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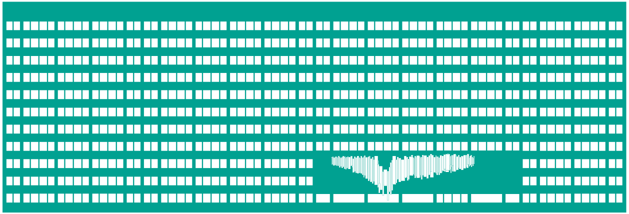
VSB TECHNICAL UNIVERSITY OF OSTRAVA



www.vsb.cz

Training QC for CLARA project

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March 21, 2025

VSB TECHNICAL UNIVERSITY OF OSTRAVA | IT4INNOVATIONS NATIONAL SUPERCOMPUTING CENTER

Název WiFi sítě/Wireless Network name (SSID): tuonet-guest

Jméno a příjmení/Full name: WiFi IT4I

Přihlašovací jméno do WiFi/Username: it4i-guest

Heslo/Password: mbfR

Program

11:45 – 12:00 **Welcome and Opening**

12:00 – 12:30 **Lunch Break**

12:30 – 14:00 **Introduction to Quantum Computing**

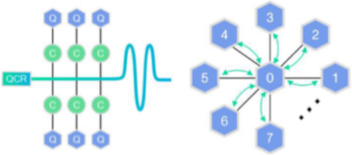
14:00 – 14:30 **Coffee Break & Showroom Tour & Photo**

14:30 – 16:00 **Hands-on Training: Practical Use Case**

16:00 – 16:15 **Coffee Break**

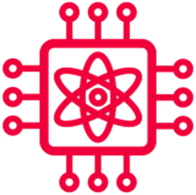
16:15 – 17:30 **Closed Discussion on Scientific Developments in the CLARA Project**

VLQ Quantum Computer - IT4Innovations VŠB-TUO



- Star-shaped qubit topology, uniform qubit connectivity
- Significant reduction in the number of SWAP operations
- Capability for highly complex quantum algorithms
- A major advancement compared to anything currently available
- Increased performance

Metric	Value
Qubits	>= 20
Qubit connectivity	one-to-all, star-shape
T1 relaxation time	typically ∼40 μs minimum for all qubits: 15 μs
T2 dephasing time	typically ∼20 μs minimum for all qubits: 15 μs
Readout fidelity	>0.95



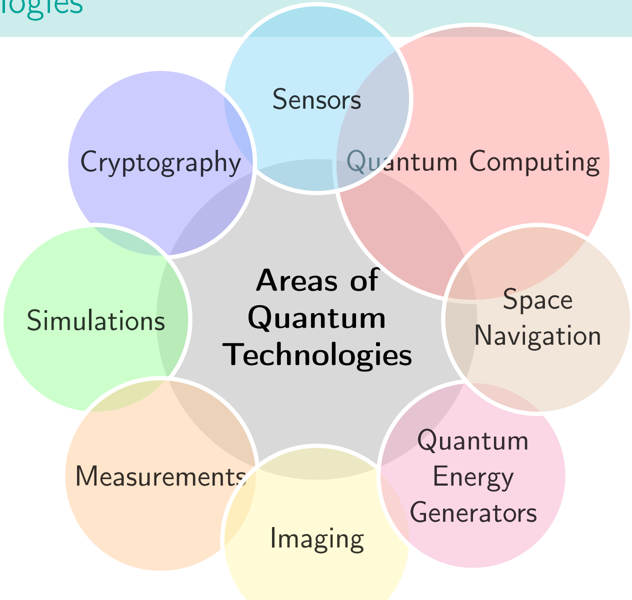
NVIDIA

CUDA QUANTUM

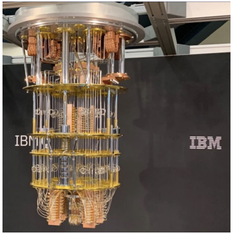
- NVIDIA CUDA Quantum
  - Platform for hybrid quantum-classical computations
  - Ability to switch between runs on CPU and QPU
  - Example of a hybrid QNN with the MNIST dataset, distinguishing between handwritten digits 0 and 1
  - Example of a hybrid QNN differentiating between various clothing images
  - Example of VQE: molecule H_2, energy

- Using CuTENSOR for GPU-based simulations with Qiskit.
  - Developed module on Karolina containing both Qiskit and CUDA with CuTENSOR (immediate execution possible)
  - Minimal functional example – measurement of a quantum circuit (2 qubits)
  - QNN example created (code in Qiskit, simulation using the CuTENSOR backend)

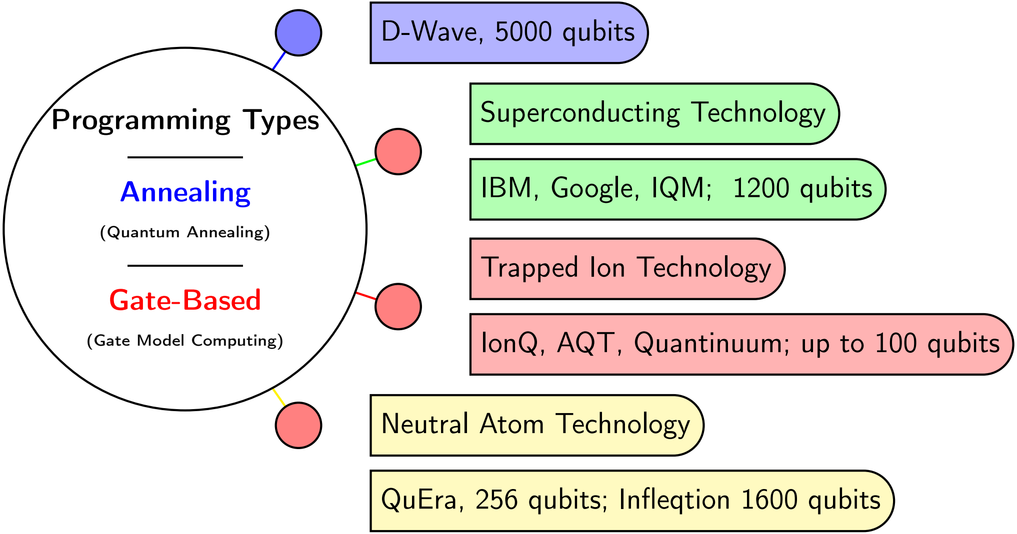
Quantum Technologies



Quantum Computer

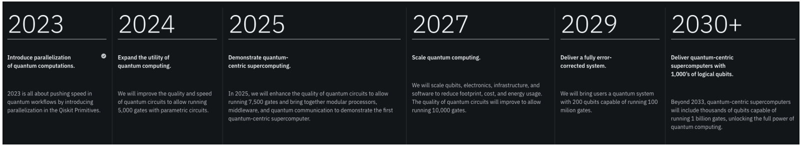


- **Quantum Computer**
  - Theoretical model of a device performing computations
  - Utilizes quantum mechanical phenomena: **superposition**, **interference**
- **Quantum Computing**
  - In a classical computer, data is represented by bits (0, 1)
  - In a quantum computer, qubits (quantum bits) are used, which can be zero, one, or a combination of both

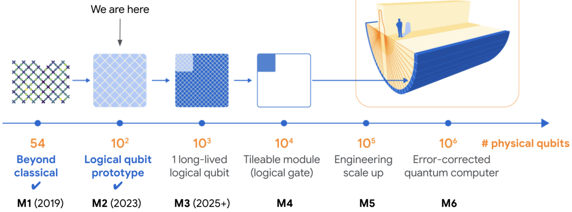

Programming Types
Annealing
(Quantum Annealing)
Gate-Based
(Gate Model Computing)
D-Wave, 5000 qubits
Superconducting Technology
IBM, Google, IQM; 1200 qubits
Trapped Ion Technology
IonQ, AQT, Quantinuum; up to 100 qubits
Neutral Atom Technology
QuEra, 256 qubits; Infleqtion 1600 qubits

"Quantum computers are here!"
"... it's not question **when** but **who** ... nobody will share it with us"
J. I. Latorre, Univ. Barcelona, CYBER WEEK, Tel Aviv, 2019

https://www.youtube.com/watch?v=40OFnZTPqyc



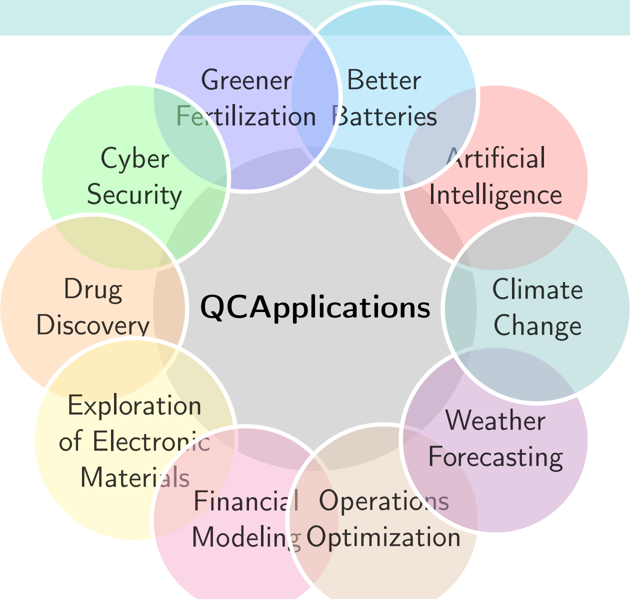
https://www.ibm.com/roadmaps/quantum/



https://quantumai.google/qecmilestone

Quasntum Computers - Future

Technology	Producer	Quantum Advantage	# Physical Qubits	# Logical Qubits
Superconducting qubits	IBM Quantum	2033	-	1000
	Google Quantum AI	-	1000 - 10000	first logical qubits
	Rigetti Computing	-	Thousands	-
	IQM	2033	1 milion	240-720
Ion Traps	IonQ	2029	Hundreds	-
	Quantinuum	2030	Thousands	Hundreds
Foton Qubits	PsiQuantum	-	-	-
	Xanadu Quantum	-	50-100	-
	Quandela	2028	-	50
Spin Qubits	Intel	-	Tisíce	-
	Silicon Quantum Computing	2030	100	-
Neutral Atoms	Pasqal	>2028	10000	-
	ColdQuanta (Infleqtion)	2028	40000	>100
	Atom Computing	-	1000	-
Quantim Annealers	D-Wave Systems	>2028	7000	-
	Qilimanjaro	-	30	-

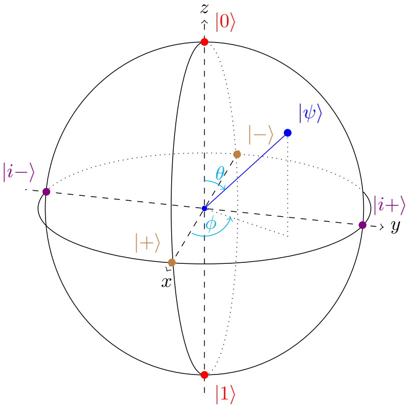

QCApplications
Greener Fertilization
Better Batteries
Artificial Intelligence
Climate Change
Weather Forecasting
Operations Optimization
Financial Modeling
Exploration of Electronic Materials
Drug Discovery
Cyber Security

Quantum Bit (abbreviated as *qubit*) is a two-dimensional quantum mechanical system, which exists in the state:

$$|\psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle\,,$$

where α and β are complex numbers, representing *amplitudes* of quantum states $|0\rangle$ and $|1\rangle$, respectively.
The squared magnitudes of these amplitudes correspond to the probabilities of measuring the quantum state in a particular basis. Therefore, the normalization condition holds: $|\alpha|^2 + |\beta|^2 = 1$.
This definition utilizes the standard *bra-ket* notation, where:

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \text{ and } |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$



Quantum Register

- Encompasses multiple qubits at once.
- A quantum register is analogous to a classical processor register, and quantum computers perform computations by manipulating qubits within a given register.
- Each qubit $|\psi\rangle$ in the register is a superposition of $\alpha|0\rangle + \beta|1\rangle$ from the computational basis elements $|0\rangle$ and $|1\rangle$.
- A register with n qubits is a superposition of all possible 2^n bit strings that can be represented with n bits.
- The state space of an n-qubit register is a linear combination of 2^n basis vectors.

$$|\psi_n\rangle = \sum_{i=0}^{2^n-1} \alpha_i |i\rangle \tag{1}$$

where i is an integer in decimal notation representing an n-bit binary number.

Quantum Registers

- For Equation (1), the normalization condition for the probability amplitudes holds:

$$\sum_{i=0}^{2^n-1} |\alpha_i|^2 = 1. \tag{2}$$

- Logically, the sum of the probabilities of all possible states must be 1, as no other state can occur and each state is mutually exclusive.
- Quantum registers are a direct extension of qubits.

- Each bit configuration in quantum superposition is represented as the tensor product of individual qubits.
- For example, $|010\rangle$, which represents the number 2 in a bit string, has the form:

$$|010\rangle = |0\rangle \otimes |1\rangle \otimes |0\rangle = \begin{pmatrix}1\\0\end{pmatrix} \otimes \begin{pmatrix}0\\1\end{pmatrix} \otimes \begin{pmatrix}1\\0\end{pmatrix} = (0\ 0\ 1\ 0\ 0\ 0\ 0\ 0)^{\mathrm{T}}.$$

$$\begin{pmatrix}1\\0\end{pmatrix} \otimes \begin{pmatrix}0\\1\end{pmatrix} = \begin{pmatrix}0\\1\\0\\0\end{pmatrix}.$$

For example, a three-qubit register has the form:

$$\begin{aligned} |\psi_3\rangle &= \alpha_0 |000\rangle + \alpha_1 |001\rangle + \alpha_2 |010\rangle + \alpha_3 |011\rangle + \alpha_4 |100\rangle + \alpha_5 |101\rangle + \alpha_6 |110\rangle + \alpha_7 |111\rangle \\ &= \sum_{i=0}^{7} \alpha_i |i\rangle . \end{aligned}$$

- Classical logic gates are mathematically described using Boolean algebra. Quantum logic gates operate on a similar principle.
- Quantum logic gates applied to quantum registers transform quantum superpositions into others, allowing the system to evolve toward a desired final state—the correct answer.
- Quantum logic gates are mathematically represented through matrix transformations (linear operations) applied to a quantum register by tensoring transformation matrices with the matrix representing the given register.
- All matrices corresponding to quantum logic gates are *unitary*[1].
- Unitary transformations applied to a single qubit can be effectively visualized on the Bloch sphere.
- Just as with classical logic gates, a standard set of commonly used quantum logic gates is established.

[1] A complex matrix U is *unitary* if and only if $U^{-1} = U^\dagger$, where $U^\dagger$ is the conjugate transpose of U ($U^\dagger = \overline{U}^T$). Additionally, it satisfies $UU^\dagger = U^\dagger U = I$.

Pauli Quantum Gates

- *Pauli Gates* X, Y, and Z correspond to rotations by an angle of π around the x, y, and z axes, respectively.
- The Pauli-X gate swaps the amplitudes of $|0\rangle$ and $|1\rangle$:

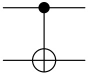
$$-\boxed{X}- = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

- $$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} |0\rangle = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} = |1\rangle$$

- $$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} |1\rangle = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} = |0\rangle$$

CNOT Quantum Gate

- The most important and widely used binary quantum gate is the CNOT (Controlled-NOT) gate.

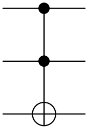


$$= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

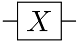
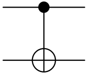
- Applying the CNOT matrix to $|11\rangle$:

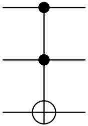
$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} |11\rangle = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} = |10\rangle$$

The most important and widely used ternary quantum gate is the Toffoli Gate (CCNOT).



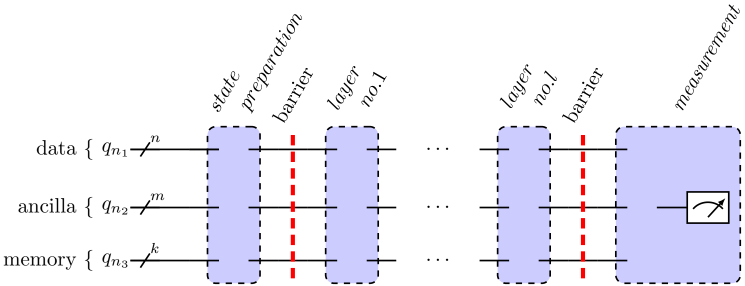
$$
= \begin{bmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0
\end{bmatrix}
$$

Gate	Symbol	Input	Output
Pauli-X		$\|0\rangle$	$\|1\rangle$
		$\|1\rangle$	$\|0\rangle$
CNOT		$\|00\rangle$	$\|00\rangle$
		$\|01\rangle$	$\|01\rangle$
		$\|10\rangle$	$\|11\rangle$
		$\|11\rangle$	$\|10\rangle$

Gate	Symbol	Input	Output
Toffoli		$\|000\rangle$	$\|000\rangle$
		$\|001\rangle$	$\|001\rangle$
		$\|010\rangle$	$\|010\rangle$
		$\|100\rangle$	$\|100\rangle$
		$\|011\rangle$	$\|011\rangle$
		$\|101\rangle$	$\|101\rangle$
		$\|110\rangle$	$\|111\rangle$
		$\|111\rangle$	$\|110\rangle$

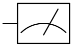
Three fundamental layers:

1. Encoding of data, which can be either classical or quantum, into the state of a set of input qubits.
2. A sequence of quantum gates applied to this set of input qubits.
3. Measurement of one or more qubits at the end to obtain a classically interpretable result.



Measurement

1. The only way to extract information from n qubits in a given state.
2. The measurement process is performed by hardware with a digital display, called an n-qubit measurement gate.
3. The n-qubit measurement gate is schematically represented by the symbol:



4. Unlike unitary gates, which have a unique output state for each input state, the state of qubits exiting the measurement gate is statistically determined only by the input qubit states.
5. The measurement action is irreversible: there is no way to reconstruct the initial state from the final state.
6. Measurement is irreversible.
7. Measurement is not linear in any sense.
8. We say that the pre-measurement state collapses/reduces to the post-measurement state due to measurement.
9. The state of n qubits is nothing more than an abstract symbol used via Born's rule to compute the probabilities of measurement outcomes.

Quantum Superposition of States

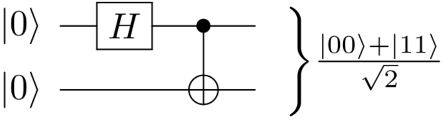
- A fundamental principle of quantum mechanics.
- Any two (or more) quantum states can be combined (superposed).
- A new quantum state is formed.

Gate	Symbol	Input	Output
Hadamard	$-\boxed{H}-$	$\|0\rangle$	$\frac{1}{\sqrt{2}}(\|0\rangle + \|1\rangle)$
		$\|1\rangle$	$\frac{1}{\sqrt{2}}(\|0\rangle - \|1\rangle)$

50% probability of measuring the value $|0\rangle$ at the output.

50% probability of measuring the value $|1\rangle$ at the output.

A simple quantum circuit that creates *entanglement* between two qubits:



The output of this circuit cannot be decomposed into individual basis states $|0\rangle$ and $|1\rangle$.

State space of a single qubit: $H_1 = \text{span}\{|0\rangle, |1\rangle\}$.
State space of two qubits: H_2:

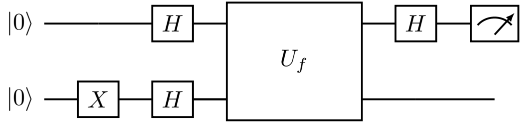
Canonical Basis	Bell Basis
$\|00\rangle$	$\|\Phi^+\rangle = \frac{1}{\sqrt{2}}(\|00\rangle + \|11\rangle)$
$\|01\rangle$	$\|\Phi^-\rangle = \frac{1}{\sqrt{2}}(\|00\rangle - \|11\rangle)$
$\|10\rangle$	$\|\Psi^+\rangle = \frac{1}{\sqrt{2}}(\|01\rangle + \|10\rangle)$
$\|11\rangle$	$\|\Psi^-\rangle = \frac{1}{\sqrt{2}}(\|01\rangle - \|10\rangle)$

Assumption: $f : \{0,1\} \longrightarrow \{0,1\}$

$$f_1 : 0 \mapsto 0 \quad f_2 : 0 \mapsto 1 \quad f_3 : 0 \mapsto 0 \quad f_4 : 0 \mapsto 1$$
$$\;\;\; 1 \mapsto 0 \qquad\;\; 1 \mapsto 1 \qquad\;\; 1 \mapsto 1 \qquad\;\; 1 \mapsto 0$$

f_1 and f_2 are constant. f_3 and f_4 are balanced.

Task: Determine whether f is constant or balanced.



$$U_f : |xy\rangle \mapsto |x, y \oplus f(x)\rangle$$

$$(H \otimes I)\, U_f\, (H \otimes H)\, (I \otimes X)\, |0\rangle \otimes |0\rangle$$

$$
\begin{aligned}
&(H\otimes I)\,U_f\,(H\otimes H)\,(I\otimes X)\;|0\rangle\otimes|0\rangle =\\
&(H\otimes I)\,U_f\,(H\otimes H)\;|0\rangle\otimes|1\rangle =\\
&(H\otimes I)\,U_f\,\frac{1}{\sqrt{2}}\,(|0\rangle+|1\rangle)\otimes\frac{1}{\sqrt{2}}\,(|0\rangle-|1\rangle) =\\
&(H\otimes I)\,U_f\,\frac{1}{2}\,(|00\rangle-|01\rangle+|10\rangle-|11\rangle) =\\
&(H\otimes I)\frac{1}{2}\,(|0,f(0)\rangle-|0,\neg f(0)\rangle+|1,f(1)\rangle-|1,\neg f(1)\rangle) =\\
&\frac{1}{2\sqrt{2}}\Big(\,(|0\rangle+|1\rangle)(|f(0)\rangle-|\neg f(0)\rangle)+(|0\rangle-|1\rangle)(|f(1)\rangle-|\neg f(1)\rangle)\Big)
\end{aligned}
$$

If f is constant $\Rightarrow |f(0)\rangle = |f(1)\rangle \Rightarrow$

$$\frac{1}{\sqrt{2}}\;|0\rangle\,(|f(0)\rangle-|\neg f(0)\rangle)$$

If f is balanced $\Rightarrow |\neg f(0)\rangle = |\ f(1)\rangle \Rightarrow$

$$\frac{1}{\sqrt{2}}\;|1\rangle\,(|f(0)\rangle-|\neg f(0)\rangle)$$

Variational Quantum Algorithms (VQA)

Variational Quantum Algorithms (VQA) are hybrid quantum-classical algorithms that use quantum circuits with optimizable parameters to solve computationally challenging problems.

Main Characteristics:

- Hybrid approach: the quantum processor performs computations while a classical optimizer adjusts parameters.
- Variational principle: the quantum circuit is designed to minimize a given objective function.
- Applications: quantum simulations, optimization, machine learning.

Examples:

- Variational Quantum Eigensolver (VQE).
- Quantum Approximate Optimization Algorithm (QAOA).

Variational Quantum Eigensolver (VQE) is an algorithm designed to find the eigenvalues and eigenvectors of a quantum system's Hamiltonian.

Principle:

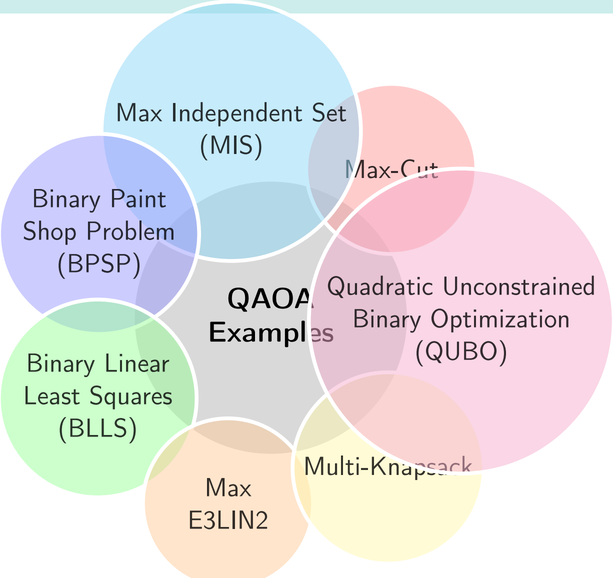
- Define the Hamiltonian H, where the lowest eigenvalue corresponds to the target energy.
- Use a parameterized quantum circuit to construct an approximate wave function $|\psi(\theta)\rangle$.
- A classical optimizer iteratively updates the parameters θ to minimize the expected energy value $\langle\psi(\theta)|H|\psi(\theta)\rangle$.

Advantages:

- More efficient than exact diagonalization methods for large systems.
- Suitable for implementation on near-term quantum devices (NISQ).

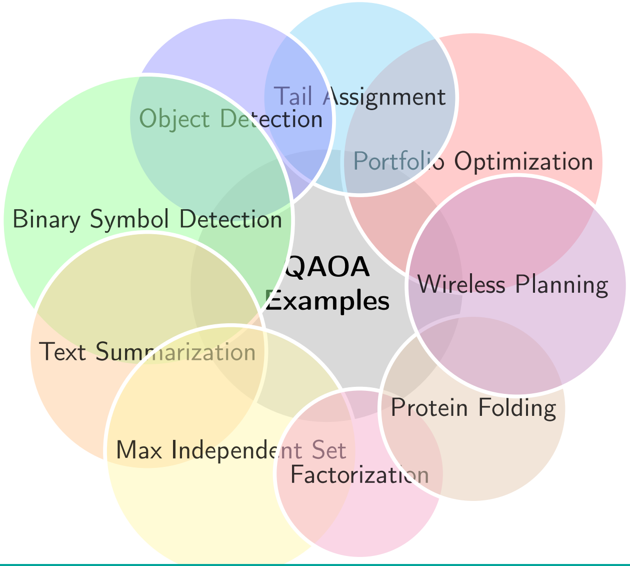
QAOA

- Suitable for finding good approximate solutions to optimization problems.
- A widely studied method for solving combinatorial optimization problems on NISQ devices.



QAOA

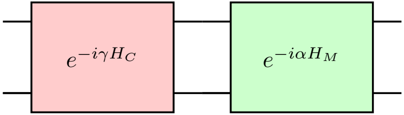
Latest application examples:



https://arxiv.org/pdf/2306.09198.pdf

QAOA is a general technique used to find approximate solutions to combinatorial optimization problems, particularly those that can be formulated as finding the optimal bitstring. QAOA consists of the following steps:

1. Define the cost Hamiltonian H_C such that its ground state encodes the solution to the optimization problem.
2. Define the mixer Hamiltonian H_M.
3. Construct the circuits $e^{-i\gamma H_C}$ and $e^{-i\alpha H_M}$, known as the cost and mixing layers.

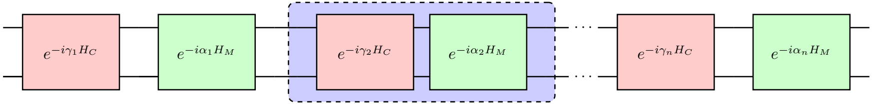


Quantum Approximate Optimization Algorithm (QAOA)

4. Choose a parameter $n \geq 1$ and construct the circuit:

$$U(\gamma, \alpha) = e^{-i\alpha_n H_M} e^{-i\gamma_n H_C} \dots e^{-i\alpha_1 H_M} e^{-i\gamma_1 H_C},$$

which consists of repeated applications of cost and mixing layers.



5. Prepare an initial state, apply $U(\gamma, \alpha)$, and optimize its parameters using classical techniques.
6. Once the circuit is optimized, measuring the output state reveals approximate solutions to the optimization problem.

Quantum Approximate Optimization Algorithm (QAOA)

In summary,

- QAOA starts by specifying cost and mixer Hamiltonians.
- By using time evolution and layering, a variational circuit is created and its parameters are optimized.
- The algorithm concludes by sampling from the circuit to obtain an approximate solution to the optimization problem.

Thank you for your attention

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