New Approaches to Simulation and Analysis of Quantum Circuits

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FI MUNI (Colloquium)

Why Quantum Computation?

Quantum computation:

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- promises to efficiently solve some problems we don't know how to efficiently solve classically

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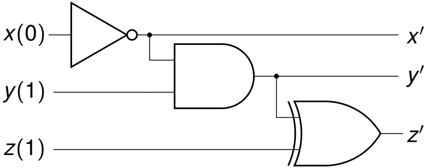
- real-world quantum computers are always 10 years away
- $\rightsquigarrow$ we need to be prepared (computer-aided analysis)
- **FUN** and thriving community!

Outline

Short Quantum Introduction

Classical vs. Quantum Circuits — State

Classical



x'	y'	z'	χ
0	0	0	0
0	0	1	0
0	1	0	0
0	1	1	0
1	0	0	0
1	0	1	0
1	**1**	**0**	**1**
1	1	1	0

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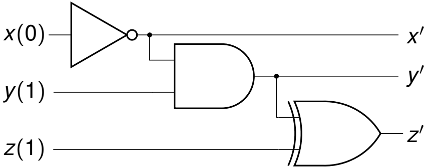

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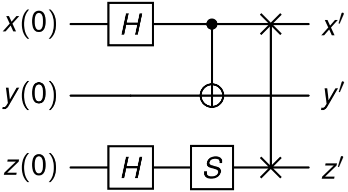

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x'	y'	z'	*amp*
0	**0**	**0**	**25 %**
0	0	1	0 %
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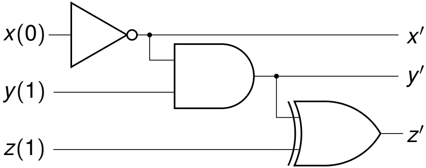

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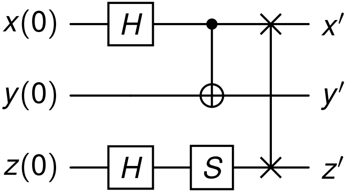

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x'	y'	z'	*amp*
0	**0**	**0**	½
0	0	1	0
0	1	0	0
0	**1**	**1**	½
1	**0**	**0**	½ *i*
1	0	1	0
1	1	0	0
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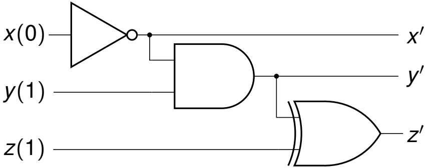
$amp(\vec{x}) \in \mathbb{C}$

$\Pr(\vec{x}) = |x|^2$

Classical vs. Quantum Circuits — Gates

Classical



A gate is a truth table

a	b	$a \oplus b$
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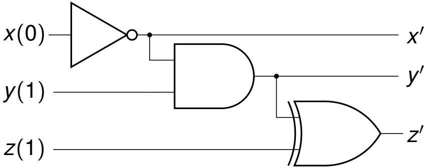

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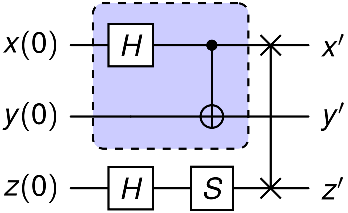

A gate is a unitary matrix

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

unitary matrix:

- conjugate transpose $U^\dagger = U^{-1}$

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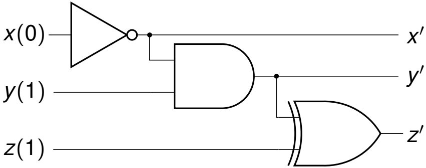

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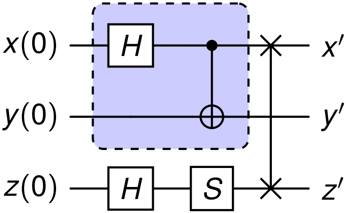

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unitary matrix:

- conjugate transpose $U^\dagger = U^{-1}$
- $\leadsto$ reversibility, norm preservation, no-cloning theorem, ...

Quantum Circuit Analysis

Reasoning over Quantum Circuits

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- exponential size of state representation
- inherently probabilistic (testing is hard!)
- need to deal with complex numbers

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Main approaches:

1. state vector simulation (strong: #**P**-complete)
2. equivalence checking (**QMA**-complete)
   - **QMA** = *Quantum Merlin Author*; the so-called “quantum NP”
3. (pre/post-condition) verification

Verification of Classical Programs

Verification of classical programs:

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$$\overset{\textit{precondition}}{\{Pre\}}\ \underset{\textit{statement}}{S}\ \overset{\textit{postcondition}}{\{Post\}}$$

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Meaning:

- If *S* is executed from a state from *Pre*
- and the execution of *S* terminates,
- then the program state after *S* terminates is in *Post*.

Verification of Quantum Circuits

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Verification of quantum circuits:

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- *Pre* and *Post* denote sets of **quantum** states

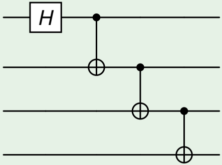
Meaning:

- If C is executed from a quantum state from *Pre*
- then the quantum state after C terminates is in *Post*.
- (termination is implicit)

Verification of Quantum Circuits

Example (GHZ)

$\{|w\rangle : w \in \{0,1\}^4\}$



$\{\frac{1}{\sqrt{2}}|0b_2b_3b_4\rangle \pm \frac{1}{\sqrt{2}}|1\bar{b}_2\bar{b}_3\bar{b}_4\rangle :$
$b_2b_3b_4 \in \{0,1\}^3\}$

Pre Circuit *Post*

$$Pre = \{|0000\rangle, |0001\rangle, \ldots, |1111\rangle\}$$
$$\text{e.g., } |0010\rangle = [0,0,1,0,0,0,0,0,0,0,0,0,0,0,0,0]^T$$

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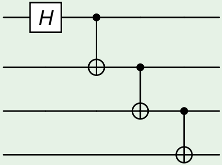

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How to efficiently represent sets of quantum states *Pre* and *Post*?

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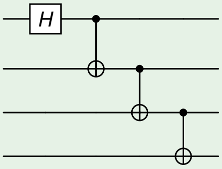

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How to efficiently represent sets of quantum states *Pre* and *Post*?

- naively $\rightsquigarrow$ double exponential size

Quantum States are Trees

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…and quantum gates are tree operations

Quantum States are Trees

x	y	z	amp
0	**0**	**0**	**½**
0	0	1	0
0	1	0	0
0	**1**	**1**	**½**
1	**0**	**0**	**½ i**
1	0	1	0
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$\Rightarrow$

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$\Rightarrow$

½	0	0	½	½i	0	0	½i

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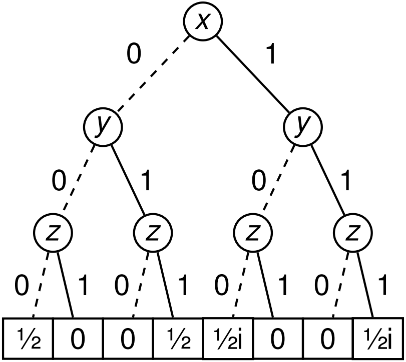

- perfect tree of height n (the number of qubits) $\rightsquigarrow 2^n$ leaves

Quantum Gates are Tree Operations

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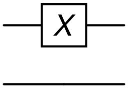
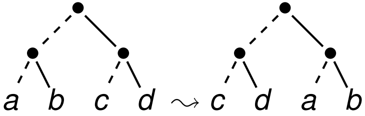
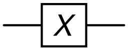


$$X_1 = \overbrace{\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}}^{X} \otimes \overbrace{\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}}^{I}$$



Quantum Gates are Tree Operations



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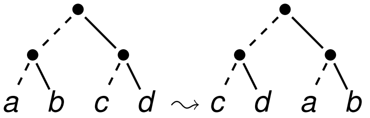
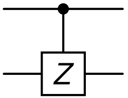
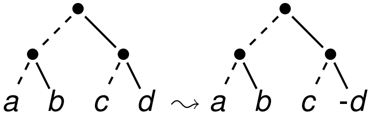




$$CZ_2^1 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$$



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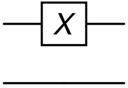

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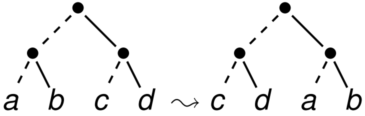

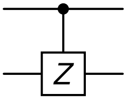

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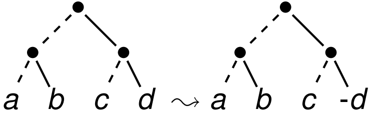
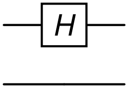
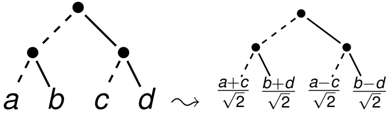




$$H_1 = \overbrace{\begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{bmatrix}}^{H} \otimes \overbrace{\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}}^{I}$$



Hadamard gate

Sets of Quantum States are Sets of Trees

- How to efficiently represent sets of trees?

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Tree automata!

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Tree automata!

- tree automata
  - finite-state automata representing sets of finite trees
  - extension of standard finite automata for regular languages

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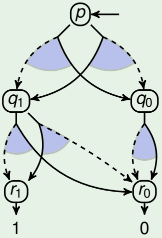
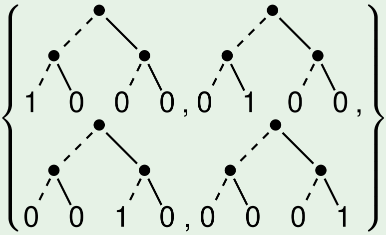
Example



represents the set



Representing *Pre* and *Post* with Tree Automata

$$\overset{\textit{precondition}}{\{\mathcal{A}_{Pre}\}} \ \underset{\textit{circuit}}{C} \ \overset{\textit{postcondition}}{\{\mathcal{A}_{Post}\}}$$

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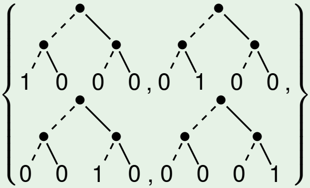
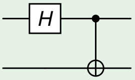
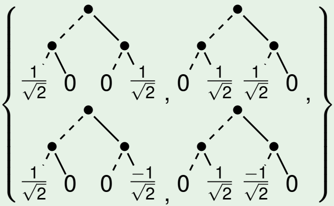


$\mathcal{L}(\mathcal{A}_{Pre})$





$\mathcal{L}(\mathcal{A}_{Post})$

Representing *Pre* and *Post* with Tree Automata

precondition $\{\mathcal{A}_{Pre}\}$ C $\{\mathcal{A}_{Post}\}$ *postcondition*

circuit

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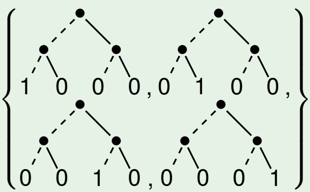

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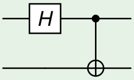
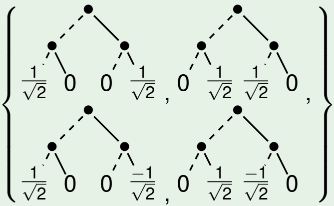




$\mathcal{L}(\mathcal{A}_{Post})$

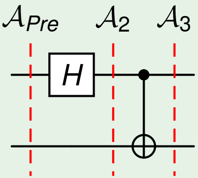
- $\mathcal{A}$'s size can be small
  - e.g., $\mathcal{A}$ for $\{|w\rangle : w \in \{0,1\}^n\}$ needs $\mathcal{O}(n)$ states/transitions

Verification with Tree Automata

$$\overset{\textit{precondition}}{\{\mathcal{A}_{Pre}\}}\ \underset{\textit{circuit}}{C}\ \overset{\textit{postcondition}}{\{\mathcal{A}_{Post}\}}$$

- Run C with $\mathcal{A}_{Pre}$:

Example



Verification with Tree Automata

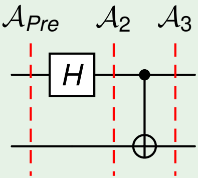
precondition *postcondition*

$$\{\mathcal{A}_{Pre}\} \quad C \quad \{\mathcal{A}_{Post}\}$$

circuit

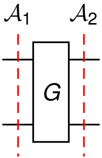
- Run C with $\mathcal{A}_{Pre}$:

Example



- …and test $\mathcal{L}(\mathcal{A}_3) \subseteq \mathcal{L}(\mathcal{A}_{Post})$
  - (tree automata inclusion is **EXPTIME**-complete)

Abstract Transformers for Quantum Gates



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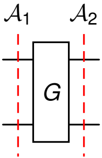

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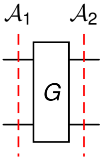

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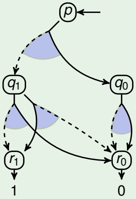
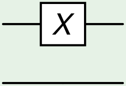
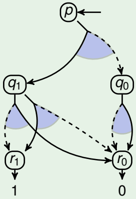
Example



$\{|00\rangle, |01\rangle\}$





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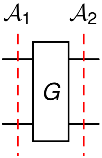

- Supported gate types:
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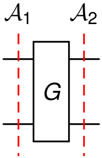

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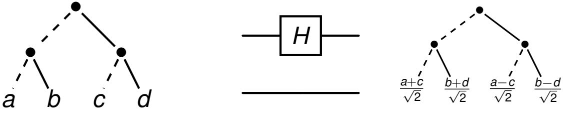
  - general: $H, R_x, R_y, \ldots$
    - need to synchronize subtrees of the same tree



    - variable reorder $\rightarrow$ leaf operation $\rightarrow$ variable reorder: $\mathcal{O}(2^{|\mathcal{A}_1|})$

Quantum Circuit Verification Algorithm

$$\underbrace{\{\mathcal{A}_{Pre}\}}_{\text{precondition}} \quad \underbrace{C}_{\text{circuit}} \quad \underbrace{\{\mathcal{A}_{Post}\}}_{\text{postcondition}}$$

- Algorithm:
  1. Start with $\mathcal{A}_{Pre}$.

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- Established a connection between **quantum** and **automata**.

[Chen, Chung, Lengál, Lin, Tsai, Yen. An Automata-Based Framework for Verification and Bug Hunting in Quantum Circuits. PLDI'23.]

Symbolic Amplitudes

Introducing Symbolic Amplitudes

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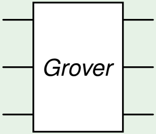

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global constraint:

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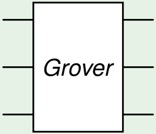

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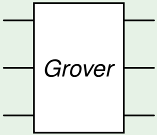

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- uncountably many quantum states
- $\rightsquigarrow$ symbolic amplitudes!

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Modifications to the verification algorithm:

- tree automata $\rightsquigarrow$ symbolic tree automata
  - alphabet contains symbolic values, terms, and predicates

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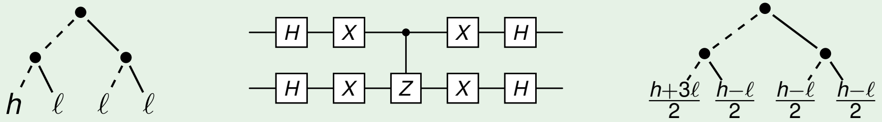

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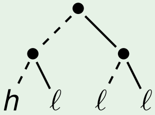

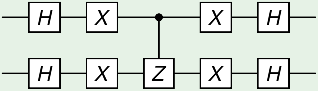

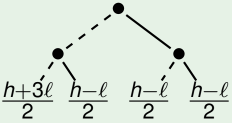

Grover's diffusion operator

- modified language inclusion test

Verifying Quantum Circuits using Symbolic Amplitudes

- More expressive specification language
- Properties such as
  - two H gates are identity
  - Bernstein-Vazirani: no imaginary component
  - $\mathit{Grover}_{\mathit{Single}}$: $\Pr(\mathit{Correct}) > 0.9$ ($n = 20$)
  - $\mathit{Grover}_{\mathit{All}}$: $\Pr(\mathit{Correct}) > 0.9$ ($n = 9$)
  - $\mathit{Grover}_{\mathit{Iter}}$: $\Pr(\mathit{Correct})$ increased ($n = 100$)

[Chen, Chung, Lengál, Lin, Tsai. AutoQ: An Automata-Based Quantum Circuit Verifier. CAV'23.]

Loop Summarization

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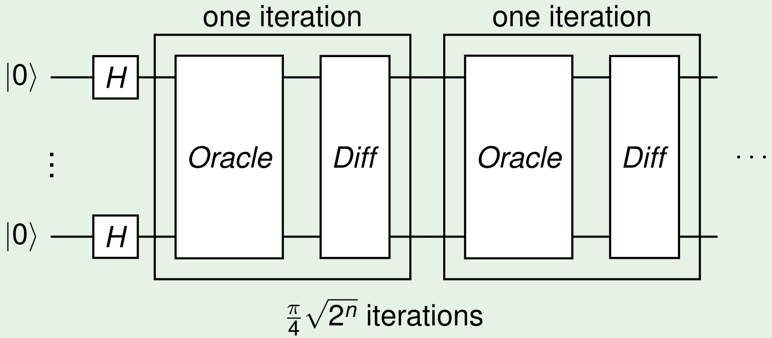
- Some algorithms use a (fixed #iterations) loop

Example (Grover's algorithm)



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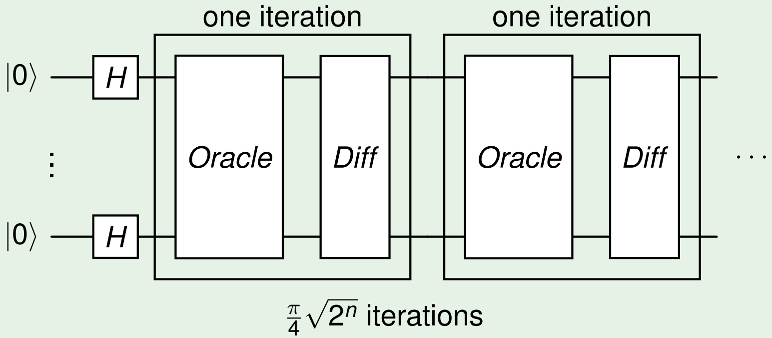
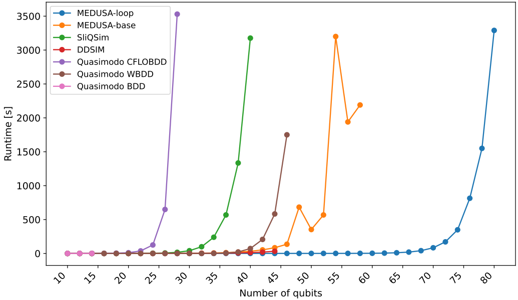


- one can use symbolic execution (with refinement) to compute the big-step semantics of the loop body
- . . . and then just use that instead of executing the gates

Loop Summarization

- Significant speed-up of simulation of amplitude amplification
  - e.g., Grover's algorithm (below), quantum counting, period finding



- chance for more speed-up (compute the closed form)
- use for analysis (WIP)

[Chen, Chen, Jiang, Jobranová, Lengál. Accelerating Quantum Circuit Simulation with Symbolic Execution and Loop Summarization. ICCAD'24.]

Level-Synchronized Tree Automata

Level-Synchronized Tree Automata (LSTAs)

Problems with the basic TA-based framework:

- time complexity of some gates is $\mathcal{O}(2^{|\mathcal{A}|})$
- doesn't support parameterized verification
  - e.g., cannot express "all perfect binary trees"

Level-Synchronized Tree Automata (LSTAs)

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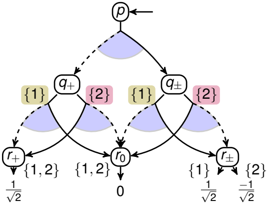
- allow synchronization across subtrees



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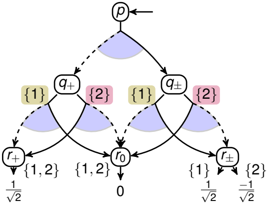

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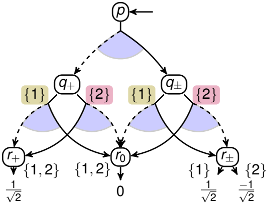

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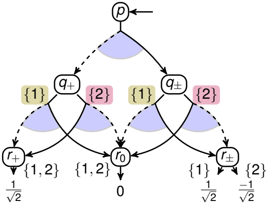

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- language operations:
  - emptiness: **PSPACE**-complete
  - inclusion: **PSPACE**-hard, in **EXPSPACE**

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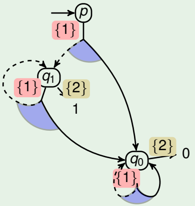
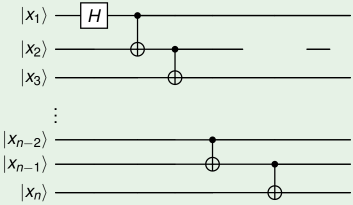
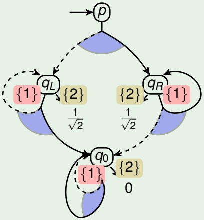
Level-Synchronized Tree Automata

- enable basic parameterized verification

Example (GHZ)







$\{|0^n\rangle : n \geq 1\}$

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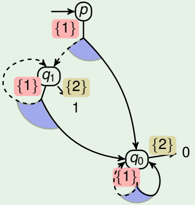

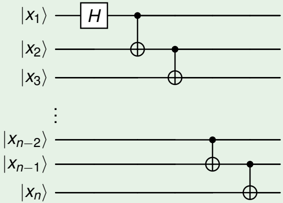

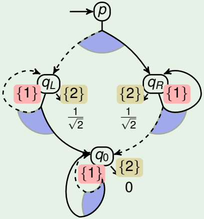

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- GHZ, fermionic unitary evolution (single/double fermionic excitation)

[Abdulla, Chen, Chen, Holík, Lengál, Lin, Lo, Tsai. Verifying Quantum Circuits with Level-Synchronized Tree Automata. POPL'25.]

Verification of Quantum Circuits with Loops

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- Common structure of quantum programs:

$$\textbf{while}\ \ (M(x_i) = 0)\\ \quad C;$$

repeat-until-success, weakly measured

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Pre: $\{1\left|0^{n+2}\right\rangle + 0\left|*\right\rangle\}$;
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Inv: $\{v_{sol1}\left|000^n\right\rangle + v_k\left|000^{n-1}1\right\rangle + \cdots +$
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- need to extend LSTAs with
  - measurements
  - symbolic values
- managed to verify:
  - weakly-measured Grover's algorithm
  - several repeat-until-success programs

[Chen, Chung, Hsieh, Huang, Lengál, Lin, Tsai. AutoQ 2.0: From Verification of Quantum Circuits to Verification of Quantum Programs. TACAS'25.]

Takeaways and Future Directions

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Quantum ♡ Automata

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  - oracle-based circuits
  - dynamic circuits
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- a good specification language
  - expressive, user-friendly
  - can compile to LSTAs quickly
- support for quantum Fourier transform
  - $\mathcal{O}(2^n)$ amplitude values
  - $\leadsto$ needs symbolic values for branches
- equivalence checking of parameterized circuits
  - oracle-based circuits
  - dynamic circuits
  - various notions of equivalence
- How to represent quantum circuits efficiently?
  - algebra over trees? logic?

Thank you!