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Hybrid Quantum Algorithms

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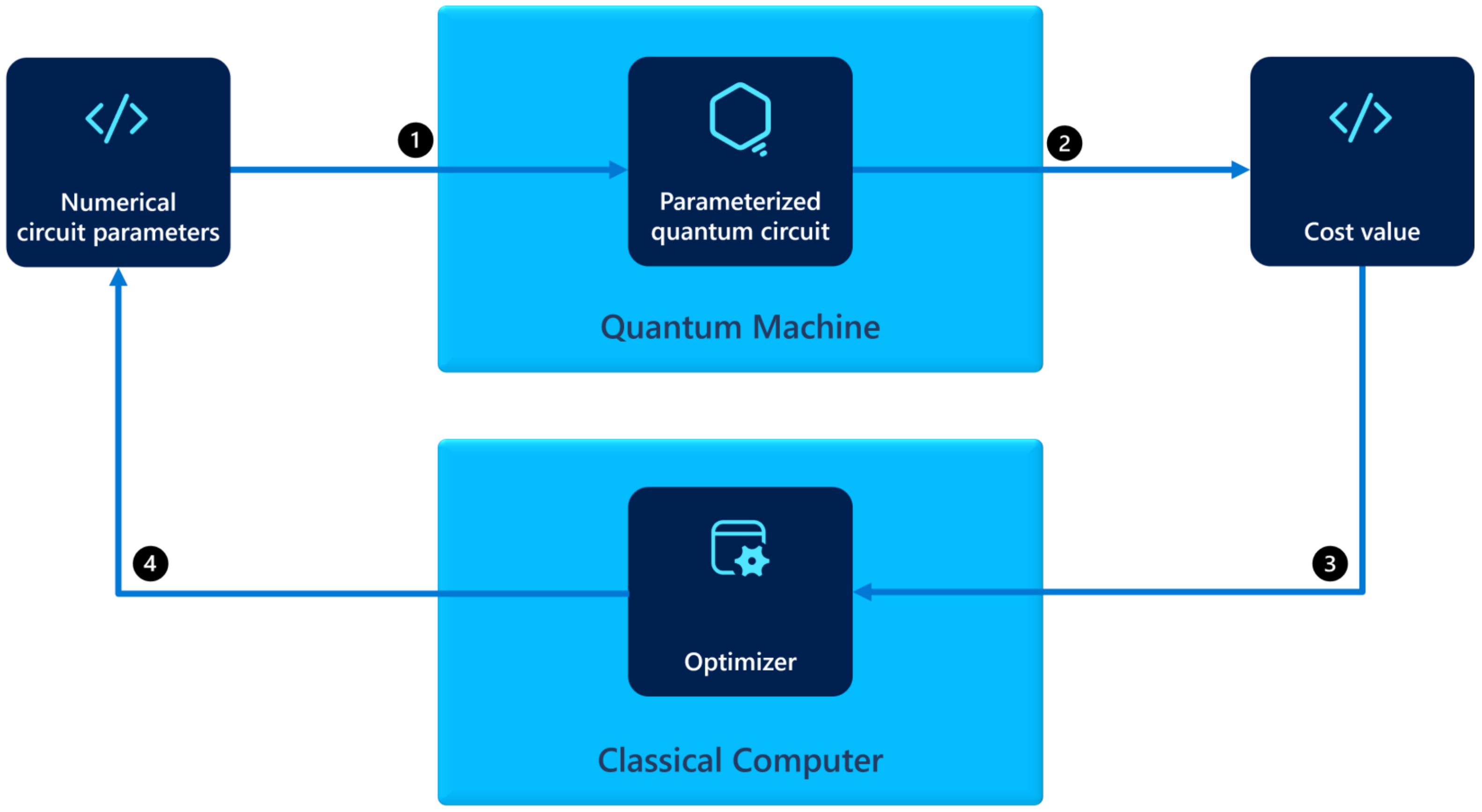

Lecture outline

- Hierarchy of hybrid quantum algorithms
- Variational quantum algorithms
- Quantum Approximate Optimization Algorithm (QAOA)
- Variational Quantum Eigensolver (VQE)

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Hierarchy of Hybrid Quantum Algorithms

Hybrid Quantum Algorithms

Quantum algorithms that combine classical and quantum computation

Most quantum algorithms are hybrid! We just don't think of them this way

1. Batch quantum computing

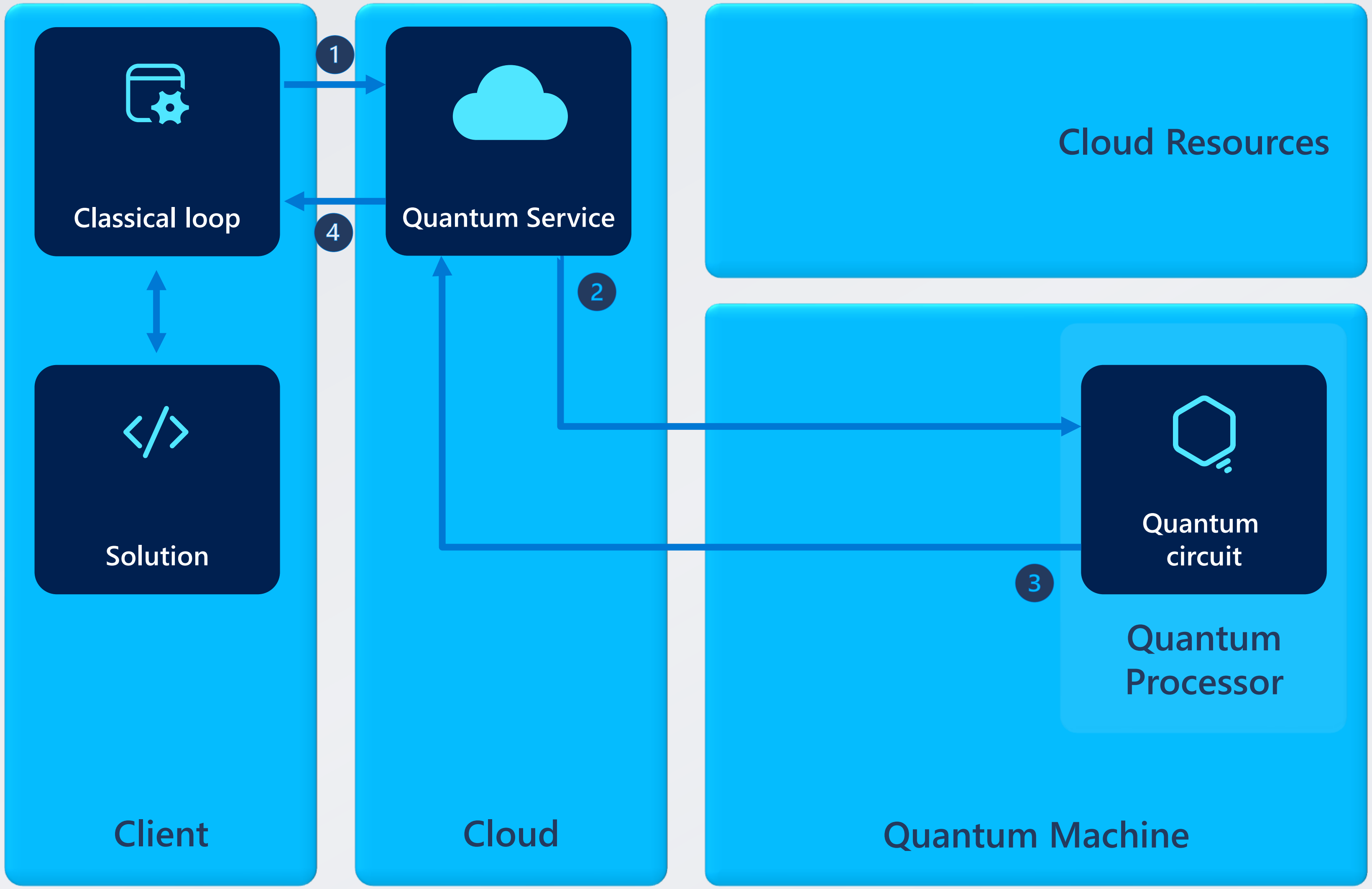
2. Interactive quantum computing

3. Integrated quantum computing

4. Distributed quantum computing

Increasingly tighter and richer integration between quantum & classical processing

Batch quantum computing

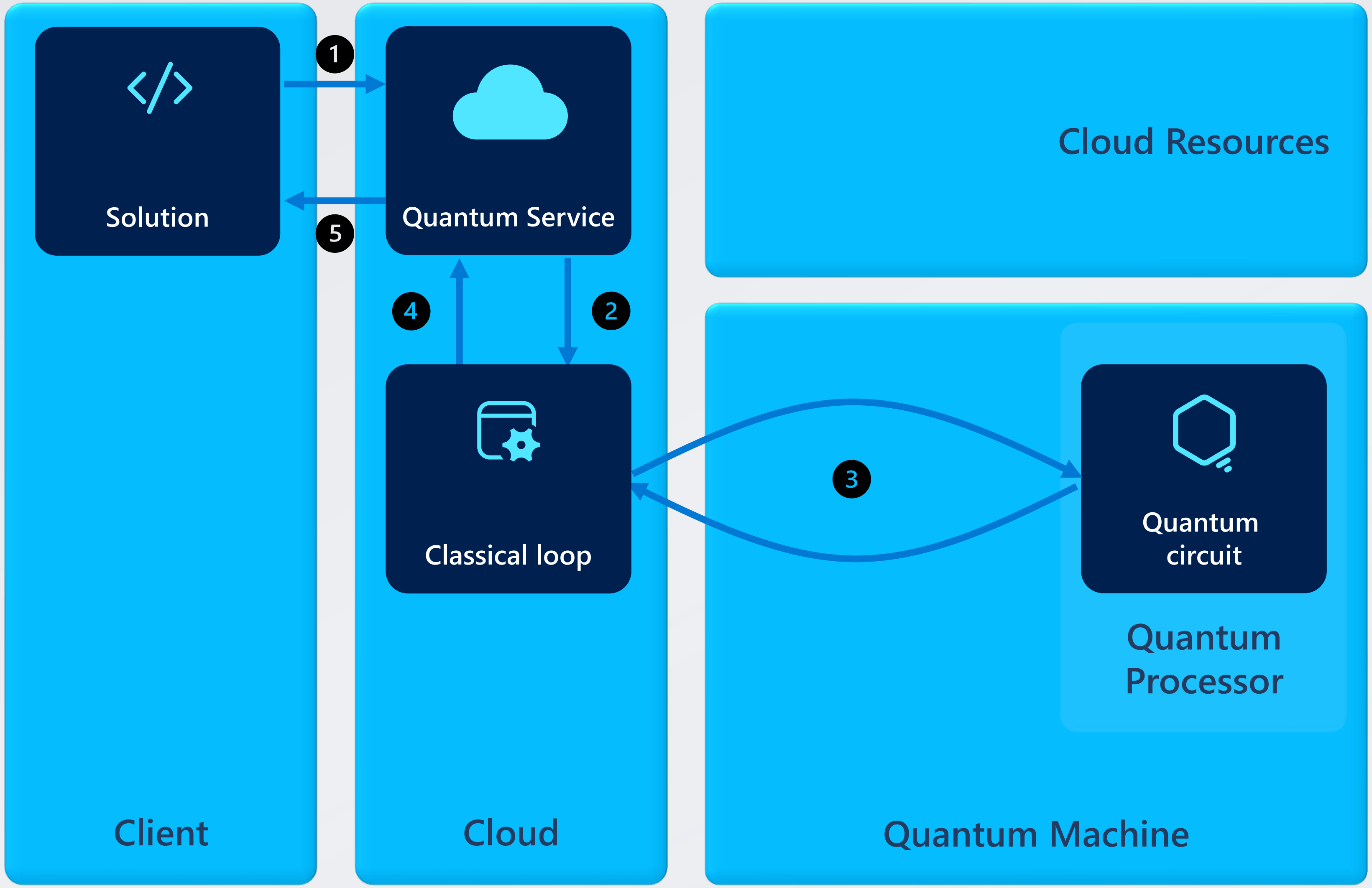


Local clients enable quantum circuits with classical pre- and post-processing

Examples:

- Deutsch-Jozsa
- Grover’s search
- Iterative phase estimation
- Quantum phase estimation (QFT-based)
- Shor’s algorithm

Interactive quantum computing



Cloud-based clients enable parameterized quantum circuits in a classical driver loop that runs in the cloud

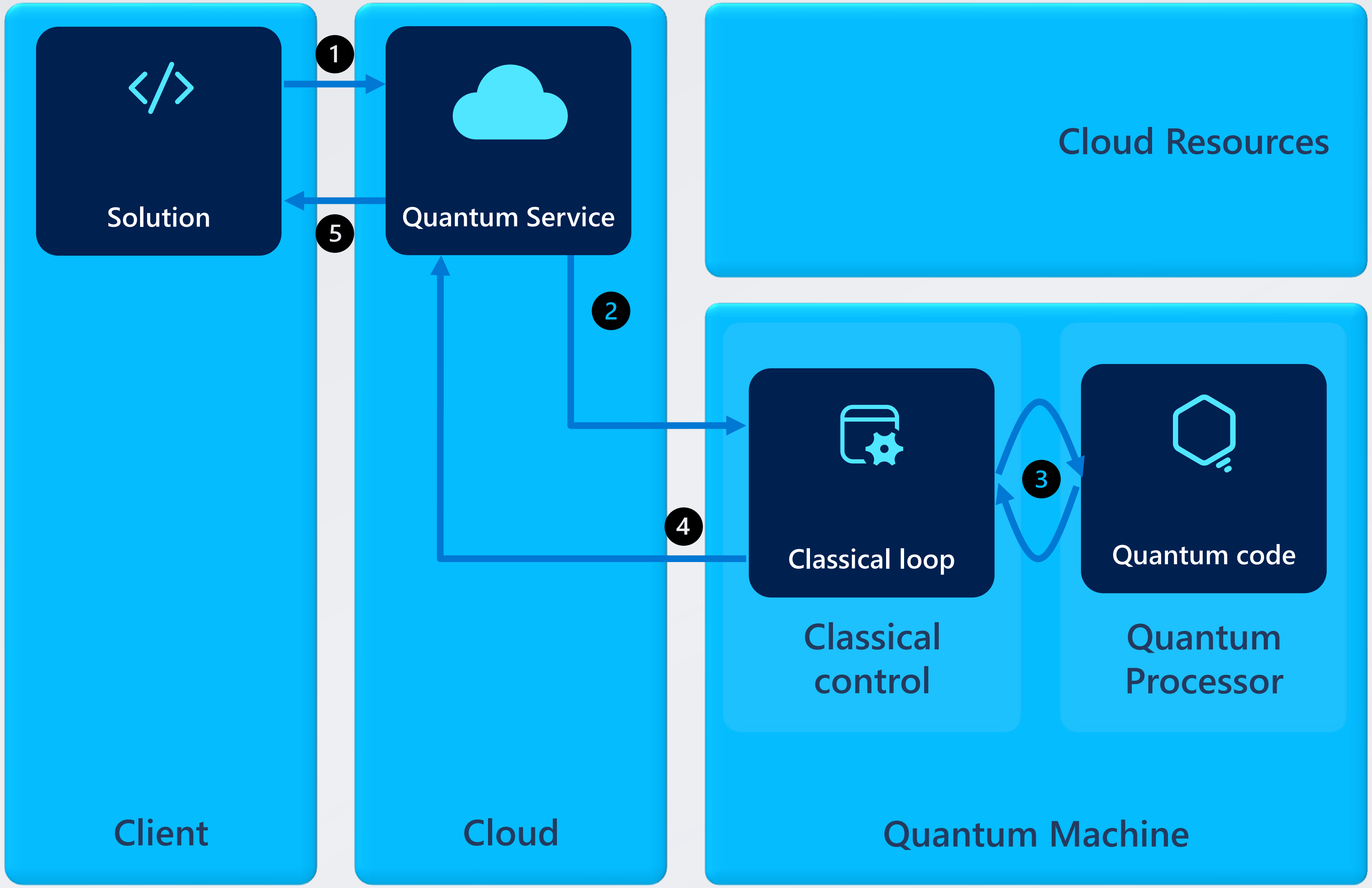
Circuit structure doesn’t change between runs, but numerical parameters do

Qubits are reset between runs

Examples:

- Variational quantum eigensolver
- Quantum approximation optimization algorithm

Integrated quantum computing

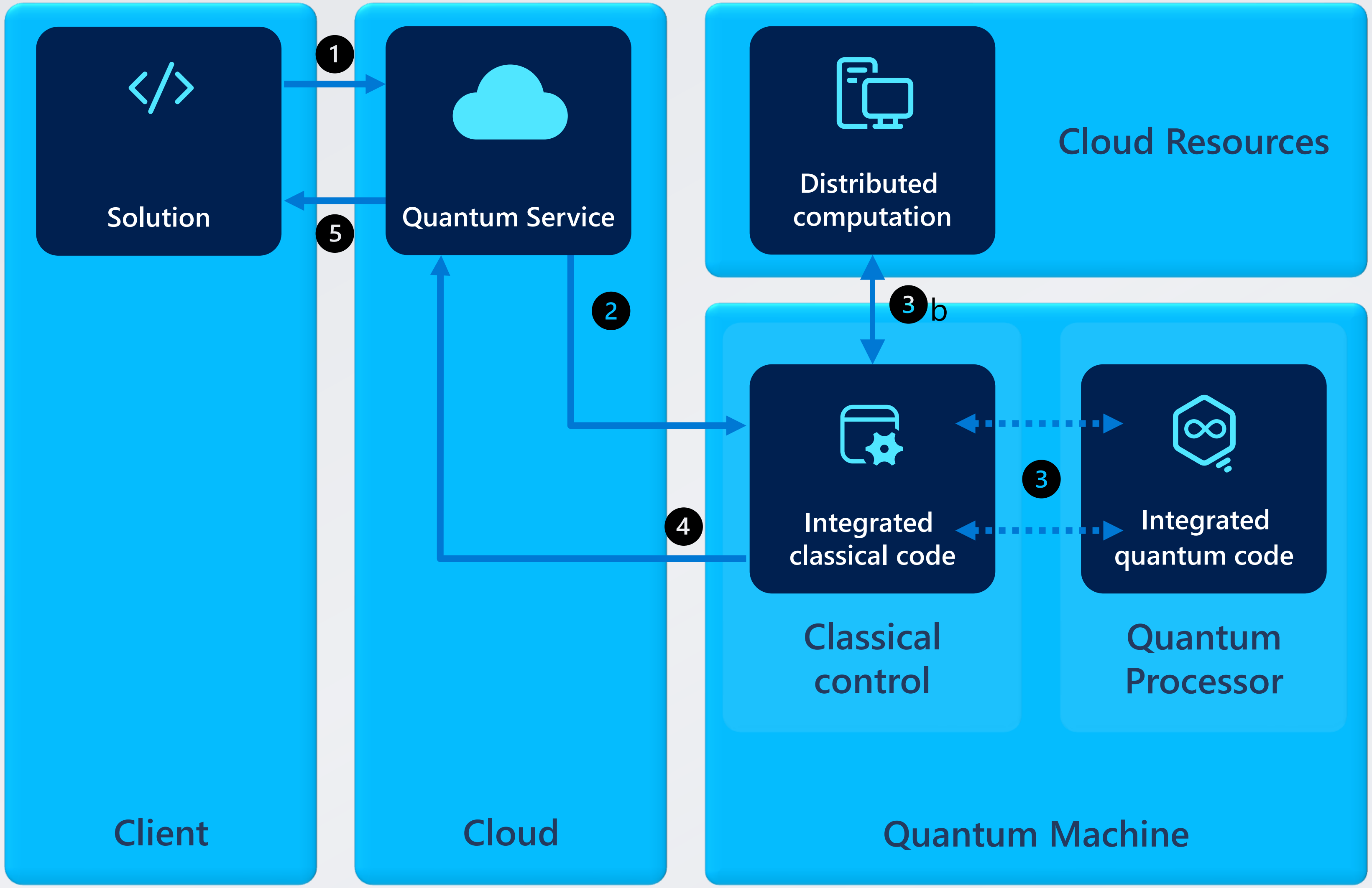


Classical code controls execution of quantum circuit while the qubits remain “alive” (maintain their state without decoherence) Circuit structure can change!

Examples:

- Teleportation: need to apply fixup to target based on measurement results
- Adaptive phase estimation with reuse of eigenstate: need to change next circuit structure based on bits learned so far
- Error correction

High-performance distributed quantum computing



Long-lived logical qubits enable full classical compute next to QPU

Full data center integration enables complex distributed hybrid jobs across quantum & HPC resources

Examples:

- Complex materials modelling
- Evaluation of a full catalytic reaction

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Variational Quantum Algorithms

Variational Quantum Algorithms: Definition

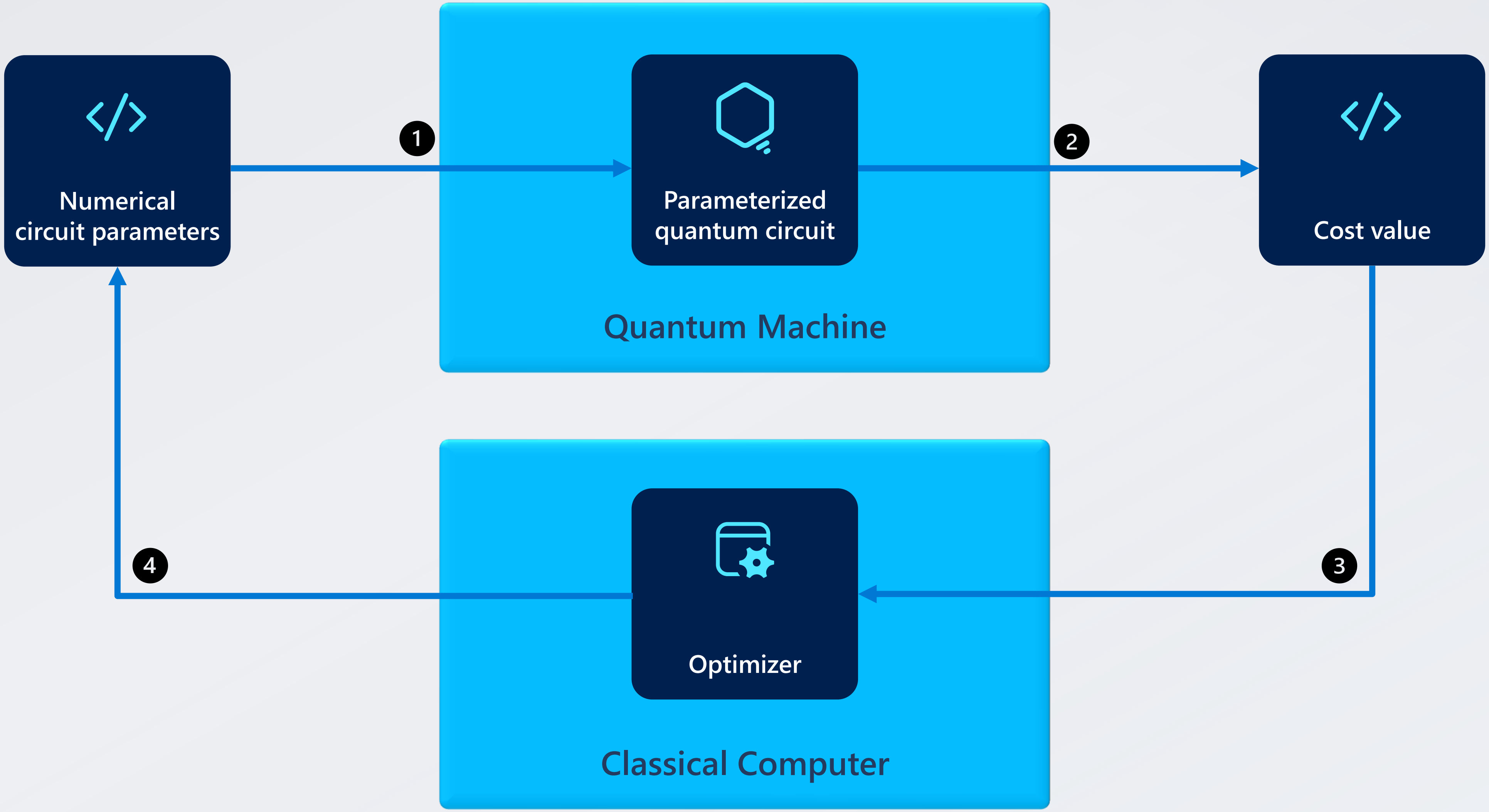
A variational quantum algorithm (VQA) is any quantum algorithm that tries to minimize some objective function by:

1. Using a parameterized quantum circuit as part of the function value estimation
2. Using classical optimization tools to find the circuit parameters that minimize the function value

Introduced in early 2010s as an attempt to get short-term practical use out of NISQ devices

Since then, they've been proposed for essentially all applications envisioned for quantum computers

Variational Quantum Algorithms: Optimization Loop



Variational Quantum Algorithms: General Considerations

Choosing ansatz - the “template” of the quantum circuit

Hyperparameters such as the circuit structure, number of gate layers, gates in each layer…

Choosing measurement strategy

How many shots to do to calculate cost value/how to do postprocessing of measurement results

Choosing initial parameters, optimizer, and optimizer hyperparameters

Classical optimizer: often gradient descent approximated using finite differences

Adaptive algorithms

Modify the structure of the circuit as the algorithm progresses

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Quantum Approximate Optimization Algorithm (QAOA)

Optimization Problem Defined on a Graph

We have an N-bit problem, described in terms of spins $s \in \{1, -1\}^N$ or Booleans $x \in \{0, 1\}^N$

$$s_k = (-1)^{x_k}, \qquad x_k = (1 - s_k)/2$$

The cost function is quadratic, defined in terms of a graph $G = (V, E)$

$$C(s) = \sum_{j \in V} a_j s_j + \sum_{(jk) \in E} b_{jk} s_j s_k$$

(In literature, a_j are called “local fields” and b_{jk} - “coupling constants”)

The goal is to find a configuration s that minimizes the cost function

Depth 1 QAOA

Depth 1 QAOA uses two parameters β and γ and consists of the following steps:

1. Prepare an even superposition of all basis states of length N

2. Apply phase change unitary

$$U_C(\gamma)|x\rangle = e^{-i\gamma C(x)}|x\rangle$$

3. Apply mixer unitary

$$U_B(\beta)|x\rangle = e^{-i\beta \sum_{j\in V} X_j}|x\rangle$$

4. Measure the resulting bit string x.

5. Repeat steps 1-4 for (the same values of β and γ) to estimate expectation of cost function

The goal is to find parameters β and γ that minimize the expectation of the cost function

Depth K QAOA

Depth K QAOA uses $2K$ parameters β_k and γ_k and consists of the following steps:

1. Prepare an even superposition of all basis states of length N

2. Apply phase change unitary $U_C(\gamma_0)$ and mixer unitary $U_B(\beta_0)$

…

K+1. Apply phase change unitary $U_C(\gamma_{K-1})$ and mixer unitary $U_B(\beta_{K-1})$

Makes the circuit more powerful, but harder to train

4. Measure the resulting bit string x.

5. Repeat steps 1-4 for (the same values of β_k and γ_k) to estimate expectation of cost function

The goal is to find parameters β_k and γ_k that minimize the expectation of the cost function

Example: MaxCut (maximum graph cut) problem

Given a graph, find a "cut" (split of vertices in two groups) that maximizes the number of edges being "cut" (the vertices of the edges ending up in different groups)

Alternatively, this minimizes the number of "uncut" edges, which is our cost to minimize

Edge (jk) is "uncut" if $s_j = s_k$, in other words, $s_j s_k = 1$. Then number of uncut edges to minimize

$$C(s) = \frac{1}{2} \sum_{(jk)\in E} \underbrace{(1 + s_j s_k)}_{\begin{array}{c} = 2 \text{ if } s_j s_k = 1 \text{ (uncut edge)} \\ = 0 \text{ if } s_j s_k = -1 \text{ (cut edge)} \end{array}}$$

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Variational Quantum Eigensolver (VQE)

VQE: High-level Overview

Allows to estimate the ground state energy of a quantum mechanical system

Knowing ground state energy is important for computational chemistry: reaction rates, reaction pathways, and binding strengths

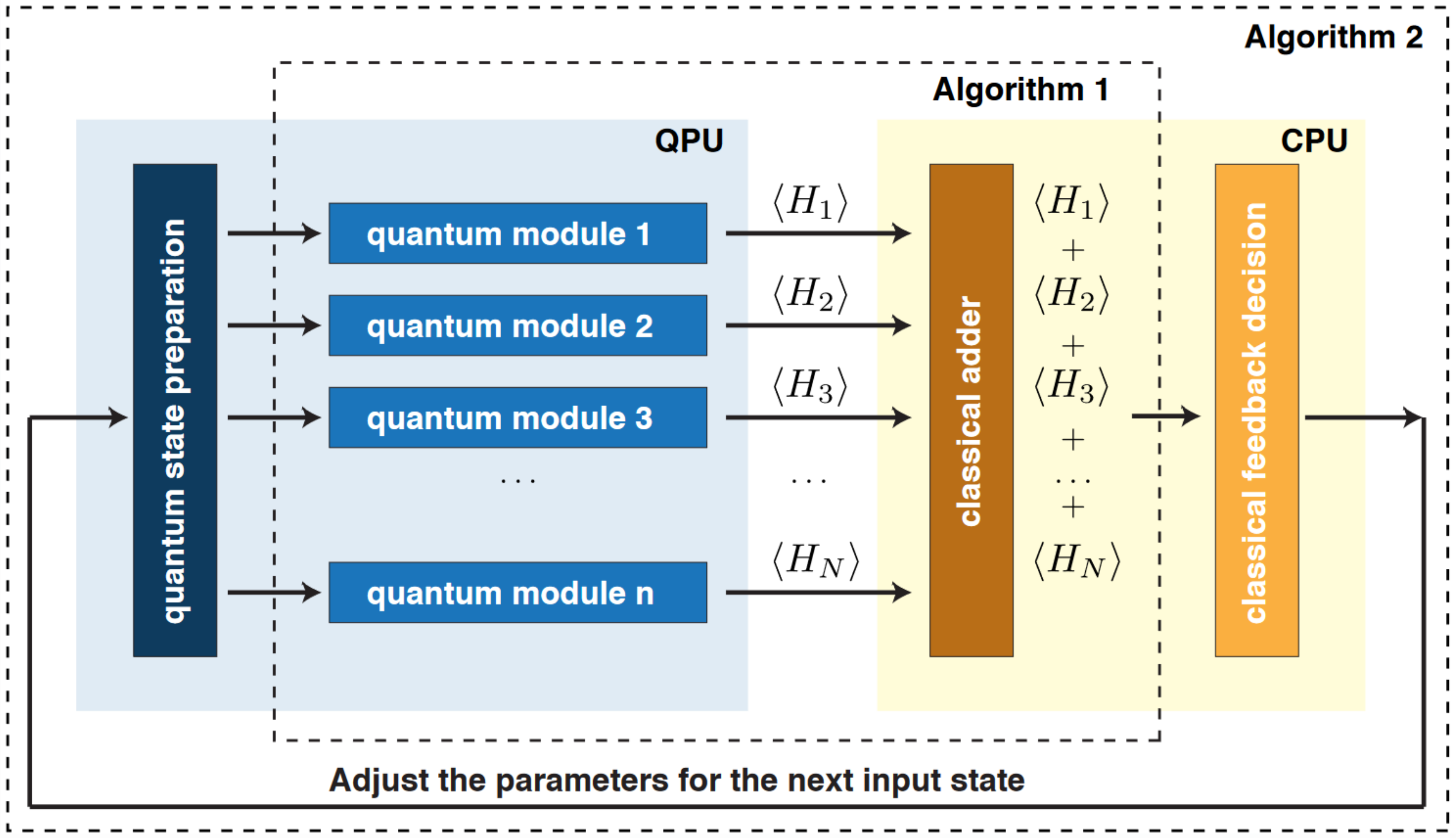
Problem is specified in terms of a unitary Hamiltonian

Ground state = one of the eigenstates, ground state energy = the lowest eigenvalue

Not the only algorithm for solving this problem!

Can be converted to a form suitable for phase estimation – but phase estimation leads to longer and more complex circuits, while VQE works with a lot of shallow circuits

VQE: Algorithm Structure



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Variational Quantum Algorithms: Challenges and State of Research

VQA: Challenges

Probabilistic nature of cost function evaluation (made worse by noise)

Any error mitigation techniques rely on a large increase in number of iterations

Barren plateaus (made worse by noise)

The more variables in the cost function, the “flatter” its landscape, the worse gradient descent works

Restructure the problem to reduce variable number, or training groups of parameters separately

Choice and analysis of circuit structure

Most “expressive” circuits (capable of preparing an arbitrary state) have a lot of parameters and are more prone to barren plateaus. Adaptive algorithms might help, but are harder to implement

Choice and analysis of optimizer

We want optimizers that work well under these conditions (probabilistic cost function, expensive iterations, noise)

VQA: State of Research

Variational algorithms looked promising for solving useful problems on NISQ machines

The last decade saw a lot of research on VQE and QAOA

Lately the consensus is that they don’t yield practical advantage

Focus is shifting back to fault-tolerant quantum computing