Simulation and Verification of Quantum Circuits

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DeiC

Overview

Motivation of two fundamental problems

Simulation of quantum circuits

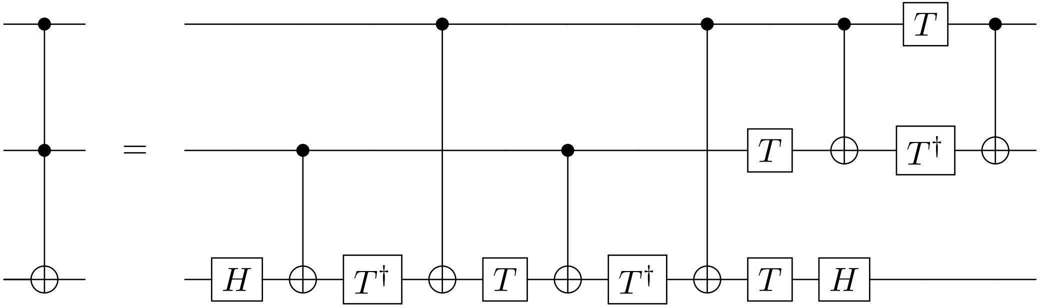
Formal verification for equivalence checking of quantum circuits

Conclusion

Overview

Circuit compilation (both conventional and quantum)

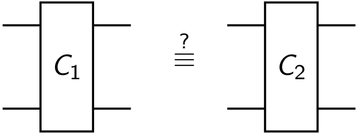
- During circuit design: use **high-level gates** and assume **arbitrary connectivity**
- **Compiler** translates to **low-level circuit** for executing on real hardware, supporting few **low-level gate types** and satisfying **connectivity constraints**



Circuit compilation (both conventional and quantum)

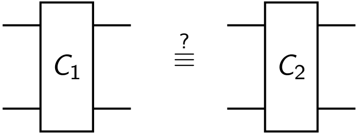
- During circuit design: use **high-level gates** and assume **arbitrary connectivity**
- **Compiler** translates to **low-level circuit** for executing on real hardware, supporting few **low-level gate types** and satisfying **connectivity constraints**
- In this process, compilers have lots of room for optimization:
  - Reduce amount of gates / operations
  - Quantum gates incur different levels of error (noise)
  - Deeper quantum circuits incur more errors
  - ...
- Important that **circuits are equivalent** before and after compilation (i.e., compute the same output for the same input)
  - How can we check **equivalence of circuits**?

Black-box equivalence check for **conventional** circuits



- Pick an input and execute both circuits
  - One-way result: Disagreement implies different circuits
  - **Exponentially many** classical inputs

Black-box equivalence check for **quantum** circuits



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- Infinitely many quantum states as input?
  - **Sufficient to check basis states**
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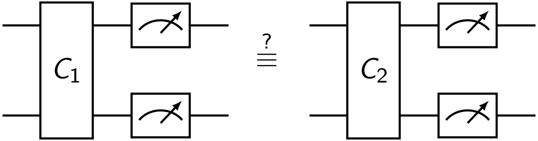

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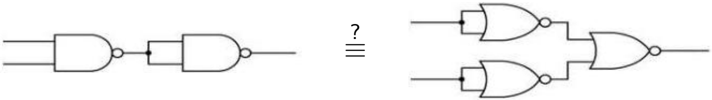
- Infinitely many quantum states as input?
  - **Sufficient to check basis states**
  - **Exponentially many** basis states
- **Can only observe basis states (via measurement)**
  - Disagreement does not imply different circuits
  - Statistical result by executing many times – **even more expensive**

Equivalence checking of circuits

- Two general directions: **testing/sampling** and **formal verification**
- **Testing**: choose an input and run the circuit
  - Single test runs are cheap, but result is **not conclusive**
  - Quantum circuits:
    - Expensive and hardly available (yet)
    - Result is probabilistic $\rightsquigarrow$ many runs for same input needed
    - Instead can **simulate circuit on conventional computer**
- **Formal verification**: mathematical proof that circuits are equivalent
  - More expensive than a few test runs, but result is **conclusive**
  - Run **on conventional computer**

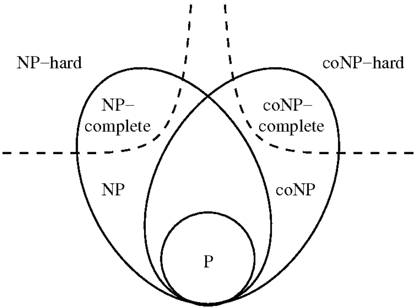
White-box equivalence check for **conventional** circuits

- What if we know the conventional circuits?



White-box equivalence check for **conventional** circuits

- Checking that two conventional circuits are equivalent is co-NP-complete
  - Believed to require exponential complexity
  - So in principle not better than checking all possible inputs



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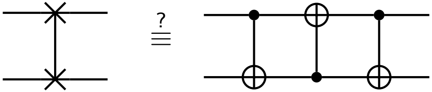

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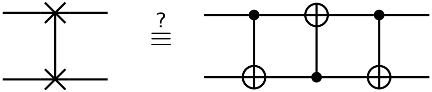

- Can simulate all basis states $\rightsquigarrow$ algorithm with definite result

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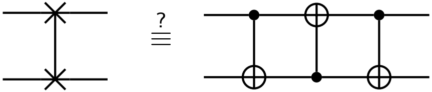

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  - Each simulation takes **exponential time**

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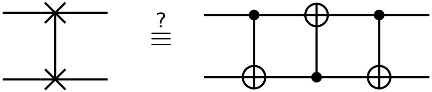

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- Alternative: compare characteristic matrices
  - Matrices are **exponentially large**

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

White-box equivalence check for **quantum** circuits

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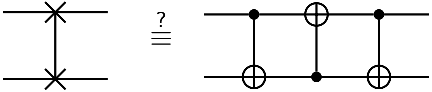


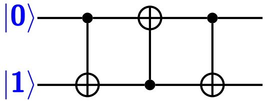
- Can simulate all basis states $\rightsquigarrow$ algorithm with definite result
  - **Exponentially** many basis states
  - Each simulation takes **exponential time**
- Alternative: compare characteristic matrices
  - Matrices are **exponentially large**
- No way around: problem is co-NQP-complete[1]
  - Believed to require exponential complexity

[1] Y. Tanaka. *Int. J. Quantum Inf.* (2010)

Overview

Simulation on conventional computer

- Simplest approach: propagate (exponentially large) state vector



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

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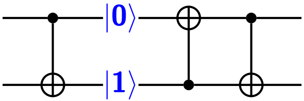

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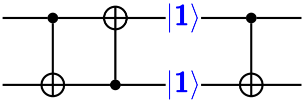

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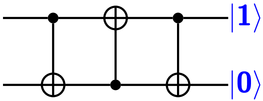
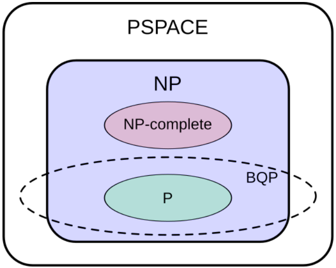


$$\begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}$$

- Now we actually have the **quantum state** (no measurements required)

Complexity of simulating a quantum circuit

- Simulation is BQP-complete
  - Believed to require exponential complexity (on conventional computer)
- **Clifford gates** (Hadamard, CNOT, phase S) can be simulated **efficiently**[1]
  - Non-universal gate set
  - Relevant for **error correction**, which will play central role in fault-tolerant era
  - **Equivalence checking** is also efficient[2]



[1] D. Gottesman. PhD thesis. 1997

[2] D. Thanos, T. Coopmans, and A. Laarman. *ATVA*. 2023

Simulation based on tensor networks

- Each step of the matrix-vector multiplications had exponential complexity
- Idea behind **tensor networks**: perform cheaper calculations when possible

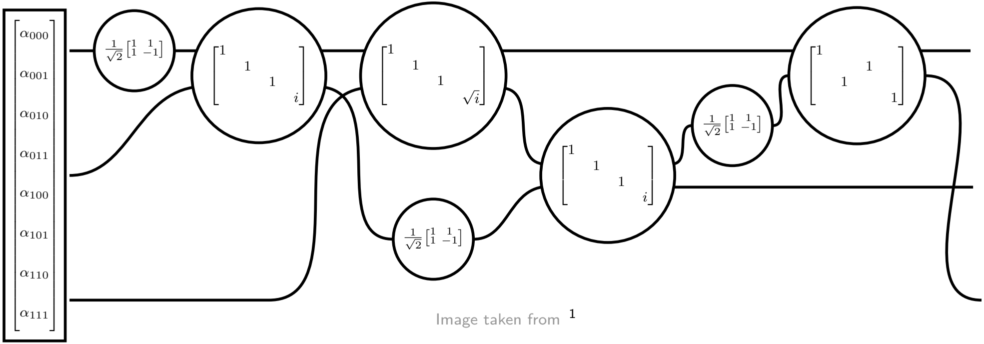
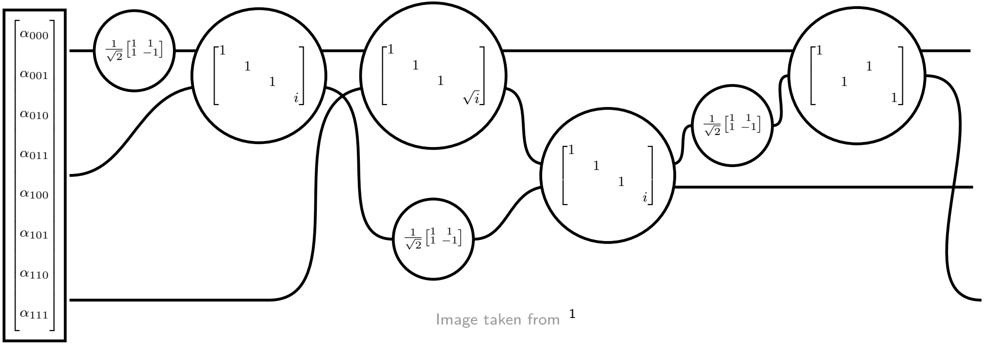


Image taken from [1]

[1] (L. Burgholzer, A. Ploier, and R. Wille. *IEEE Trans. Comput. Aided Des. Integr. Circuits Syst.* [2023])

Simulation based on tensor networks

- **Tensor network**: graph of tensors, initially corresponding to gates in circuit
- Nodes with shared edges can be **contracted** (= merged) **in any order**



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Simulation based on tensor networks

- **Tensor network**: graph of tensors, initially corresponding to gates in circuit
- Nodes with shared edges can be **contracted** (= merged) **in any order**
- Finding the optimal contraction order is NP-hard[1]
- Practice: use of good enough and efficient solutions (heuristics)[2]

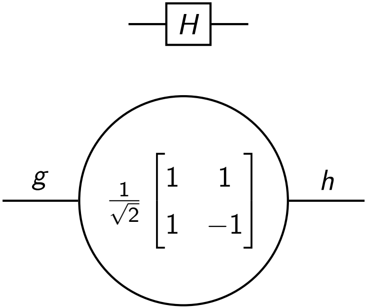
---

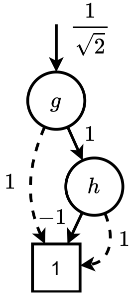
[1] C. Lam, P. Sadayappan, and R. Wenger. *Parallel Process. Lett.* (1997).
[2] J. Gray and S. Kourtis. *Quantum* (2021).

Tensor decision diagrams (TDDs)[1]

- Alternative representation of a tensor
- Sometimes avoids exponential size of matrix / vector representation

Example: Hadamard gate with tensor and tensor decision diagram





[1]X. Hong, X. Zhou, S. Li, Y. Feng, and M. Ying. *ACM Trans. Design Autom. Electr. Syst.* (2022).

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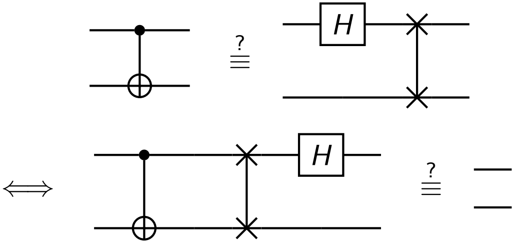
Reverse scheme for equivalence checking[1]

$$C_1 \equiv C_2 \stackrel{\text{def}}{\Longleftrightarrow} \exists\theta\colon U_1 = e^{i\theta}\cdot U_2 \Longleftrightarrow \exists\theta\colon U_1 \cdot U_2^\dagger = e^{i\theta}\cdot I \stackrel{\text{def}}{\Longleftrightarrow} C_1 C_2^{-1} \equiv C_I$$

- C_2^{-1} is the inverted C_2 (reversed and each gate inverted)



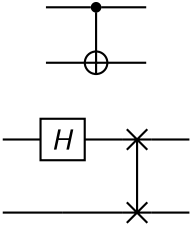
(Coincidentally, the swap and Hadamard gates are self-inverse)

[1] G. F. Viamontes, I. L. Markov, and J. P. Hayes. *ICCAD*. 2007.

TDD-based algorithm for equivalence checking[1]

Algorithm combines reverse scheme, tensor networks, and TDDs

Given: Quantum circuits C_1, C_2



[1] C. B. Larsen, S. B. Olsen, K. G. Larsen, and C. Schilling. *Entropy* (2024).

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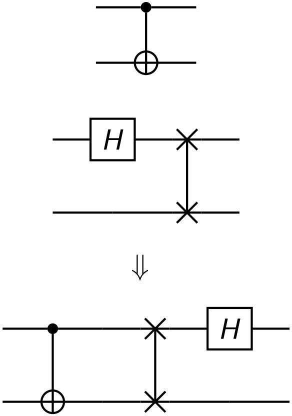

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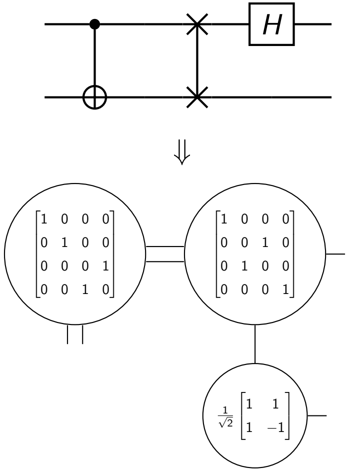
Given: Quantum circuits C_1, C_2

1. Construct circuit $C_1 C_2^{-1}$
2. Convert $C_1 C_2^{-1}$ to tensor network



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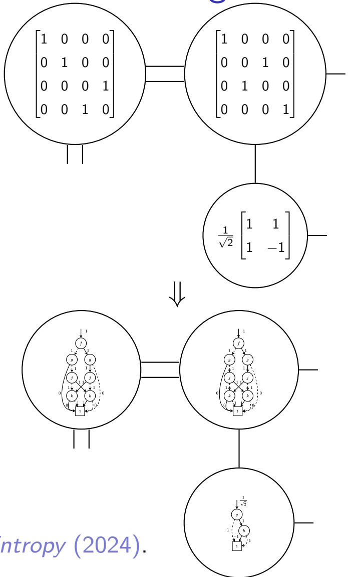
1. Construct circuit $C_1 C_2^{-1}$
2. Convert $C_1 C_2^{-1}$ to tensor network
3. Convert all tensors to TDDs



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Given: Quantum circuits C_1, C_2

1. Construct circuit $C_1 C_2^{-1}$
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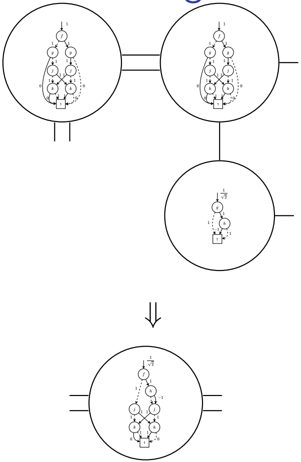
3. Convert all tensors to TDDs
4. Contract TDD network



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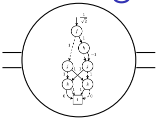
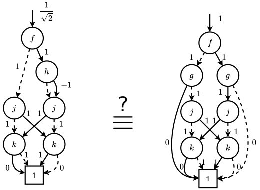


$\Downarrow$



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5. Compare final TDD to identity TDD

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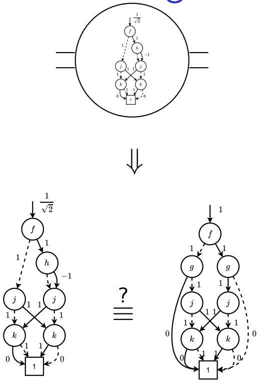

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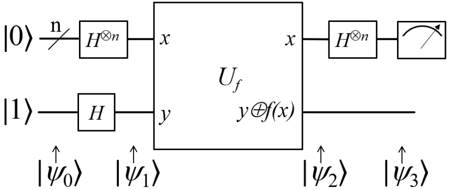
Empirical evaluation on circuits from three quantum algorithms

- Circuits from MQT Bench[1] with varying number of qubits at two compilation levels (level 1 and 3 (out of 4)) with significantly different gate sets and layouts
  - Deutsch-Jozsa algorithm (DJ)
  - Greenberger-Horne-Zeilinger state preparation (GHZ)
  - Graph state preparation (GS)

[1] N. Quetschlich, L. Burgholzer, and R. Wille. *Quantum* (2023).

Deutsch-Jozsa algorithm (DJ)[1,2]

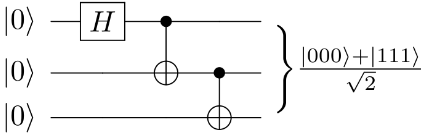
- Given $f: \{0,1\}^n \to \{0,1\}$ with promise that it is either
  - constant (100% "0" or 100% "1") or
  - balanced (50% "0" and 50% "1")
- Task: Determine which of the two cases it is
- Demonstrates exponential speed-up (requires a single shot)



[1] D. Deutsch and R. Jozsa. *Proc. R. Soc. A* (1992).
[2] R. Cleve, A. Ekert, C. Macchiavello, and M. Mosca. *Proc. R. Soc. A* (1998).

Greenberger-Horne-Zeilinger state preparation (GHZ)[1]

- The **GHZ state** generalizes the Bell state
- For 3 qubits: $\dfrac{|000\rangle + |111\rangle}{\sqrt{2}}$
- For k qubits: $\dfrac{|0\rangle^{\otimes k} + |1\rangle^{\otimes k}}{\sqrt{2}}$
- Used in quantum communication and cryptography protocols



[1] D. M. Greenberger, M. A. Horne, and A. Zeilinger. *Bell's theorem, quantum theory and conceptions of the universe.* 1989.

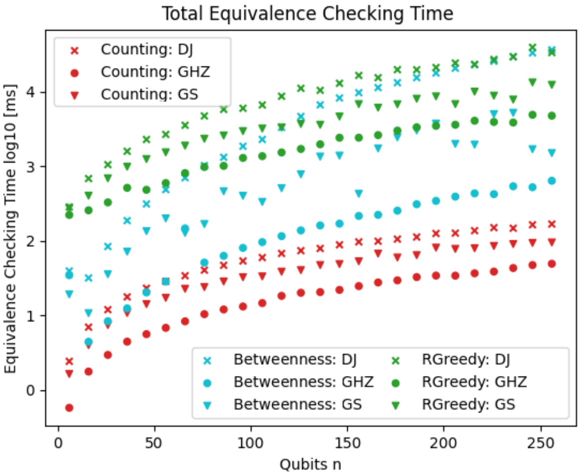
Graph state preparation (GS)[1]

- A **graph state** is a state that can be represented by a graph
- Each vertex corresponds to a qubit
- $|G\rangle = \prod_{(u,v)\in E} CZ^{(u,v)} |+\rangle^{\otimes |V|}$

  where $CZ^{(u,v)}$ is the corresponding controlled-Z gate
- Useful, e.g., in quantum error-correcting codes

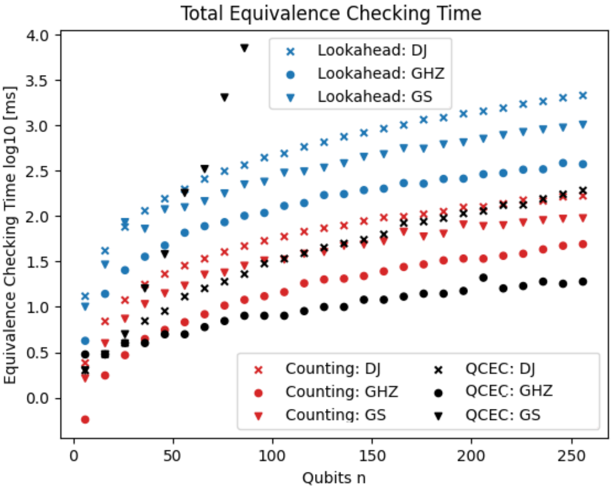
[1] M. Hein et al. *arXiv preprint quant-ph/0602096* (2006).

Comparison to cotengra[1]



[1] J. Gray and S. Kourtis. *Quantum* (2021).

Comparison to QCEC[1]



[1] L. Burgholzer and R. Wille. *Softw. Impacts* (2021).

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- **Equivalence checking** is a central problem
  - Both for conventional and quantum computers
  - Theoretically intractable, but practical solutions often work
- **Simulation** and **formal verification** are powerful technologies
- **Promising tools** are being developed
  - Tensor networks
  - Decision diagrams
  - . . . many more!

More about quantum from Aalborg University

- At Digital Tech Summit
  - Aalborg University booth @ UNI3
  - Petar Popovski: *Low-Latency Classical Communications for Quantum Applications* (tomorrow 9:30)
- In 2026
  - Hosting Danisch Quantum Community's *Scientific Quantum Conference*
  - Hosting IEEE *Int. Conference on Quantum Control, Computing and Learning*
  - Organizing Workshop on *Formal Methods in Quantum Computing*
- In general
  - AAU Quantum Hub
  - CLASSIQUE: *Center for Classical Communication in the Quantum Era*