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Graph Partitioning Approach for Fast Quantum Circuit Simulation

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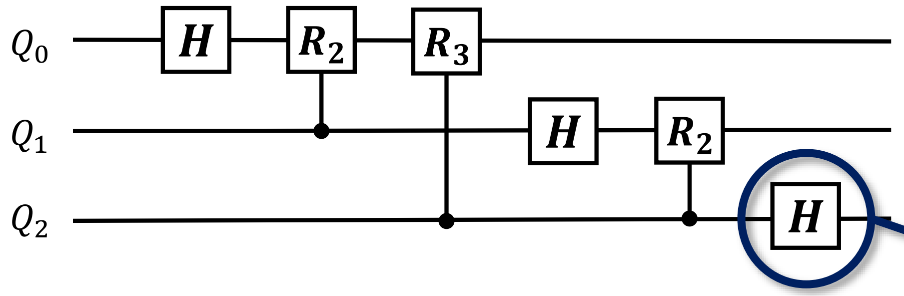
INTRODUCTION

What is Quantum Circuit?

Example) **3-Qubit Quantum Fourier Transform**



"***Quantum Circuit*** is an efficient and powerful method of ***describing quantum computation*** procedures."

M. Nielsen and I. Chuang,
"***Quantum Computation and Quantum Information***."

- **Hadamard Gate**

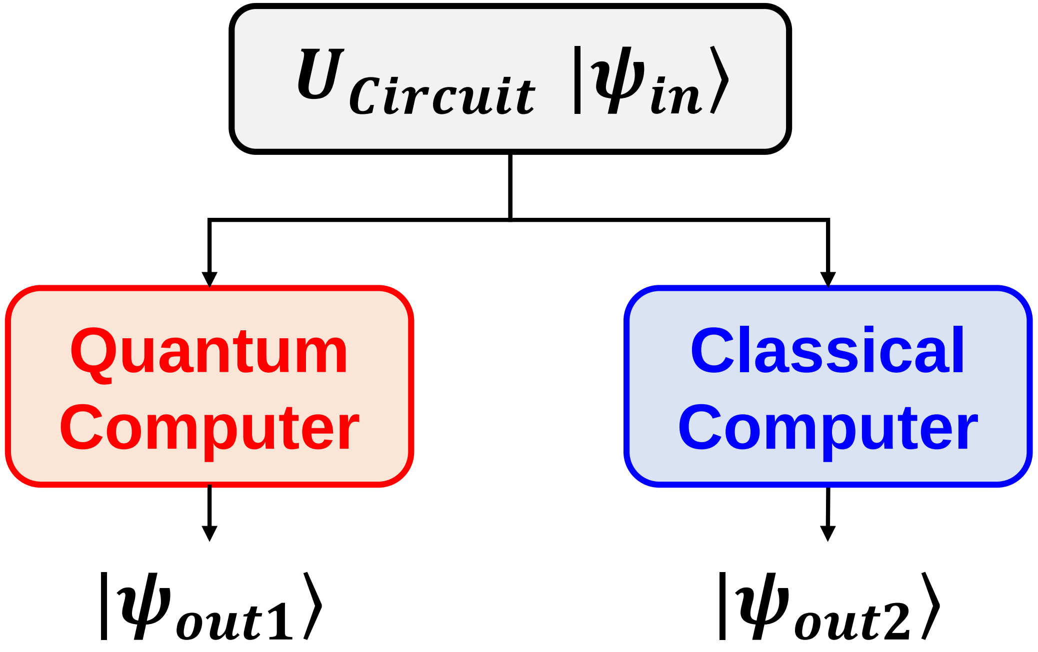
$$H = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

- **Unitary Matrix**

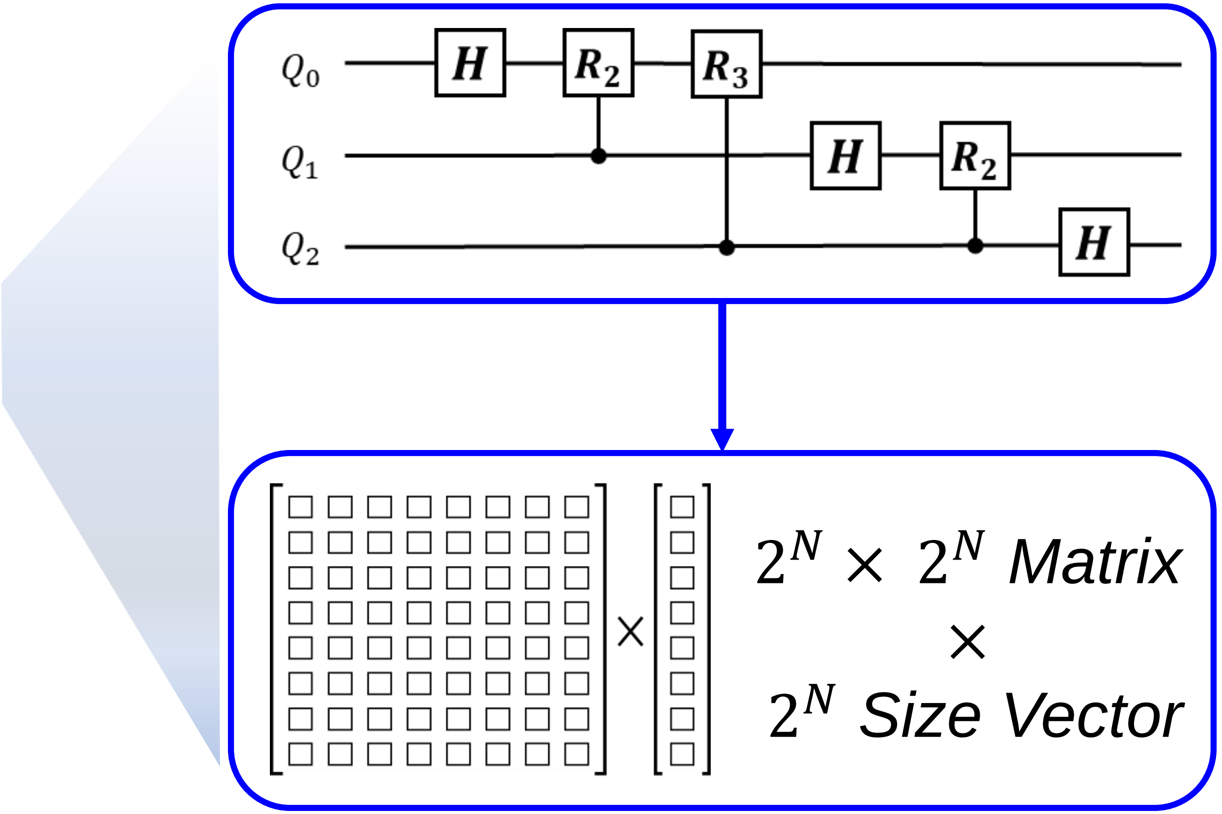
$$HH^{\dagger} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = I$$

- **Quantum circuit describes quantum computation procedures**.
- It consists of **quantum gates**, which can be represented by **unitary matrix**.

What is Quantum Circuit Simulation and Why it is difficult?

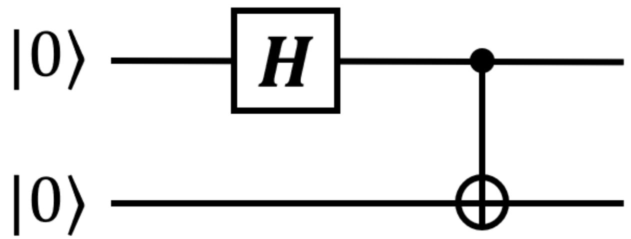


$$|\psi_{out1}\rangle == |\psi_{out2}\rangle\,?$$



- Simulation plays a key role in **verification** of quantum computing.
- But it is heavily **time-consuming**.

Two different Simulation Methods



Schrödinger-Style Simulation

$$|\psi_{out}\rangle = CNOT \times H \otimes I \times |00\rangle$$

$$= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \times \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \end{bmatrix} \times \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

Feynman-Style Simulation

$$Path1: CNOT \cdot \frac{1}{\sqrt{2}}|00\rangle = \frac{1}{\sqrt{2}}|00\rangle$$

$$Path2: CNOT \cdot \frac{1}{\sqrt{2}}|10\rangle = \frac{1}{\sqrt{2}}|11\rangle$$

$$|\psi_{out}\rangle = Path1 + Path2 = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$

- Schrödinger-Style: **Fast** but exponentially increasing **memory usage**.
- Feynman-Style: **Memory-efficient** but its **runtime depends on # of Paths.**

Hybrid Schrödinger-Feynman (HSF) Simulation

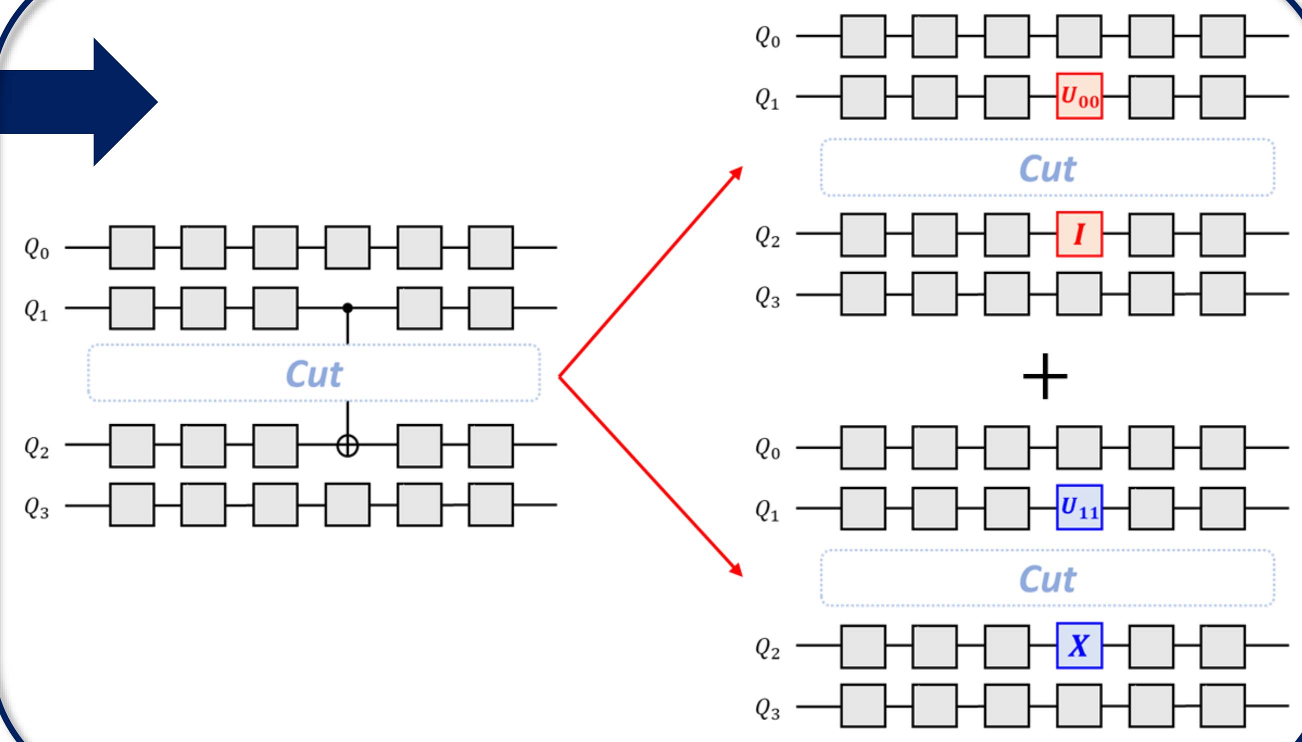
Gate Decomposition

$$\mathbf{G} = |0\rangle\langle 0| \otimes \mathbf{G}_{00} + |0\rangle\langle 1| \otimes \mathbf{G}_{01} + |1\rangle\langle 0| \otimes \mathbf{G}_{10} + |1\rangle\langle 1| \otimes \mathbf{G}_{11}$$

Example)

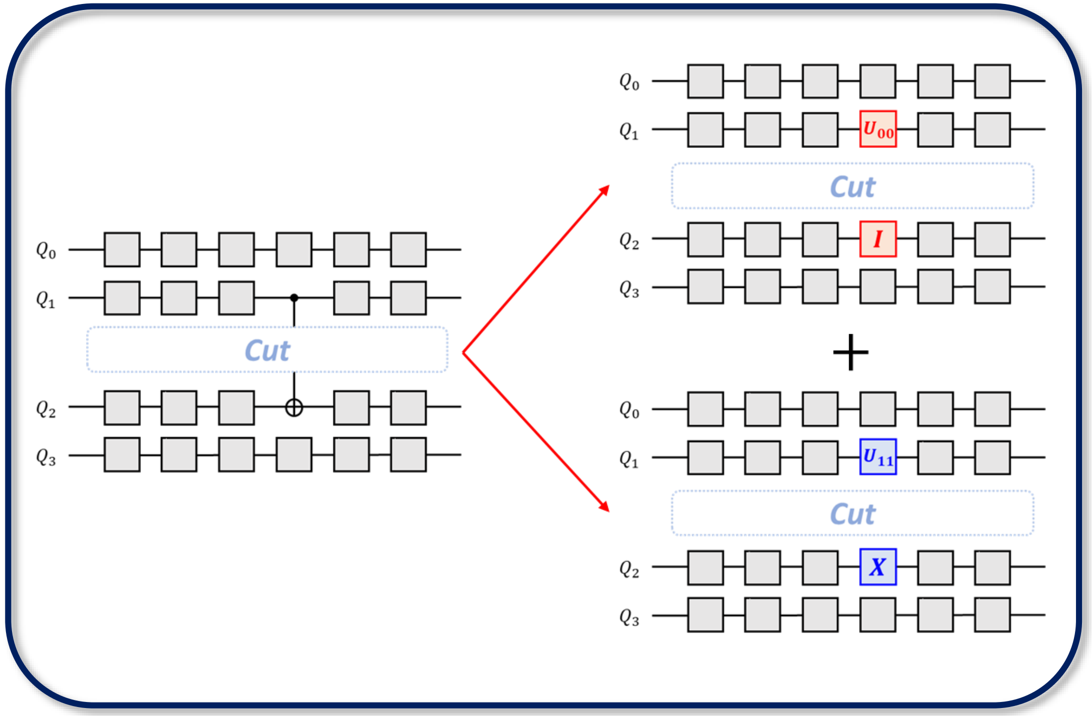
$$CNOT = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \otimes I + \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \otimes X$$

$$\rightarrow U_{00} \qquad \rightarrow U_{11}$$

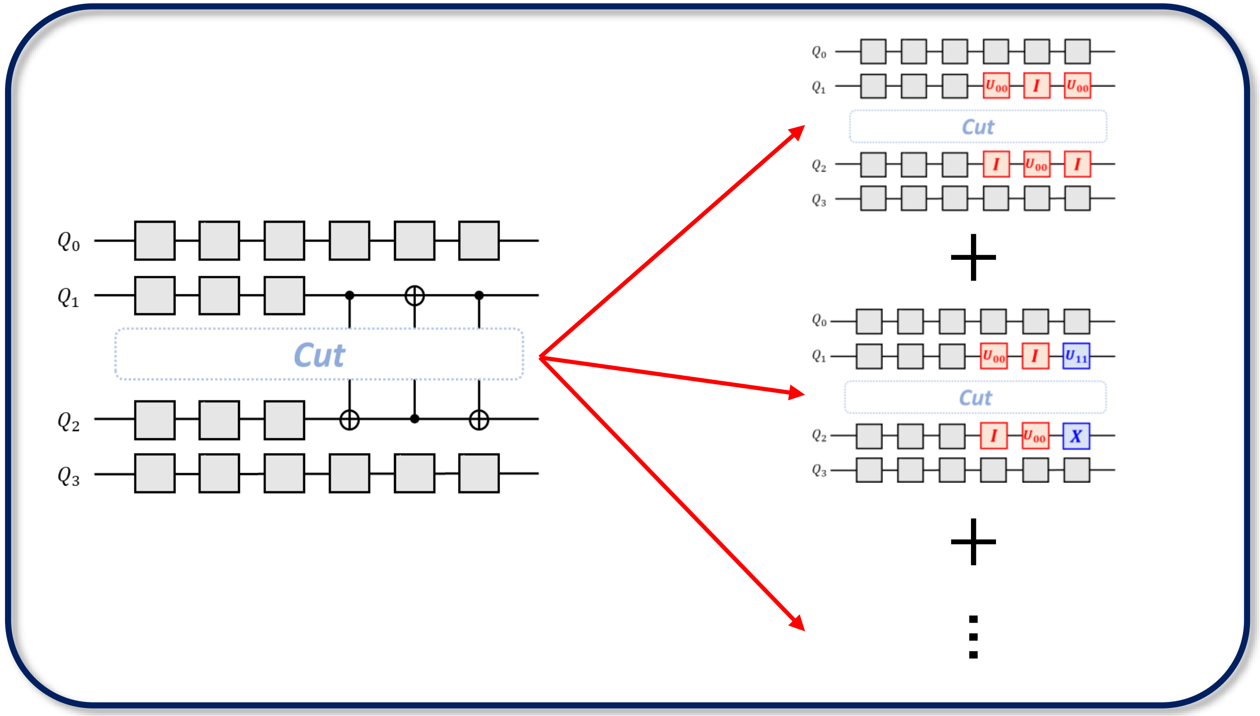


- **HSF** is a **mixture** of Schrodinger and Feynman Simulation.
- It can deal with circuits of smaller size.

Motivation



$\mathbf{1}$ Crossing Gates $\longrightarrow$ $\mathbf{2^1}$ Branches



$\boldsymbol{N}$ Crossing Gates $\longrightarrow$ $\mathbf{2^N}$ Branches

- HSF does not do well when there are too many crossing gates.
- **How can we reduce the the number of Crossing Gates?**

PROPOSED METHOD

Overall Flow

1. Graph Partitioning

- Build Weighted-Graph
- Fidducia-Mattheyses Algorithm

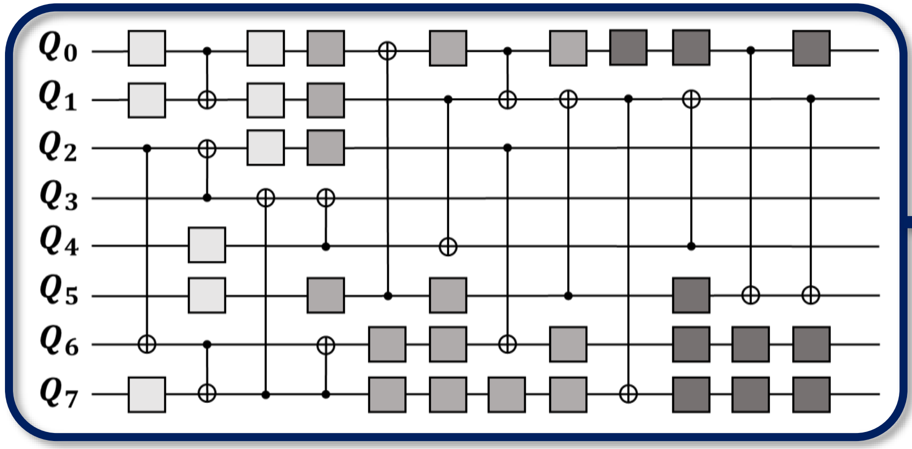
2. Layered Simulation

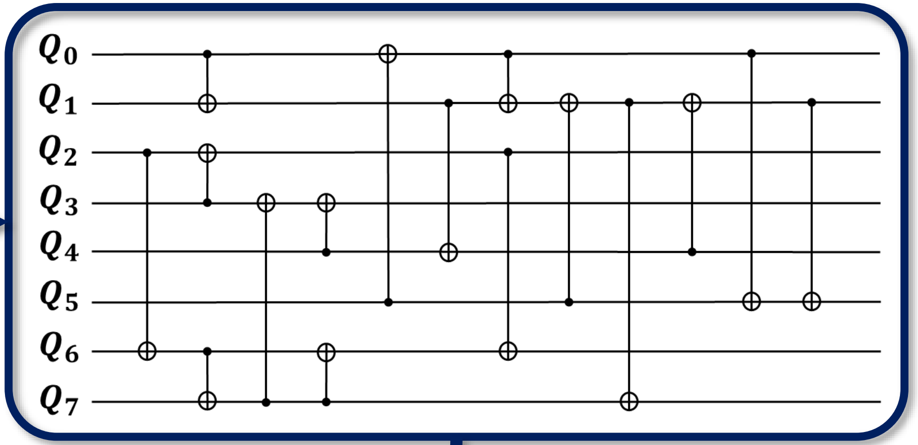
- Layer Assignment
- DFS Order Simulation

3. Qubit Re-Ordering

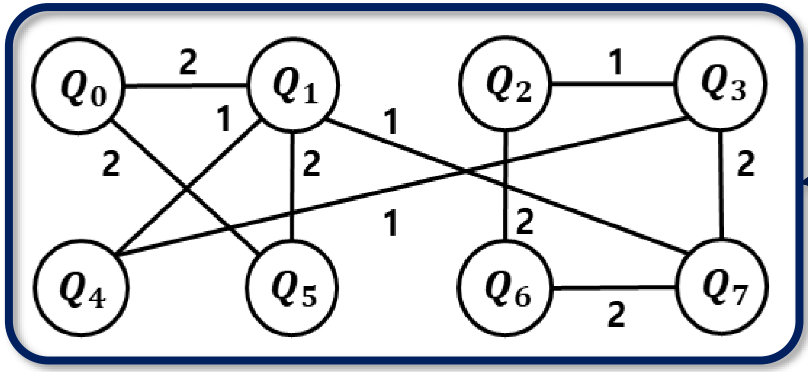
- Fast Qubit SWAP Procedure

1. Graph Partitioning - (1) Build Weighted-Graph



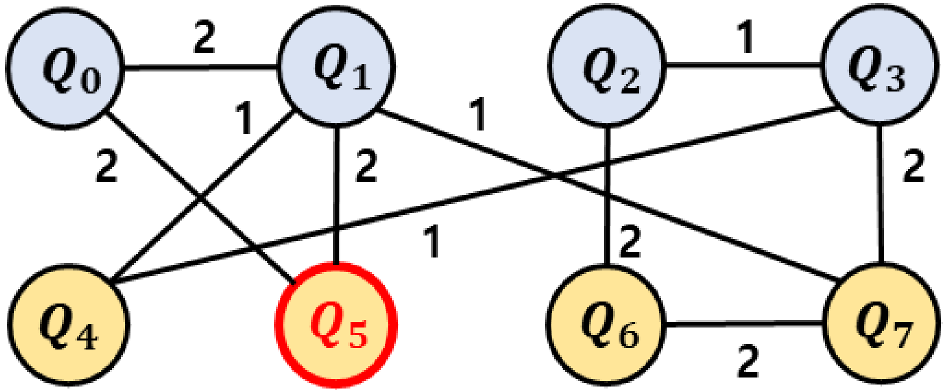


Weighted Graph



- **Ignore single-qubit gates**.
- **1)** Qubit ⟶ Vertex, **2)** # of two-qubit gates ⟶ Weight of edge.

1. Graph Partitoining – (2) FM Partitioning



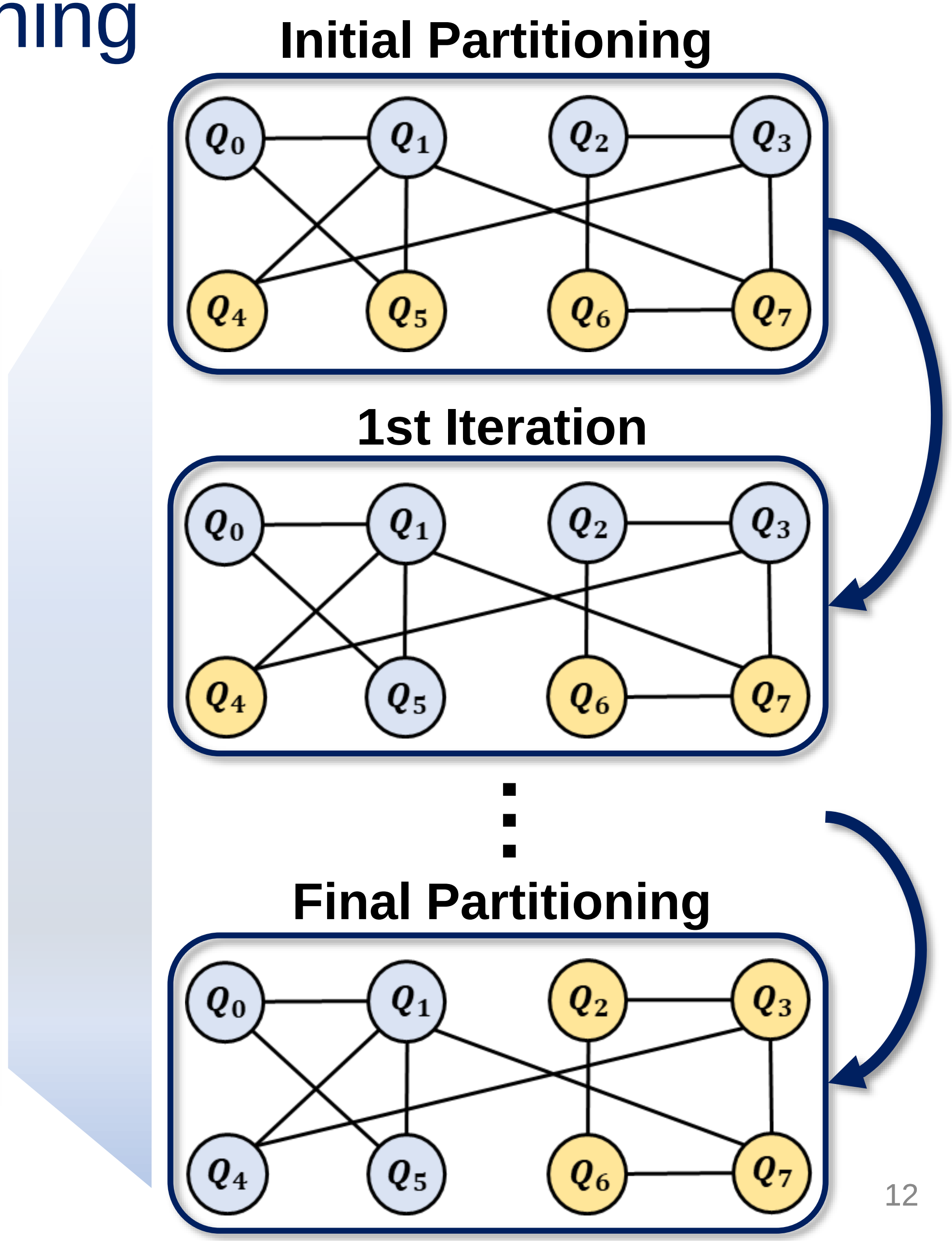
Gain of moving Q_5 to the opposite partition

$$= \sum(\textit{uncut edges}) - \sum(\textit{cut edges})$$

$$= 4 - 0 = 4$$

Qubit	*Gain*	*Status*
Q_0	0	*free*
Q_1	2	*free*
Q_2	0	*free*
Q_3	2	*free*
Q_4	2	*free*
Q_5	4	*free* → *fixed*
Q_6	-1	*free*
Q_7	1	*free*

Iteration	*Qubit*	*ΣGain*
1	Q_5	4
2	Q_3	6
3	Q_2	8
4	Q_4	**8**
5	Q_6	6
6	Q_0	2
7	Q_7	3
8	Q_1	0



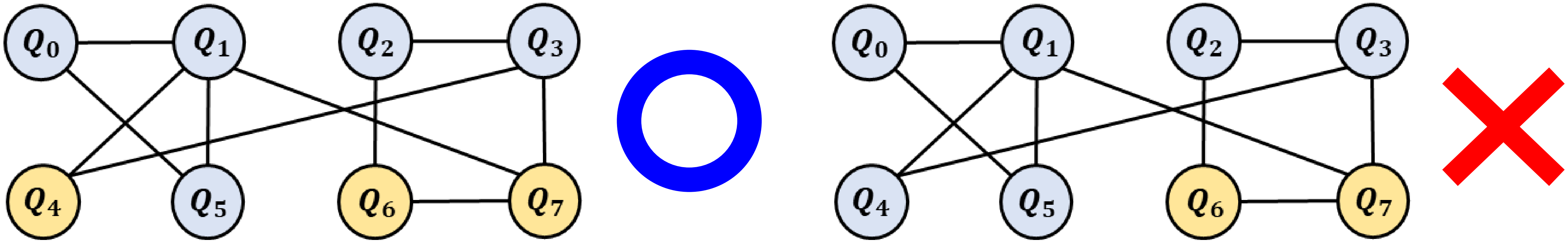
Why FM Algorithm?

- **Low Complexity**
  - Fast (Linear time-complexity)
  - Easy to implement

- **Balance Ratio**
  - Can control the partition balance

Example

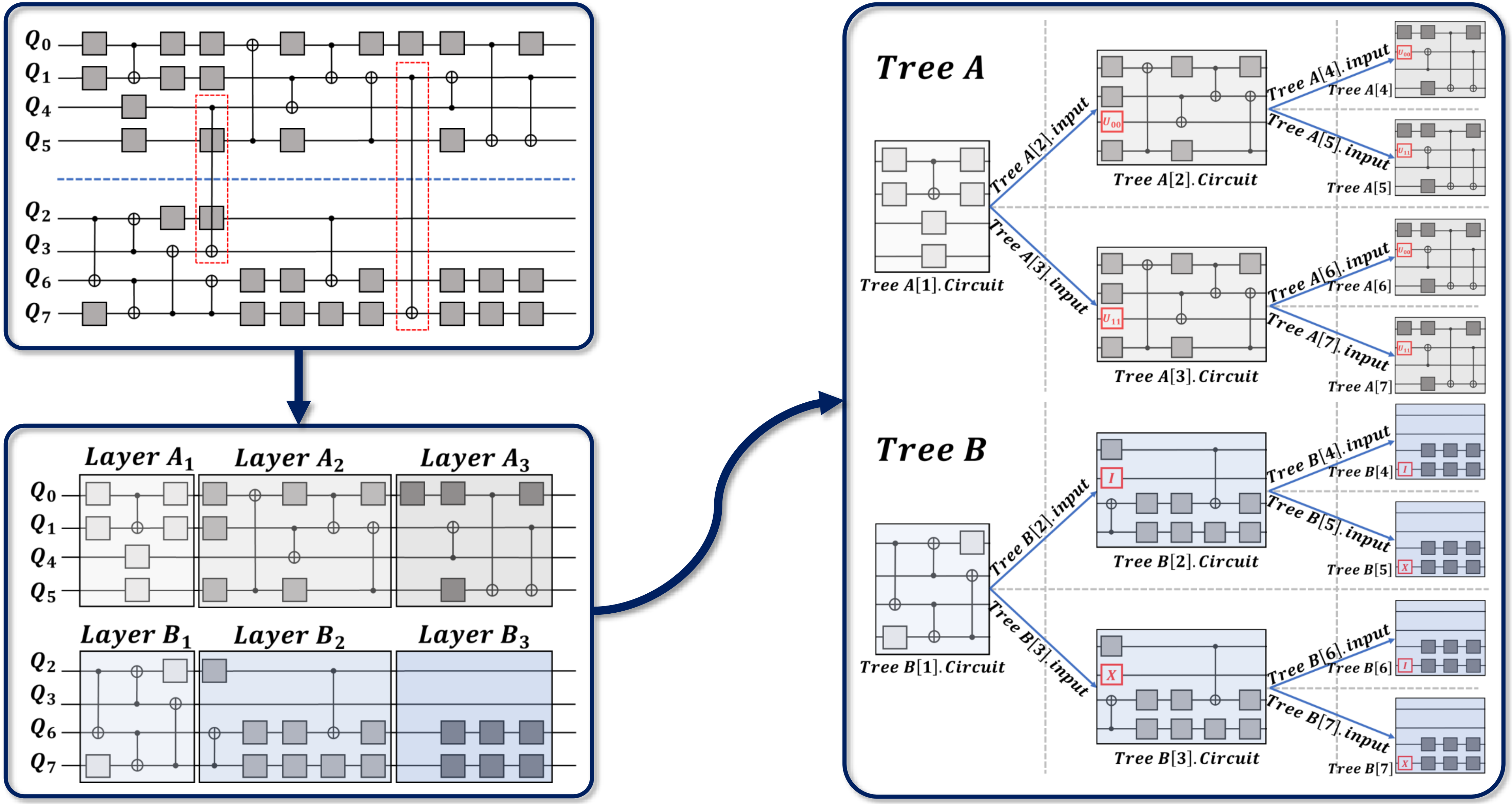
If balance ratio $\boldsymbol{r = 0.3}$



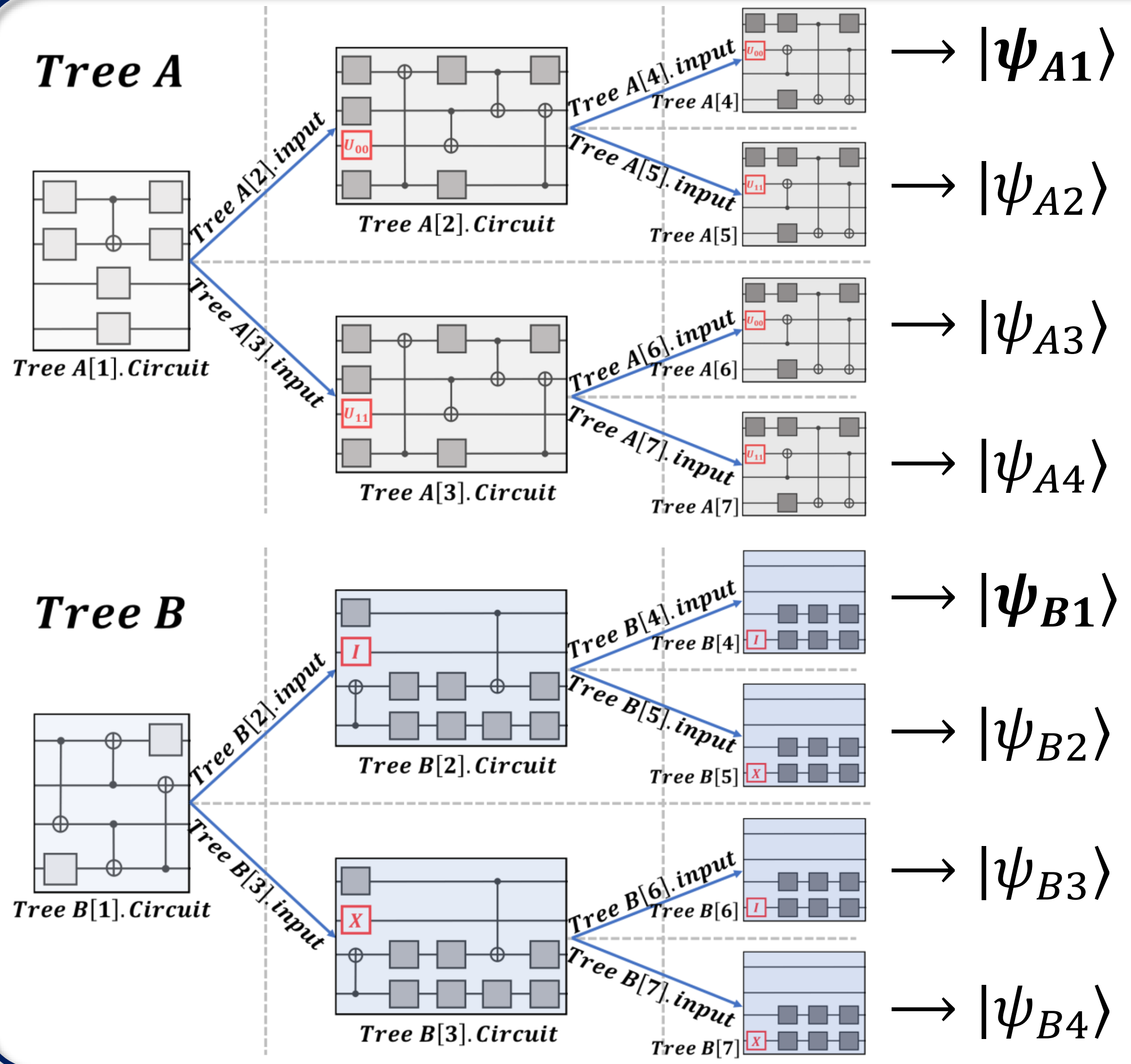
$$\boldsymbol{min\left(\frac{5}{8}, \frac{3}{8}\right) = 0.375 > 0.3}$$

$$\boldsymbol{min\left(\frac{6}{8}, \frac{2}{8}\right) = 0.25 < 0.3}$$

2. Layered Simulation - (1) Layer Assignment



2. Layered Simulation - (2) DFS Order Simulation



$$|\psi_1\rangle = |\psi_{A1}\rangle \otimes |\psi_{B1}\rangle$$

$$\begin{aligned}|\boldsymbol{\psi}_{\boldsymbol{Final}}\rangle &= |\psi_{A1}\rangle \otimes |\psi_{B1}\rangle \\ &+ |\psi_{A2}\rangle \otimes |\psi_{B2}\rangle \\ &+ |\psi_{A3}\rangle \otimes |\psi_{B3}\rangle \\ &+ |\psi_{A4}\rangle \otimes |\psi_{B4}\rangle \\ &= \sum |\psi_{Ai}\rangle \otimes |\psi_{Bi}\rangle \\ &= \sum |\boldsymbol{\psi}_{\boldsymbol{i}}\rangle\end{aligned}$$

3. Qubit Re-Ordering – Why do we need SWAP?

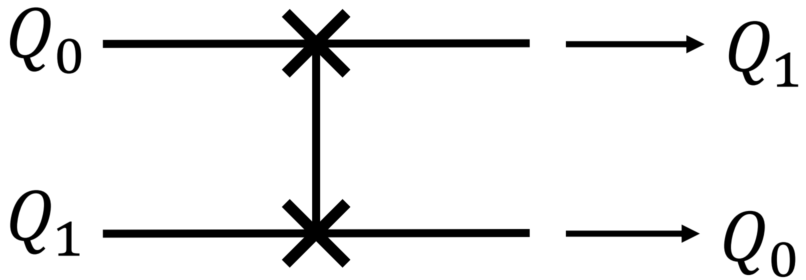
$$|\psi_{Final}\rangle = |Q_7 Q_6 Q_3 Q_2 Q_5 Q_4 Q_1 Q_0\rangle$$

$$\boldsymbol{SWAP(Q_3, Q_5)}$$
$$\boldsymbol{SWAP(Q_2, Q_4)}$$

$$|\psi_{Final}\rangle = |Q_7 Q_6 Q_5 Q_4 Q_3 Q_2 Q_1 Q_0\rangle$$

Approach #1. Applying SWAP Gate

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



- We have to restore the initial qubit order.
- Our unsuccessful first approach was applying SWAP gates.

3. Qubit Re-Ordering – Fast Qubit SWAP

Approach #2. Fast SWAP with bit-masking

Algorithm 3: SWAP(i, j, Amp)

Input :Qubit index $i, j\,(i > j)$, Amplitude Vector $Amp[\,]$

```
Set TargetMask1 ← 000...001 << i
Set TargetMask2 ← 000...001 << j
Set MaskR ← (111...111 >> N − j)
Set MaskL ← (111...111 << i + 1)
Set MaskM ← 111...111 ⊕ (MaskR ∨ MaskL ∨ TargetMask1 ∨ TargetMask2)
Set Idx ← 0
while Idx < 2^(N−2) do
    Set RealIdx ←
      (Idx ∧ MaskR) ∨ ((Idx << 1) ∧ MaskM) ∨ ((Idx << 2) ∧ MaskL)
    Set TargetIdx1 ← RealIdx ∨ TargetMask1
    Set TargetIdx2 ← RealIdx ∨ TargetMask2
    Exchange(Amp[TargetIdx1], Amp[TargetIdx2])
    Idx ← Idx + 1
end
```

Example) **SWAP**(3, 5, $|\psi\rangle$)

$$|Q_7Q_6\mathbf{Q_3}Q_2\mathbf{Q_5}Q_4Q_1Q_0\rangle = \boldsymbol{\alpha_0}|00000000\rangle$$

$$\ldots$$

$$+\ \boldsymbol{\alpha_8}|00001000\rangle$$
$$+\ \boldsymbol{\alpha_9}|00001001\rangle$$
$$\ldots$$
$$+\ \boldsymbol{\alpha_{32}}|00100000\rangle$$
$$+\ \boldsymbol{\alpha_{33}}|00100001\rangle$$
$$\ldots$$
$$+\ \boldsymbol{\alpha_{223}}|11011111\rangle$$
$$\ldots$$
$$+\ \boldsymbol{\alpha_{247}}|11110111\rangle$$

$\boldsymbol{Idx} = 0$: Exchange Amplitudes ($\alpha_8 \leftrightarrow \alpha_{32}$)

$\boldsymbol{Idx} = 1$: Exchange Amplitudes ($\alpha_9 \leftrightarrow \alpha_{33}$)

$\boldsymbol{Idx} = 2^6 - 1$: Exchange Amplitudes ($\alpha_{223} \leftrightarrow \alpha_{247}$)

Experimental Results

Experimental Setup

- **Benchmark**
  - Google Supremacy Circuits **[1]**
- **Implementation**
  - Base: Decision-Diagram Simulator (DDSim) **[2]**
  - C++, OpenMP
- **Comparison**
  - Hybrid Schrodinger-Feynman Decision-Diagram Simulator (HSF-DDSim) **[3]**

[1] Google Random Circuit Samplings, https://github.com/sboixo/GRCS

[2] A. Zulehner and R. Wille, "*Advanced Simulation of Quantum Computations*", IEEE Transactions on CAD, 2019 https://github.com/cda-tum/ddsim

[3] L. Burgholzer, H. Bauer and R. Wille, "Hybrid Schrodigner-Feynman Simulation of Quantum Circuits with Decision Diagrams", International Conference on Quantum Computing and Engineering, 2021

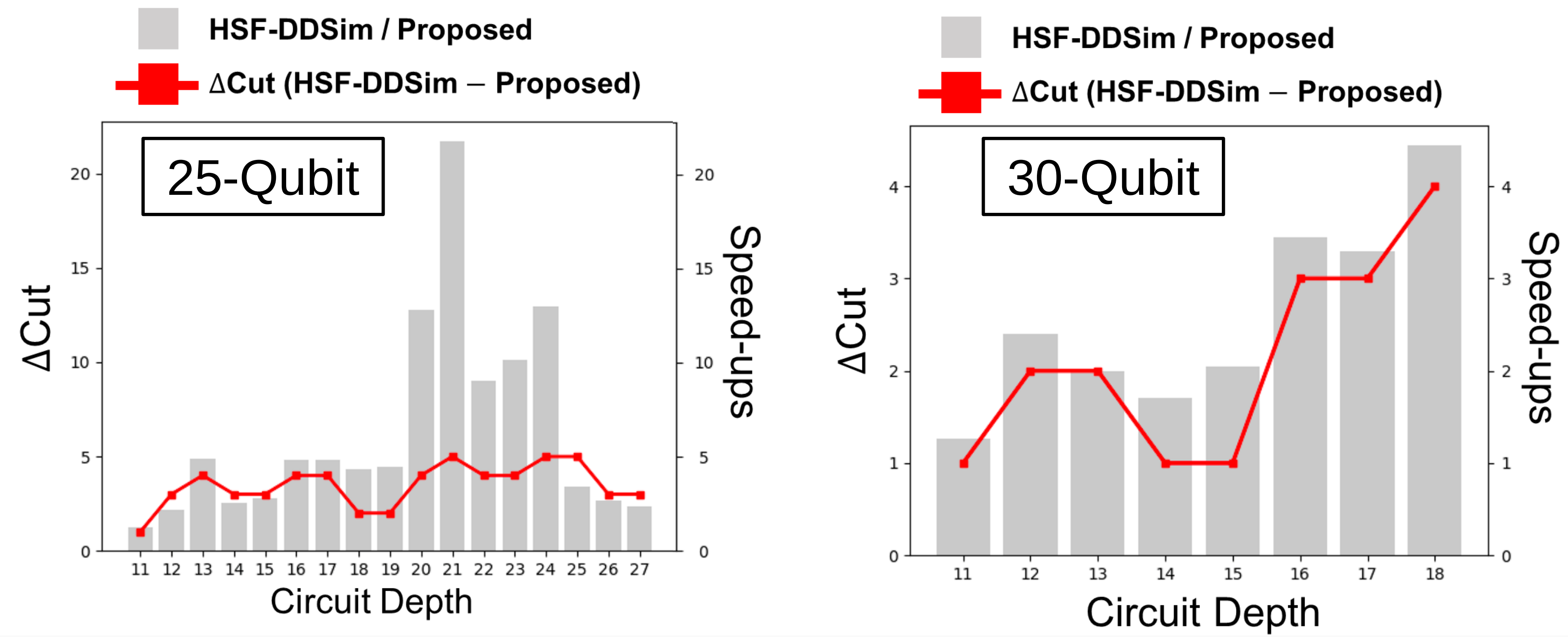
Experimental Results (1) Effectiveness of fast SWAP

Benchmark	Baseline - DDSim	Graph Partitioning + Applying SWAP gate	Graph Partitioning + Optimized SWAP
Name	Runtime [s]	Runtime [s]	Runtime [s]
inst_4x5_10_0	244.9	2.3	1.4
inst_4x5_12_0	803.4	15.7	0.7
inst_4x5_16_0	1374.5	164.6	7.4
inst_4x5_20_0	2748.2	12680.0	57.2
inst_5x5_14_0	>24 h	816.7	87.5

* $inst\_A\text{x}B\_C$ means a circuit of $A * B$ qubits and C depths

- HSF with graph partitioning can bring a huge speed-up.
- The overhead of applying swap gates can make it disappear.
- Our fast SWAP procedure can be a solution for the problem.

Experimental Results (2) Comparison with HSF-DDSim



- FM partitioning makes fewer cuts than the half slicing.
- Our approach achieved runtime improvement up to 20X times.

CONCLUSION

Conclusion

Summary

- Traditional HSF simulation uses simple half slicing.
- The number of crossing gates increases the simulation time exponentially.
- Partitioning approach can make fewer crossing gates than half slicing.
- This leads to significant speed-up of simulation.

Future Work

- How can we consider noise in the partitioning approach?
- How about other benchmarks?

THANK YOU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