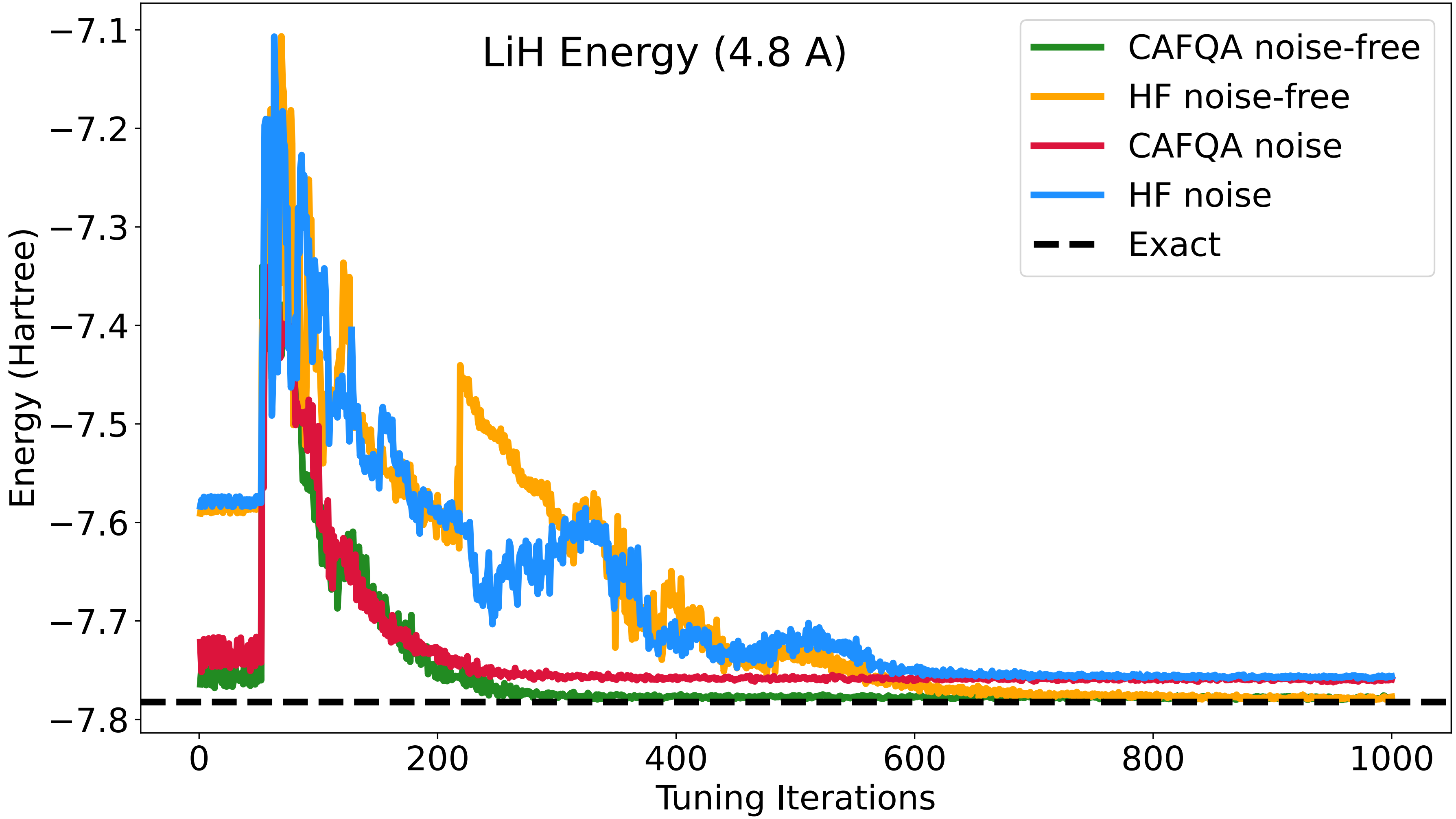
Overall Accuracy



Search Iterations



Post-CAFQA Quantum Exploration



Conclusions

- CAFQA builds a Clifford ansatz by tuning a HW-efficient parameterized circuit in the Clifford space, producing a stabilizer initial state for high accuracy VQA estimations.

- CAFQA's benefits are significant because it is classically scalable, it searches the search space efficiently (through BO) and its per-iteration expectation measurements are ideal.

- Results:
  - ✓ Stand-alone Clifford search achieves 99% mean accuracy across VQE chemistry and optimization problems.
  - ✓ Recovers up to 99.99% of the correlation energy that cannot be estimated by SOTA methods like Hartree-Fock.
  - ✓ Scalability showcased by tackling large / complex systems like Chromium Dimer.

Thank you!

gravi@uchicago.edu