國家實驗研究院
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Scalable Quantum Circuit Simulation with CUDA-Q

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About me

- 李泰岳博士 (Dr. Tai-Yue Li)
- 服務單位：國家高速網路與計算中心 (Since 2025/01~)
- 學歷：國立東華大學物理博士
- 專長：
  - X 光影像重建、稀疏視角影像重建
  - 機器學習、深度學習
  - 大規模量子計算、量子機器學習、張量網路

Position

The National Science and Technology Council (NSTC)

is the government ministry of the Republic of China (Taiwan) for the promotion and funding of **academic research**, development of science and technology and science parks.

The National Institutes of Applied Research (NIAR)

is the institution resulted from the combination of national laboratories into an independent nonprofit institute.

One of 7 national-level research laboratories under NARL

國家高速網路與計算中心

National Center for High-performance Computing

Founded In 1991

National Center for High-performance Computing (NCHC)

Taiwan's only national-level supercomputing center.
The NCHC possesses a large computing and networking platform facilities for use by domestic academia and the general public.

Position

新竹本部

台南分部

台中分部

• Milestones

1991
Taiwan's first National level supercomputer Center

2011
御風者 WINDRIDER
177 TF

2017
台灣杉一號
TAIWANIA 1
1.7 PF

2018
台灣杉二號
TAIWANIA 2
9 PF
AI-HPC
NV_V100*2016

2021
台灣杉三號
TAIWANIA 3
2.7 PF

2023
TAIDE Project
Trustworthy AI Dialogue Engine
3.8 PF
NV_ H100*9

2024
Forerunner 1
is expected to begin services
3.53 PF

2025-2029
Computing power plan
Target 480 PF

2003
NPO under NARLabs

2004
TWAREN Services 10G

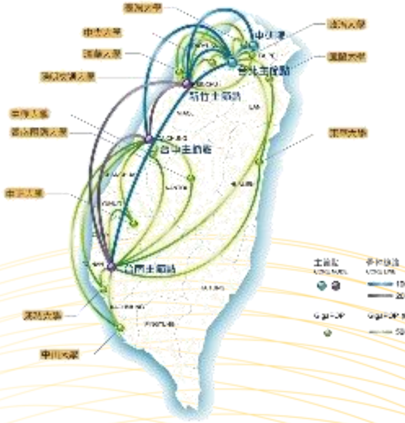
2016
100G Network Backbone

2021
Forward-looking Infrastructure Development Program
→ Start building self-build fiber backbone (phase1)

2022
*information security level A
*Formosa Open Internet Exchange activated

2023
self-build fiber backbone (phase1) activated

2025
NCHC IDC (Tainan)
scheduled for opening



• Computing Power Plan

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2024-2028

Taiwan CHIP-BASED Industrial Innovation Program

To support the Taiwan Chip-based Industrial Innovation Program, NCHC will develop a shared heterogeneous architecture supercomputer for general-purpose AI (GPU), large-scale scientific research (CPU), and future quantum computing. We aim to create a user-friendly cloud service platform to improve application efficiency.

2024 — 16 PF GPU
- 400+ GPUs
- 10 PB storage
- InfiniBand 200Gbps
- PUE <1.35

2025 — 100 PF GPU
- 1680+ GPUs
- 25 PB storage
- InfiniBand 200Gbps
- PUE <1.3

2026 — 80 PF GPU+CPU
- 1200+ GPUs
- 20 PB storage
- InfiniBand 400Gbps
- PUE <1.27

Total 200 PF

2027 — 35 PF GPU+CPU
- 520+ GPUs
- 10 PB storage
- InfiniBand 400Gbps
- PUE <1.25

2027 — 60 PF GPU+CPU
- 1000+ GPUs
- 15 PB storage
- InfiniBand 400Gbps
- PUE <1.25

2028 — 49 PF GPU+CPU+Quantum
- 700+ GPUs
- 10 PB storage
- InfiniBand 800Gbps
- PUE <1.25

Total 280 PF

2028 — 75 PF GPU+CPU
- 1260+ GPUs
- 25 PB storage
- InfiniBand 800Gbps
- PUE <1.25

2029 — 65 PF GPU+CPU
- 1020+ GPUs
- 20 PB storage
- InfiniBand 800Gbps
- PUE <1.25

2027-2029

"New Silicon Valley" in southern Taiwan Project

The National Science and Technology Council announced the launch of a new national program in August 2024, planning to invest in the development of Taiwan's own artificial intelligence platform over the next five years to promote the smart technology industry ecosystem in southern Taiwan. The plan will establish 200 PF of computing power and increase the nation's overall computing power to 480 PF.

National Quantum Team in Taiwan

Phase1	2022~2026	$250M
Phase2	2026~2030	TBD

Primary Missions

- Constructing quantum computing systems with practical problem-solving capabilities.
- Developing reliable quantum communication systems.
- Cultivating quantum talent and fostering industrial applications.

Taiwan Quantum Program office

Hardware Technology for Universal Quantum Computer

Photonic Quantum Technology

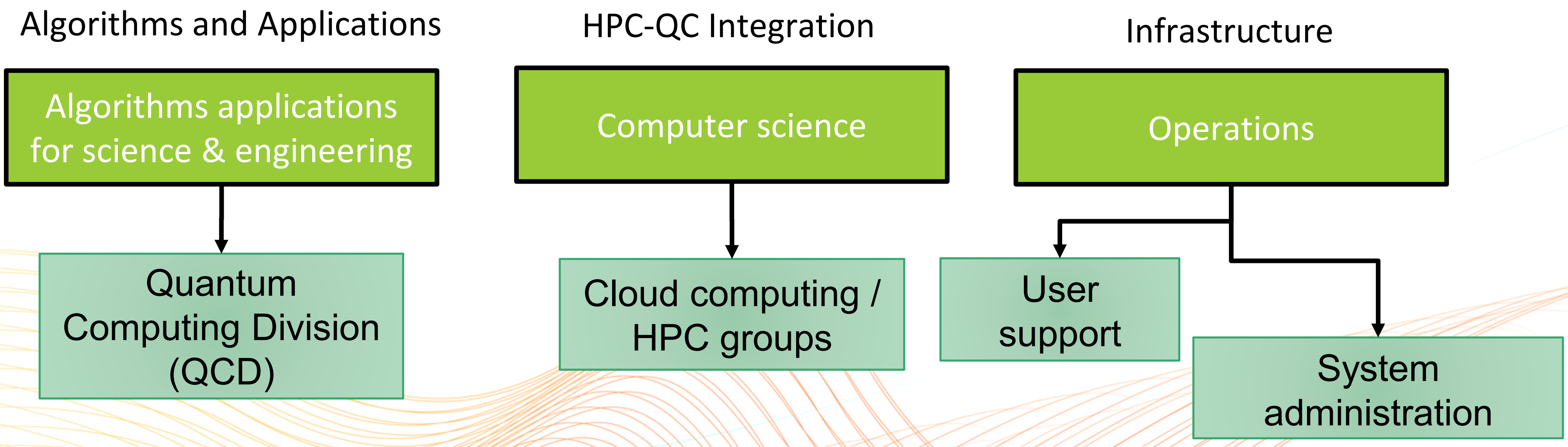
Quantum Software Technology and Application

Planning Project for the Testbed of the Quantum Computing Subsystems

Quantum Simulator / QC-HPC

Quantum computing in NCHC (planning)

- 負責量子電腦主機的建置，於台灣本土提供量子計算的服務；
- 整合既有HPC資源，提供量子與HPC運算的整合服務；
- 培育新一代量子+HPC計算人才；
- 促進量子計算應用於各種科學研究領域。



Now

Future

Applications

- Open Quantum System
- Optimization
- Quantum Chemistry
- Quantum Machine Learning

Algorithms

- HHL algorithm
- Quantum Fourier Transform
- Error Suppression
- Error Mitigation
- Error Correction

QC-HPC integration

- Scheduler HPC queue QC queue
- Resource Management
- Compiler / Programming Model
- Software Environment
- Benchmark
- Web Portal

QC Hardware

- Commercial QC (On site)
- Self-Developed QC (Remote)
- Quantum Simulator
- Quantum Emulator
- Quantum Network

Quantum Computing /Computer Introduction

Gate-based QC vs Annealing-based QC

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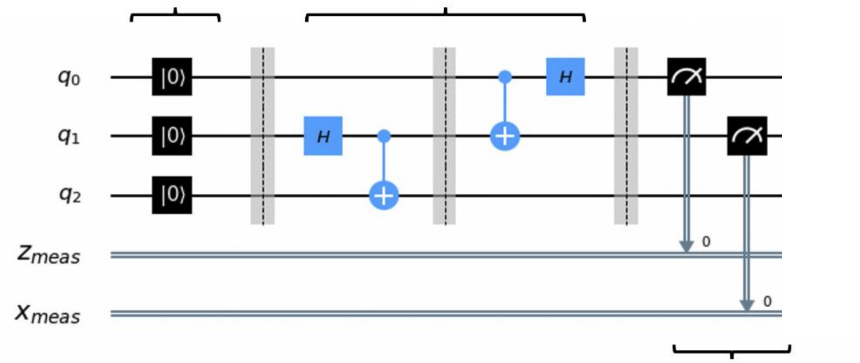
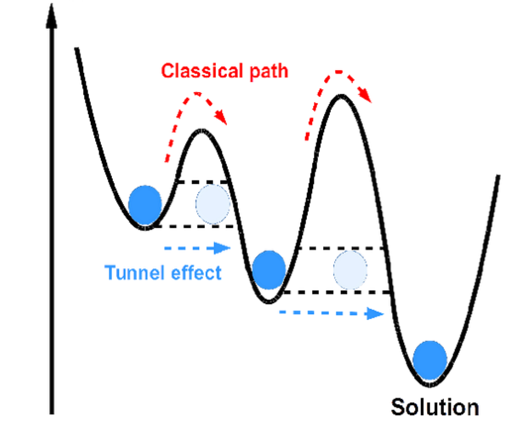
Gate-based

Quantum algorithm



Annealing-based

QUBO form



Quantum Tunnelling

Gate-based QC vs Annealing-based QC

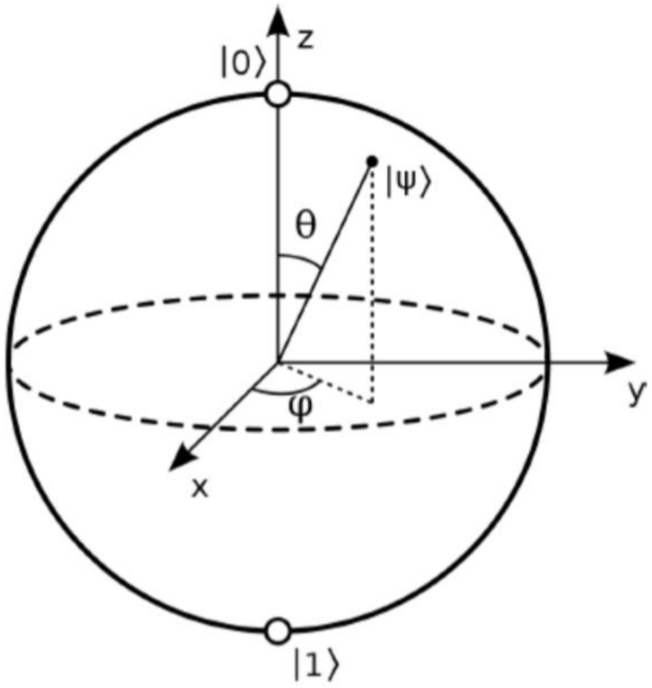
Feature	Gate-Based Method	Annealing-Based Method
Universality	Universal: can implement a wide range of quantum algorithms	Specialized: designed primarily for optimization problems
Algorithm Flexibility	Supports arbitrary quantum circuits (e.g., Shor's, Grover's)	Limited to problems mapped to QUBO/Ising models
Hardware Requirements	Demands precise control and low-noise conditions fewer qubits (~100 qubits)	Can scale to thousands of qubits with simpler control mechanisms D-wave (~5640 qubits)
Robustness to Noise	Highly sensitive to decoherence; requires complex error correction	More robust in its adiabatic evolution against certain noise types
Result Accuracy	Capable of yielding exact results with error correction	Provides approximate, probabilistic solutions

Superposition

Bit

Qubit

(Bloch Sphere)



0

0	1

1	0	1

$$c_0|0\rangle + c_1|1\rangle = \begin{bmatrix} c_0 \\ c_1 \end{bmatrix}$$

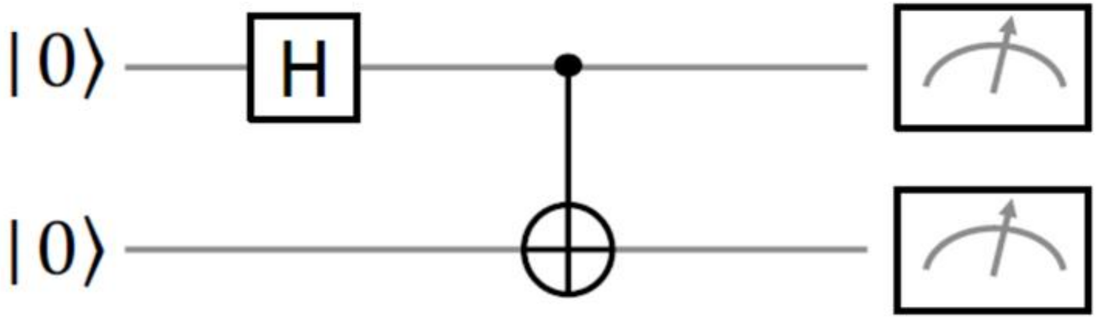
$$c_{00}|00\rangle + c_{01}|01\rangle + c_{10}|10\rangle + c_{11}|11\rangle = \begin{bmatrix} c_{00} \\ c_{01} \\ c_{10} \\ c_{11} \end{bmatrix}$$

$$\begin{aligned} & c_{000}|000\rangle + c_{001}|001\rangle + c_{010}|010\rangle + c_{011}|011\rangle + \\ & c_{100}|100\rangle + c_{101}|101\rangle + c_{110}|110\rangle + c_{111}|111\rangle \end{aligned} = \begin{bmatrix} c_{000} \\ c_{001} \\ c_{010} \\ c_{011} \\ c_{100} \\ c_{101} \\ c_{110} \\ c_{111} \end{bmatrix}$$

Entanglement

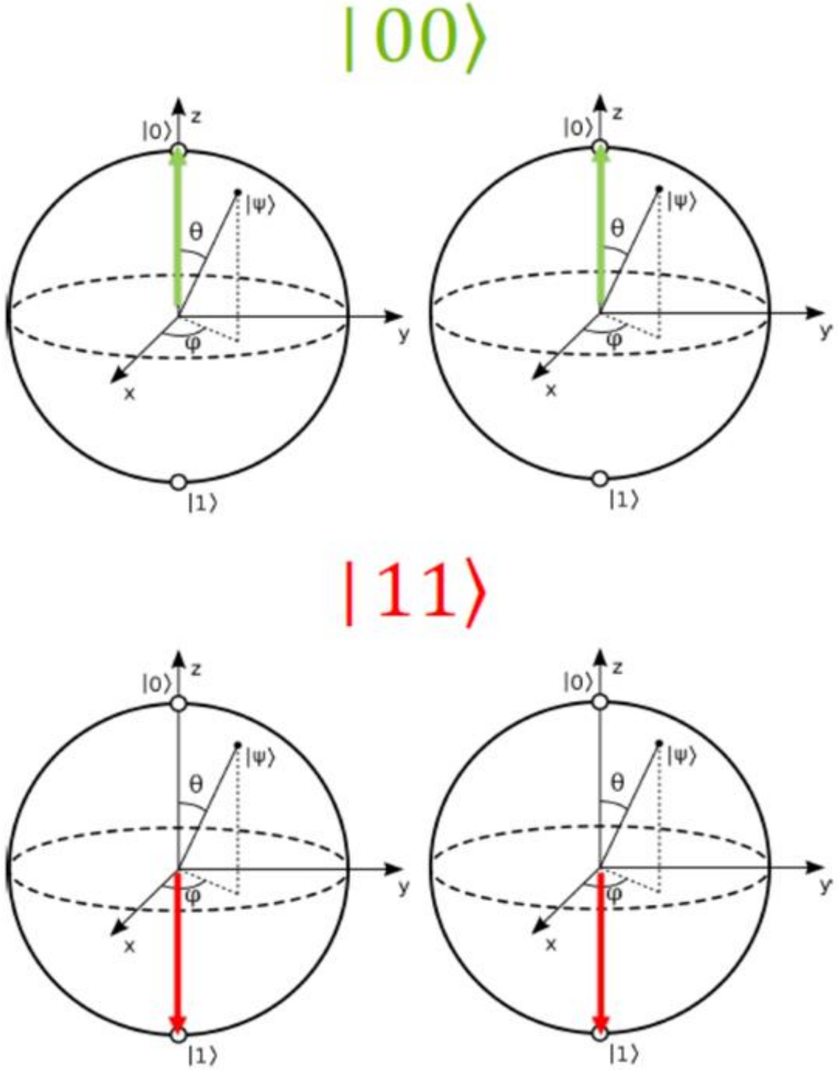
Hadamard Gate:
$\text{Had}|0\rangle = |0\rangle + |1\rangle$
$\text{Had}|1\rangle = |0\rangle - |1\rangle$

CNOT Gate:
$\text{CNOT}|10\rangle = |11\rangle$
$\text{CNOT}|11\rangle = |10\rangle$



$$|00\rangle \rightarrow |00\rangle + |11\rangle$$

(Bell state)



Single Qubit

二進制：$|0\rangle$、$|1\rangle$

十進制：$|0\rangle$、$|1\rangle$

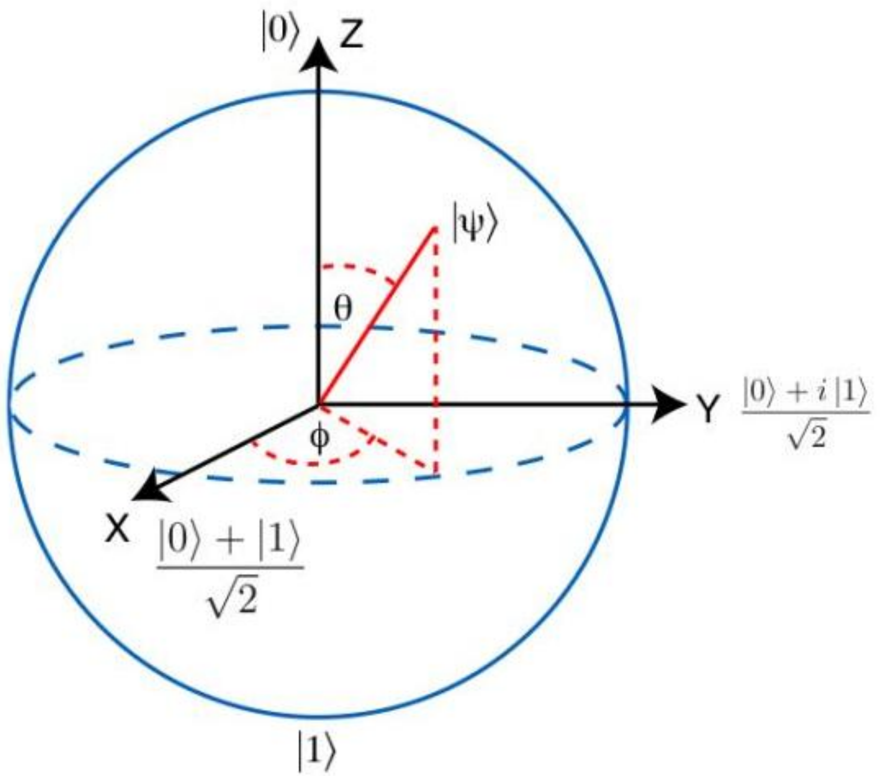
$$|0\rangle = \begin{pmatrix}1\\0\end{pmatrix}, |1\rangle = \begin{pmatrix}0\\1\end{pmatrix}$$

X軸：$\dfrac{|0\rangle + |1\rangle}{\sqrt{2}} = \dfrac{1}{\sqrt{2}}\begin{pmatrix}1\\0\end{pmatrix} + \dfrac{1}{\sqrt{2}}\begin{pmatrix}0\\1\end{pmatrix} = \dfrac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}$

Y軸：$\dfrac{|0\rangle + i|1\rangle}{\sqrt{2}} = \dfrac{1}{\sqrt{2}}\begin{pmatrix}1\\0\end{pmatrix} + \dfrac{i}{\sqrt{2}}\begin{pmatrix}0\\1\end{pmatrix} = \dfrac{1}{\sqrt{2}}\begin{pmatrix}1\\i\end{pmatrix}$

Z軸：$|0\rangle = \begin{pmatrix}1\\0\end{pmatrix}$

Bloch sphere

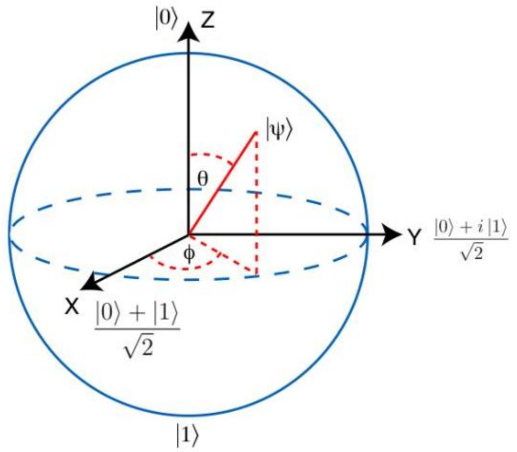


Two Qubits

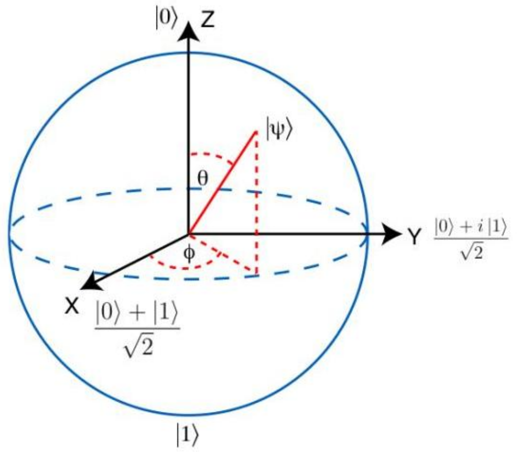
二進制：$|00\rangle$、$|01\rangle$、$|10\rangle$、$|11\rangle$
十進制：$|0\rangle$、$|1\rangle$、$|2\rangle$、$|3\rangle$

$$|00\rangle = \begin{pmatrix}1\\0\\0\\0\end{pmatrix}、|01\rangle = \begin{pmatrix}0\\1\\0\\0\end{pmatrix}、|10\rangle = \begin{pmatrix}0\\0\\1\\0\end{pmatrix}、|11\rangle = \begin{pmatrix}0\\0\\0\\1\end{pmatrix}$$

Bloch sphere



Bloch sphere



N Qubits

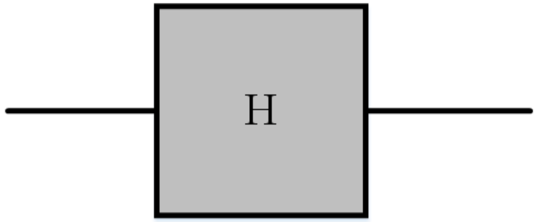
二進制：$|00\ldots00\rangle$、$|00\ldots01\rangle$、$|00\ldots10\rangle$、$|11\ldots11\rangle$
十進制：$|0\rangle$、$|1\rangle$、$|2\rangle$、$|3\rangle$、…、$|2^n-1\rangle$

$$|00\ldots00\rangle=\begin{pmatrix}1\\0\\0\\\vdots\\0\end{pmatrix}、|00\ldots01\rangle=\begin{pmatrix}0\\1\\0\\\vdots\\0\end{pmatrix}、|00\ldots10\rangle=\begin{pmatrix}0\\0\\1\\\vdots\\0\end{pmatrix}、|11\ldots11\rangle=\begin{pmatrix}0\\0\\0\\\vdots\\1\end{pmatrix}$$

Single Qubit Gate

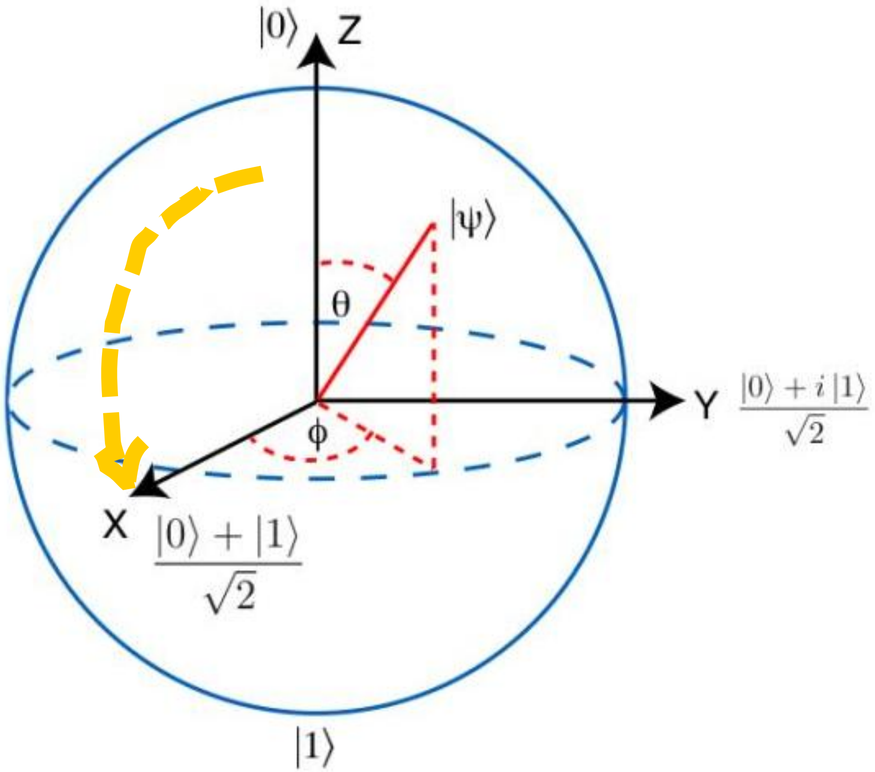
Hadamard Gate

$$H = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$



Input	Output
|0>	$(\|0> + \|1>)/\sqrt{2}$
|1>	$(\|0> - \|1>)\ /\sqrt{2}$

Bloch sphere



Single Qubit Gate

S Gate

$$S = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}$$

$\mathbf{S}^{\dagger}$ Gate

$$S^{\dagger} = \begin{pmatrix} 1 & 0 \\ 0 & -i \end{pmatrix}$$

T Gate

$$T = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{pmatrix}$$

$T^{\dagger}$ Gate

$$T^{\dagger} = \begin{pmatrix} 1 & 0 \\ 0 & e^{-i\pi/4} \end{pmatrix}$$

U_2 Gate

$$U_2(\varphi, \lambda) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -e^{i\lambda} \\ e^{i\varphi} & e^{i(\lambda+\varphi)} \end{pmatrix}$$

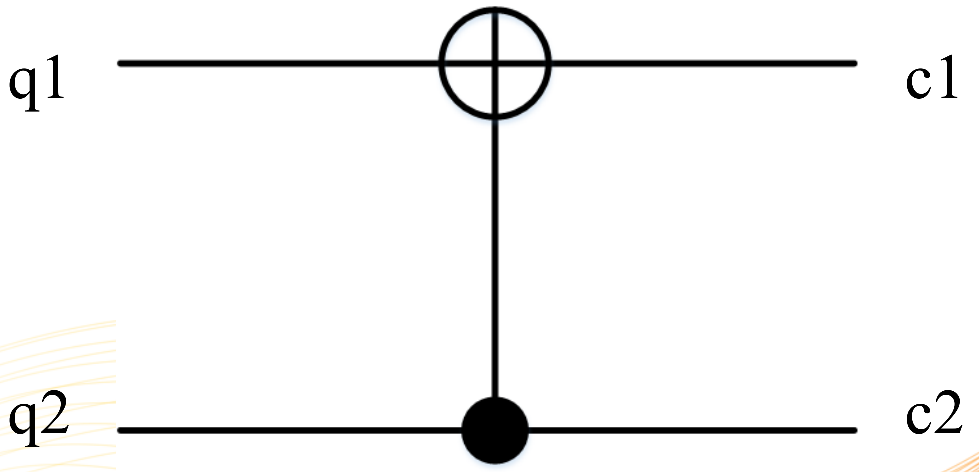
U_3 Gate

$$U_3(\theta, \varphi, \lambda) \\ = \begin{pmatrix} cos(\theta/2) & -e^{i\lambda} sin(\theta/2) \\ e^{i\varphi} sin(\theta/2) & e^{i(\lambda+\varphi)} cos(\theta/2) \end{pmatrix}$$

Two Qubits Gate

CNOT Gate

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

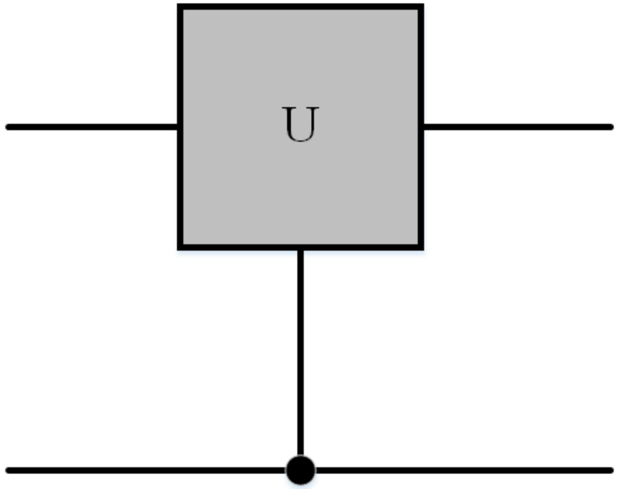


q2	q1	c2	c1
|0>	|0>	|0>	|0>
|0>	|1>	|0>	|1>
|1>	|0>	|1>	|1>
|1>	|1>	|1>	|0>

Two Qubits Gate

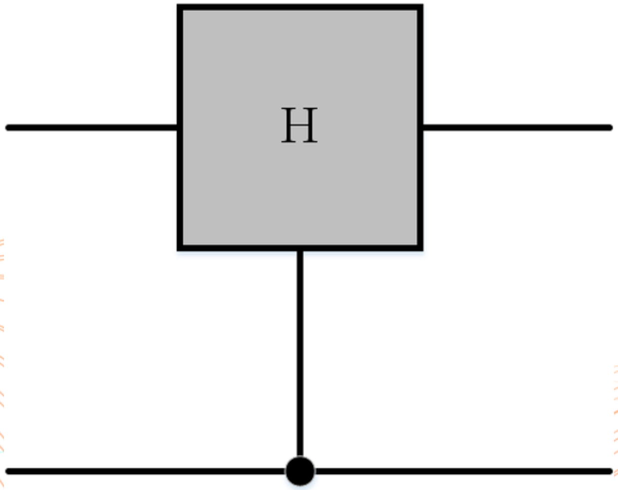
CU Gate

$$CU = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & u_{11} & u_{12} \\ 0 & 0 & u_{21} & u_{22} \end{pmatrix}$$



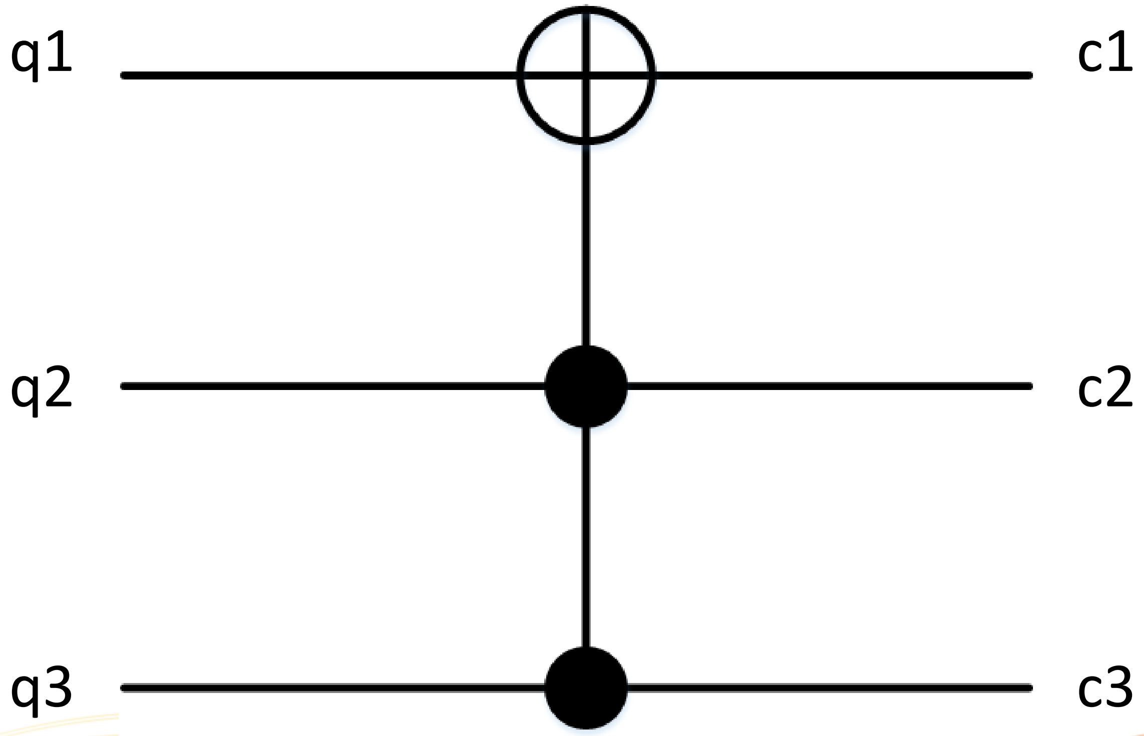
CH Gate

$$CH = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 0 & 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix}$$



Three Qubits Gate

CCNOT Gate

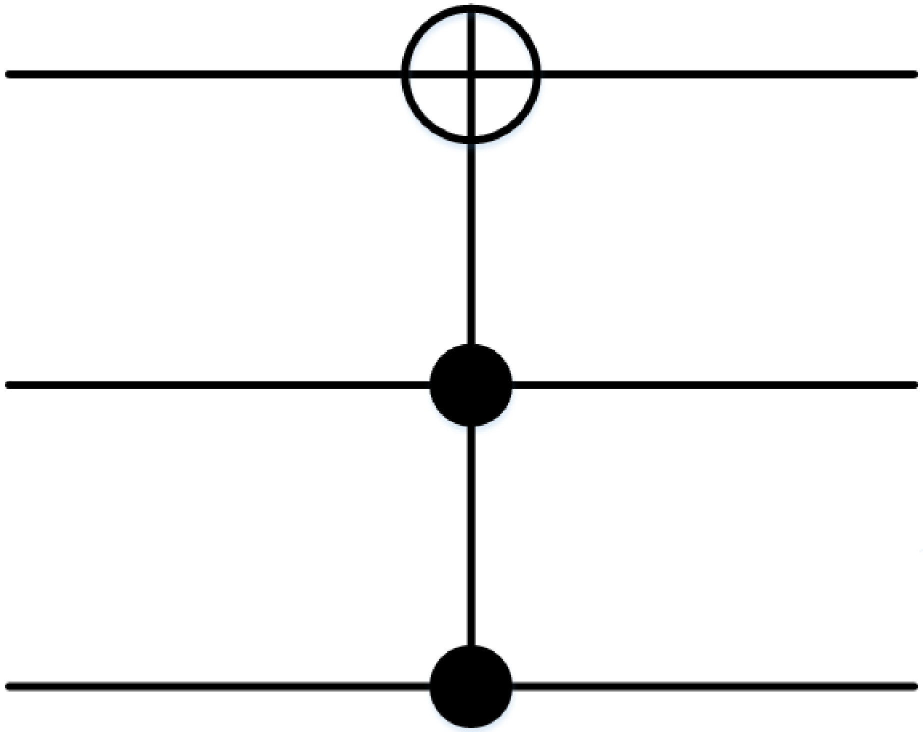


q3	q2	q1	c3	c2	c1
|0>	|0>	|0>	|0>	|0>	|0>
|0>	|0>	|1>	|0>	|0>	|1>
|0>	|1>	|0>	|0>	|1>	|0>
|0>	|1>	|1>	|0>	|1>	|1>
|1>	|0>	|0>	|1>	|0>	|0>
|1>	|0>	|1>	|1>	|0>	|1>
|1>	|1>	|0>	|1>	|1>	|1>
|1>	|1>	|1>	|1>	|1>	|0>

Three Qubits Gate

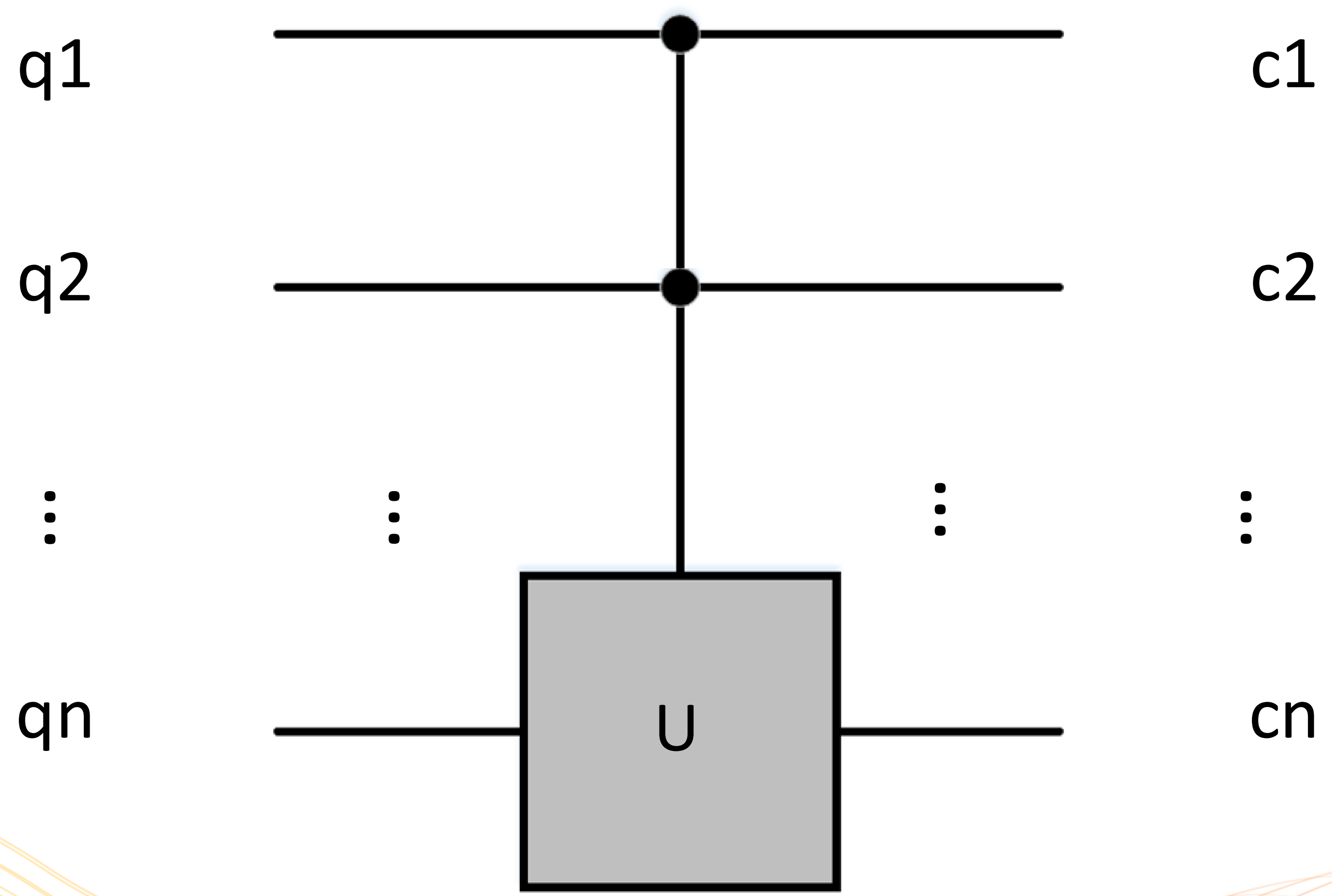
CCNOT Gate

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



N Qubits Gate

<u>**NCU Gate**</u>



Quantum Circuit

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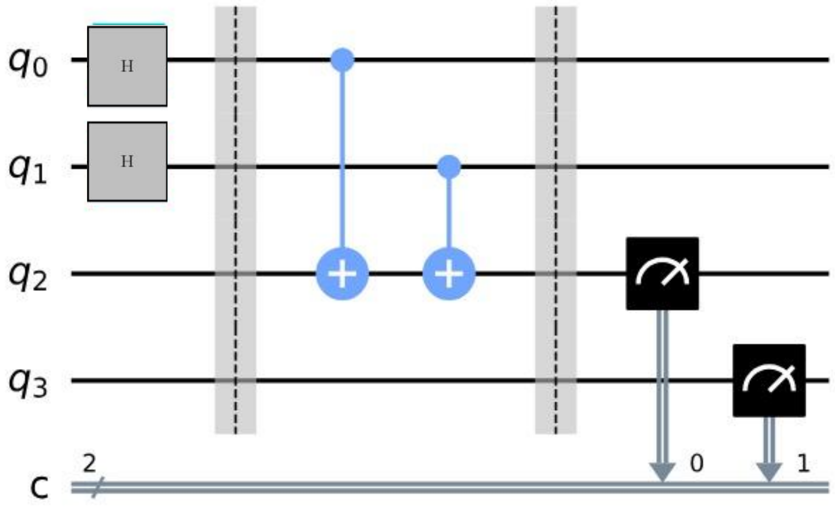
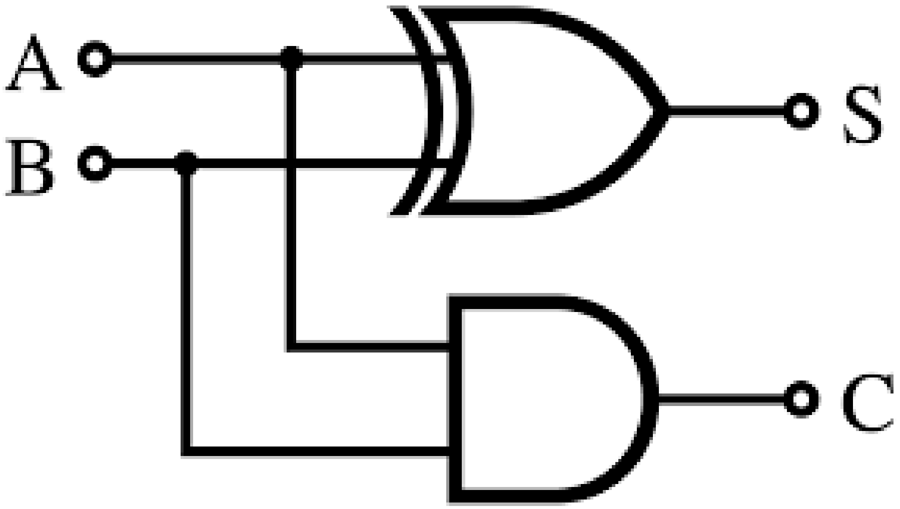
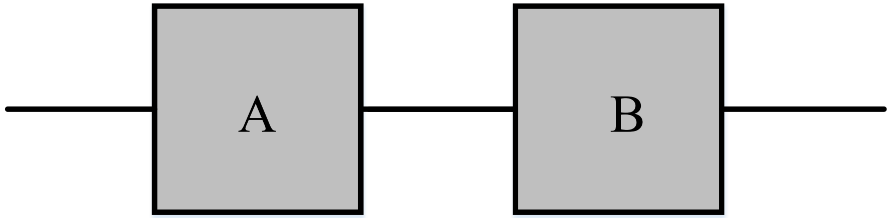


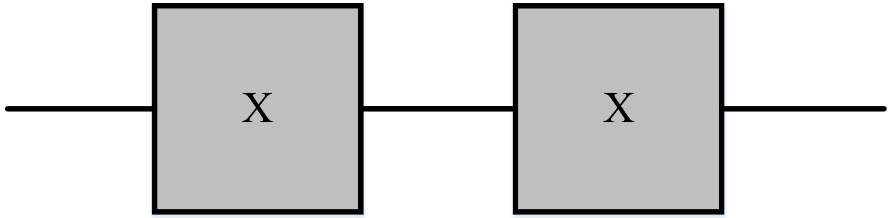


q1 (B)	q0 (A)	q3 (C)	q2 (S)
|0>	|0>	|0>	|0>
|0>	|1>	|0>	|1>
|1>	|0>	|0>	|1>
|1>	|1>	|1>	|0>

Quantum Circuit Series Connection

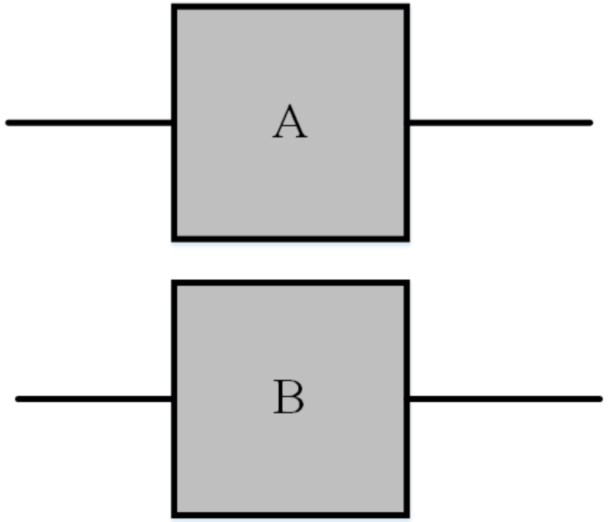


$$B \cdot A = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \cdot \begin{pmatrix} e & f \\ g & h \end{pmatrix} = \begin{pmatrix} ae + bg & af + bh \\ ce + dg & cf + dh \end{pmatrix}$$



$$x \cdot x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \cdot \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Quantum Circuit Parallel Connection

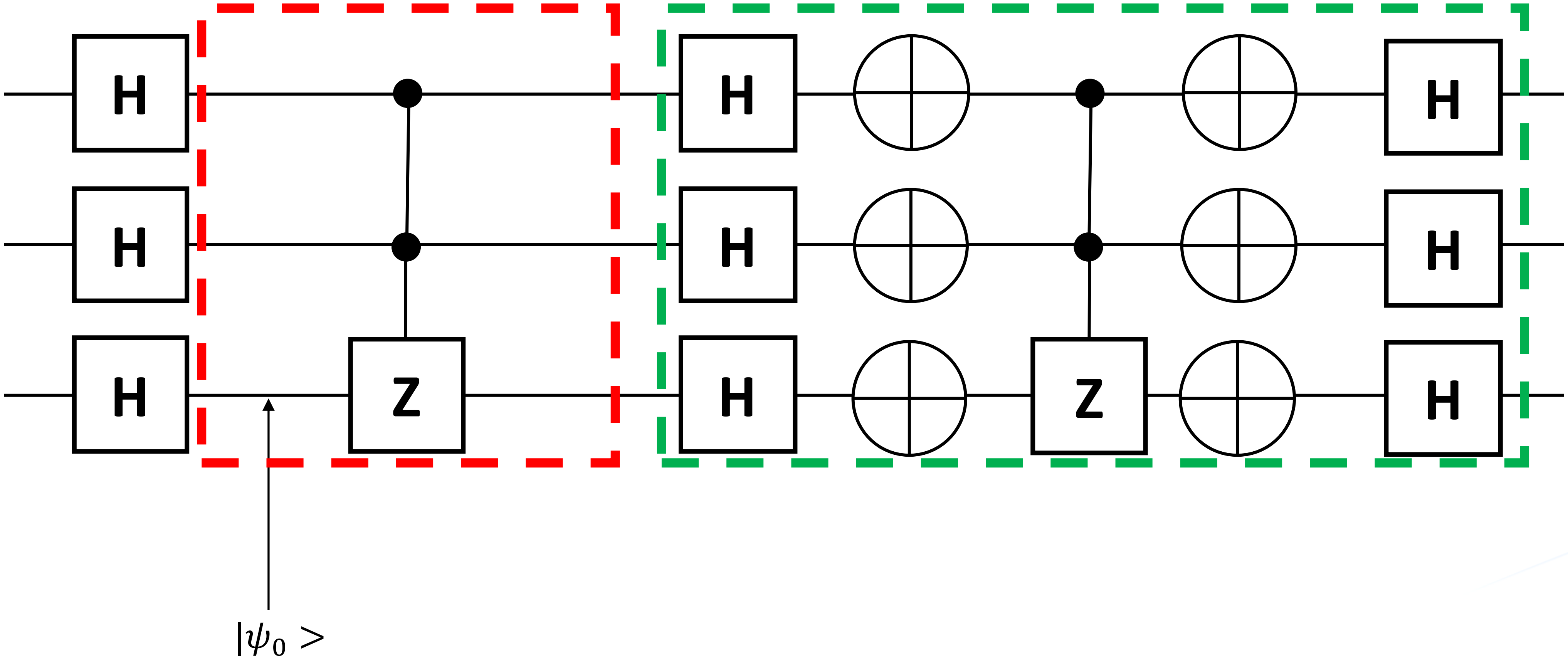


C = B ⊗ A

$$A = \begin{bmatrix} a_{1,1} & a_{1,2} \\ a_{2,1} & a_{2,2} \end{bmatrix}, \qquad B = \begin{bmatrix} b_{1,1} & b_{1,2} \\ b_{2,1} & b_{2,2} \end{bmatrix},$$

$$\begin{bmatrix} a_{1,1} & a_{1,2} \\ a_{2,1} & a_{2,2} \end{bmatrix} \otimes \begin{bmatrix} b_{1,1} & b_{1,2} \\ b_{2,1} & b_{2,2} \end{bmatrix} = \begin{bmatrix} a_{1,1} \begin{bmatrix} b_{1,1} & b_{1,2} \\ b_{2,1} & b_{2,2} \end{bmatrix} & a_{1,2} \begin{bmatrix} b_{1,1} & b_{1,2} \\ b_{2,1} & b_{2,2} \end{bmatrix} \\ a_{2,1} \begin{bmatrix} b_{1,1} & b_{1,2} \\ b_{2,1} & b_{2,2} \end{bmatrix} & a_{2,2} \begin{bmatrix} b_{1,1} & b_{1,2} \\ b_{2,1} & b_{2,2} \end{bmatrix} \end{bmatrix} = \begin{bmatrix} a_{1,1}b_{1,1} & a_{1,1}b_{1,2} & a_{1,2}b_{1,1} & a_{1,2}b_{1,2} \\ a_{1,1}b_{2,1} & a_{1,1}b_{2,2} & a_{1,2}b_{2,1} & a_{1,2}b_{2,2} \\ a_{2,1}b_{1,1} & a_{2,1}b_{1,2} & a_{2,2}b_{1,1} & a_{2,2}b_{1,2} \\ a_{2,1}b_{2,1} & a_{2,1}b_{2,2} & a_{2,2}b_{2,1} & a_{2,2}b_{2,2} \end{bmatrix}.$$

StateVector Simulation



StateVector Simulation

$$H^{\otimes 3} = H \otimes H \otimes H = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \otimes \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \otimes \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} = \frac{1}{2\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \otimes \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{bmatrix}$$

$$= \frac{1}{2\sqrt{2}}\begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 \\ 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 \\ 1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 \end{bmatrix} = \frac{1}{\sqrt{8}}\begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 \\ 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 \\ 1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 \end{bmatrix}$$

$$|000> = |0> \otimes |0> \otimes |0> = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \otimes \begin{bmatrix} 1 \\ 0 \end{bmatrix} \otimes \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \otimes \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

StateVector Simulation

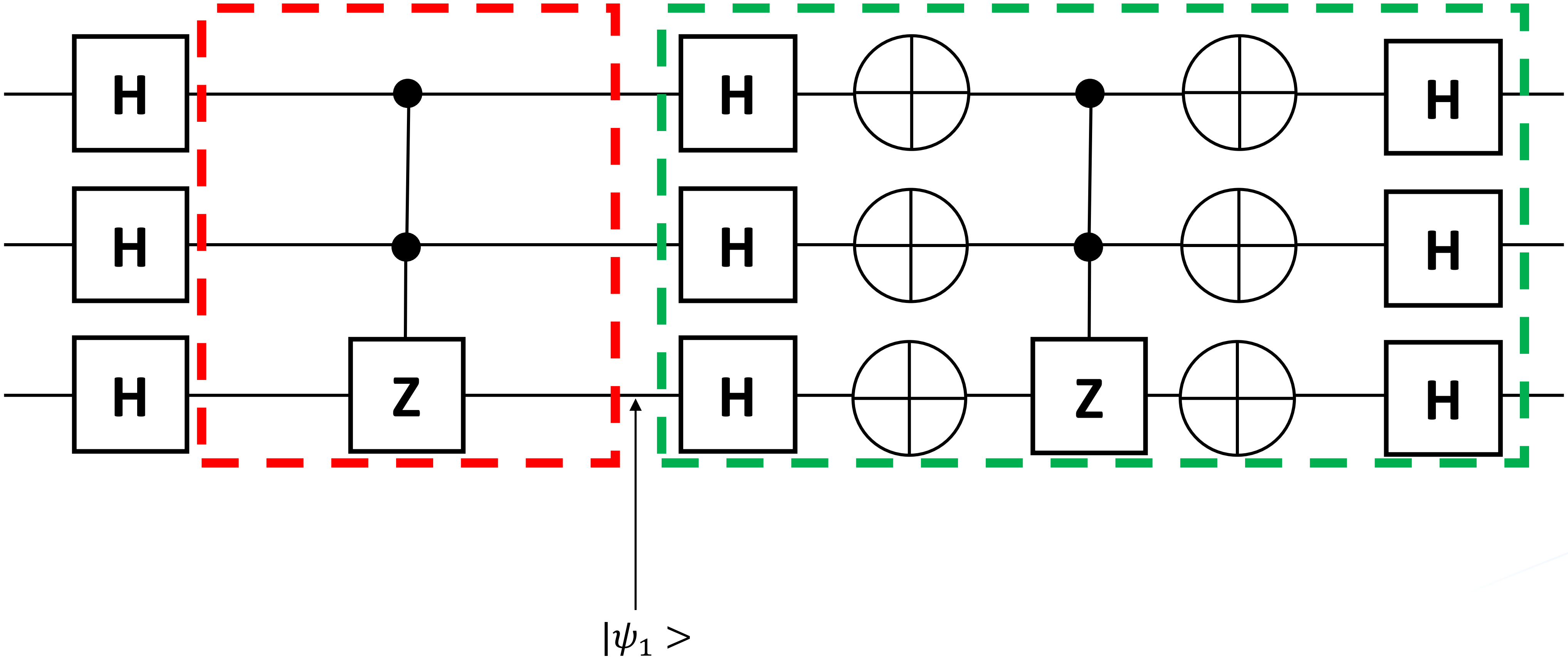
$$|\boldsymbol{\psi_0}> = H^{\otimes 3}\ |000> = \frac{1}{\sqrt{8}}\begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 \\ 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 \\ 1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 \end{bmatrix}\begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} = \frac{1}{\sqrt{8}}\begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$

$$= \frac{1}{\sqrt{8}}(\begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{bmatrix})$$

$$= \frac{1}{\sqrt{8}}(|000> + |001> + |010> + |011> + |100> + |101> + |110> + |111>)$$

$$= \boxed{\frac{1}{\sqrt{8}}(|0> + |1> + |2> + |3> + |4> + |5> + |6> + |7>)}$$

StateVector Simulation



StateVector Simulation

$$|\psi_1> = U_f|\psi_0>$$

$$= U_f H^{\otimes 3}\ |000>$$

$$= \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \end{bmatrix} \frac{1}{\sqrt{8}} \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} = \frac{1}{\sqrt{8}} \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ -1 \end{bmatrix}$$

$$= \frac{1}{\sqrt{8}}(|000> +|001> +|010> +|011> +|100> +|101> +|110> -|111>)$$

$$= \frac{1}{\sqrt{8}}(|0> +|1> +|2> +|3> +|4> +|5> +|6> \boxed{-|7>})$$

StateVector Simulation

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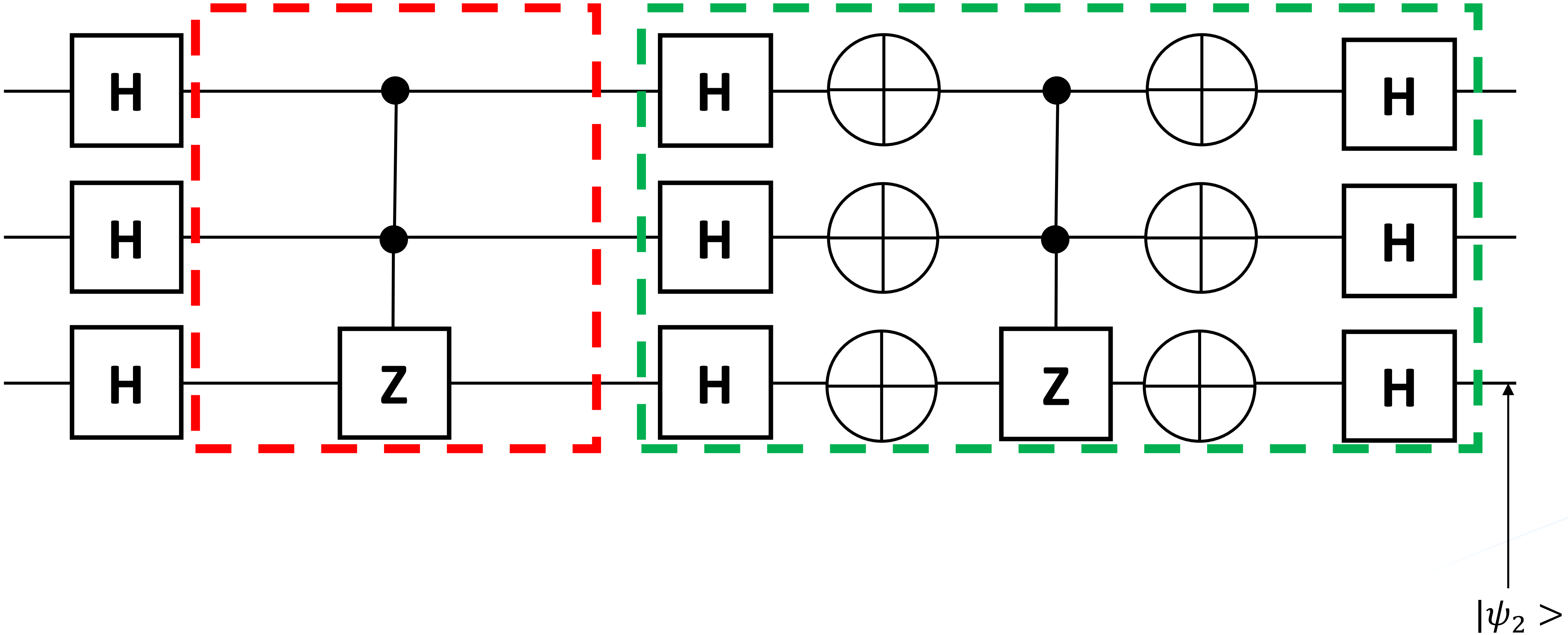

StateVector Simulation

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$$|\psi_2> = (2|\psi><\psi| - \mathbb{I})\ |\psi_1>$$

$$= (2|\psi><\psi| - \mathbb{I})U_f H^{\otimes 3}\ |000>$$

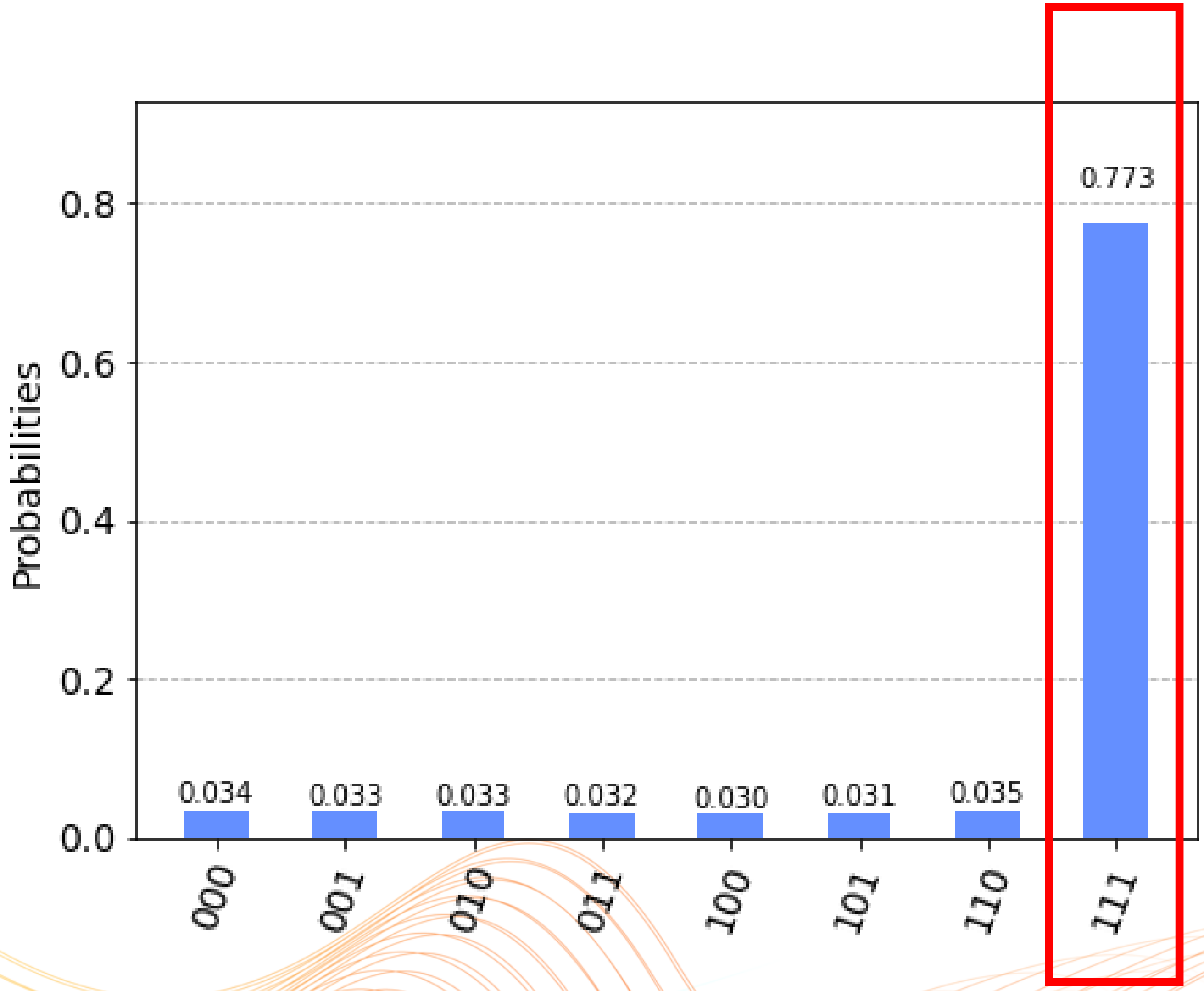
$$= \frac{1}{4}\begin{bmatrix} -3 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & -3 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & -3 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & -3 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & -3 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & -3 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & -3 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & -3 \end{bmatrix} \frac{1}{\sqrt{8}} \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ -1 \end{bmatrix} = \frac{1}{4\sqrt{8}} \begin{bmatrix} 2 \\ 2 \\ 2 \\ 2 \\ 2 \\ 2 \\ 2 \\ 10 \end{bmatrix} = \frac{1}{2\sqrt{8}} \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ \boxed{5} \end{bmatrix}$$

$$= \frac{1}{2\sqrt{8}}(|000> + |001> + |010> + |011> + |100> + |101> + |110> + 5|111>)$$

$$= \frac{1}{2\sqrt{8}}(|0> + |1> + |2> + |3> + |4> + |5> + |6> \boxed{+5|7>)}$$

狀態$|7>$的機率和其他的比起來最大，所以我們找到$|7>$

StateVector Simulation

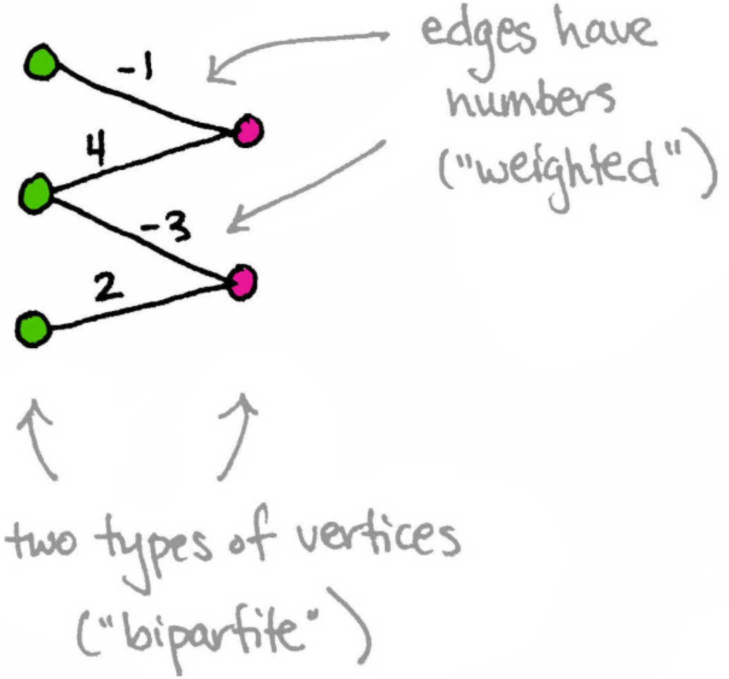


Tensor Network Representation

Tensor Network

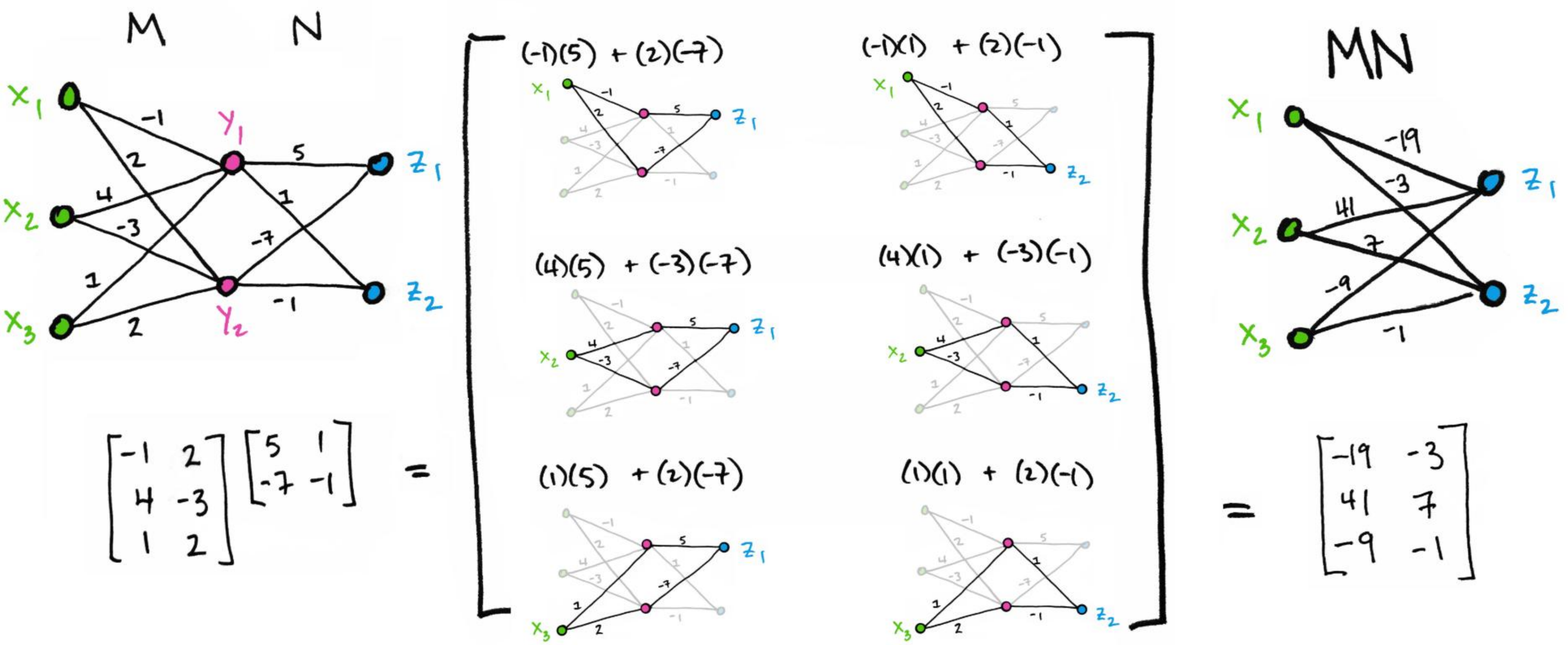
M has three rows & two columns and corresponds to this weighted bipartite graph:

$$M = \begin{bmatrix} -1 & 0 \\ 4 & -3 \\ 0 & 2 \end{bmatrix} = \begin{bmatrix} -1 & 0 \\ 4 & -3 \\ 0 & 2 \end{bmatrix}$$



https://www.math3ma.com/blog/matrices-probability-graphs

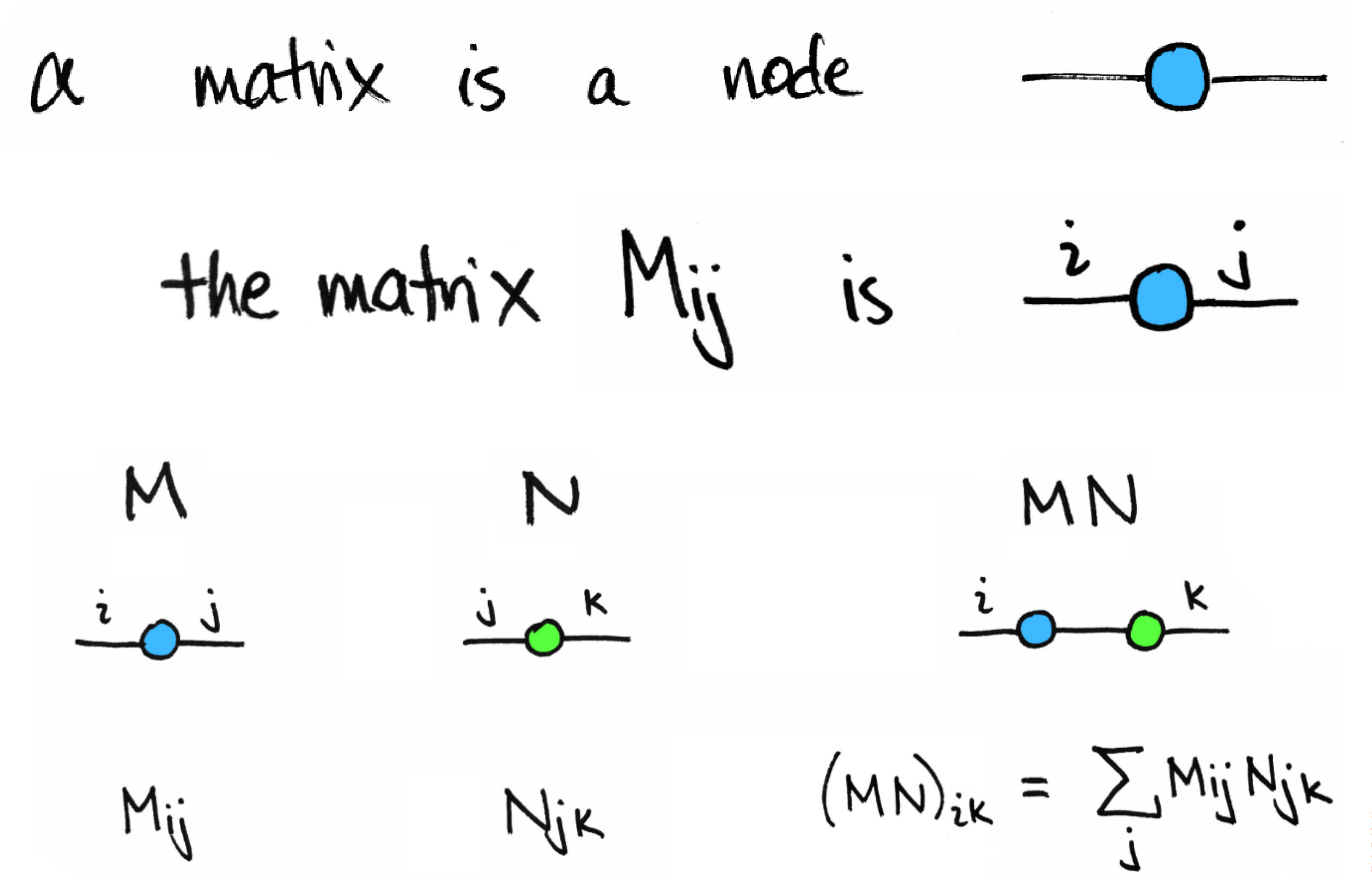
Tensor Network



$$\begin{bmatrix} -1 & 2 \\ 4 & -3 \\ 1 & 2 \end{bmatrix}\begin{bmatrix} 5 & 1 \\ -7 & -1 \end{bmatrix} = \begin{bmatrix} (-1)(5)+(2)(-7) & (-1)(1)+(2)(-1) \\ (4)(5)+(-3)(-7) & (4)(1)+(-3)(-1) \\ (1)(5)+(2)(-7) & (1)(1)+(2)(-1) \end{bmatrix} = \begin{bmatrix} -19 & -3 \\ 41 & 7 \\ -9 & -1 \end{bmatrix}$$

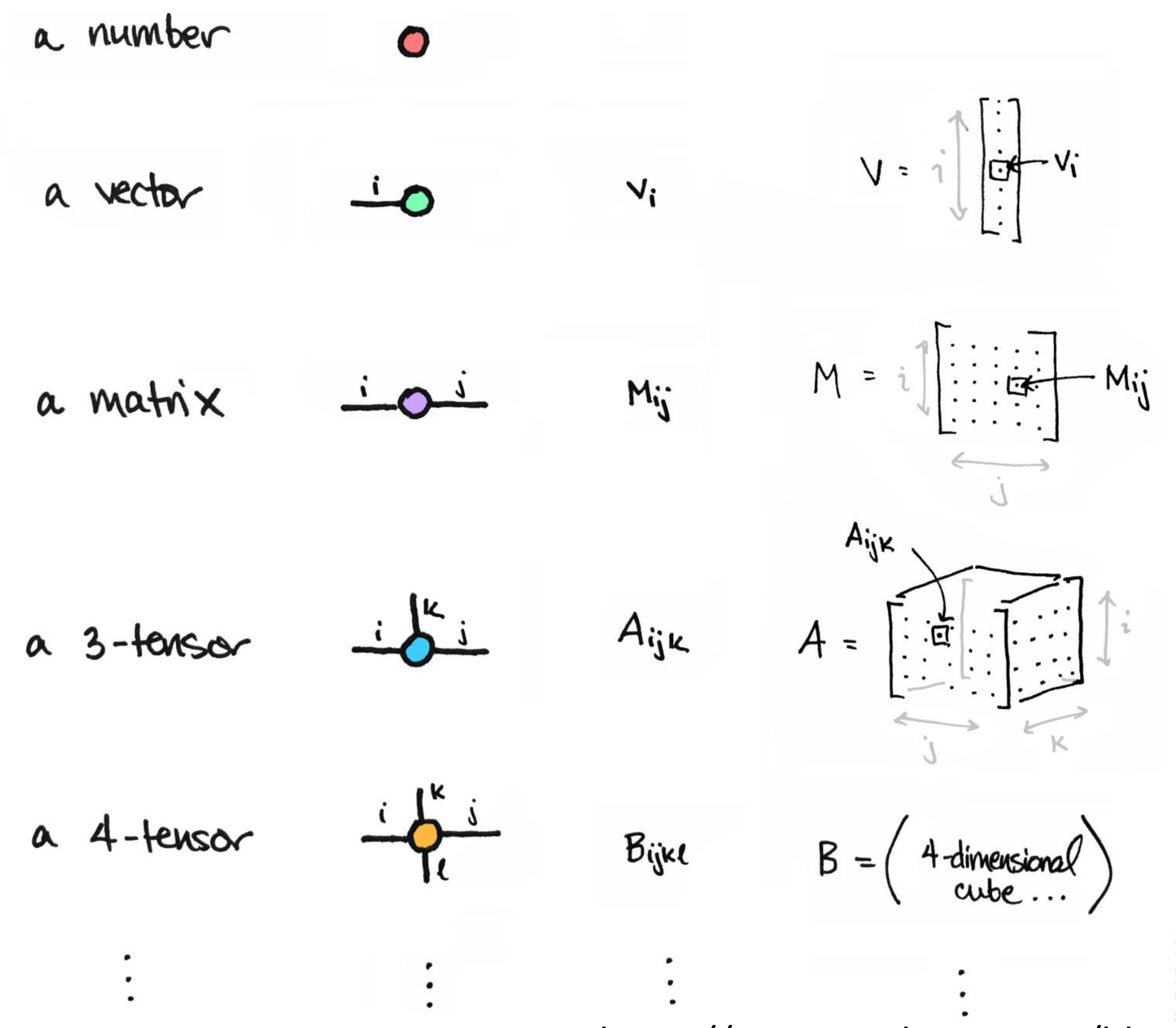
https://www.math3ma.com/blog/matrices-probability-graphs

Tensor Network



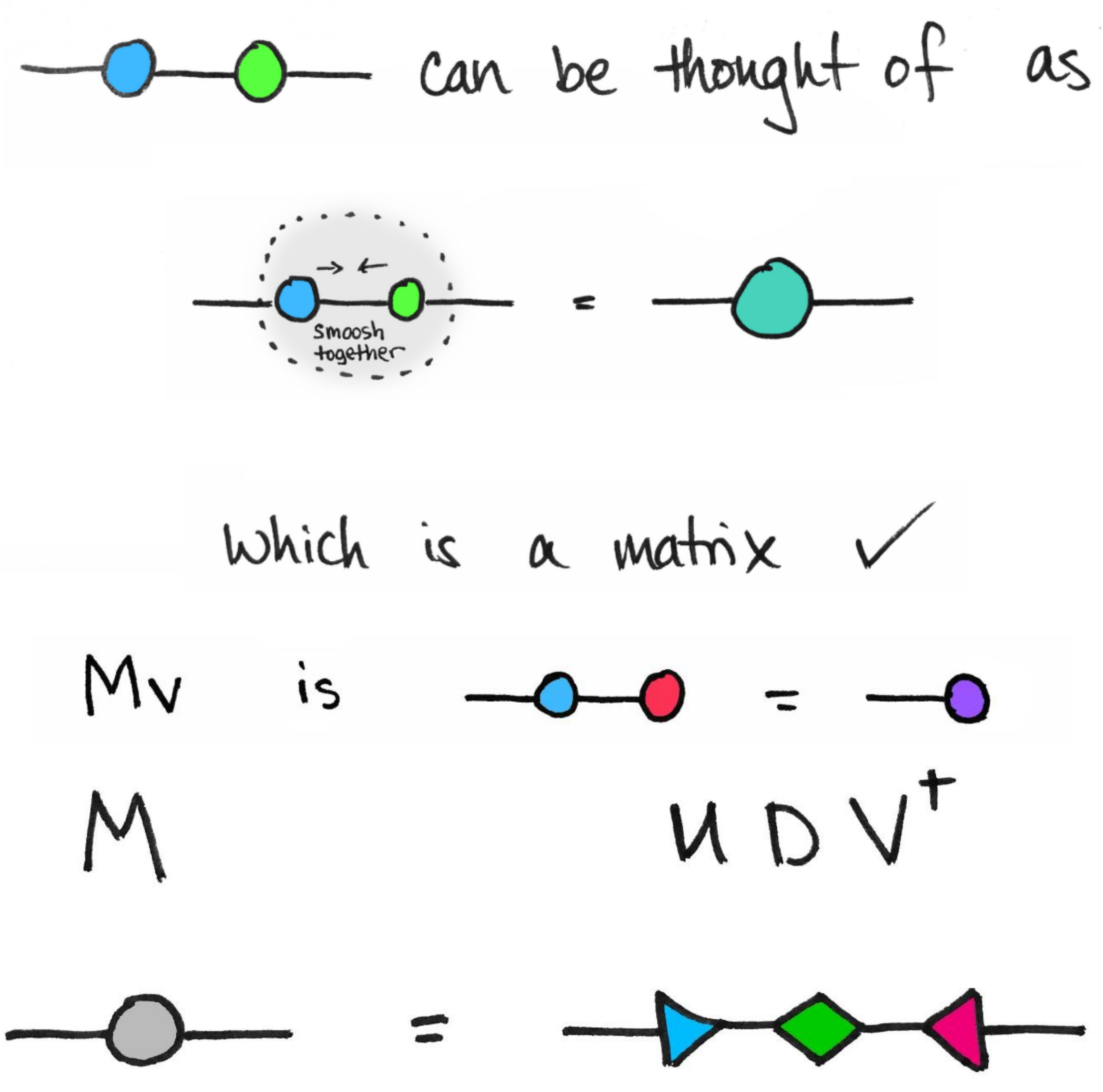
https://www.math3ma.com/blog/matrices-probability-graphs

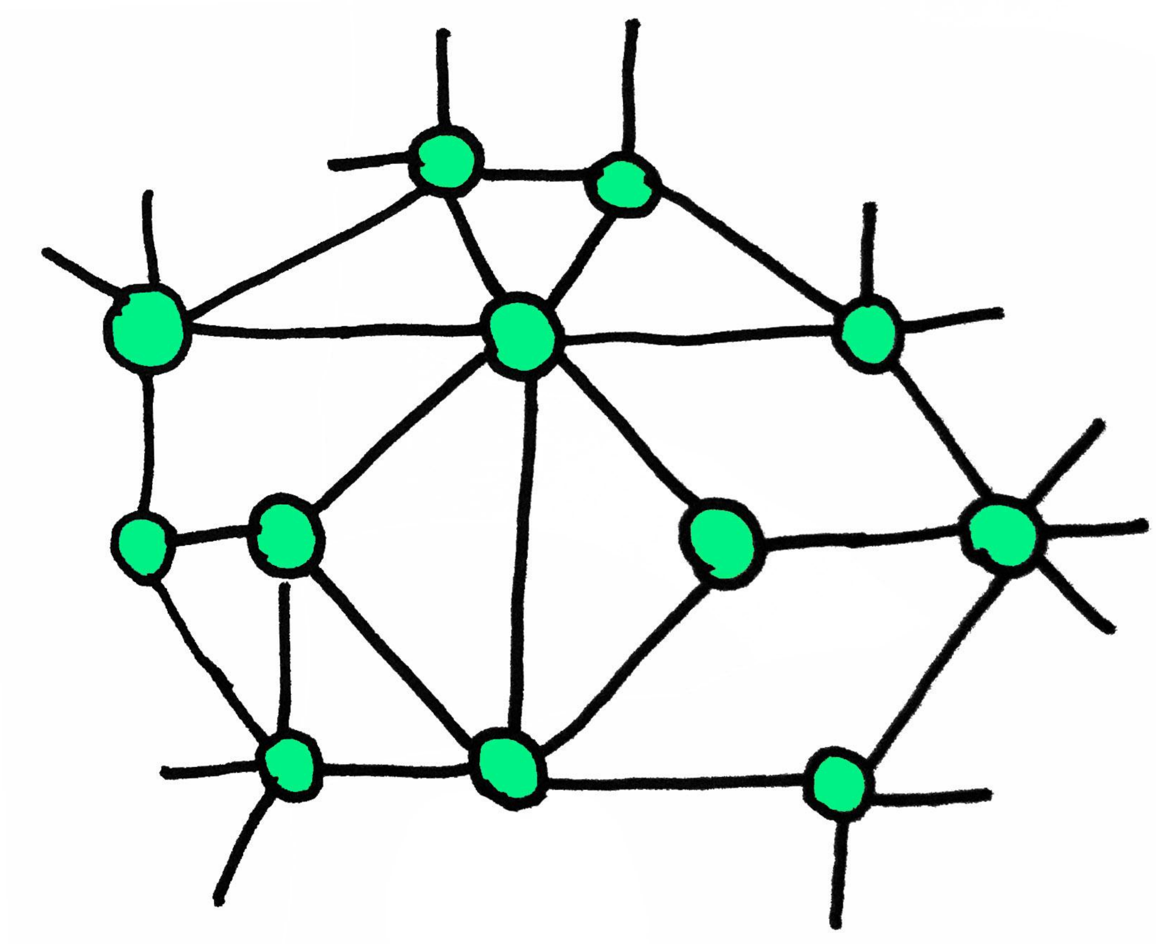
Tensor Network



https://www.math3ma.com/blog/matrices-probability-graphs

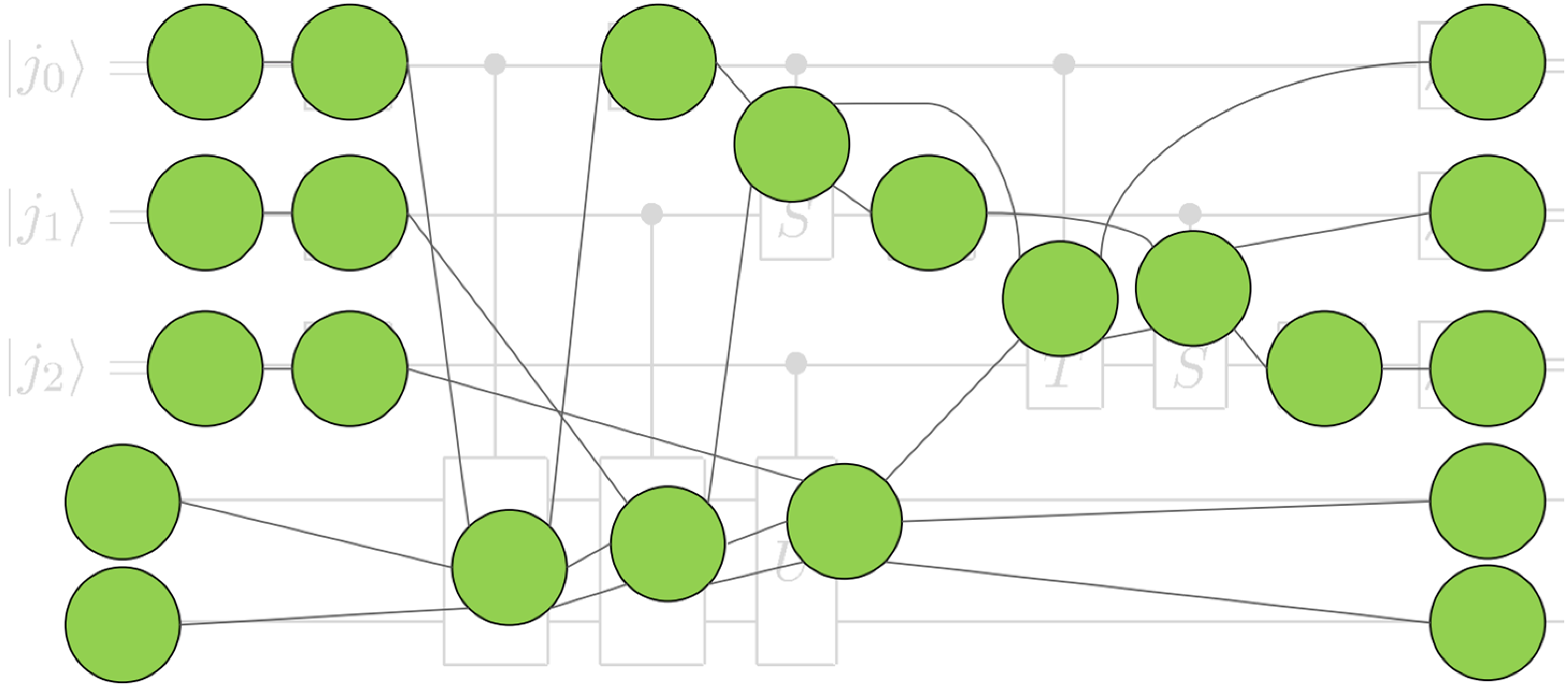
Tensor Network





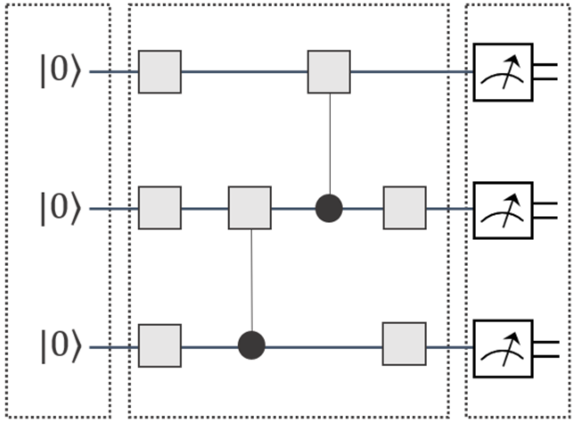
https://www.math3ma.com/blog/matrices-probability-graphs

Tensor Network Representation



Quantum Circuit Simulation

Quantum Circuit
(Gate-Based Quantum Computing)

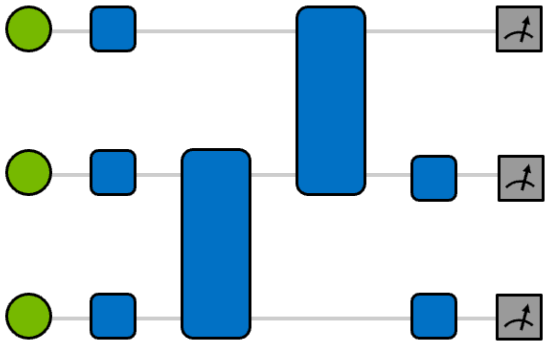


Put **dataset** (Classical or Quantum) **into Quantum Algorithm**

Noisy Intermediate-Scale QC
(QPU)

Limited qubits and gates with insufficient accuracy

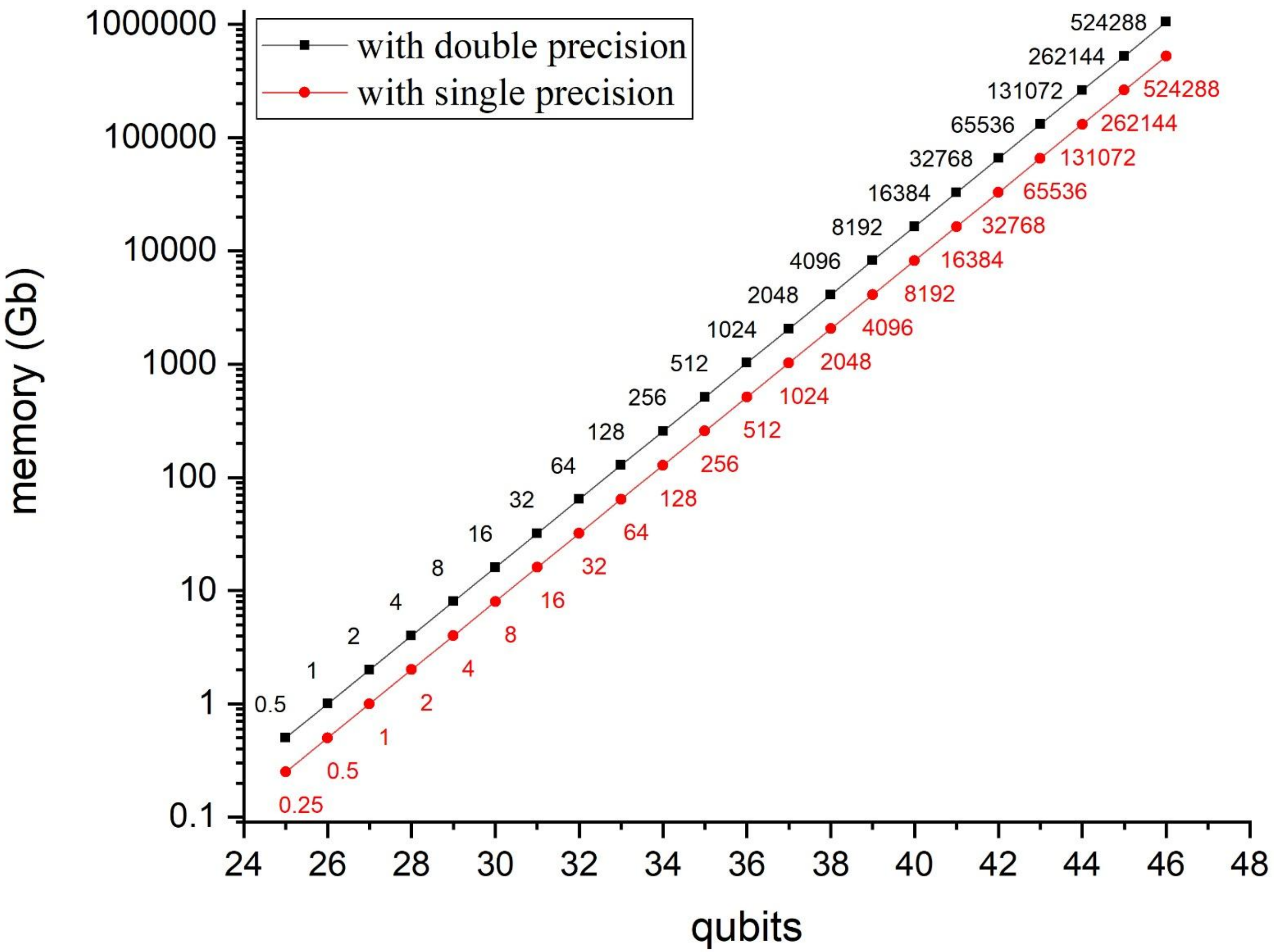
Quantum Circuit Simulation
(HPC platform)



A series of matrix operations on CPUs and GPUs
Scalable with accurate results

Quantum Circuit Simulation

2^(qubits)*16(complex values[Bytes])



Quantum Circuit Simulation

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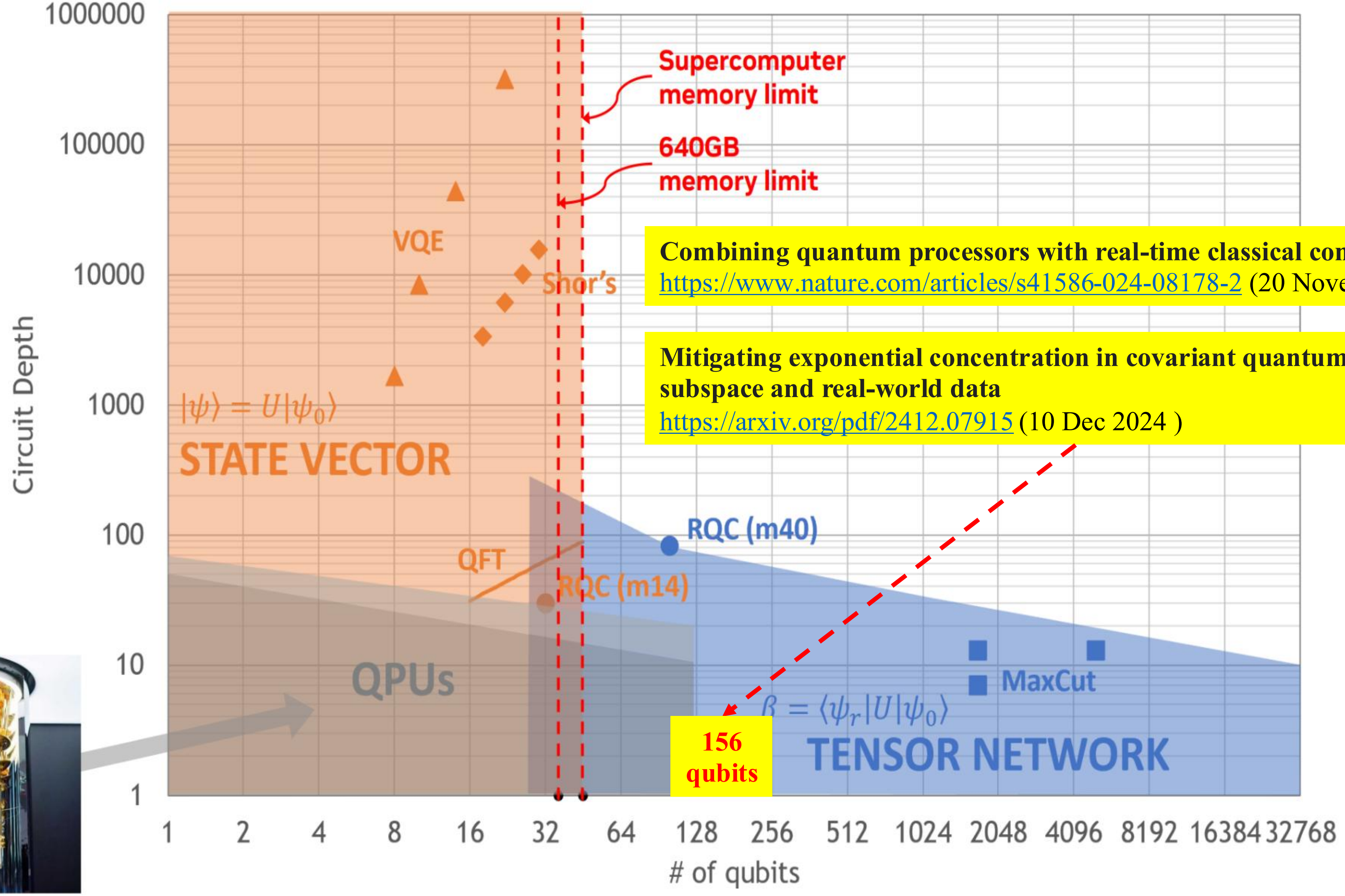

Combining quantum processors with real-time classical communication
https://www.nature.com/articles/s41586-024-08178-2 (20 November 2024)

Mitigating exponential concentration in covariant quantum kernels for subspace and real-world data
https://arxiv.org/pdf/2412.07915 (10 Dec 2024)

Why CUDA-Q ?

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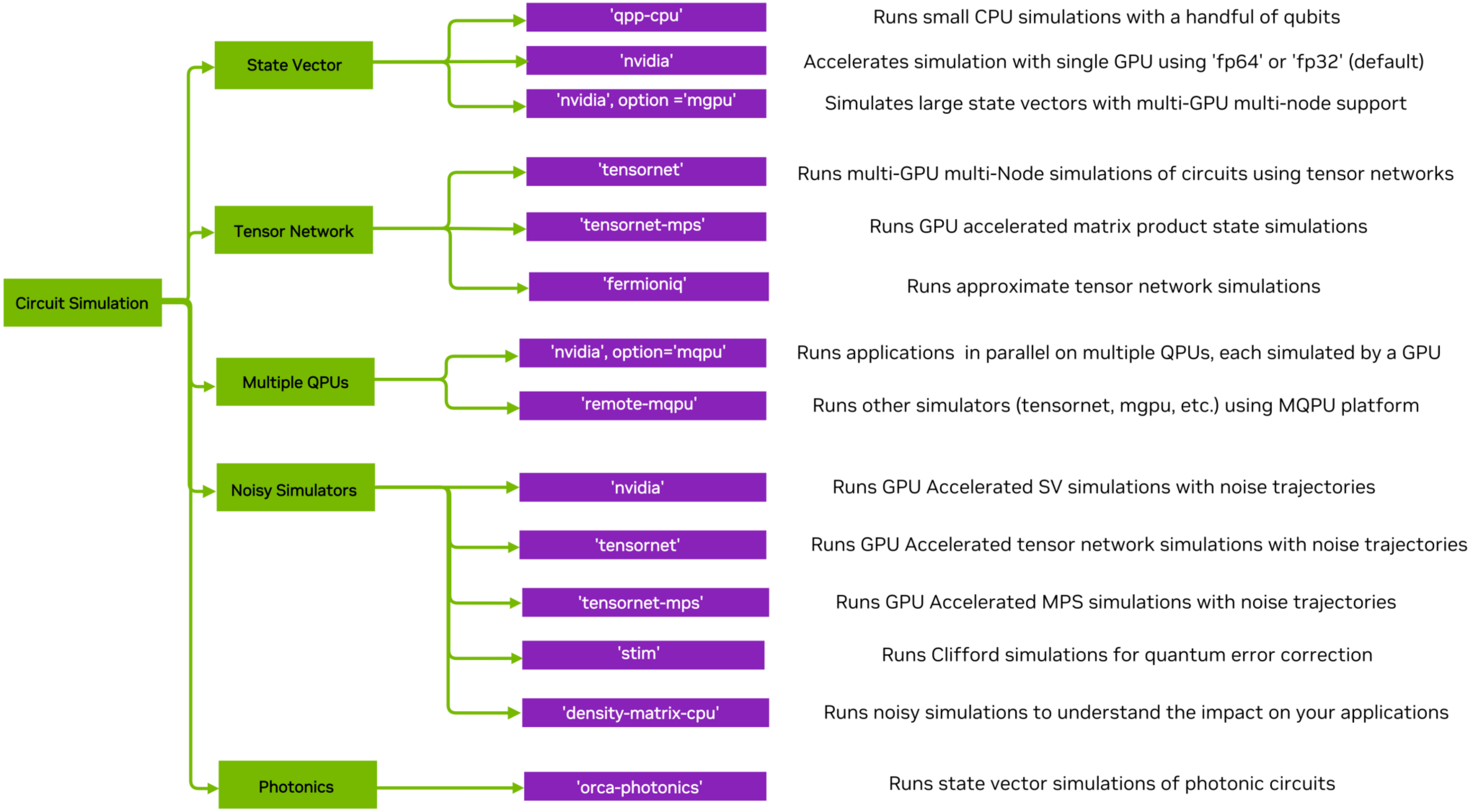

https://nvidia.github.io/cuda-quantum/latest/using/backends/simulators.html

Why CUDA-Q ?

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Physical QPUs

Ion Trap	Neutral Atom	Superconducting	Photonic	Aggregators
IONQ	Infleqtion		ORCA COMPUTING	Amazon Braket aws
QUANTINUUM	Pasqal	IQM		
	QuEra Computing Inc.	OQC		

https://nvidia.github.io/cuda-quantum/latest/using/backends/hardware.html

Research of Quantum Machine Learning in NCHC

Scalable Quantum Support Vector Machine Simulation

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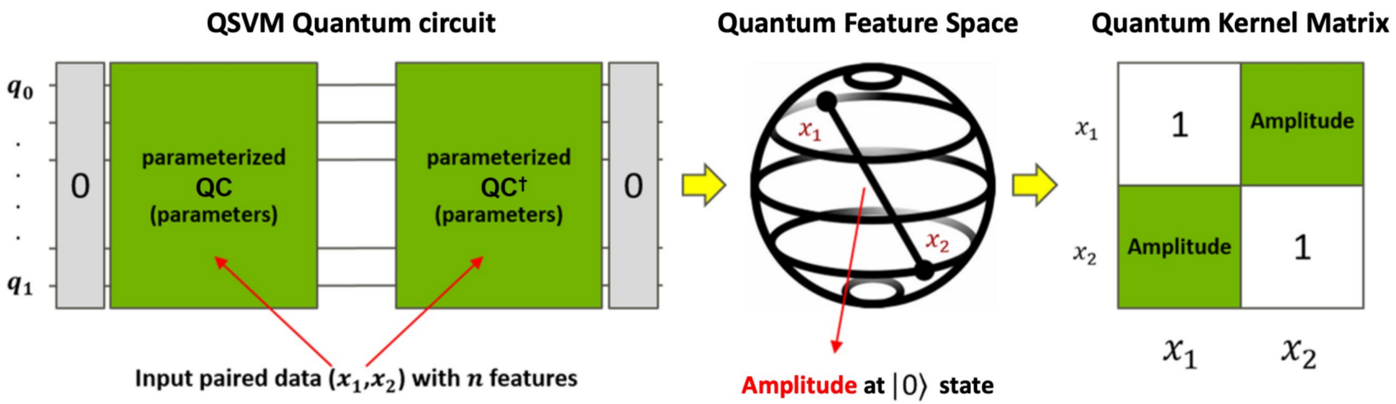
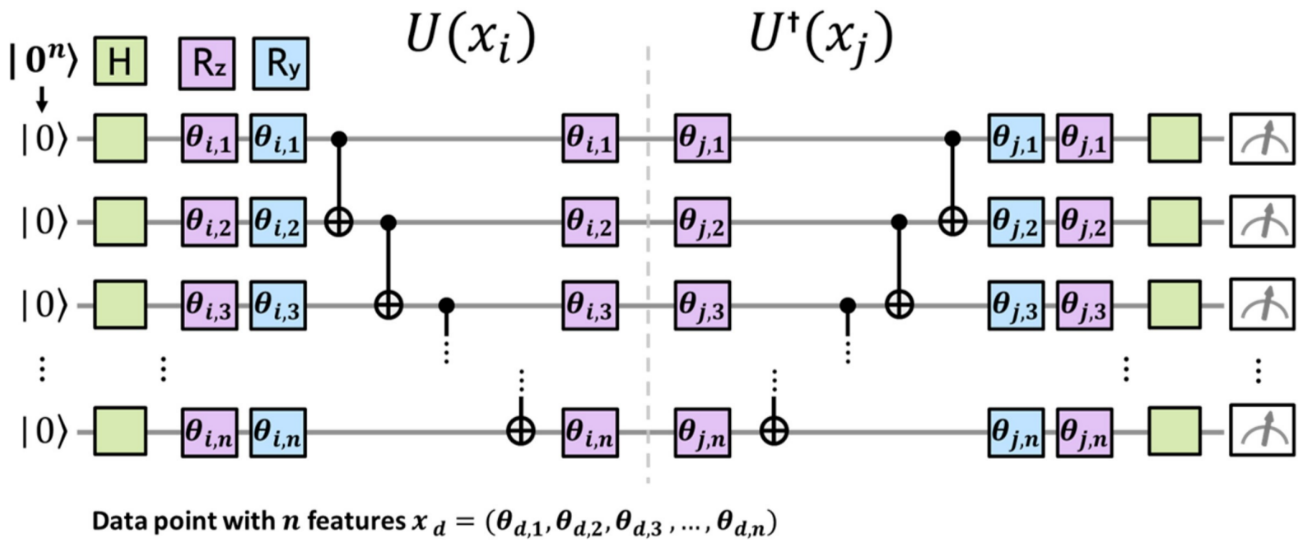
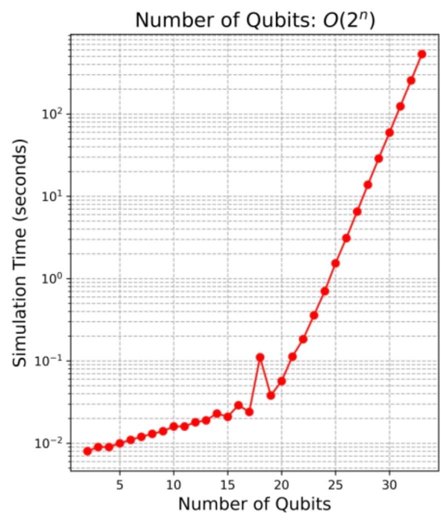
QSVM Workflow and Computational Complexity on HPC Platform

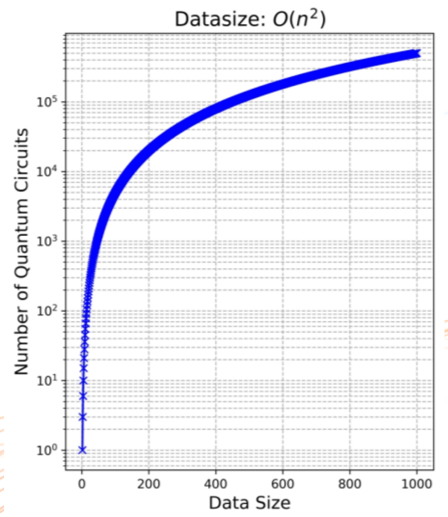
(a)



(b)







Scalable Quantum Support Vector Machine Simulation

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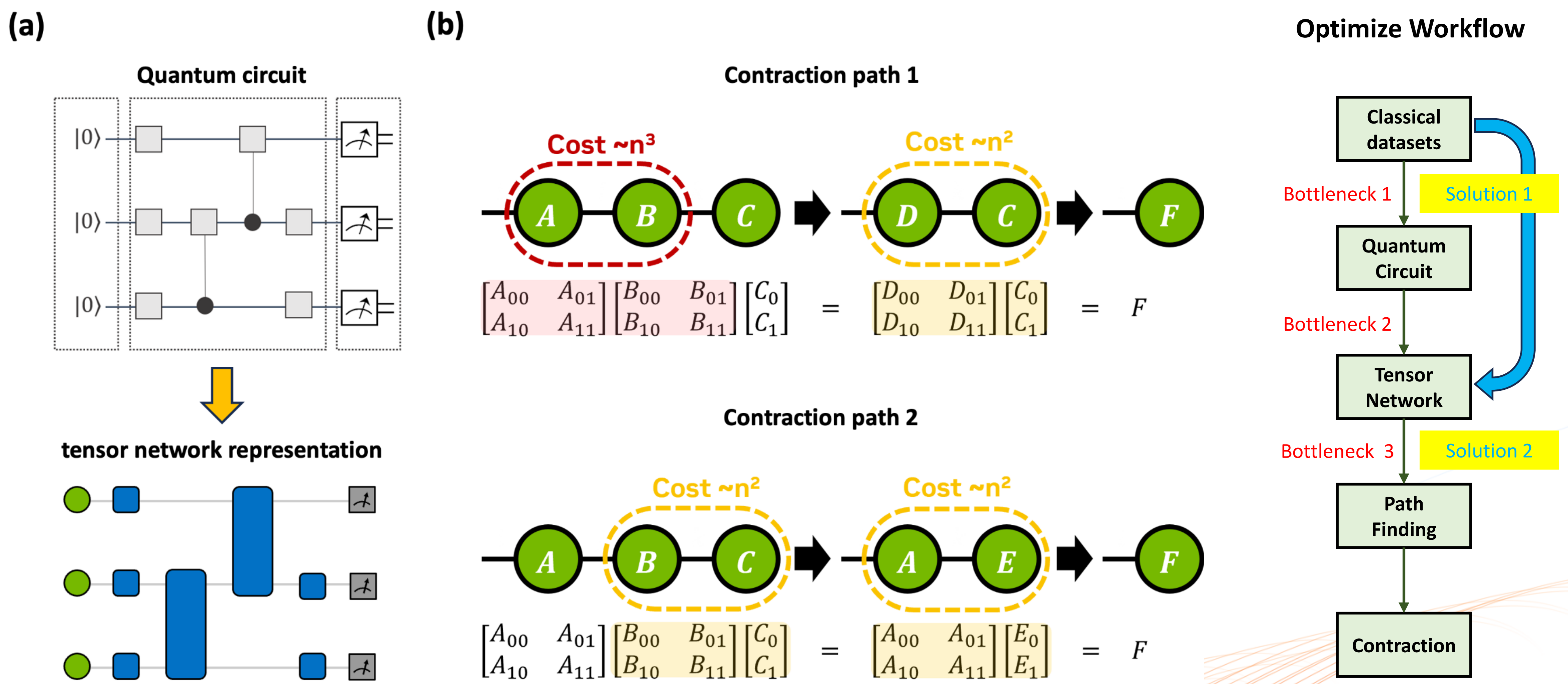
Tensor Network Simulation using cuQuantum



“Validating Large-Scale Quantum Machine Learning: Efficient Simulation of Quantum Support Vector Machines Using Tensor Networks”, Machine Learning: Science and Technology **6**, 015047, 2025.

Scalable Quantum Support Vector Machine Simulation

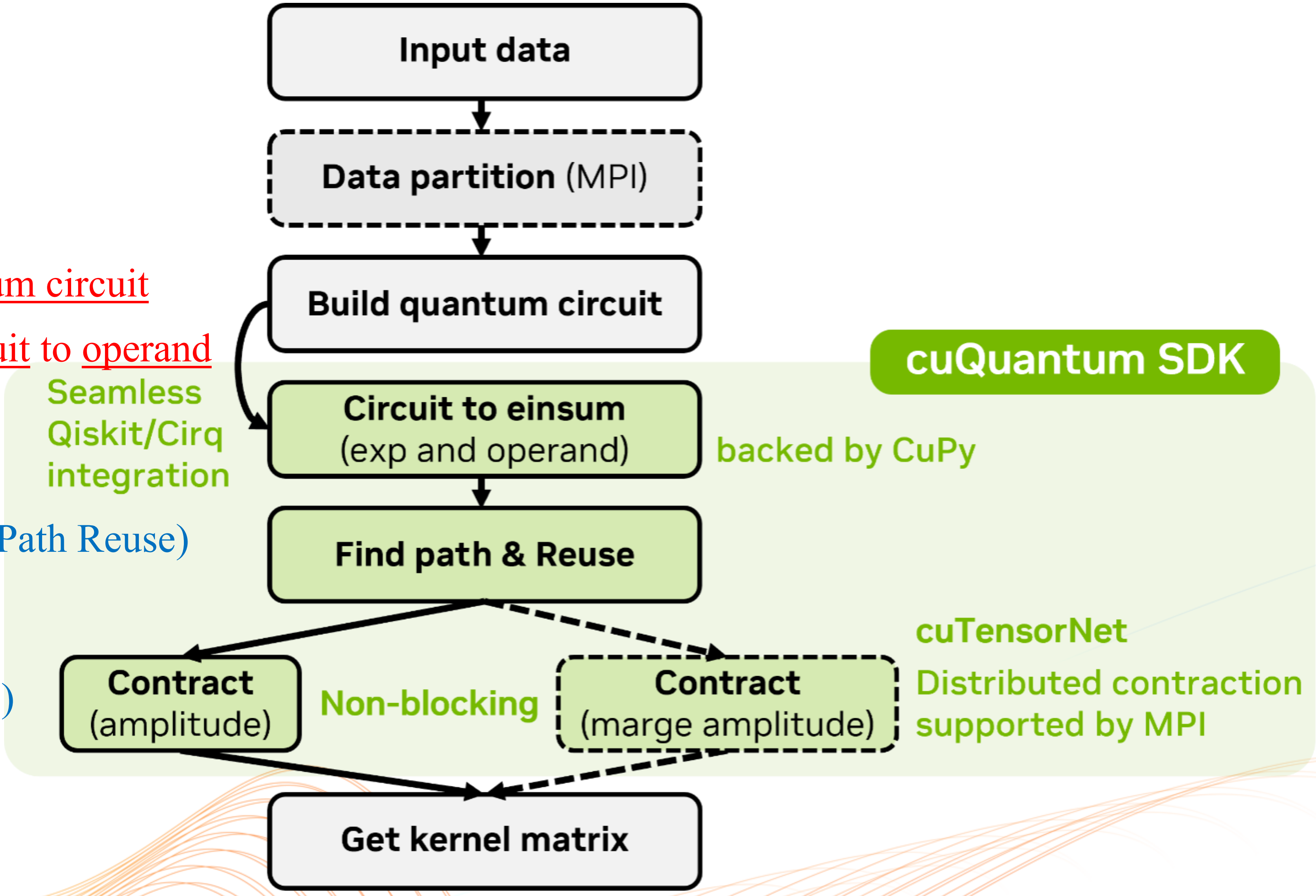
Bottleneck1: data to quantum circuit

Bottleneck2: quantum circuit to operand

data to operand

Bottleneck3: path finding (Path Reuse)

Bottleneck4: contract (MPI)



"Validating Large-Scale Quantum Machine Learning: Efficient Simulation of Quantum Support Vector Machines Using Tensor Networks", Machine Learning: Science and Technology **6**, 015047, 2025.

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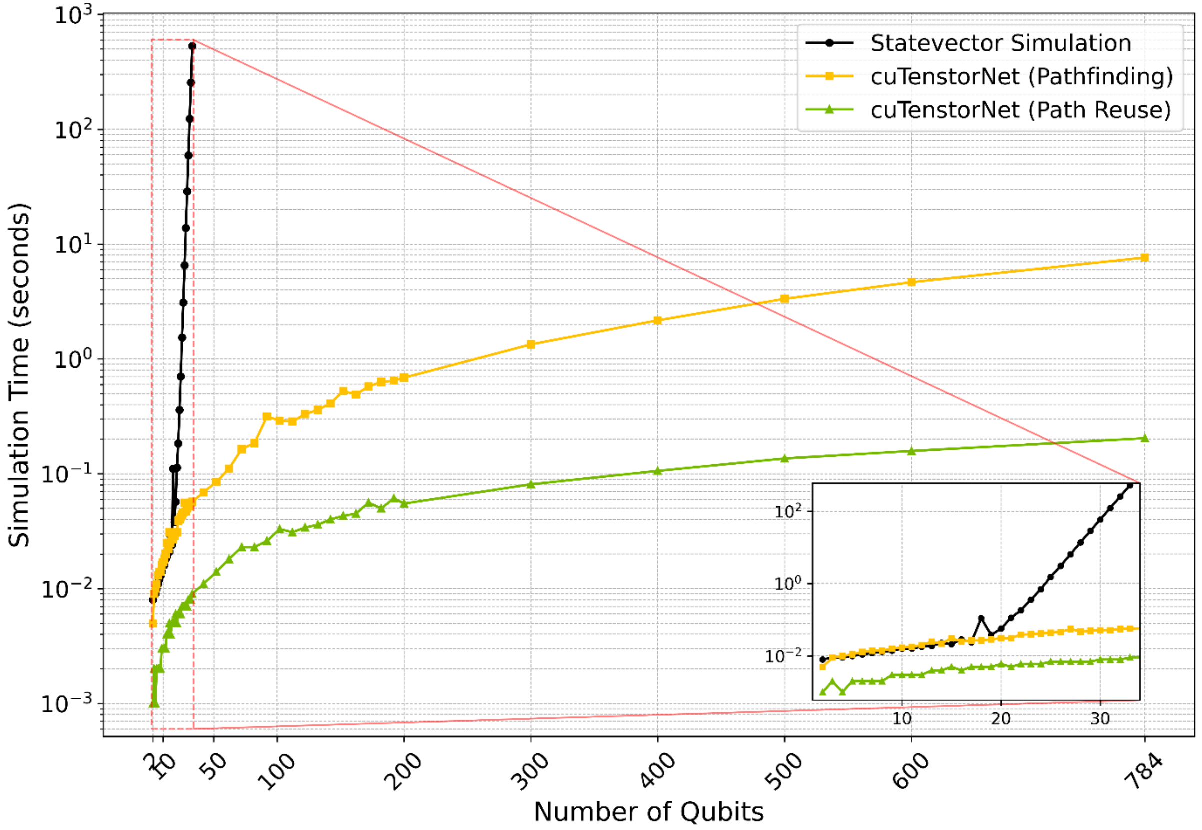
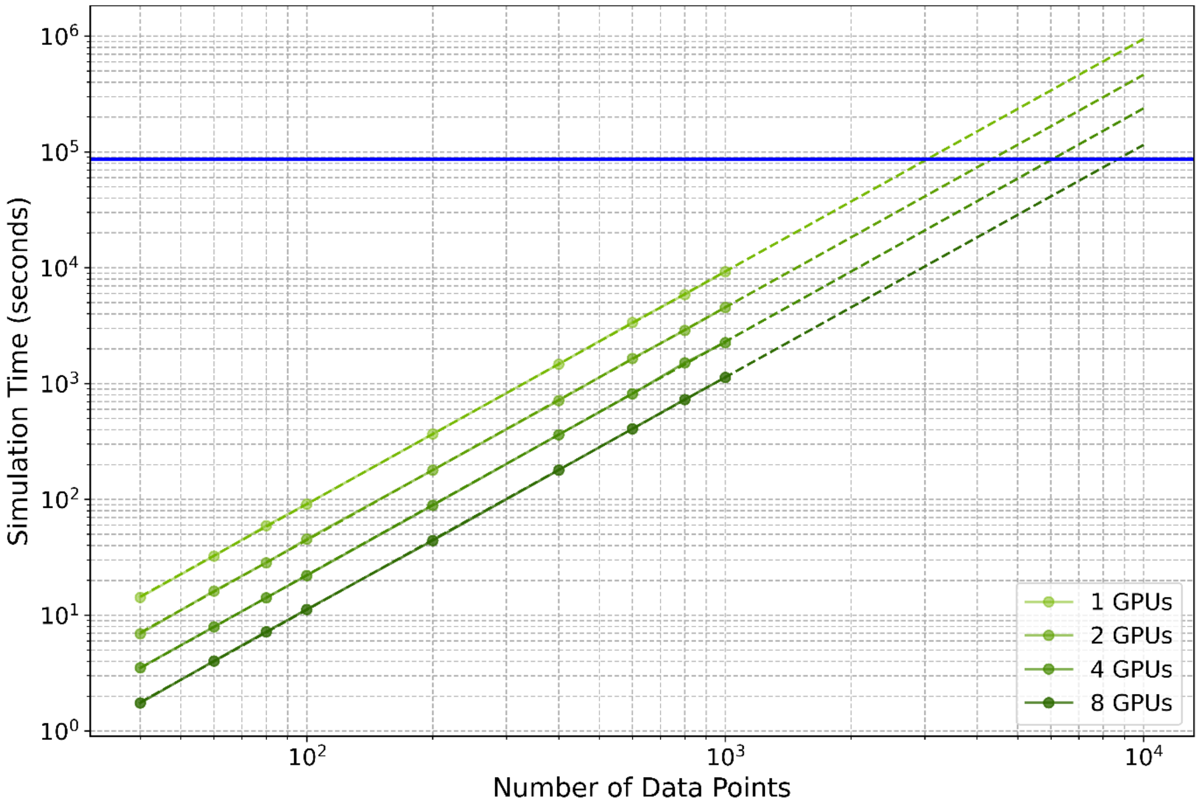
Single-GPU and Multi-GPUs Benchmark





"Validating Large-Scale Quantum Machine Learning: Efficient Simulation of Quantum Support Vector Machines Using Tensor Networks", Machine Learning: Science and Technology **6**, 015047, 2025.

Scalable Quantum Support Vector Machine Simulation

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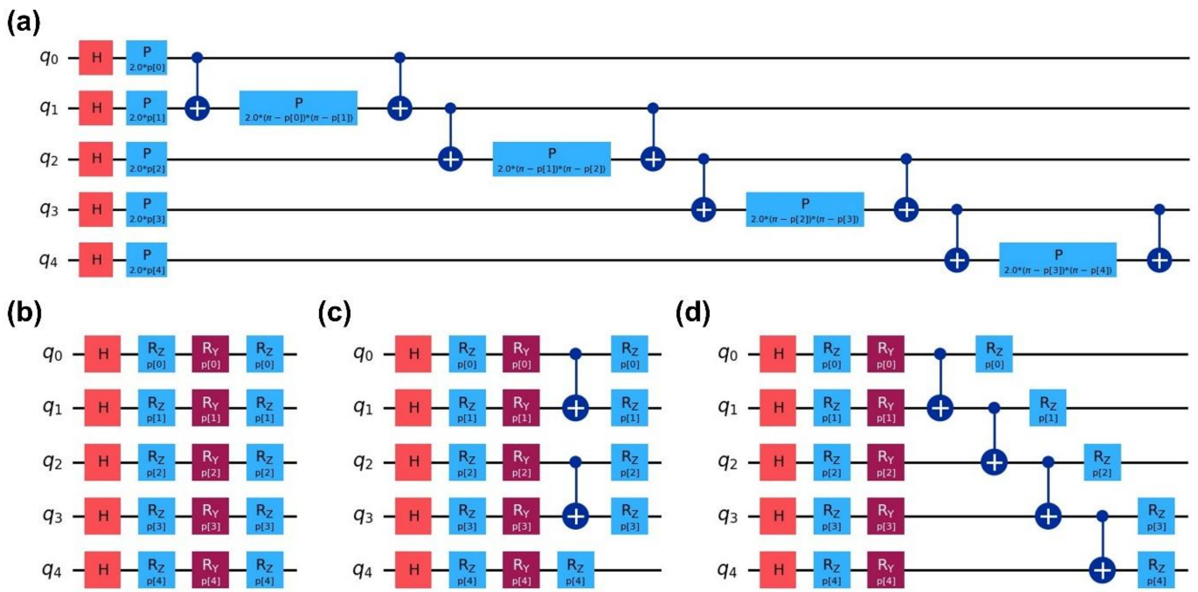
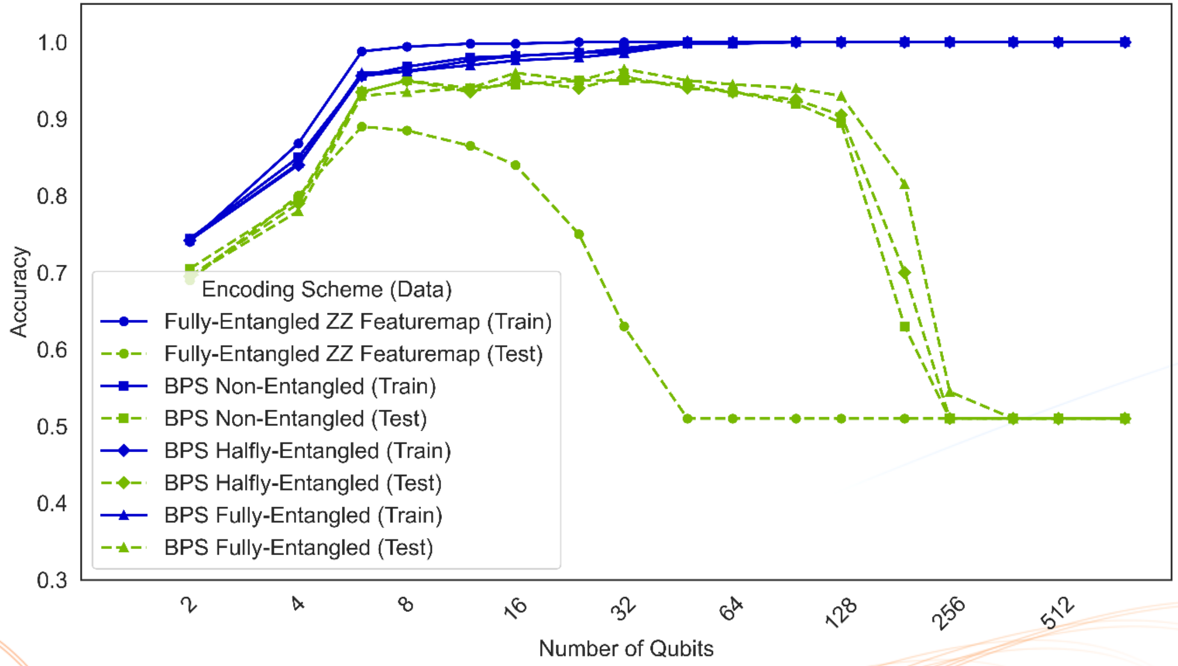
Performance of Quantum Circuit Architectures and Entanglement Levels

Different Quantum Circuit Architectures and Entanglement Levels



Performance



"Validating Large-Scale Quantum Machine Learning: Efficient Simulation of Quantum Support Vector Machines Using Tensor Networks", Machine Learning: Science and Technology **6**, 015047, 2025.

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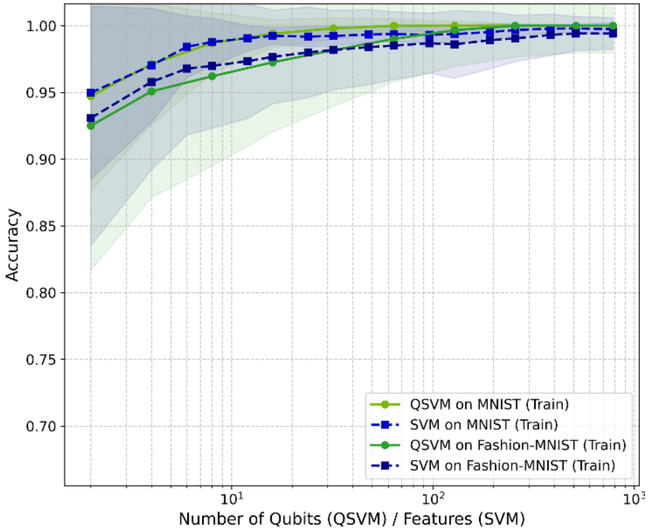
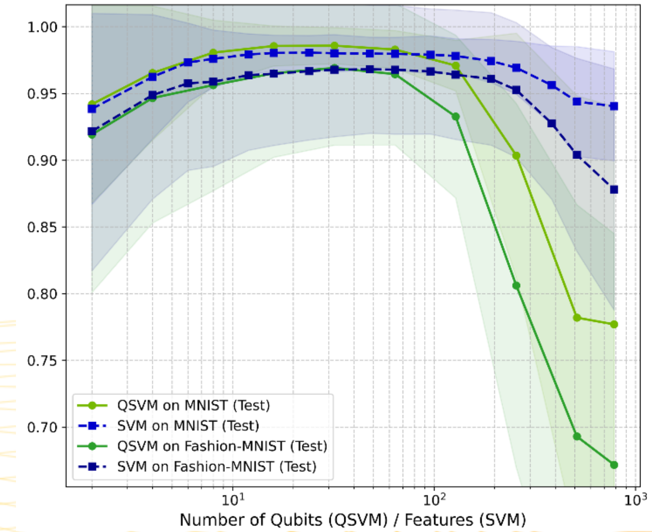
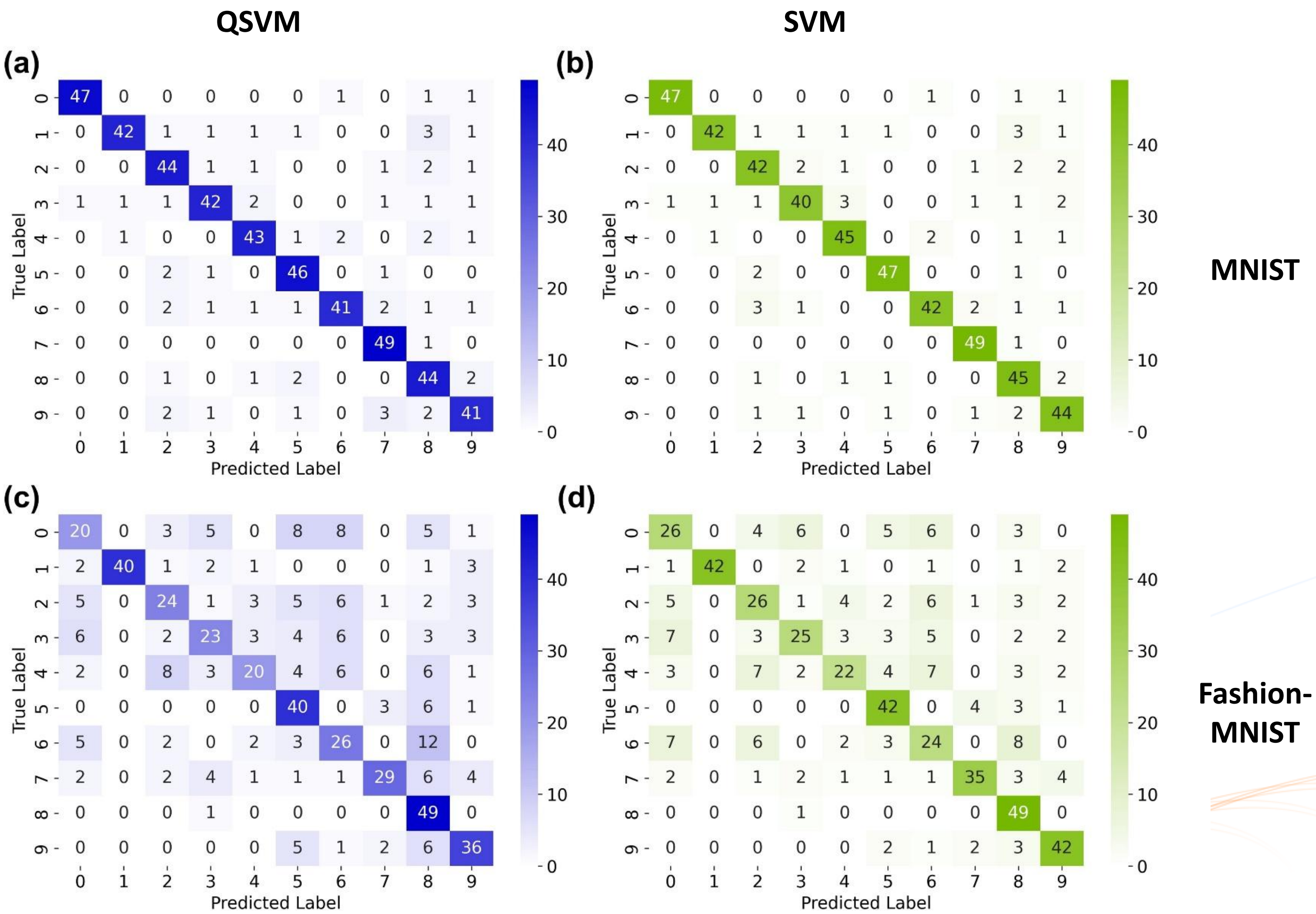
Multi-class Classification







“Validating Large-Scale Quantum Machine Learning: Efficient Simulation of Quantum Support Vector Machines Using Tensor Networks”, Machine Learning: Science and Technology **6**, 015047, 2025.

Scalable Quantum Support Vector Machine Simulation

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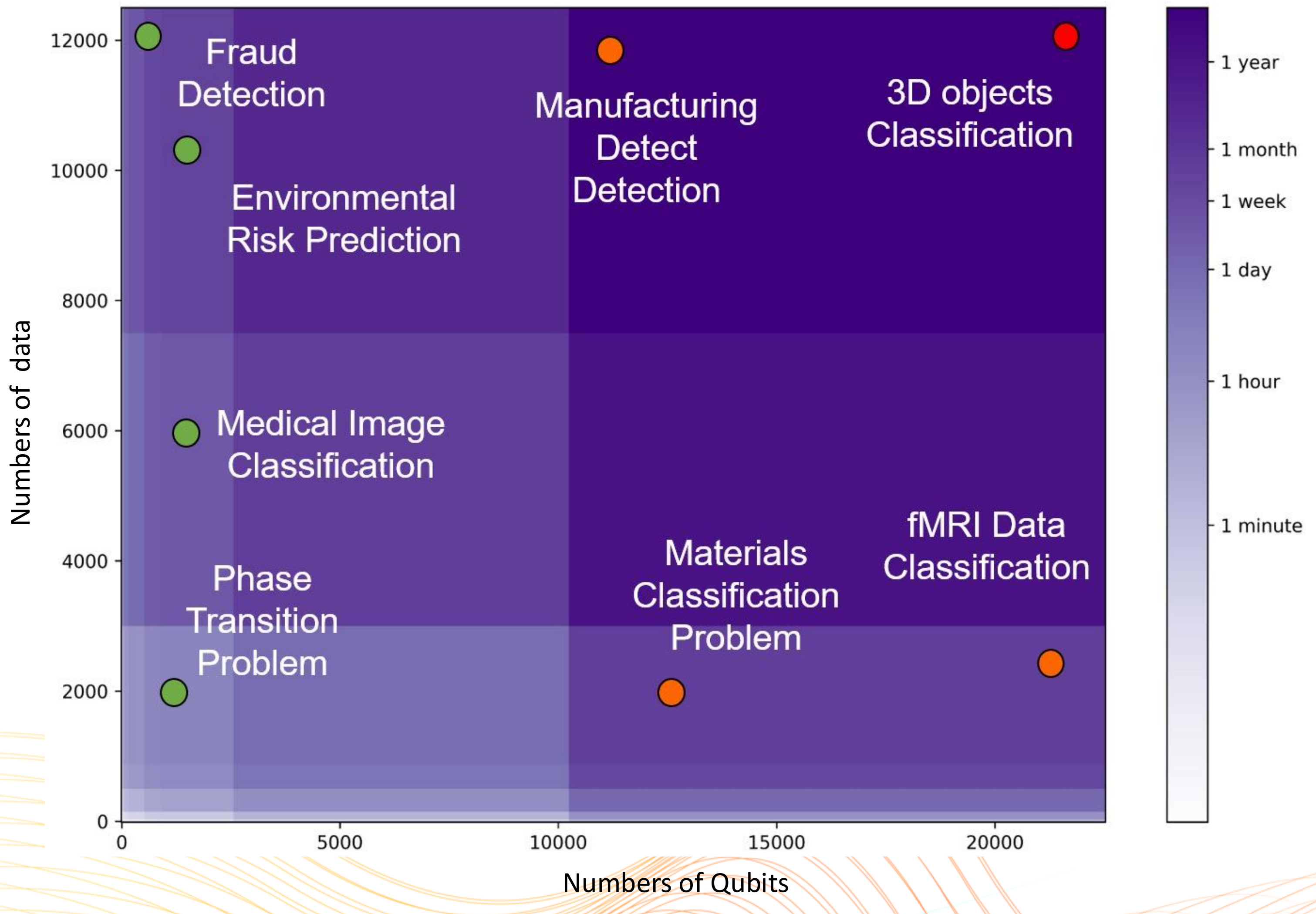
Call for Various Datasets



(we are ready!)

GitHub Code

Paper

"Validating Large-Scale Quantum Machine Learning: Efficient Simulation of Quantum Support Vector Machines Using Tensor Networks", Machine Learning: Science and Technology **6**, 015047, 2025.

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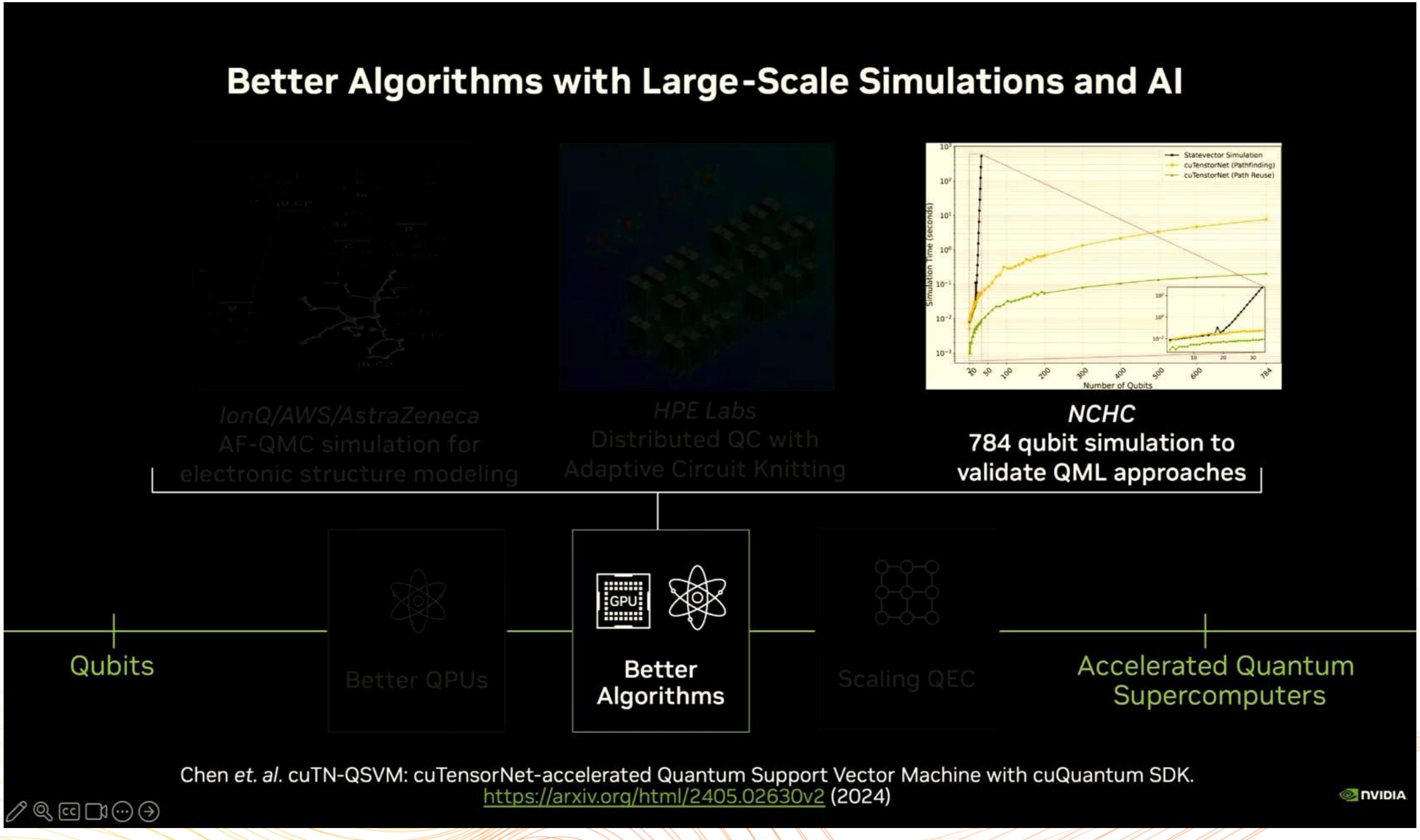
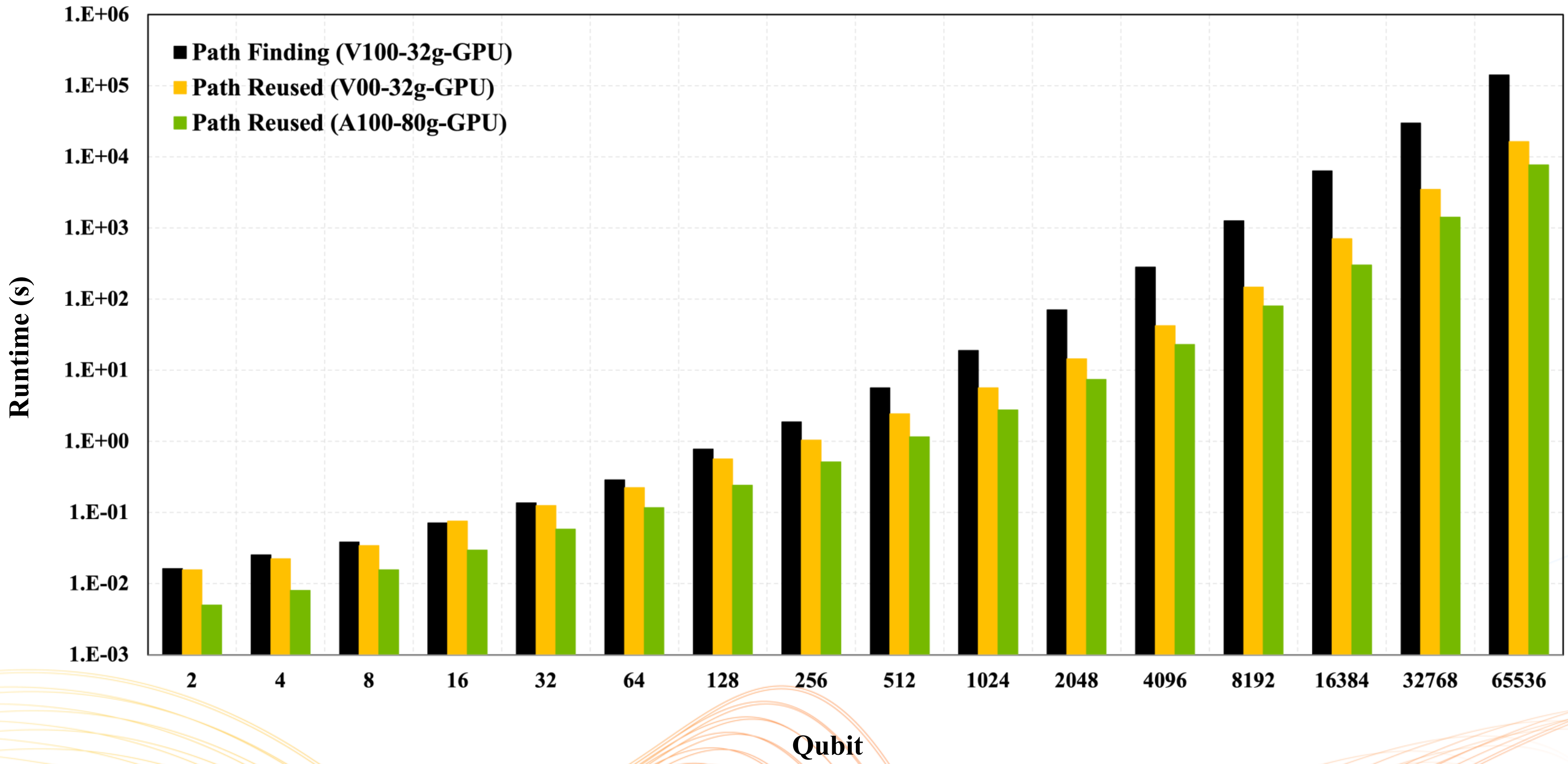


"Validating Large-Scale Quantum Machine Learning: Efficient Simulation of Quantum Support Vector Machines Using Tensor Networks", Machine Learning: Science and Technology **6**, 015047, 2025.

Scalable Quantum Support Vector Machine Simulation



Scalable Quantum Support Vector Machine Simulation

Qubit	Build QC and TN (s)	Renew TN (s)	Build Environment (s)	Get Path (s)	Contraction (s)	Total Time (s)
2	0.01	0.00	0.00	0.00	0.00	0.02
4	0.00	0.00	0.00	0.01	0.00	0.02
8	0.01	0.01	0.00	0.01	0.00	0.03
16	0.01	0.01	0.04	0.03	0.00	0.10
32	0.03	0.02	0.03	0.05	0.01	0.14
64	0.05	0.04	0.02	0.11	0.01	0.23
128	0.26	0.07	0.01	0.22	0.02	0.58
256	0.19	0.29	0.03	0.46	0.05	1.03
512	0.61	0.58	0.07	1.06	0.10	2.41
1024	1.41	1.17	0.17	2.56	0.19	5.50
2048	3.24	2.21	0.31	7.03	0.38	13.17
4096	6.65	4.50	1.07	22.03	1.01	35.26
8192	13.39	9.06	3.50	79.15	1.47	106.57
16384	28.29	18.25	11.57	299.87	2.82	360.80
32768	56.86	39.26	36.61	1420.52	5.76	1559.01
65536	123.92	87.08	159.42	7724.41	11.32	8106.16

Scalable Quantum Support Vector Machine Simulation

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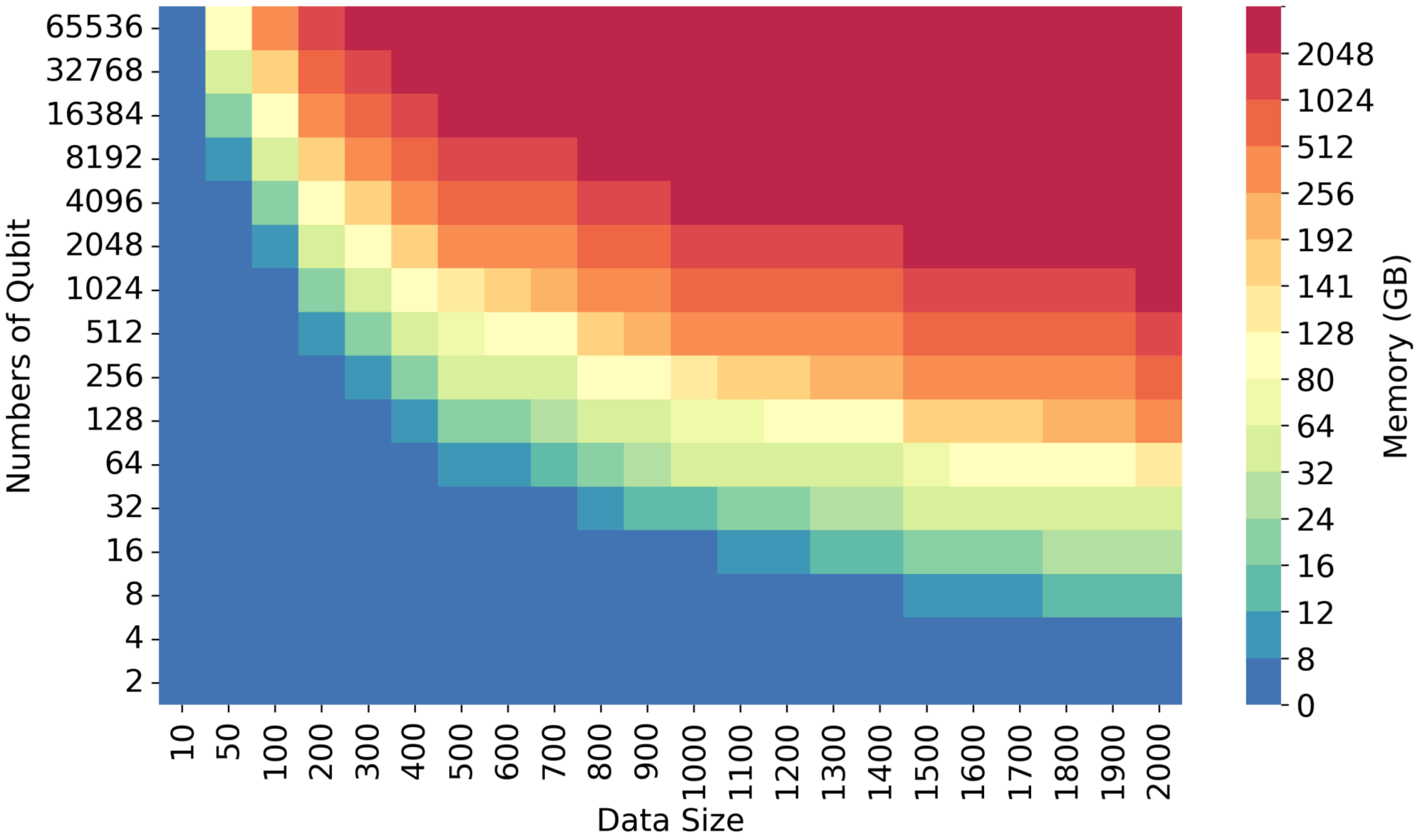
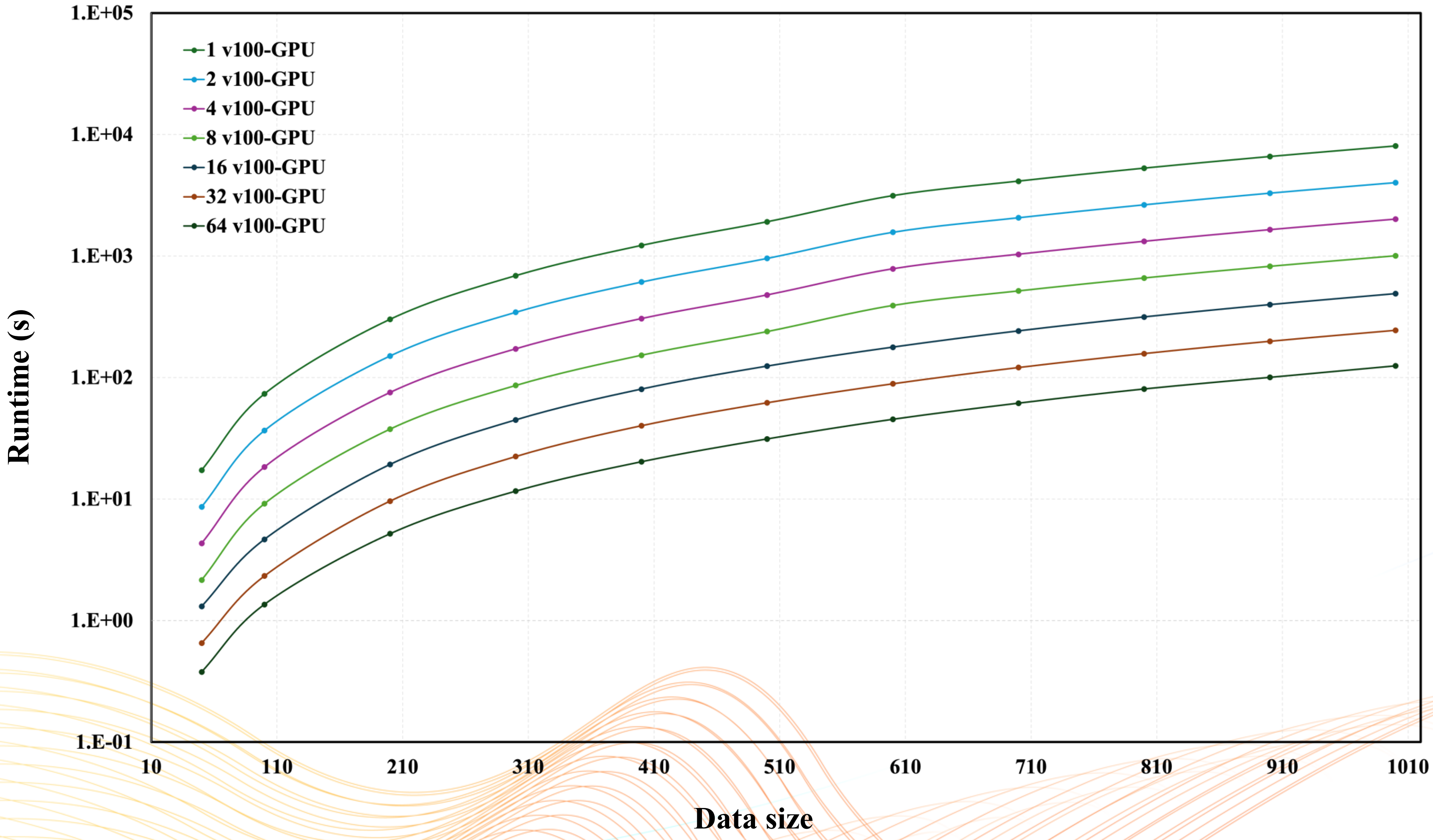


Scalable Quantum Support Vector Machine Simulation



Scalable Quantum Support Vector Machine Simulation

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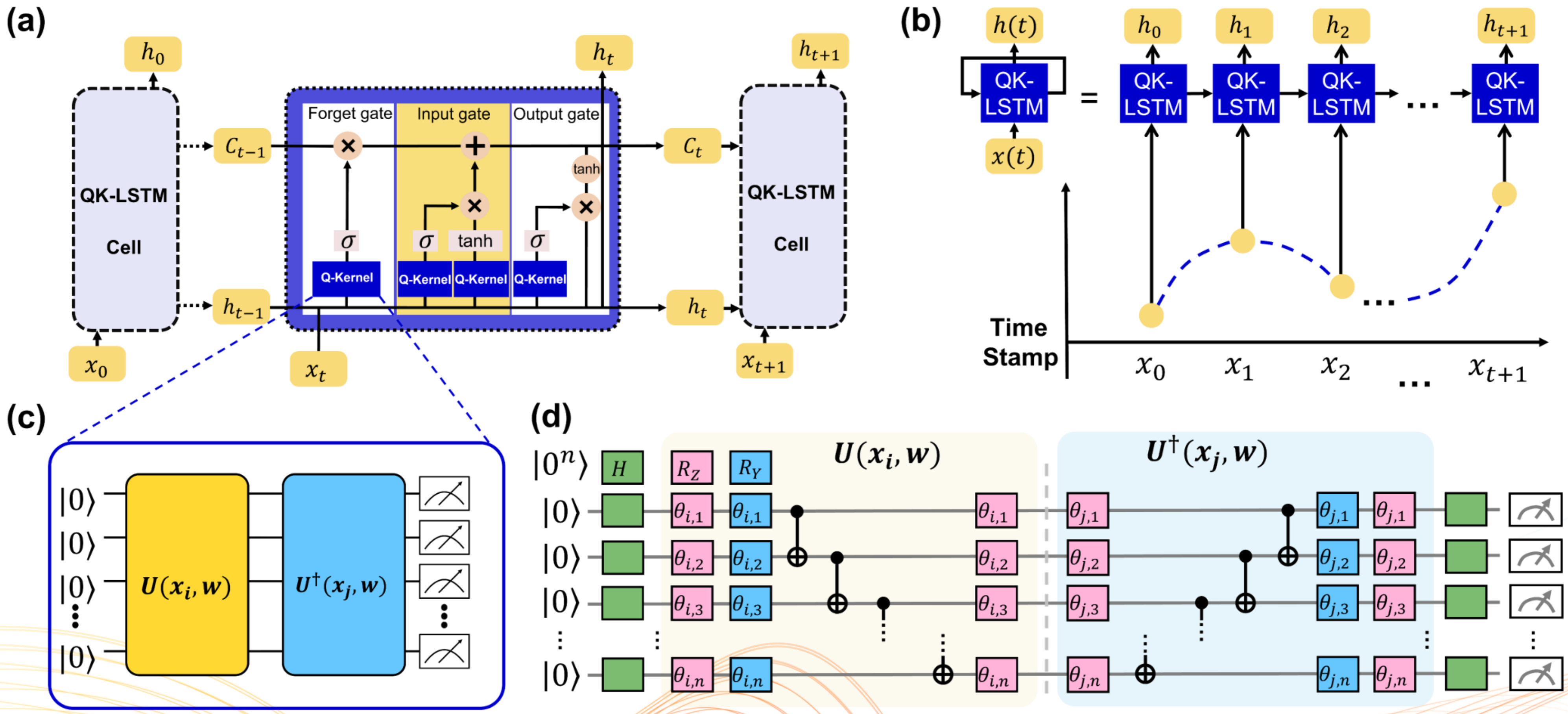
Qubit	Data Size	Quantum Circuit	Quantum Circuit/GPU	GPUs	Build QC and TN (s)	Renew TN (s)	Build Environment (s)	Get Path (s)	Contraction (s)	Total Time (s)
2048	50	1225	20	64	1.374	3.098	0.37	8.637	4.845	18.324
2048	100	4950	78	64	1.348	5.716	0.382	8.673	18.647	34.766
2048	200	19900	311	64	1.36	16.201	0.373	8.698	83.4	110.032
2048	300	44850	701	64	1.38	41.769	0.406	8.789	183.441	235.785
2048	400	79800	1247	64	1.375	73.437	0.394	8.962	326.574	410.742
2048	500	124750	1950	64	1.382	110.838	0.396	8.923	513.117	634.656
2048	600	179700	2808	64	1.392	156.375	0.418	9.28	739.758	907.223
2048	700	244650	3823	64	1.397	212.694	0.405	9.241	1003.388	1227.125
2048	800	319600	4994	64	1.386	288.6	0.419	9.728	1317.922	1618.055
2048	900	404550	6322	64	1.404	350.633	0.424	9.746	1671.988	2034.195
2048	1000	499500	7805	64	1.389	447.505	0.432	10.242	2072.545	2532.113

Quantum Kernel-based Long Short-Term Memory

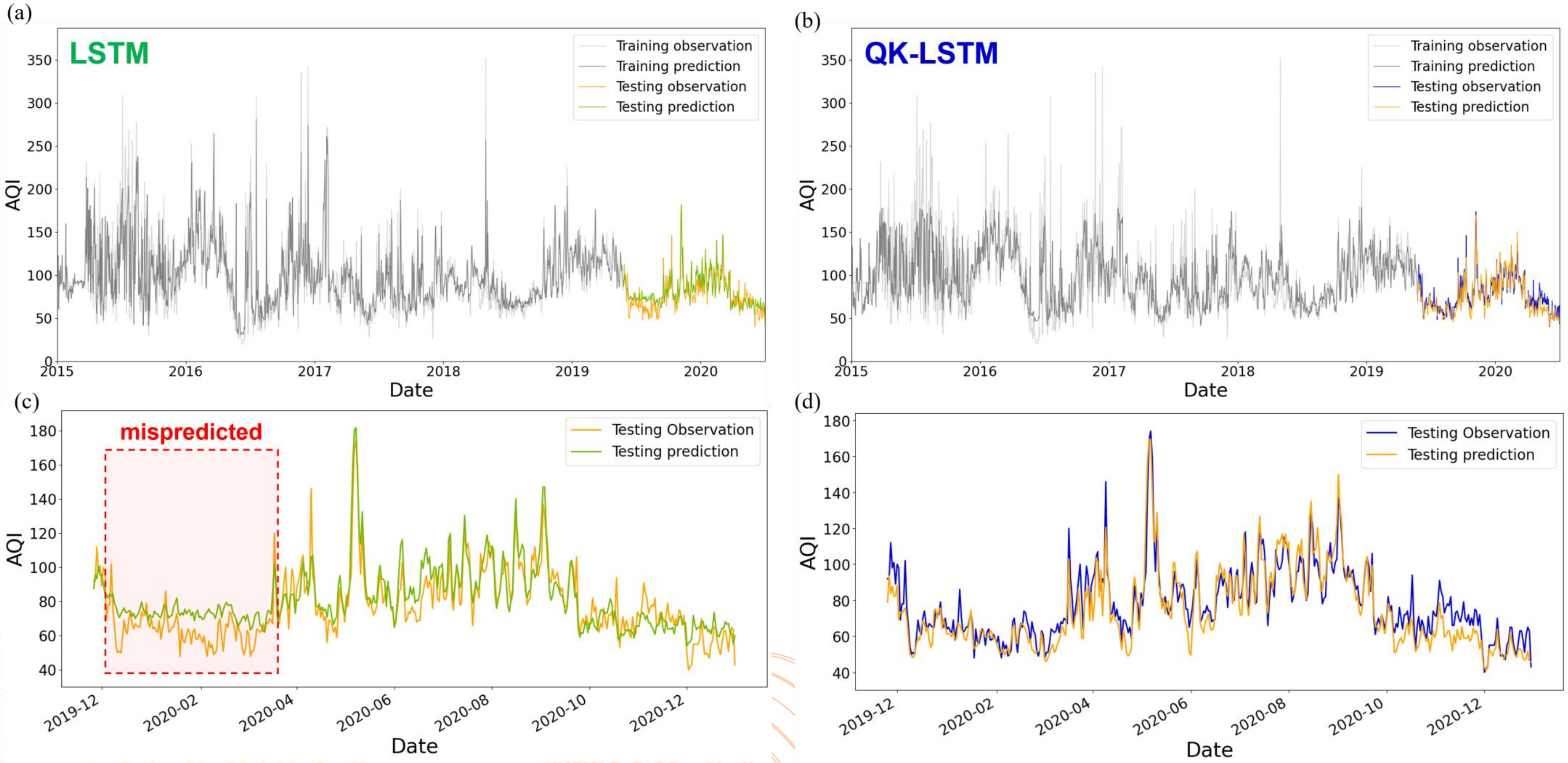
Overview of the QK-LSTM architecture



“Quantum Kernel-Based Long Short-term Memory for Climate Time-Series Forecasting”, IEEE QCNC 2025

Quantum Kernel-based Long Short-Term Memory

Comparative analysis of air quality prediction performance using classical LSTM and QK-LSTM models



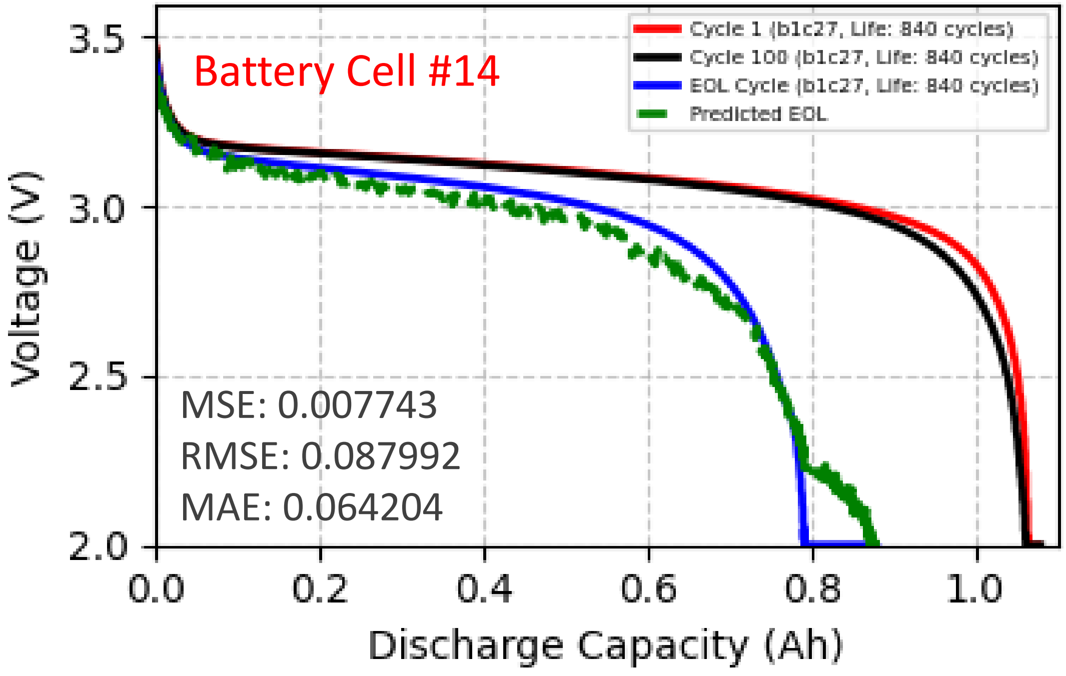
"Quantum Kernel-Based Long Short-term Memory for Climate Time-Series Forecasting", IEEE QCNC 2025

Quantum Kernel-based Long Short-Term Memory

- Input: The first 100 cycles of each battery [capacitance, voltage, current, temperature]
- Target: V(Q) of each batter's EOL (last discharge curve)

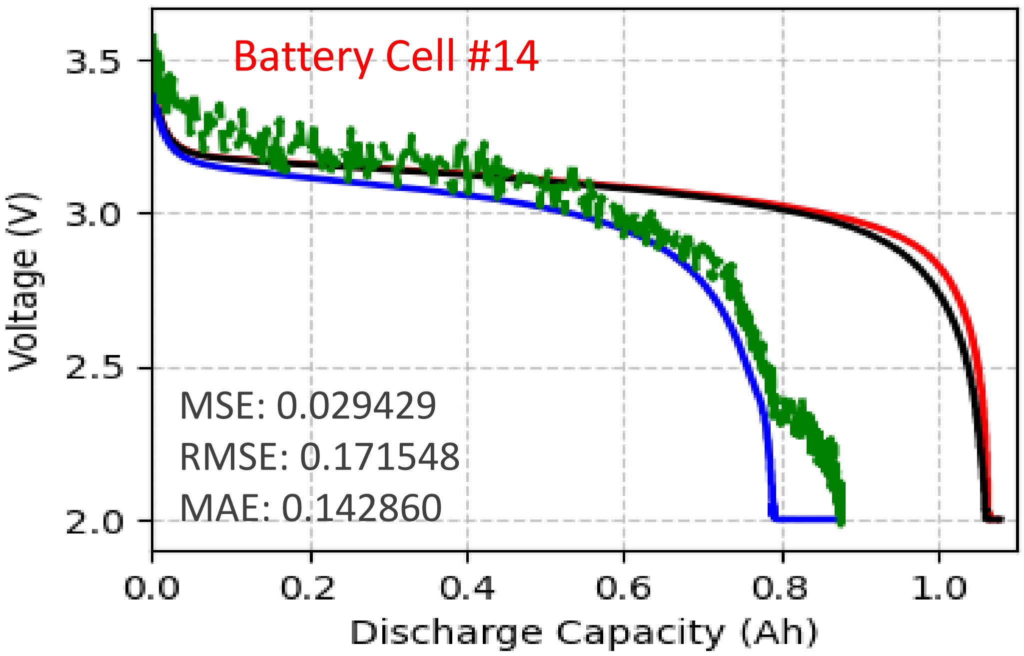
- Training dataset: 91 batteries
- Testing dataset: 23 batteries

QKLSTM :The Best Battery Cell #14



Number of QKLSTM Layer parameter:164

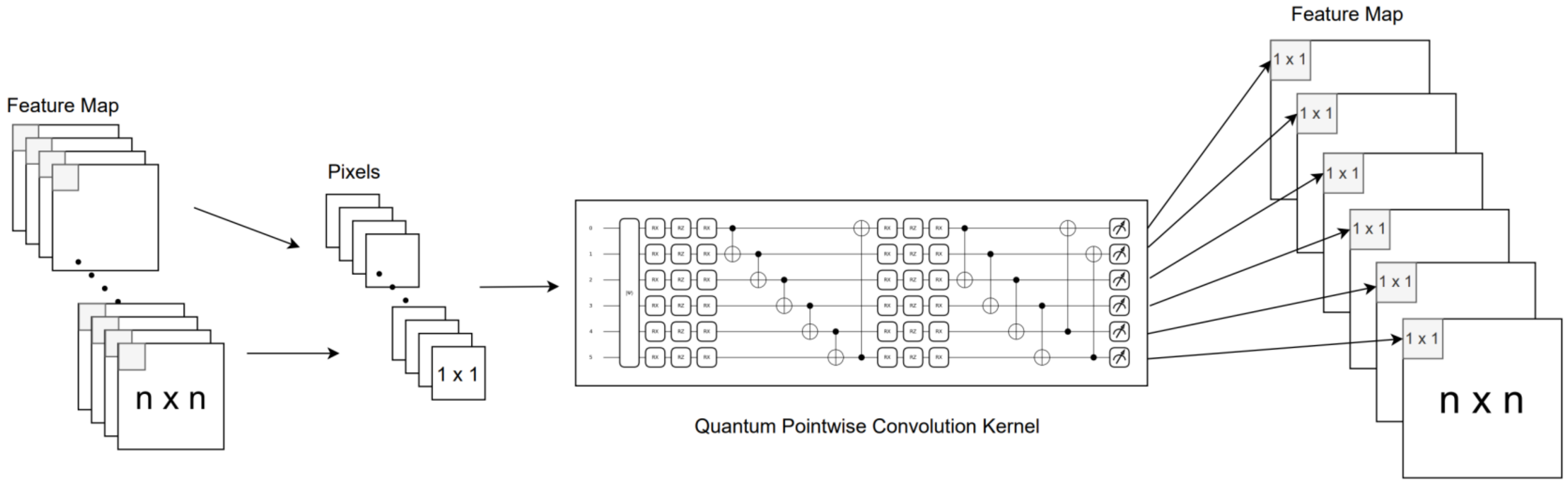
LSTM :The Best Battery Cell #14



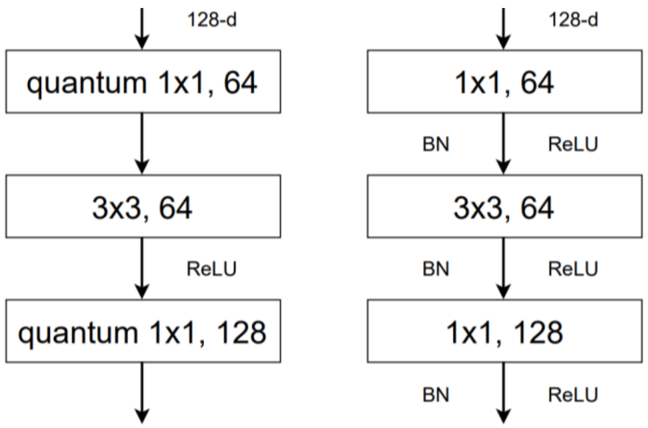
Number of LSTM Layer parameter:17920

Quantum Pointwise Convolution Networks

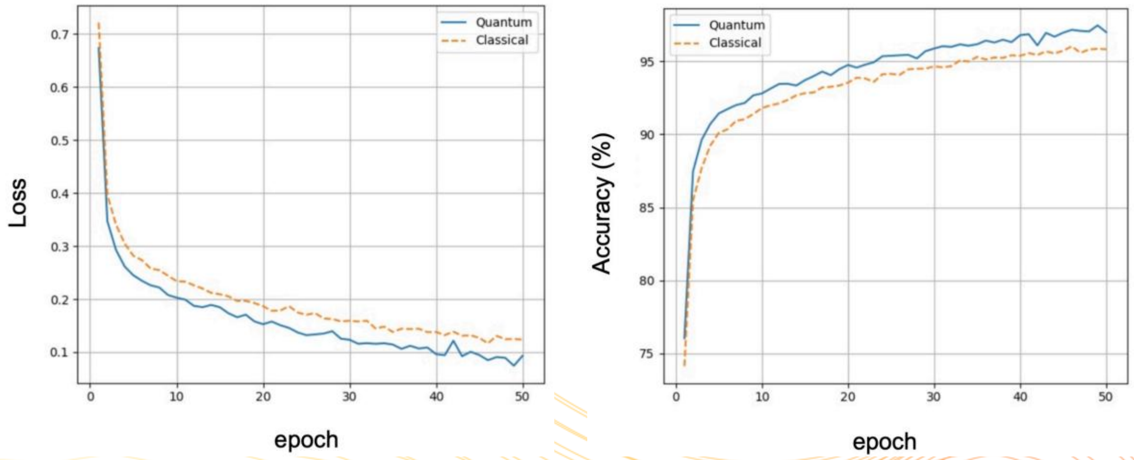
(a) Overview of the Quantum Pointwise Convolution Networks (QPWCNN)



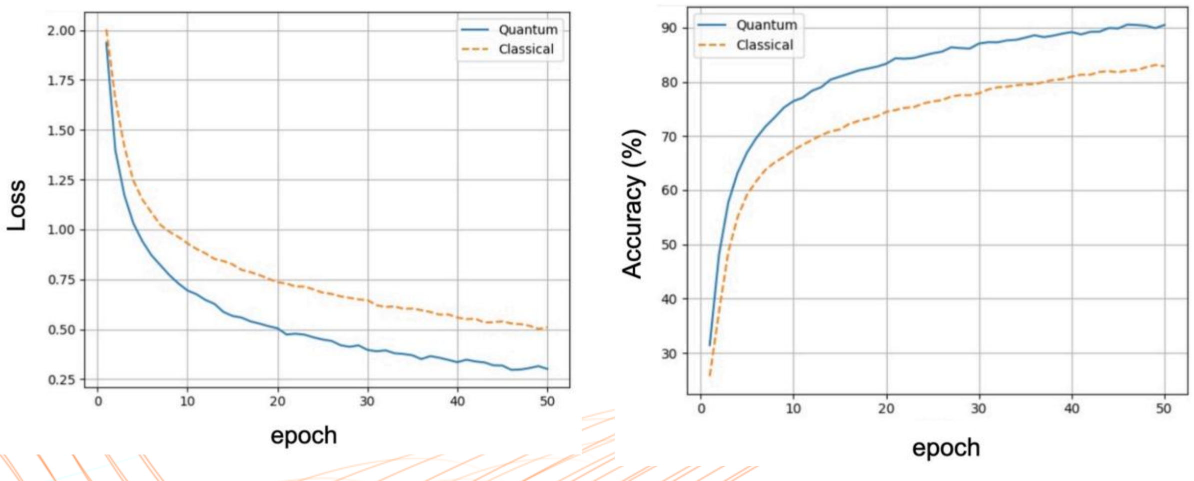
(b) With and without QPWCNN layer



(c) Fashion mnist Result



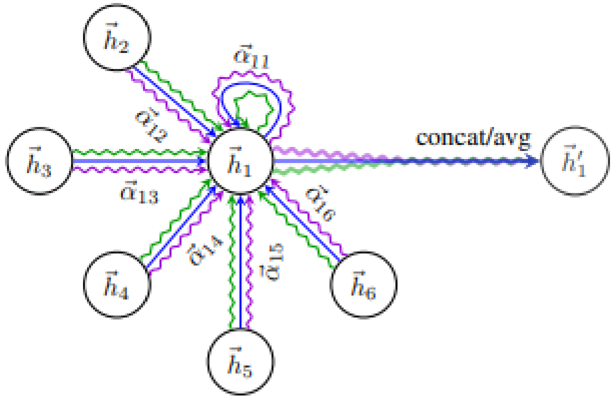
(d) Cifar10 Result



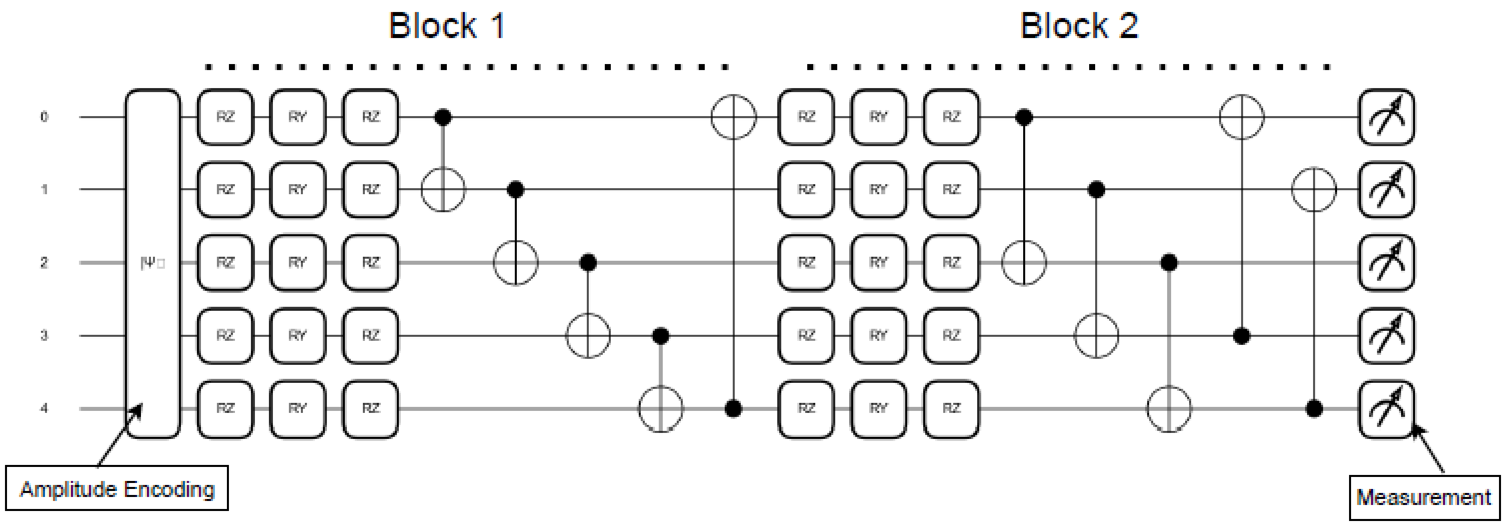
"Quantum Pointwise Convolution: A Flexible and Scalable Approach for Neural Network Enhancement", IEEE QCNC 2025

Quantum Graph Attention Network

A Novel Quantum Multi-Head Attention Mechanism for Graph Learning



An illustration of multi-head attention (with K = 3 heads) by node 1 on its neighborhood. Different arrow styles and colors denote independent attention computations. The aggregated features from each head are concatenated or averaged to obtain $\overrightarrow{h_1'}$. (https://arxiv.org/abs/1710.10903)



Example of a quantum circuit used in QGAT

"Quantum Graph Attention Network: A Novel Quantum Multi-Head Attention Mechanism for Graph Learning", Submitted to NeurIPS

Quantum Graph Attention Network

Benchmark results

Table 1: Accuracy (%) on transductive node classification benchmarks. All results are averaged over 5 runs; standard deviations are reported.

Model	Pubmed	ogbn-arxiv	ogbn-products
GAT [11]	78.1 ± 0.59	71.54 ± 0.3	79.04 ± 1.54
GATv2 [11]	78.5 ± 0.38	71.87 ± 0.25	80.63 ± 0.7
QGAT	$\mathbf{79.2 \pm 0.62}$	$\mathbf{73.62 \pm 0.42}$	$\mathbf{82.10 \pm 2.31}$

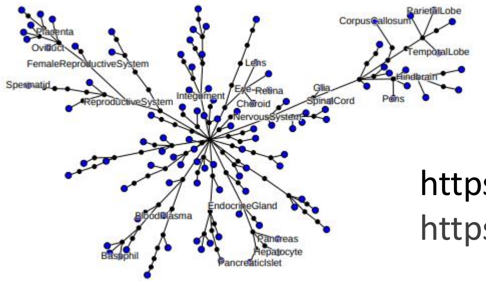
Table 2: Inductive node classification performance on PPI and ogbn-proteins. Metric: Micro-F1 (PPI) and ROC-AUC (ogbn-proteins). All results are averaged over 5 runs; standard deviations are reported.

Model	PPI (Micro-F1)	ogbn-proteins (ROC-AUC)
GAT [6]	97.3 ± 0.20	78.63 ± 1.62
GATv2	98.2 ± 0.25	$\mathbf{79.52 \pm 0.55}$ [11]
QGAT	$\mathbf{98.9 \pm 0.12}$	79.41 ± 0.21

Table 3: Link prediction performance on OGB benchmarks. Metric: Hits@50 (%) for *ogbl-collab*, and Mean Reciprocal Rank (MRR) for *ogbl-citation2*. All results are averaged over 5 runs; standard deviations are reported.

Model	ogbl-collab	ogbl-citation2
GAT [11]	46.63 ± 2.80	75.95 ± 1.31
GATv2 [11]	49.7 ± 3.08	80.14 ± 0.71
QGAT	$\mathbf{51.2 \pm 1.92}$	$\mathbf{82.2 \pm 1.27}$

https://arxiv.org/abs/2005.00687



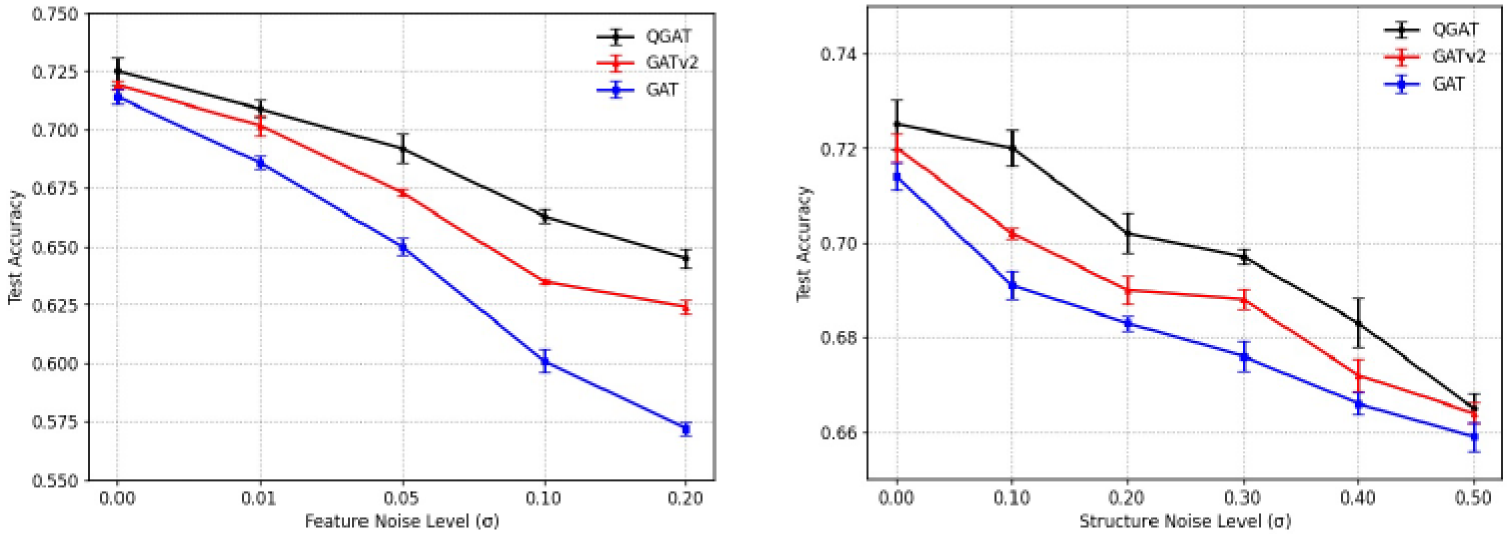
https://arxiv.org/abs/1707.04638
https://arxiv.org/abs/1706.02216

https://snap.stanford.edu/

"Quantum Graph Attention Network: A Novel Quantum Multi-Head Attention Mechanism for Graph Learning", Submitted to NeurIPS

Quantum Graph Attention Network

Robustness to Noise



(a) Feature noise. Test accuracy under Gaussian perturbation with σ.

(b) Structural noise. Test accuracy under random edge insertion with σ.

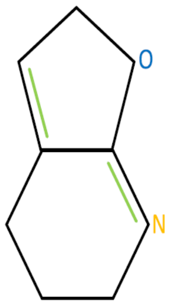
Figure 2: Robustness comparison of QGAT, GATv2, and GAT under feature and structural noise. Each point is averaged over 5 runs with standard deviation shown as error bars.

“Quantum Graph Attention Network: A Novel Quantum Multi-Head Attention Mechanism for Graph Learning”, Submitted to NeurIPS

Quantum Circuit for Molecular Generation

Overview of the quantum-based molecular generator (QMG)

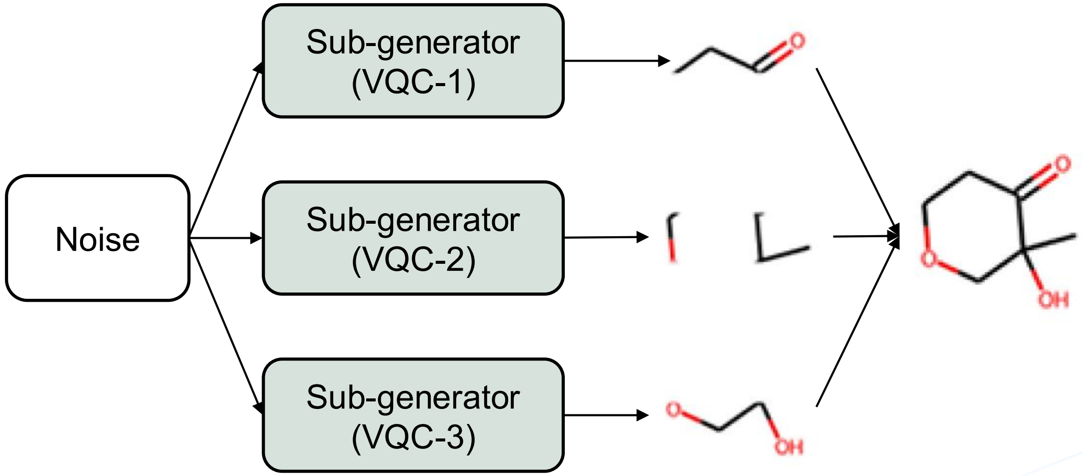
QM9 datastes: Only C,N,O atoms and 9 heavy atoms at most (ignore F atom).



$$B = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 2 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 2 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 2 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 \end{bmatrix}$$

$$A = [1 \quad 3 \quad 1 \quad 2 \quad 1 \quad 1 \quad 1 \quad 1 \quad 1]$$

$$a_i \in \{\text{None}, \text{C}, \text{N}, \text{O}\}^9$$
$$b_{ij} \in \{\text{None}, \text{single}, \text{double}, \text{triple}\}^{36}$$
$$\log_2 4^9 + \log_2 4^{36} = 90 \text{ qubits}$$

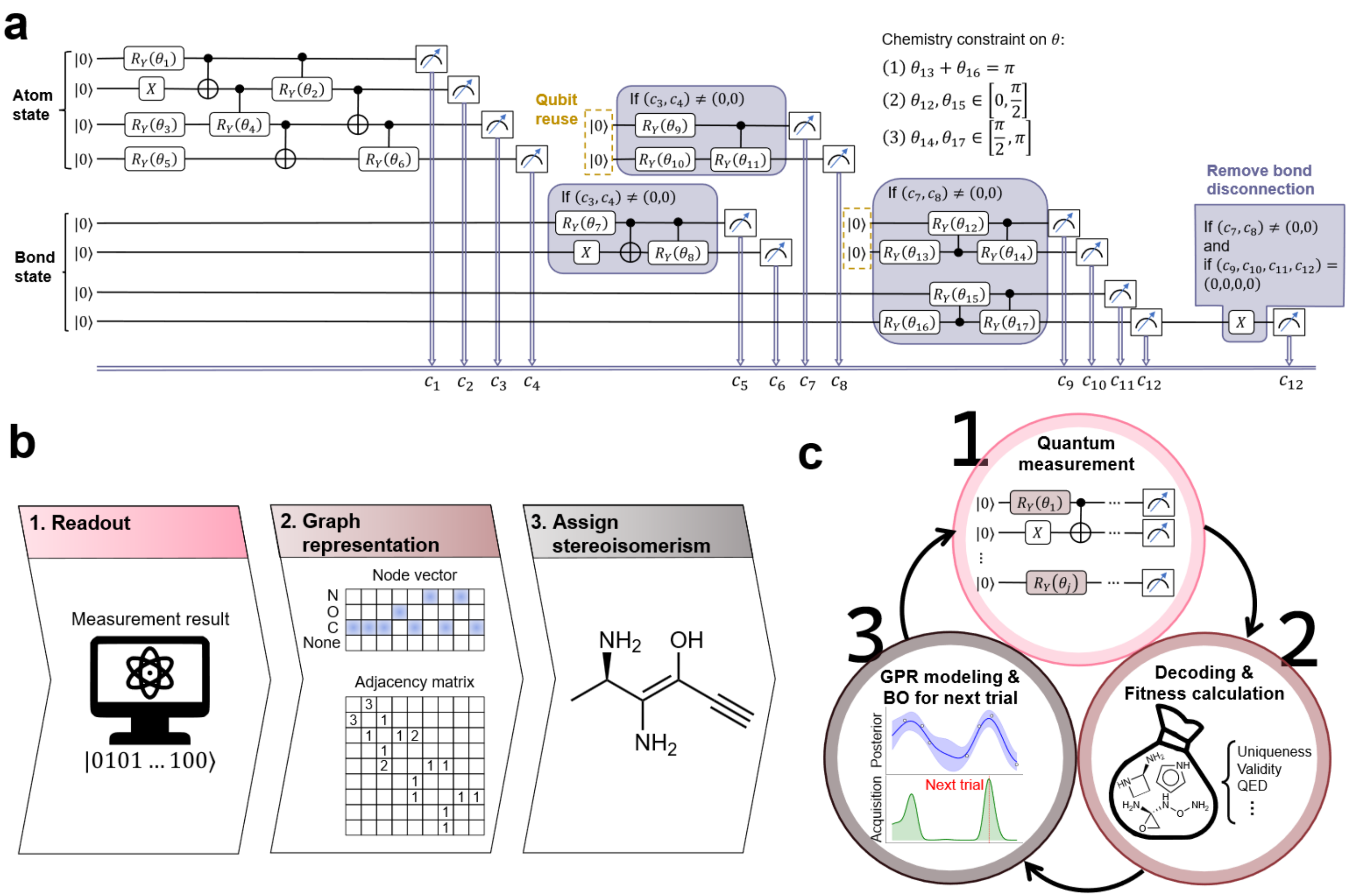


“Exploring Chemical Space with Chemistry-Inspired Dynamic Quantum Circuits in the NISQ Era”, ACS Journal of Chemical Theory and Computation (Accpeted)

Quantum Circuit for Molecular Generation

國家實驗研究院
NATIONAL INSTITUTES OF APPLIED RESEARCH

Overview of the quantum-based molecular generator (QMG)



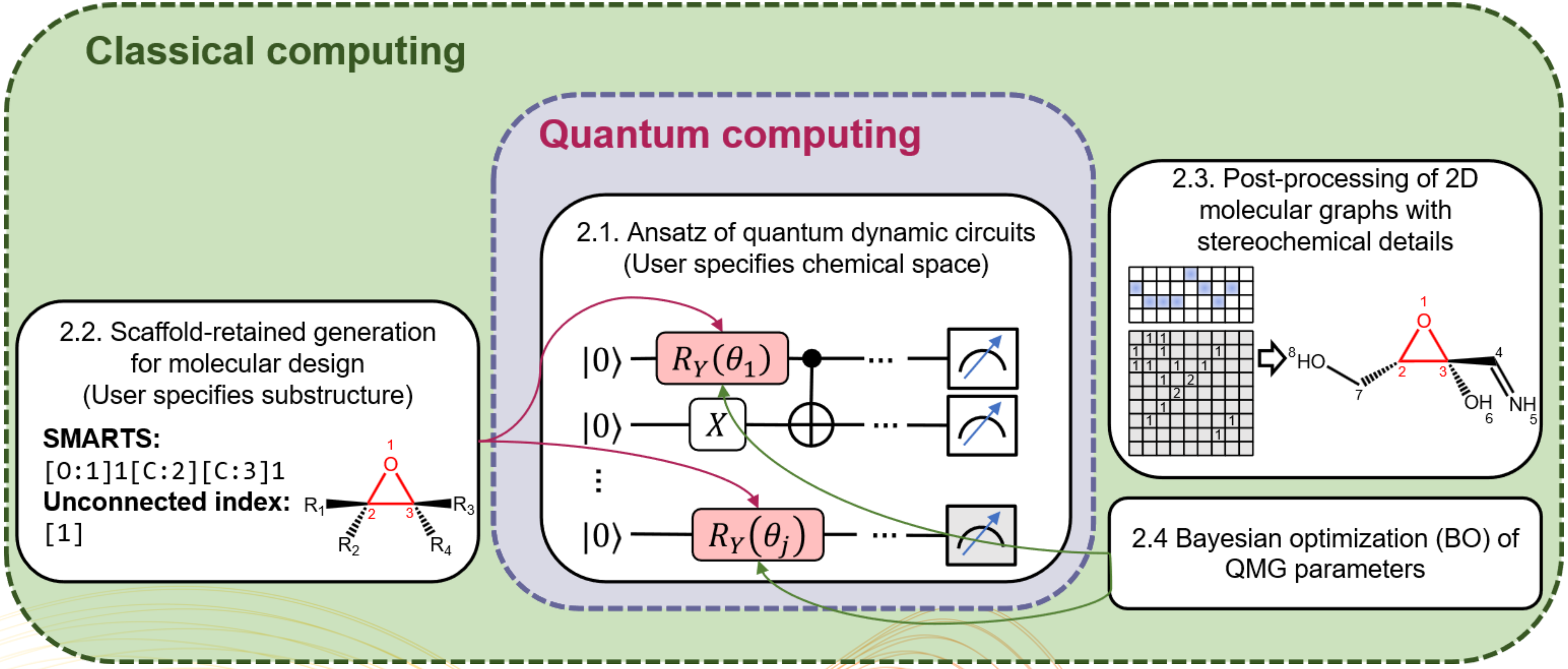
Overview of the molecular structure generation and using dynamic quantum circuit. (a) An illustration figure of 3-heavy atom quantum-based molecule generator (QMG). (b) The measurement outcome (binary value) would be post-processed to molecular structures on classical computers. (c) The parameters in quantum generator take the Bayesian optimization (BO) routine for enhancing properties and validity.

"Exploring Chemical Space with Chemistry-Inspired Dynamic Quantum Circuits in the NISQ Era", ACS Journal of Chemical Theory and Computation (Accpeted)

Quantum Circuit for Molecular Generation

国家實驗研究院
NATIONAL INSTITUTES OF APPLIED RESEARCH

Overview of the quantum-based molecular generator (QMG)

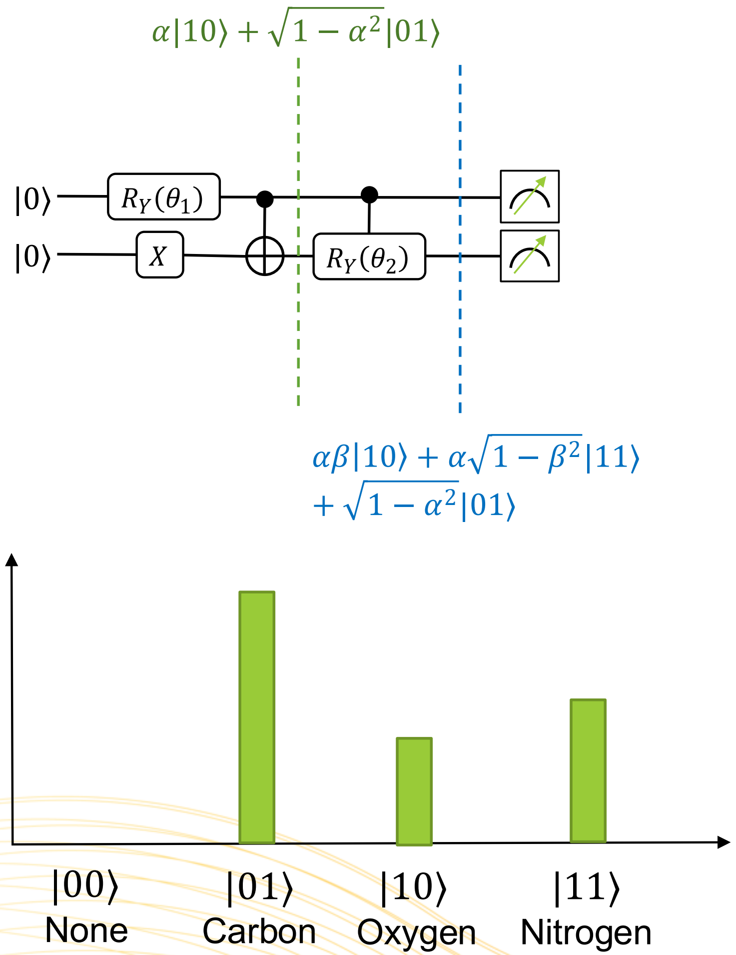


Overview of the quantum-based molecular generator (QMG) construction process.

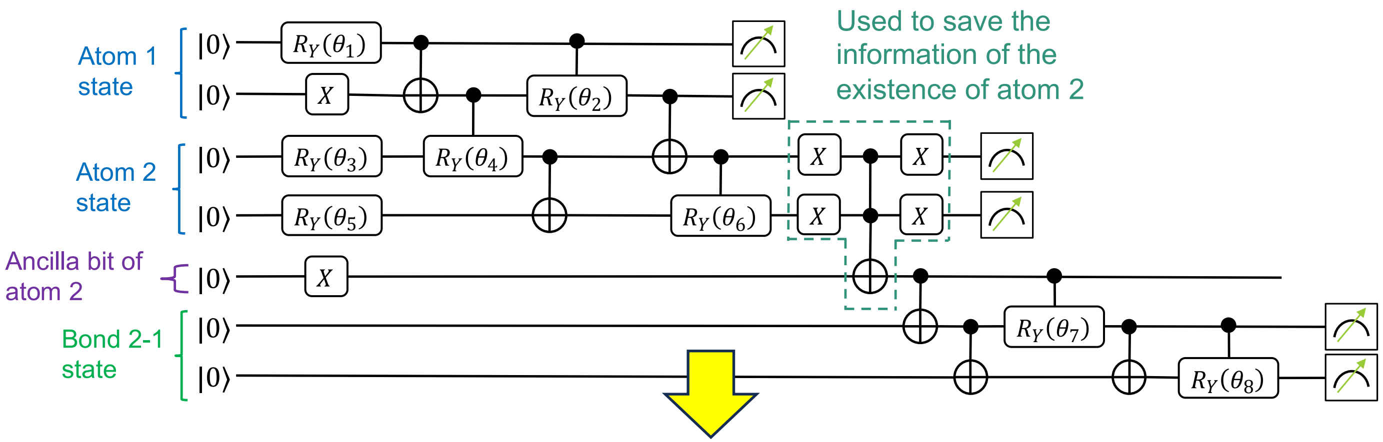
"Exploring Chemical Space with Chemistry-Inspired Dynamic Quantum Circuits in the NISQ Era", ACS Journal of Chemical Theory and Computation (Accpeted)

Quantum Circuit for Molecular Generation

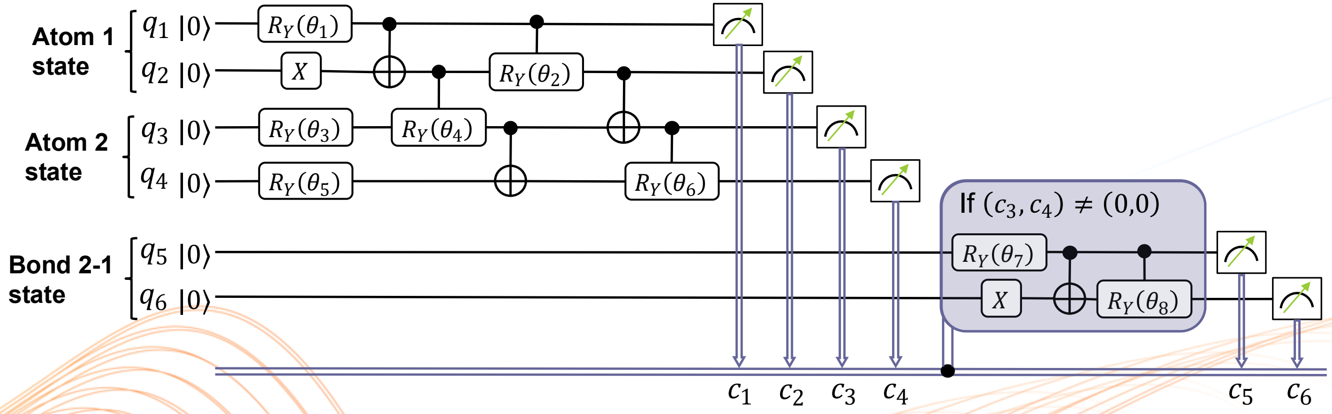
(a) One-heavy atom system



(b) Two-heavy atom system：Static Circuit



(c) Two-heavy atom system： Dynamic Circuit



"Exploring Chemical Space with Chemistry-Inspired Dynamic Quantum Circuits in the NISQ Era", ACS Journal of Chemical Theory and Computation (Accpeted)

Quantum Circuit for Molecular Generation

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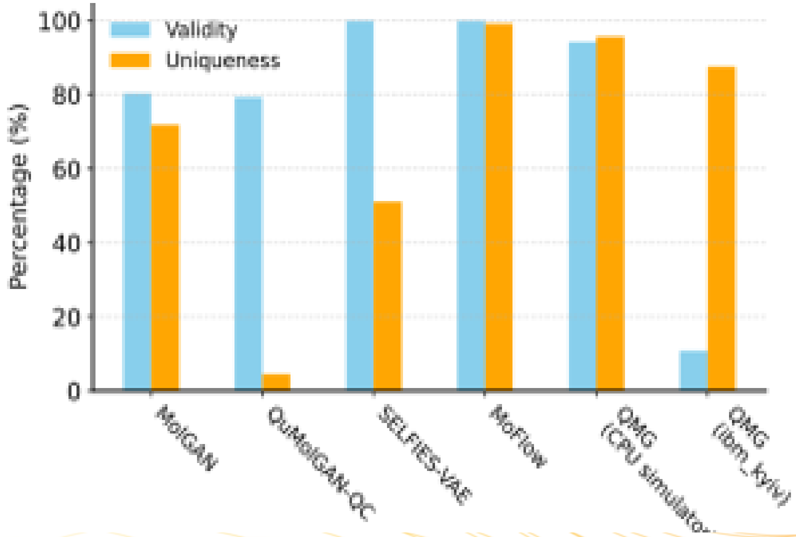
No. of heavy atoms	No. of qubits required for **static** circuit	No. of qubits required for **dynamic** circuit	No. of parameters in dynamic circuit	Valid proportion of quantum state (%)
2	6	6	8	45.32
3	12	8	17	10.67
4	20	10	29	1.10
5	30	12	44	0.04
6	42	14	62	-
7	56	16	83	-
8	72	18	107	-
9	90	20	134	-
N	$N(N+1)$	$2(N+1)$	$8+3(N-2)(N+3)/2$	-

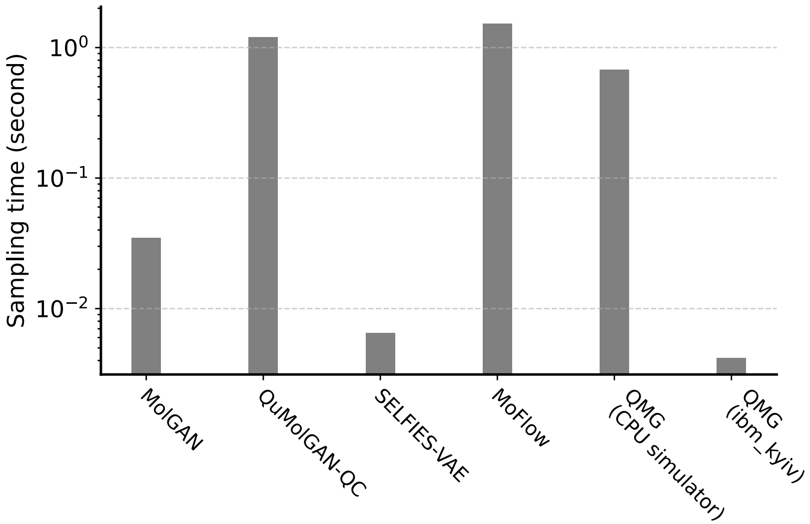
“Exploring Chemical Space with Chemistry-Inspired Dynamic Quantum Circuits in the NISQ Era”, ACS Journal of Chemical Theory and Computation (Accpeted)

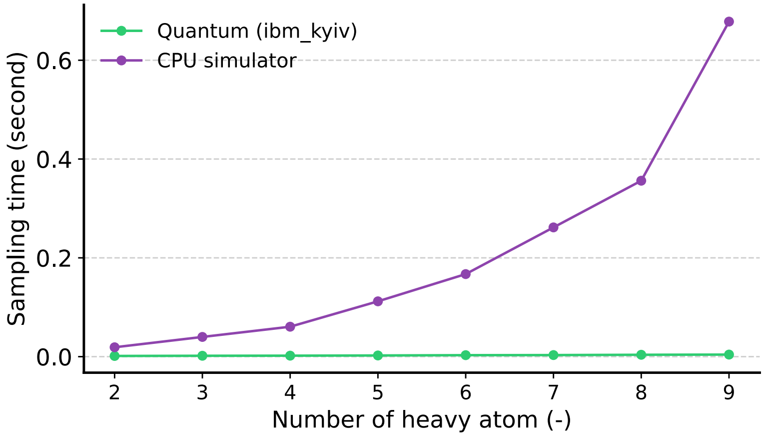
Quantum Circuit for Molecular Generation

Benchmark Result

Model	Validity (%) (↑)	Uniqueness (%) (↑)	No. of parameters (↓)
MolGAN [1]	80.40	71.89	~576,000
QuMolGAN-QC [2]	79.39	4.49	~90,000
SELFIES-VAE [3]	100	51.08	~77,000
MoFlow [4]	100	99.26	~2,712,000
QMG (Ours)	93.9	94.6	**134**







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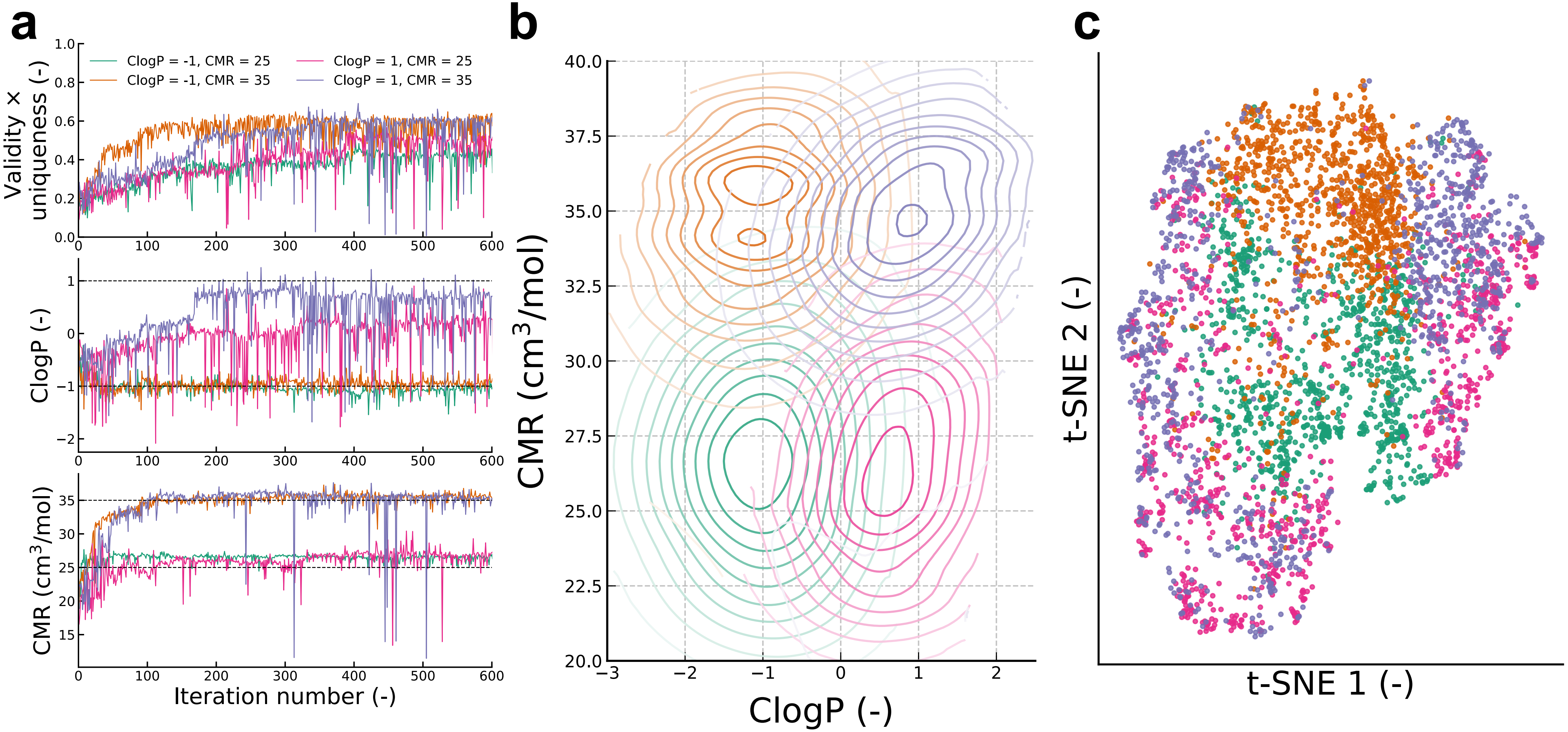
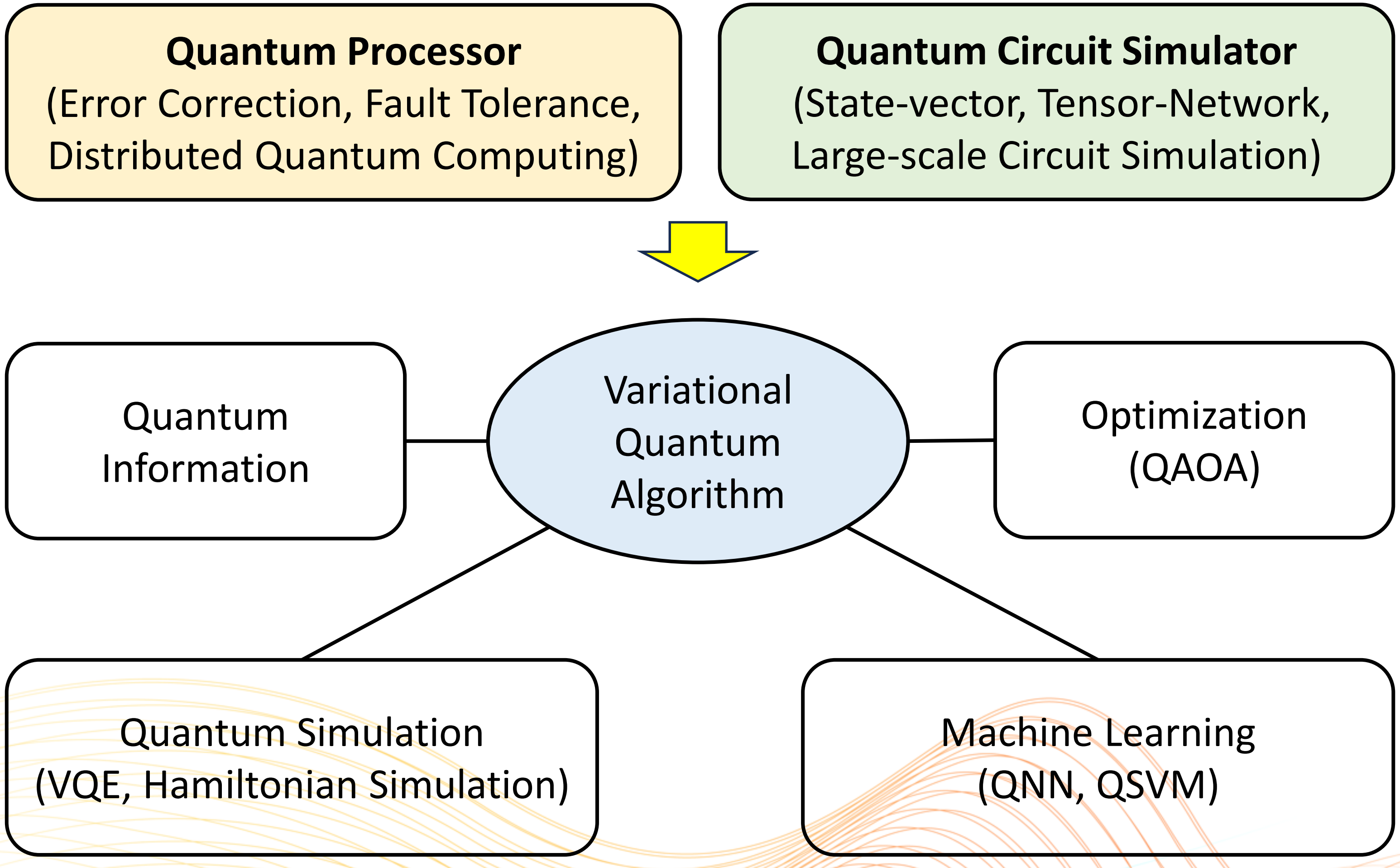
Quantum Circuit for Molecular Generation



"Exploring Chemical Space with Chemistry-Inspired Dynamic Quantum Circuits in the NISQ Era", ACS Journal of Chemical Theory and Computation (Accpeted)

Future Works

Gate-base system



Annealing-base system

- QUBO
- Quantum Annealing (QA)
- Simulated Quantum Annealing (SQA)
- Hybrid Quantum–Classical Annealing
- Classical Simulated Annealing (SA)

Collaborators

陳南佑/國網中心
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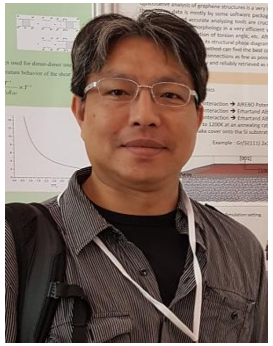
陳冠朋/國網中心
楊安正/國網中心
林俊鈺/國網中心

陳隆奕/台大化學系
甯安/KAIST
徐育兆/成大不分系
董甄茵/台大電機系

王允遠/NVIDIA
陳冠丞/QuEST

關於我們

科學計算小組

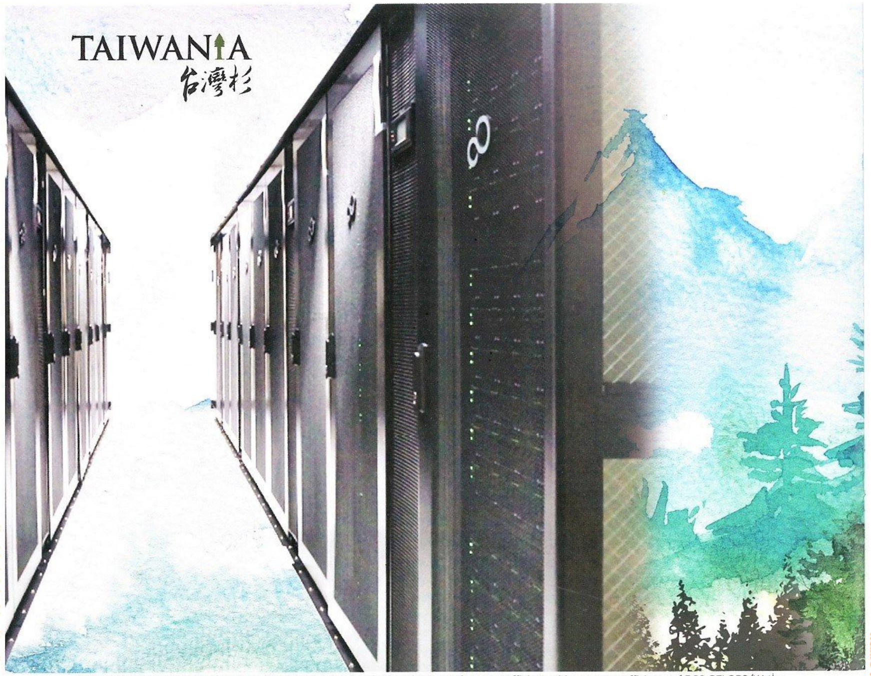




陳南佑 博士	李玟頡 博士	楊安正 博士	陳冠朋	李泰岳
清華大學物理博士	中山大學機械博士	成功大學機械博士	中央大學應數碩士	東華大學物理博士
影像資訊學、材料資訊學、半導體計算 機器學習、深度學習、大尺度平行計算 量子機器學習	微觀模擬、材料計算與材料資訊、平行計算、半導體量子傳輸模擬、機器學習與深度學習	微觀模擬、材料計算與材料資訊、平行計算、機器學習與深度學習、系統整合	統計分析、機器學習與深度學習、量子計算	深度學習、機器學習、X光斷層掃描重建、量子機器學習、大規模量子計算模擬

Thank you for your attention!

boost scientific insights and engineering ingenuity



▲ Taiwan's new Peta level high performance computing host: This host is extremely power-efficient, with an energy efficiency of 3.99 GFLOPS/W, the computation capacity of which is nearly 10 times more per watt than Windrider.