Quantum Chemistry on NISQ Quantum Computers

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Outline

- QChem Applications
- HPC Limitations & QComp Potential
- Electronic Structure Problem
- Quantum Phase Estimation
- NISQ
- Quantum Noise(s)
- Variational Quantum Eigensolver
- Correction, Mitigation and Suppression

Google colab

Hands-On Prep

1. Login to you Google account
2. https://drive.google.com/drive/folders/1akj_35QyrPzhlE6L1YpH2OksdRfEGK5o?usp=drive_link
3. Run 1_install_test.ipynb
   - Runtime -> Run all

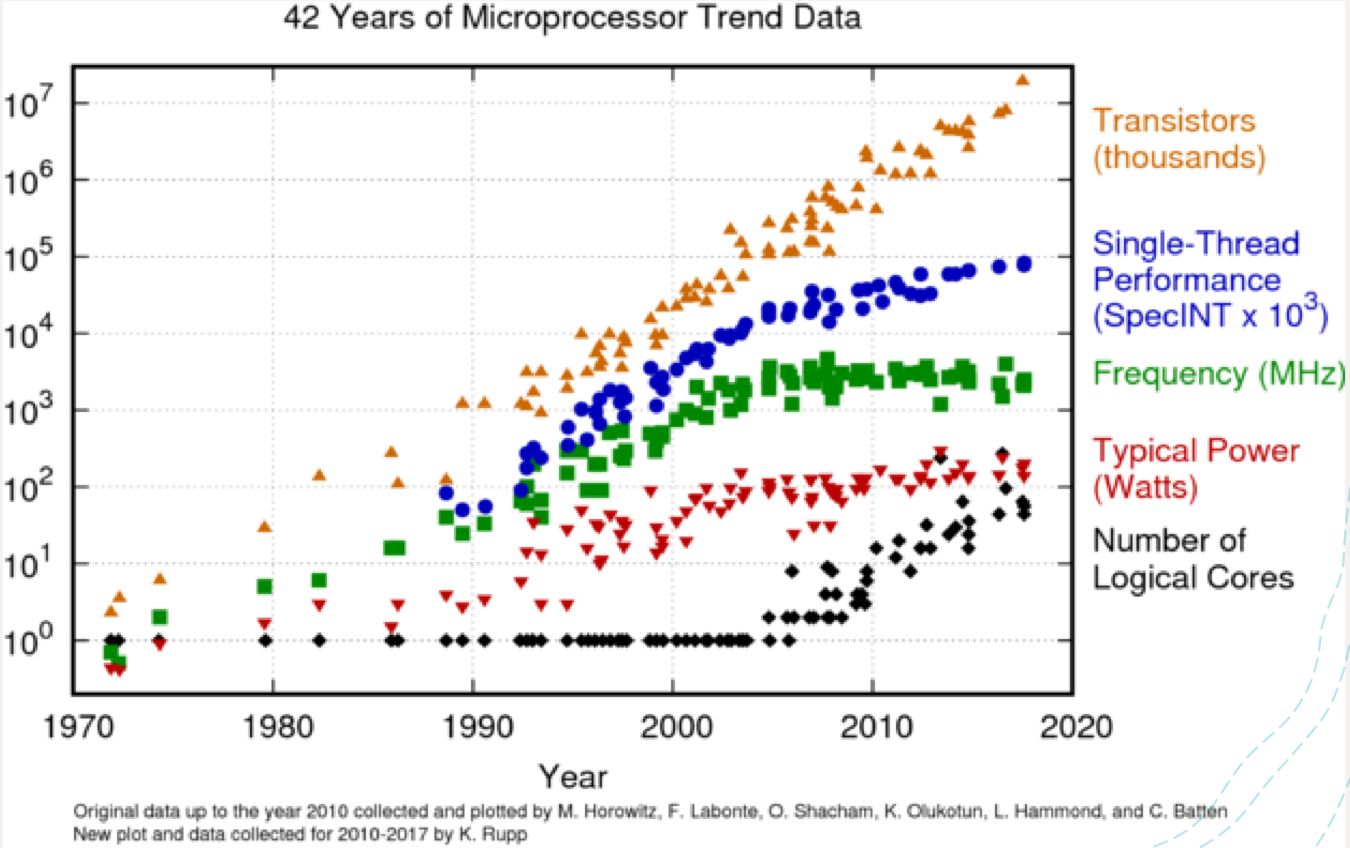
Quantum Chemistry Applications

- Drug Design
- Rocket Fuels
- Material Science
- Plasma Medicine

Source: Stanford U, HIV Drug Resistance Database

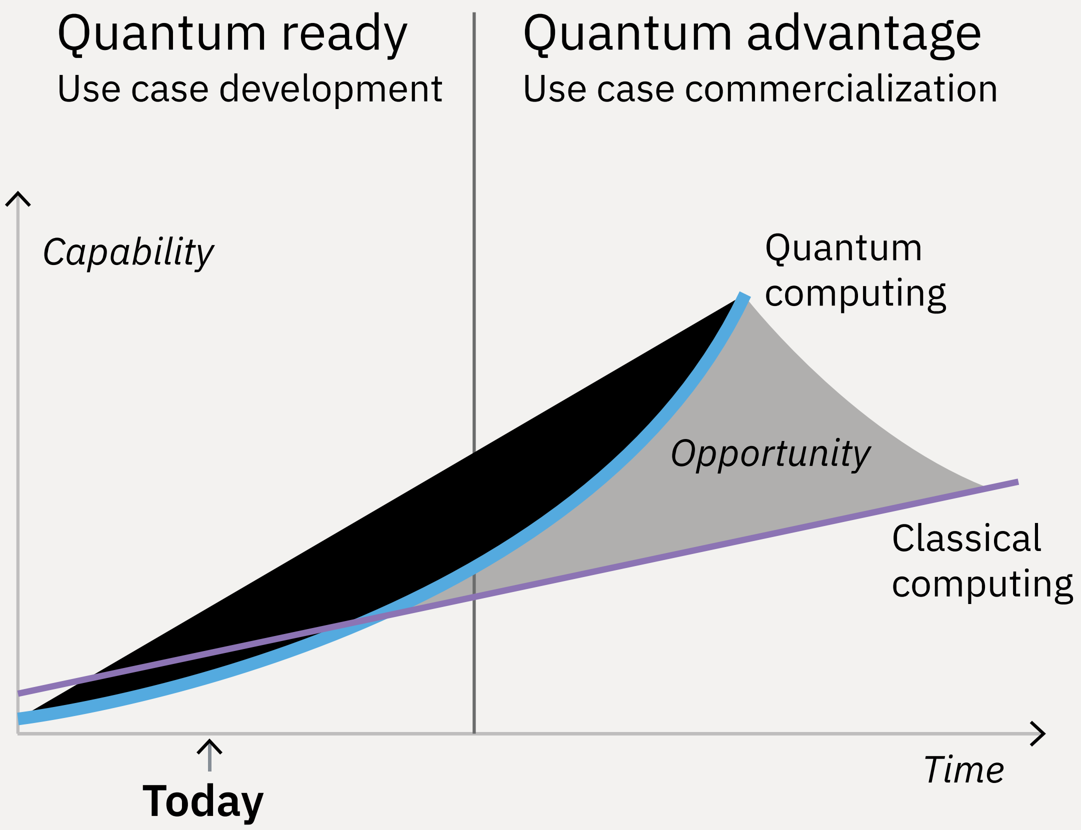
Current HPC Challenges

+ Limits of Moore's law
  + Power wall (Limit to clock speed)
  + Transistor-size limits
+ Logical difficulties in multi-level parallelization
+ Computationally-demanding applications



Quantum Advantage

- Superpolynomial speedup (?)
- Manin (1980), Feynman (1981), Preskill (2012)
- Feasible under different assumptions
- Not with current computers



Source: IBM

Integer factorization (Shor's algorithm)

Boson sampling

Sampling the output distribution of random quantum circuits

QC Approaches

Boson Sampling

- Non-universal
- Utilizes boson scattering
- Expectation values of matrix permanent
- Few physical resources
- Clique problem, max-cut, …

Quantum Annealing

- Adiabatic Theorem
- Slow evolution
- Staying in ground-state
- QUBO

Gate-based Programming

- Similar to logical gates
- Every gate represent a unitary operator
- Reversible computing

Quantum Bits

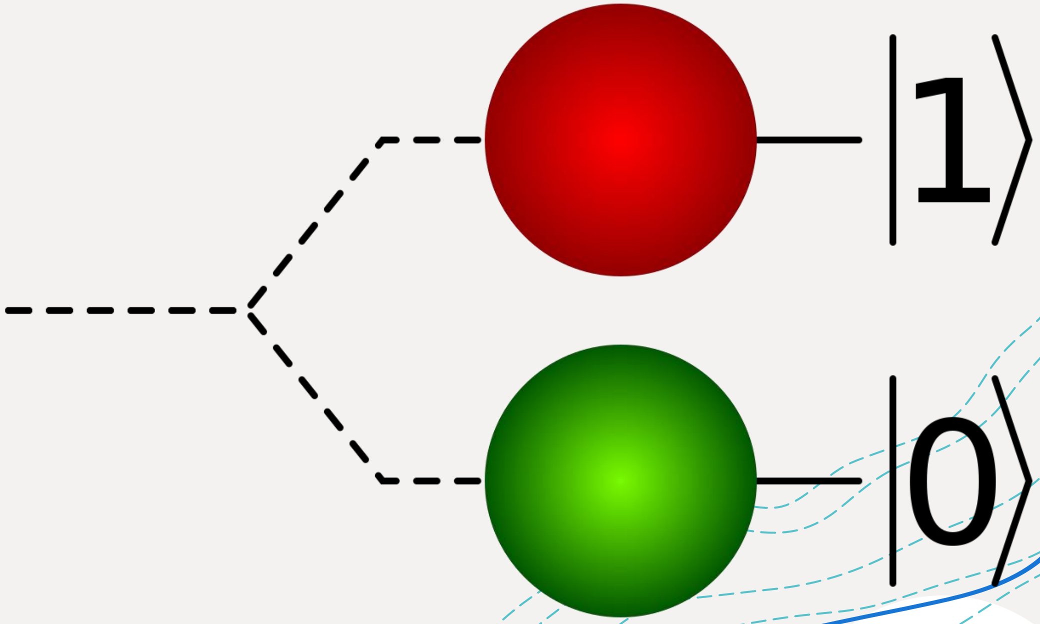
$$|\psi\rangle = c_0|\psi_0\rangle + c_1|\psi_1\rangle$$

$$|0\rangle = 1|\psi_0\rangle + 0|\psi_1\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$$|1\rangle = 0|\psi_0\rangle + 1|\psi_1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

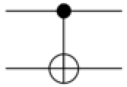
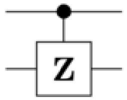
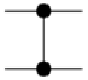
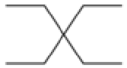
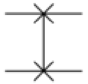
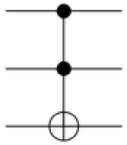
+ Quantum unit, interest in its ground and the first excited state
+ Possible extensions to qutrits, qudits, etc.
+ Computational basis |0>, |1>

- Photon polarizations
- Energy levels of ion / **superconducting circuit**
- Nuclear spin-states of atom
- Spin states of electron

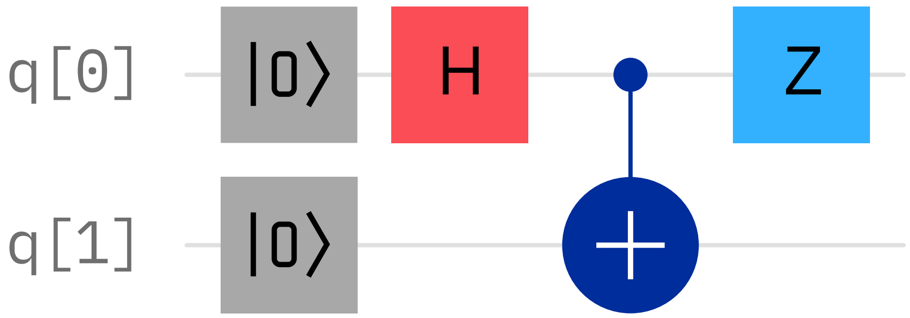


Quantum Gate

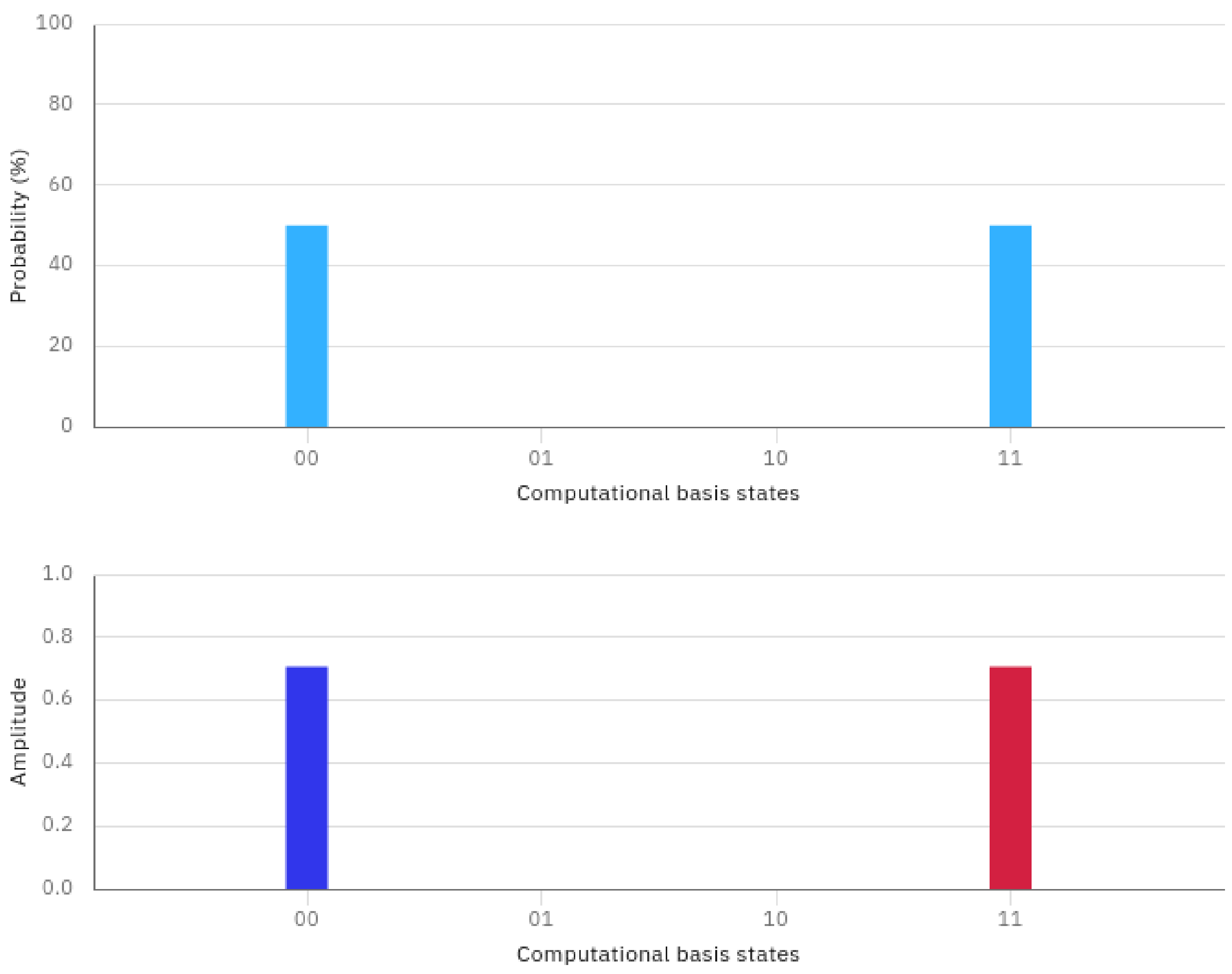
+ Representing unitary operators
+ Can be thought of as matrices
+ Realized via lasers, microwaves, …

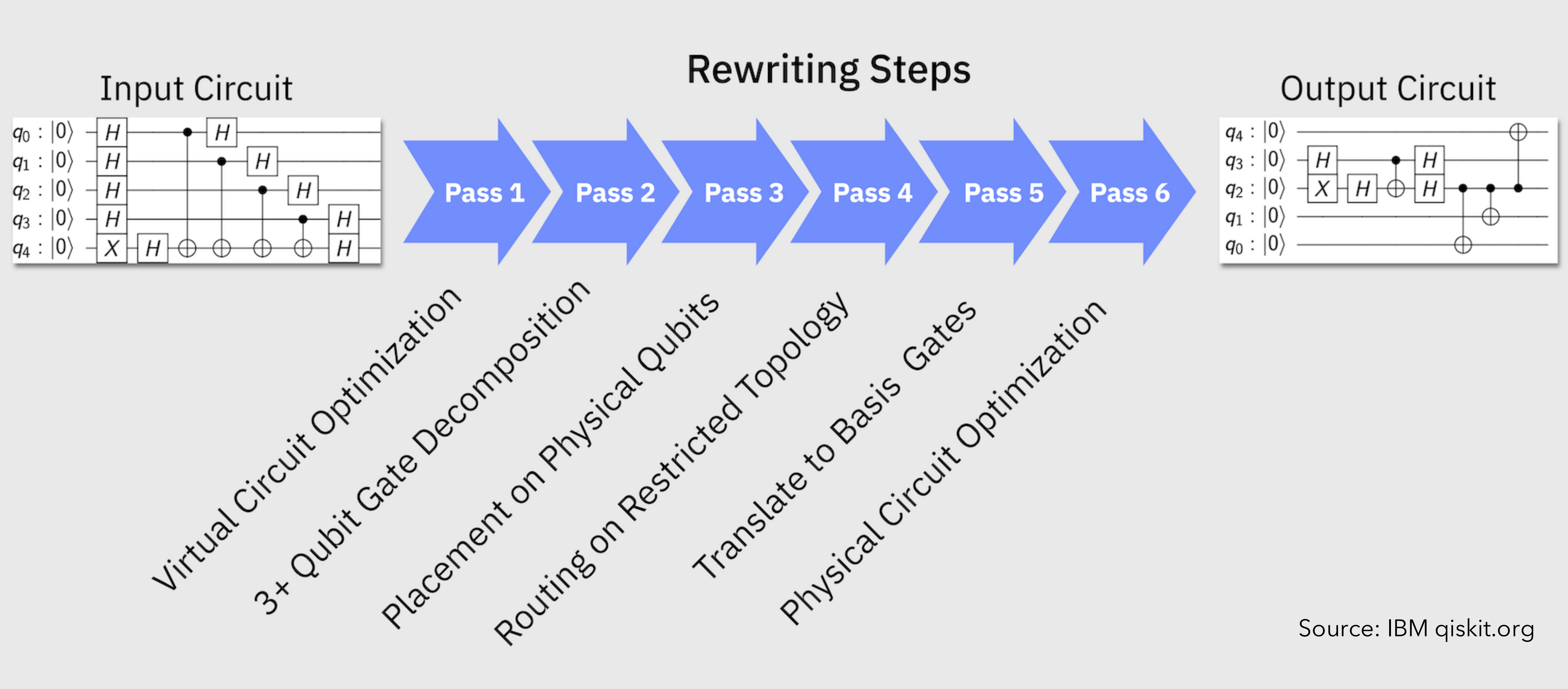
Operator	Gate(s)		Matrix
Pauli-X (X)	**X**	$\oplus$	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
Pauli-Y (Y)	**Y**		$\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$
Pauli-Z (Z)	**Z**		$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
Hadamard (H)	**H**		$\frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$
Phase (S, P)	**S**		$\begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}$
$\pi/8$ (T)	**T**		$\begin{bmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{bmatrix}$
Controlled Not (CNOT, CX)			$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$
Controlled Z (CZ)			$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$
SWAP			$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$
Toffoli (CCNOT, CCX, TOFF)			$\begin{bmatrix} 1&0&0&0&0&0&0&0 \\ 0&1&0&0&0&0&0&0 \\ 0&0&1&0&0&0&0&0 \\ 0&0&0&1&0&0&0&0 \\ 0&0&0&0&1&0&0&0 \\ 0&0&0&0&0&1&0&0 \\ 0&0&0&0&0&0&0&1 \\ 0&0&0&0&0&0&1&0 \end{bmatrix}$

Quantum Circuit



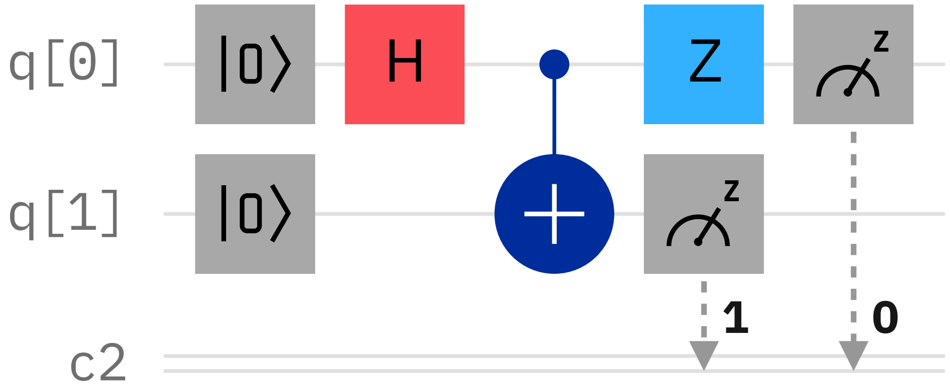
$$|\psi\rangle = Z \otimes I \cdot CX \cdot H \otimes I \cdot |0\rangle \otimes |0\rangle$$
$$= \left[\frac{1}{\sqrt{2}},\quad 0,\quad 0,\quad -\frac{1}{\sqrt{2}}\right]$$



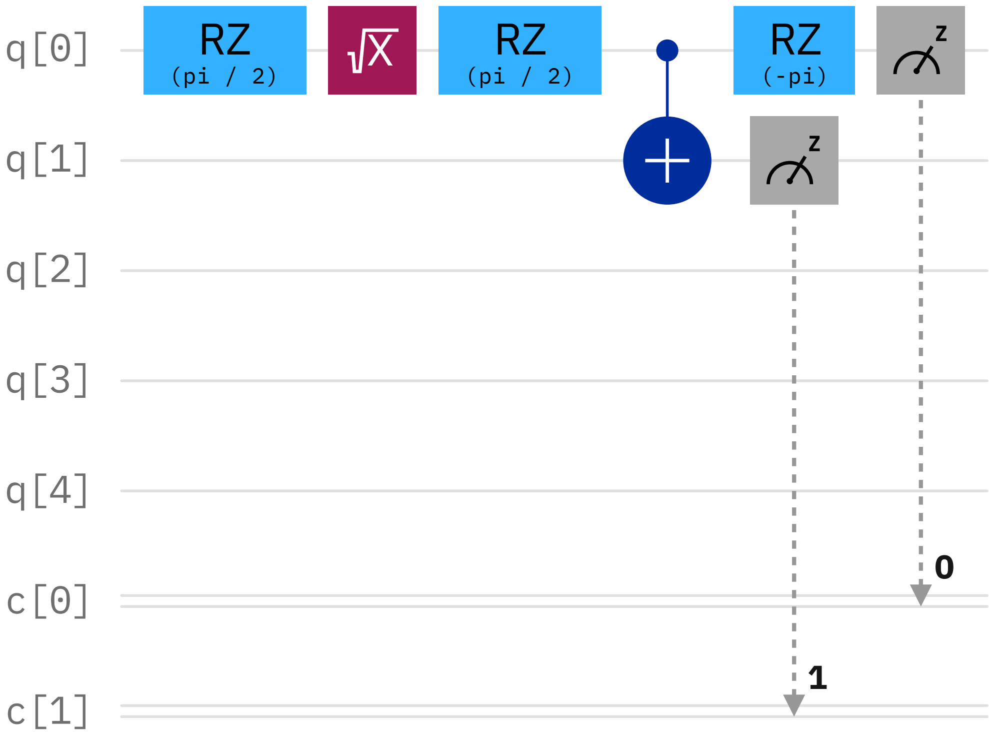


Transpilation

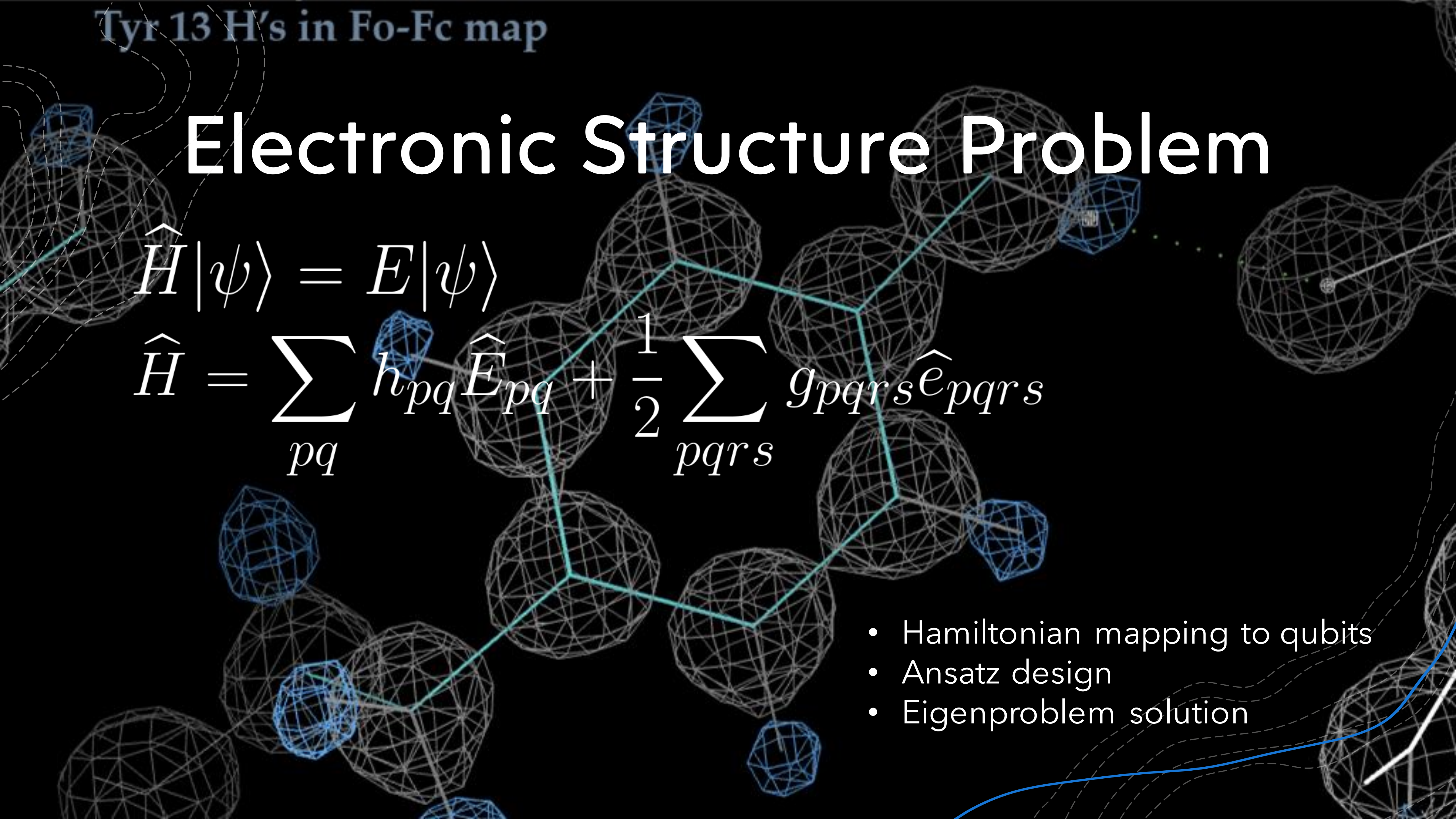
"REWRITING" OF OUR CIRCUITS TO THE SET OF INSTRUCTIONS THE COMPUTER OFFERS



Original



IBMQ Quito



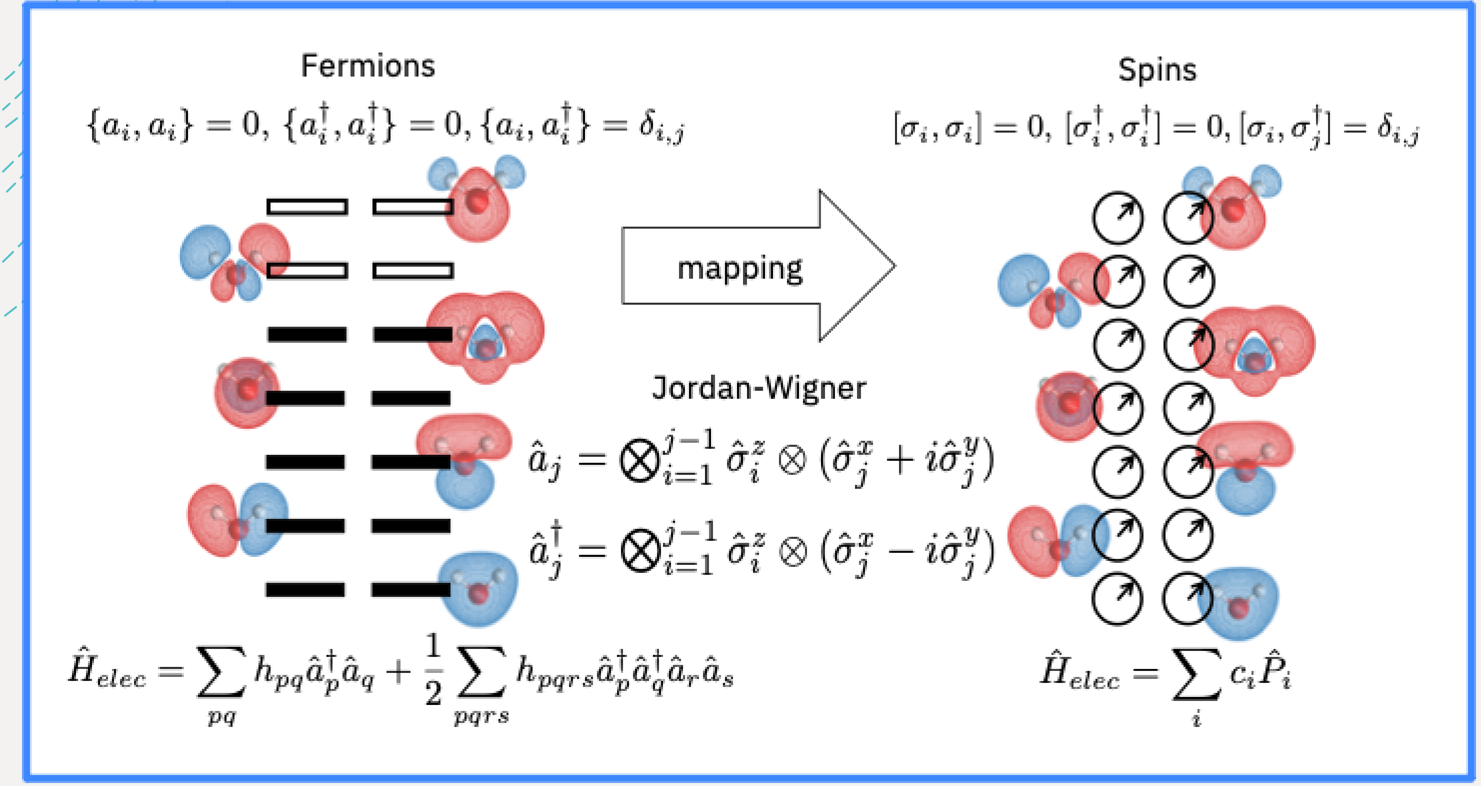
Electronic Structure Problem

$$\hat{H}|\psi\rangle = E|\psi\rangle$$

$$\hat{H} = \sum_{pq} h_{pq}\hat{E}_{pq} + \frac{1}{2}\sum_{pqrs} g_{pqrs}\hat{e}_{pqrs}$$

- Hamiltonian mapping to qubits
- Ansatz design
- Eigenproblem solution

Hamiltonian Mapping

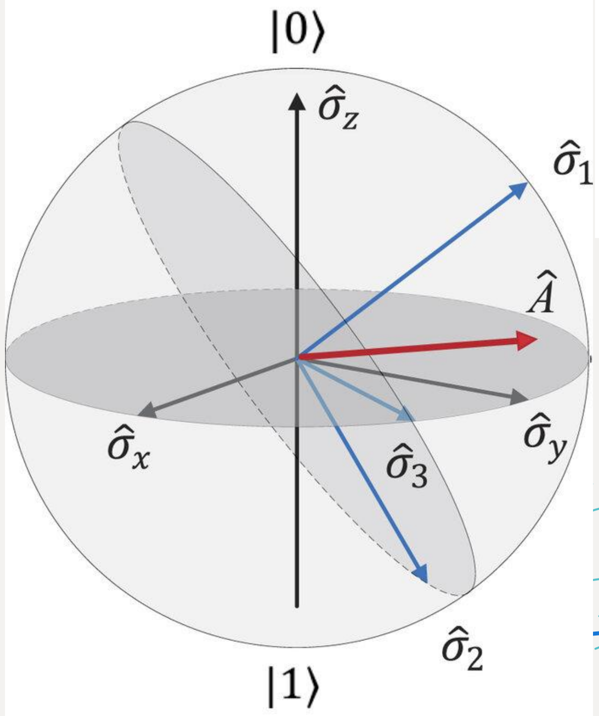


- Mapping of Hamiltonian to Pauli matrices
- Jordan-Wigner
- Parity mapping
- Bravyi-Kitaev

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

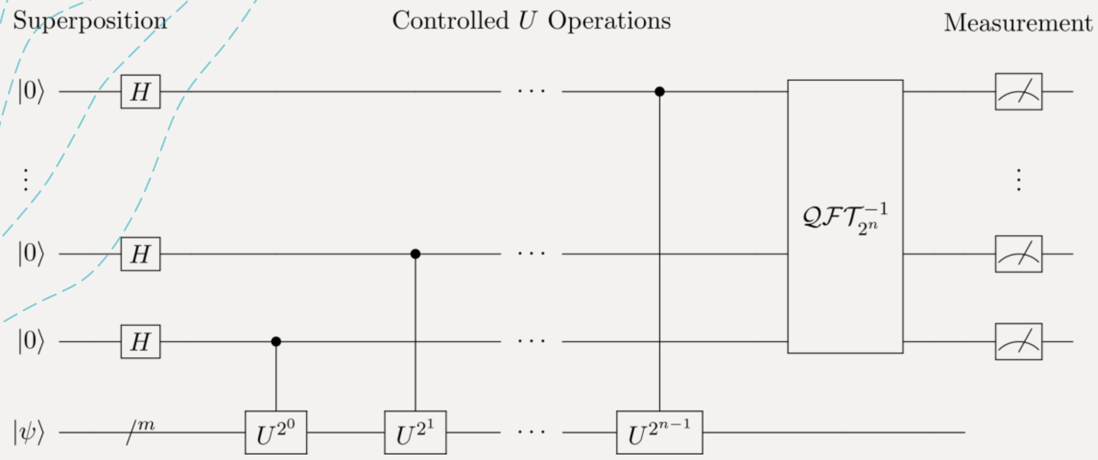
$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$



Ansatz Design

- Representing statevectors
- Similar to Artificial Neural Networks
- Points of freedom to-be-fitted
- Physics-based (UCC)
  - Problem-specific
  - Visibly encoded information
  - Rather simple & shallow
- Hardware-efficient
  - General
  - Information is scattered
  - Deep circuits
  - More points-of-freedom



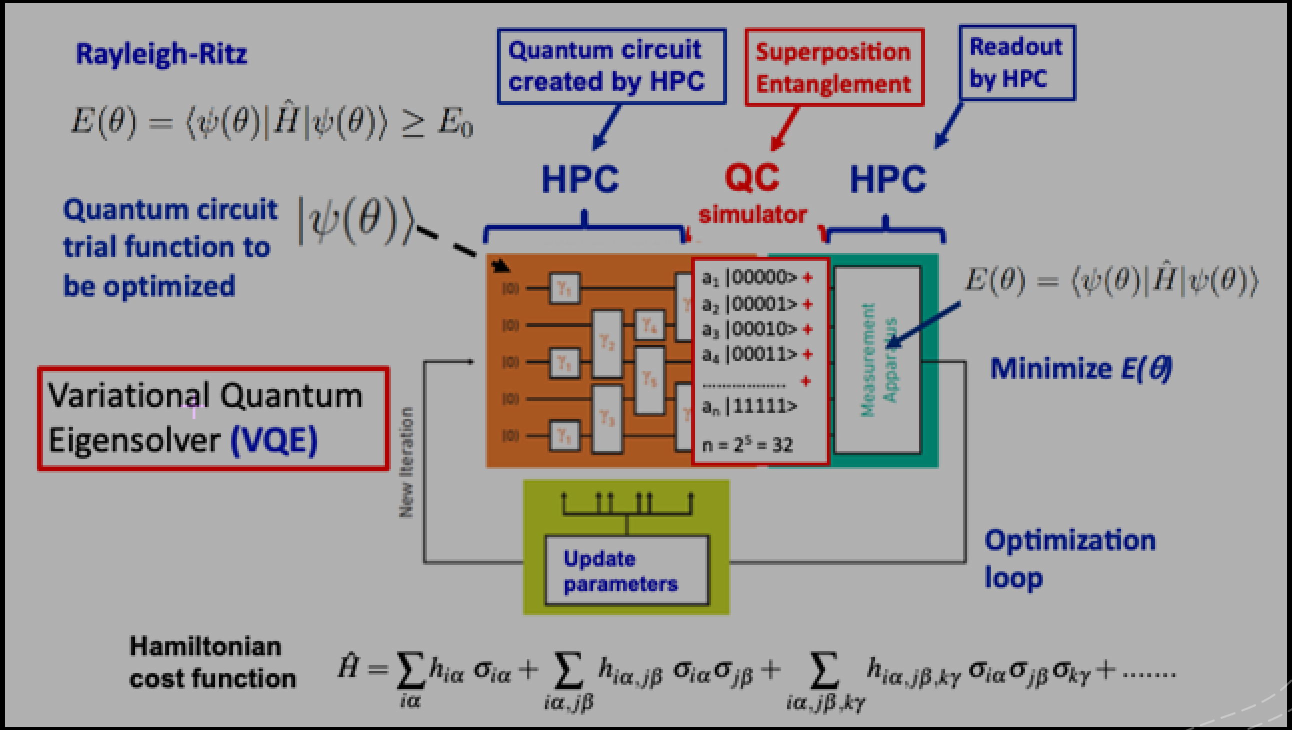
$$\widehat{U}|\psi\rangle = e^{2\pi i\theta}|\psi\rangle$$

Solving Eigenproblem via QPE

- Obtaining a local phase of unitary operator
- Uses Inverse Quantum Fourier Transform
- Demanding many qubits

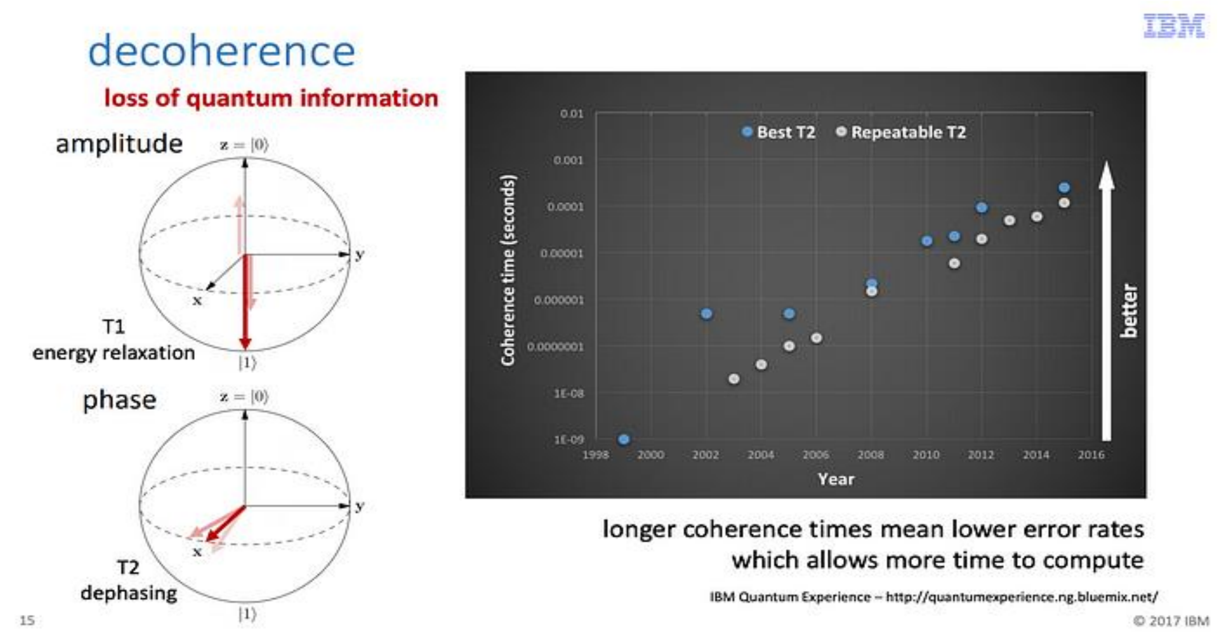
Solving Eigenproblem via VQE

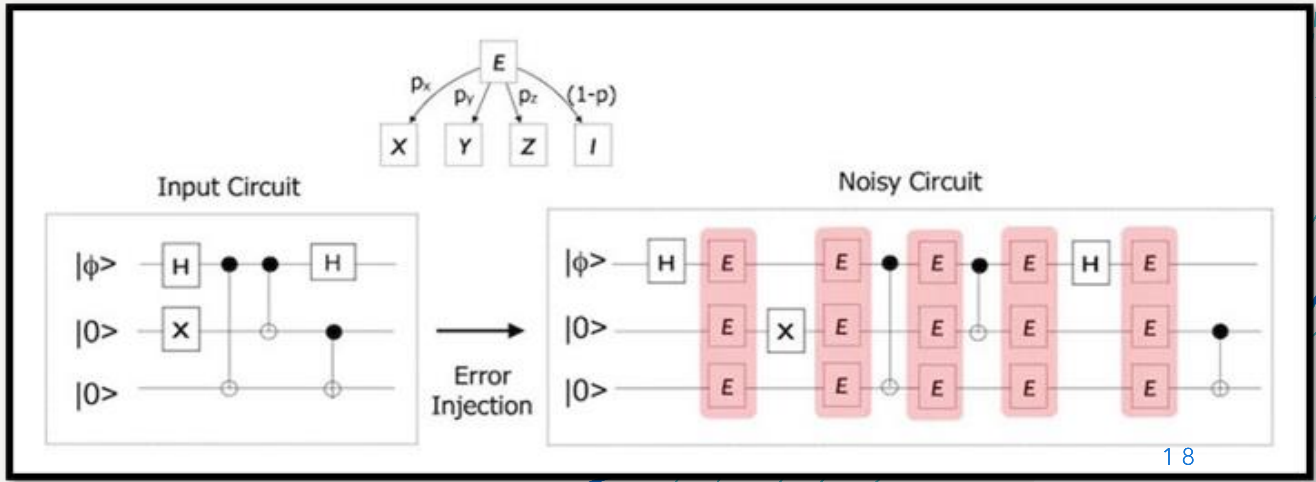
- Based on variational principle
- Hybrid quantum-classical approach
- Ansatz approximates statevector
- Potentially efficient also on NISQ infrastructures



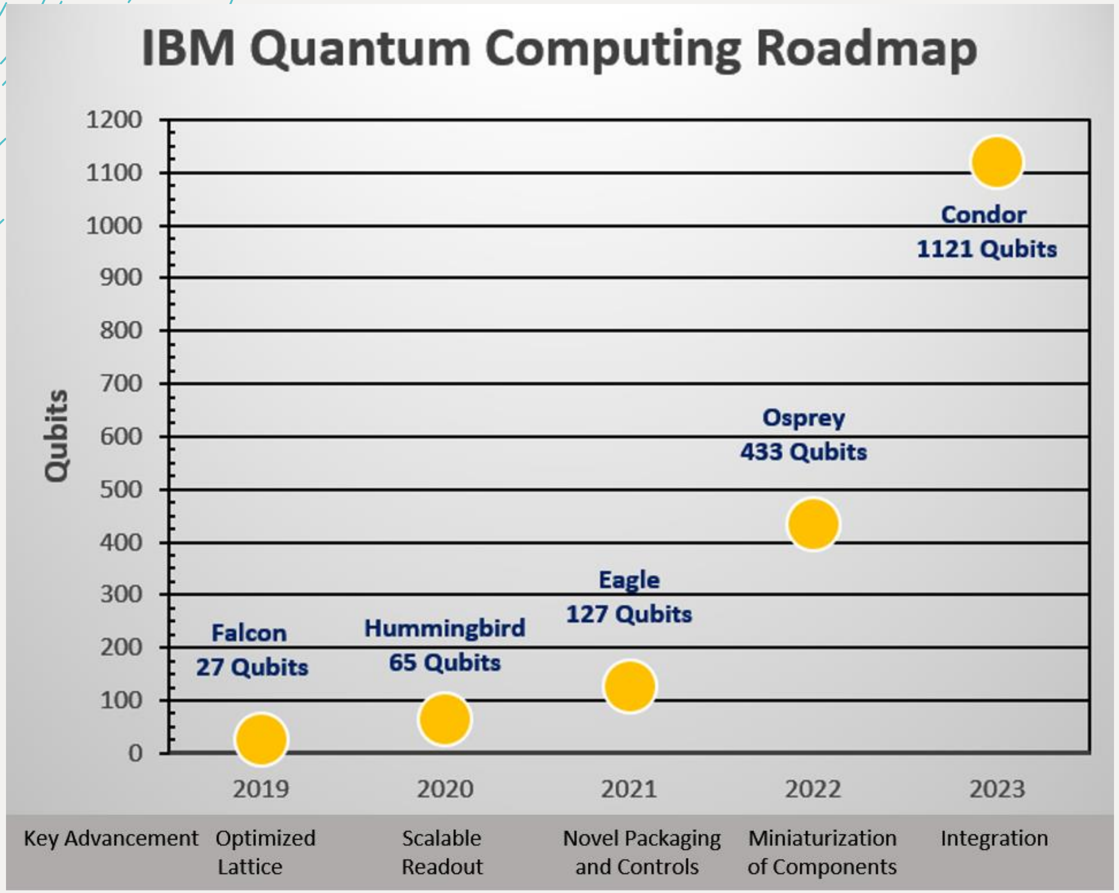
Emerging problems

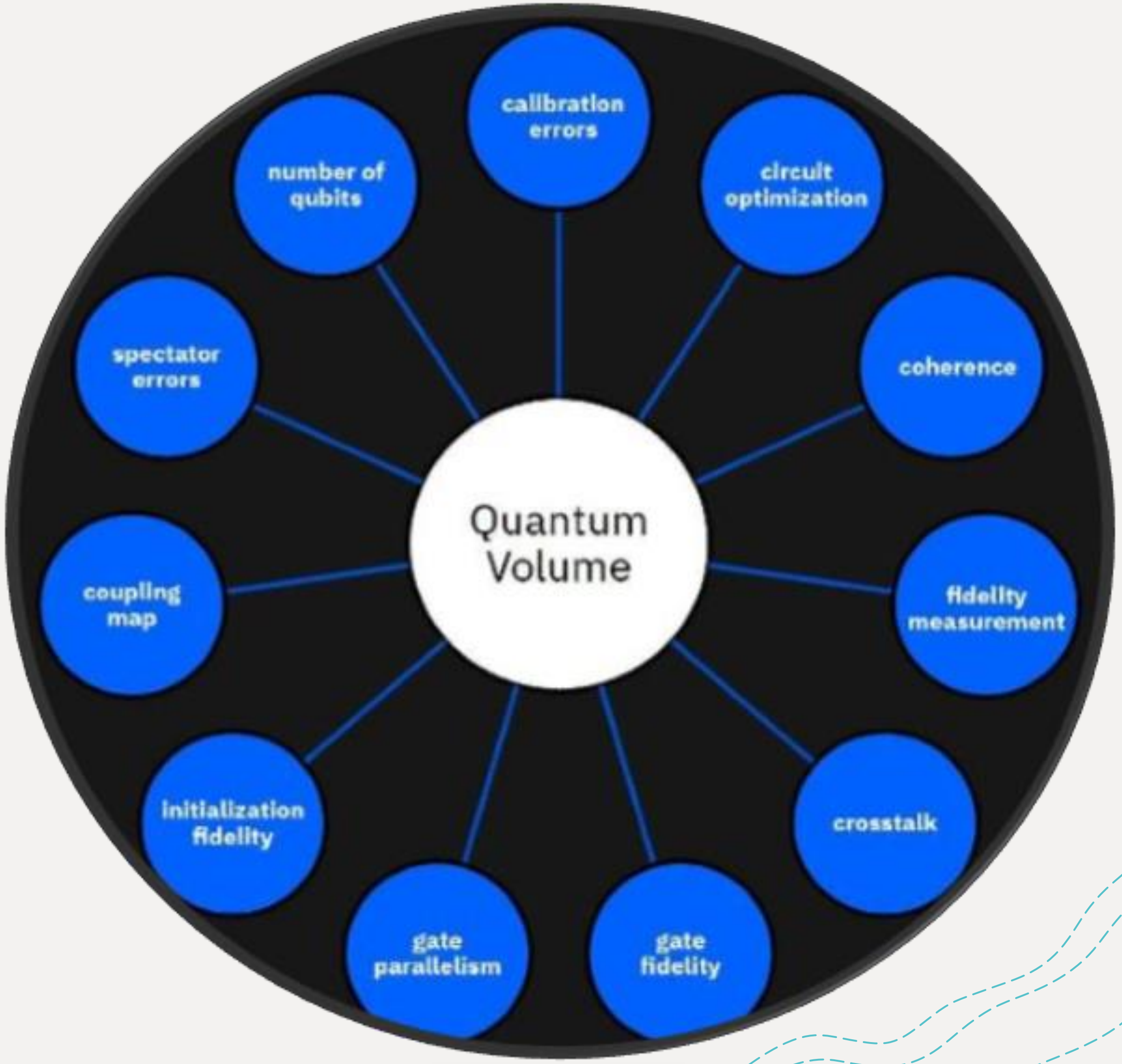
- Sampling noise
  - Optimization problems
- Decoherence
  - Temperature fluctuations
  - Mechanical vibrations
  - Thermal noise (Brownian motion)
  - Cosmic rays
  - Interaction among qubits
  - Energy relaxation (spin-lattice)
  - Dephasing (spin-spin)





Quantum Volume

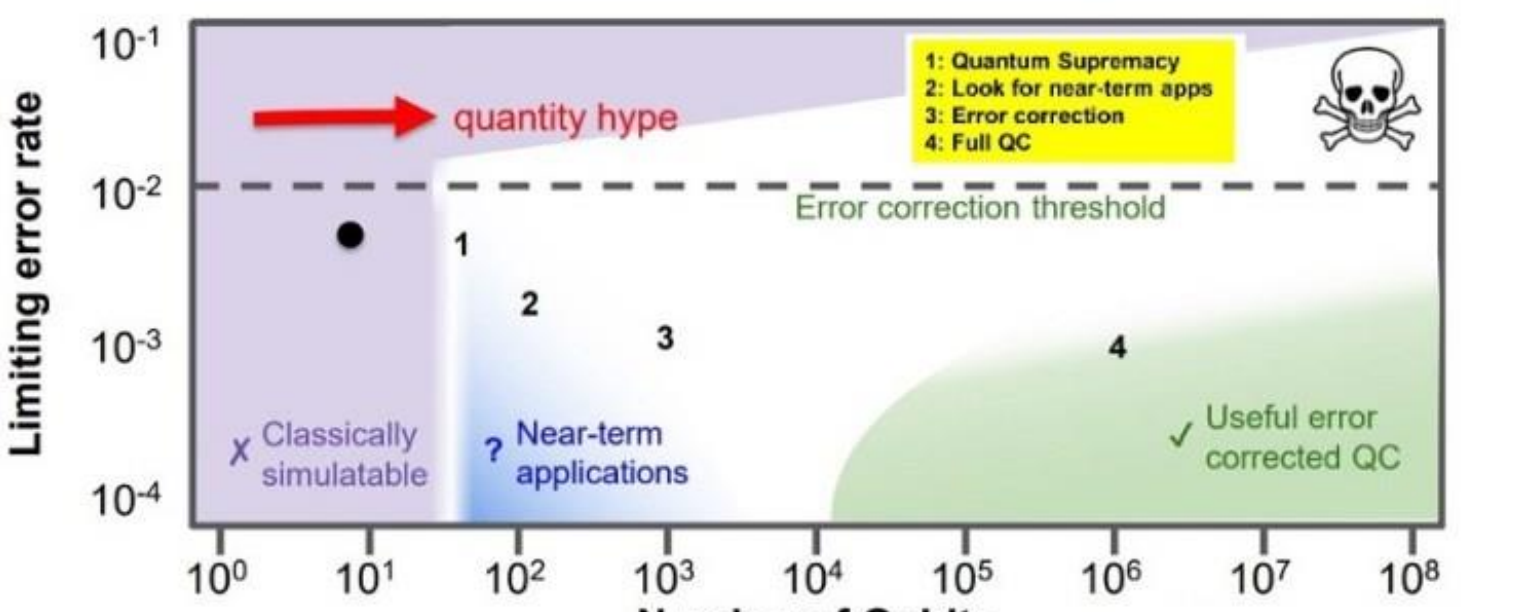




Source: IBM

NISQ Machines

+ Noisy Intermediate-Scale Quantum
+ 50 – hundreds of qubits (*Preskill*)
+ NO fault tolerance
+ NO general quantum supremacy
+ QAOA, VQE, QML, …



Source: John Martinis, Google

Classical Error Correction

- Redundant encoding via *error correction code*
- *Repetition encoding*
  - Possible to repair (n-1)/2 mistakes

$$\{0, 1\}_B \rightarrow \{000, 111\}_{C3}$$

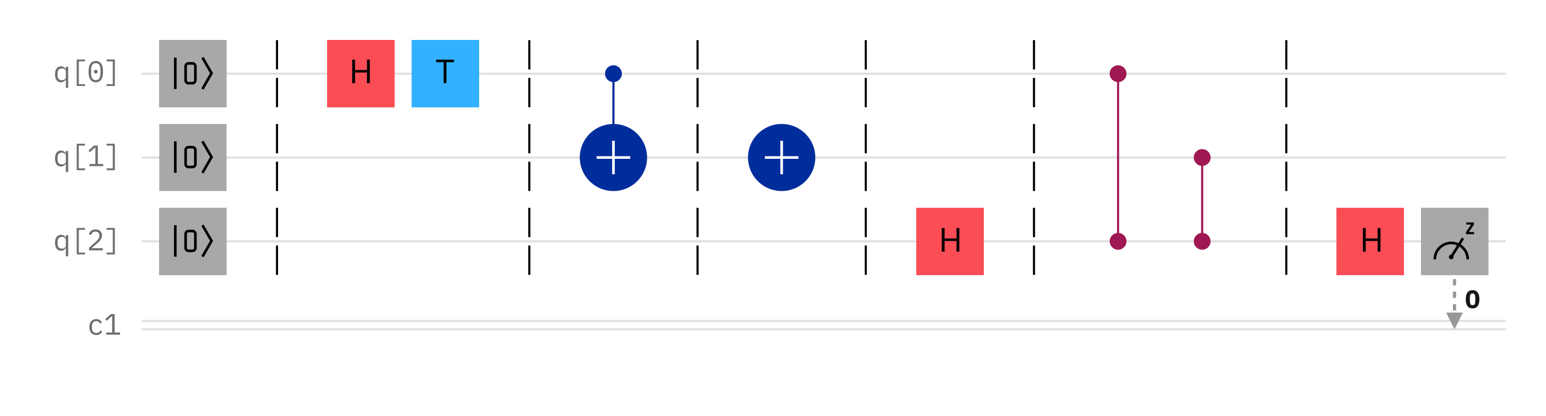
Quantum Error Correction

+ No-cloning theorem
+ Statevector collapse
+ Infinite number of mistakes
+ Incoherent state evolution (decoherence)
+ Bit-flip (X-error), Phase-flip (Z-error)
+ Example 1, Example 2, Example 3

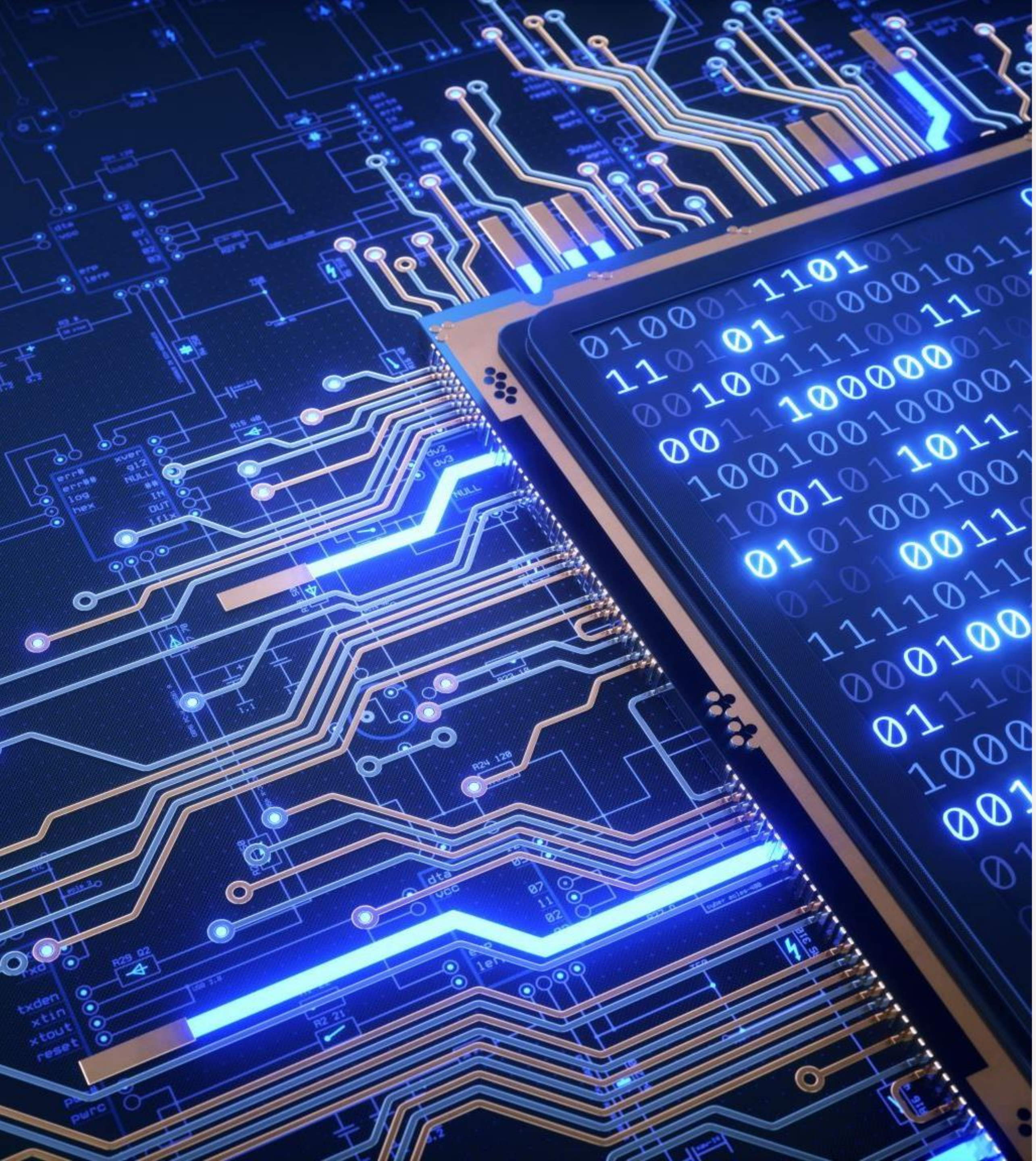
$$X|\psi\rangle = c_1 X|0\rangle + c_2 X|1\rangle \rightarrow c_1|1\rangle + c_2|0\rangle$$
$$Z|\psi\rangle = c_1 Z|0\rangle + c_2 Z|1\rangle \rightarrow c_1|0\rangle - c_2|1\rangle$$

- Error detection (location + type)
- Error correction
- Prevention of error propagation

Fault Tolerance



- So far assuming…
  - Coherent errors
  - Localized errors
- In reality…
  - Incoherent evolution of a state (interaction with outer environment)
  - Error can emerge everywhere
- Truly fault tolerant systems need many qubits and repeated stabilizer measurements

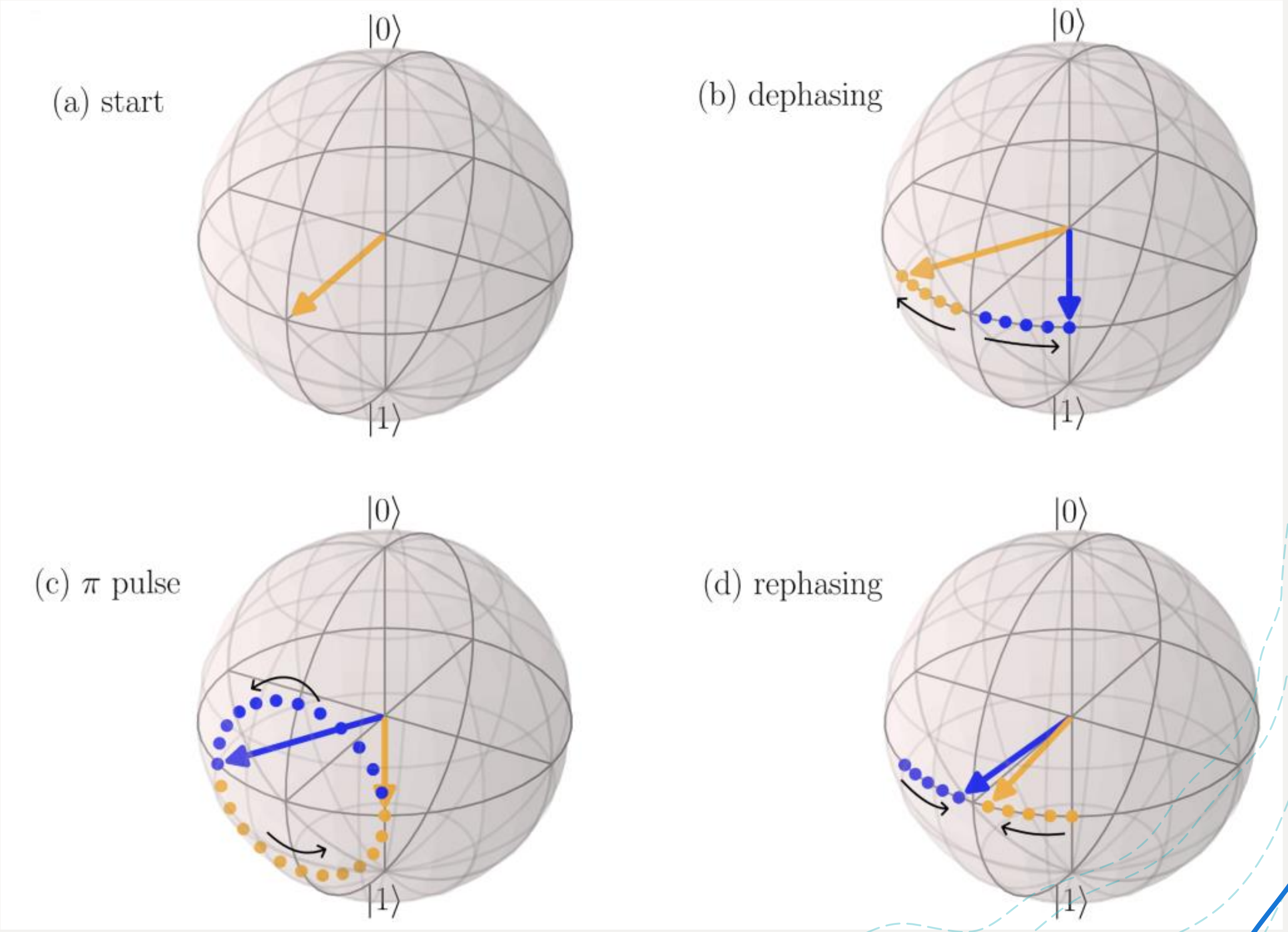


NISQ & Decoherence

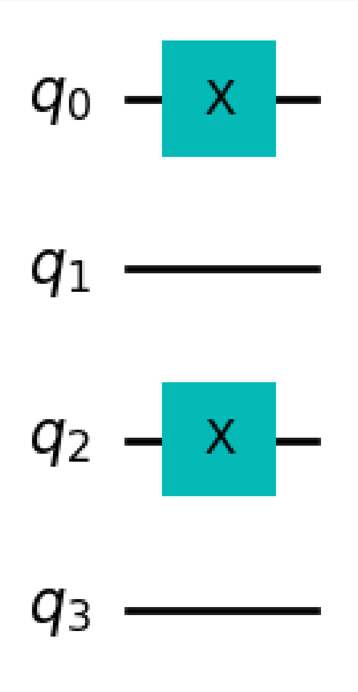
+ Quantum Error Suppression
+ Quantum Noise Mitigation
+ Noise-robust Optimization

Dynamical Decoupling

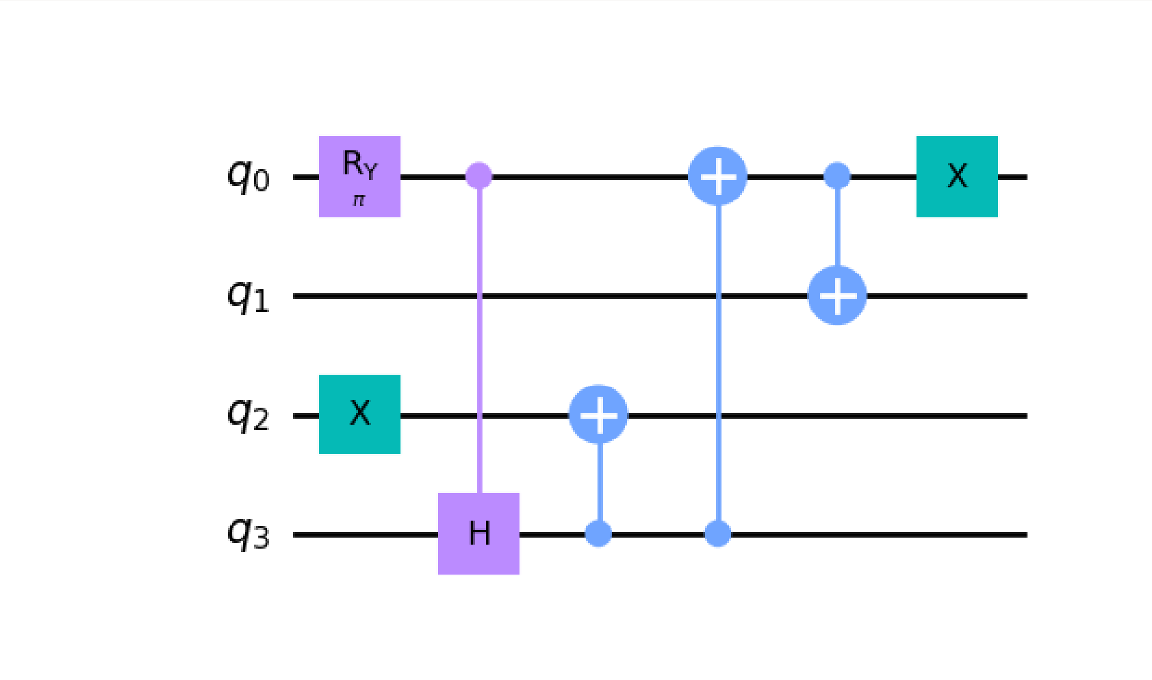
- Patological interactions can be also seen as state rotations
- Mitigation via rotations cancelling the decoherence out
- Commonly used with magnetic resonance imaging, etc.
- Spin-echo, CPGM, …, protocols
- Animation



Source: aws.amazon.com

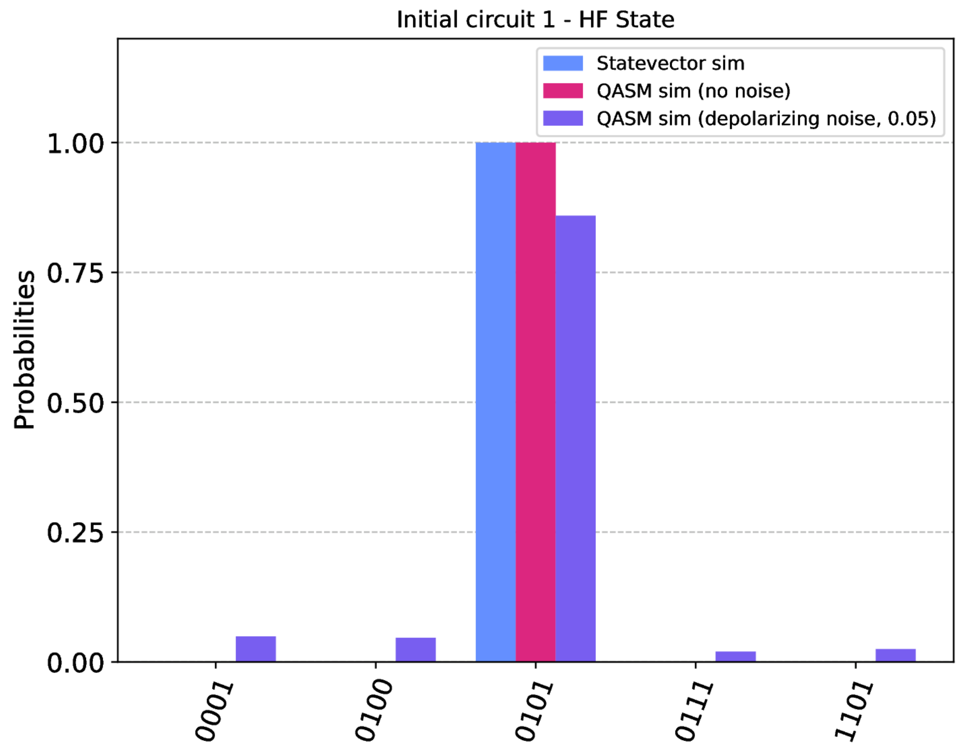


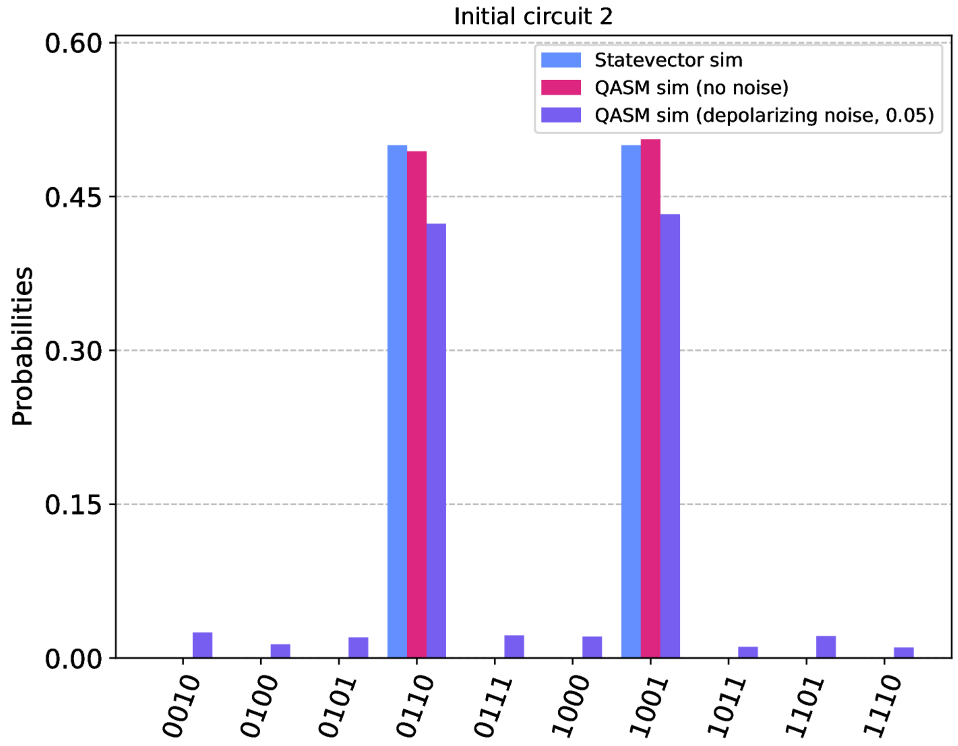
Initial circuit 1

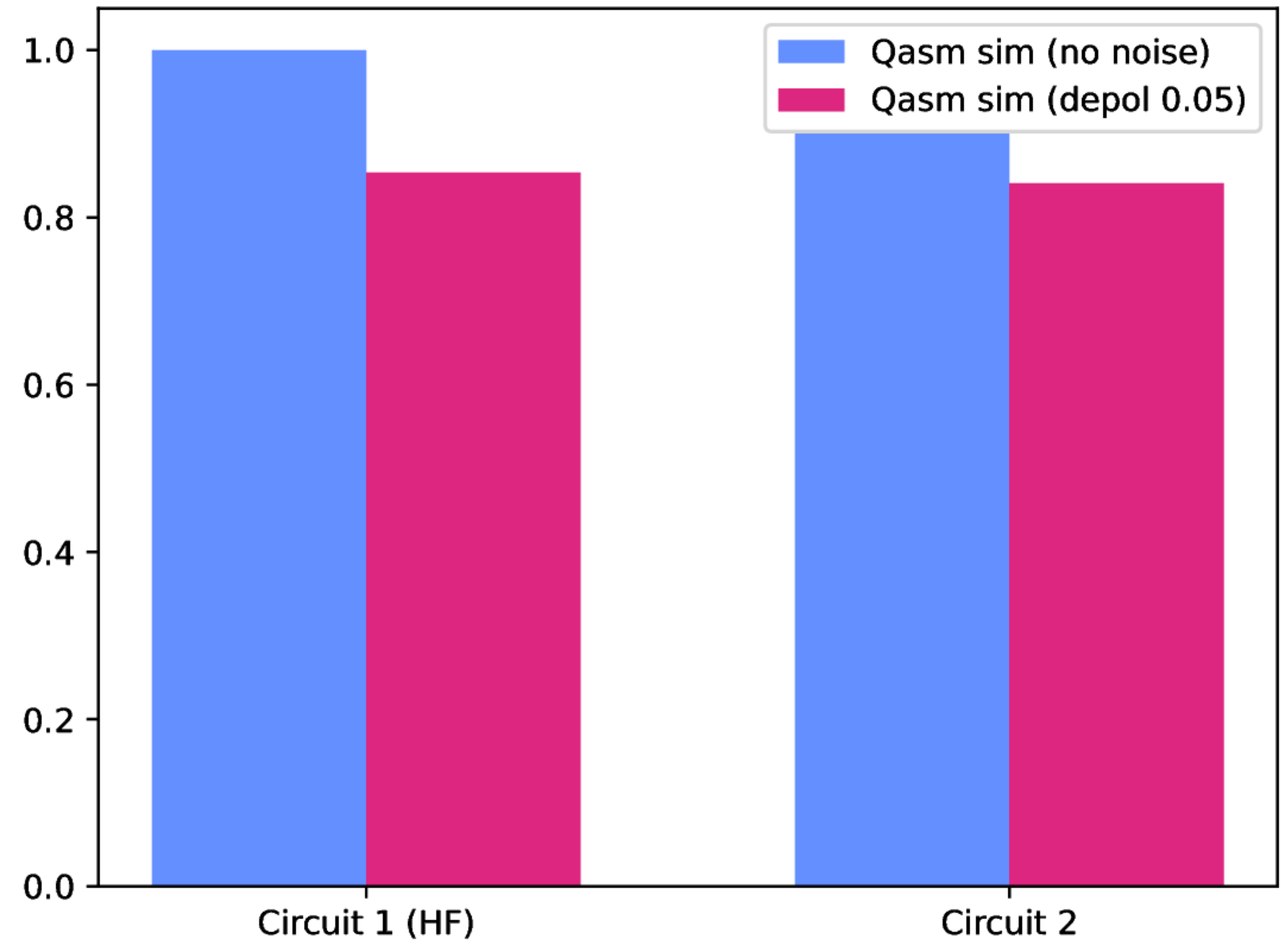


Initial circuit 2

Testing Circuits


Initial circuit 1 - HF State
Statevector sim
QASM sim (no noise)
QASM sim (depolarizing noise, 0.05)
Probabilities
1.00
0.75
0.50
0.25
0.00
0001
0100
0101
0111
1101

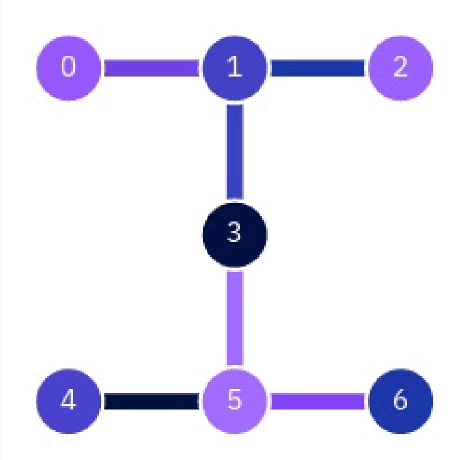

Initial circuit 2
Statevector sim
QASM sim (no noise)
QASM sim (depolarizing noise, 0.05)
Probabilities
0.60
0.45
0.30
0.15
0.00
0010
0100
0101
0110
0111
1000
1001
1011
1101
1110


1.0
0.8
0.6
0.4
0.2
0.0
Qasm sim (no noise)
Qasm sim (depol 0.05)
Circuit 1 (HF)
Circuit 2

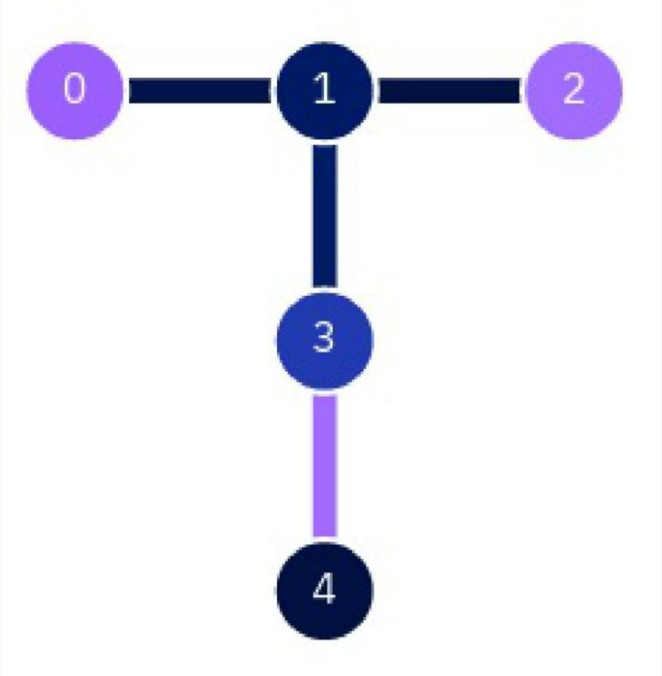
Real Machines

+ Quito (Falcon r4T)
+ Manila (Falcon r5.11L)
+ Nairobi (Falcon r5.11H)

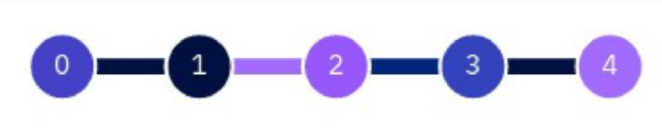
Nairobi

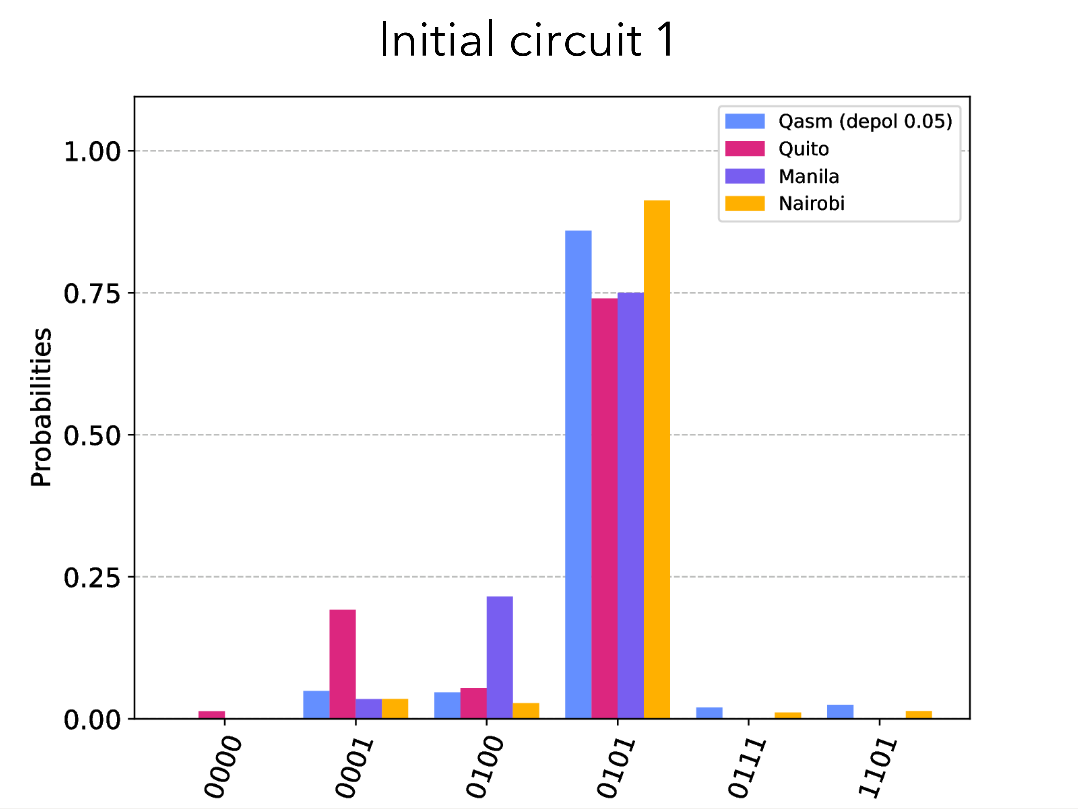


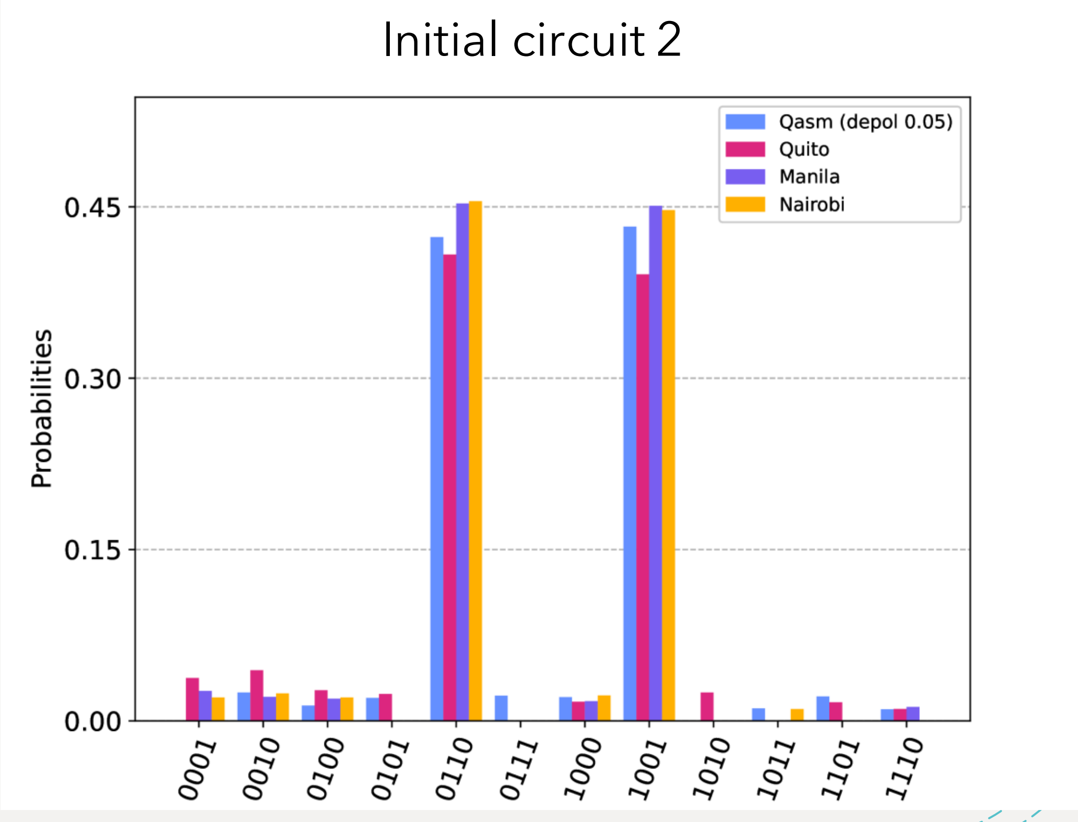
Quito



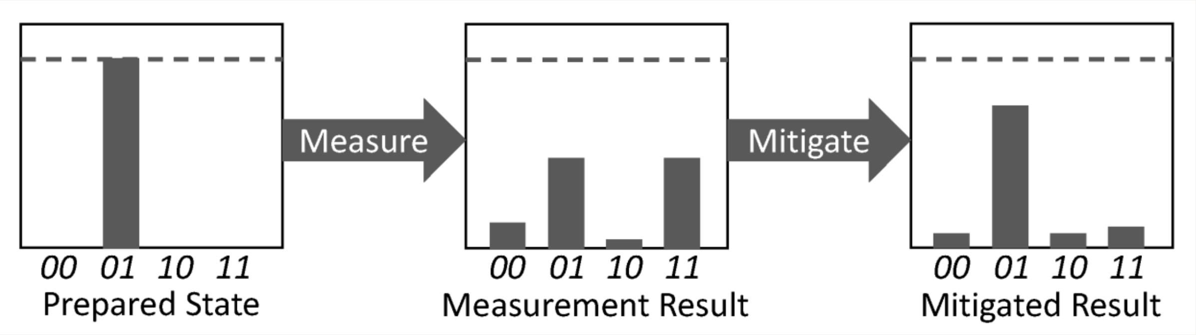
Manila




Initial circuit 1
Qasm (depol 0.05)
Quito
Manila
Nairobi
Probabilities
1.00
0.75
0.50
0.25
0.00
0000
0001
0100
0101
0111
1101

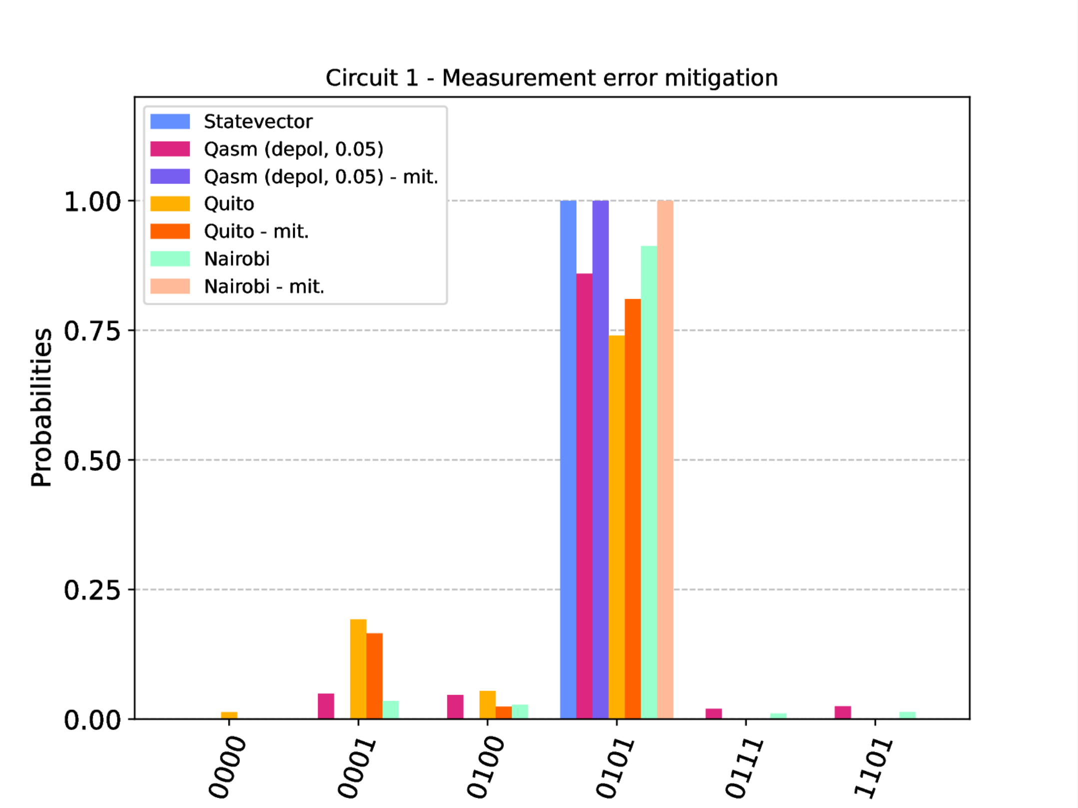

Initial circuit 2
Qasm (depol 0.05)
Quito
Manila
Nairobi
Probabilities
0.45
0.30
0.15
0.00
0001
0010
0100
0101
0110
0111
1000
1001
1010
1011
1101
1110

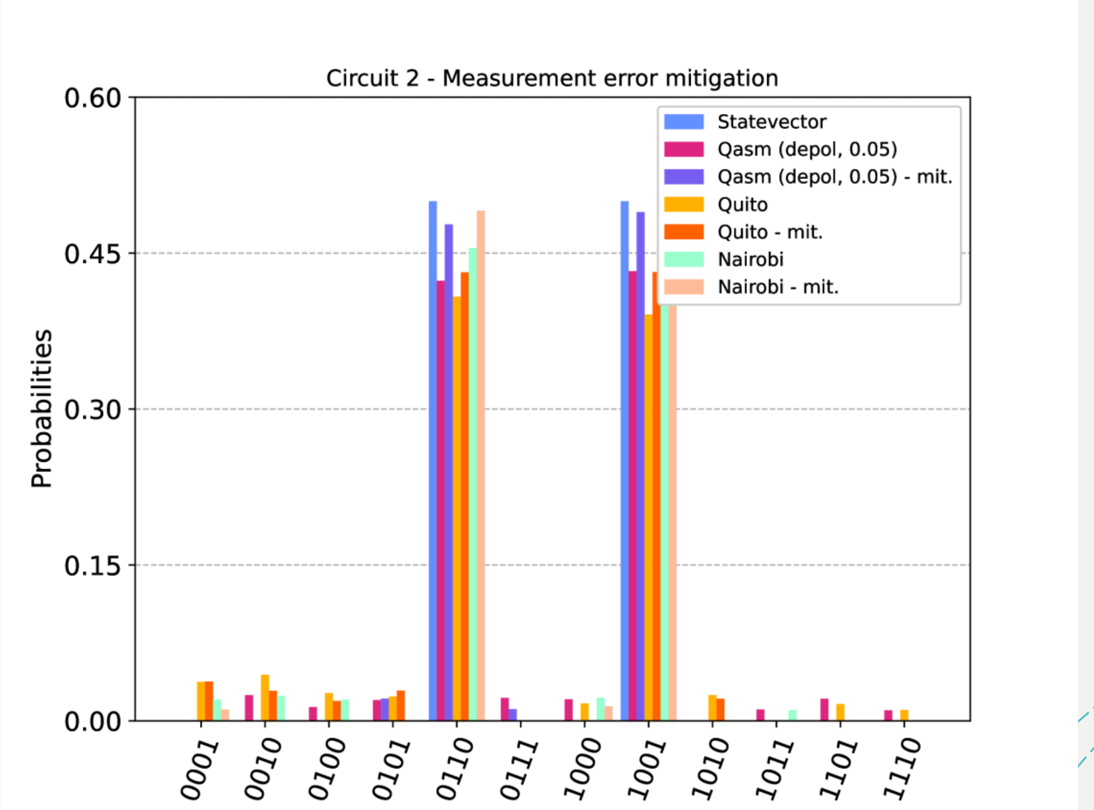
Measurement Error Mitigation



- Assumes, that errors emerge at the measurement only
- Describes errors w.r.t. measurements of initial states via *calibration matrix*
- Tries to mitigate the noise via inverse calibration matrix
  - Possible to use Moore-Penrose pseudoinv., Neumann series, ...

$$\begin{bmatrix} Pr(00|00) & Pr(00|01) & Pr(00|10) & Pr(00|11) \\ Pr(01|00) & Pr(01|01) & Pr(01|10) & Pr(01|11) \\ Pr(10|00) & Pr(10|01) & Pr(10|10) & Pr(10|11) \\ Pr(11|00) & Pr(11|01) & Pr(11|10) & Pr(11|11) \end{bmatrix}$$

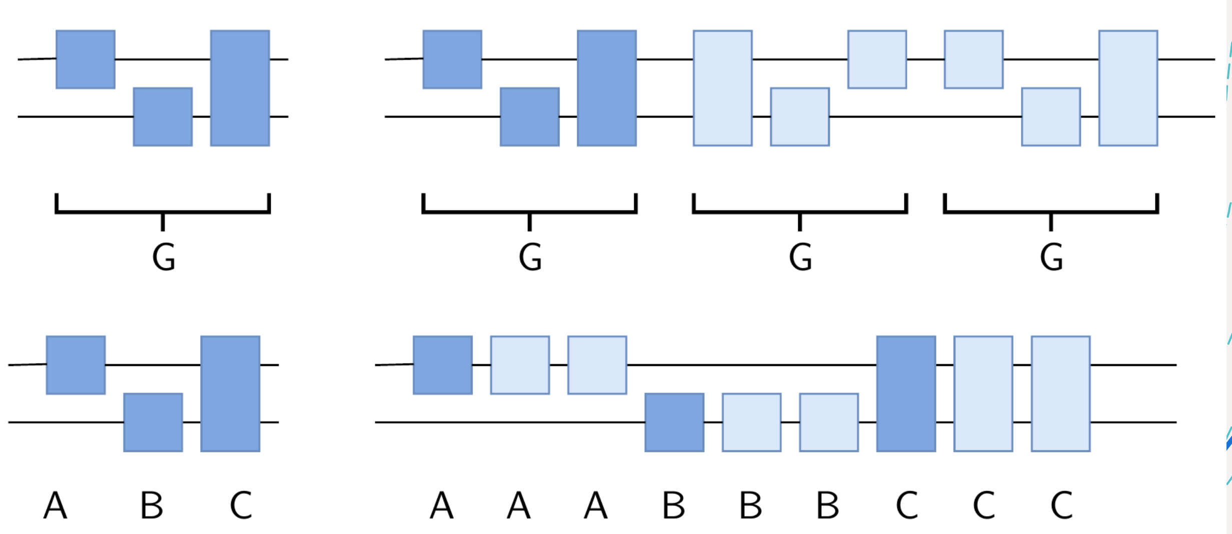

Circuit 1 - Measurement error mitigation
Statevector
Qasm (depol, 0.05)
Qasm (depol, 0.05) - mit.
Quito
Quito - mit.
Nairobi
Nairobi - mit.
Probabilities
1.00
0.75
0.50
0.25
0.00
0000
0001
0100
0101
0111
1101

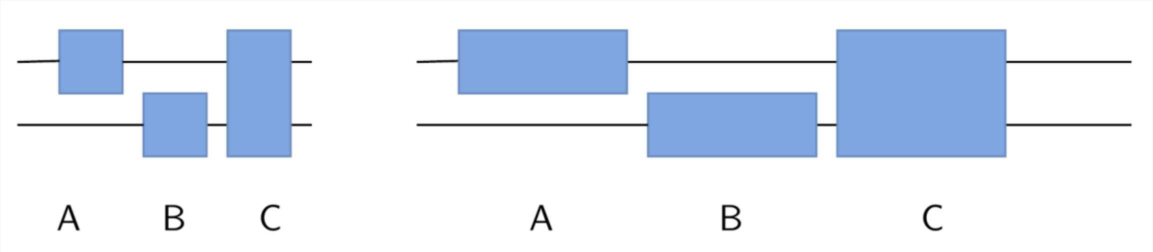

Circuit 2 - Measurement error mitigation
Statevector
Qasm (depol, 0.05)
Qasm (depol, 0.05) - mit.
Quito
Quito - mit.
Nairobi
Nairobi - mit.
Probabilities
0.60
0.45
0.30
0.15
0.00
0001
0010
0100
0101
0110
0111
1000
1001
1010
1011
1101
1110

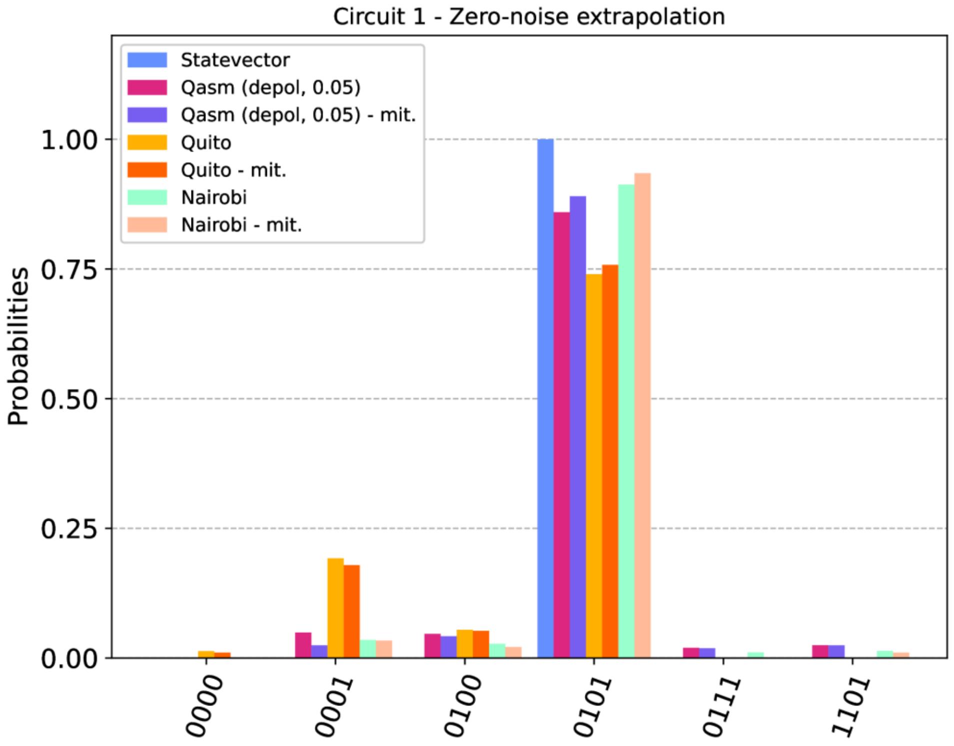
Zero-Noise Extrapolation

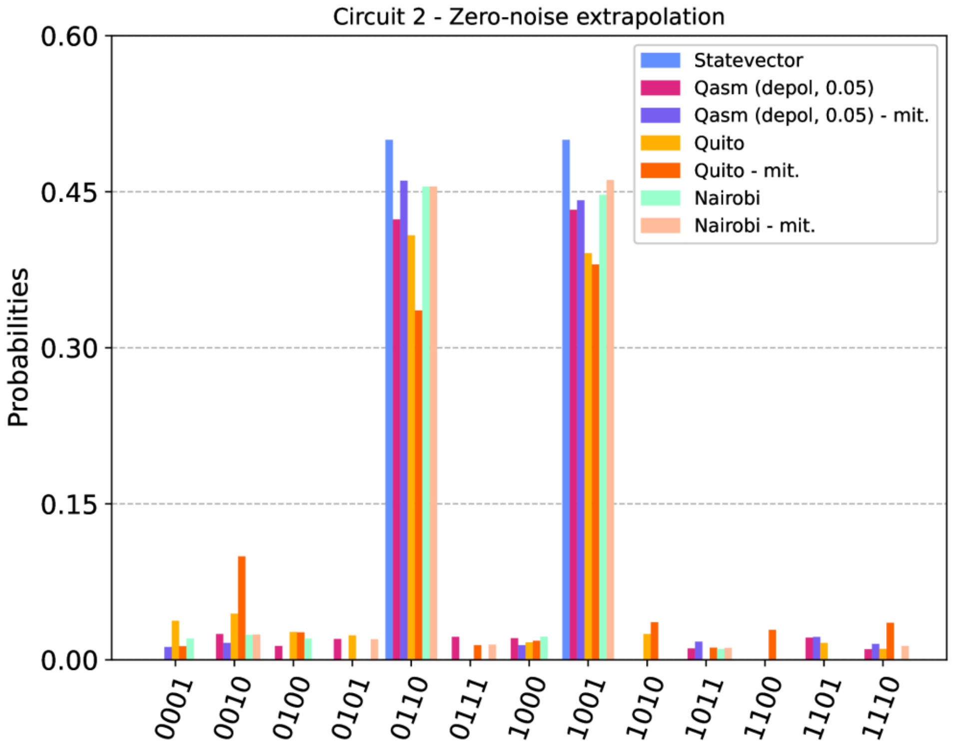
+ Extrapolates noiseless exp. value from a range with different values of noise
+ Noise is artificially increased in a systematic manner
  + Unitary folding
  + Pulse-stretching

$$G \to GG^{\dagger}G$$



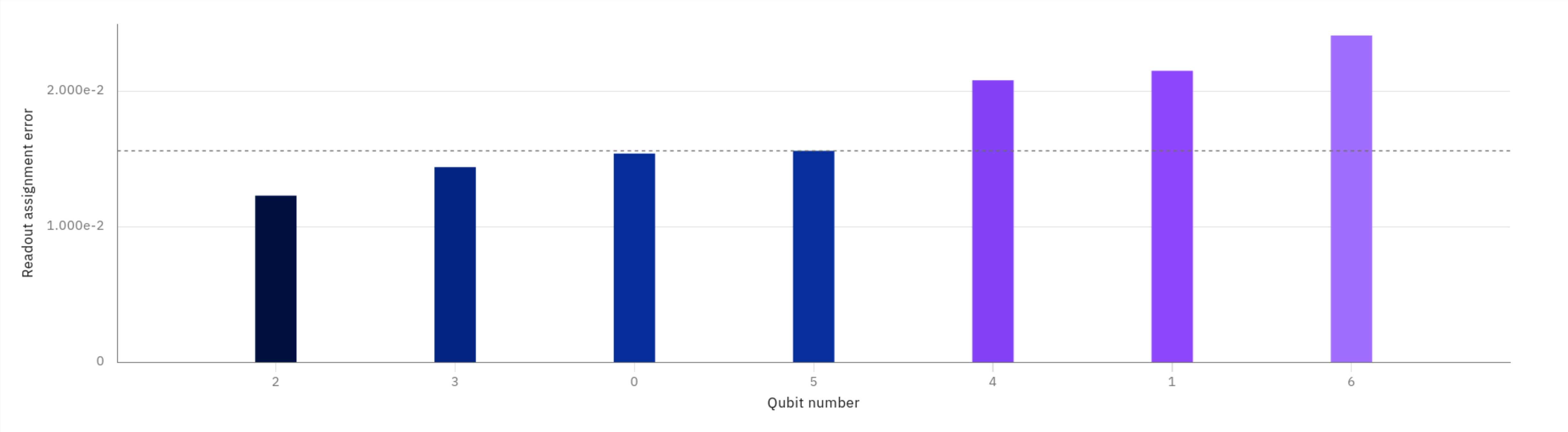


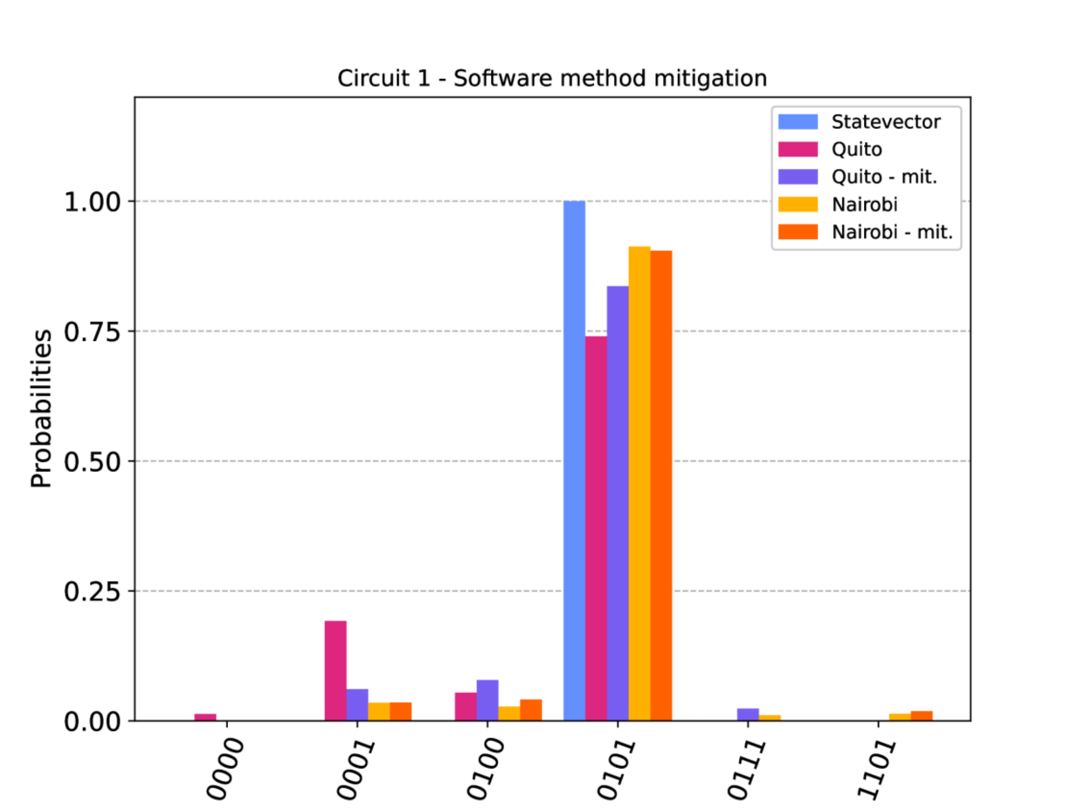

Circuit 1 - Zero-noise extrapolation
Statevector
Qasm (depol, 0.05)
Qasm (depol, 0.05) - mit.
Quito
Quito - mit.
Nairobi
Nairobi - mit.
Probabilities
1.00
0.75
0.50
0.25
0.00
0000
0001
0100
0101
0111
1101

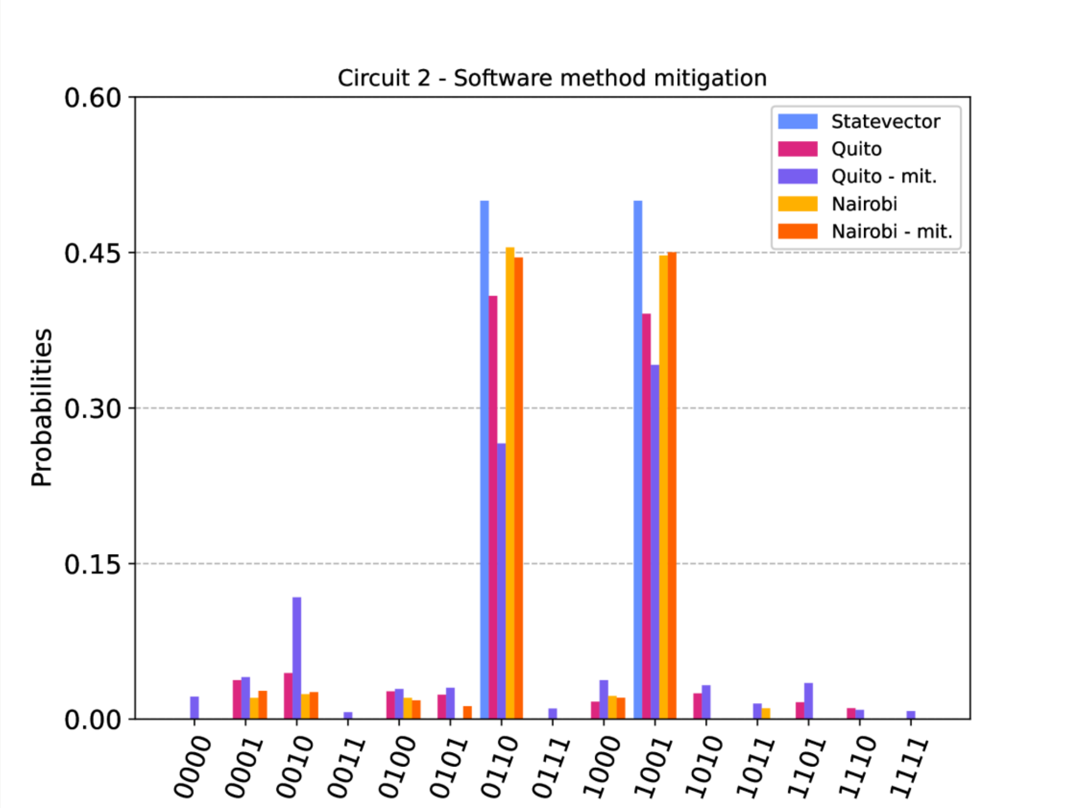

Circuit 2 - Zero-noise extrapolation
Statevector
Qasm (depol, 0.05)
Qasm (depol, 0.05) - mit.
Quito
Quito - mit.
Nairobi
Nairobi - mit.
Probabilities
0.60
0.45
0.30
0.15
0.00
0001
0010
0100
0101
0110
0111
1000
1001
1010
1011
1100
1101
1110

Software Method

- Intuitively close to thread-core binding (pinning)
- Mapping of virtual qubits to physical qubits
- Usually prioritizes diminishing of readout (measurement) or U3 (rotation) error




Circuit 1 - Software method mitigation
Statevector
Quito
Quito - mit.
Nairobi
Nairobi - mit.
Probabilities
1.00
0.75
0.50
0.25
0.00
0000
0001
0100
0101
0111
1101


Circuit 2 - Software method mitigation
Statevector
Quito
Quito - mit.
Nairobi
Nairobi - mit.
Probabilities
0.60
0.45
0.30
0.15
0.00
0000
0001
0010
0011
0100
0101
0110
0111
1000
1001
1010
1011
1101
1110
1111

TL; DL

Quantum Error Correction

- Too many qubits necessary

Quantum Error Suppression

- Requires detailed knowledge of the system
- Requires access to low-level computer control

Measurement Error Mitigation

- Works only for shallow circuits

Zero-Noise Extrapolation

- Introduces large runtime overhead

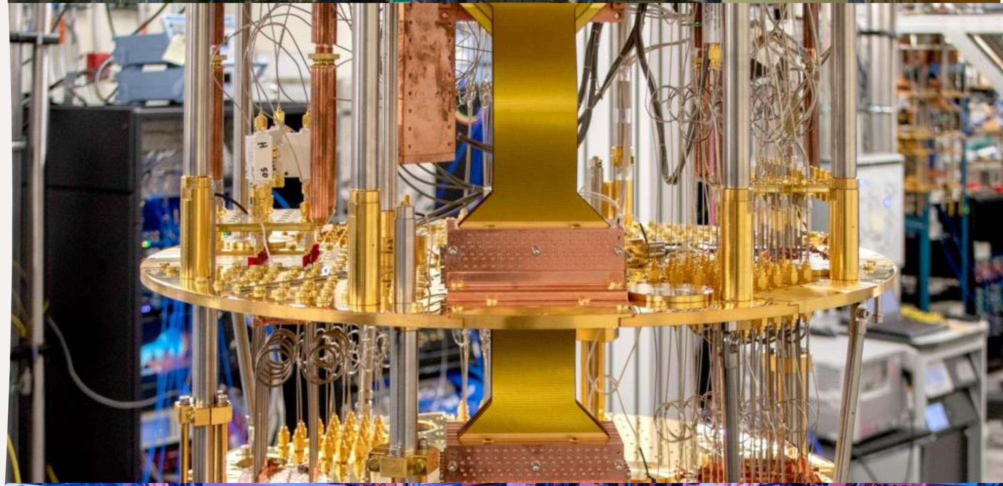
Software Method

- Requires careful analysis of the problem
- Sometimes can't be used efficiently, if mapping introduces another source of errors

Current Situation with QC & Future Outlook

- Still noisy
- No clear quantum advantage in
- Increasing number of qubits

- Probable usage as accelerators
- Hybrid quantum-classical algorithms (VQE, QAOA, …)



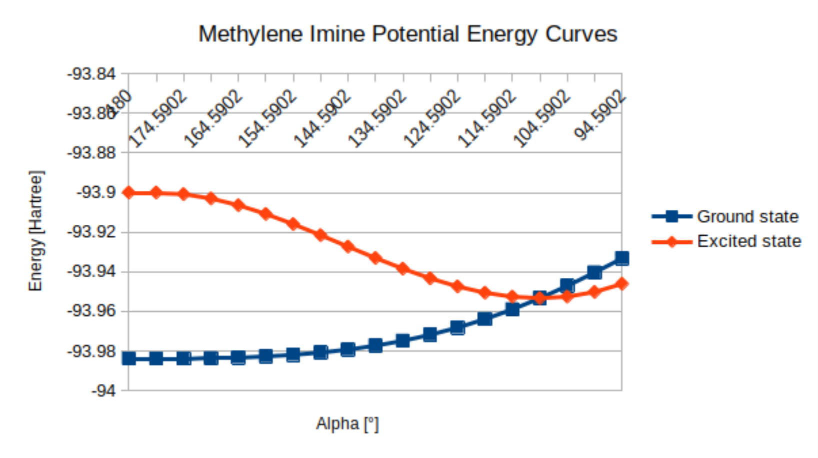
My Work

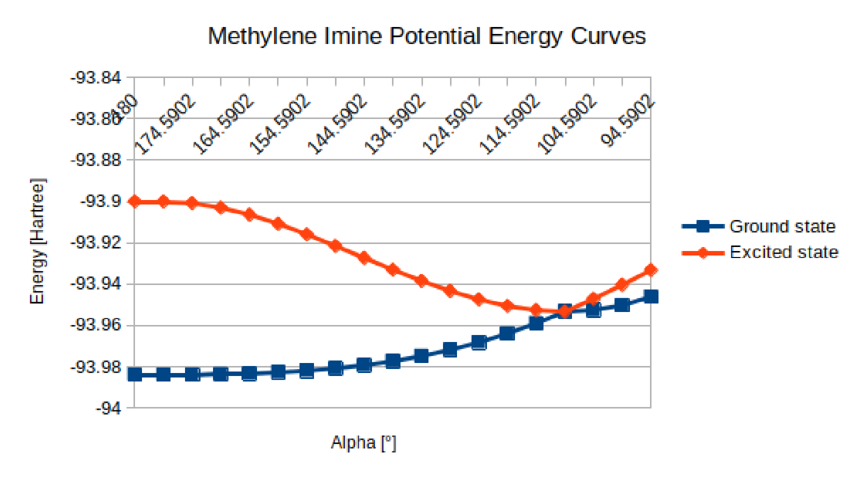
GitLab

- SA-OO-VQE method for Quantum Chemistry
- Ground & excited states
- Analytical gradients
- Non-adiabatic couplings
- Orbital diabatization
- **https://gitlab.com/MartinBeseda/sa-oo-vqe-qiskit.git**

S **SA-OO-VQE Qiskit**

main sa-oo-vqe-qiskit





Thank you for your attention!