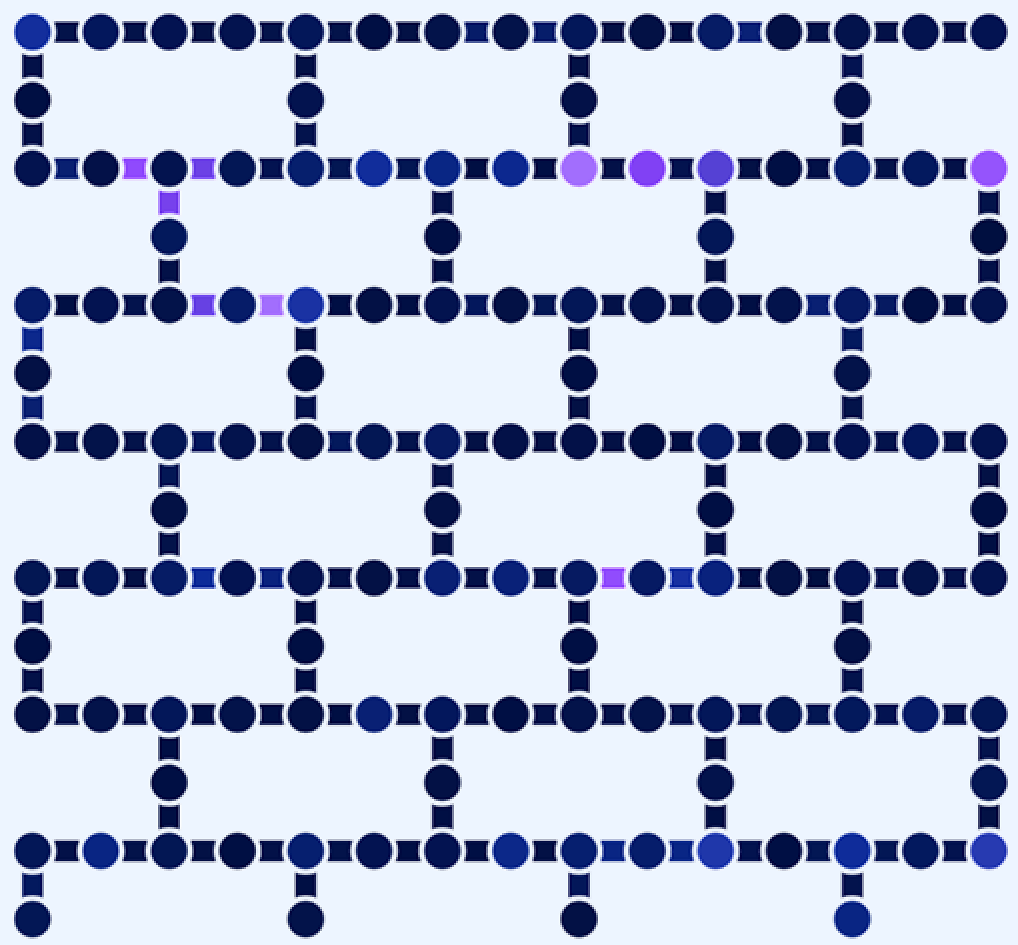
Practical quantum algorithms

Joana Fraxanet Morales
Quantum Algorithm
Engineering team

IBM **Quantum**

Motivation for variational quantum algorithms



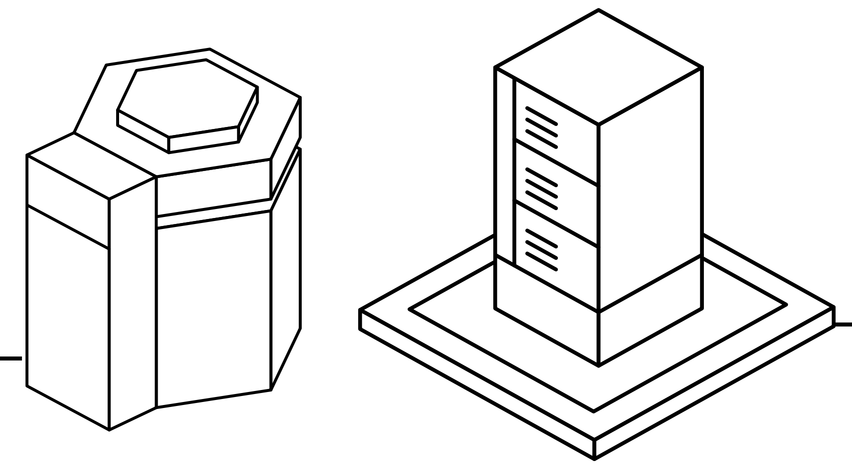
Leveraging Near-Term Quantum Hardware

- Access to 100+ qubit devices
- No quantum error correction
- Limited circuit depth and qubit connectivity

Requires *noise-resilient*, *shallow*, and *adaptable* quantum algorithms.

Hybrid approach

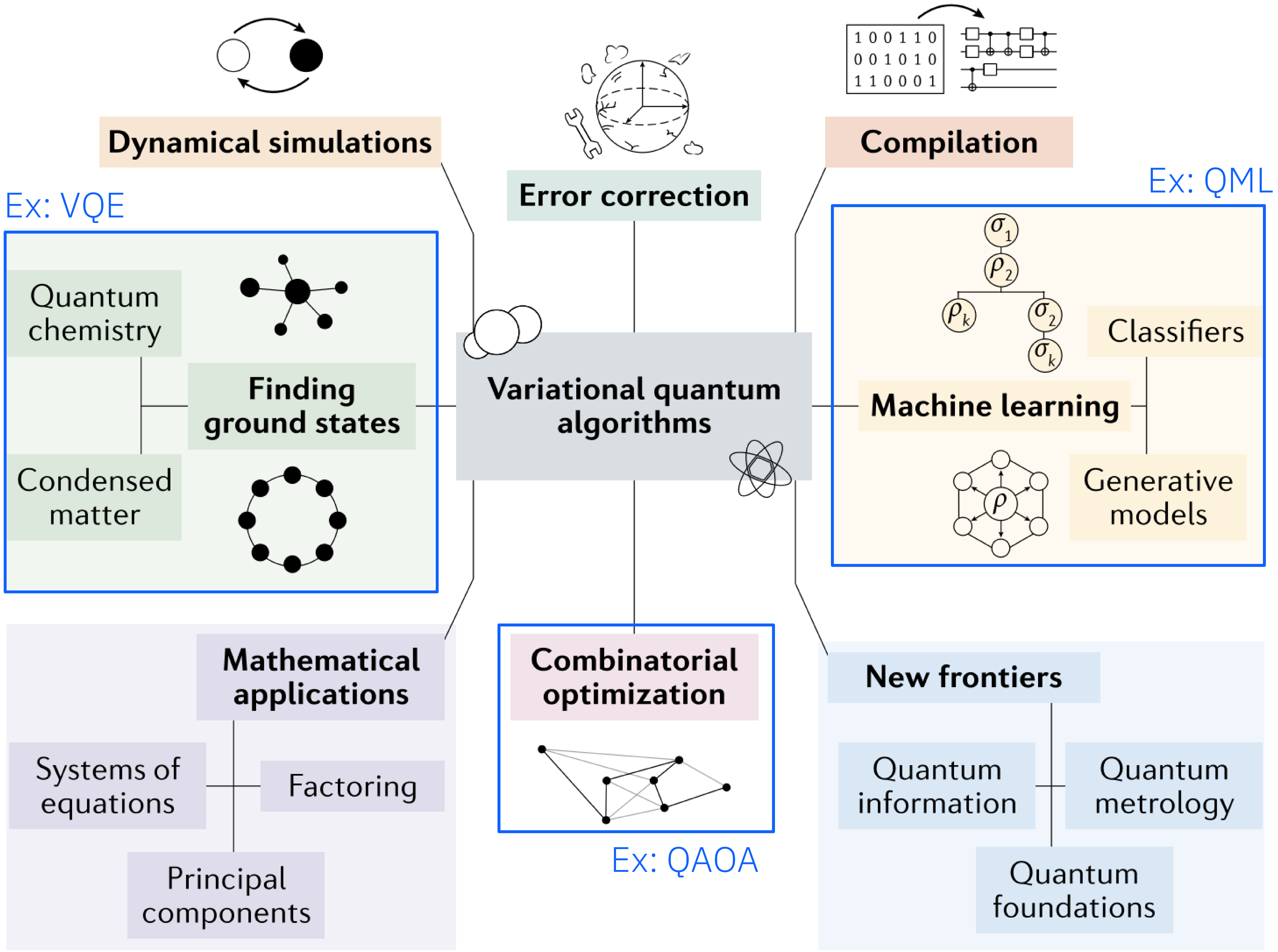
Quantum:
State preparation, entanglement, and measurement



Classical:
Parameter optimization and/or post-processing

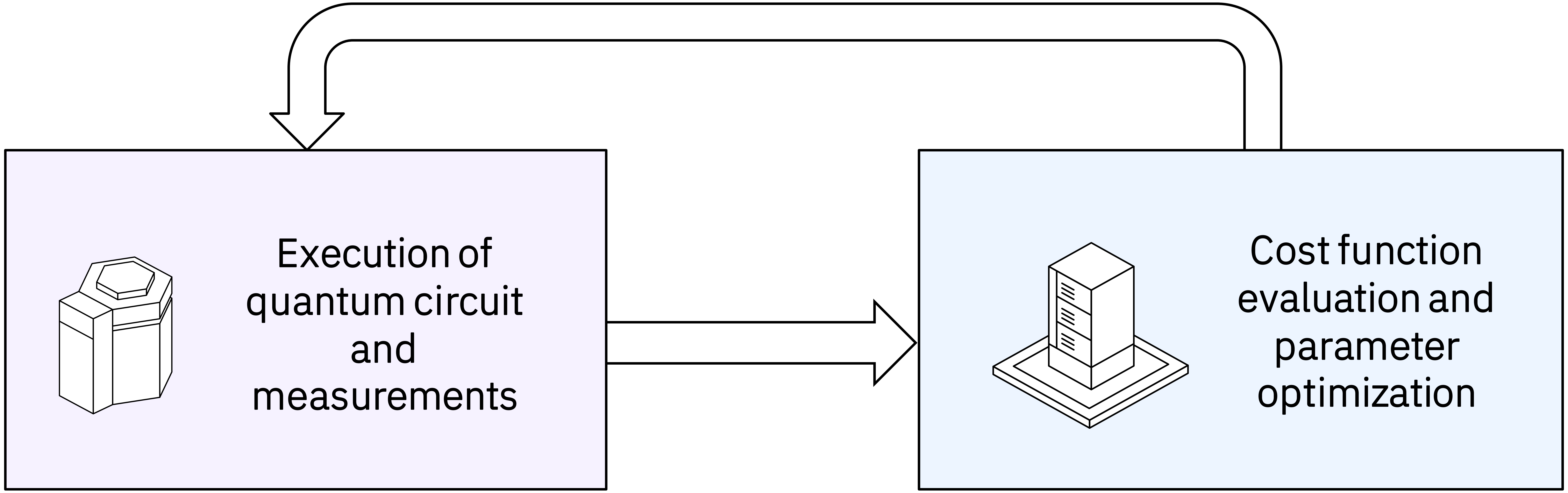
But… variational quantum algorithms (VQAs) present challenges in scalability and reliability both in near-term and fault-tolerant settings.

Motivation for variational quantum algorithms



M Cerezo *et al*, *Nat Rev Phys* **9**, 625 (2021)

Overview of Variational Quantum Algorithms



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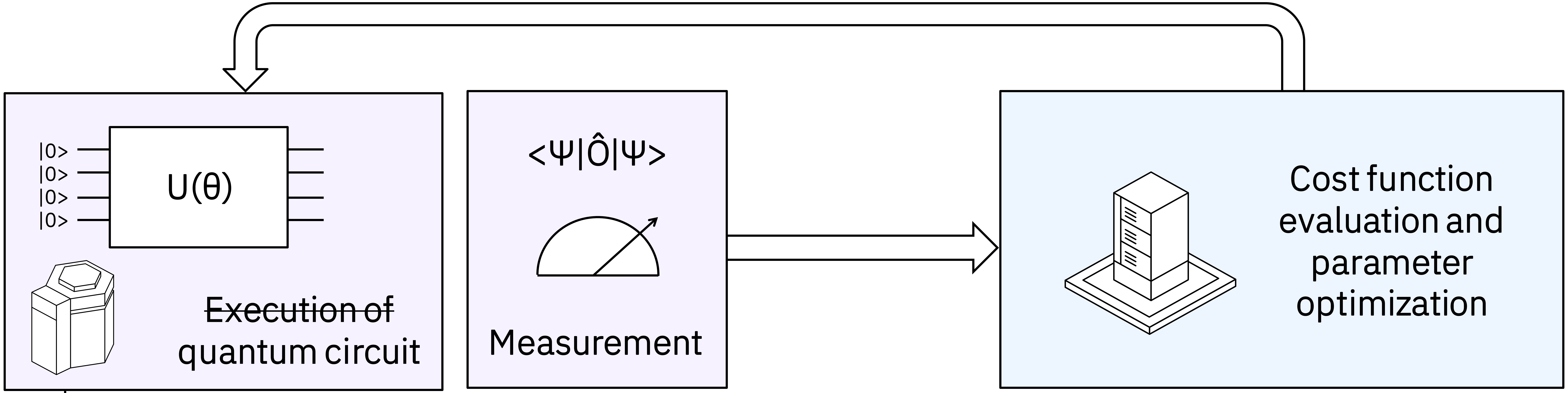
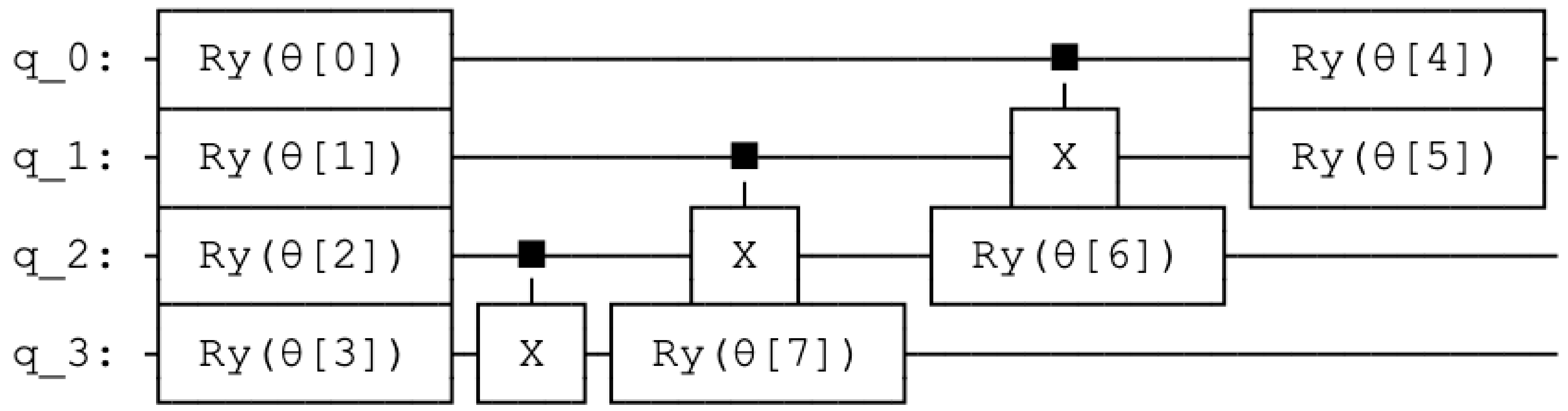
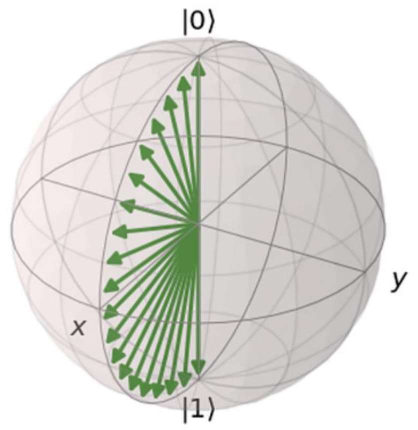


- Choice of ansatz

RealAmplitudes(4, reps=1)





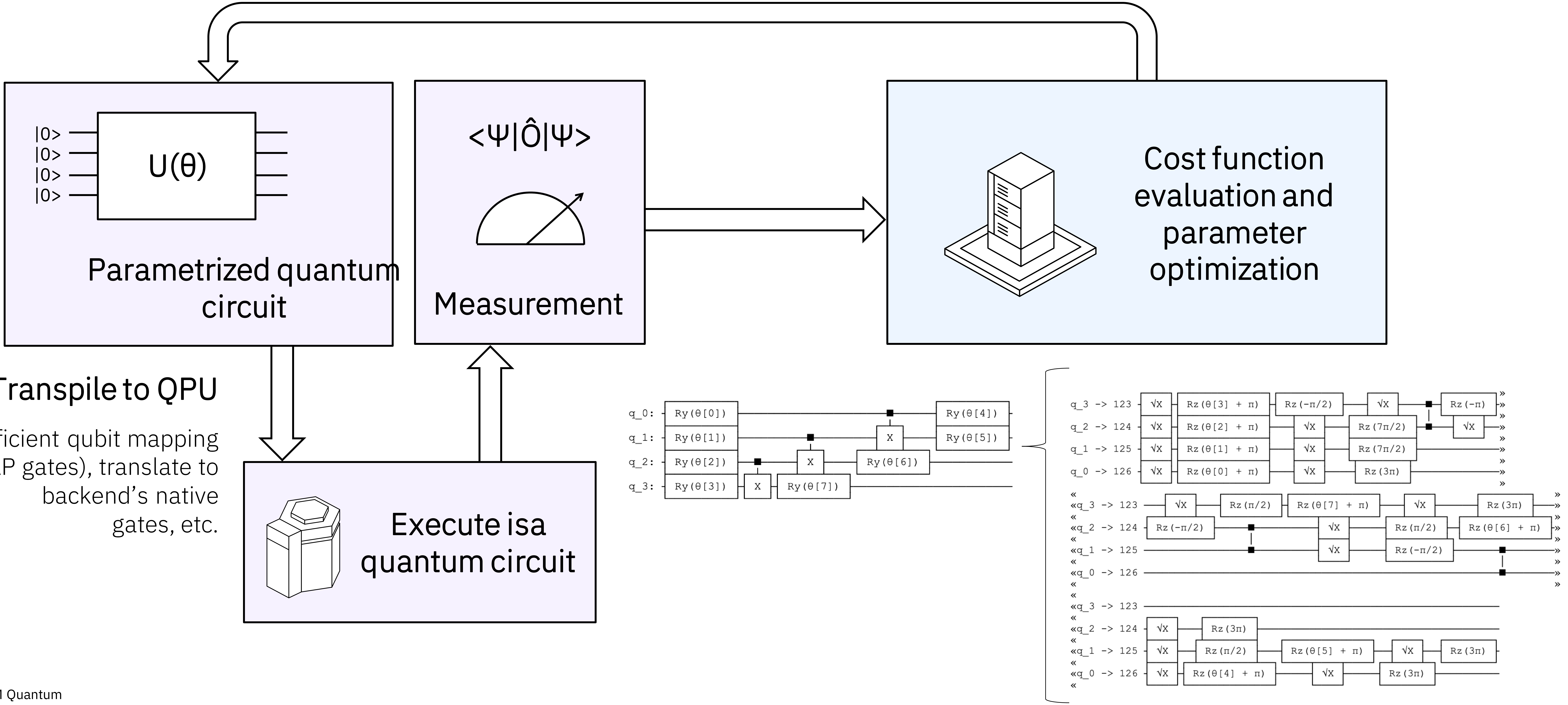
- Choice of initial parameters θ_0 (are there any constraints?)

Qiskit circuit library

`n_local` (num_qubits, rotation_blocks, ...[, ...])	Construct an n-local variational circuit.
`efficient_su2` (num_qubits[, su2_gates, ...])	The hardware-efficient $SU(2)$ 2-local circuit.
`real_amplitudes` (num_qubits[, entanglement, ...])	Construct a real-amplitudes 2-local circuit.
`pauli_two_design` (num_qubits[, reps, seed, ...])	Construct a Pauli 2-design ansatz.
`excitation_preserving` (num_qubits[, mode, ...])	The heuristic excitation-preserving wave function ansatz.
`qaoa_ansatz` (cost_operator[, reps, ...])	A generalized QAOA quantum circuit with a support of custom initial states and mixers.
`hamiltonian_variational_ansatz` (hamiltonian)	Construct a Hamiltonian variational ansatz.
`evolved_operator_ansatz` (operators[, reps, ...])	Construct an ansatz out of operator evolutions.

arxiv.2402.15879

Overview of Variational Quantum Algorithms



Transpile to QPU

Efficient qubit mapping (SWAP gates), translate to backend's native gates, etc.

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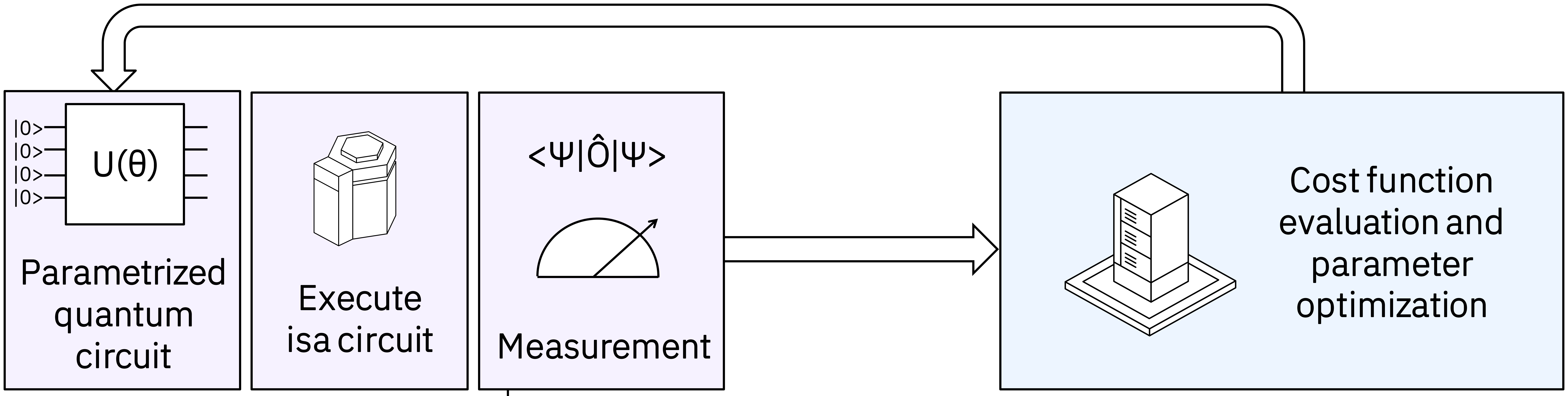


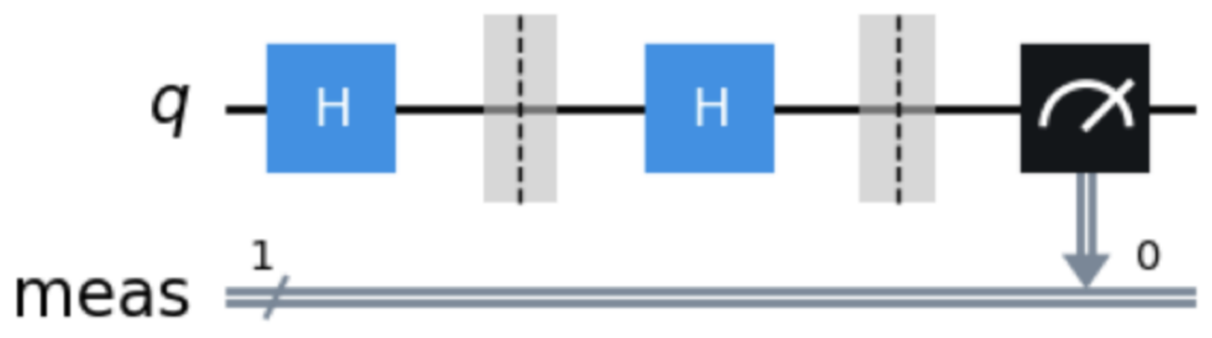
- Observable is given by the problem
- Expectation value is computed with finite num. of shots

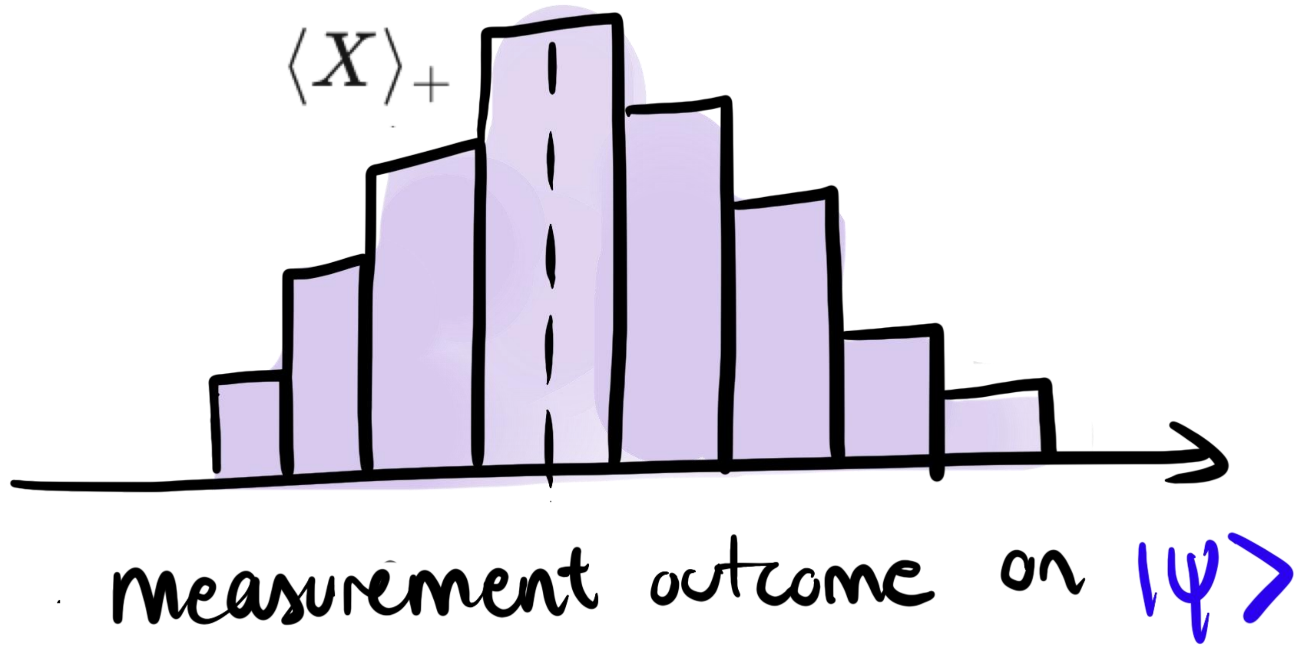
Quantum state

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right)$$

Observable

$$\hat{X} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$





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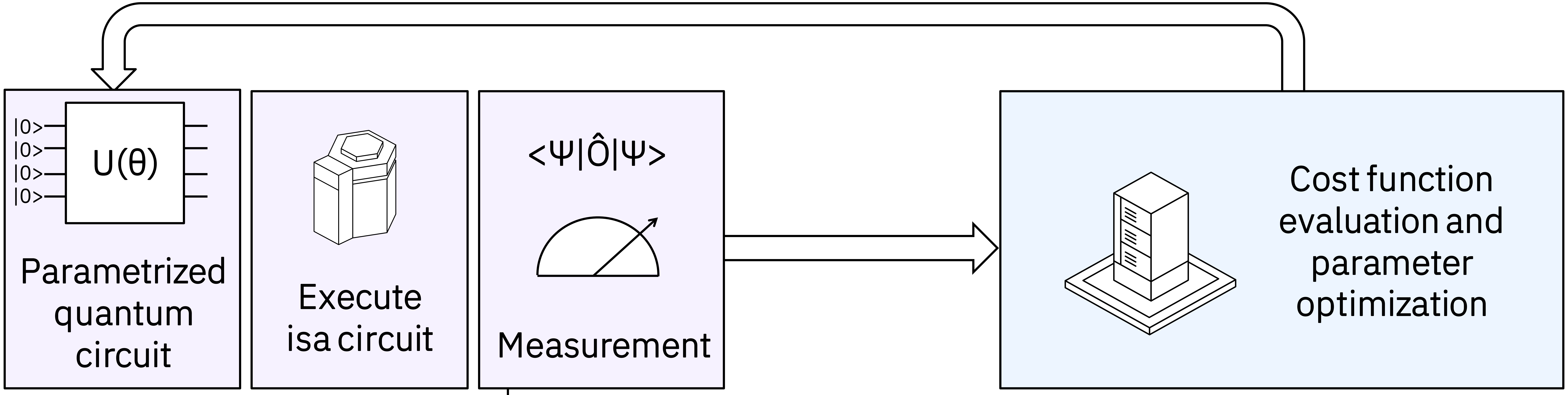
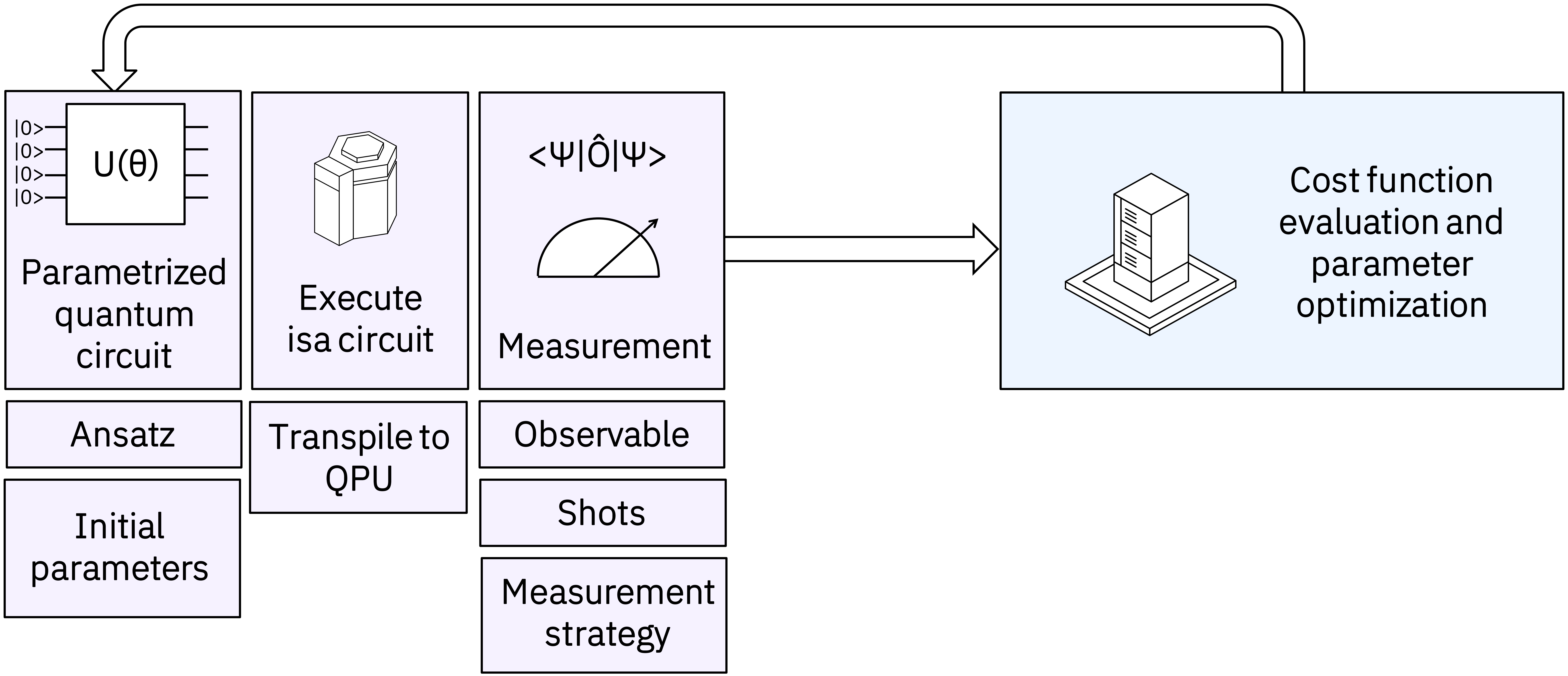


- Observable is given by the problem
- Expectation value is computed with finite num. of shots
- For complex observables we need grouping strategies

$\hat{O} = Z_0 \cdot X_1 + Y_1 \cdot X_2 + X_2 \cdot X_3 + X_0 + Z_3$ (5 terms)

Group 1: $Z_0 \cdot X_1 + X_2 \cdot X_3$
Group 2: $Y_1 \cdot X_2 + X_0 + Z_3$

Overview of Variational Quantum Algorithms



Inspired in “Introduction to VQAs”,
By Michał Stęchły, arxiv.2402.15879

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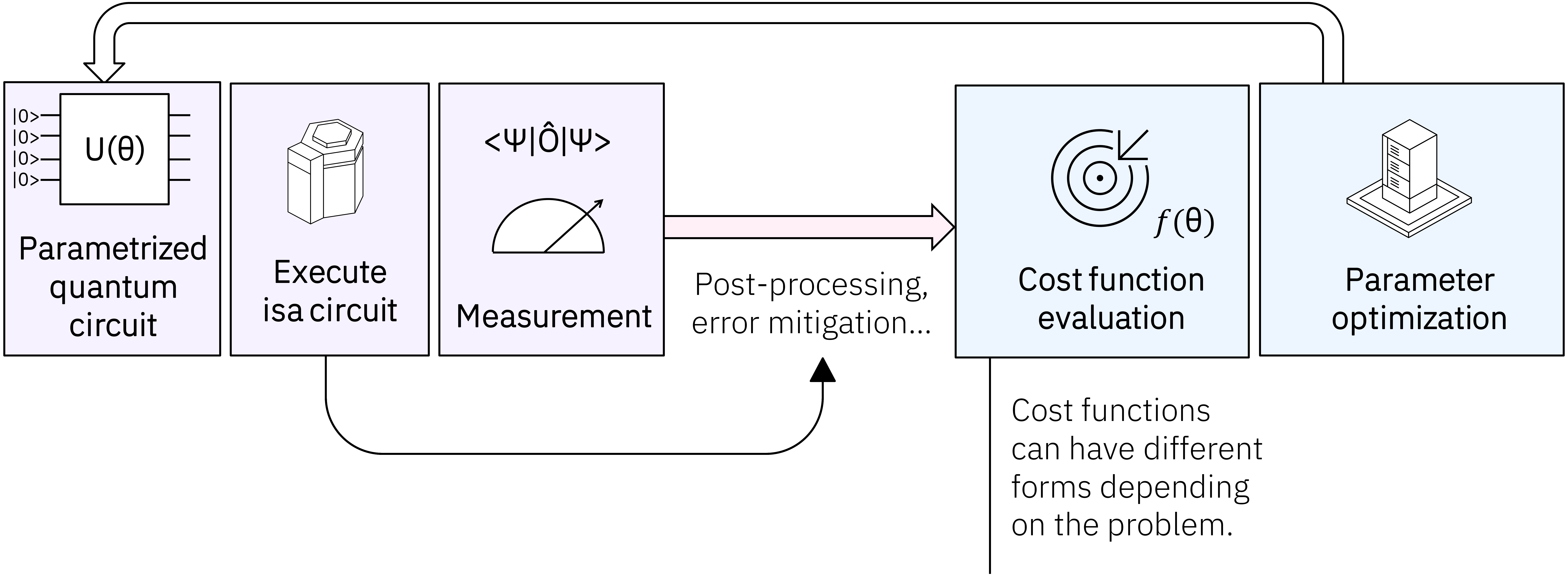

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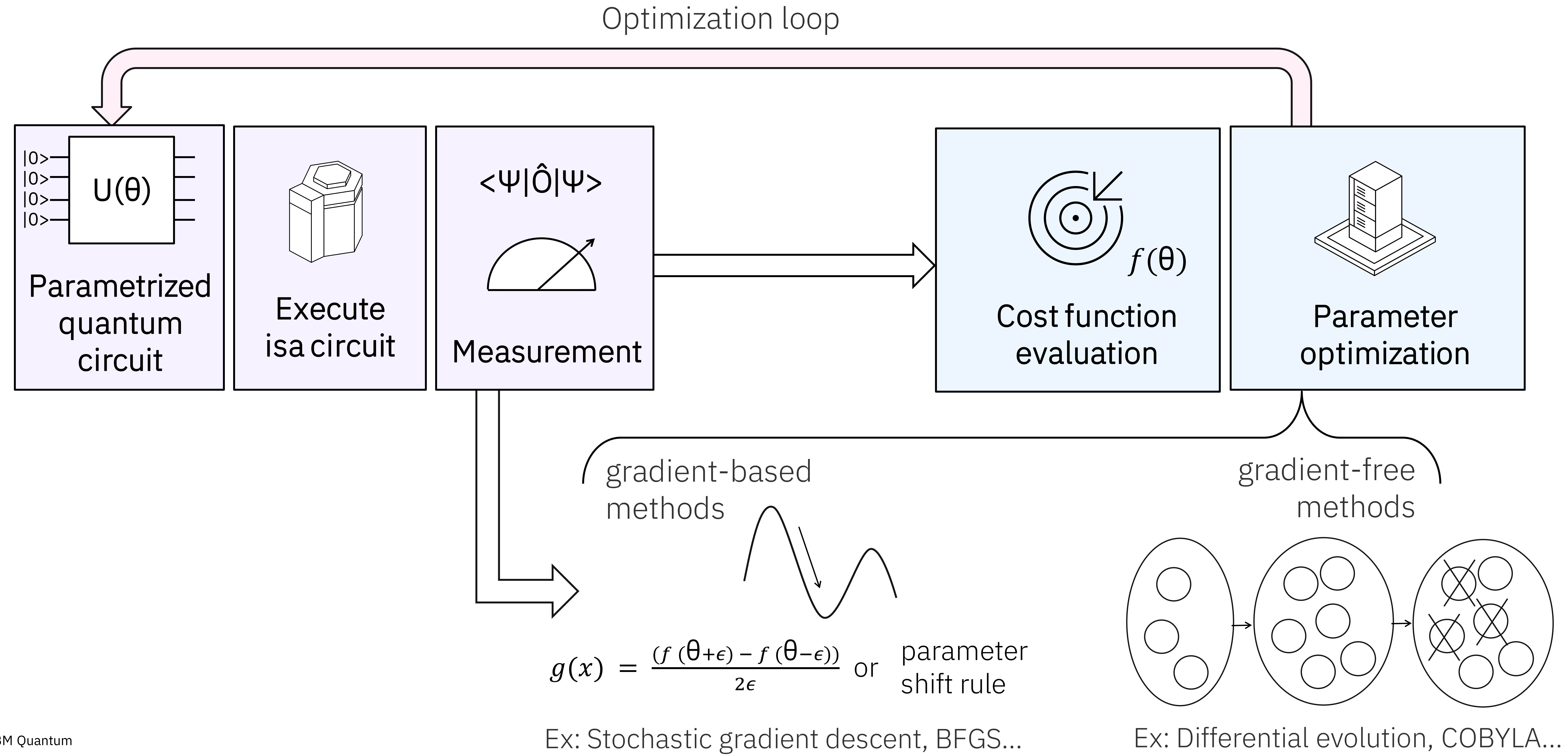

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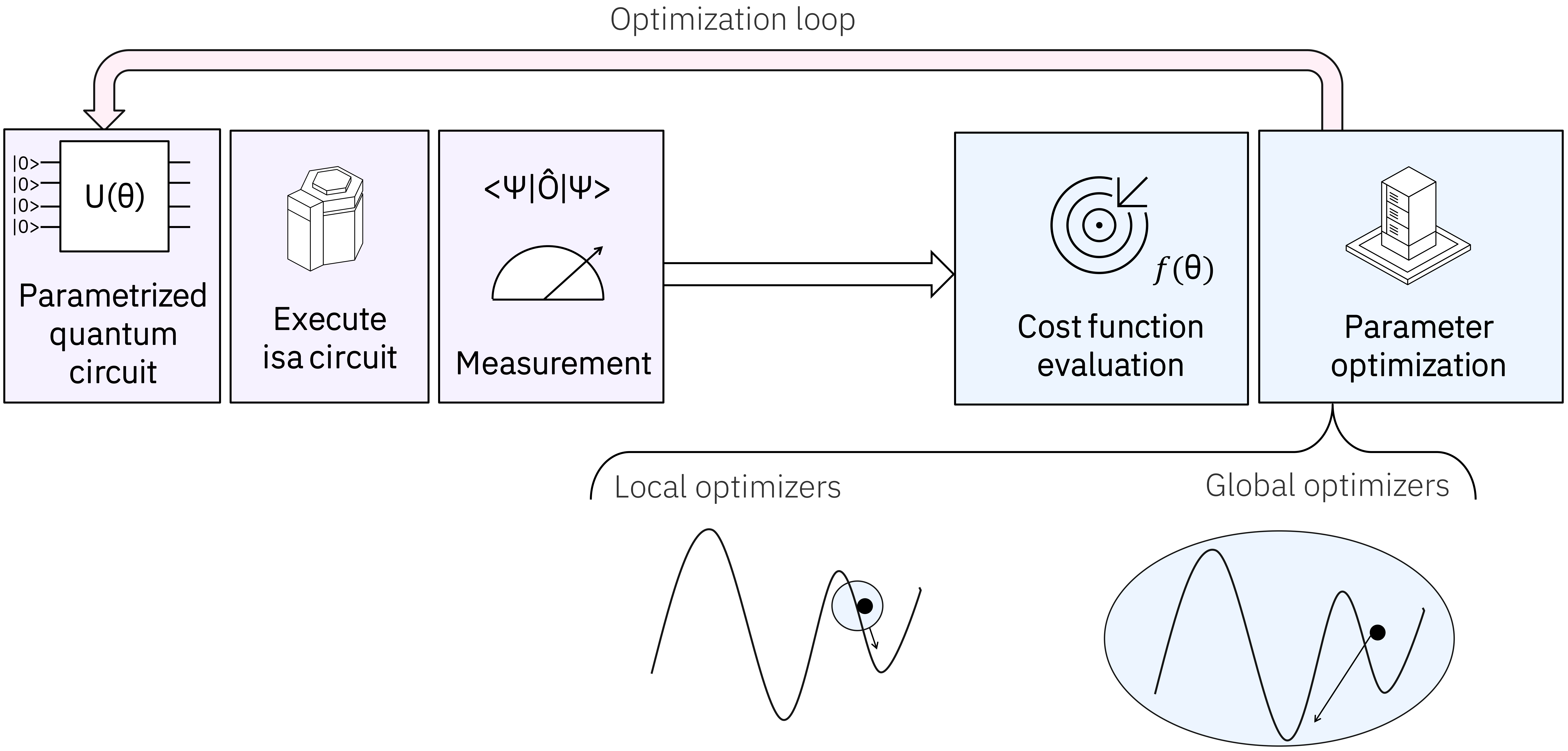

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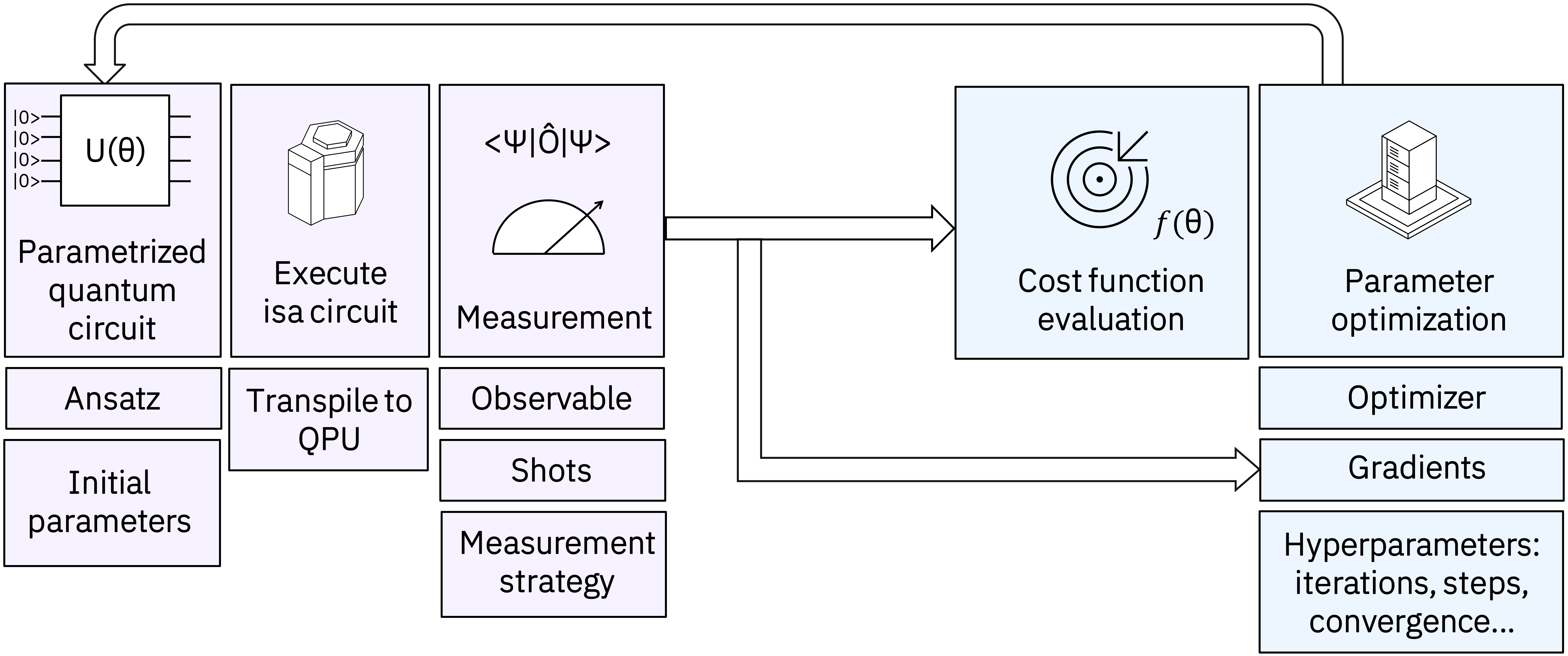

Inspired in “Introduction to VQAs”, by Michał Stęchły, arxiv.2402.15879

Key Examples of Variational Quantum Algorithms

Variational Quantum Eigensolver (VQE)

A variational eigenvalue solver on a quantum processor

Alberto Peruzzo,[1,*] Jarrod McClean,[2,*] Peter Shadbolt,[1] Man-Hong Yung,[2,3]
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April 2013

Quantum Approximate Optimization Algorithm (QAOA)

A Quantum Approximate Optimization Algorithm

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Sam Gutmann

November 2014

QML examples: Variational Quantum Classifiers (VQCs), generative models...

Variational Quantum Eigensolver

VQE is used to estimate an upper bound of the energy of the ground state of a given quantum mechanical system.

High-Energy Physics
Understanding the fundamental nature of particles and forces

Materials
Predicting and understanding material behavior

Healthcare & Life Sciences
Understanding biochemical interactions and reactions

Ground state energies are fundamental in **quantum chemistry** and hard to obtain with classical computers.

The variational principle:

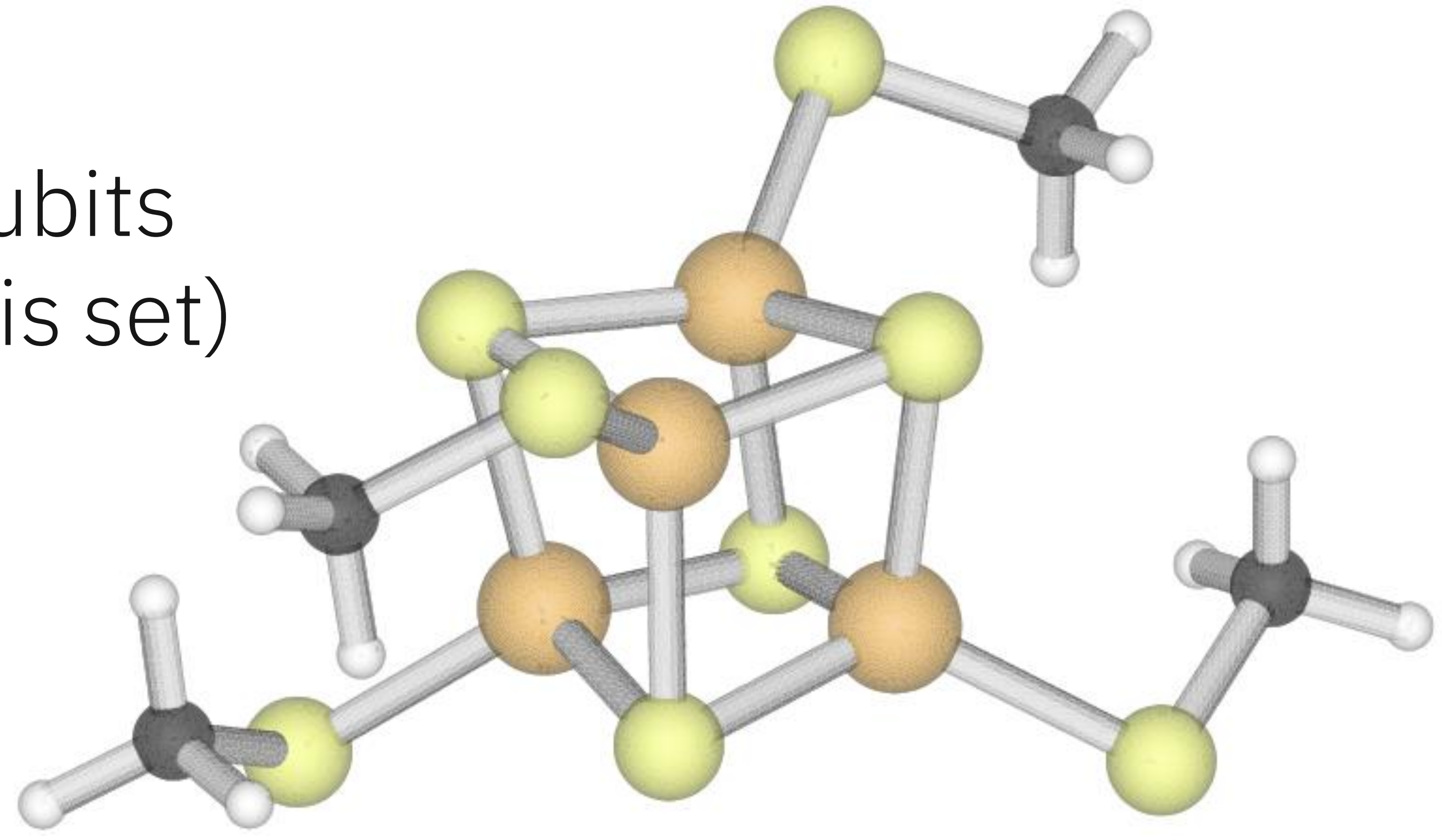
If we take an arbitrary state $|\psi\rangle$ with an associated energy E_ψ, we know that $E_\psi \geq E_0$ (GS energy):

$$\langle\psi|H|\psi\rangle \geq E_0$$

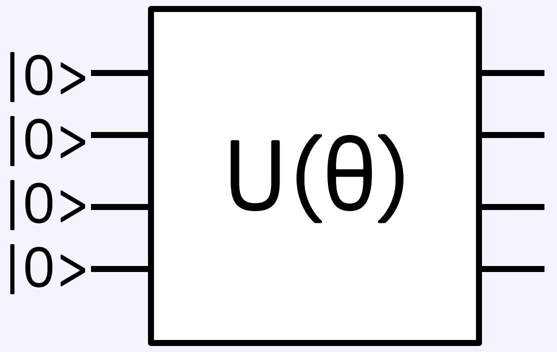
Trying all the possible states and picking the one with lowest energy is not a possibility!

Example of a VQE implementation – Quantum Chemsitry

Fe_4S_4 on 72 qubits
(TZP-DKH basis set)



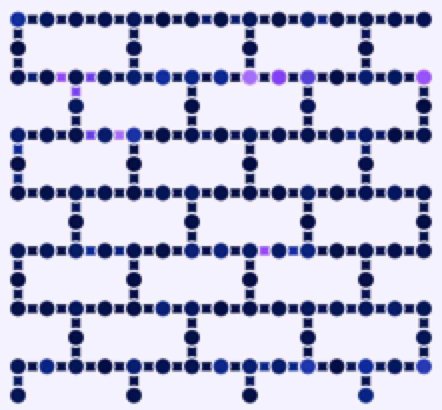
Initial parameters:
- Start with Hartree-Fock product state
  |11100000>
- Initialize parameters randomly/using previous classical computations.



Parametrized quantum circuit

$$\hat{H} = \sum_{\substack{pr\\ \sigma}} h_{pr}\, \hat{a}^\dagger_{p\sigma}\hat{a}_{r\sigma} + \sum_{\substack{prqs\\ \sigma\tau}} \frac{(pr|qs)}{2}\, \hat{a}^\dagger_{p\sigma}\hat{a}^\dagger_{q\tau}\hat{a}_{s\tau}\hat{a}_{r\sigma}$$

Hardware efficient ansatz

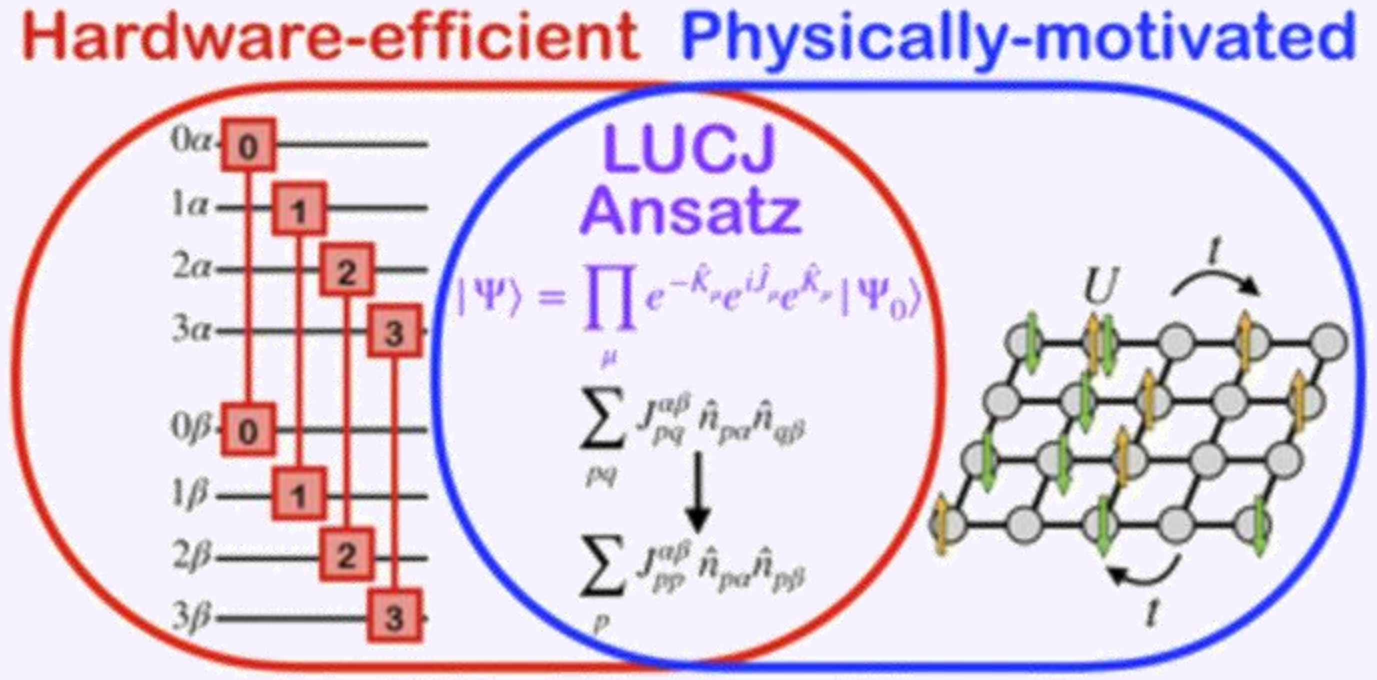


qUCCSD: Physically motivated ansatz for Quantum Chemistry.

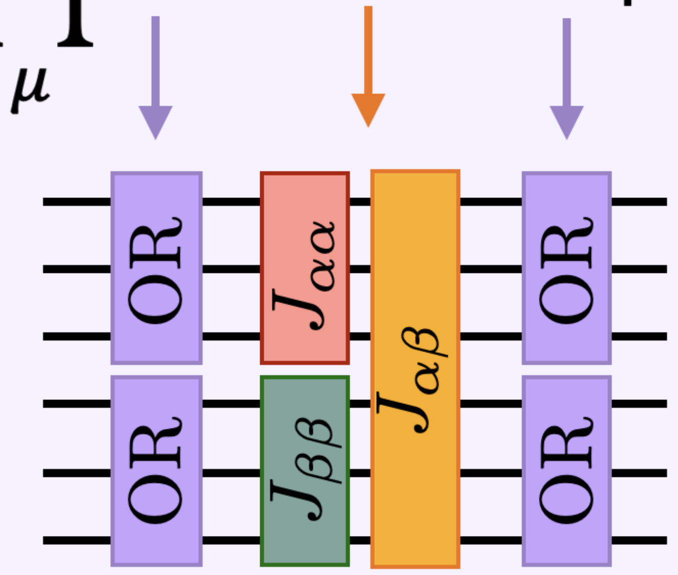
$$|\psi\rangle = e^{\hat{T}-\hat{T}^\dagger}|\Phi_0\rangle$$

$$\hat{T} = \sum_{ia} t_i{}^a \hat{a}^\dagger_a \hat{a}^\dagger_i + \sum_{ijab} t_{ij}{}^{ab} \hat{a}^\dagger_a \hat{a}^\dagger_b \hat{a}^\dagger_j \hat{a}^\dagger_i$$

LUCJ:



$$|\Psi\rangle \simeq \prod_\mu e^{-K_\mu}\, e^{iJ_\mu} e^{K_\mu}\, |\Phi_0\rangle$$



Motta, Sung, Whaley, Head-Gordon, Shee, Chem. Sci. 14, 40, 11213-11227 (2023).

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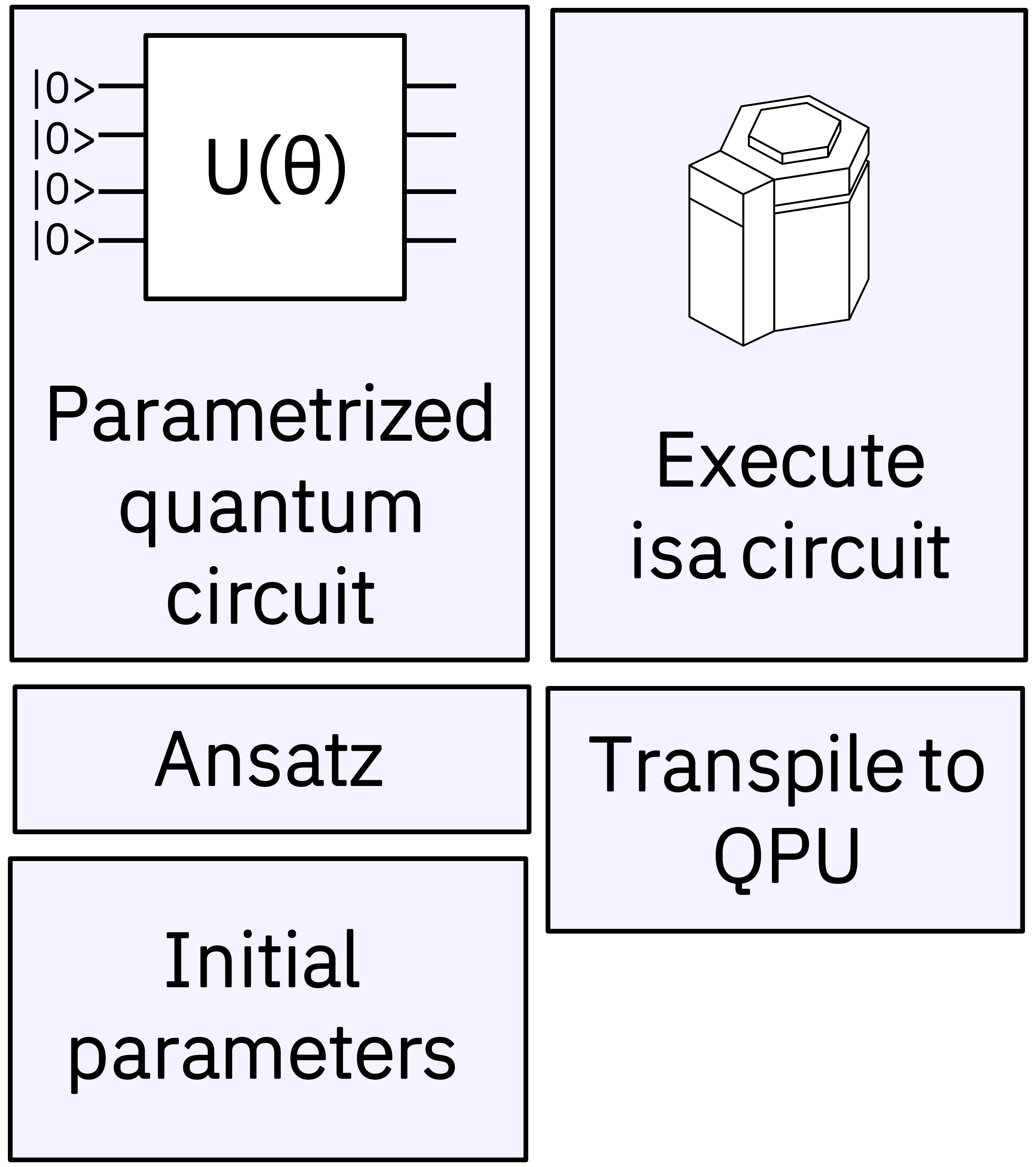

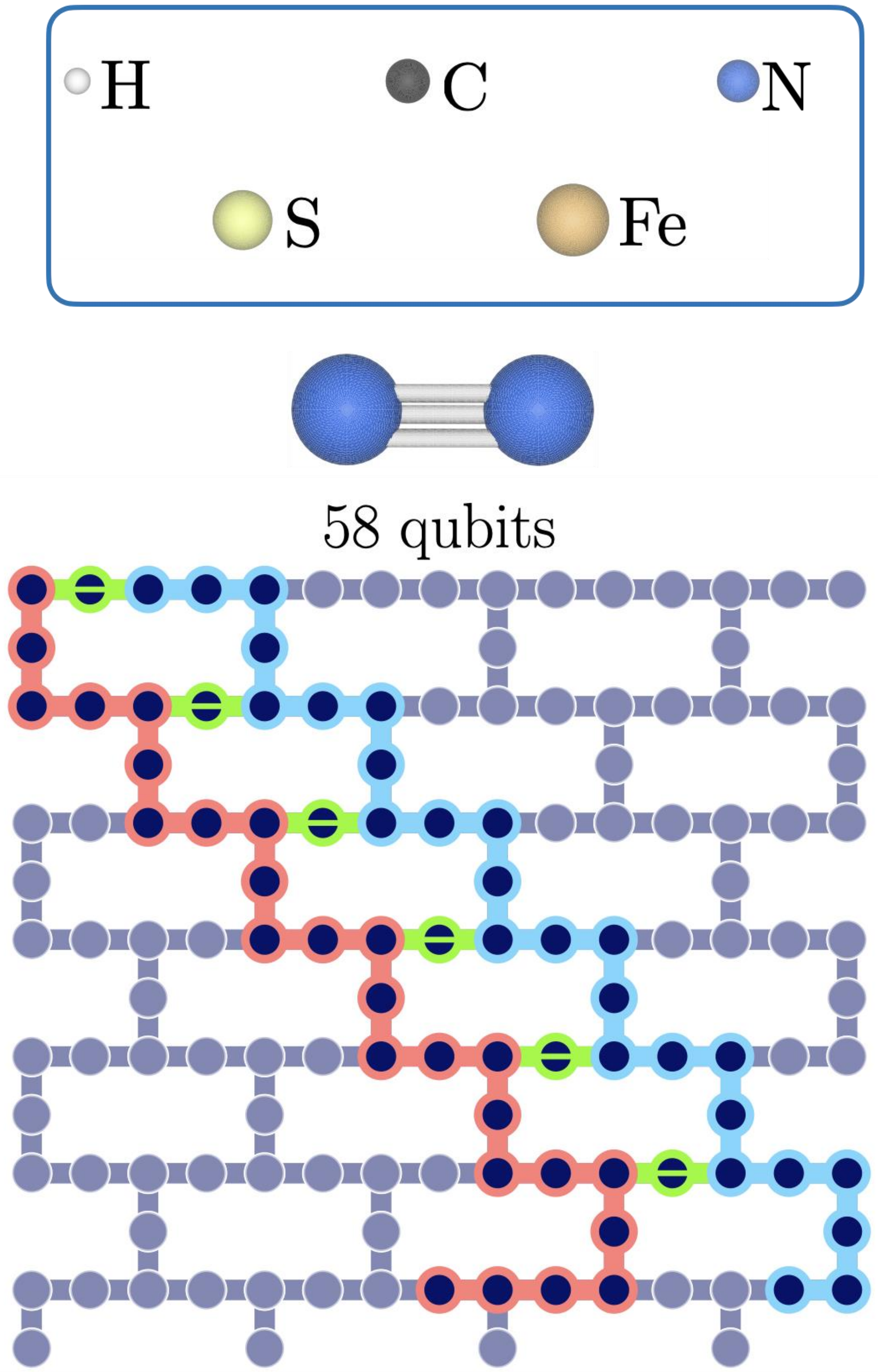

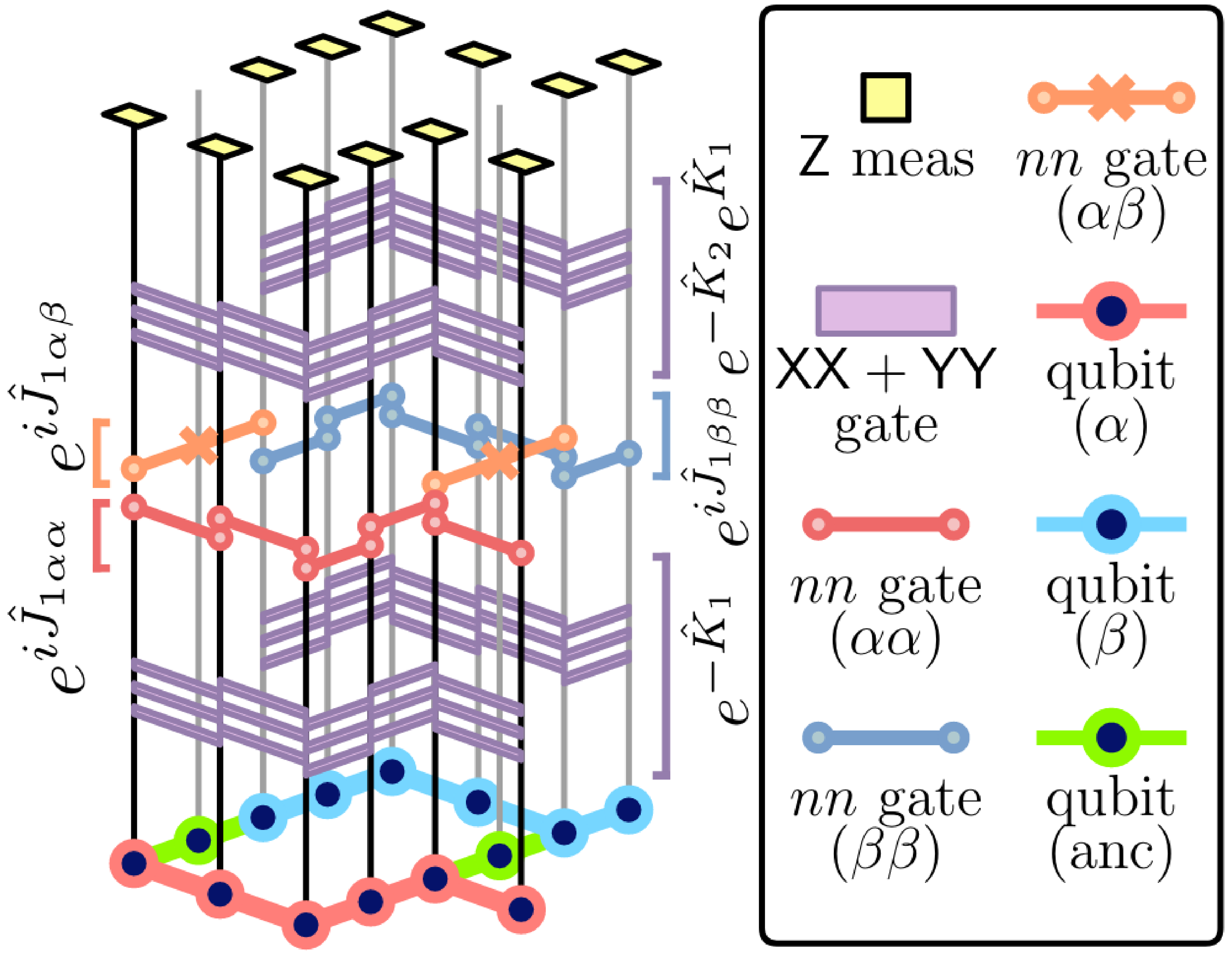

Chemistry Beyond Exact Solutions on a Quantum-Centric Supercomputer, arXiv.2405.05068

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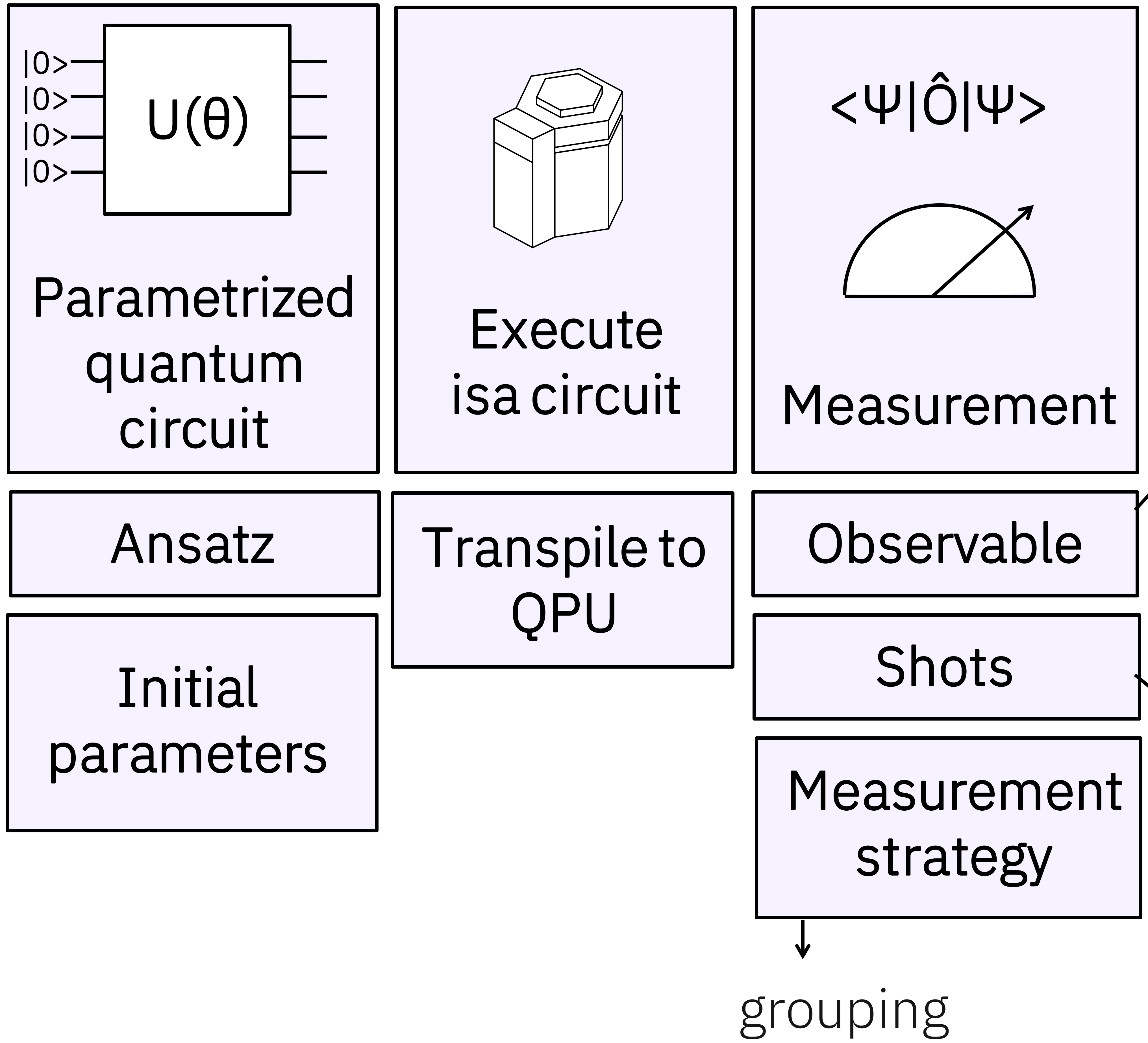

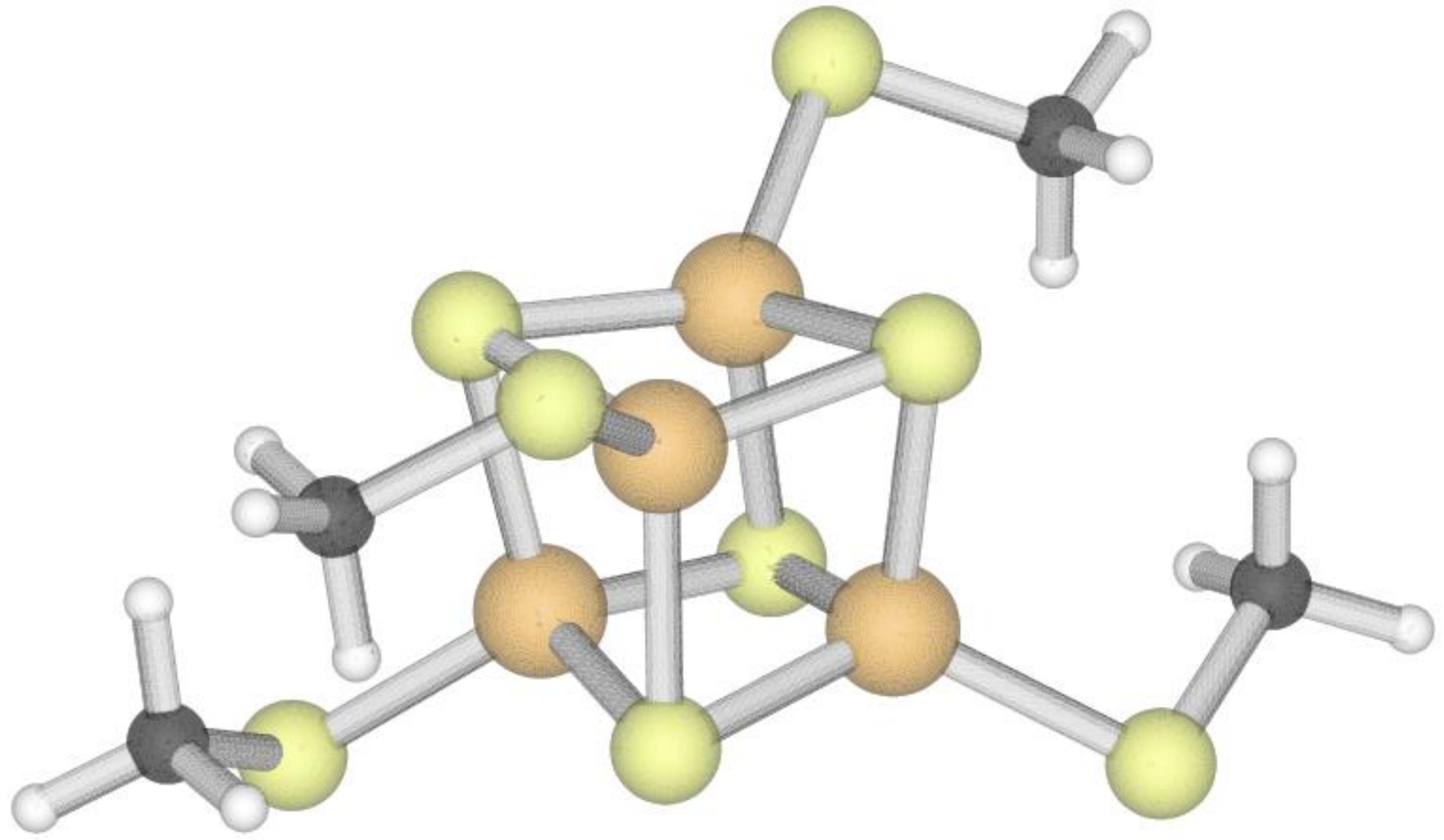

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Measurement and cost function:

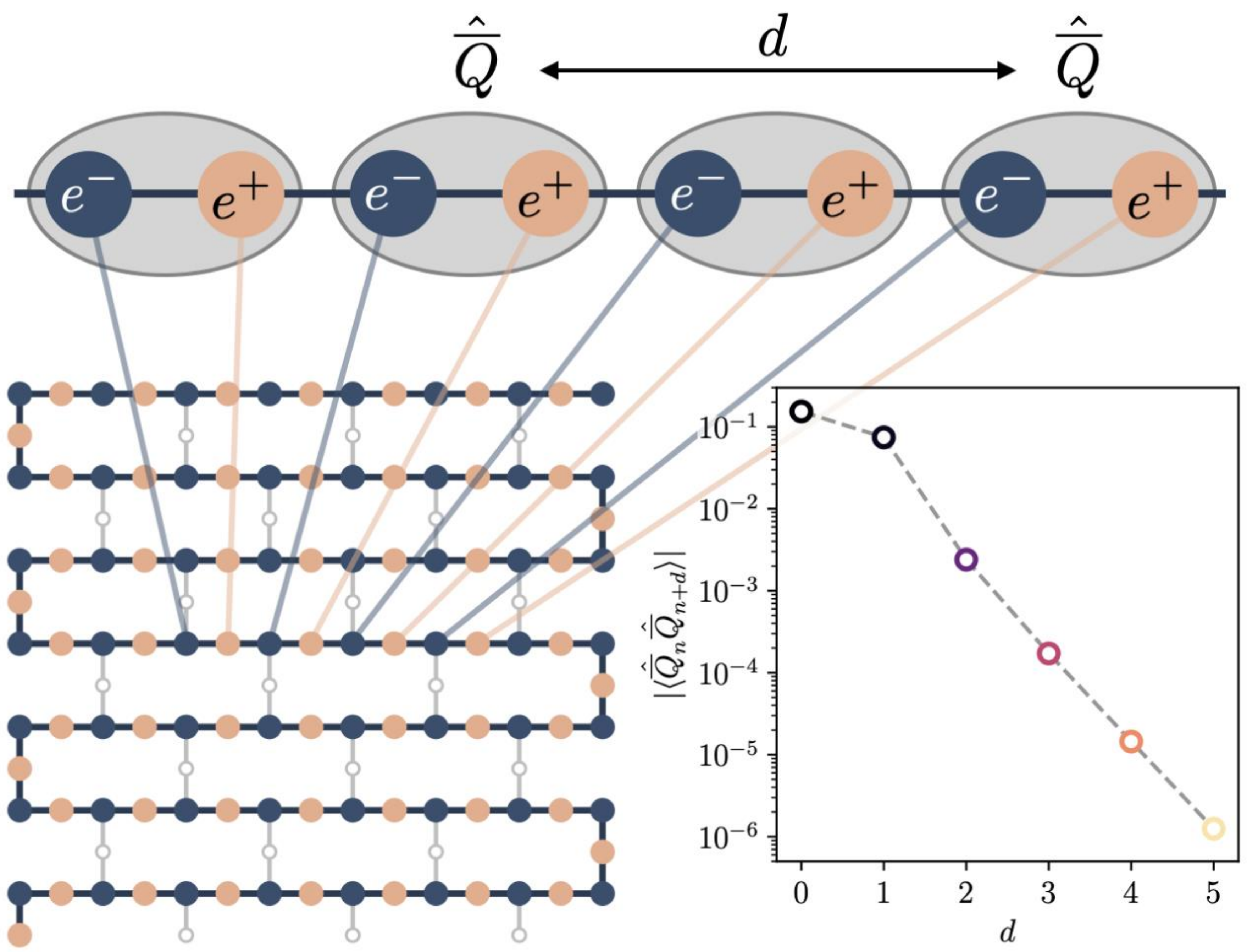
- Fe_4S_4 on 72 qubits (TZP-DKH basis set): 6.7M Pauli operators
- 10^{-7} precision on each operator for milliHartree precision
- Each circuit must be executed 10^{14} times

VQE estimation at 10µs/circuit ~30 years

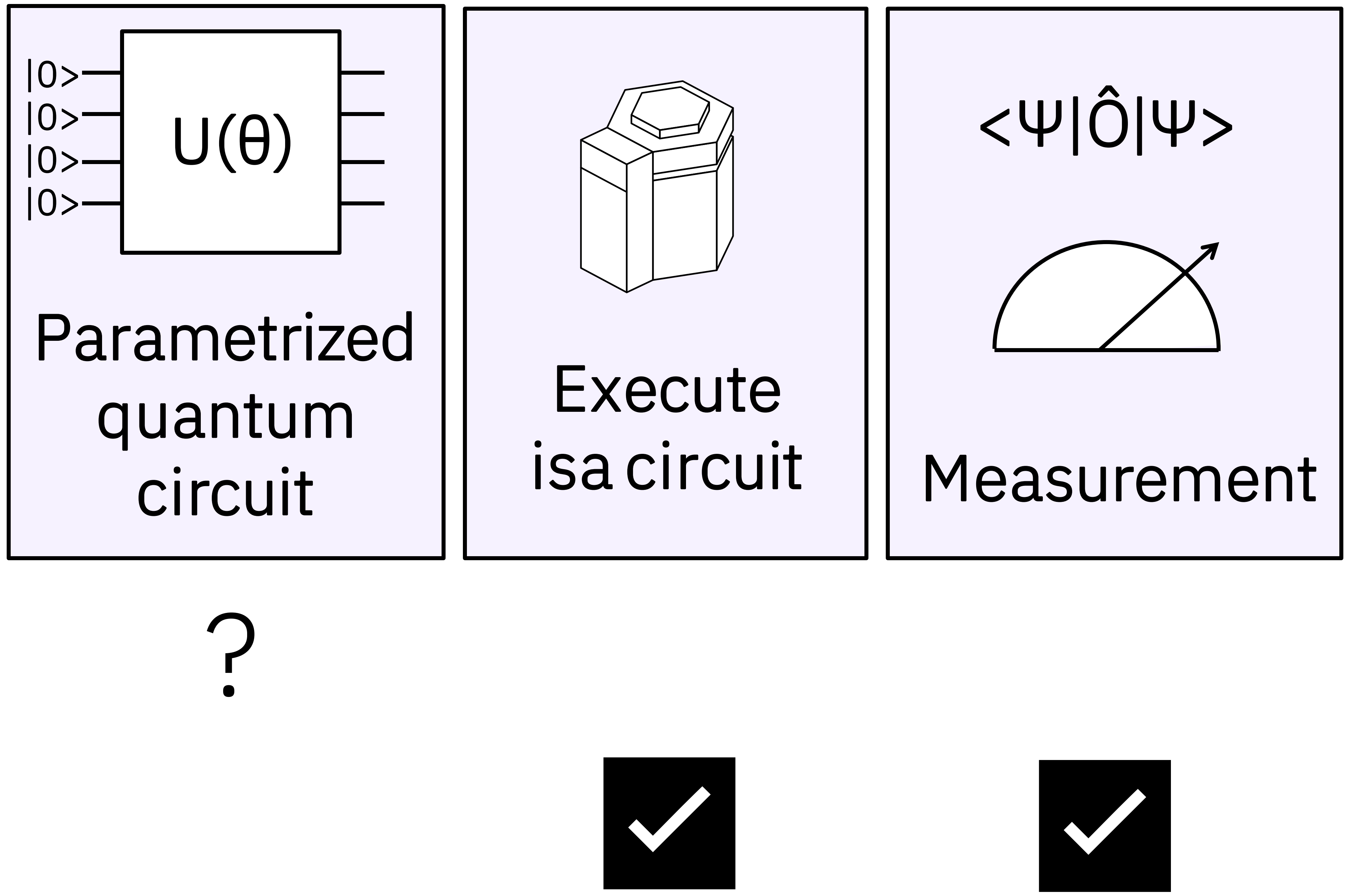
Chemistry Beyond Exact Solutions on a Quantum-Centric Supercomputer, arXiv.2405.05068

Other VQE implementations – ADAPT-VQE

Scalable Circuits-ADAPT-VQE: Groundstate preparation for Schwinger Model using 112 Qubits
Roland C. Farrell, Marc Illa, Anthony N. Ciavarella, Martin J. Savage, arXiv:2401.08044



Schwinger Model follows the heavy-hex lattice connectivity and the Hamiltonian has a smaller number of Pauli operators.



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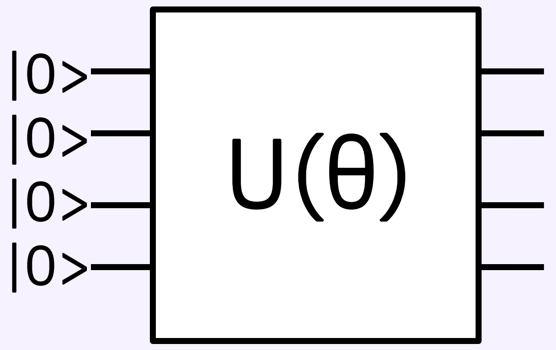
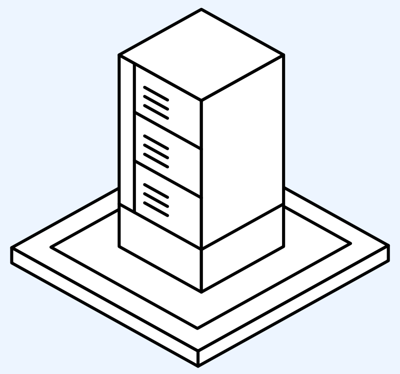
Building an ansatz with ADAPT-VQE:

1. Define a pool of operators $\hat{O}_i$ (symmetries, scalability).
2. Initialize a state with the symmetries of target state.
3. For each $\hat{O}_i$, determine the gradient of the cost function between the target and evolved ansatz states.
4. Identify the operator $\hat{O}_n$ with the largest magnitude gradient and update the ansatz with the parameterized evolution of the operator.
5. Optimize the new variational ansatz to minimize the cost function.



Parametrized quantum circuit



Parameter optimization

Keeping number of parameters small.

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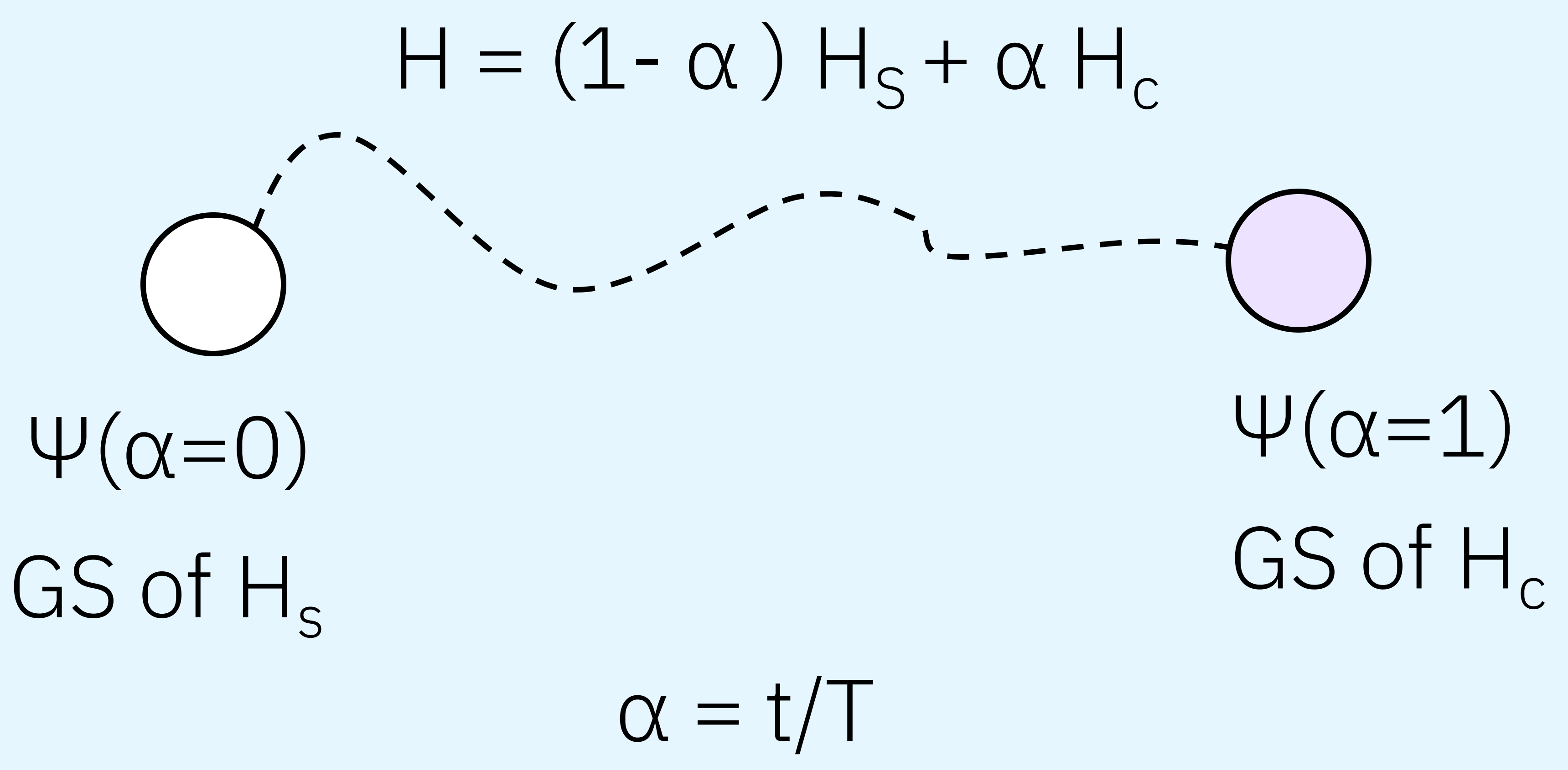
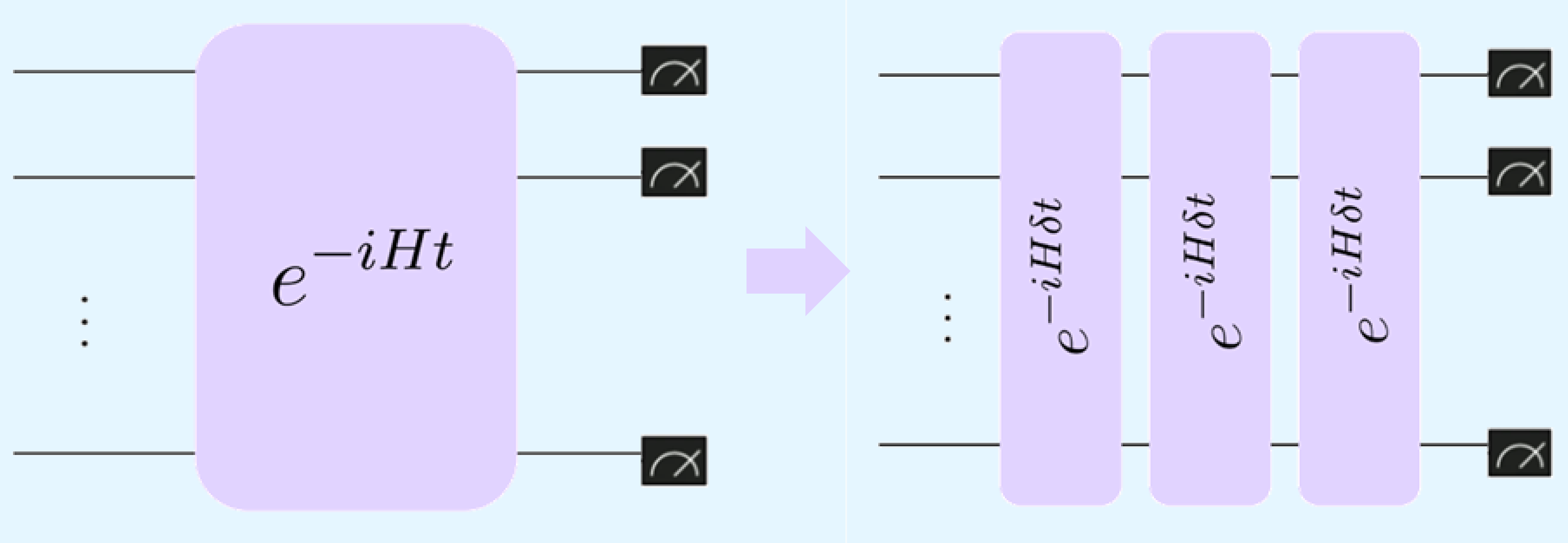
Quantum Approximate Optimization Algorithm

QAOA is a VQE-based approach to combinatorial optimization that draws on principles from Adiabatic Quantum Computing (AQC) and trotterized time evolution.

Adiabatic Quantum Computing solves optimization problems by initializing a quantum system in the ground state of an easy Hamiltonian and adiabatically evolving it into a problem Hamiltonian, whose ground state encodes the solution.



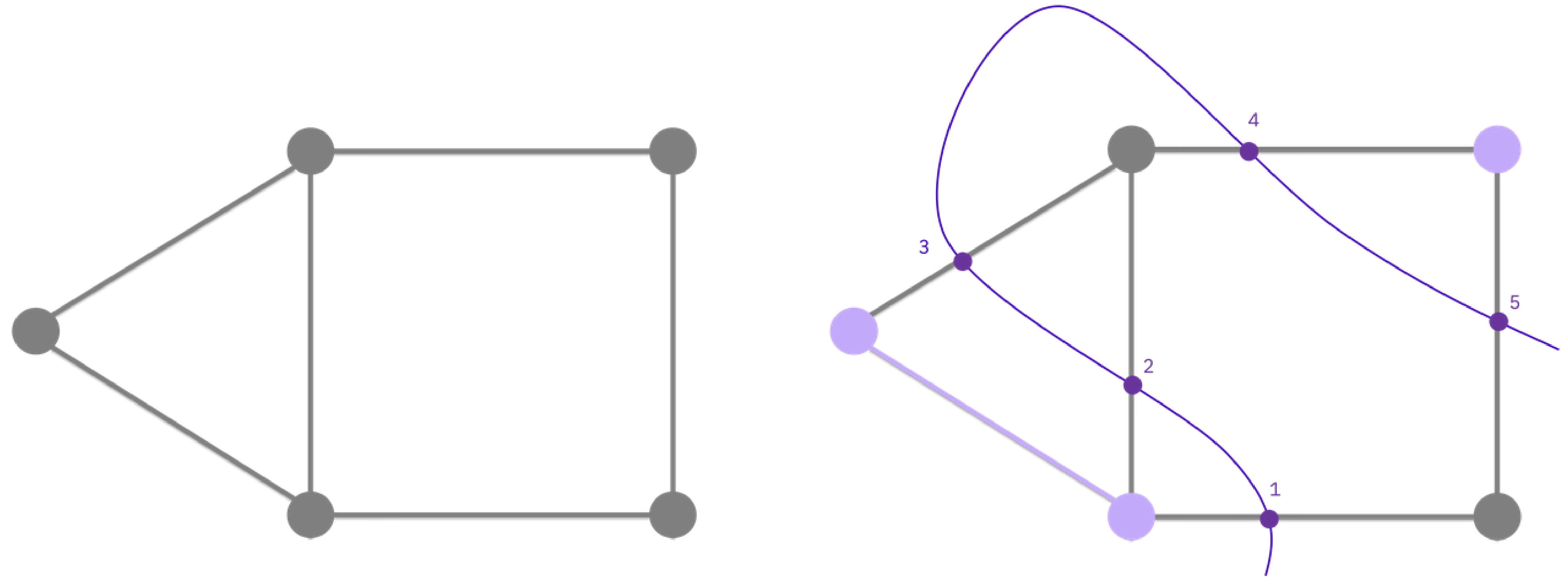
Trotterized time evolution



$$|\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle, \quad H = \sum_j a_j H_j,$$

$$|\psi(t)\rangle \approx \left(\prod_j e^{-ia_jH_jt/r}\right)^r |\psi(0)\rangle \qquad r \to \infty$$

QAOA – The MaxCut problem



The MaxCut problem

$$\min_{x\in\{0,1\}^n} \sum_{(i,j)} 2x_i x_j - x_i - x_j$$

↓

QUBO formulation

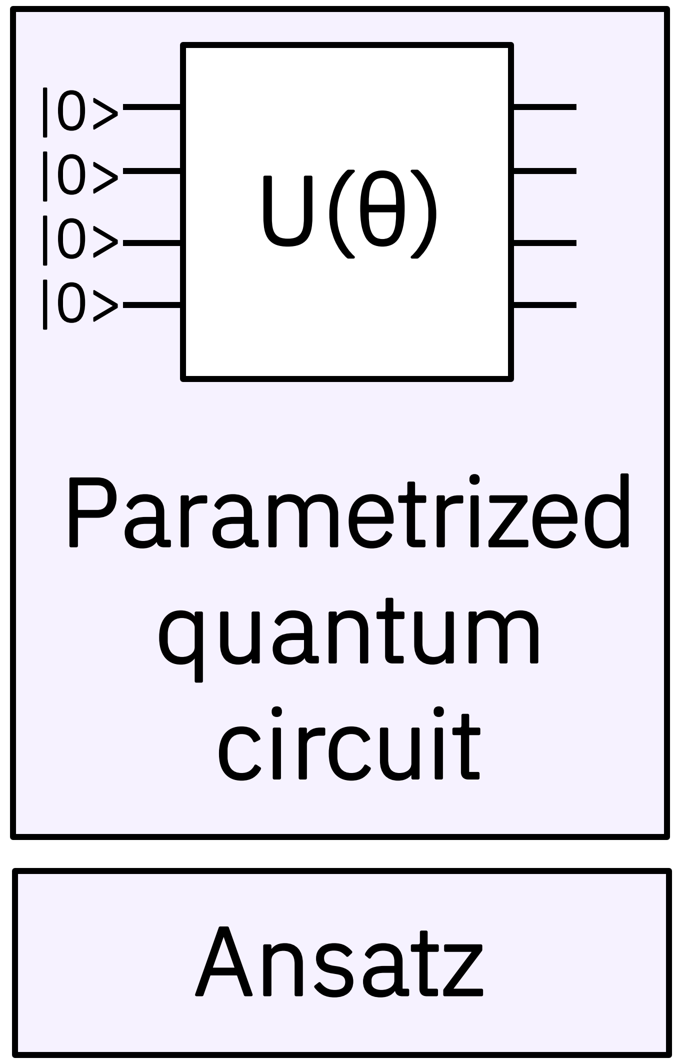
$$\min_{x\in\{0,1\}^n} x^T Q x$$

↓

Ising Hamiltonian

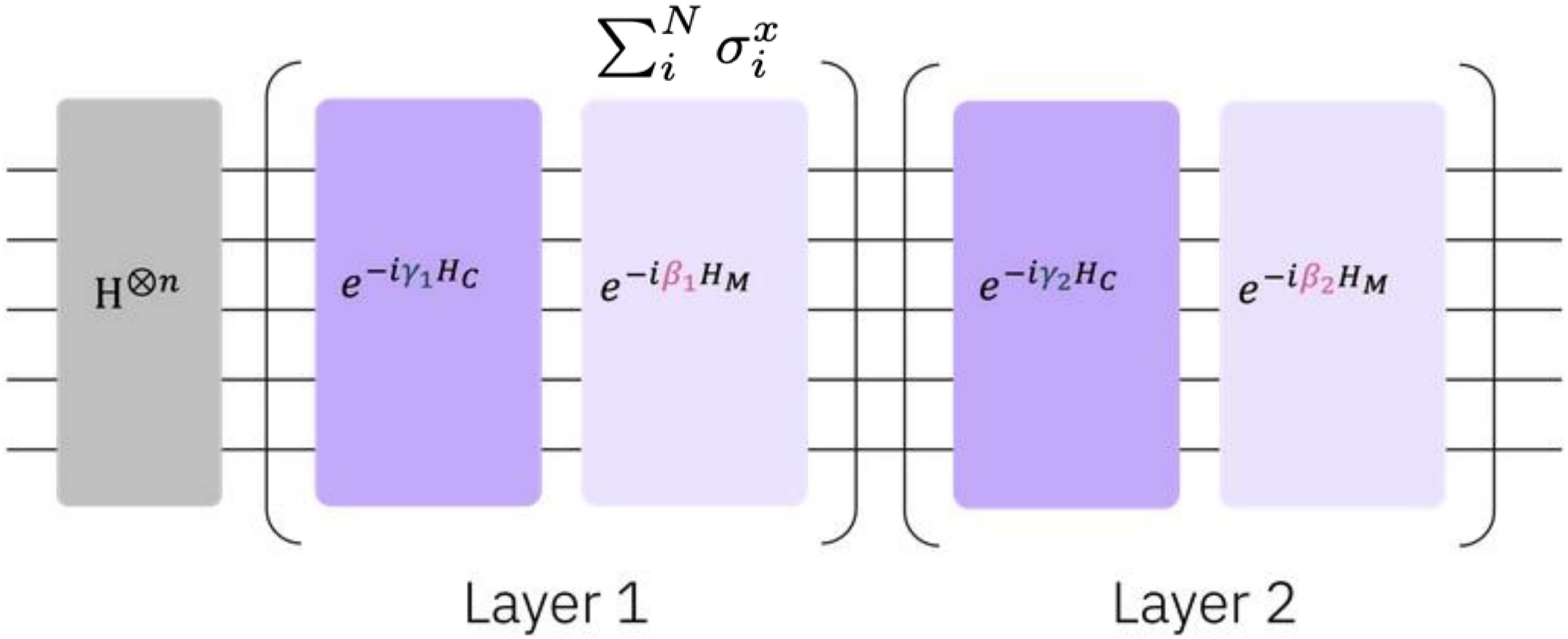
$$H_C = \sum_{ij} Q_{ij} Z_i Z_j + \sum_i b_i Z_i$$

Problem encoding



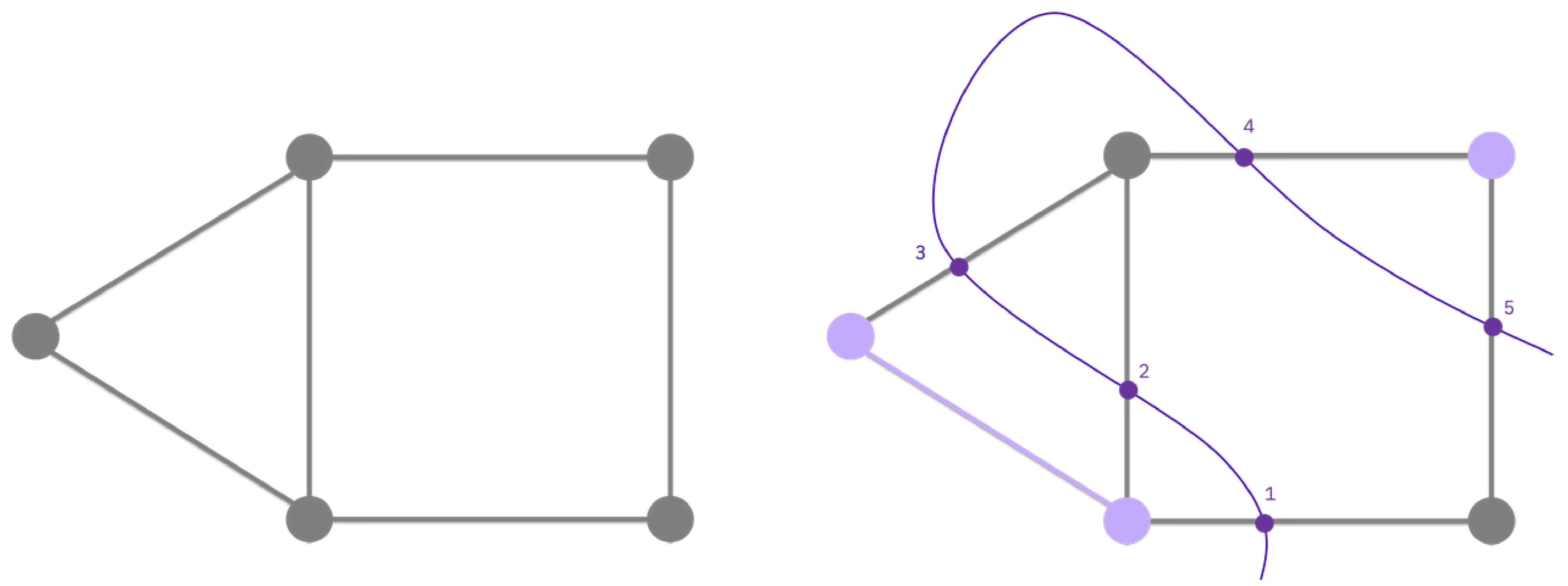
”Picewise” approximation of trotterized evolution of H = (1- α) H_M + α H_C :

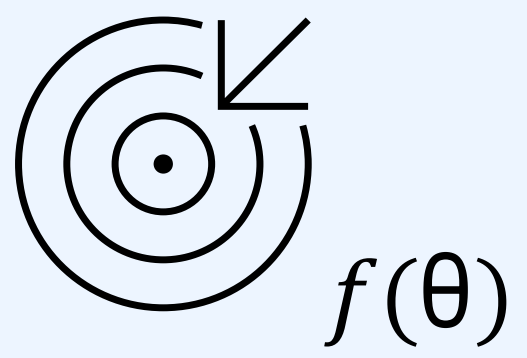
- Parameters angles γ_i and β_i are trained to keep the depth low.
- H_C is the cost Hamiltonian, while H_M is the mixing Hamiltonian. They do not commute.
- Initial state is the groundstate of H_M.



https://learning.quantum.ibm.com/tutorial/quantum-approximate-optimization-algorithm

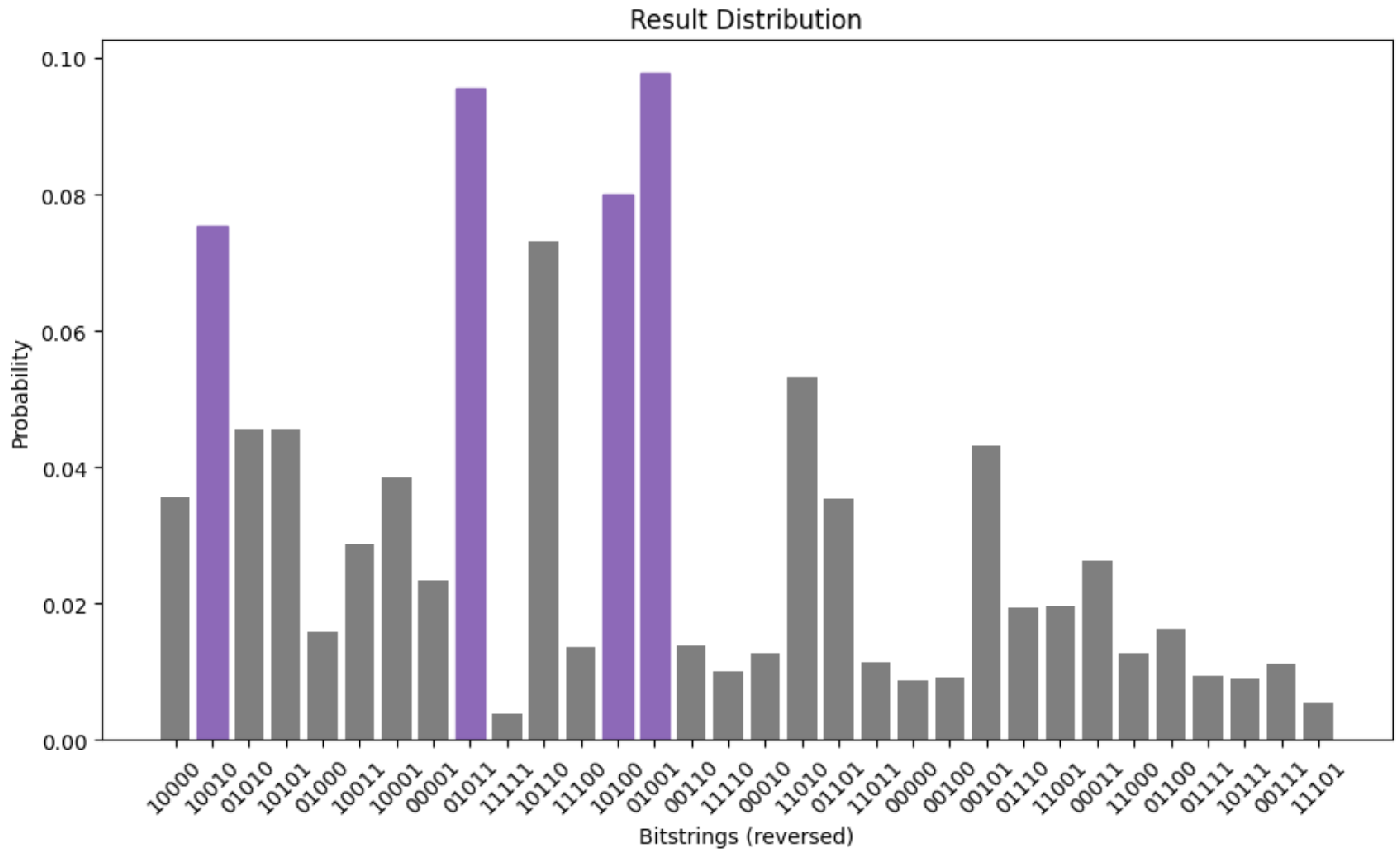
Quantum Approximate Optimization Algorithm





Cost function evaluation

The result are the bitstrings with highest probability.



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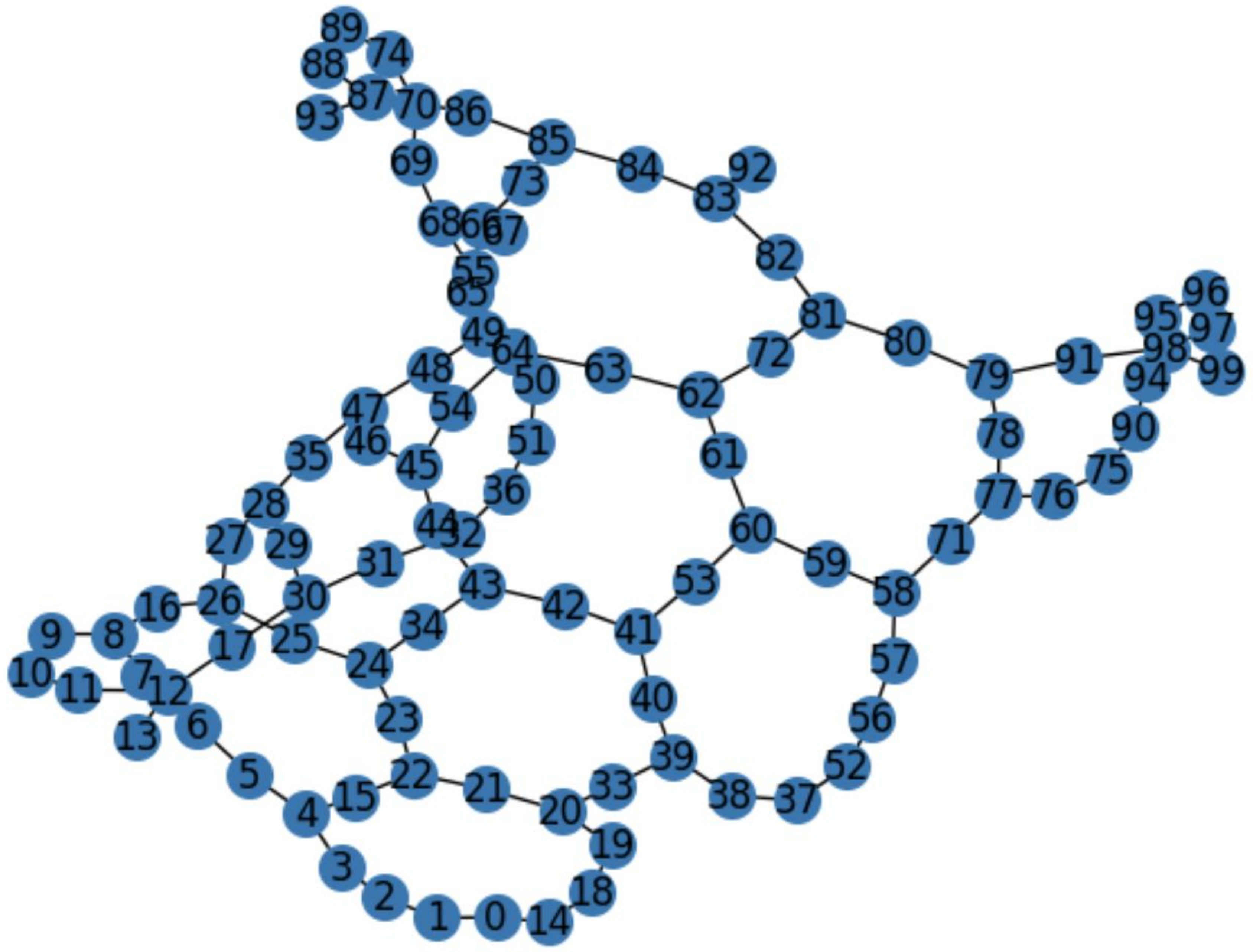
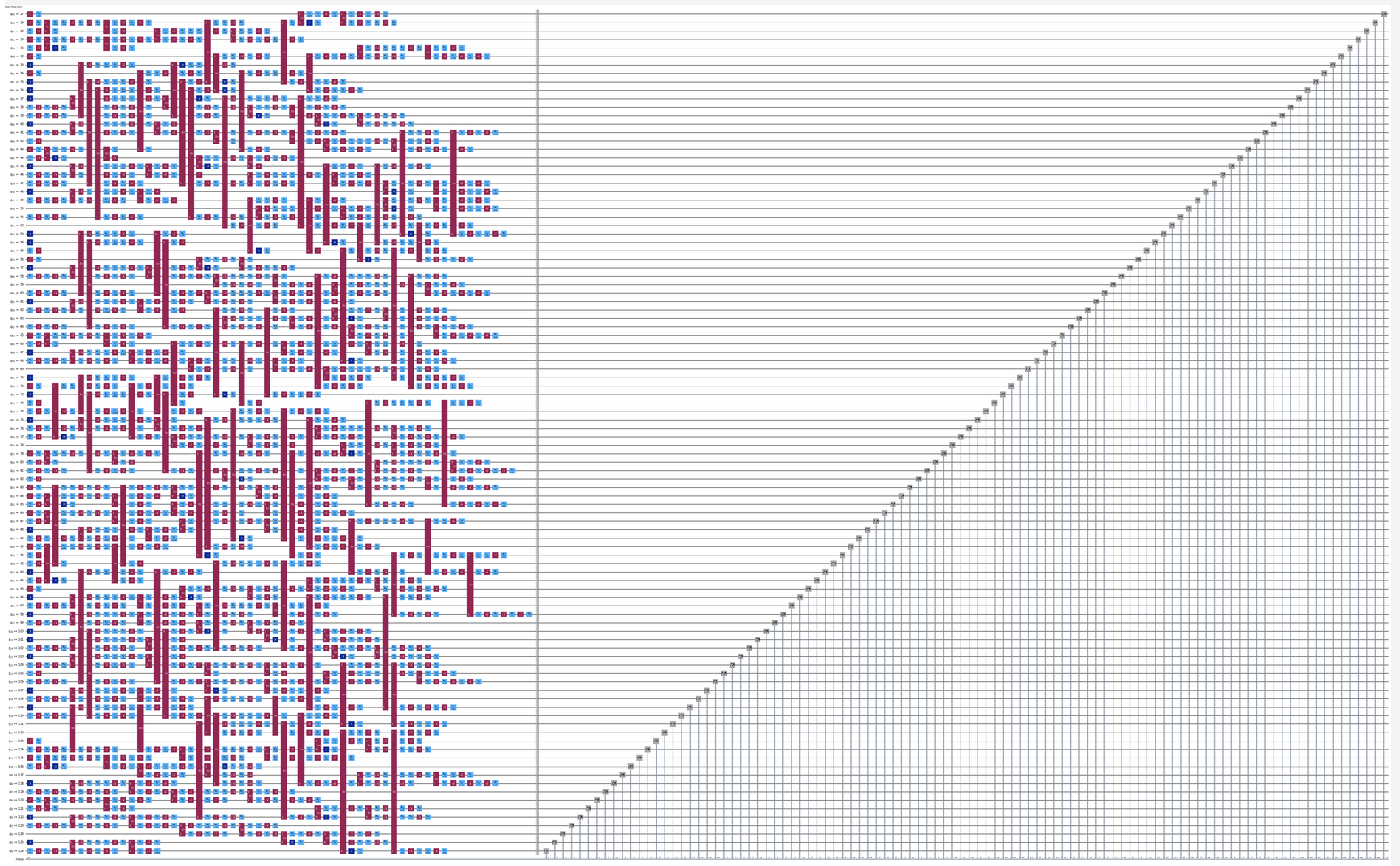
Quantum Approximate Optimization Algorithm

For some specific instances, QAOA
can be scaled to solve large graphs!





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Quantum Approximate Optimization Algorithm

There are many improvements over QAOA in the literature:

Warm start QAOA: Using classical pre-processing for clever parameter initializations
arXiv:2009.10095, September 2020

Quantum alternating operator ansatz: Use mixing Hamiltonian which allows you to evolve your state only within feasible subspace
arXiv:1709.03489, September 2017

Hardware implementations of large-scaling QAOA: Error mitigation and swap strategies
arXiv:2202.03459, February 2022
arXiv:2307.14427, July 2023

...

April 2025

Quantum Optimization Benchmark Library
The Intractable Decathlon

Thorsten Koch [*1, 2], David E. Bernal Neira[3], Ying Chen[4], Giorgio Cortiana[5], Daniel J. Egger[6], Raoul Heese[7], Narendra N. Hegade[8], Alejandro Gomez Cadavid[8,9], Rhea Huang[10], Toshinari Itoko[11], Thomas Kleinert[12], Pedro Maciel Xavier[3, 13], Naeimeh Mohseni[5], Jhon A. Montanez-Barrera[14], Koji Nakano[15], Giacomo Nannicini[10], Corey O'Meara[5], Justin Pauckert[16], Manuel Proissl[6], Anurag Ramesh[3], Maximilian Schicker[1], Noriaki Shimada[11], Mitsuharu Takeori[11], Víctor Valls[17], David Van Bulck[18], Stefan Woerner [†6], and Christa Zoufal [‡6]

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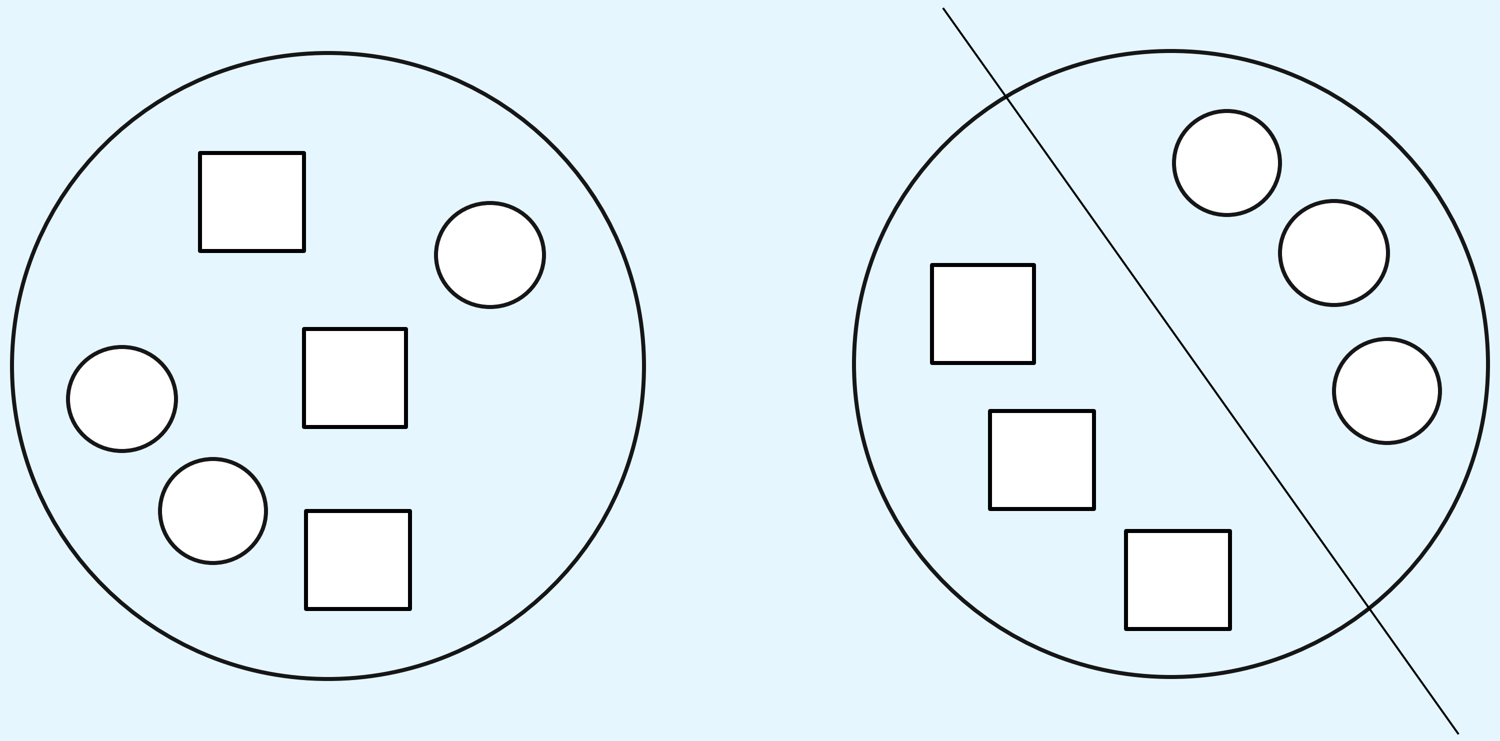
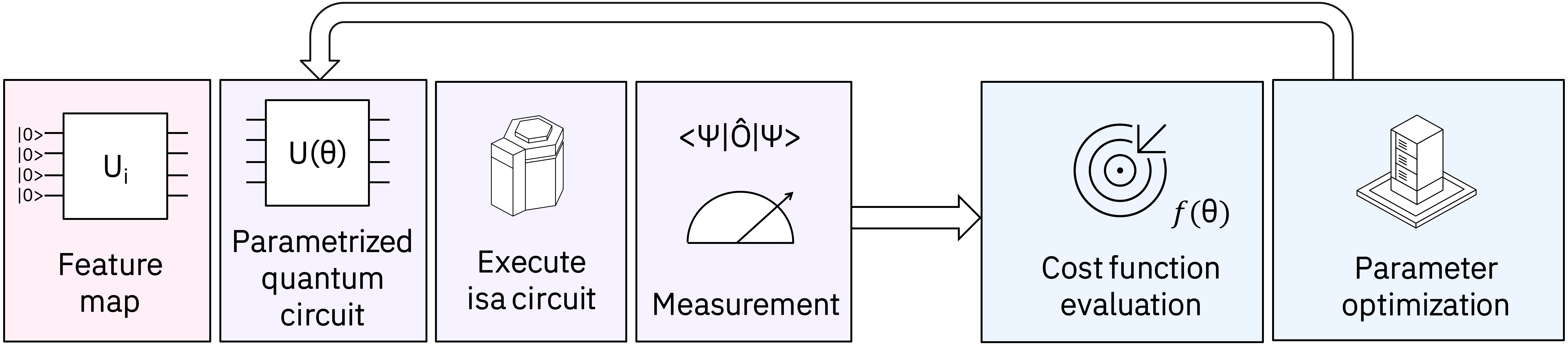
Variational Quantum Machine Learning



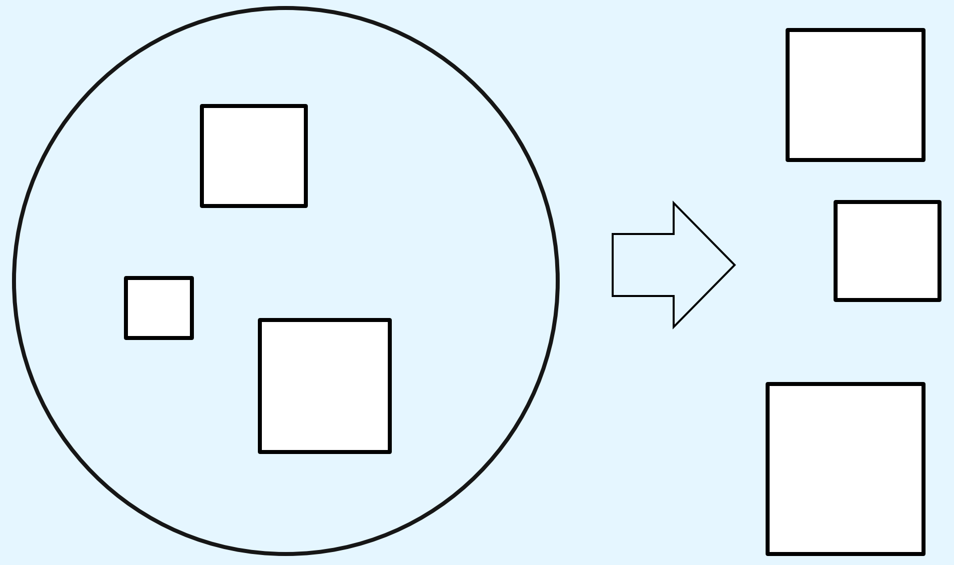
Variational Quantum Classifiers (VQCs)

- Encode the data into a quantum state.
- Train the parametrized quantum circuit to classify the test data (supervised learning).
- Once the parameters have been optimized, the VQC can be used to classify new data points.

arXiv:1802.06002 (2018)



Variational Quantum Machine Learning

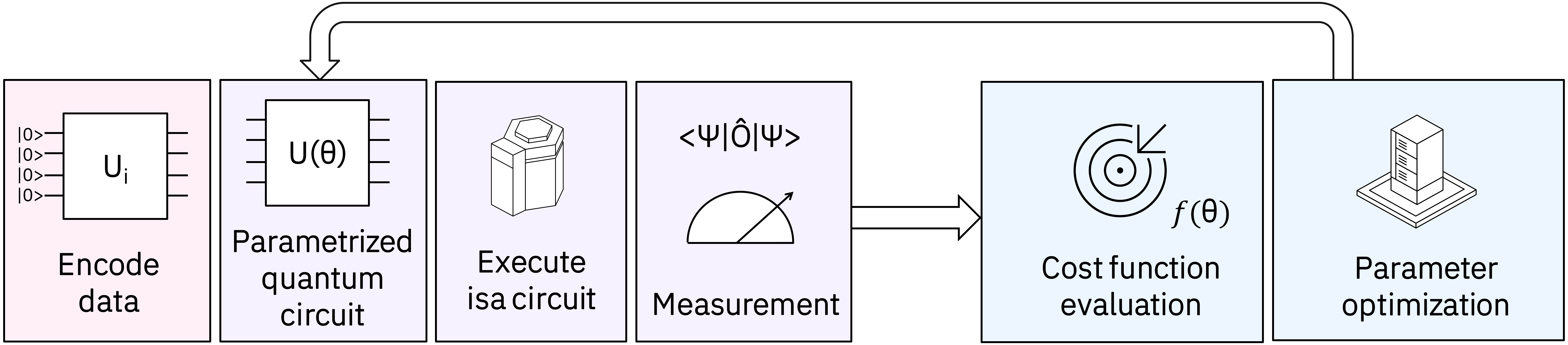


Generative models (ex: Quantum Boltzmann machine)

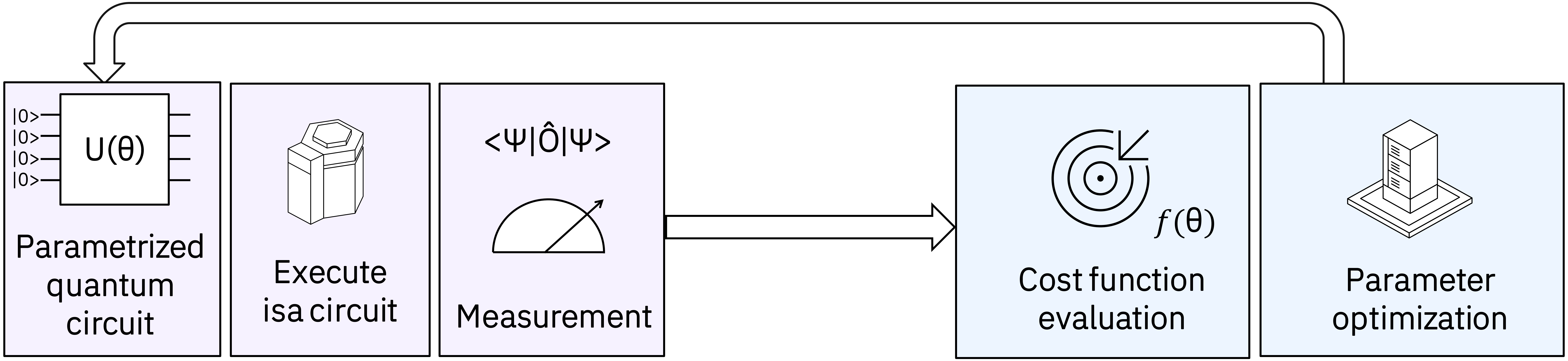
- Define a quantum Hamiltonian that encodes the energy of the system
- Encode the data into a quantum state
- Compute the expectation value of the Hamiltonian for both the model distribution and the data distribution using quantum measurements.
- Minimize cost function

$$\Delta\theta = -\eta\left(\langle O_\theta\rangle_{\text{data}} - \langle O_\theta\rangle_{\text{model}}\right)$$

Phys. Rev. X 8, 021050 (2018)



Review of challenges and Open Questions in VQAs



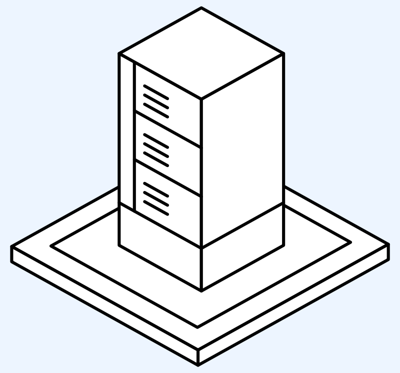
Ansatz design: expressibility versus trainability

Hardware limitations: Noise, connectivity, size of the device...

Measurement bottleneck

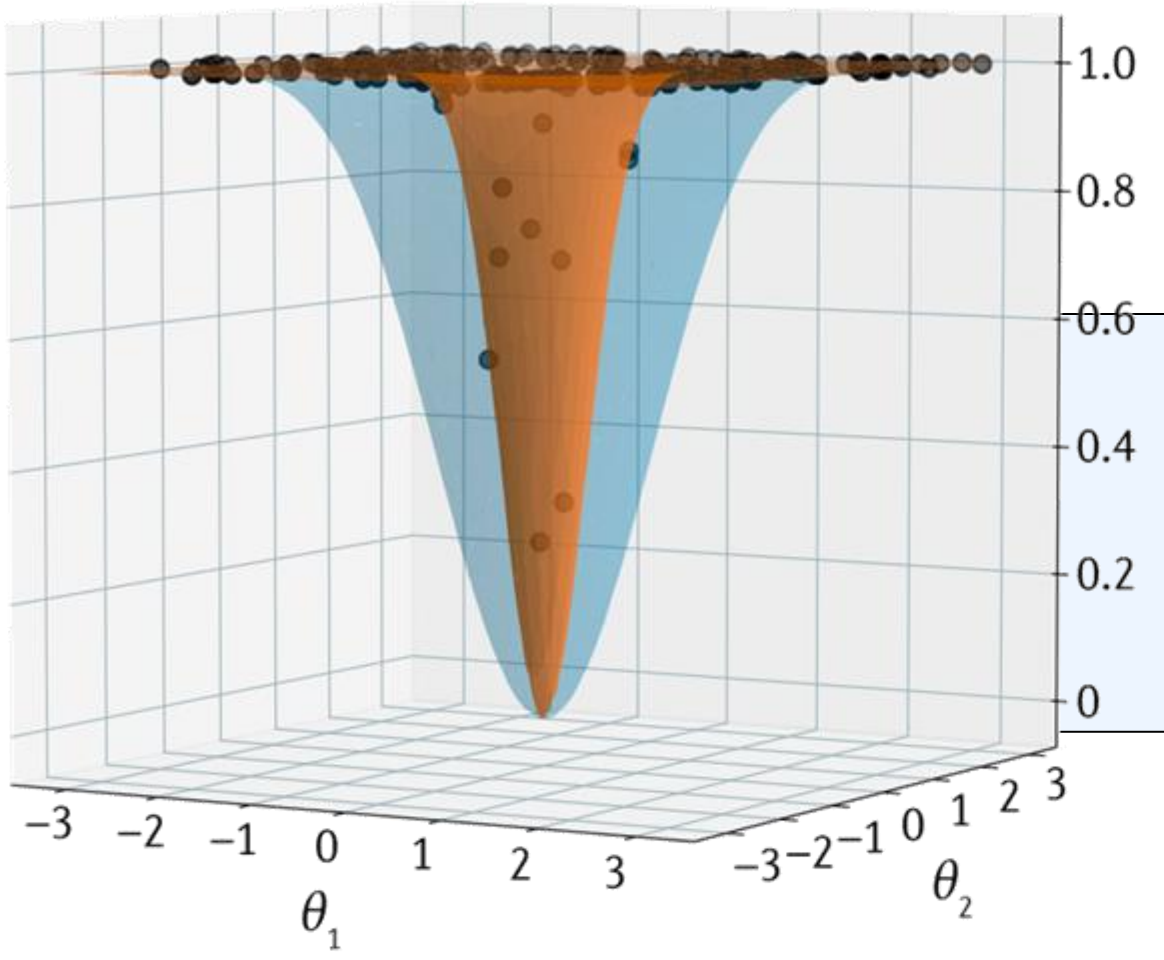
Trainability issues: Barren plateaus and poor local minima

Review of challenges and Open Questions in VQAs



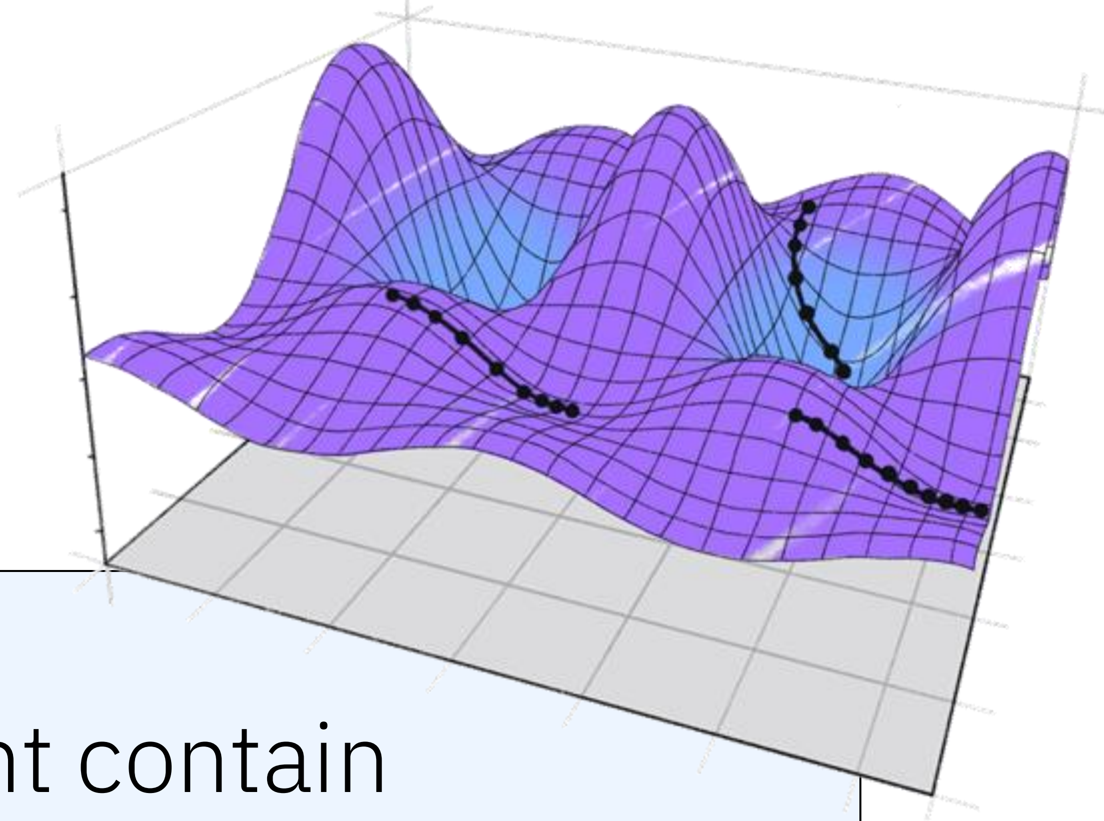
Parameter optimization

Trainability issues: Barren plateaus and poor local minima



M Cerezo *et al*, *Nat Rev Phys* **9**, 625 (2021)

Barren Plateaus are vanishing gradients in high-dimensional energy landscapes



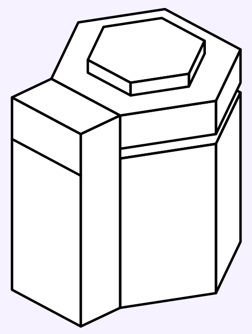
Energy landscapes might contain many local minima.

Potential solutions:

- Layer by layer training to initialize params close enough to the minimum
  Quantum Mach. Intell. 3, 5 (2021)
- Find good initializations.
- Study models with provable absence of barren plateaus
  Nat. Comm. 12, 1791 (2021)
  - shallow circuits with local measurements
  - dynamics with small Lie algebras
  - embedding symmetries into the circuit's architecture
  - …

But such models have been proven to be classically simulable.
arXiv:2312.09121

Review of challenges and Open Questions in VQAs

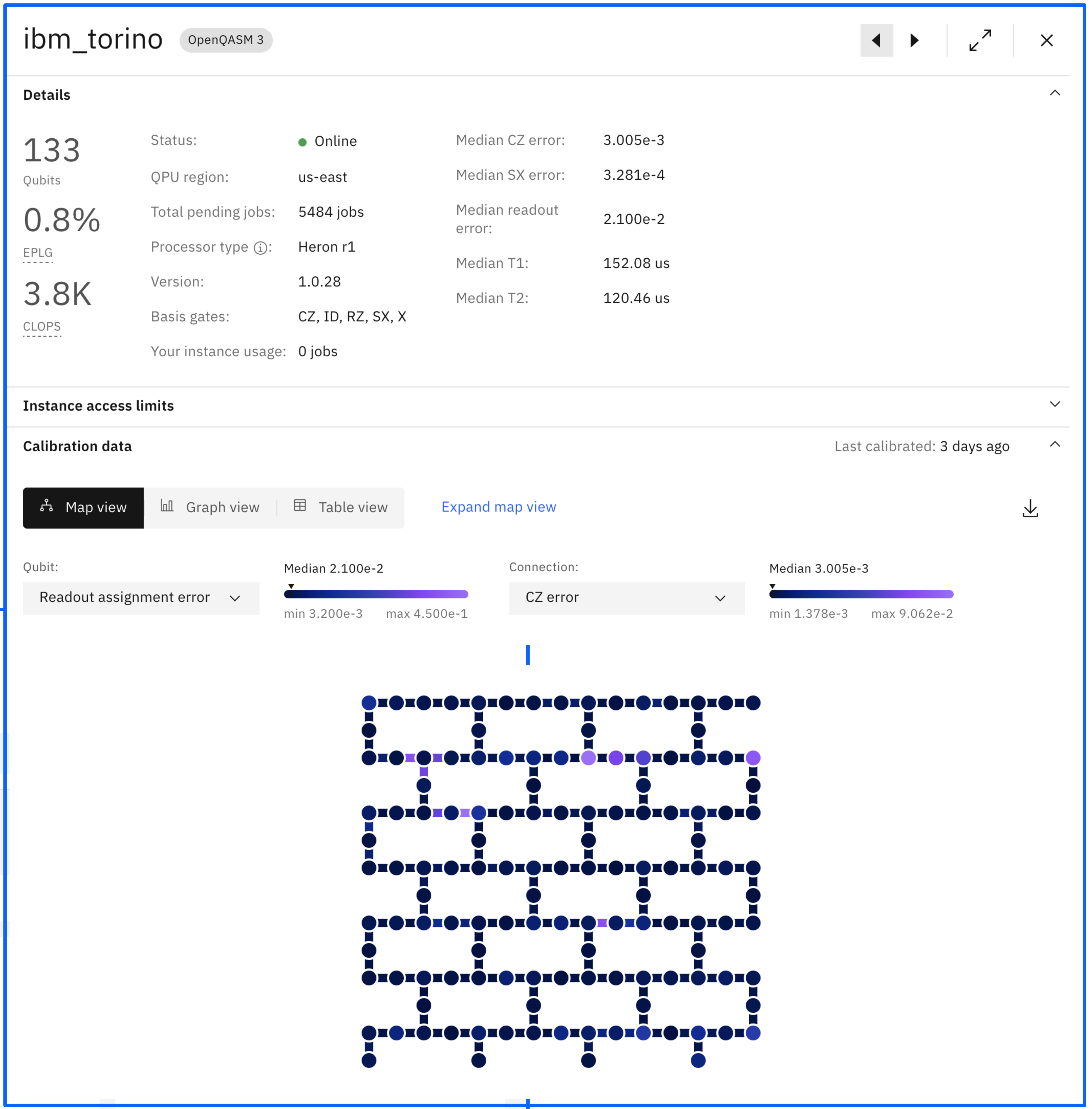


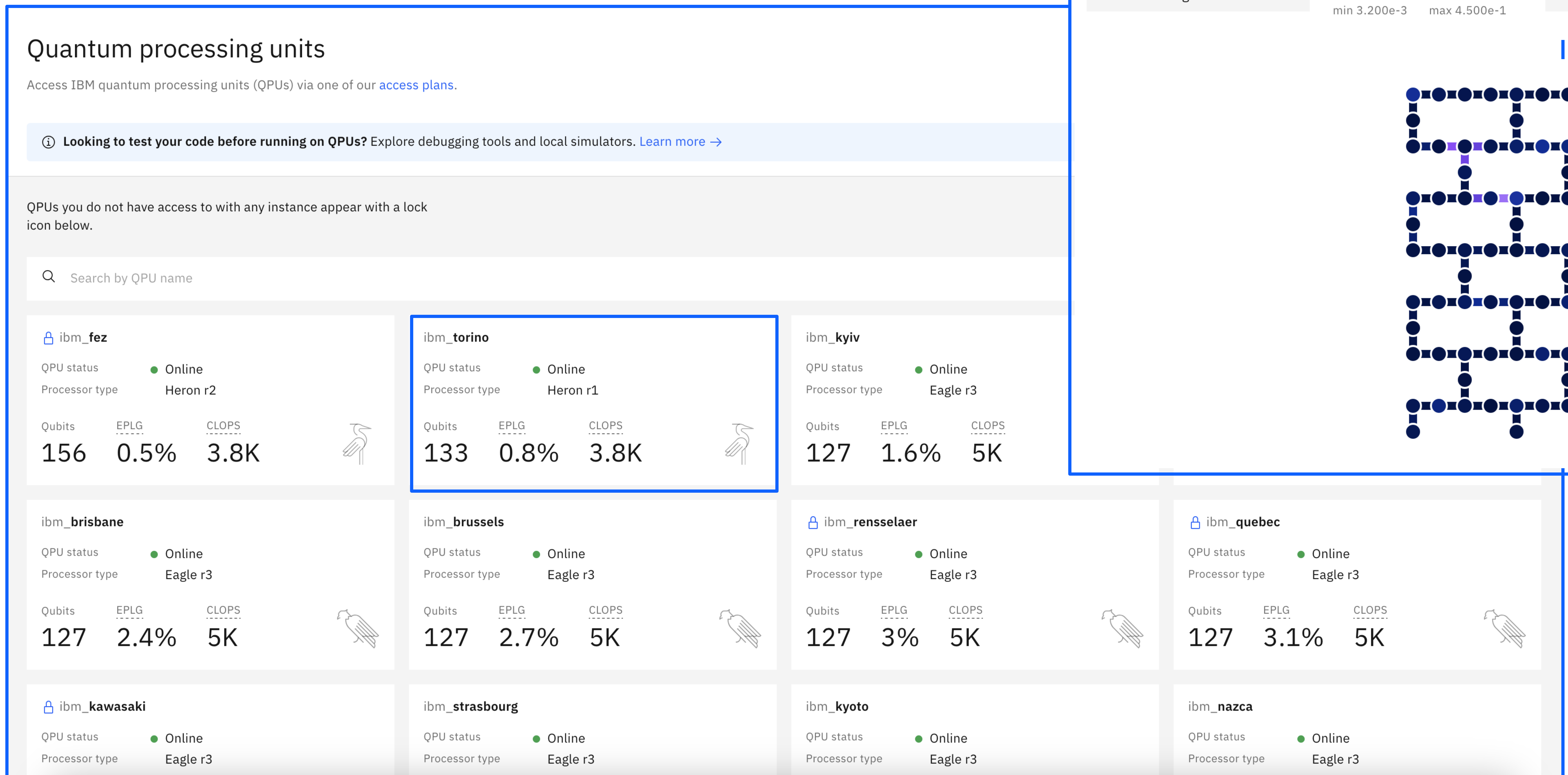
Execute isa circuit

Hardware limitations: Noise, connectivity, size of the device…

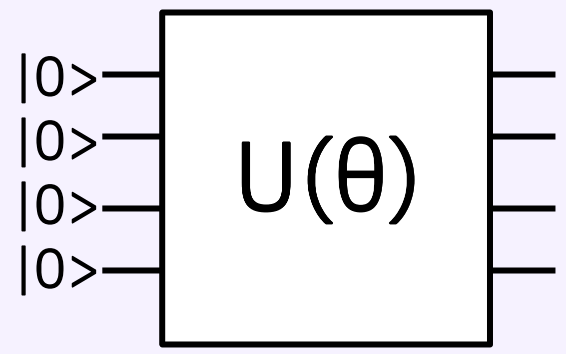
Potential solutions:

- Build adaptable ansätze.
- Asses the effect of noise and error mitigation techniques on the performance/trainability of VQAs. Quantum 8, 1287 (2024)





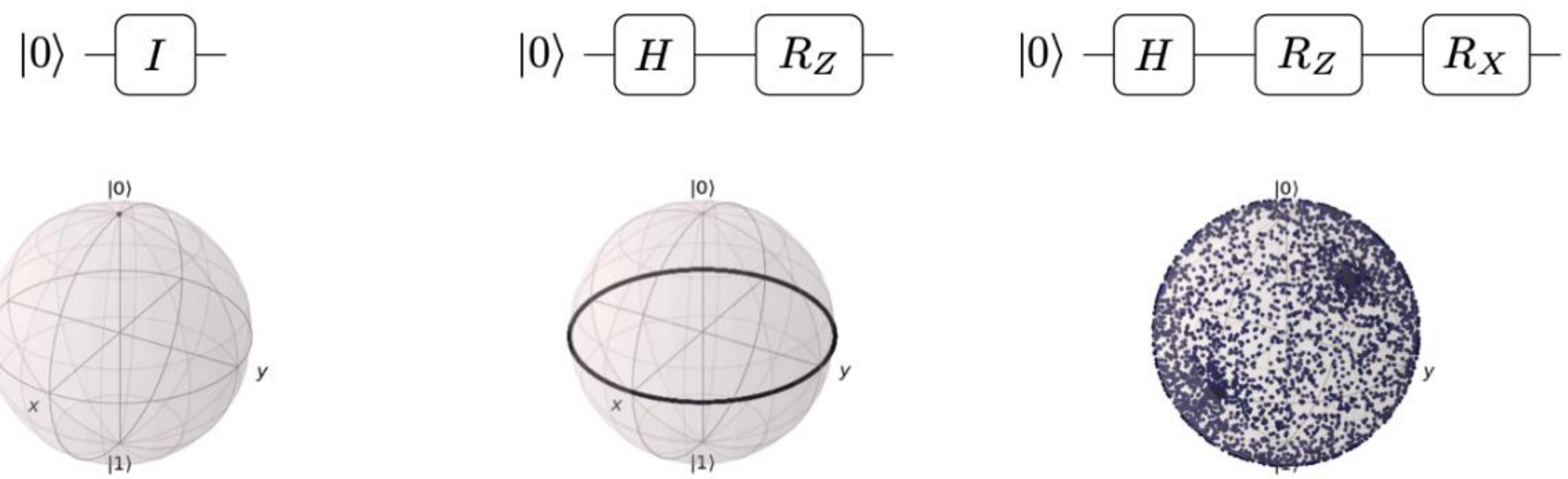
Review of challenges and Open Questions in VQAs



Parametrized quantum circuit

Ansatz design: expressibility versus trainability

Definition of ansatz expressibility:



Alan Aspuru-Guzik et al, Advanced quantum technologies 2, 12, December 2019

vS

Shallow depth and trainability

Problem-motivated ansatz:

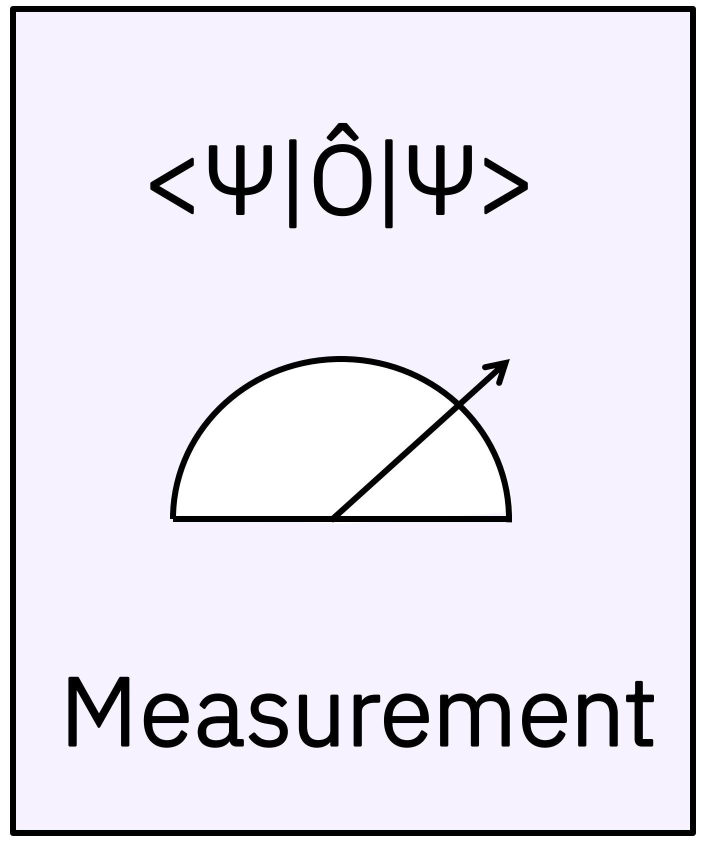
- Inspired by the phsyics of the problem: symmetries and structure.
- Inspired by already existing classical ansatze.

Hardware-motivated ansatz:

- Device connectivity and noise model.
- Taking into account the strenghts of the device.

It is possible to combine both approaches ✓

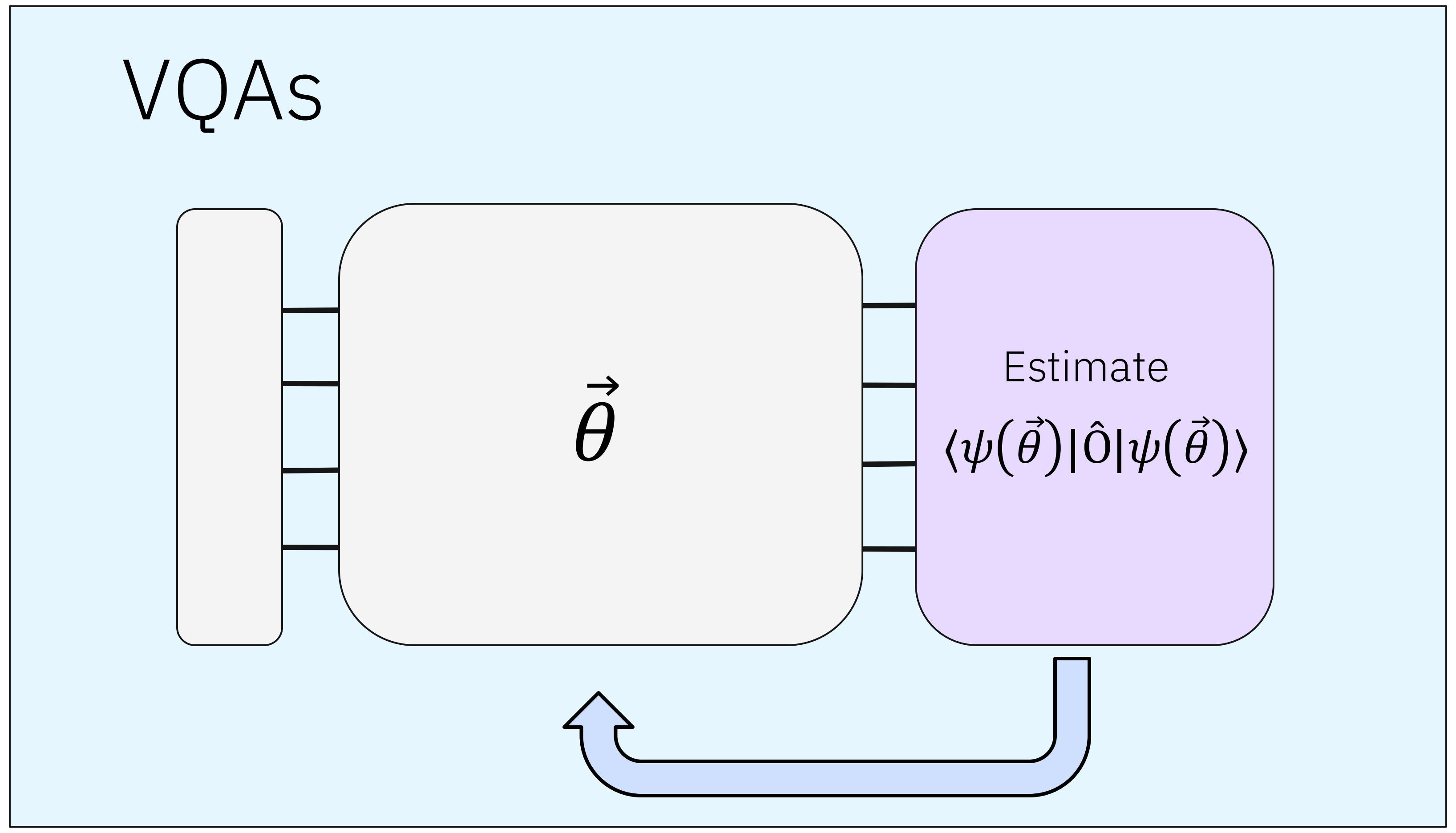
Review of challenges and Open Questions in VQAs

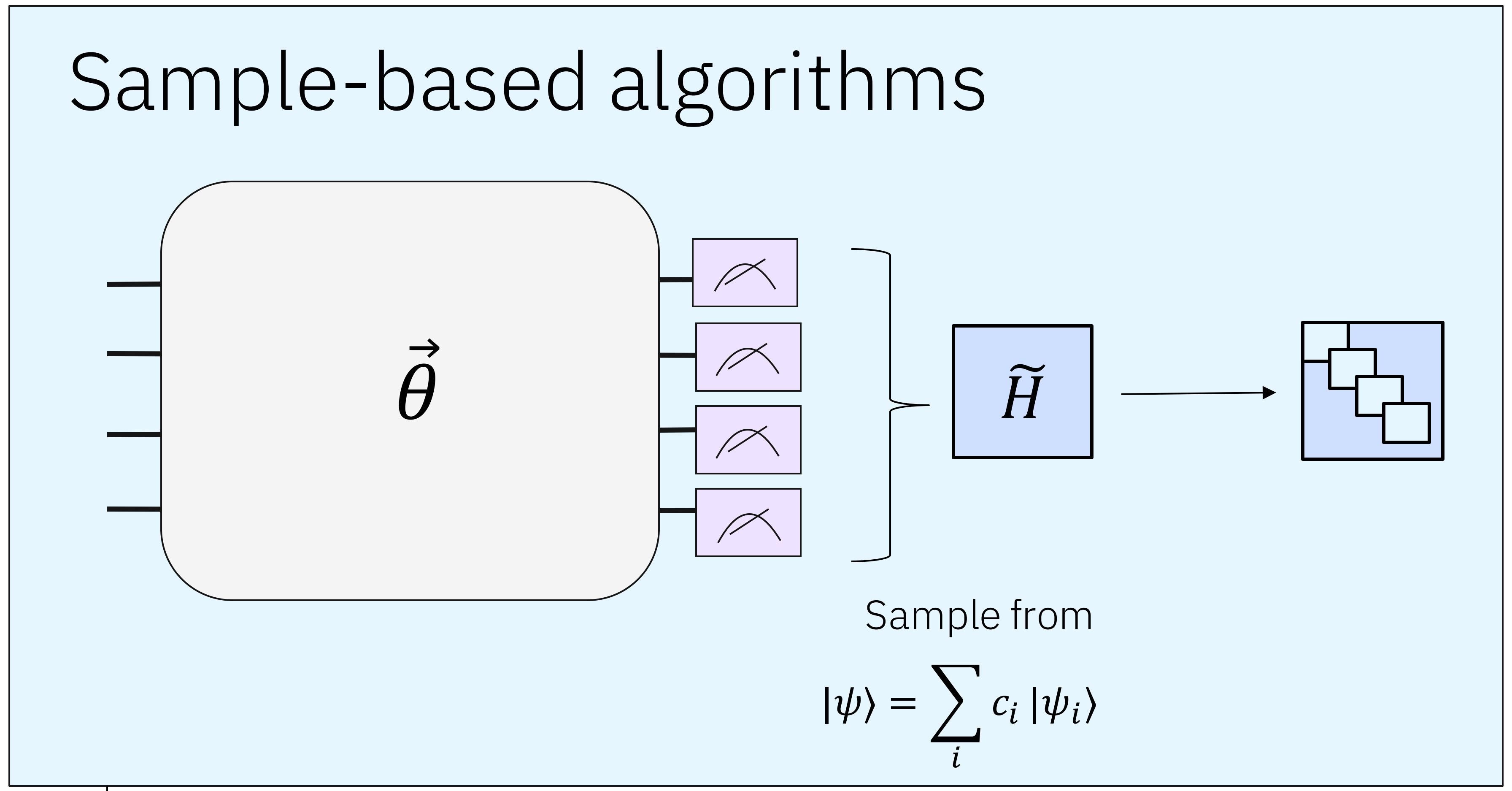


Measurement bottleneck

Potential solutions:

- Operator grouping and commutativity strategies.
- Avoid computing expectation values, sample bitstrings instead:





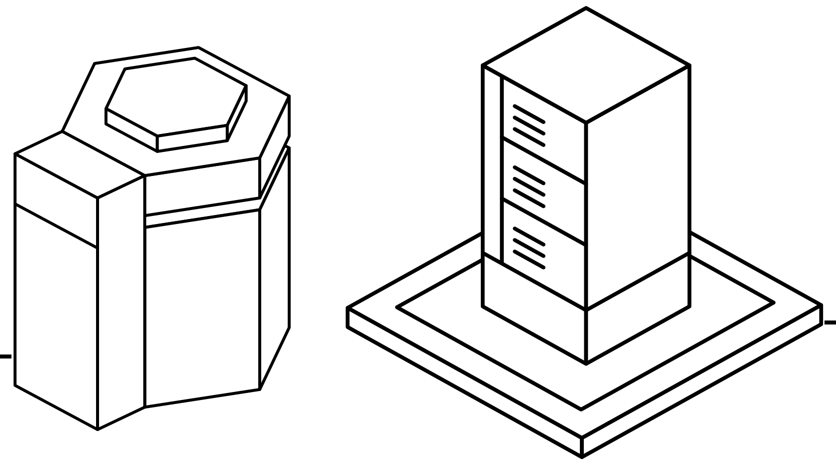
- Sample-based Quantum Diagonalization (**SQD**)
  arXiv:2405.05068, May 2024
- Sample-based Krylov Quantum Diagonalization (**SKQD**)
  arXiv:2501.09702, January 2025

Near term quantum hardware requires noise-resilient, shallow, and adaptable quantum algorithms.

Variational quantum algorithms have been a key ingredient to leverage near-term quantum hardware, but currently present challenges in terms of scalability.

Other approaches to harness hybrid architectures, such as QCSC, show promise in the near future:

Quantum: State preparation, entanglement, and measurement



HPC: Parameter optimization and/or post-processing

QGSS, 2025

Practical quantum algorithms

Joana Fraxanet Morales
Quantum Algorithm
Engineering team

IBM **Quantum**