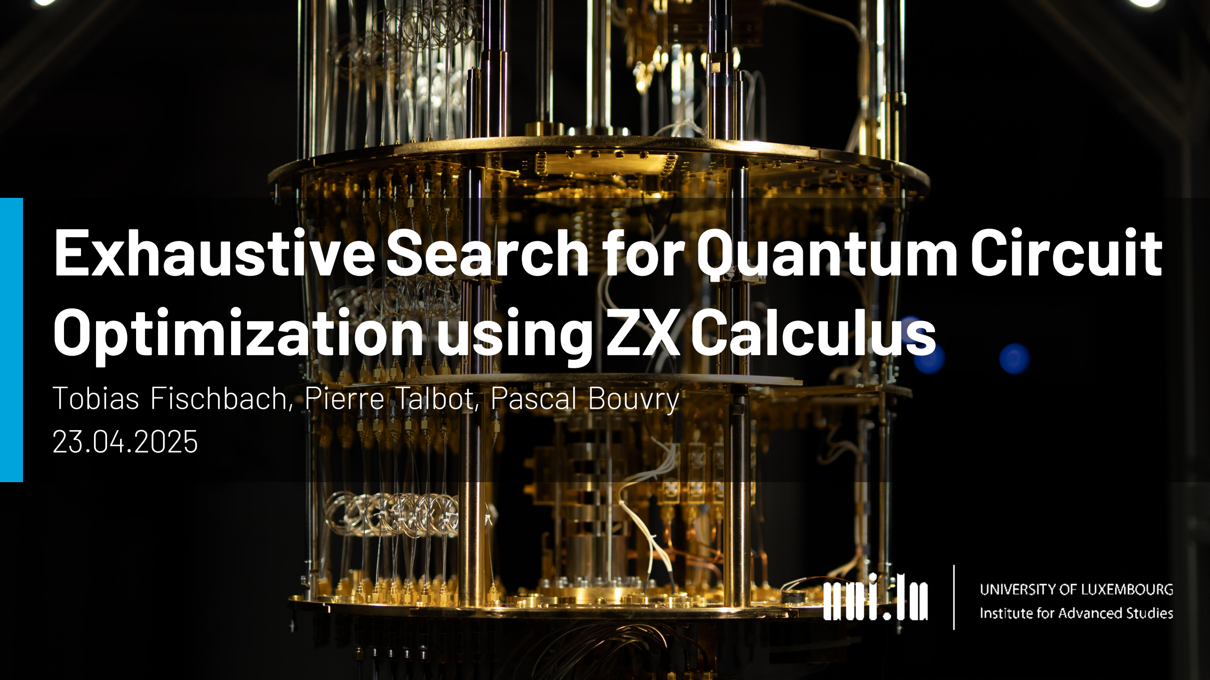

Exhaustive Search for Quantum Circuit Optimization using ZX Calculus

Tobias Fischbach, Pierre Talbot, Pascal Bouvry

23.04.2025

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Quantum Computing

Applications

- Factorization
  - Shor [21] $\mathcal{O}(\log N^3)$ vs. GNFS [17] $\mathcal{O}(\exp\sqrt{\frac{64}{9}}\log N^{\frac{1}{3}}\log\log N^{\frac{2}{3}})$
- Unstructured search
  - Grover [8] $\mathcal{O}(\sqrt{N})$ vs. linear search [12] $\mathcal{O}(N)$
- Simulation of quantum systems
  - Molecular interaction [1]
- Quantum artificial intelligence
  - Perovskite structure prediction [16]
  - Climate modelling [25]

$\Rightarrow$ Near exponential speedup for certain applications

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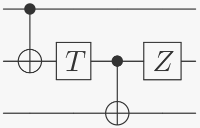
Quantum Circuits [18]

- Analagous to classical logic gates
- But **reversible**
- Input is reconstructable from output
- Gates are unitary operators
- Not all gates have classical counter part (eg. Hadamard)



$\Rightarrow$ **Near exponential speedup for certain applications**

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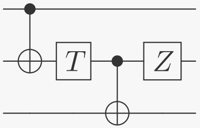
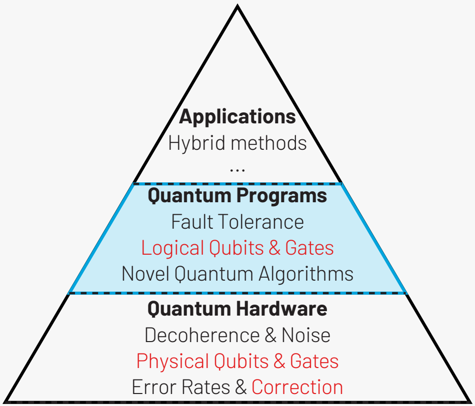


What is the catch?

Quantum Computing

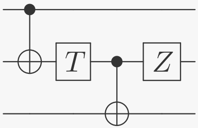
- **Ressource restrictions**:
  - 127 logical qubits [6]
  - up to ≈ 5000 logical gates
  - short coherence time ($80[\mu s]$ to $1[ms]$) [22]
- **Error correction**:
  - noise drives gate error rate [24]
  - limits the number of usable gates
  - overhead varies by an order of magnitude for different gates [20]
- **Quantum computing limited to artificial problems**



$\Rightarrow$ **Architecture-independent QC optimization**

QC Optimization

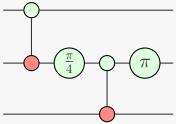
- Infinite universal gate sets
- Infinite gate commutation rules
- Equivalence verification computational expensive



$\Rightarrow$

ZX Calculus [2, 3]

- 8 generators
- 9 well defined rewriting rules
- Rewriting rules preserve semantics



$\Rightarrow$ State-space for combinatorial optimization is (infinitely) large

Contribution

- **Formalization** of ZX diagram optimization
- New set of **pruning conditions** for state-space reduction
- Reproducible **framework** that integrates in standard quantum compilation pipelines (≈ 7000 LOC)

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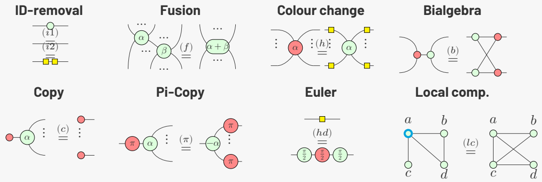
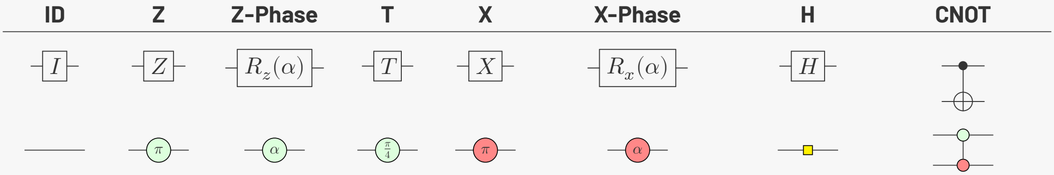
ZX calculus

Diagrammatic Reasoning Framework

- Every QC can be expressed as a ZX diagram [26]
- **Semantic preserving rewriting rules**
- Circuit extraction is # P-hard [4]
- Applied for QC optimization and verification





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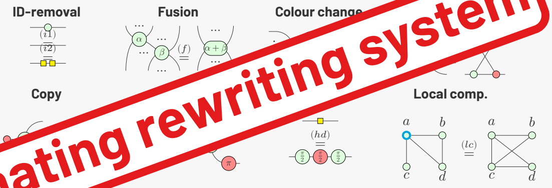
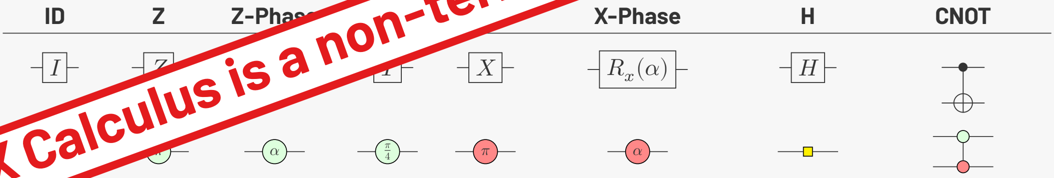
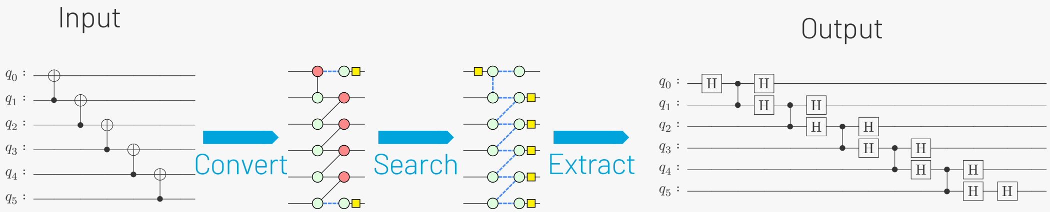


ZX Calculus is a non-terminating rewriting system



Optimization Pipeline



Formal ZX diagram optimization

Quantum Circuit Optimization

- Input & output quantum circuit
  - Let **QC** be the set of quantum circuits
- opt is a function that maps a quantum circuit to a metric
  - $opt : \mathbf{QC} \to \mathbb{Z}$

Define quantum circuits

Formal ZX diagram optimization

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Define quantum circuits

- Linear map of qubits
  - Let **LM** be the set of the linear map of qubits
- γ is a function that maps a quantum circuit to its linear map
  - $\gamma : \mathbf{QC} \to \mathbf{LM}$

Quantum circuits implement a linear map of qubits

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Quantum circuits implement a linear map of qubits

- f is a function to transform quantum circuits
  - $f : \mathbf{QC} \rightarrow \mathbf{QC}$
  - f is semantic-preserving $\forall q \in \mathbf{QC},\ \gamma(q) = \gamma(f(q))$
  - f minimizes the objective function $\min opt$

Functions that transform quantum circuits need to **keep the same** linear map of qubits

$\Rightarrow f$ is a quantum circuit optimization algorithm

Formal ZX diagram optimization

- ZX diagrams
  - Let **ZX** be the infinite set of all finite ZX diagrams
- α is a function that converts quantum circuits to ZX diagrams
  - $\alpha : \mathbf{QC} \rightarrow \mathbf{ZX}$

Every quantum circuit can be converted to a ZX diagram

Formal ZX diagram optimization

ZX-based Quantum Circuit Optimization

- ZX diagrams
  - Let **ZX** be the infinite set of all finite ZX diagrams
- α is a function that converts quantum circuits to ZX diagrams
  - $\alpha : \mathbf{QC} \rightarrow \mathbf{ZX}$
- $extract$ is a function that converts ZX diagrams to quantum circuits
  - $extract : \mathbf{ZX} \rightarrow \mathbf{QC} \cup \{\bot\}$
  - A ZX diagram is extractable if $zx \in \mathbf{ZX}, extract(zx) \neq \bot$

Every quantum circuit can be converted to a ZX diagram

Not every ZX diagram can be extracted

Formal ZX diagram optimization

ZX-based Quantum Circuit Optimization

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  - α : **QC** $\rightarrow$ **ZX**

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  - $extract$: **ZX** $\rightarrow$ **QC** $\cup \{\bot\}$
  - A ZX diagram is extractable if $zx \in$ **ZX**, $extract(zx) \neq \bot$

Not every ZX diagram can be extracted

- Rewriting rules
  - Let **R** $= \{i1, i2, f, h, b, c, \pi, hd, lc\}$ be the set of rewriting rules
- $r \in R$ is a function that transforms a ZX diagram
  - $r \in R$: **ZX** $\rightarrow$ **ZX**

Rules are functions that transform ZX diagrams

$\Rightarrow$ A ZX based QC algorithm searches for extractable ZX diagrams that improves QC metric(s)

Formal ZX diagram optimization

ZX-based Quantum Circuit Optimization

State-space formed by finite sequence of rules on converted quantum circuit

- W is the ZX state-space
  - $q \in QC, W \subseteq$ **ZX** s.t. $w \in W$ exists for a finite sequence of rewriting rules
  - $w = (r_n \circ ... \circ r_1 \circ \alpha)(q)$

- w is a function that converts a QC to a ZX diagram and applies a finite sequence of rewriting rules
  - $w = (r_n \circ ... \circ r_1 \circ \alpha)(q)$

Formal ZX diagram optimization

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  - $w = (r_n \circ \ldots \circ r_1 \circ \alpha)(q)$
- Solutions are all extractable ZX diagrams in the state-space W:
  - $S \subseteq W$
  - $\forall w \in W, \; \mathit{extract}(w) \neq \bot \Leftrightarrow w \in S$

Extractable ZX diagrams of the state-space are solutions

Formal ZX diagram optimization

ZX-based Quantum Circuit Optimization

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Extractable ZX diagrams of the state-space are solutions

- **Optimal solutions** is the largest subset of solutions such that a metric is minimized
  - $O \subseteq S$
  - $\forall o \in O, s \in S, opt(extract(o)) \leq opt(extract(s))$

All solutions ZX diagrams that minimize a metric are optimal

Experimental Setup

Challenges

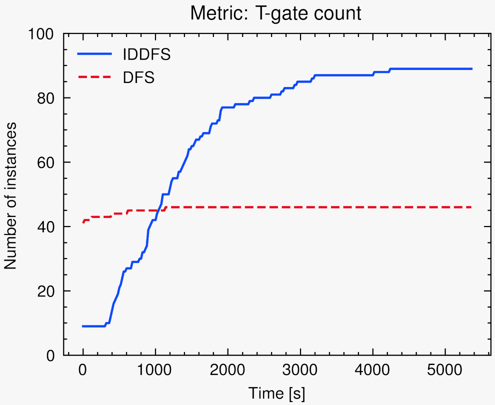
- Non-termination $\rightarrow$ select efficient pruning conditions
- Failed circuit extraction $\rightarrow$ compute metrics on ZX diagram; ensure graph-likeness
- High-memory requirement $\rightarrow$ open question

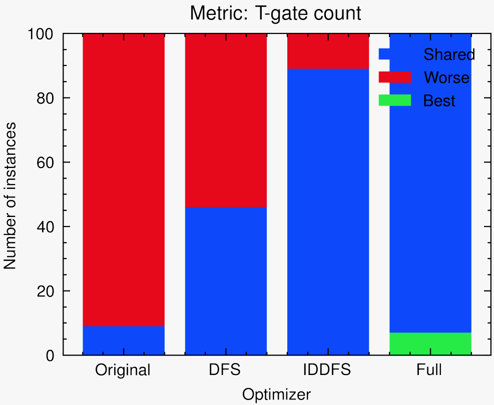
Benchmark

- 100 standard quantum circuits
- 1.5 hour global timeout
- Pruning conditions:
  - No colour cycle
  - No spider unfusion
  - Rule bundling
- DFS & IDDFS
- Connectivity change takes precedent over spider count

Results

T-gate reduction





Results

T-gate reduction

DFS

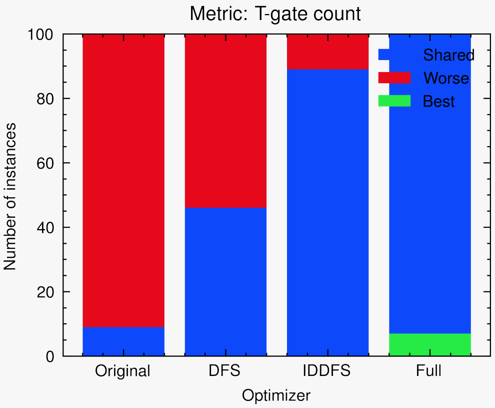
- reduces T-gate count by $\approx 10\%$
- equates Full reduce on 46% of the instances

IDDFS

- reduces T-gate count by $\approx 26\%$
- equates Full reduce on 89% of the instances

Full reduce [11]

- reduces T-gate count by $\approx 27\%$
- always leads to the best result



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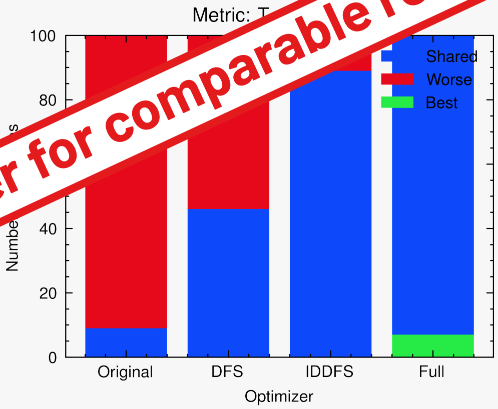
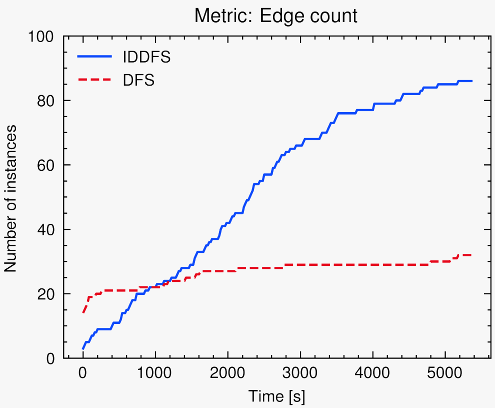
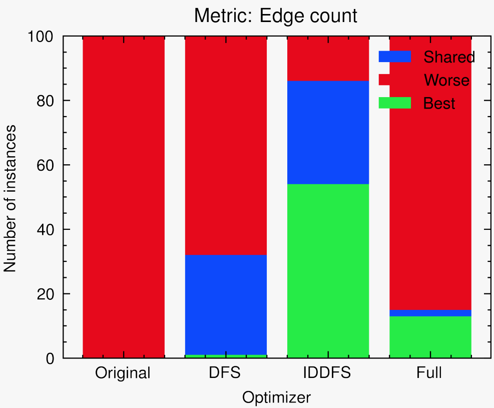


Orders of magnitudes slower for comparable results

Results

Edge count reduction





Results

Edge count reduction

DFS

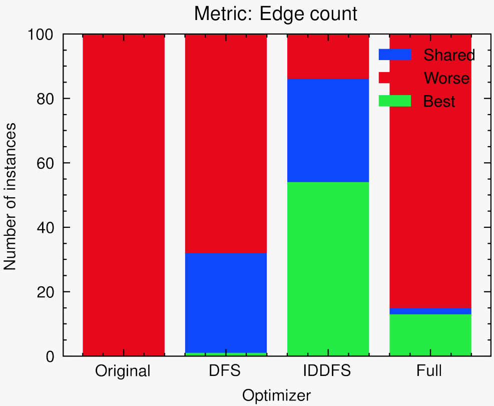
- reduces Edge count by $\approx 11\%$
- best solution on 32% of the instances

IDDFS

- reduces Edge count by $\approx 22\%$
- best solution on 86% of the instances
- comparable to SOTA algorithms that target Edge count (29% reduction) [23]

Full reduce

- not designed for edge count reduction
- reduces Edge count by $\approx 2\%$
- best solution on 15% of the instances



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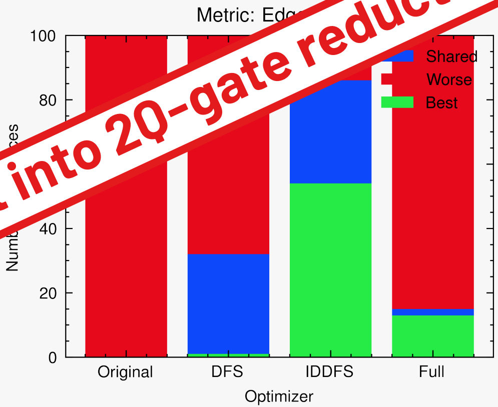

How to translate Edge count into 20-gate reduction?

Implementation

- ≈ 7000 LOC
- Integrates with pre-existing quantum compilation pipelines (Qiskit and PyZX)
- Solver and metric independent
- Currently supported solvers:
  - DFS, IDDFS, Local-Elimination
- New pruning conditions
- Snapshots for time-evolution
- Extensible code base
- Pre-defined benchmark with standard circuits

Code available on Gitlab.

Summary

Conclusion

- **Formalization** of ZX diagram optimization
- New set of **pruning conditions** for state-space reduction
- Reproducible **framework** that integrates in standard quantum compilation pipelines (≈ 7000 LOC)
- **Exhaustive search**:
  - **Equals T-gate count of SOTA** on 89% of the instances
  - **Reduces the edge count** by 22% on average **close to SOTA** (29%)

Outlook

- Improved solvers
  - **Limited-Discrepancy search**
  - Lexiographic search
  - **Better Local-Elimination implementation**
- New pruning conditions
- Target two-qubit gates from edge count

Thank you for your attention.

Check out the Framework.

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