Classical Simulation and Modeling to Advance Quantum Frontiers

Gokul Subramanian Ravi

Postdoctoral Scholar, University of Chicago (- Aug ‘23)

Assistant Professor, University of Michigan (Sep ‘23 -)

EPiQC CCF-1730449; STAQ NSF Phy-1818914; NSF 2110860; US DOE Office of Advanced Scientific Computing Research, Accelerated Research for Quantum Computing Program; NSF QLCI HQAN (#2016136); U.S. DOE Office of Science, National Quantum Information Science Research Centers; NSF #2030859 CIFellows Project

ModSim 08/09/23

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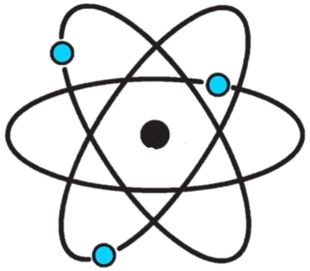
What is quantum good for?



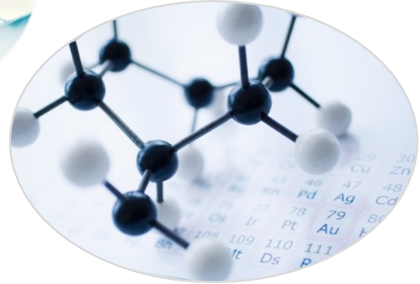
https://ggos.org/intro/geodesy-and-quantum-mechanics/

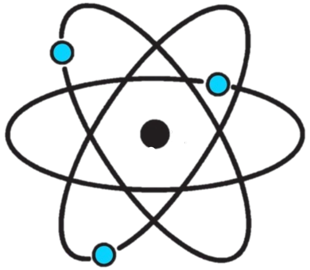
What is quantum good for?

Drug discovery

Security

Industrial chemistry





Finance

Optimization tasks

Artificial Intelligence

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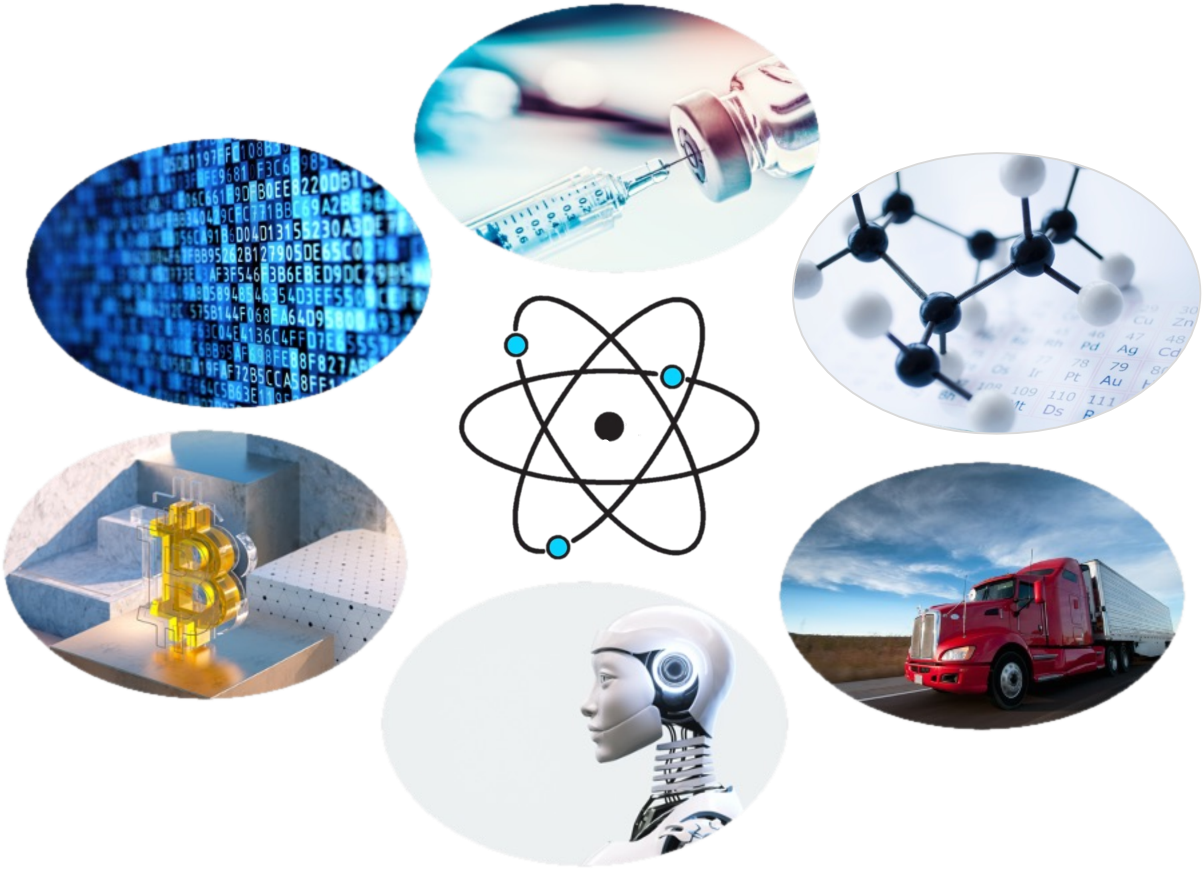

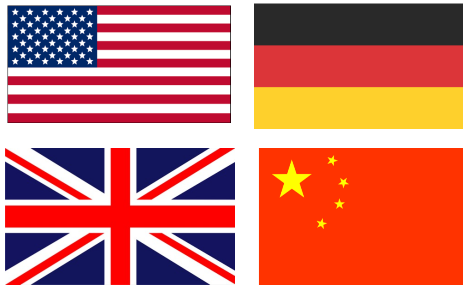

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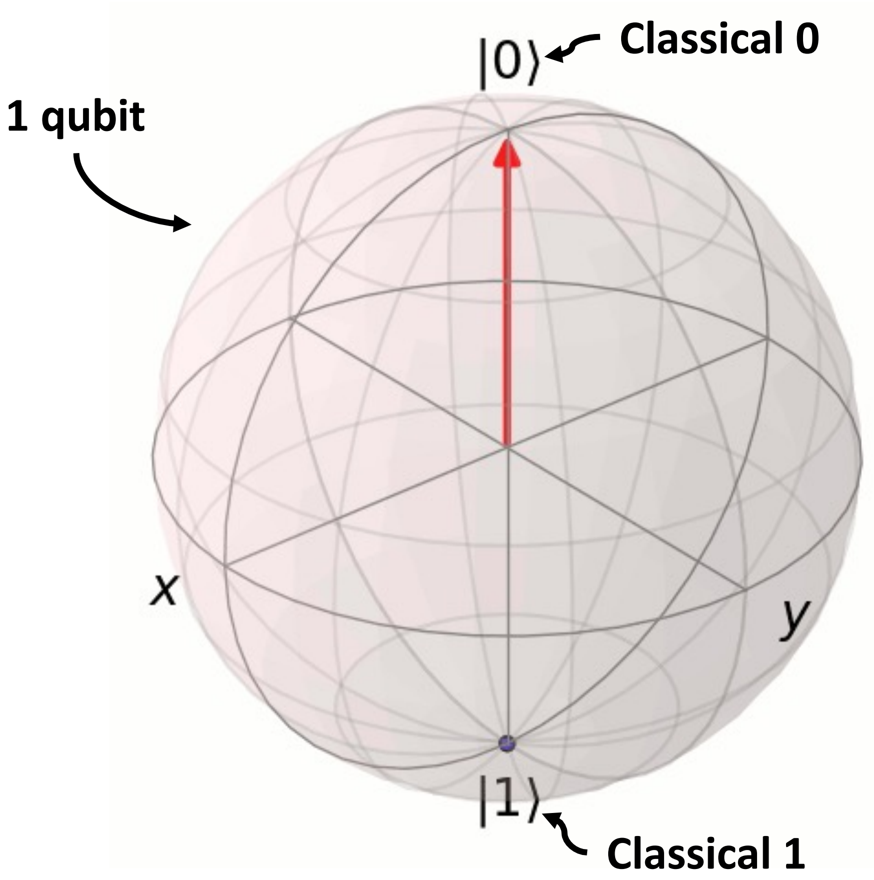
How does quantum work?



https://desireevl.com/posts/quantum-intro

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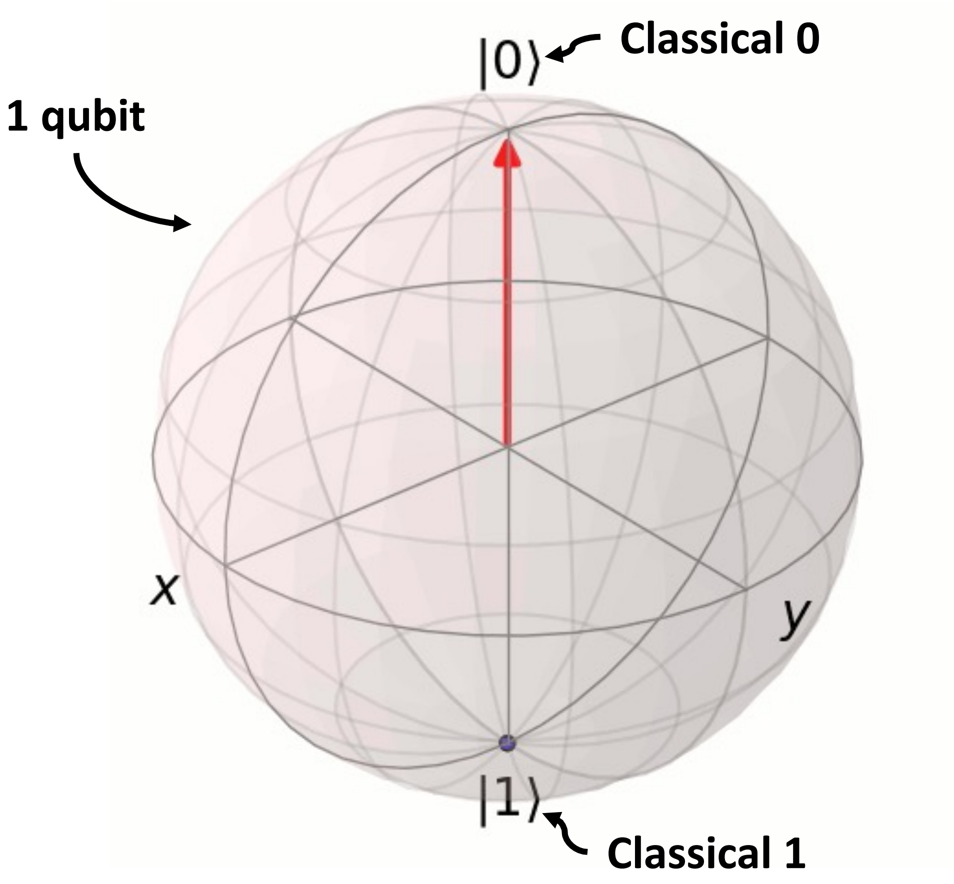


1 qubit → simultaneous 2^1 classical 1-bit states *
N qubits → simultaneous 2^N classical N-bit states *

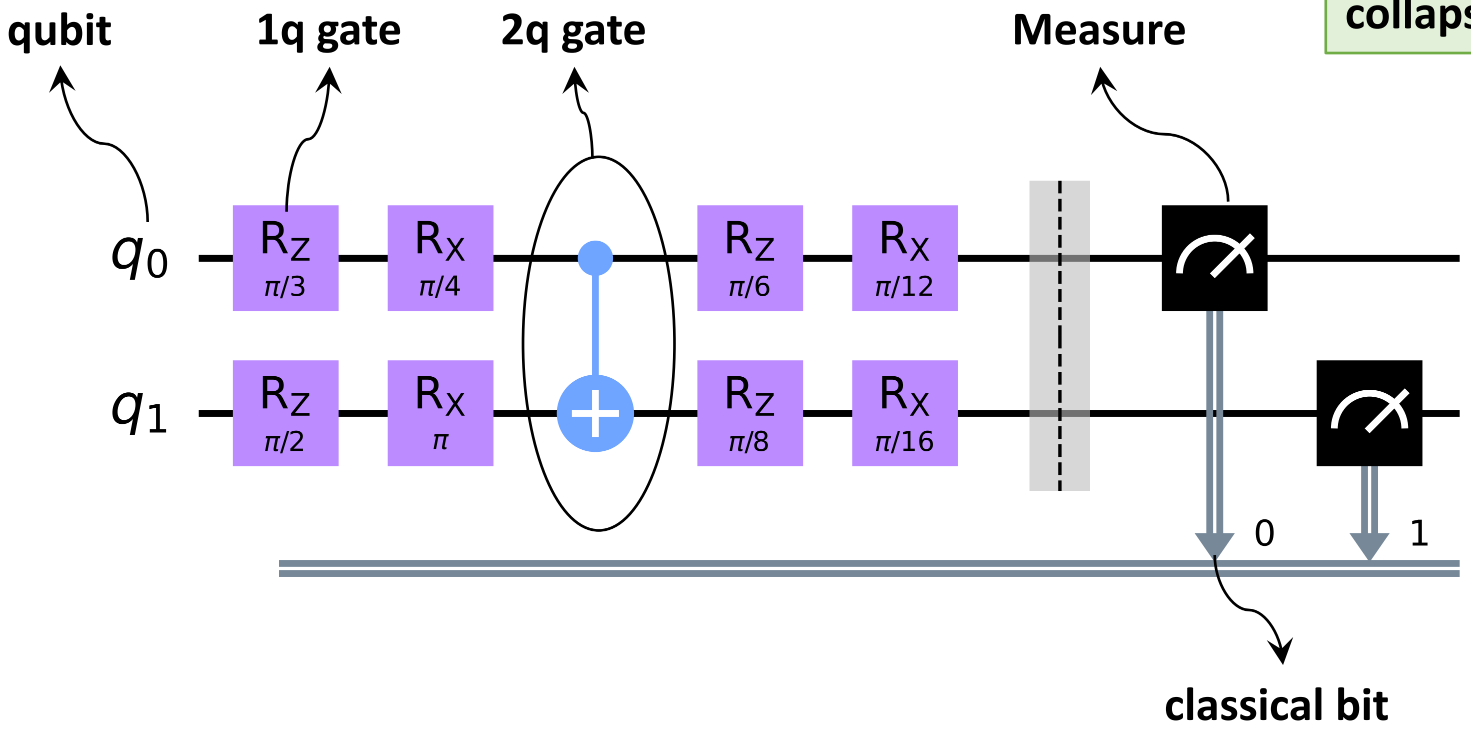
Quantum Advantage

https://desireevl.com/posts/quantum-intro

*** with some constraints**

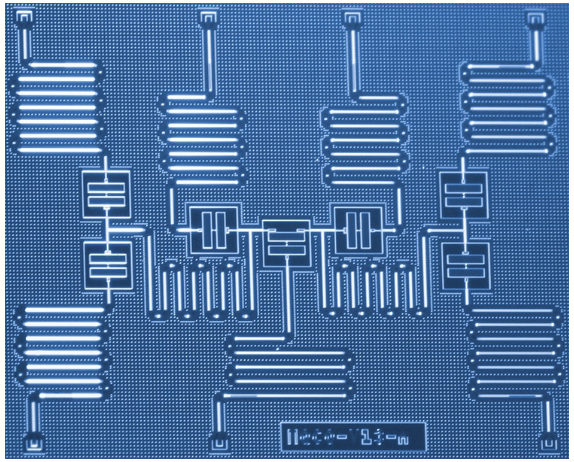
How does quantum work?

Internally computes on 2^N N-bit states, but collapses at measurement to 1 N-bit state.

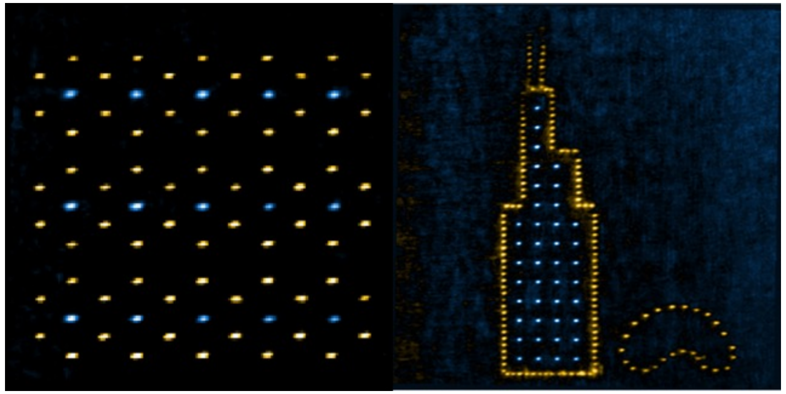


NISQ era: Many promising but imperfect quantum technologies

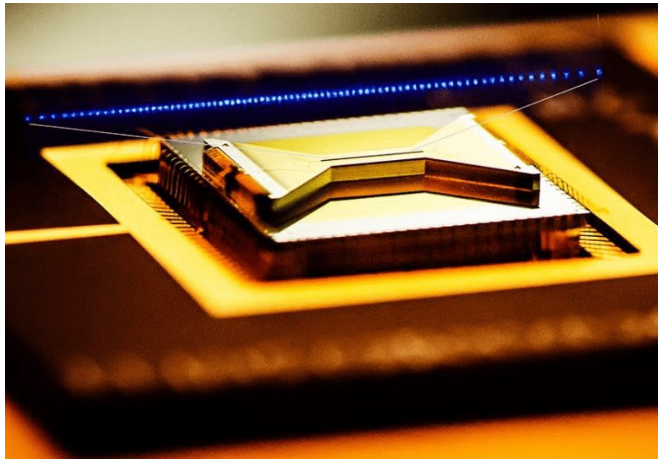
NISQ: Noisy Intermediate Scale Quantum → Few qubits, poor quality



Superconducting



Neutral atom



Trapped Ion

Gambetta:2017 npj Quantum Information; Singh:2022 Phys. Rev. X; STAQ / Duke University

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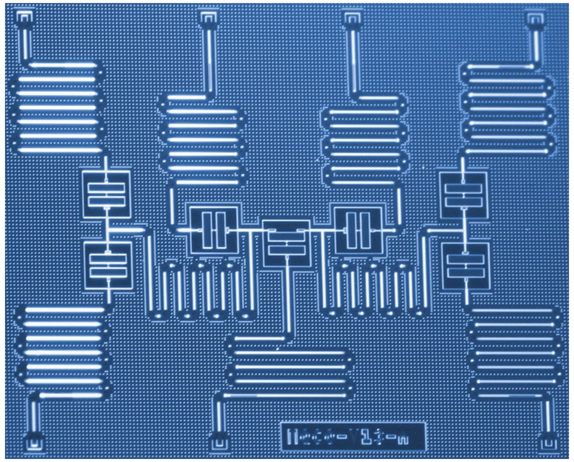
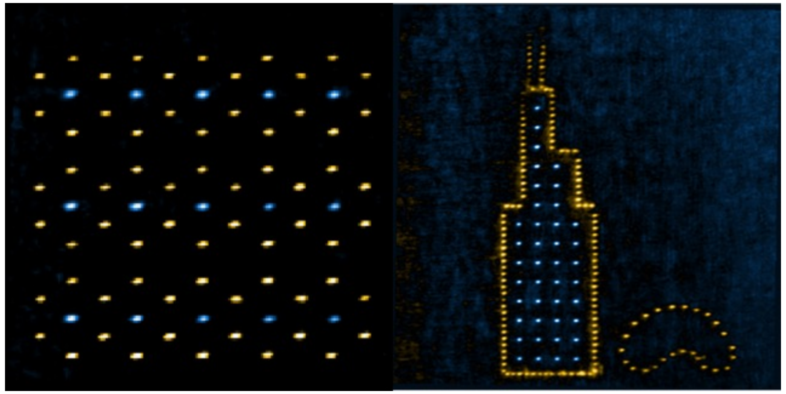


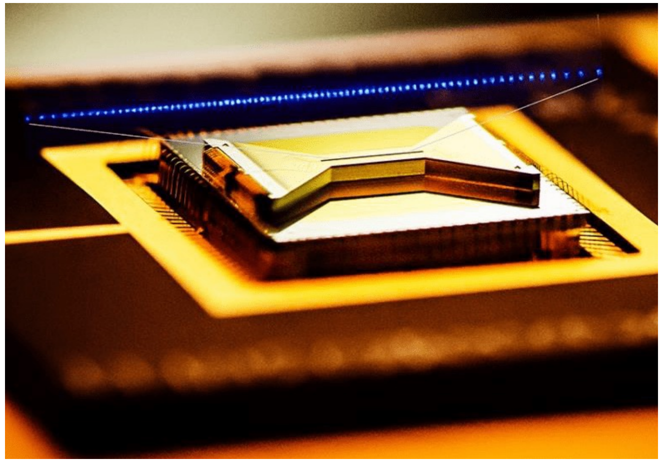
Superconducting

Qubit Lifetime
Gate Fidelity



Neutral atom

Gate Fidelity
Measurement

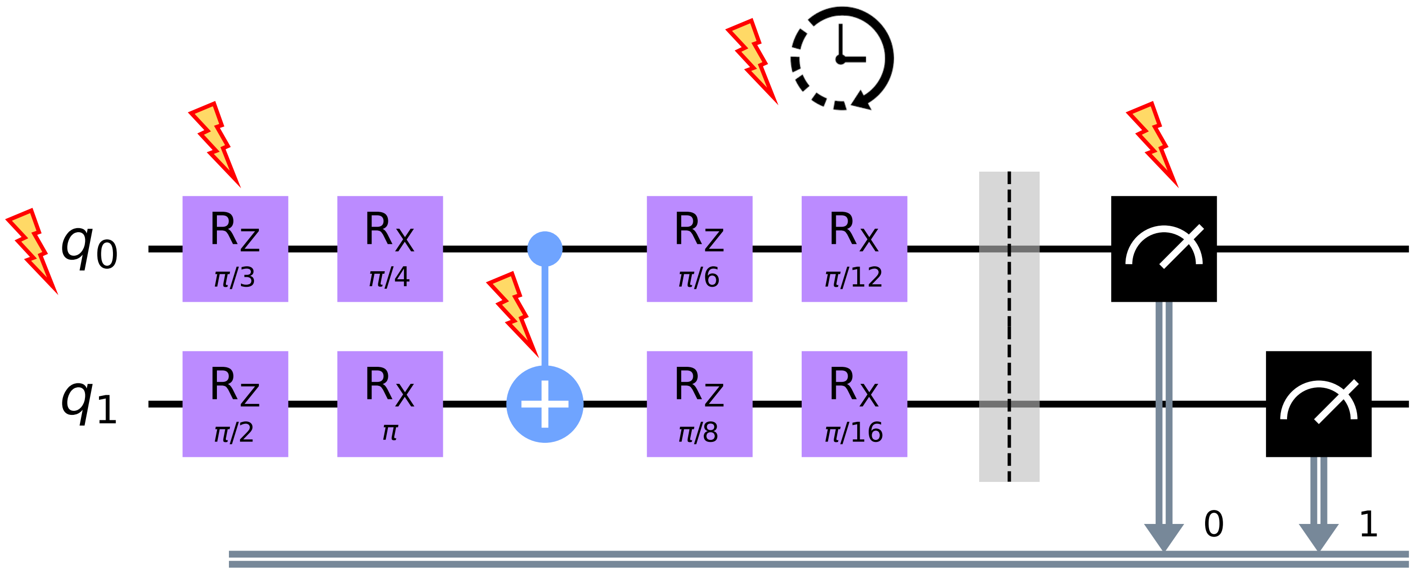


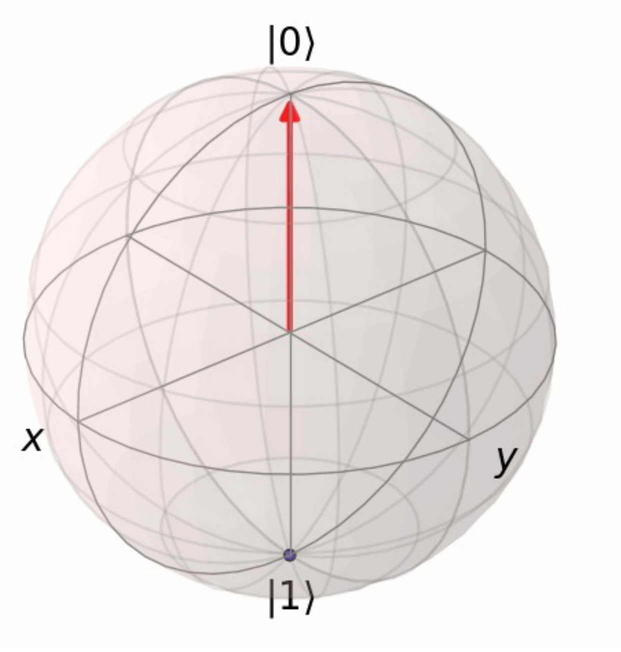
Trapped Ion

Scalability
Gate Speed

Gambetta:2017 npj Quantum Information; Singh:2022 Phys. Rev. X; STAQ / Duke University

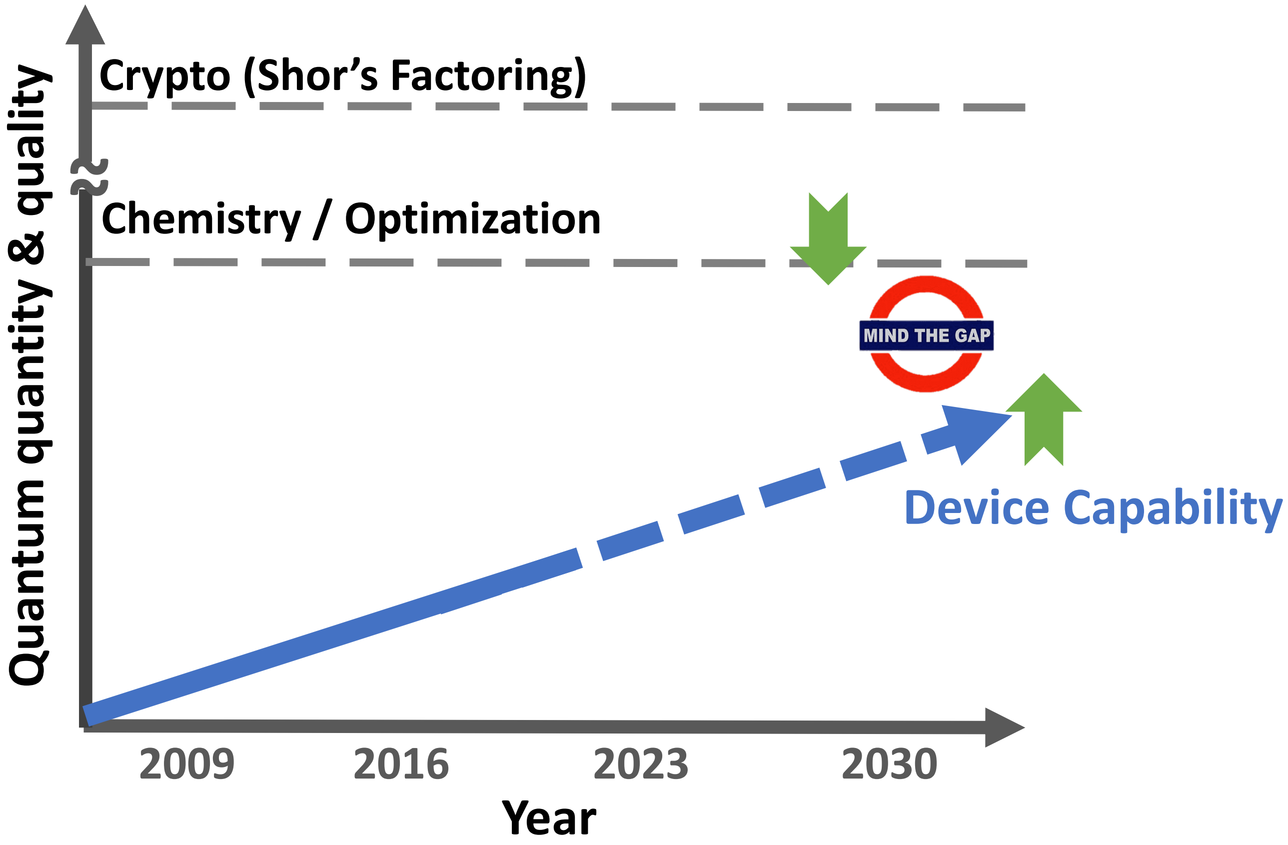
Noisy quantum circuits



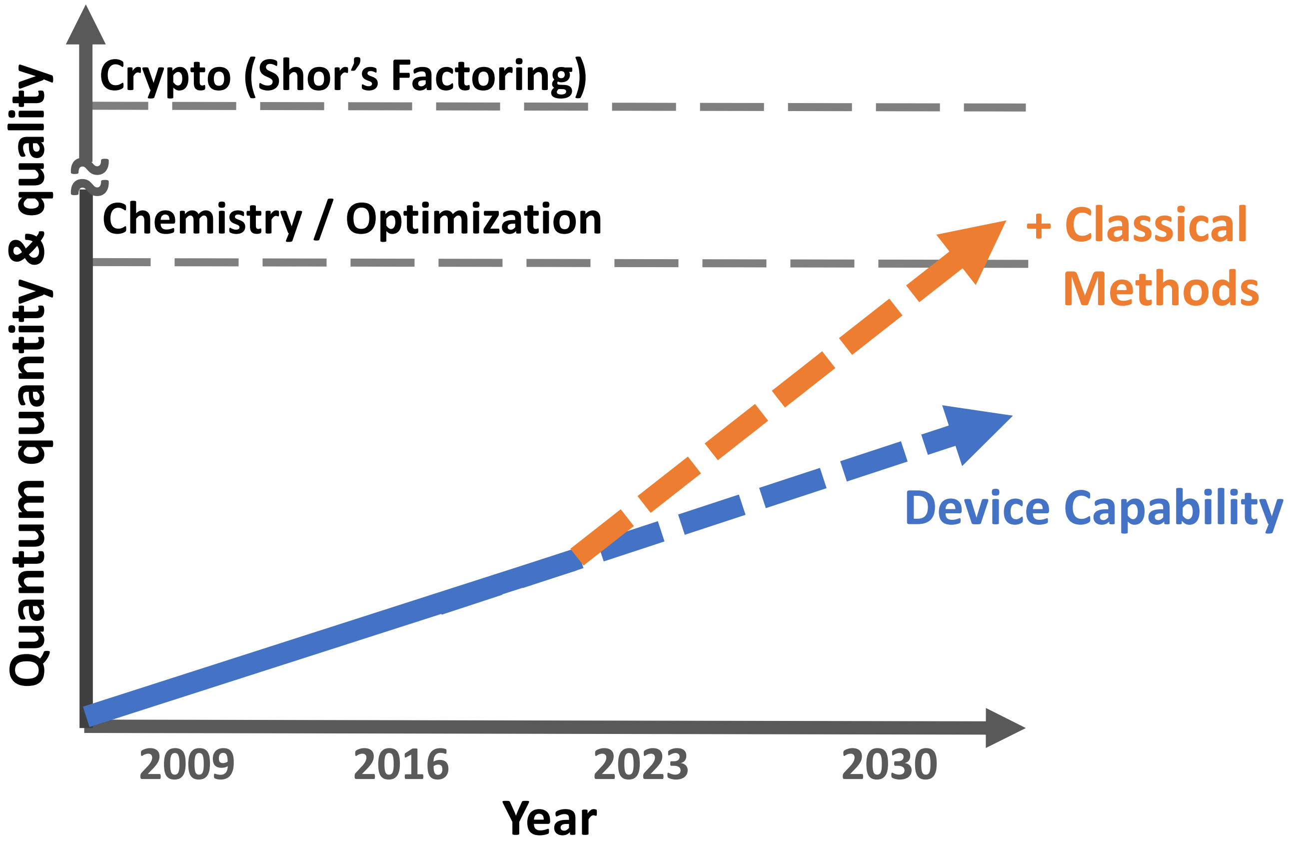


State prep error
qubit decoherence,
1Q/2Q gate errors,
crosstalk errors,
measurement errors

Bridging the quantum gap: Reduced application requirements + better technology?



Bridging the quantum gap: Classical computing approaches



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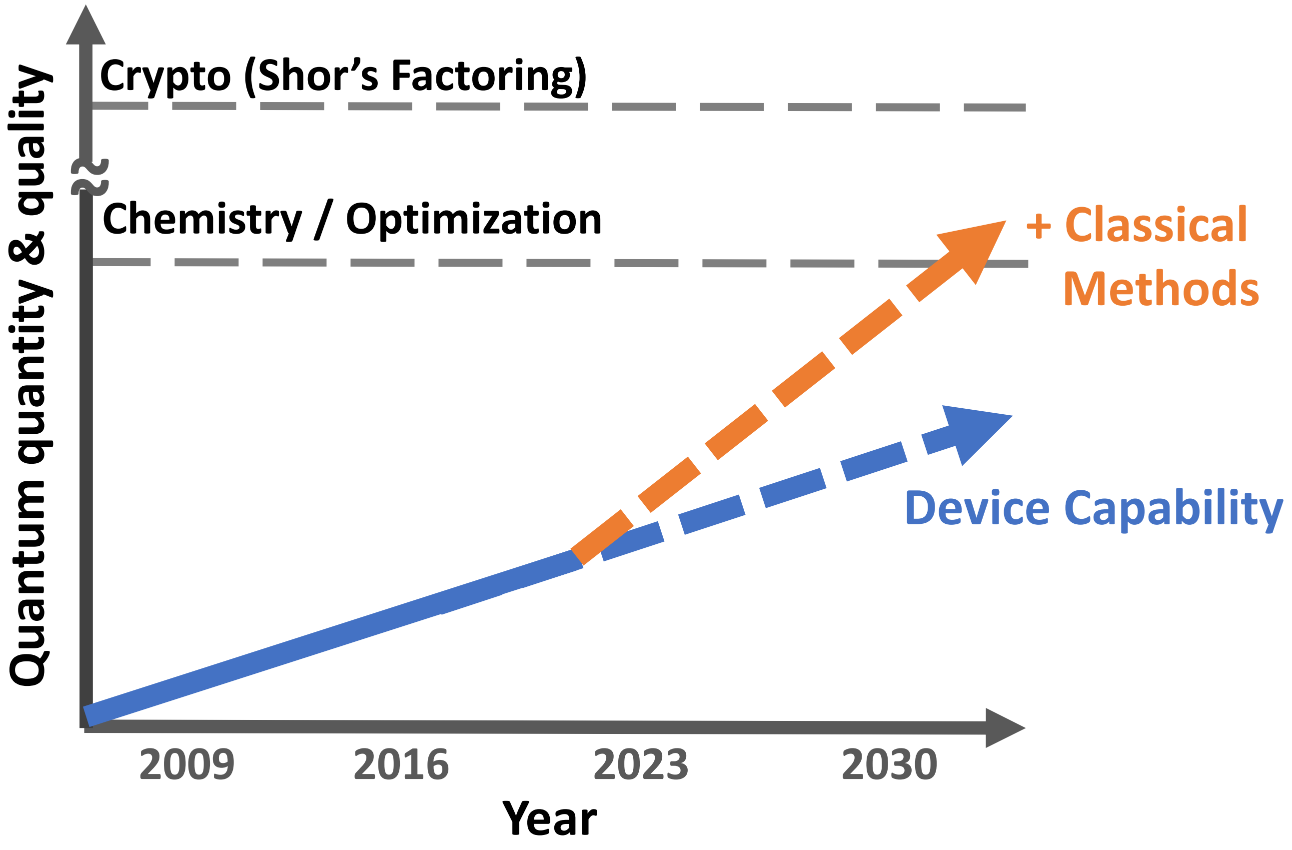
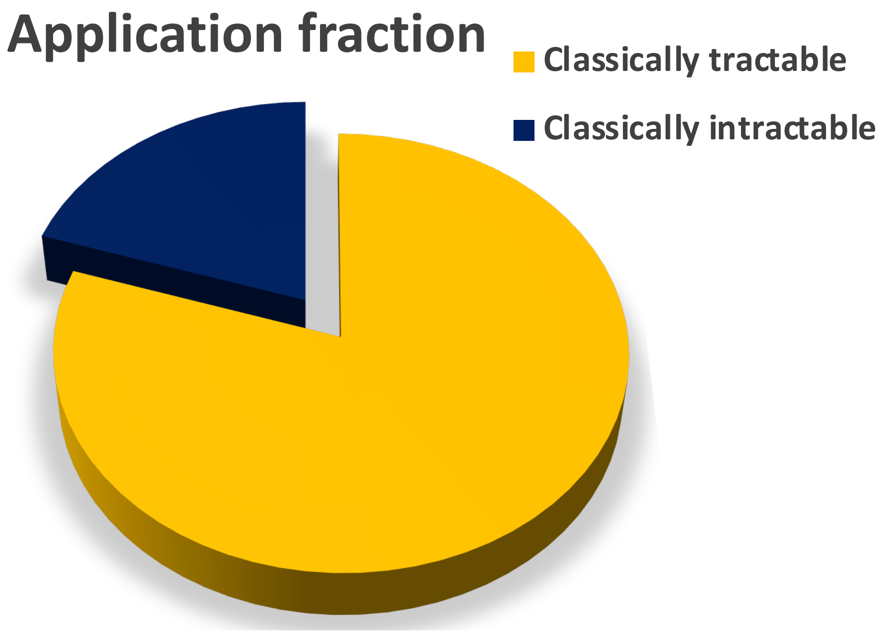


1. PL and Compilation
2. Computer Architecture
3. Classical simulation
4. High performance computing
5. Cryogenic hardware design
6. Noise modeling and Optimization
7. Multi-chip / distributed computing
8. Cloud resource modeling and management

#1) Classical simulation to alleviate quantum challenges



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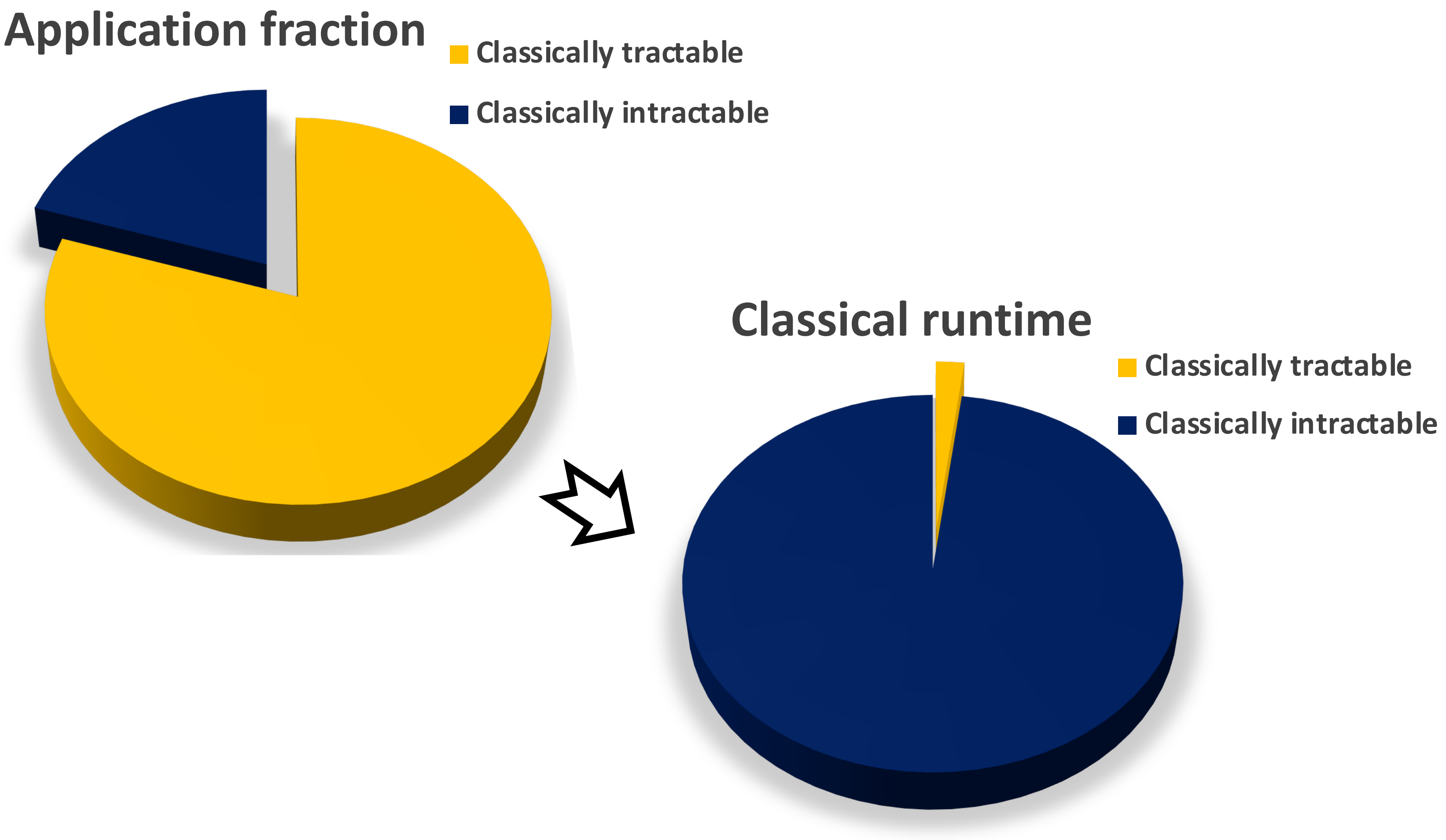

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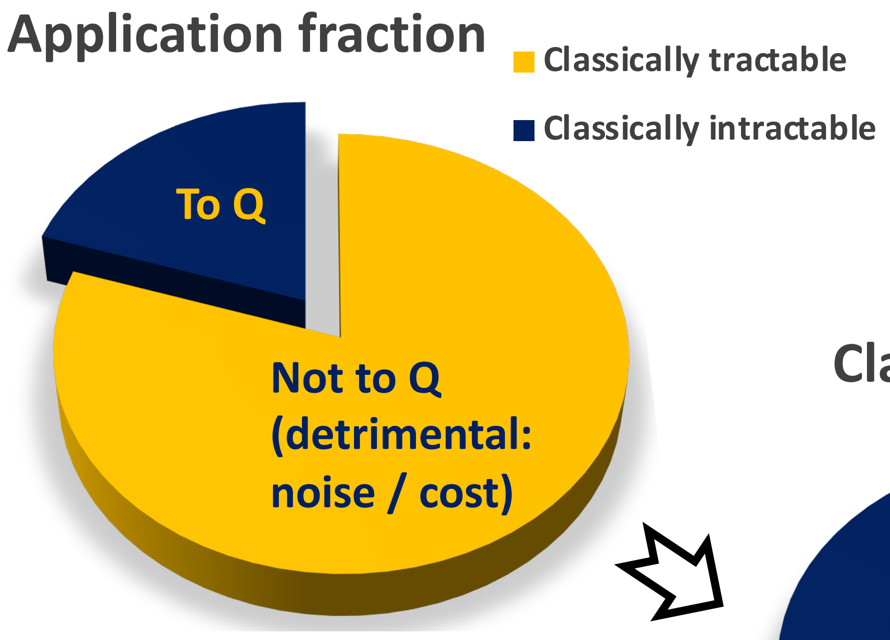

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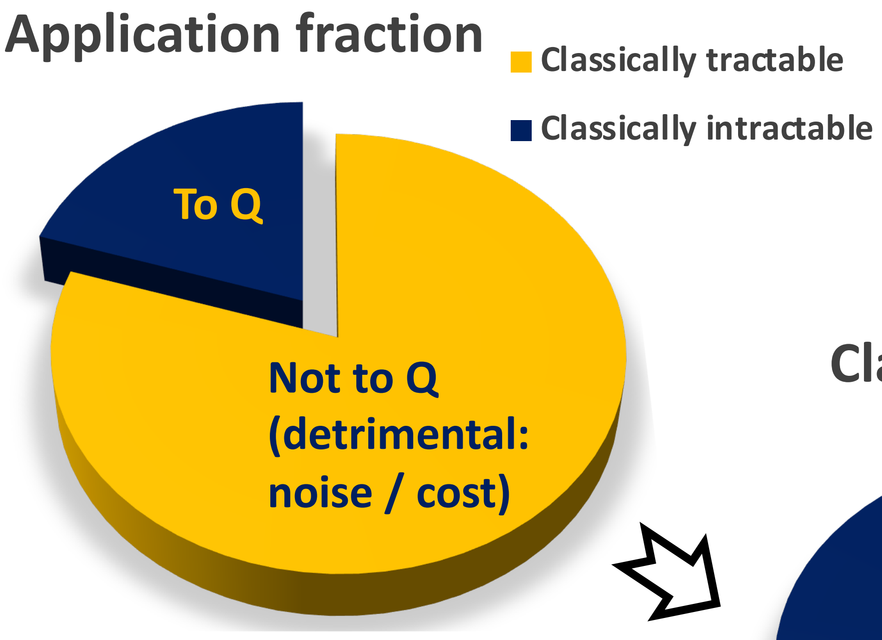
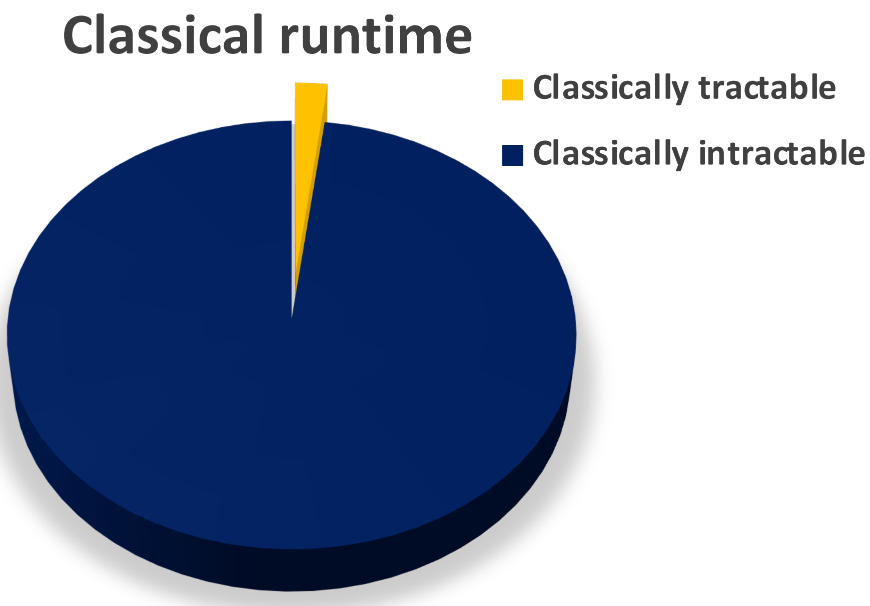
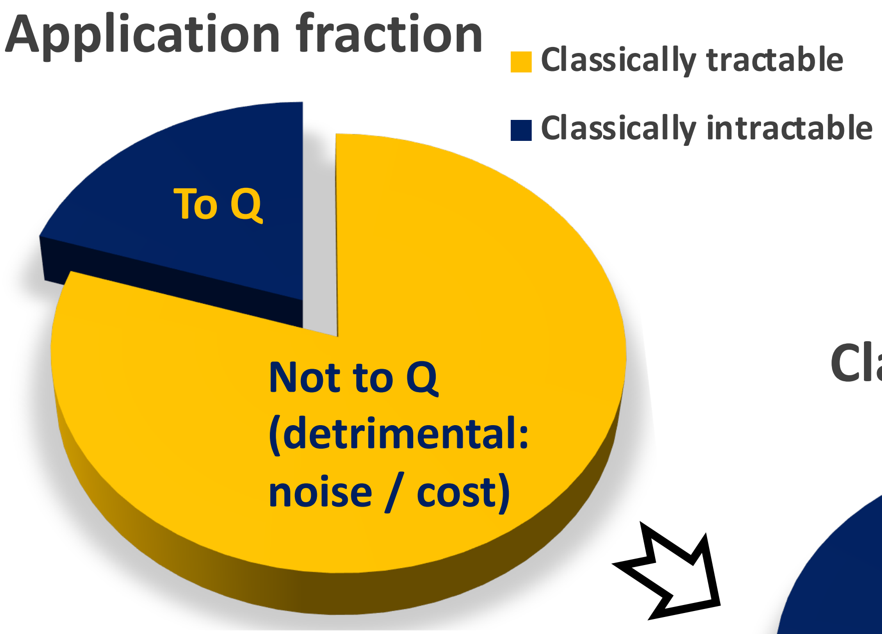


- *No clear separation between classical and quantum components.*
- *The classical tractability depends on the simulation platform.*

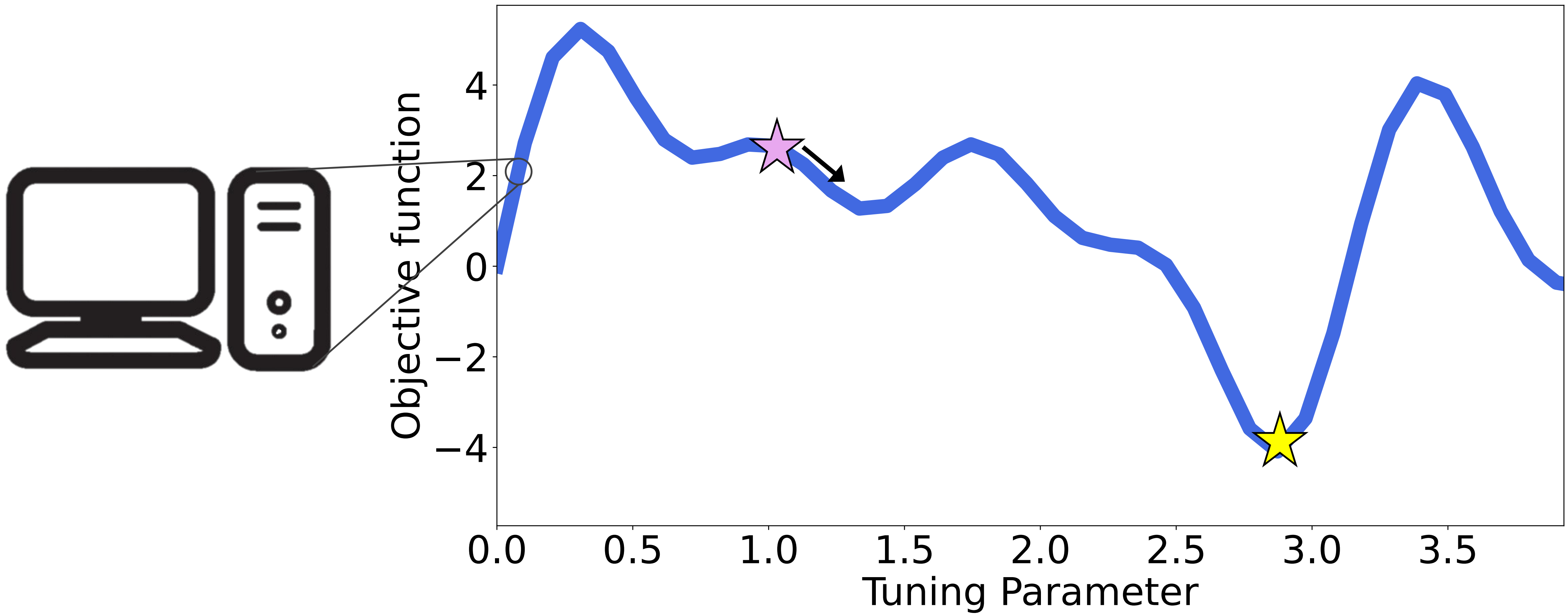


CAFQA: A Classical Simulation Bootstrap for Variational Quantum Algorithms

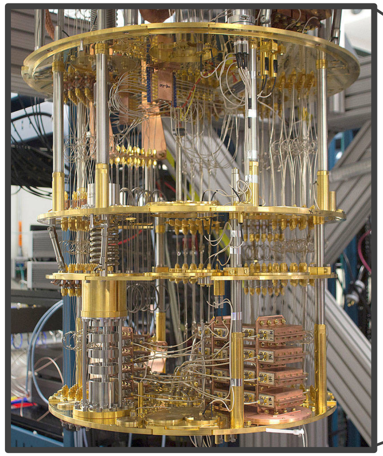
Gokul Ravi, Pranav Gokhale, Yi Ding, William Kirby, Kaitlin Smith, Jonathan Baker, Peter Love, Hank Hoffmann, Kenneth Brown, Frederic Chong. ASPLOS 2023 + QIP 2022

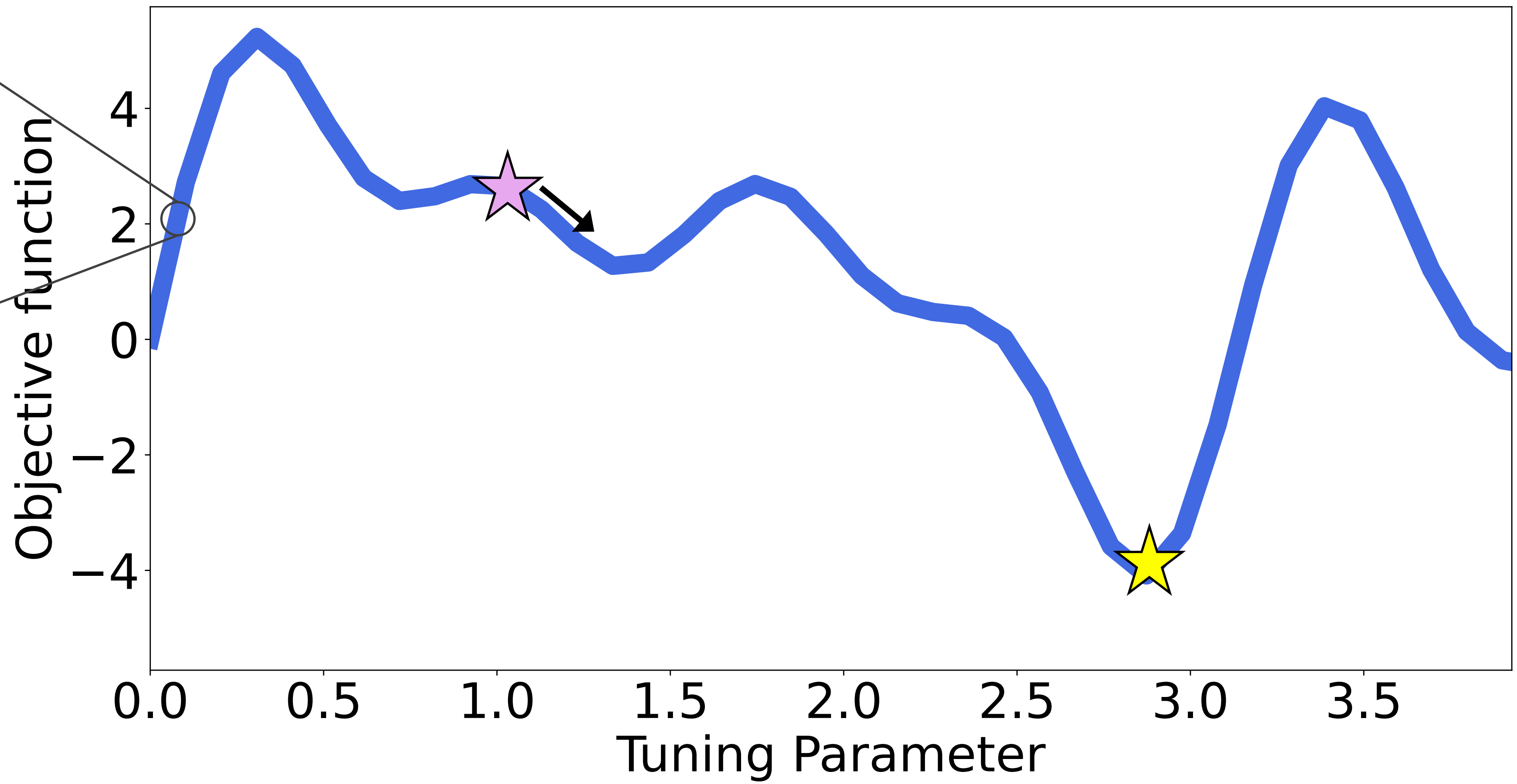


Navigating a classical optimization contour

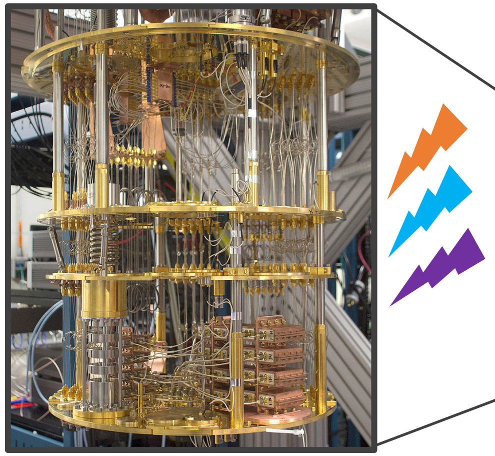


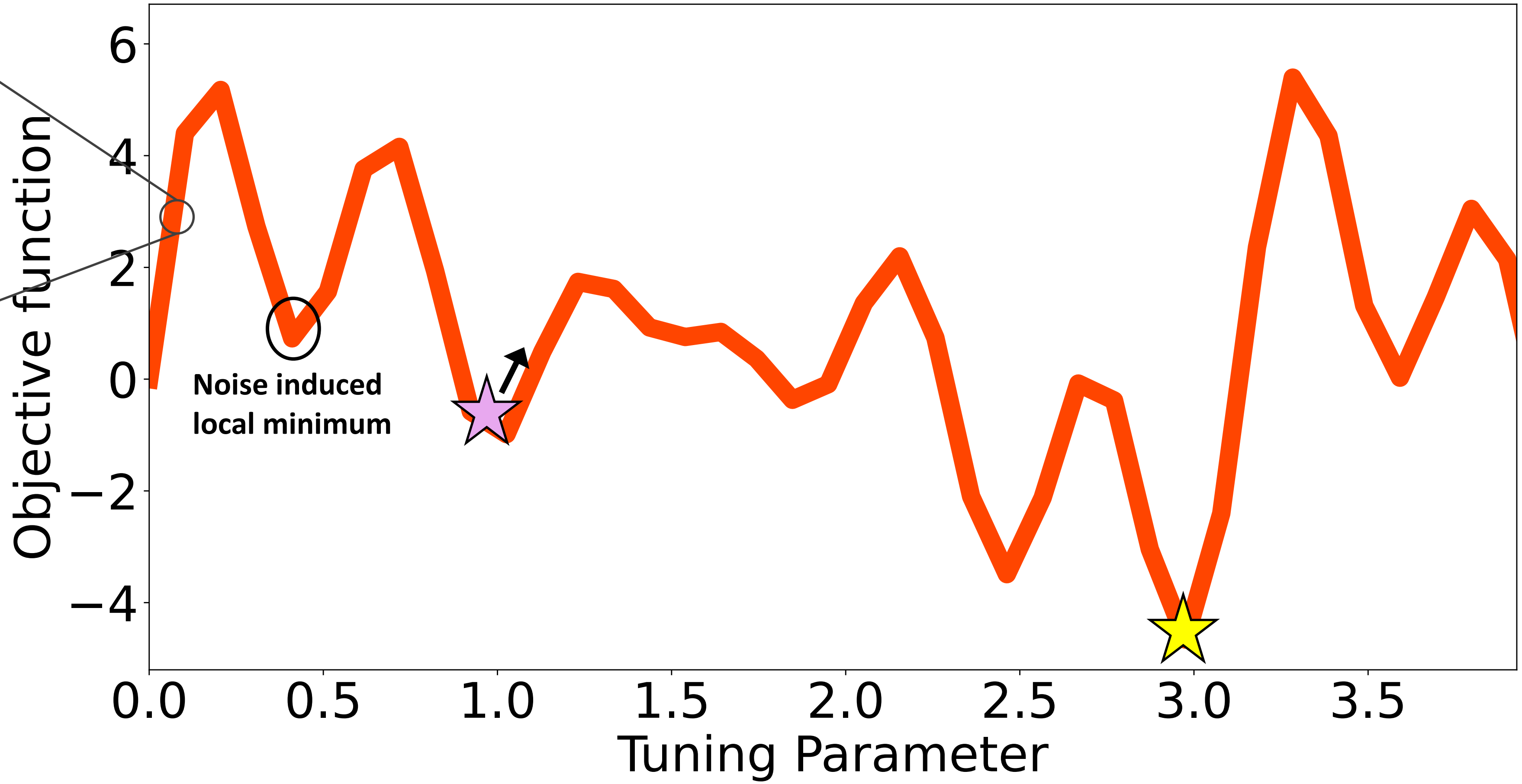
Navigating an ideal Variational Quantum Algorithm contour





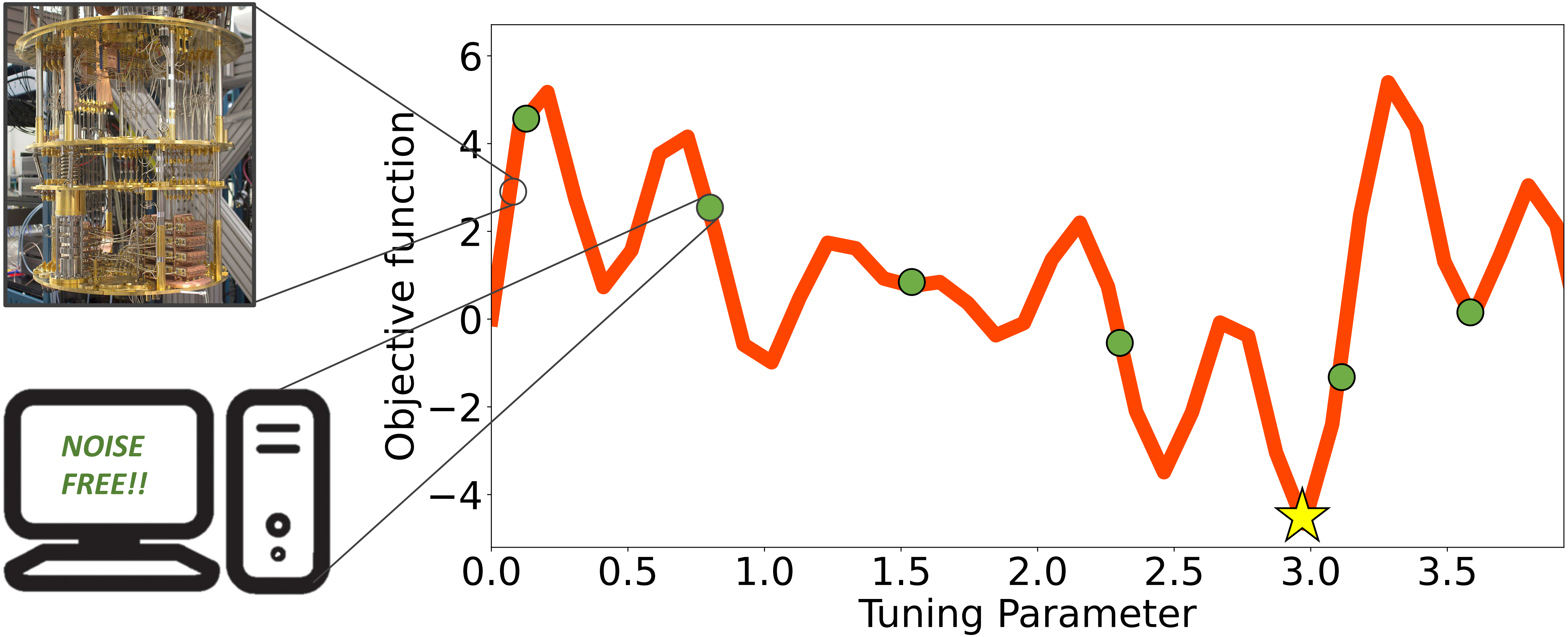
Navigating a noisy Variational Quantum Algorithm contour





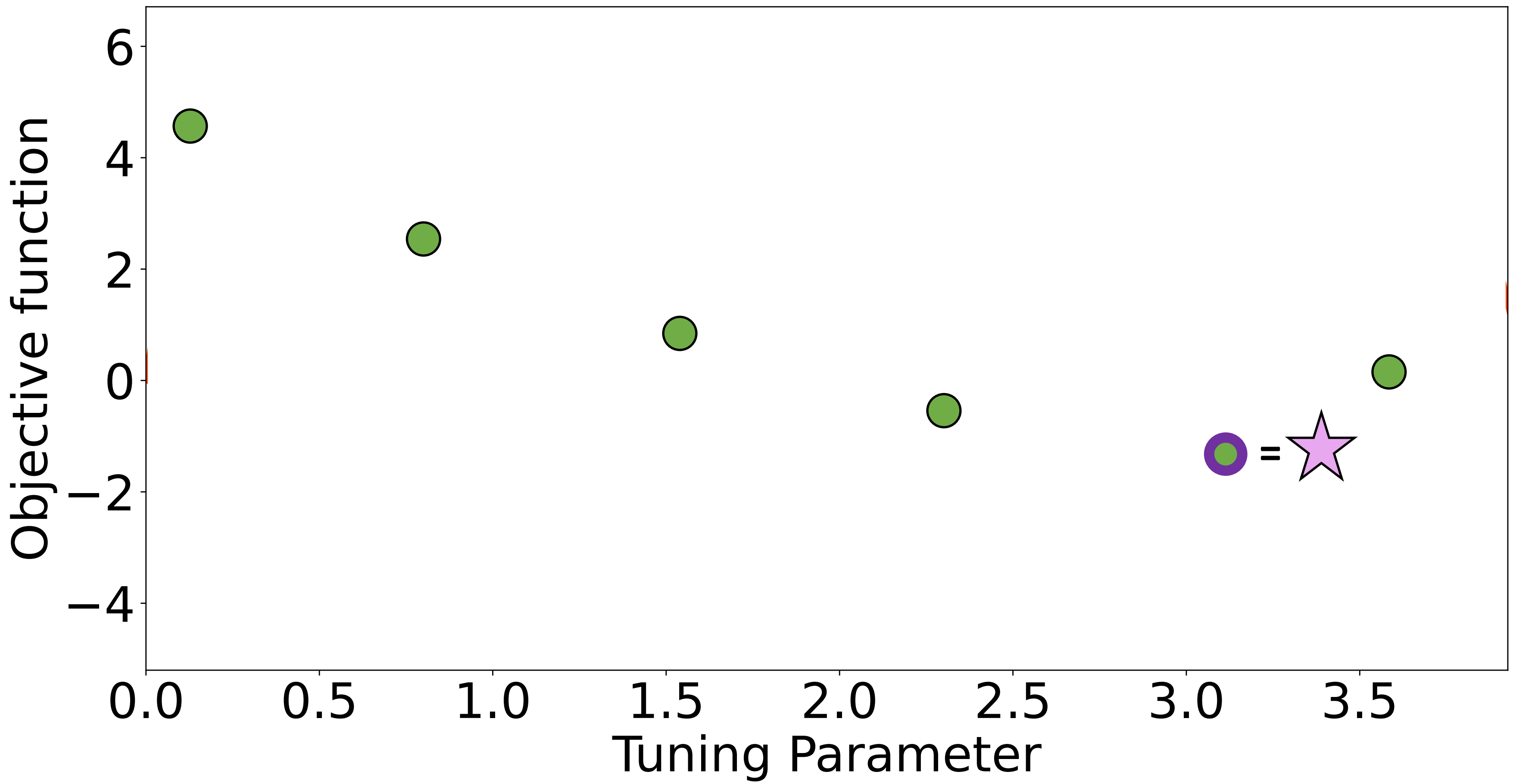
CAFQA: Clifford Ansatz For Quantum Accuracy

CAFQA Insight #1: Portion of the quantum space is classically simulable (Clifford space).



CAFQA: Clifford Ansatz For Quantum Accuracy

CAFQA Insight #2: Efficiently search the discrete space classically to find the lowest objective (w/ Bayesian Optimization).



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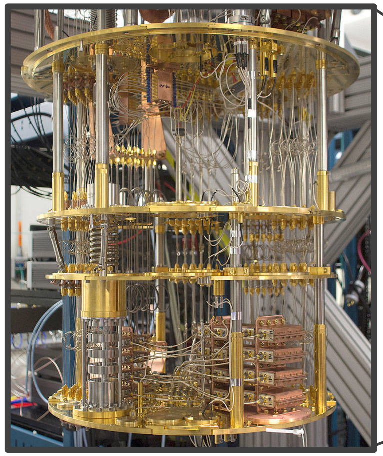

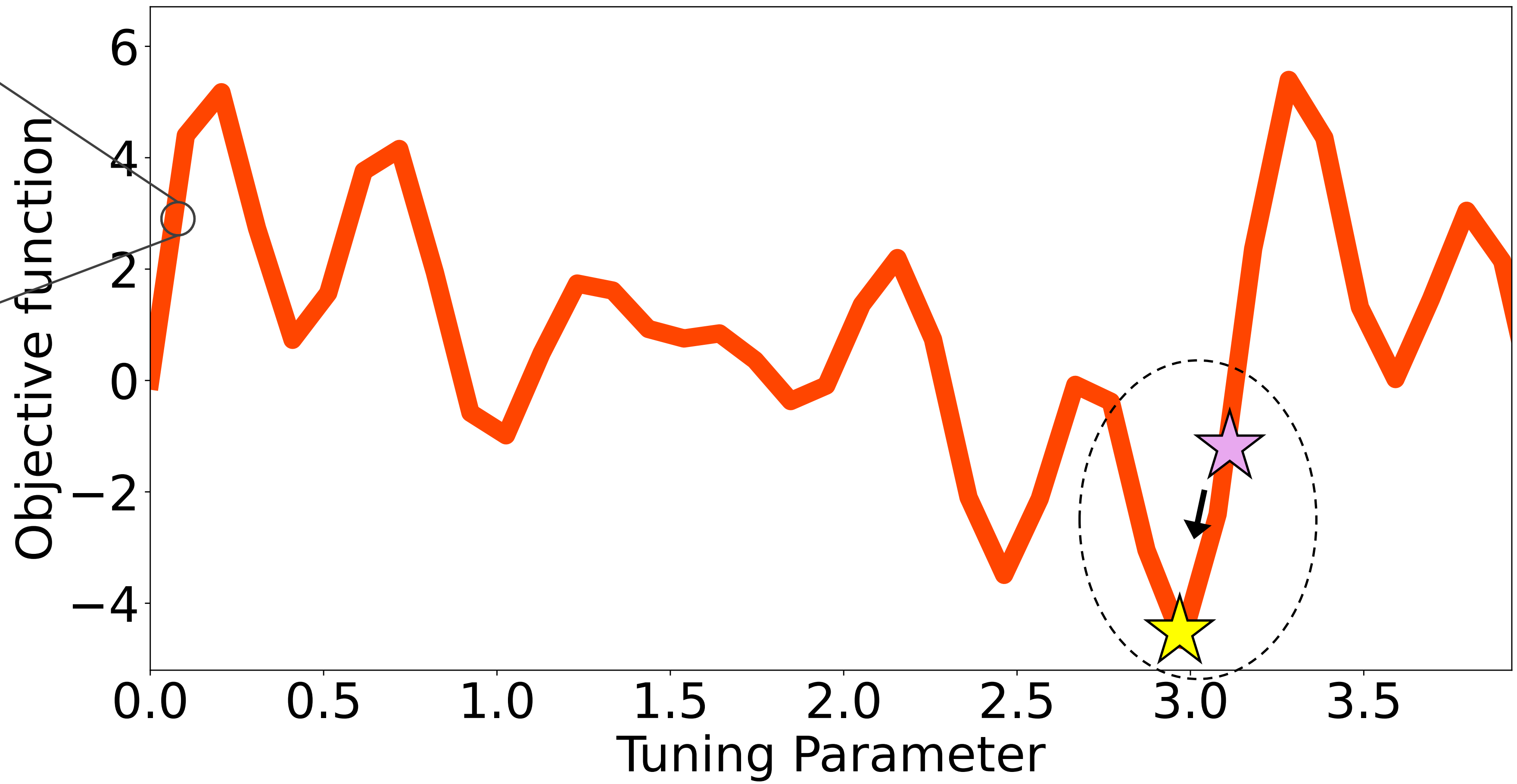

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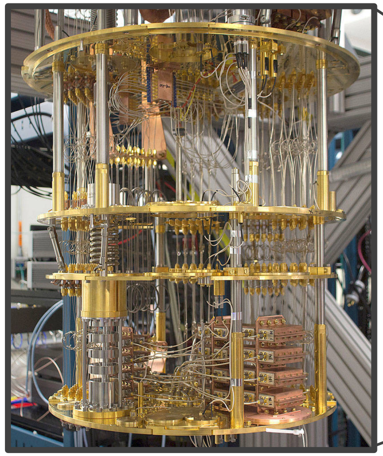
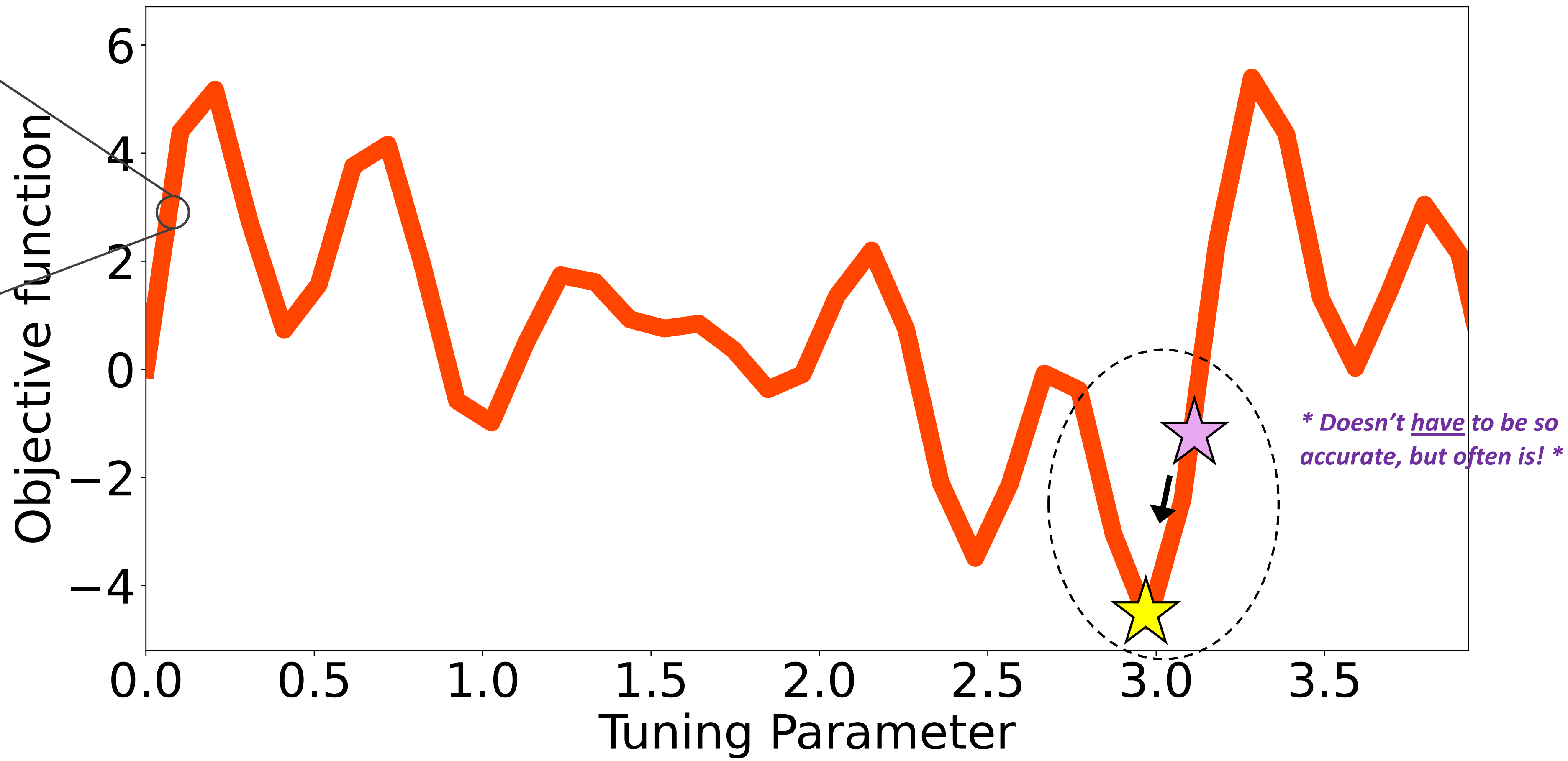
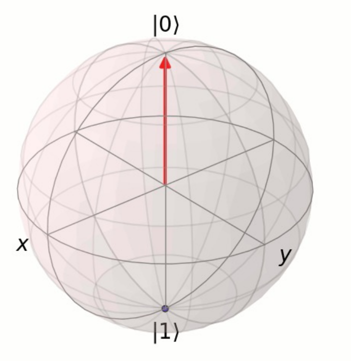
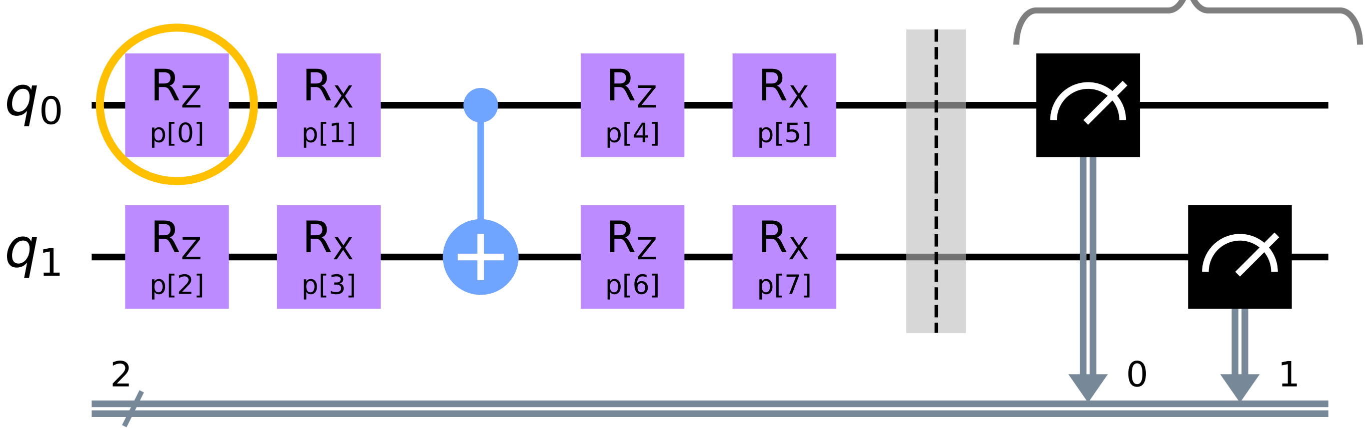


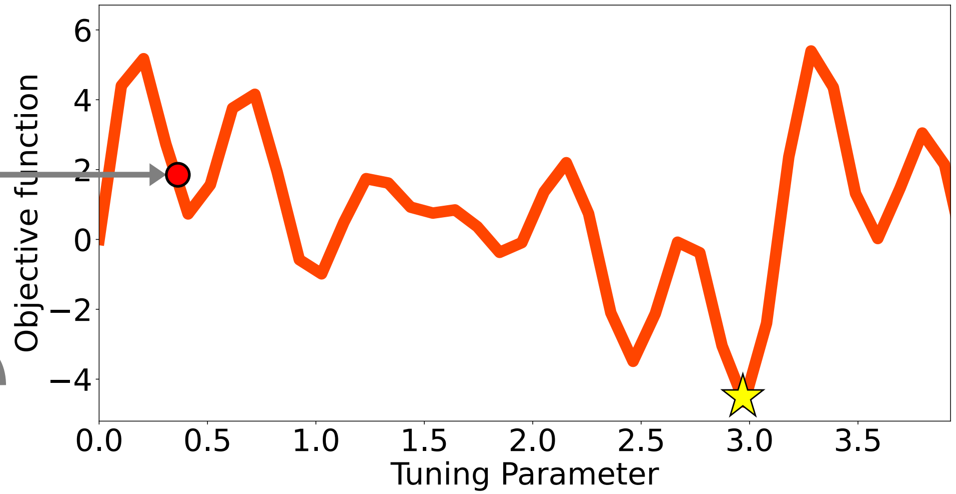


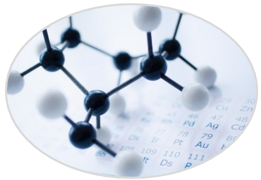
How VQA works



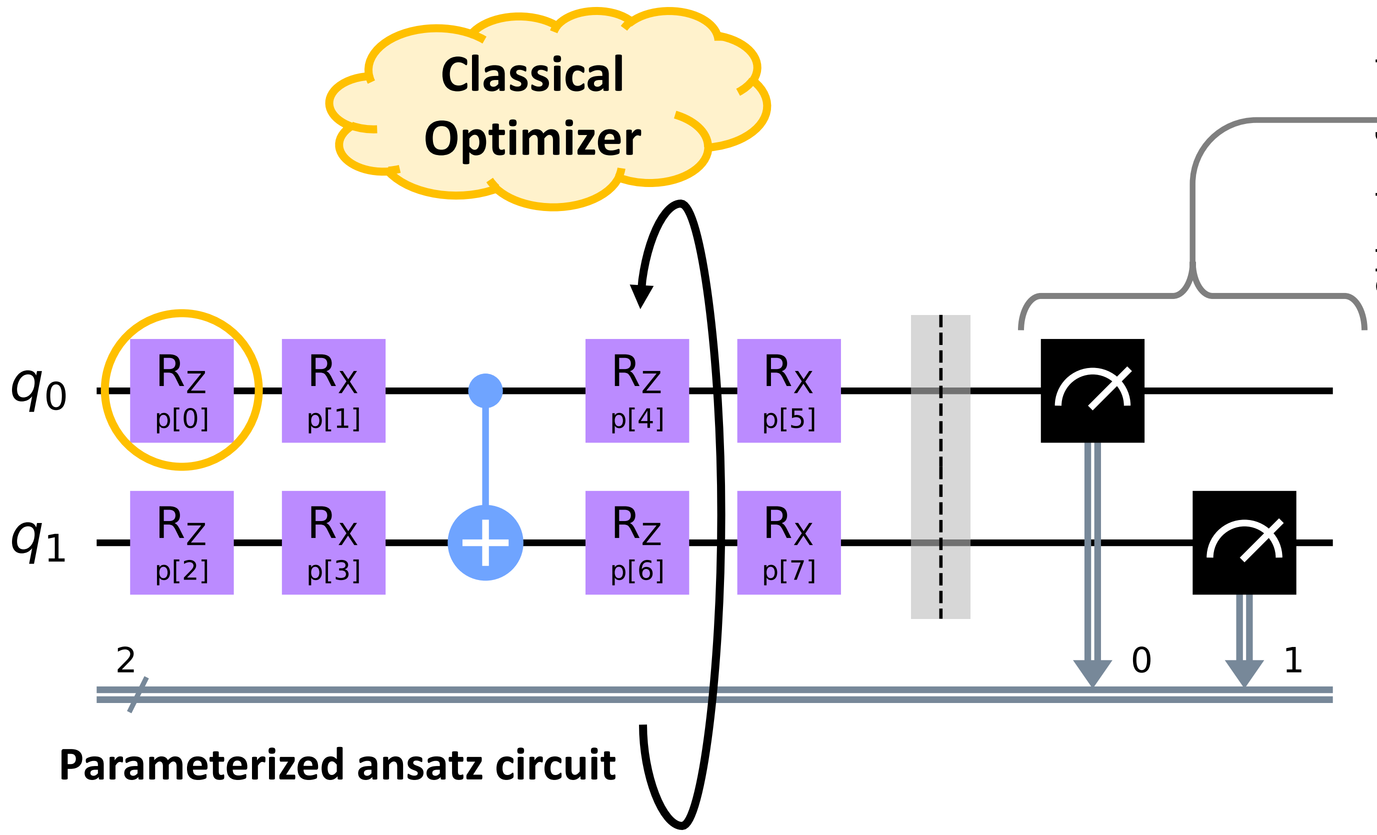


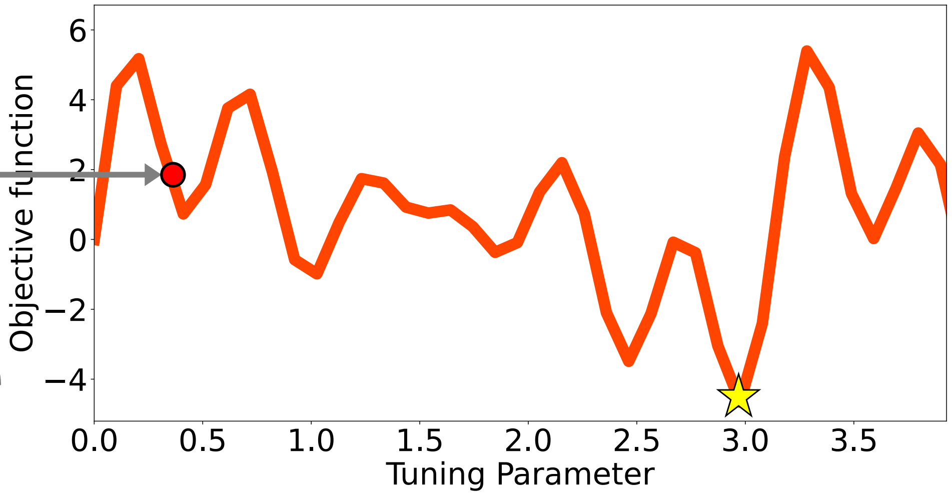
Parameterized ansatz circuit

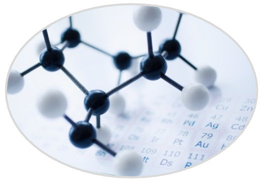




How VQA works

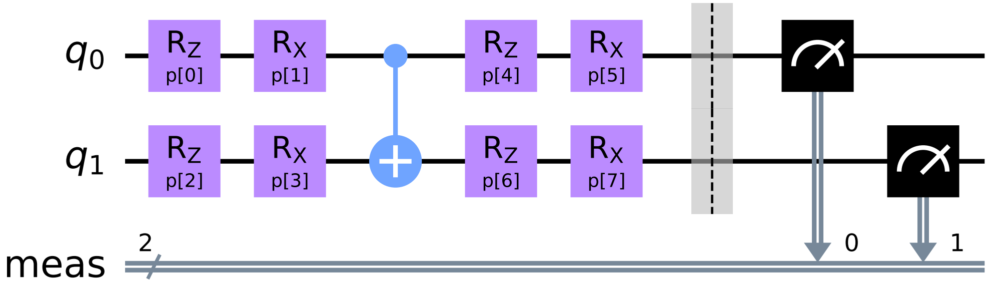






Classical simulability of Clifford quantum circuits

Parameterized ansatz circuit



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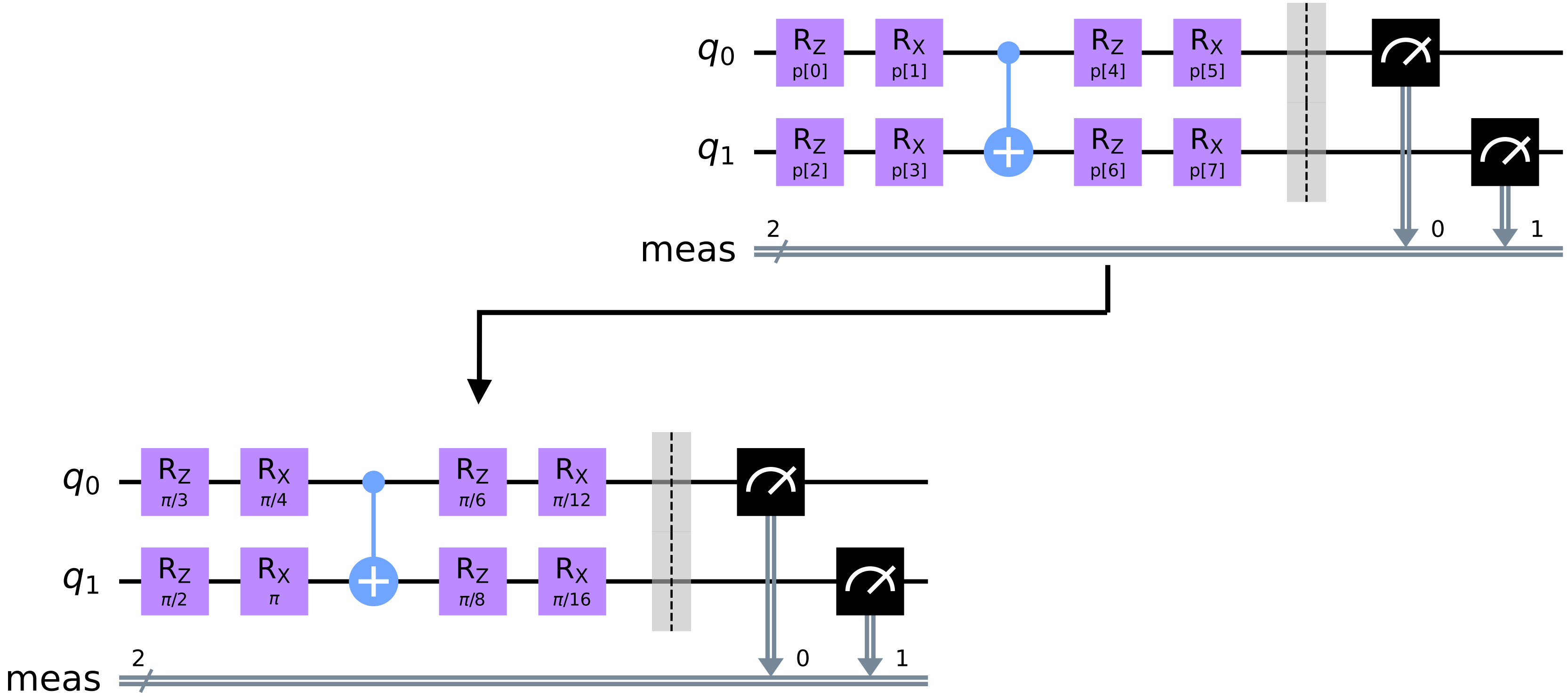


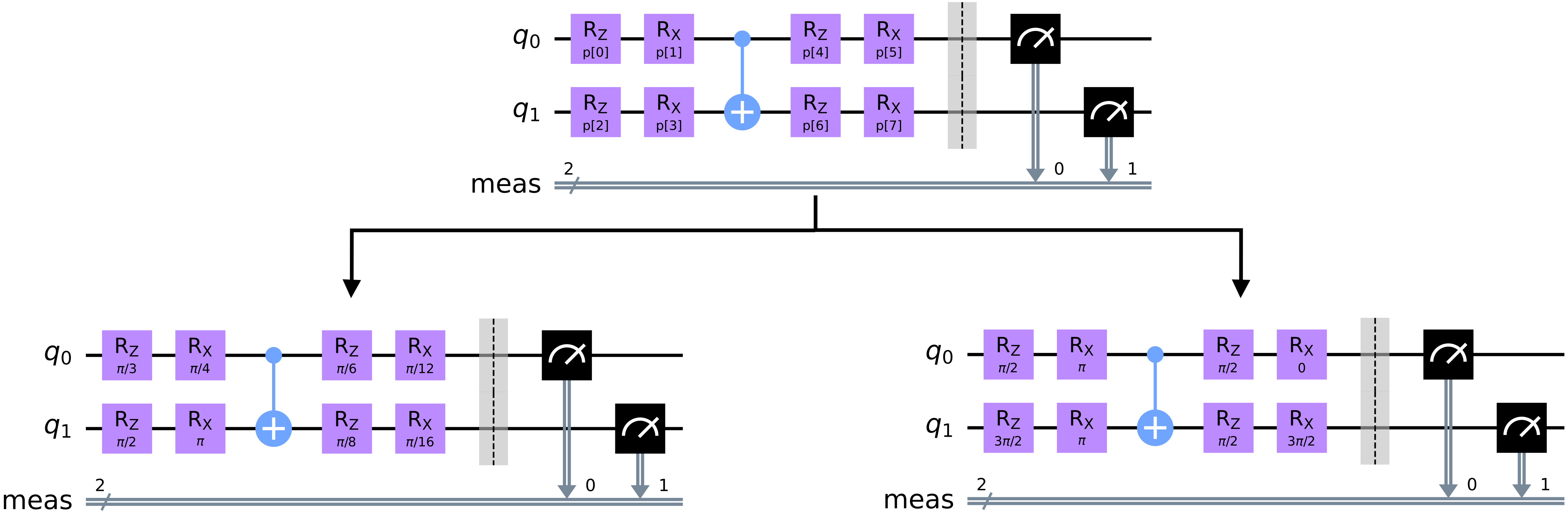
A classically <u>intractable general</u> circuit

Continuous angles = [0, 2*pi]

Classical simulability of Clifford quantum circuits

Gottesman–Knill theorem [‘98] - A QC circuit can be classically simulated efficiently if: (a) it has only Clifford gates, (b) classical qubit prep and measurement.

Parameterized ansatz circuit



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Continuous angles = [0, 2*pi]

A classically <u>simulable Clifford</u> circuit

Discrete angles = {0, pi/2, pi, 3*pi/2}

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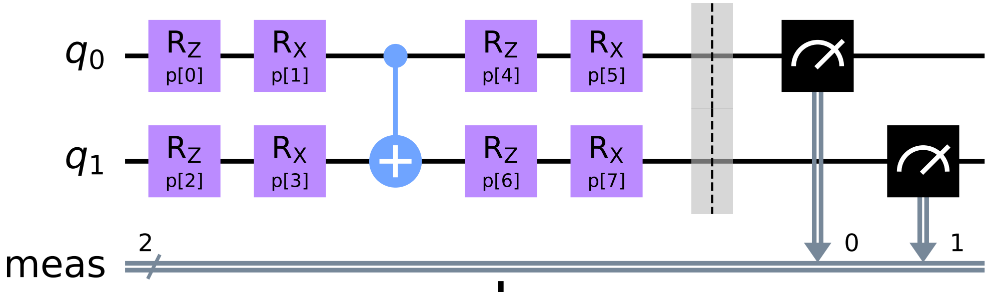

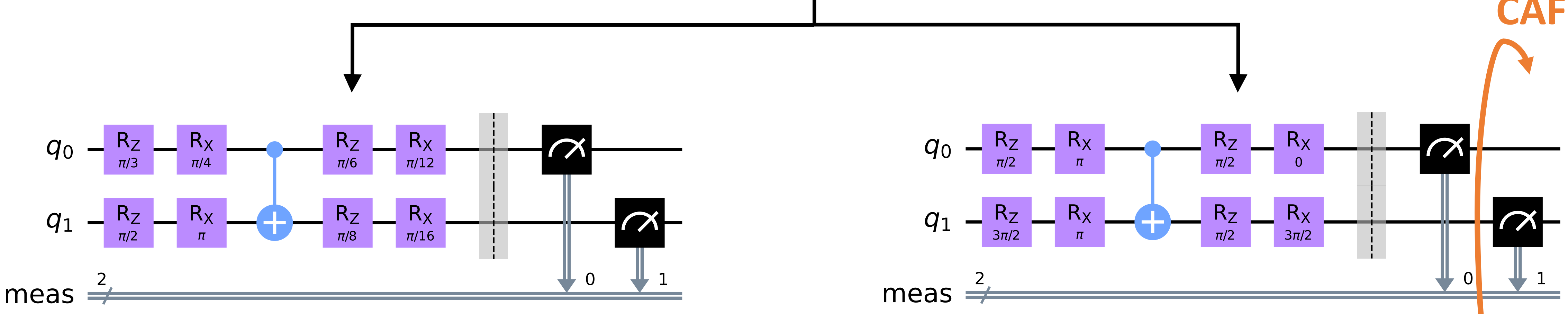

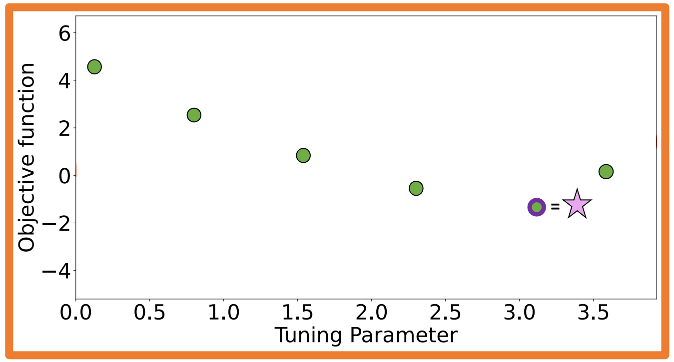

CAFQA

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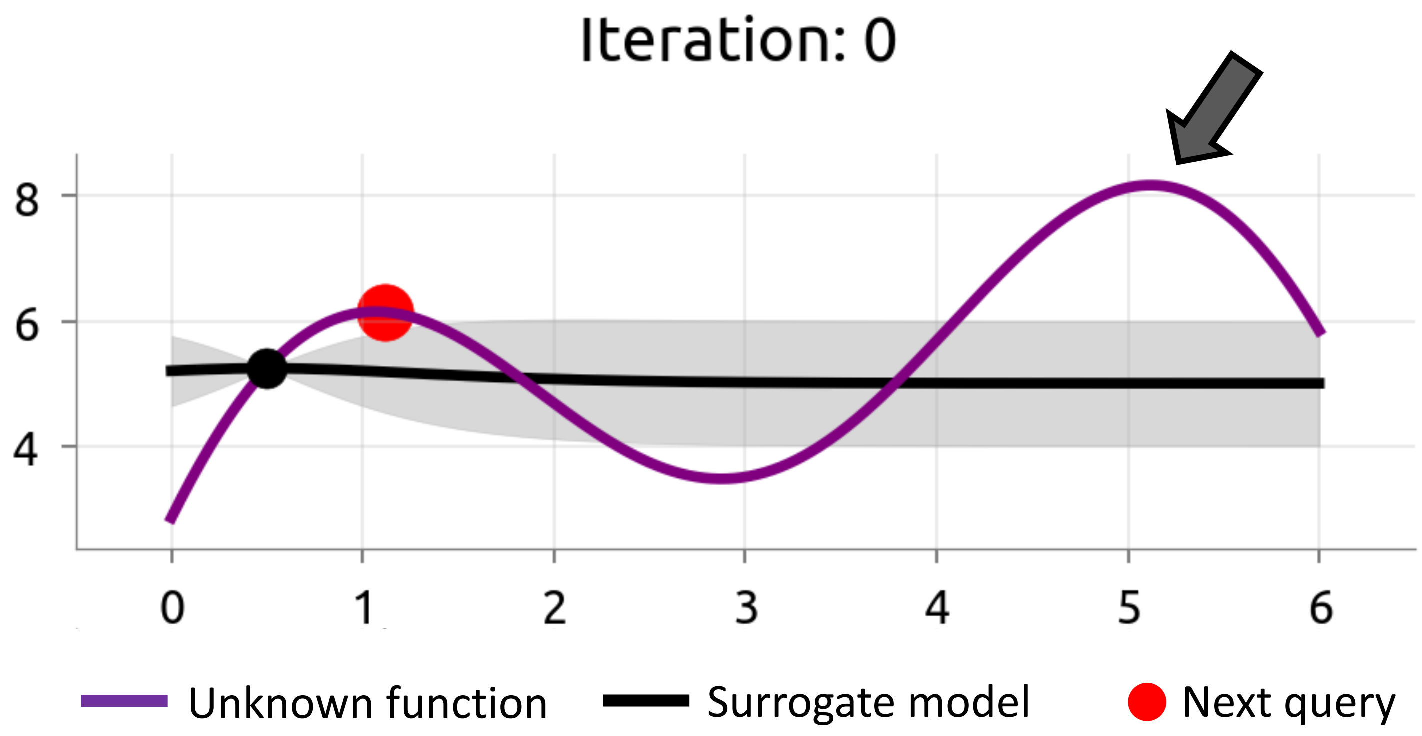
Finding the optimal Clifford point: Bayesian Optimization



https://distill.pub/2020/bayesian-optimization/

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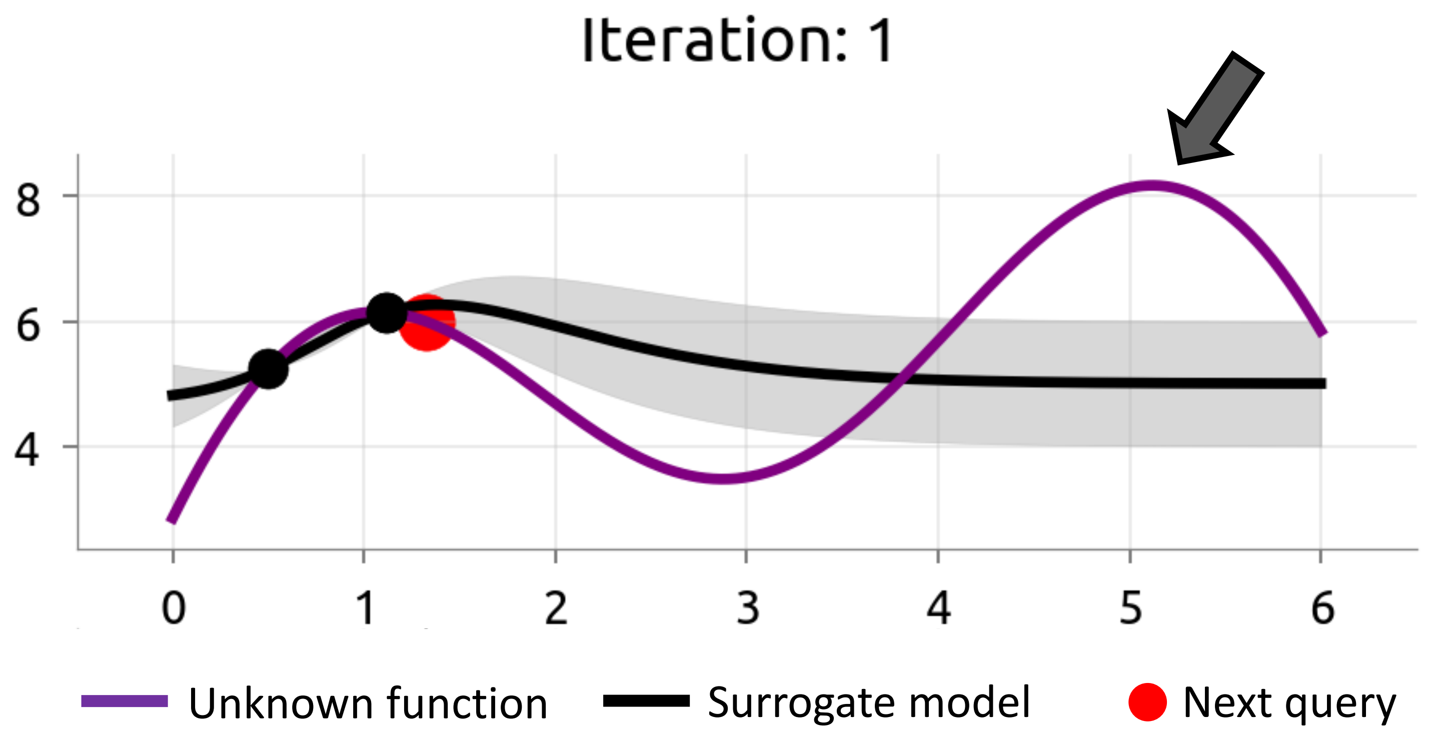

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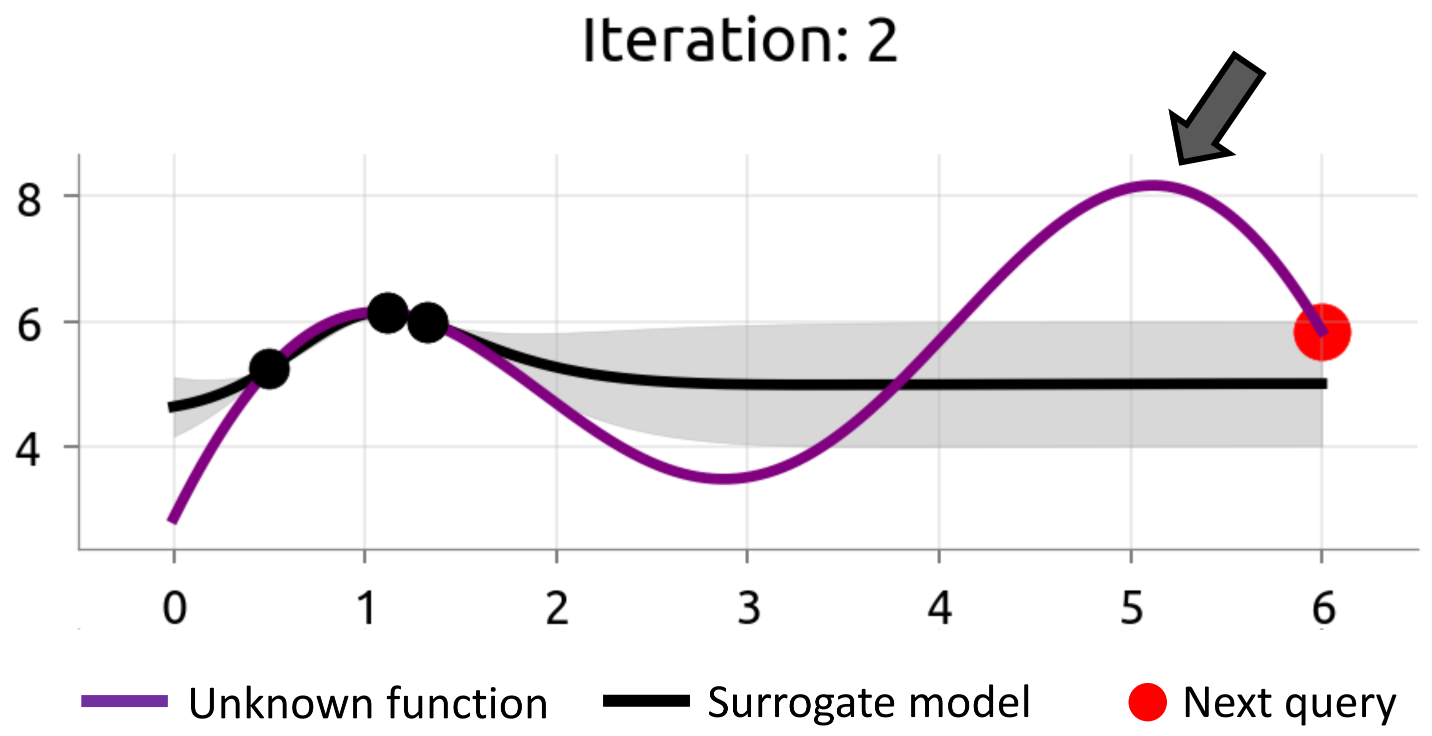

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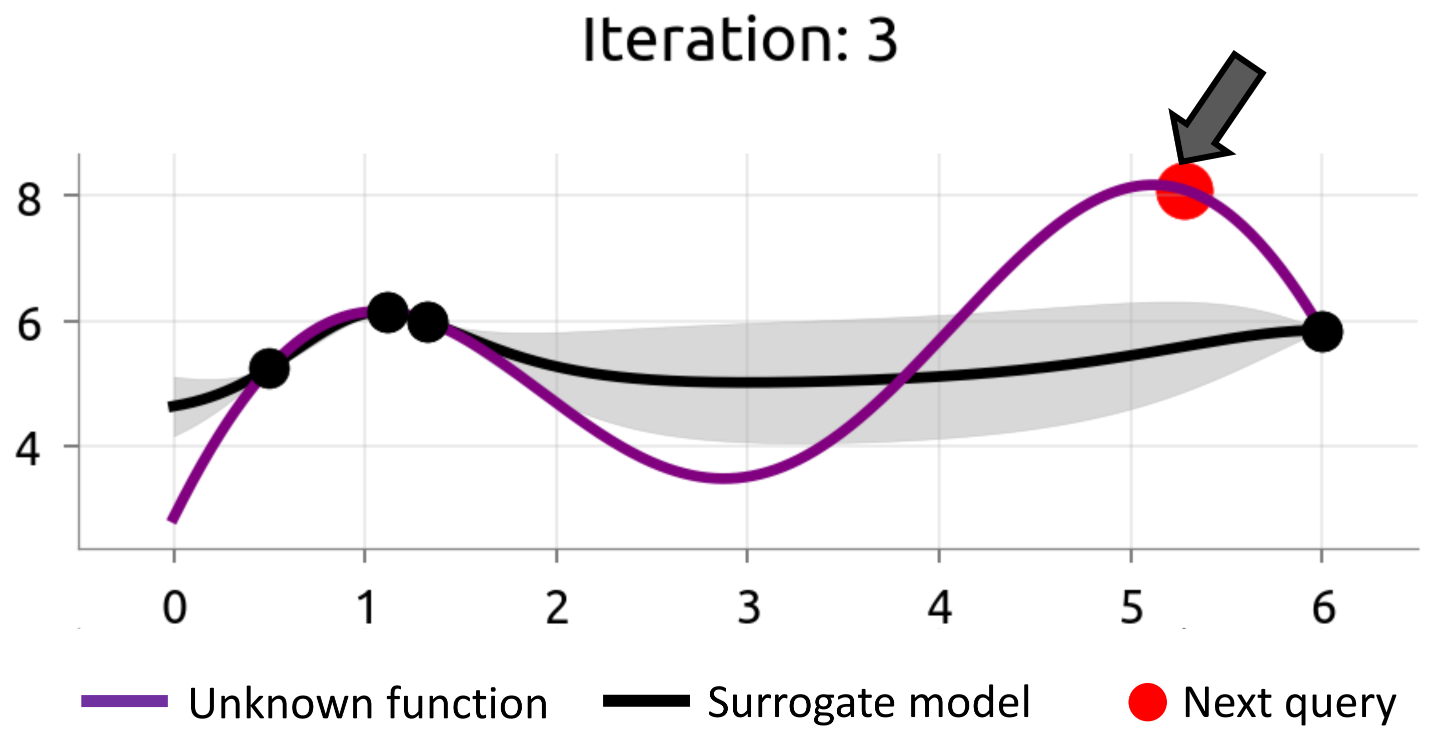

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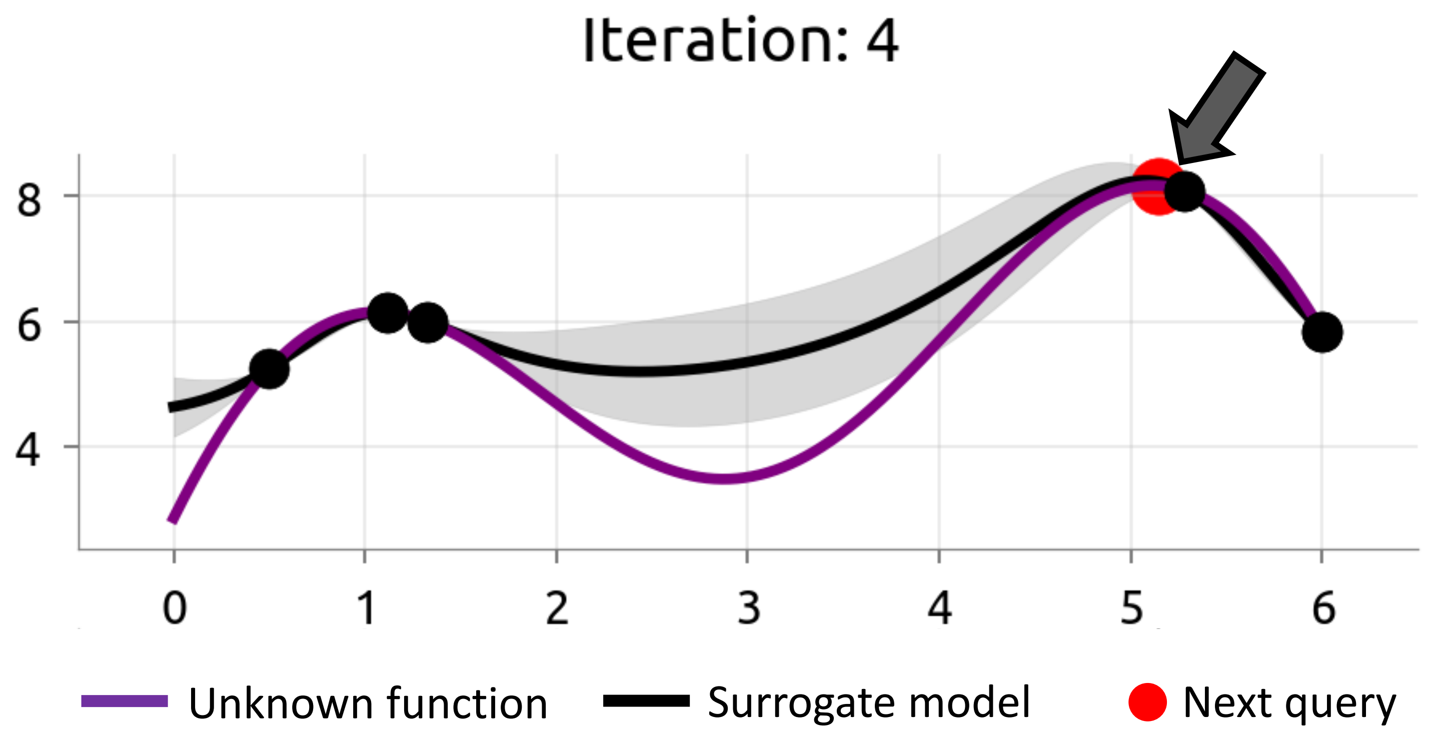

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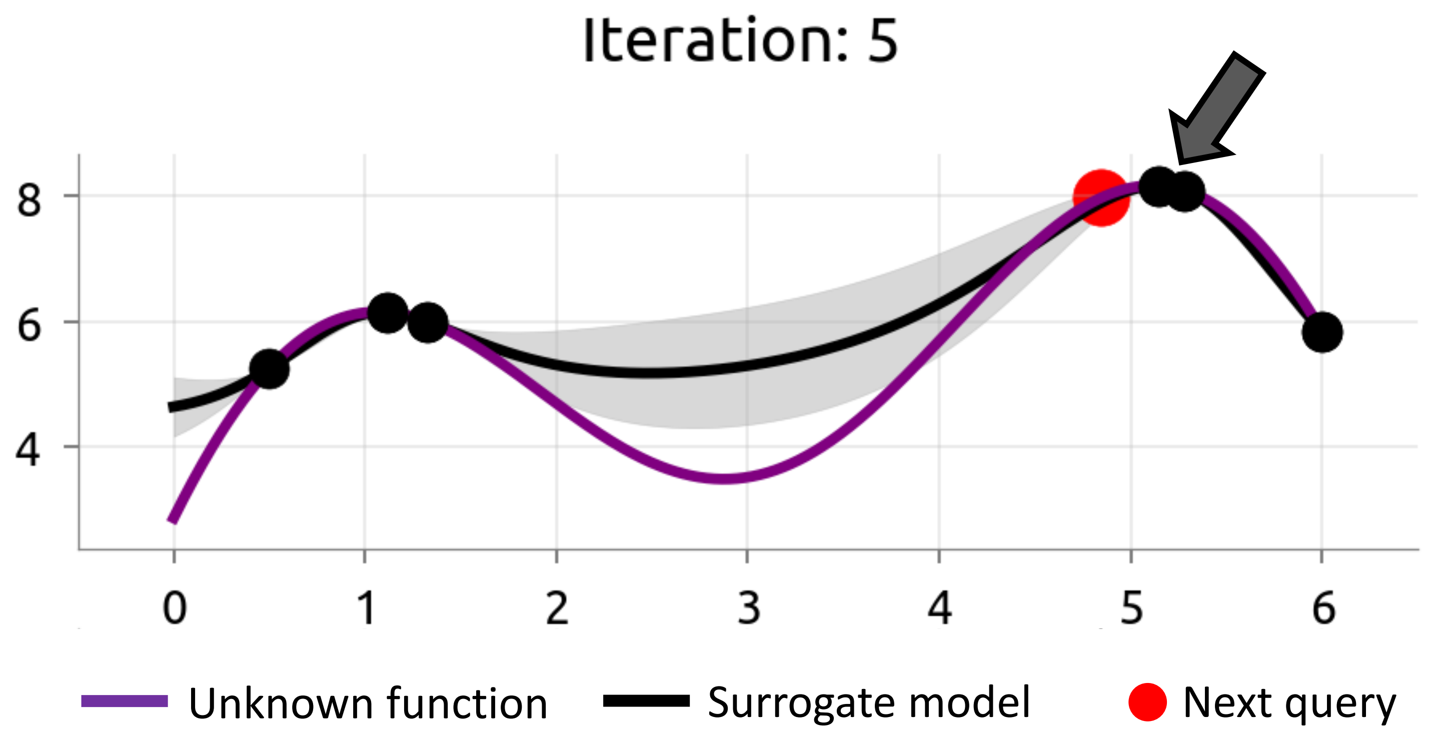

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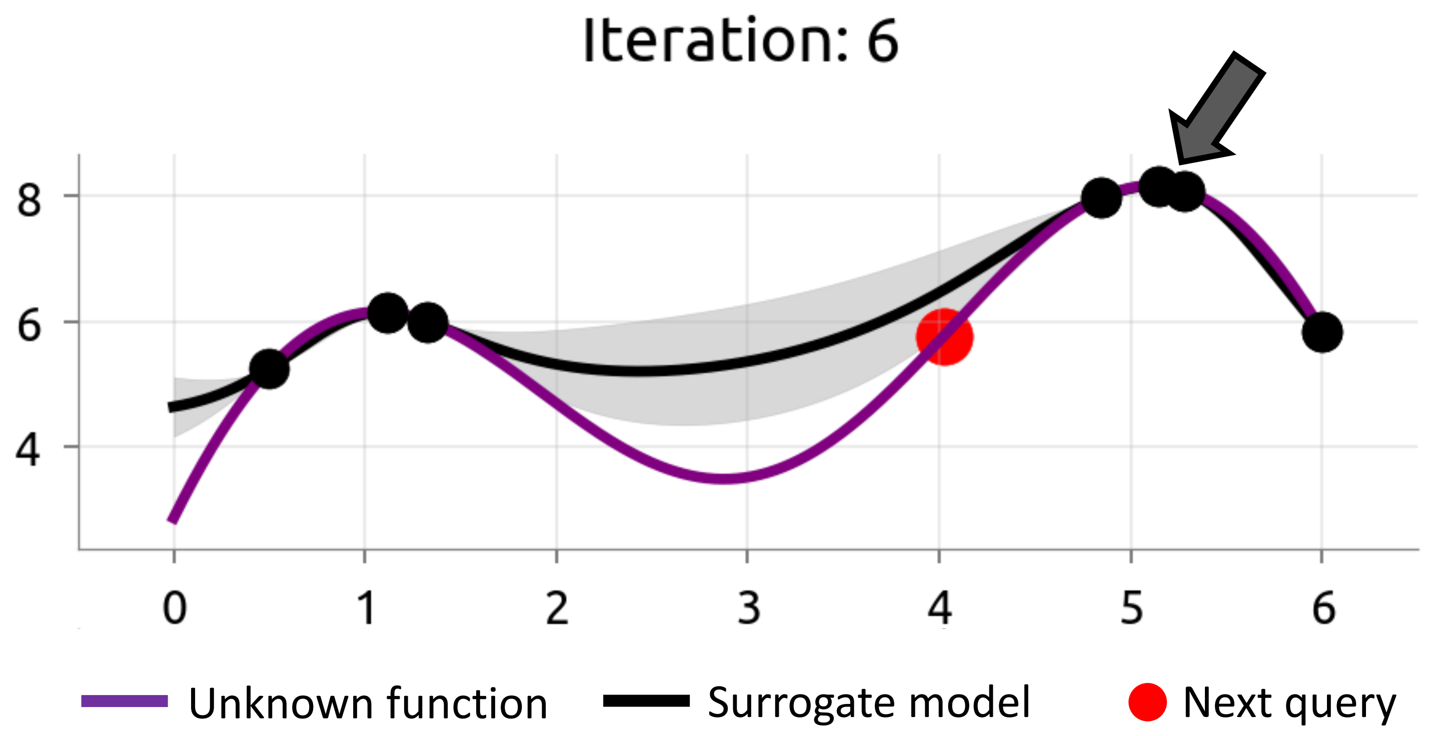

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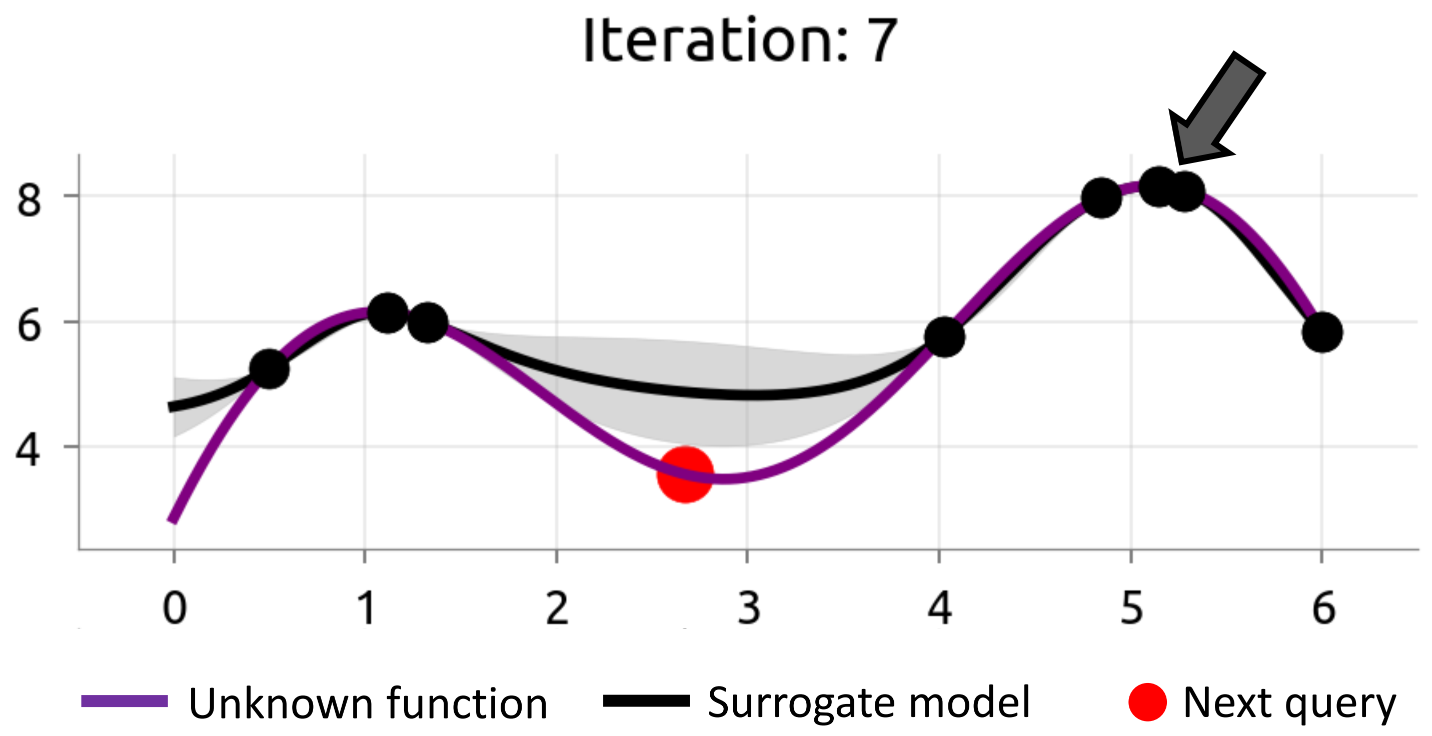

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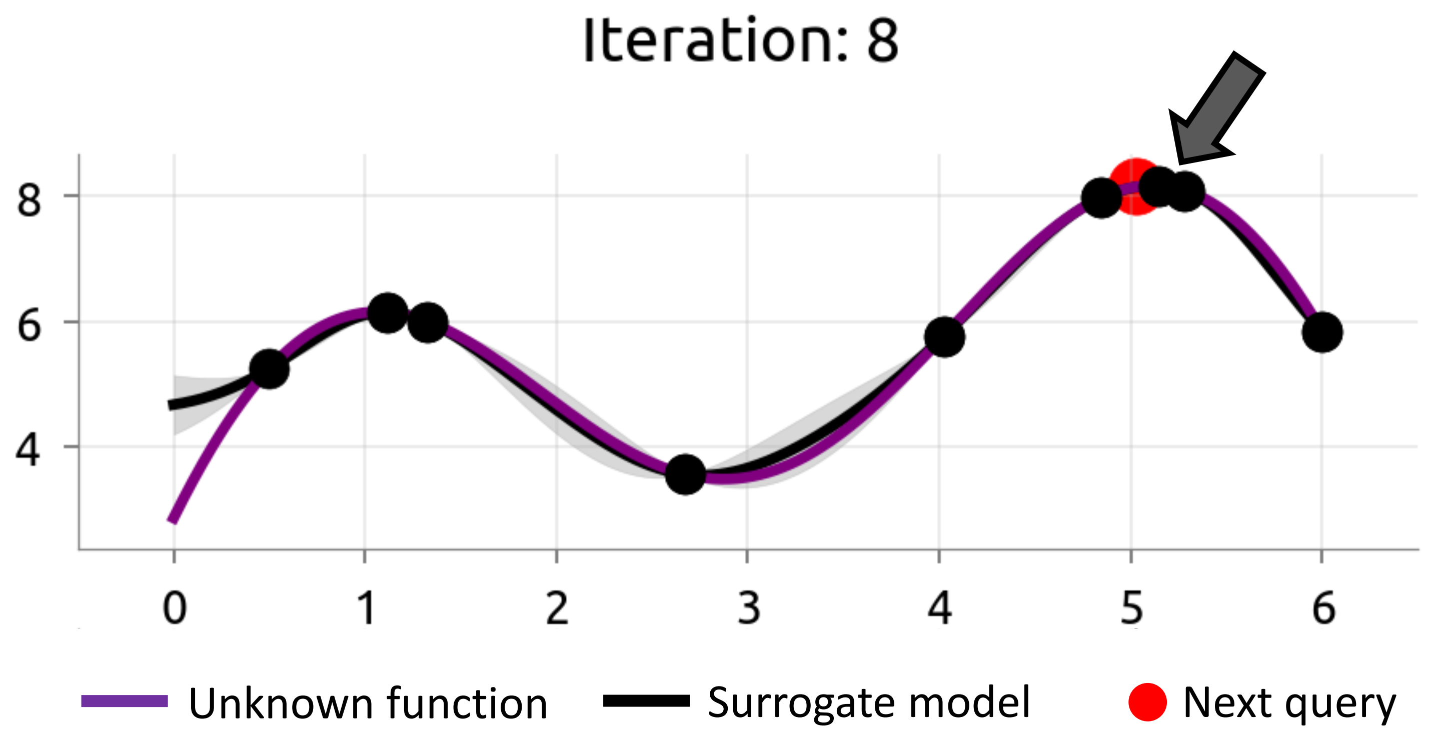

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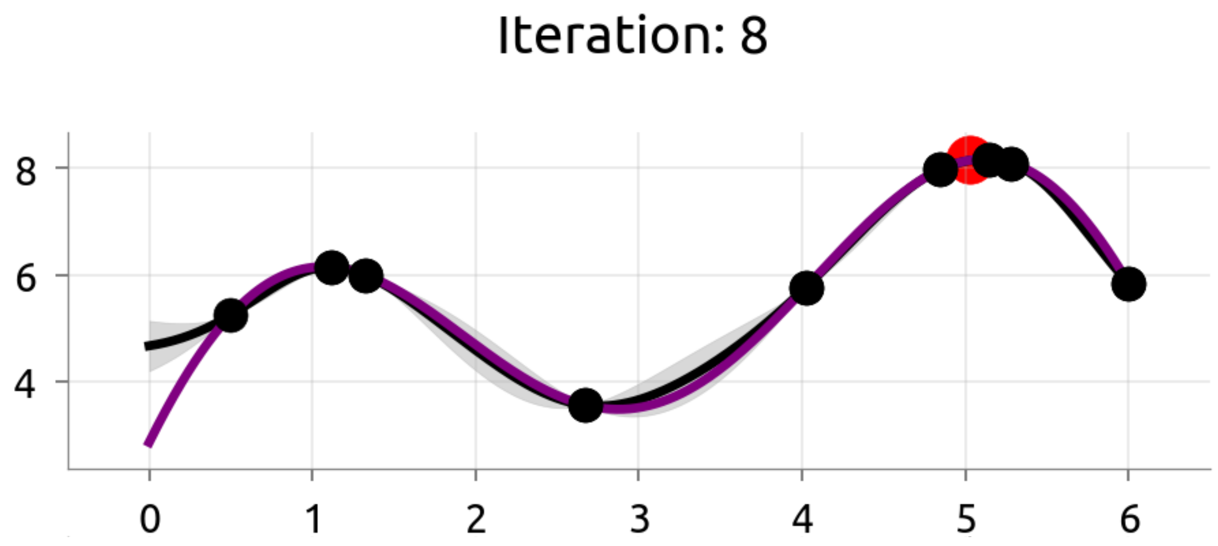


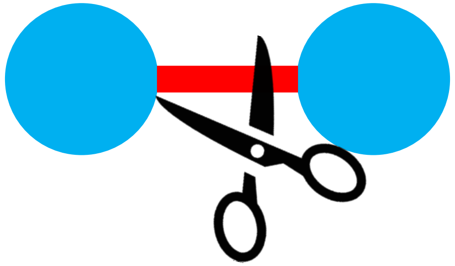
<u>HyperMapper</u> [Nardi 2019]: A Practical Design Space Exploration Framework.

(1) Random forests surrogate model (discrete search space).

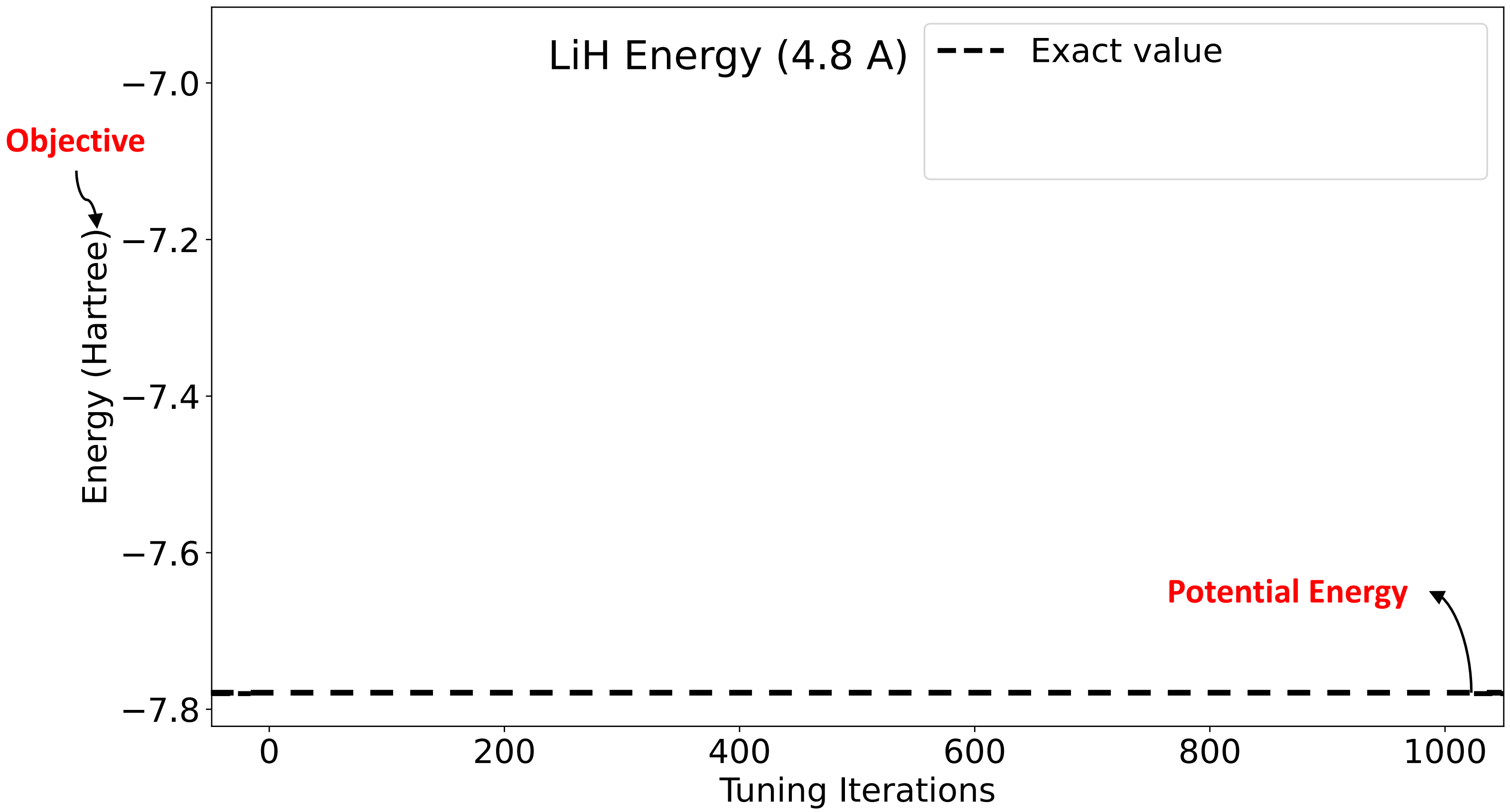
(2) Semi-greedy acquisition function.

Quantitative benefits for chemistry applications

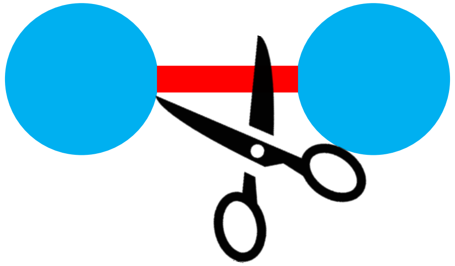
Potential Energy



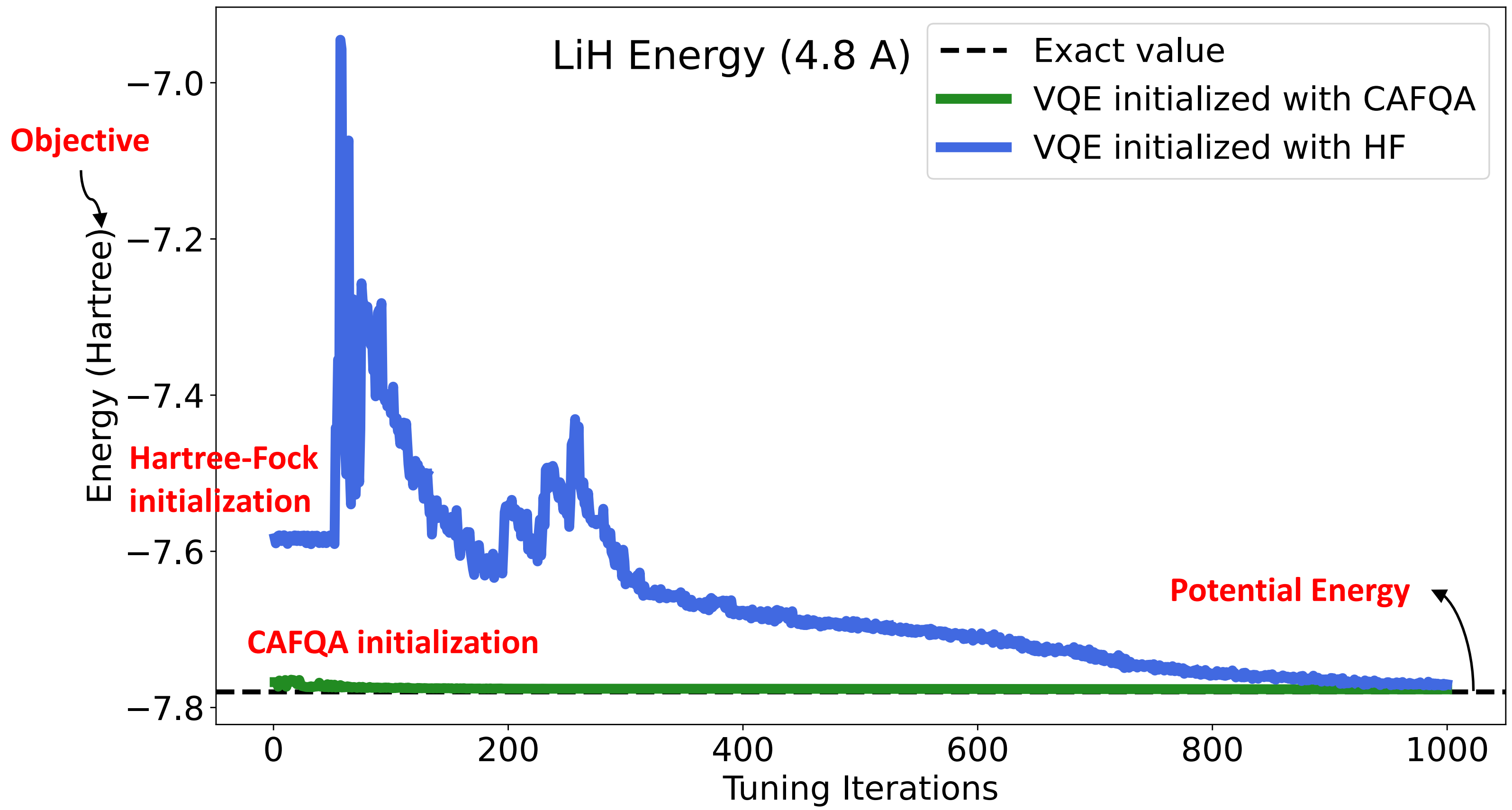
Quantitative benefits for chemistry applications



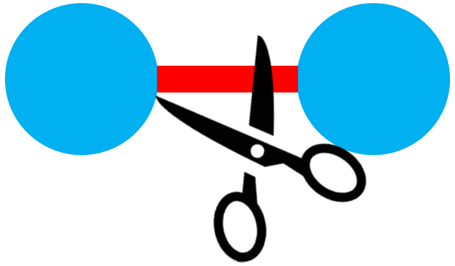
Potential Energy



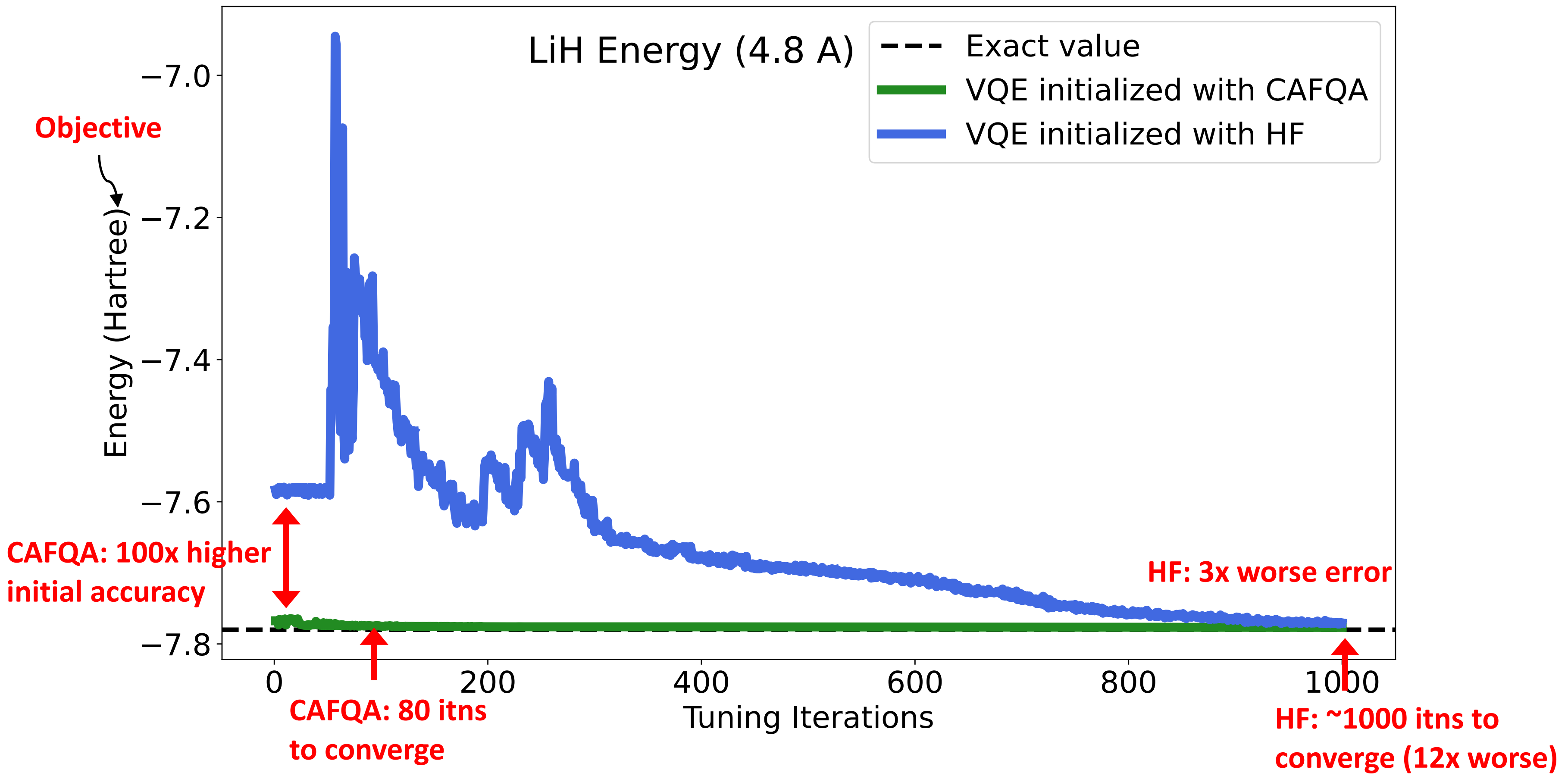
Quantitative benefits for chemistry applications

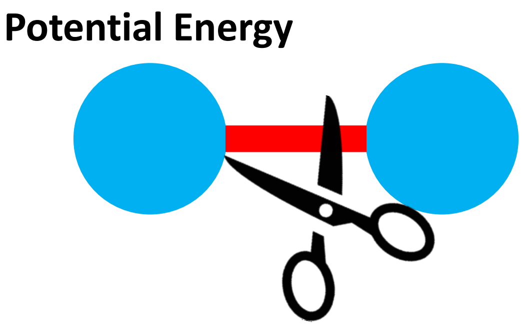


Potential Energy

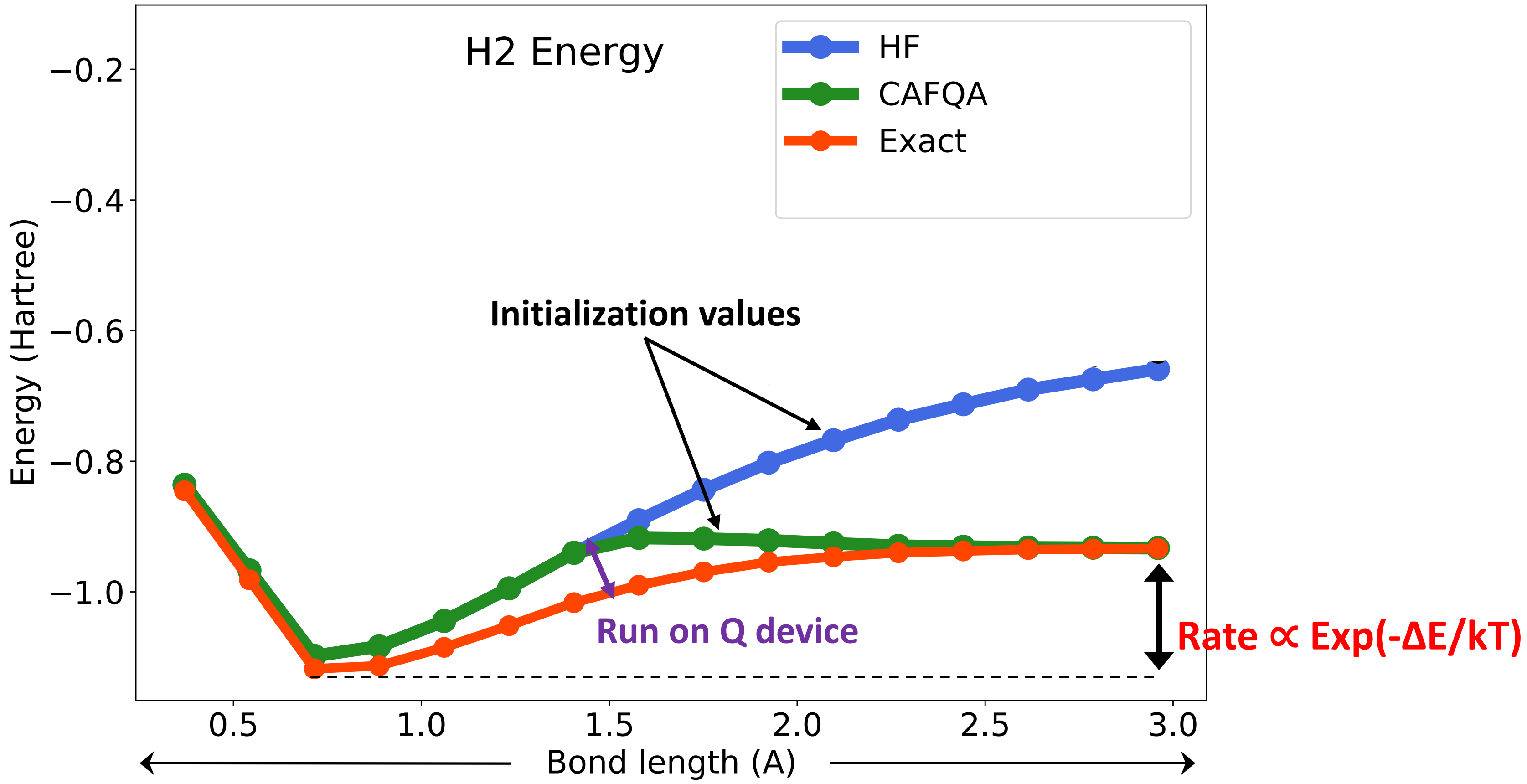


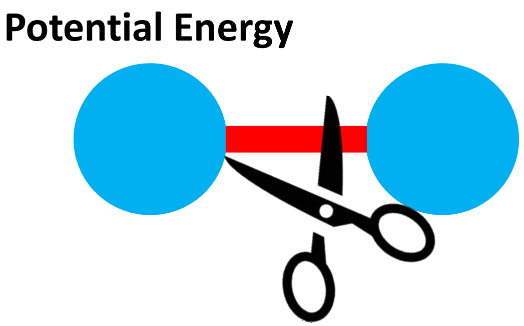
Quantitative benefits for chemistry applications



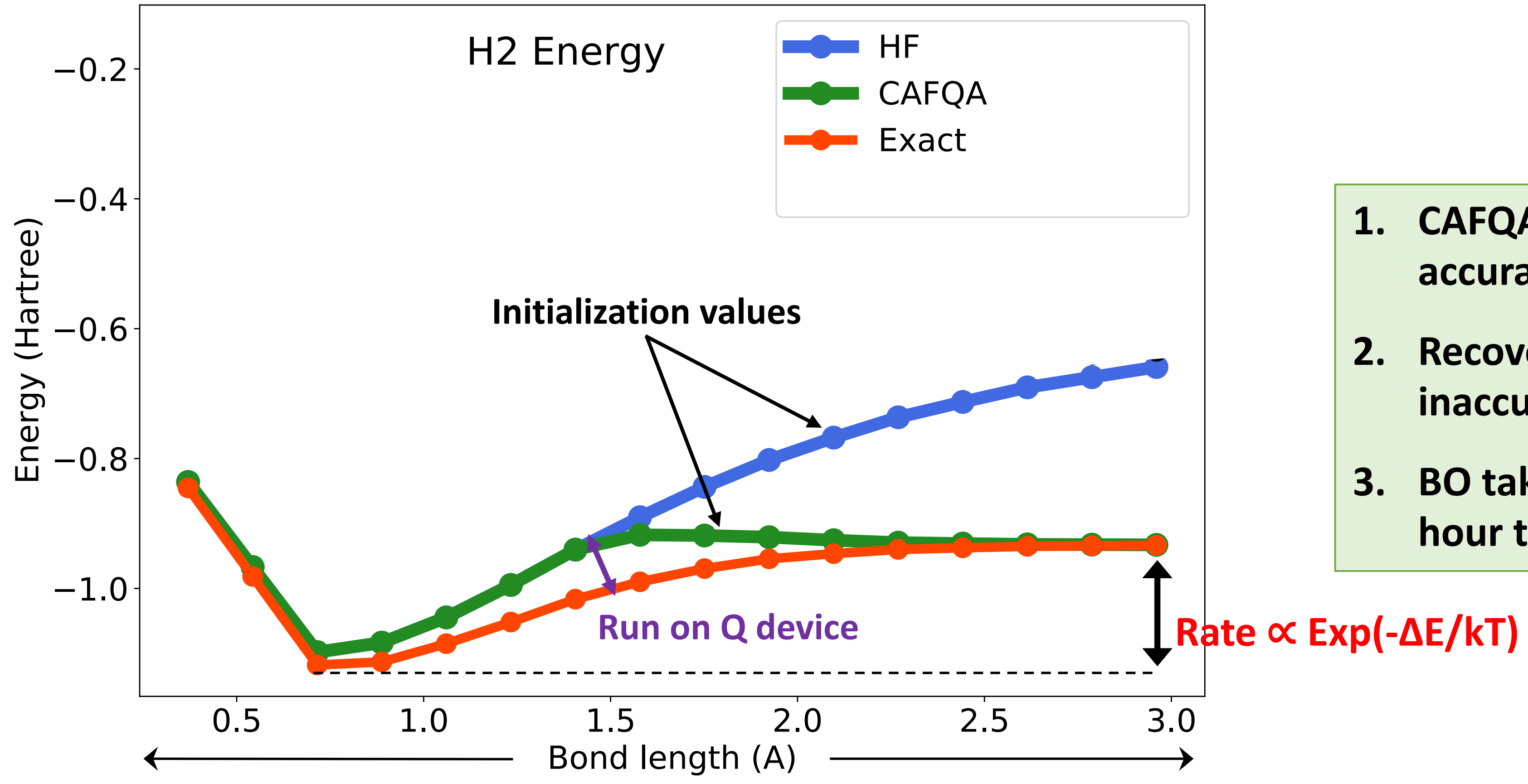


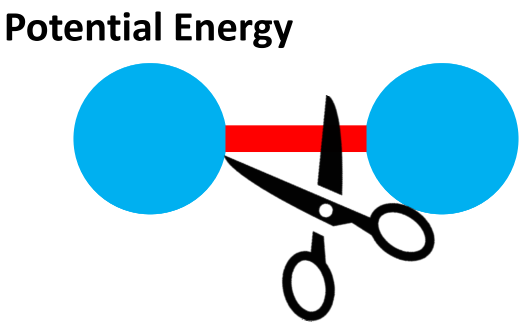
Quantitative benefits for chemistry applications





Quantitative benefits for chemistry applications



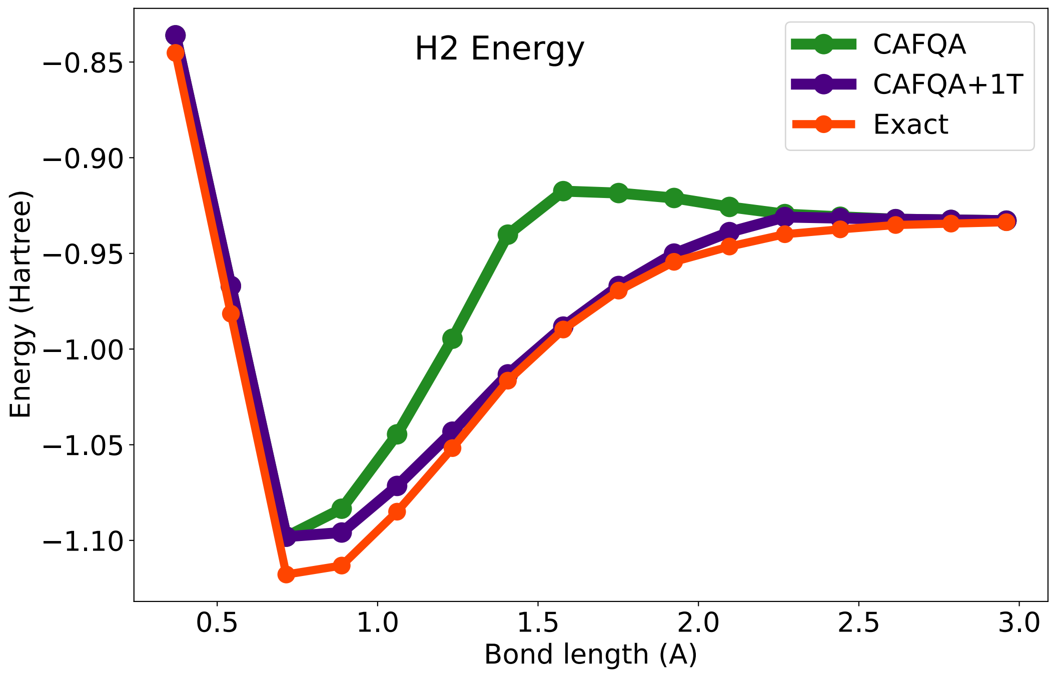


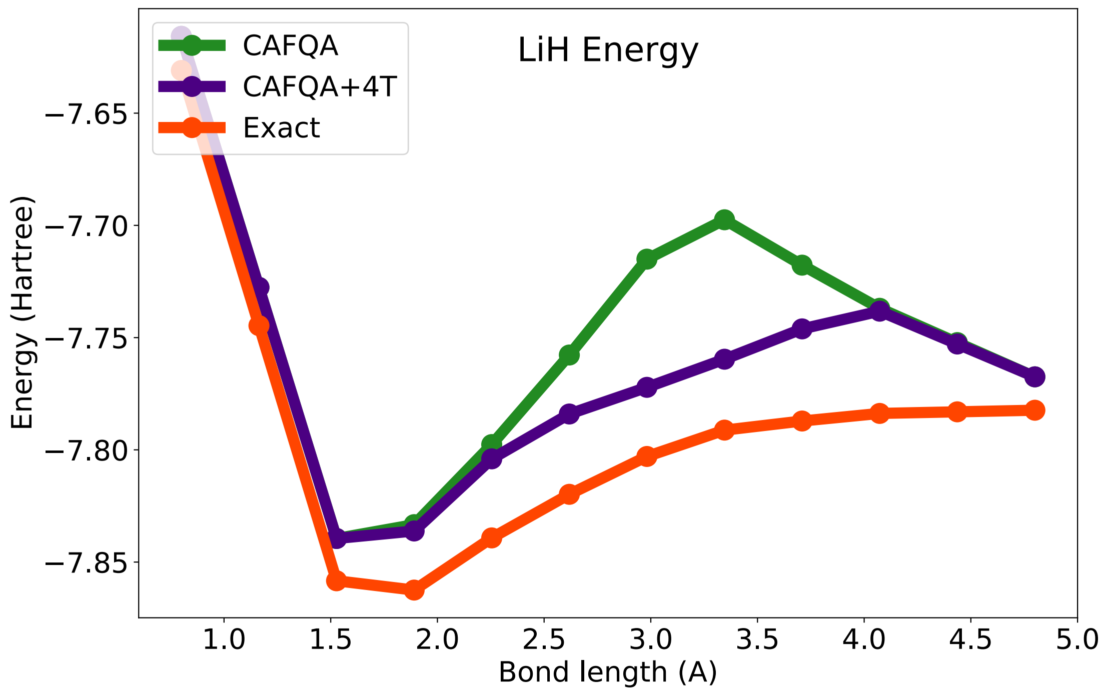
1. CAFQA achieves 99% mean initialization accuracy (systems up to 34 qubits).
2. Recovers up to 99.99% of Hartree-Fock inaccuracy (57x mean).
3. BO takes ~2000 iterations (mean), 1 hour to a week in wall-clock time.

CAFQA 2.0: Reducing the constants and tackling new applications.

- Bare-metal Hamiltonian expectation compute on Cliffords: 10x speedup.
- Genetic Algorithm – inefficient but much faster: 10x speedup.
- Parallelization of GA population: 10-100x speedup.
- 100-qubit *physics spin models*:
  - CAFQA 1.0: NA vs. CAFQA 2.0: 1 hour
- Cr2 molecule (34 qubits, 30k terms):
  - CAFQA 1.0: 1+ week vs. CAFQA 2.0: 10 hours (and order of magnitude higher accuracy)
- Exploiting Clifford symmetry in designing the ansatz: ??? speedup

CAFQA-*ish*: Classical sim to the compute limit





Systematically push to max classical limit
What is the classical limit?: Laptop vs Desktop vs Supercomputer
Interesting optimization problems

Working with classical simulators

Build new theory-inspired simulators, <u>accelerate with application-tailoring, software, hardware optimizations, integrate with SOTA classical/AI tools</u>

CAFQA: A classical simulation bootstrap for variational quantum algorithms

Gokul Subramanian Ravi*
University of Chicago

Pranav Gokhale
Super.tech (a division of ColdQuanta)

Yi Ding
MIT

William M. Kirby
Tufts University

Kaitlin N. Smith
University of Chicago

Jonathan M. Baker
University of Chicago

Peter J. Love
Tufts University

Henry Hoffmann
University of Chicago

Kenneth R. Brown
Duke University

Frederic T. Chong
University of Chicago
Super.tech (a division of ColdQuanta)

Simulating quantum circuit expectation values by Clifford perturbation theory

Tomislav Begušić, Kasra Hejazi, and Garnet Kin-Lic Chan

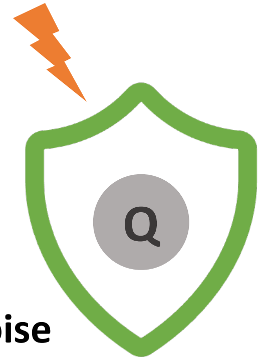
Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, California 91125,

Efficient tensor network simulation of IBM's Eagle kicked Ising experiment

Joseph Tindall,[1] Matthew Fishman,[1] E. Miles Stoudenmire,[1] and Dries Sels[1,2]

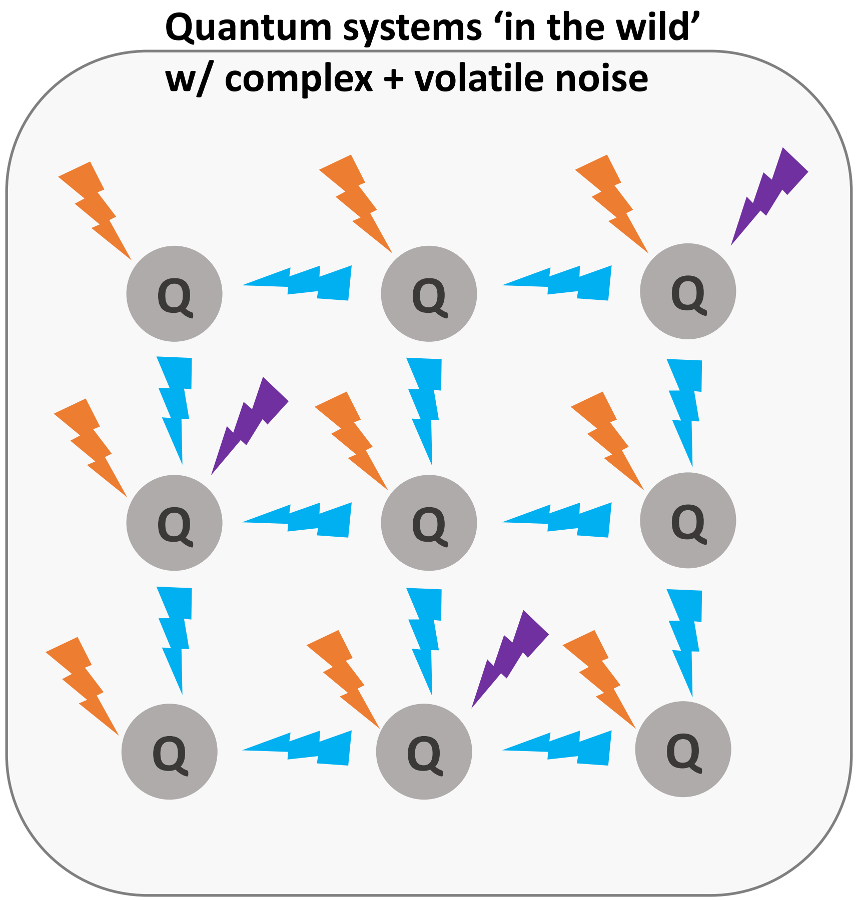
[1] *Center for Computational Quantum Physics, Flatiron Institute, New York, New York 10010, USA*
[2] *Center for Quantum Phenomena, Department of Physics, New York University, 726 Broadway, New York, NY, 10003, USA*

#2) Adaptive noise mitigation through modeling and optimization

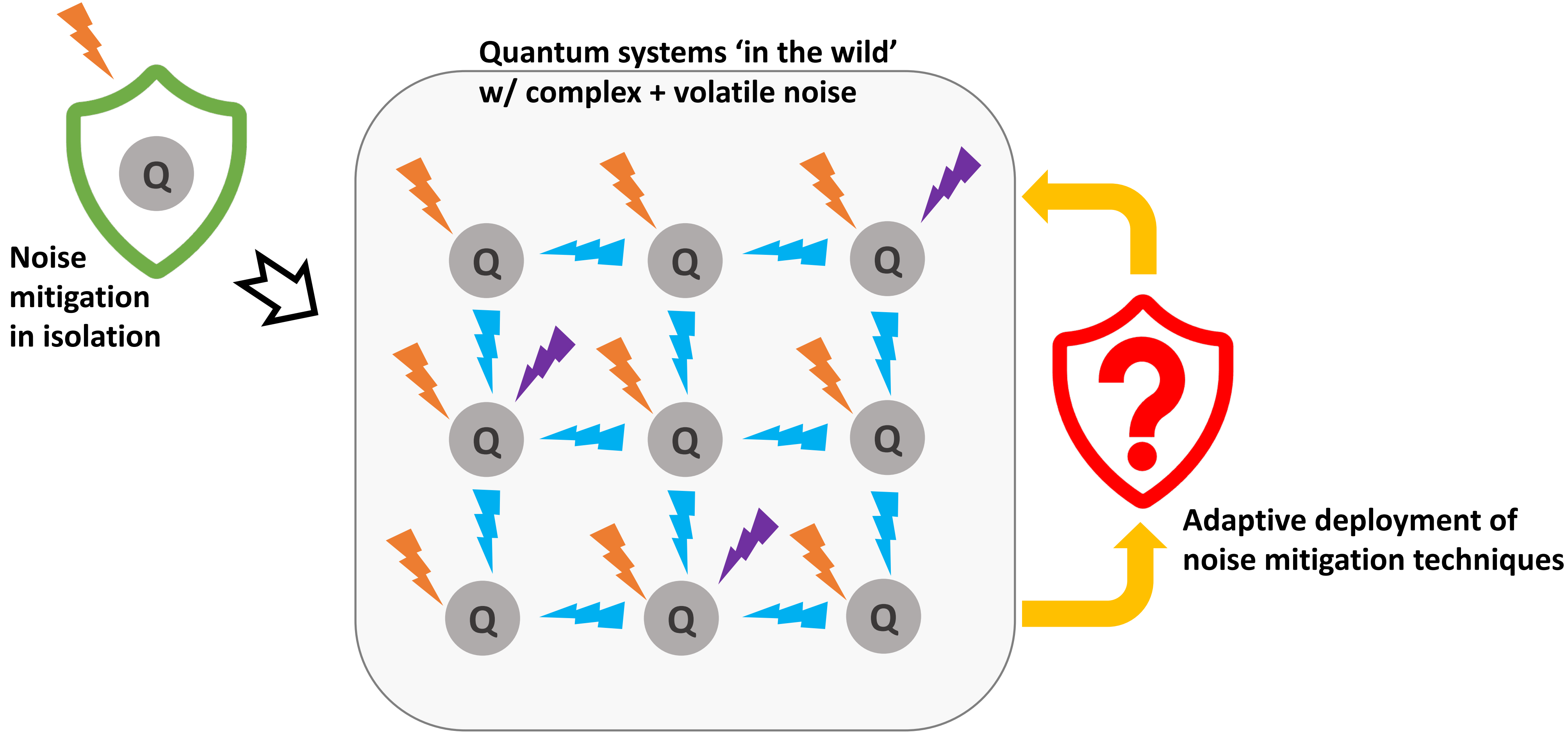


Noise mitigation in isolation

#2) Adaptive noise mitigation through <u>modeling</u> and optimization

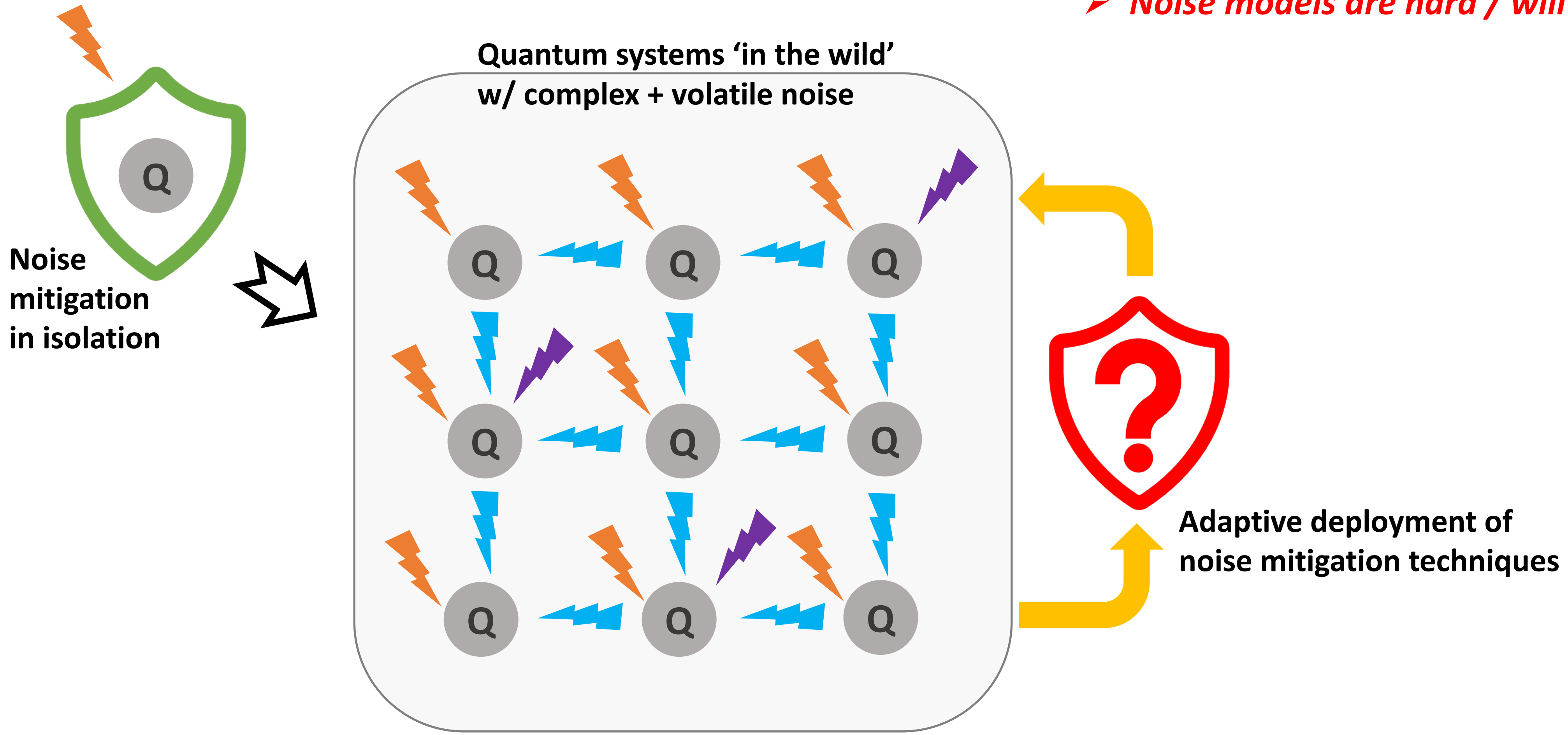


#2) Adaptive noise mitigation through modeling and optimization



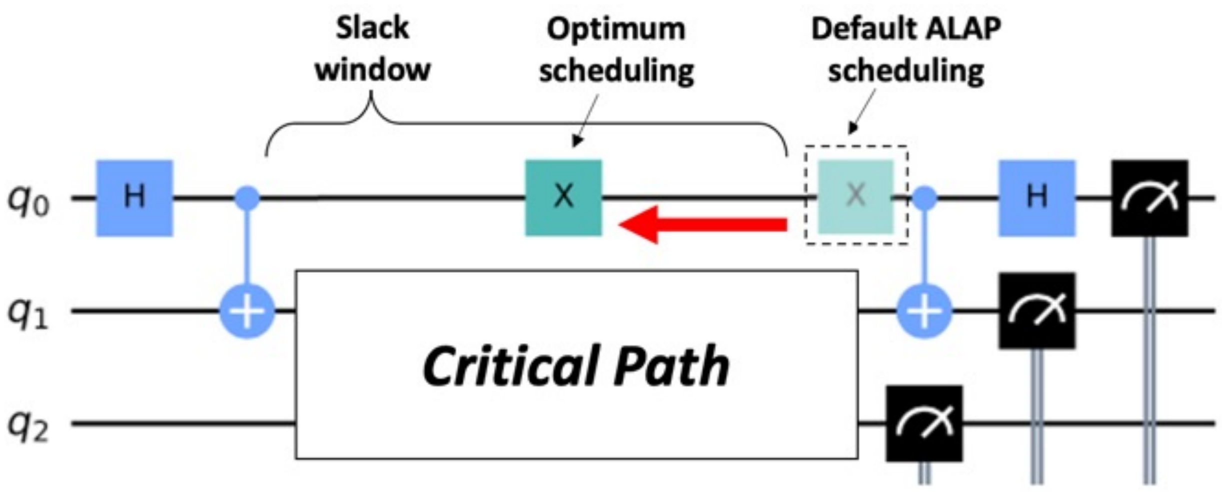
#2) Adaptive noise mitigation through modeling and optimization

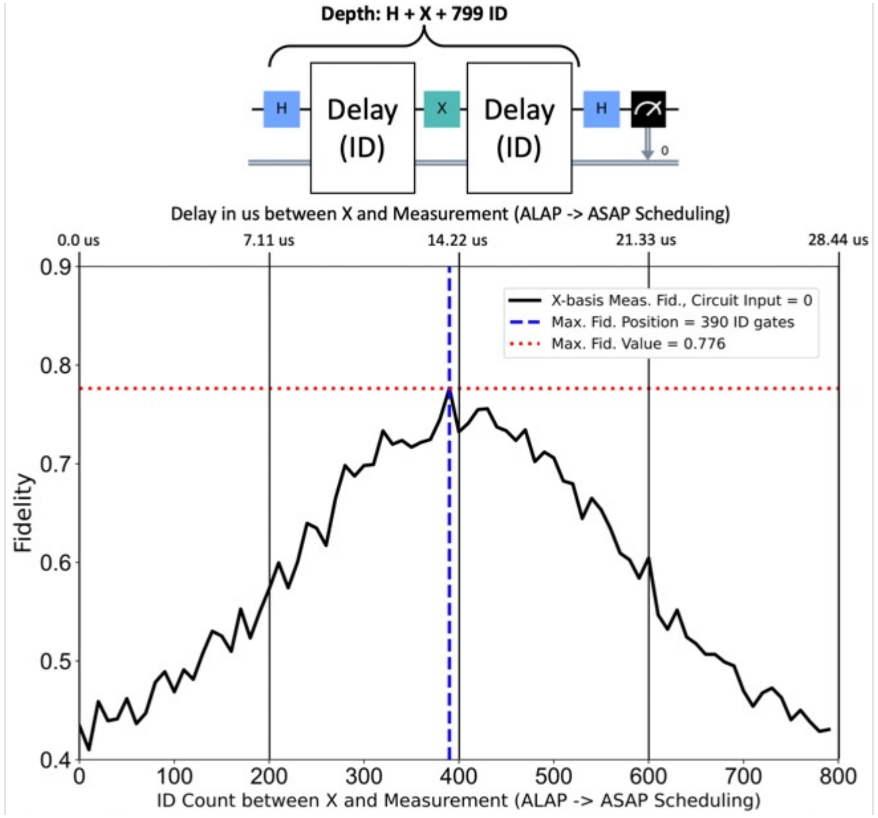
- ***Noise models are important.***
- ***Noise models are hard / will not suffice.***



Gate scheduling and insertion for noise mitigation

Error Mitigation in Quantum Computers through Instruction Scheduling. Smith, Ravi, et al. ACM TQC. 2022

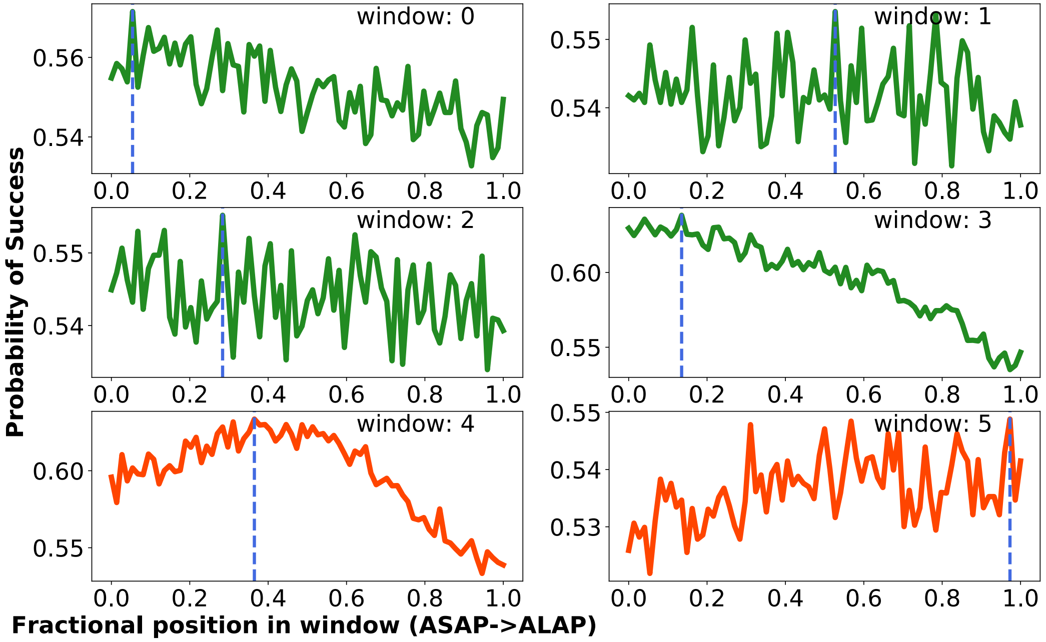




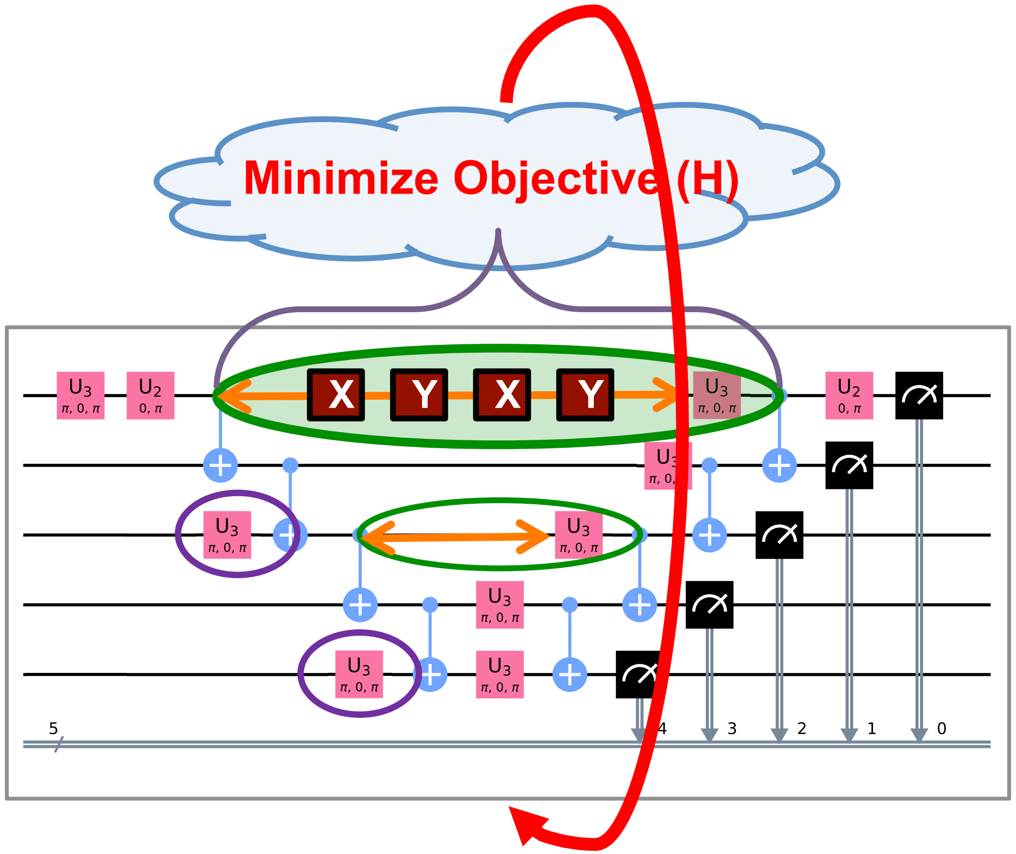
Noise modeling is critical to study new error mitigation techniques!

Optimizing VQA noise mitigation 'in the loop'

VAQEM: A Variational Approach to Quantum Error Mitigation. Ravi et al., HPCA '22



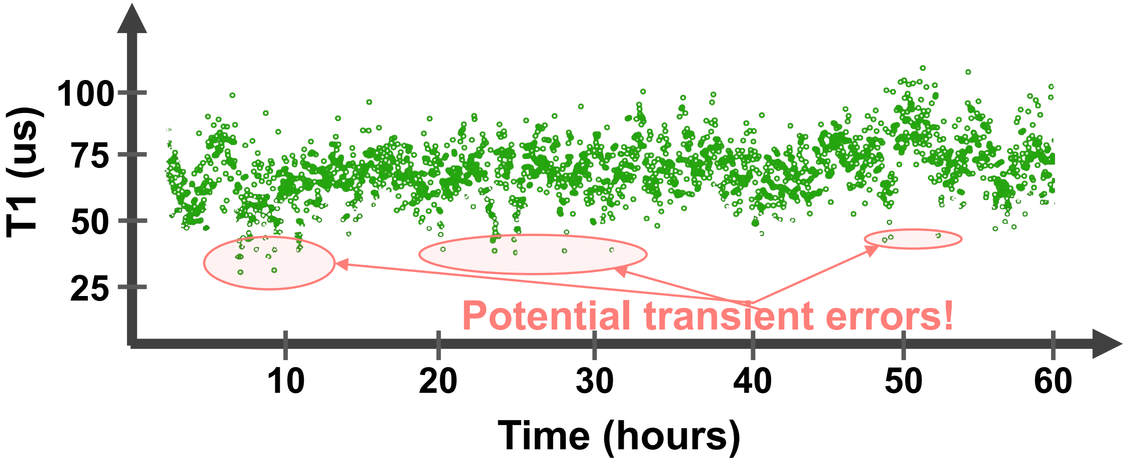
Gate scheduling / DD seq. insertion



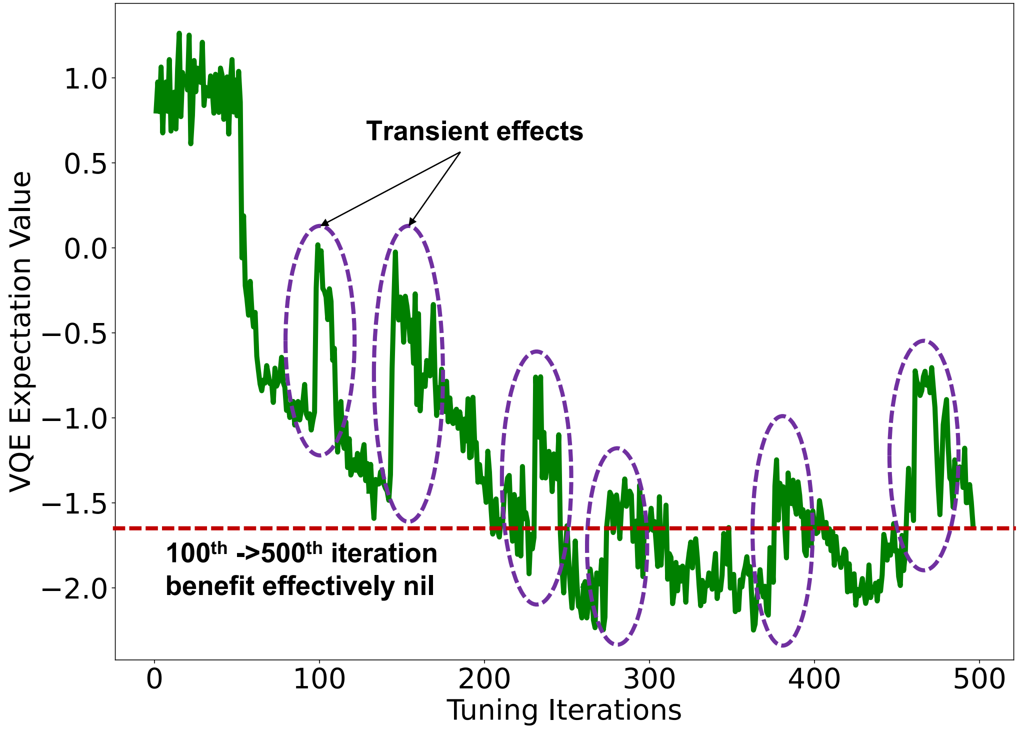
Noise models don't capture complex interactions but can help strategize and reduce search space for dynamic optimization schemes!

Mitigating transient noise effects in VQA

QISMET: Navigating the Dynamic Noise Landscape of Variational Quantum Algorithms. Ravi et al., ASPLOS '23

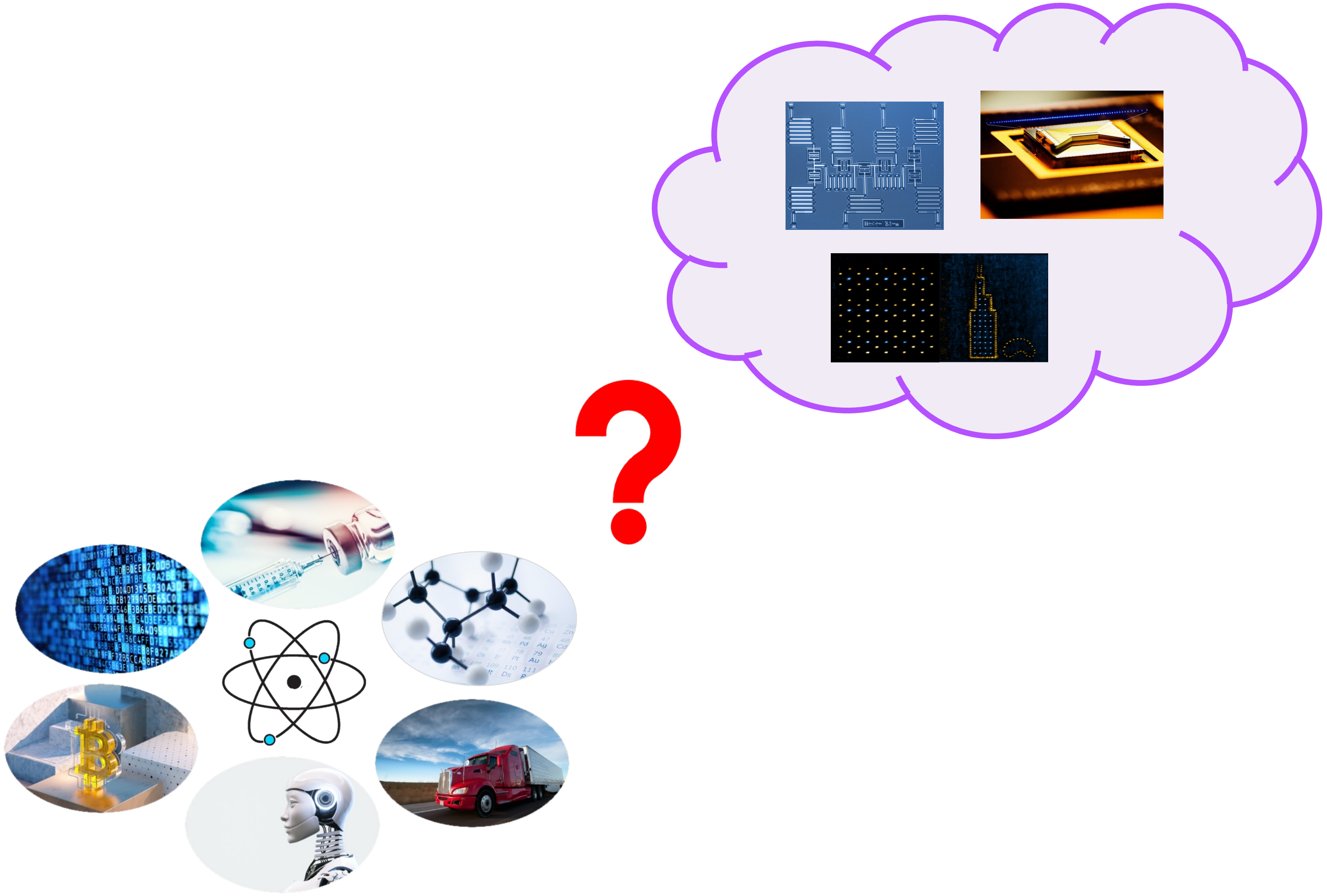


JJ Burnett, et al. **Decoherence benchmarking of superconducting qubits**. NPJ Quantum 2019

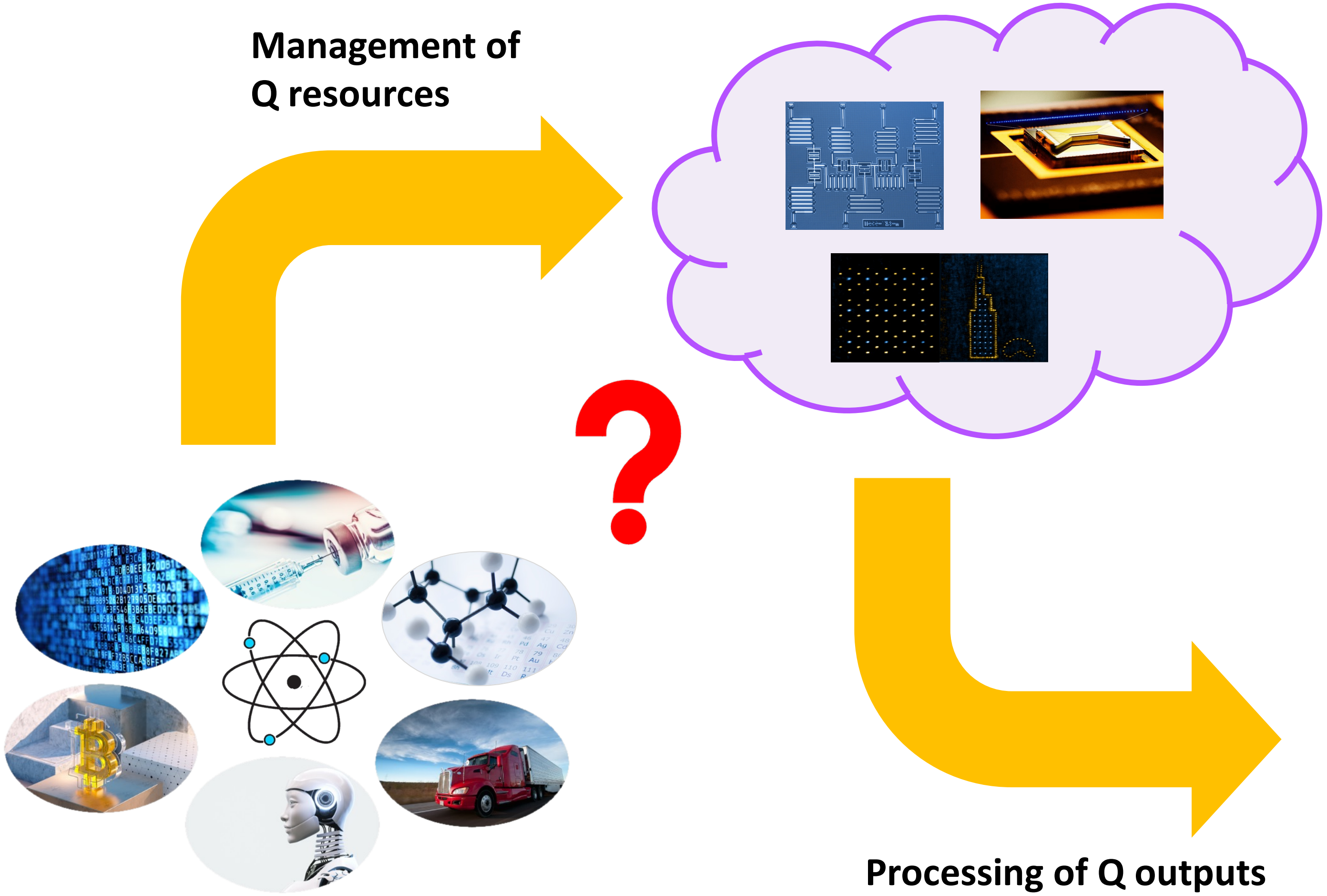


Noise models are poor for transient noise but profiling can help learn thresholds for dynamic optimization schemes!

#3) Resource modeling in the cloud

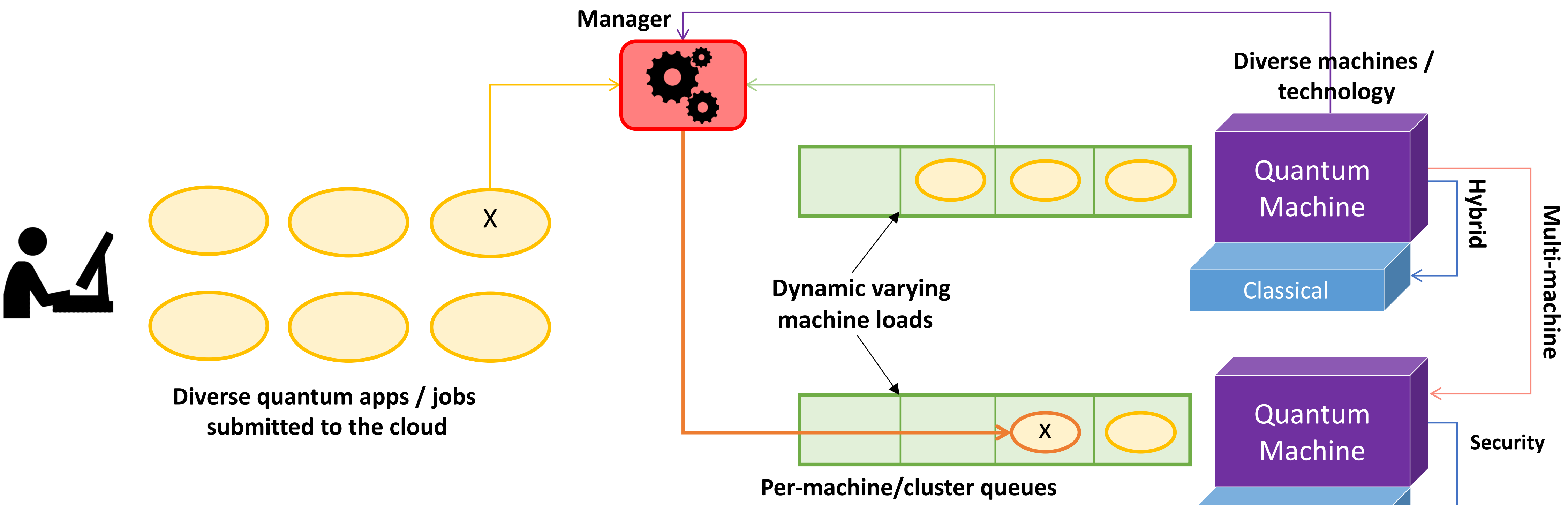


#3) Resource modeling in the cloud



Managing cloud resources

Best Q machines for app? Best hybrid systems for app? Throughput vs fidelity? FT + NISQ? QOS guarantees?

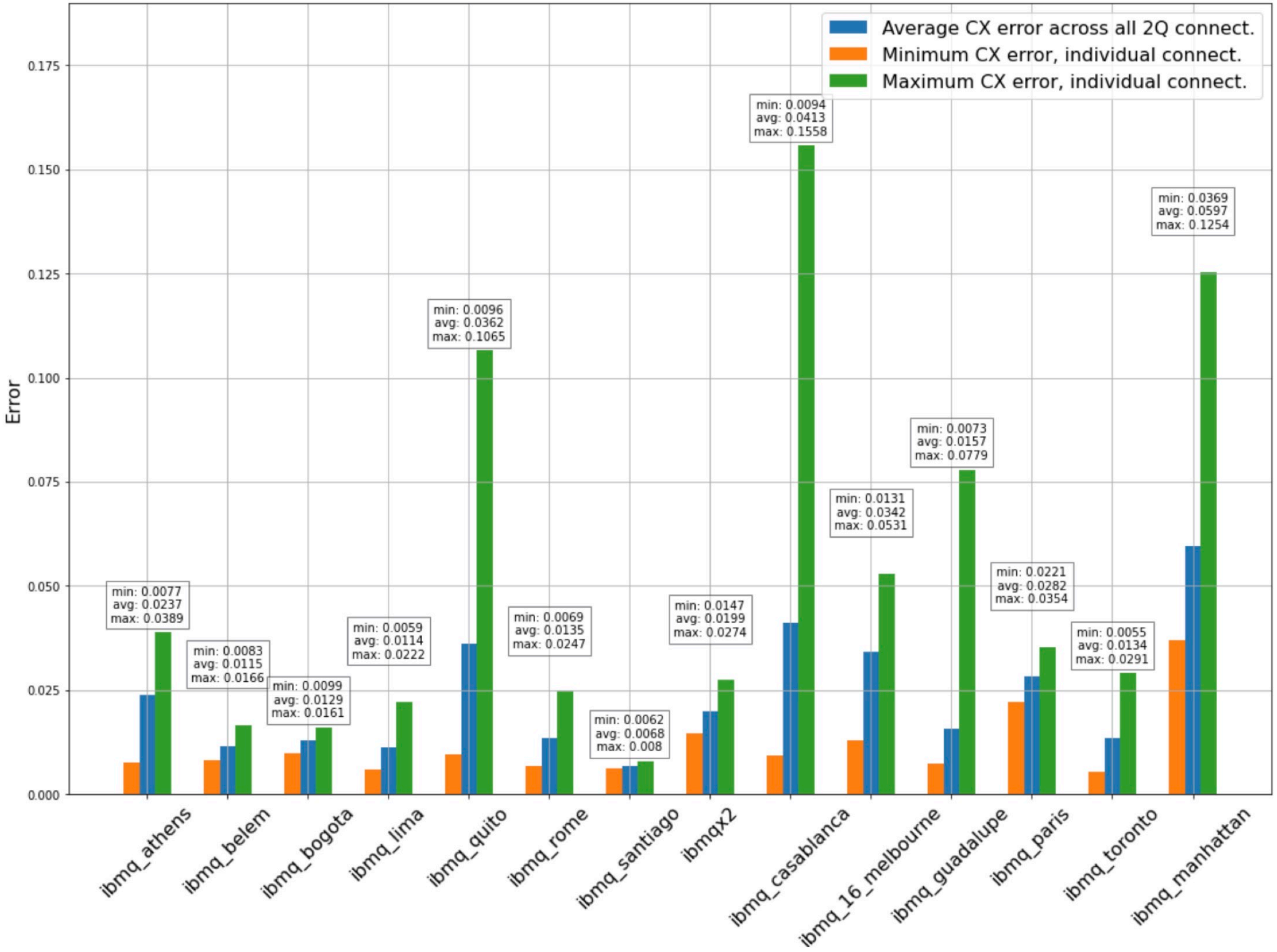


Quancorde: Boosting fidelity with Quantum Canary Ordered Diverse Ensembles. Ravi et al., ICRC '22 + Patent filed

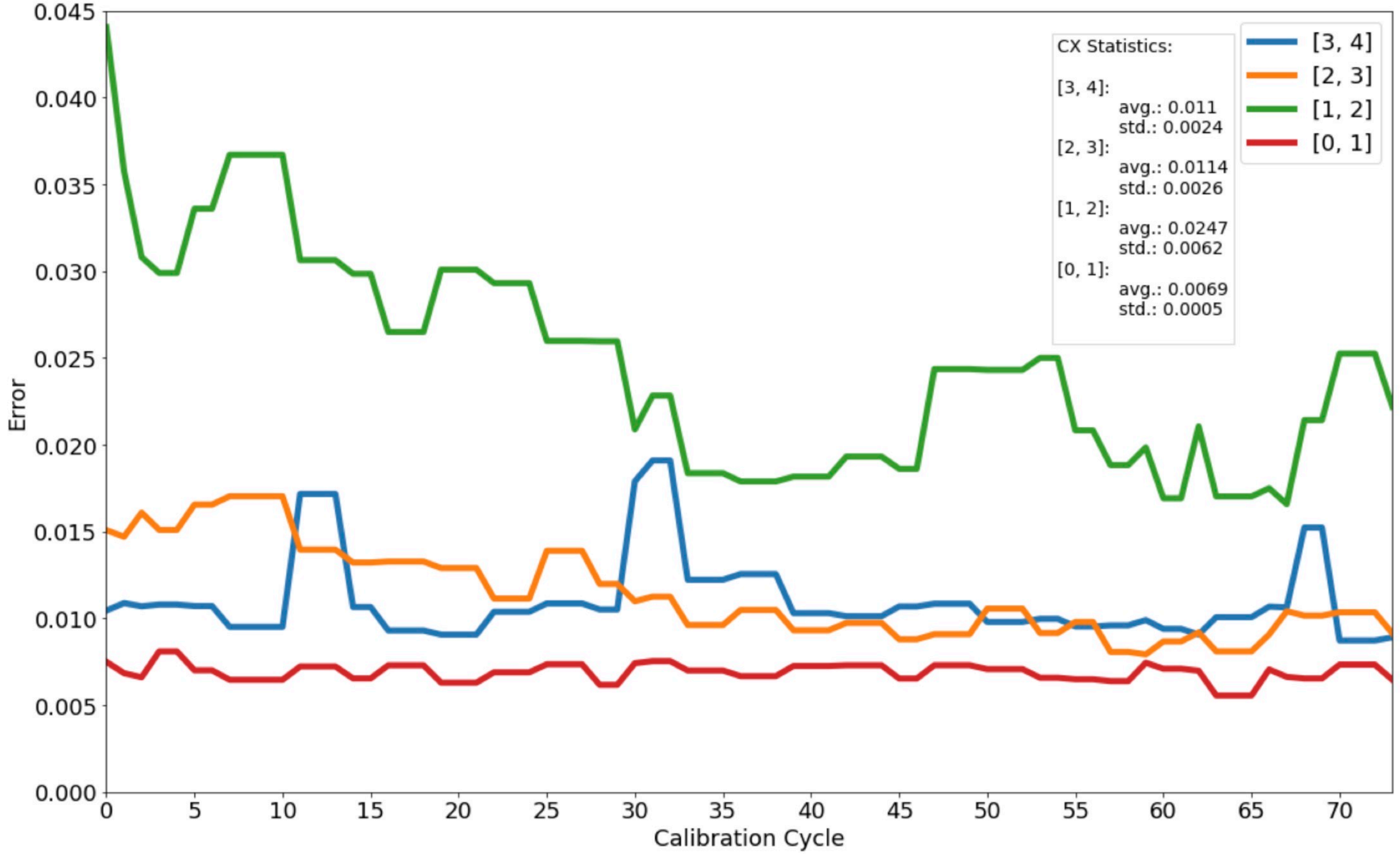
Adaptive job and resource management for the growing quantum cloud. Ravi et al., QCE '21 + Patent filed

Quantum Computing in the Cloud: Analyzing job and machine characteristics. Ravi et al., IISWC '21

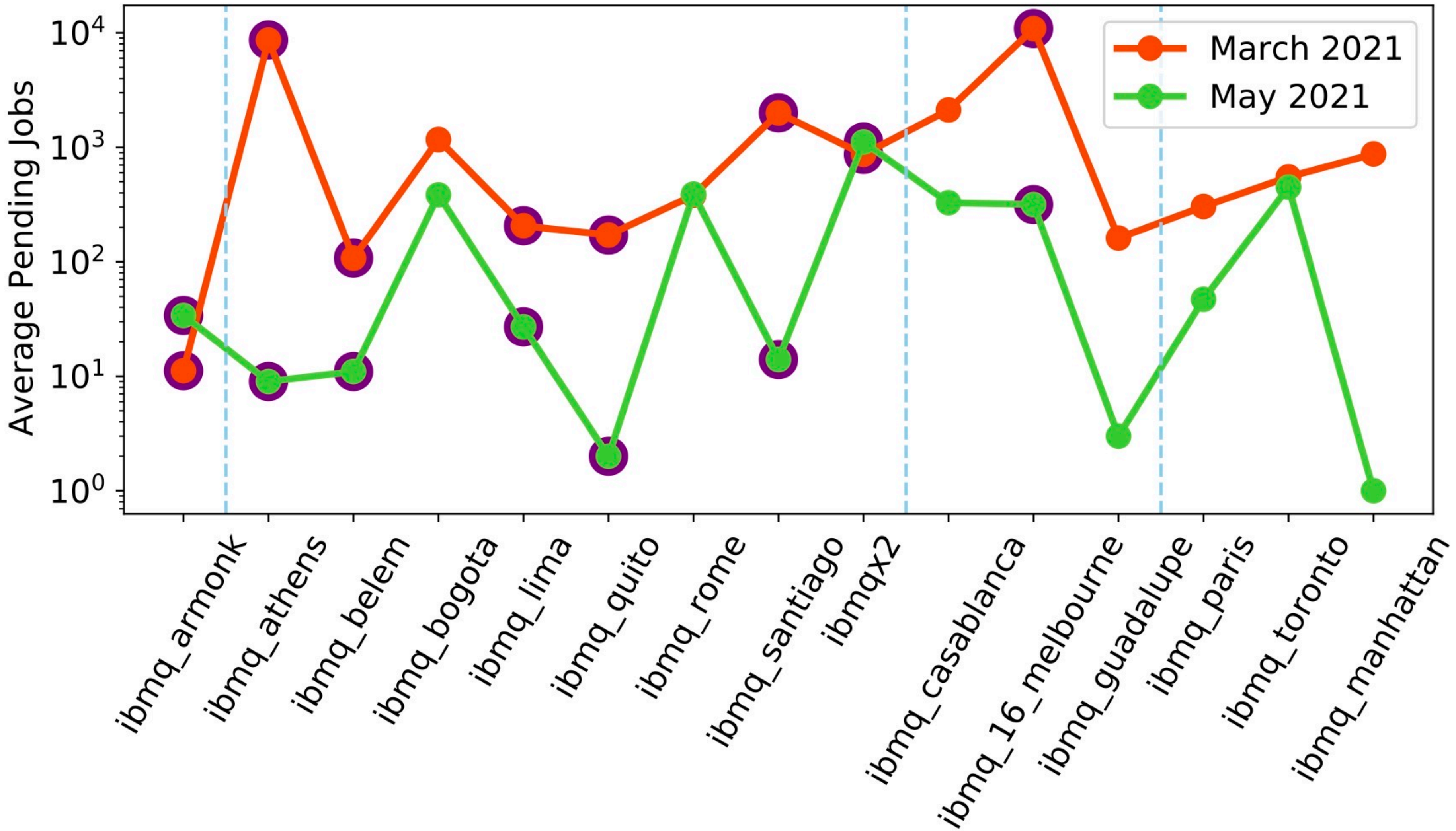
Quantum Cloud: Error diversity (Spatial)



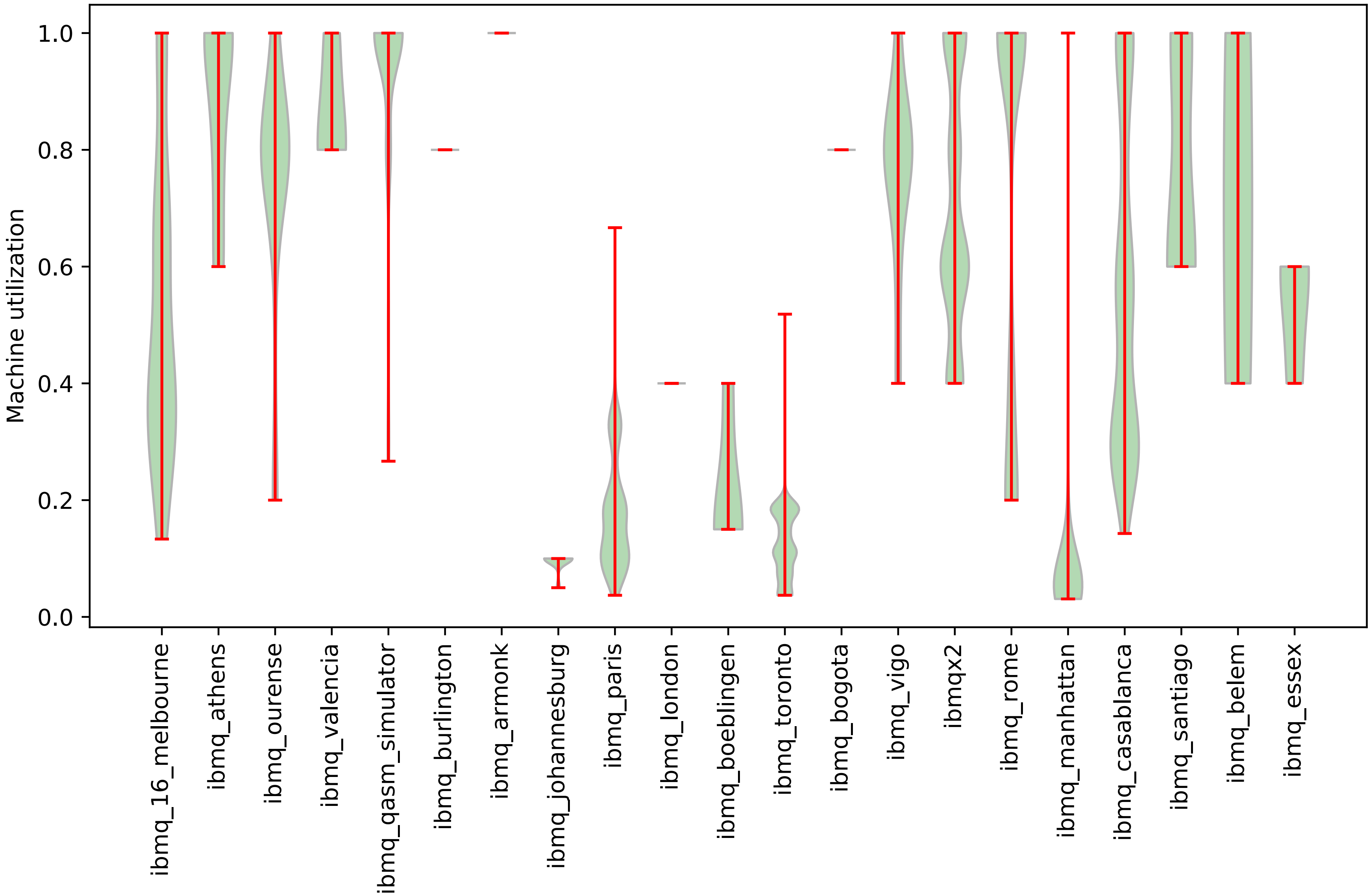
Quantum Cloud: Error diversity (Temporal)



Quantum Cloud: Machine loads and wait times



Quantum Cloud: Machine utilization



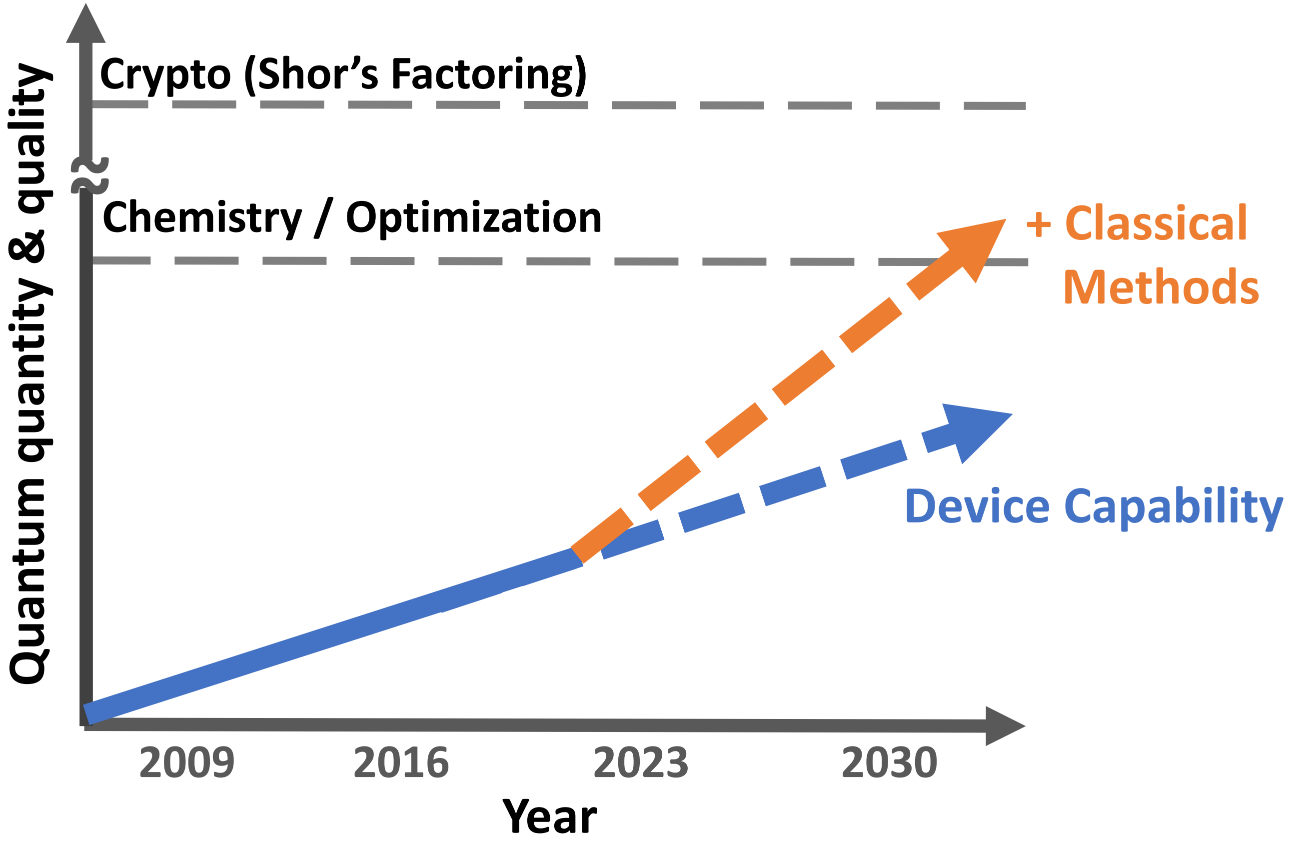
Bonus: Cryogenic chip design

IBM scientists cool down the world's largest quantum-ready cryogenic concept system

Project Goldeneye pushes the limits of low-temperature refrigeration while laying the groundwork for the quantum industry's ability to scale to larger experiments.

https://research.ibm.com/blog/goldeneye-cryogenic-concept-system

Bridging the quantum gap: Classical computing approaches



1. PL and Compilation
2. Computer Architecture
3. Classical simulation
4. High performance computing
5. Cryogenic hardware design
6. Noise modeling and Optimization
7. Multi-chip / distributed computing
8. Cloud resource modeling and management

applied sciences

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Current Developments in Quantum Hybrid Systems

Guest Editors

Prof. Dr. Frederic Chong, Dr. Gokul Subramanian Ravi

Deadline

20 November 2023

Special Issue

Thank you!

gsravi@umich.edu

Project	**Arxiv**	**Software**
CAFQA	arXiv:2202.12924	github.com/rgokulsm/CAFQA
VAQEM	arXiv:2112.05821	github.com/rgokulsm/VAQEM
QISMET	arXiv:2209.12280	Coming Soon
VarSaw	arXiv:2306.06027	https://github.com/siddharthdangwal/VarSaw
QCloud	arXiv:2203.13121	https://github.com/rgokulsm/QuantumQueue