

Special Meeting 2

Tobias Fischbach, Pierre Talbot, Pascal Bouvry

20.06.2025



UNIVERSITY OF LUXEMBOURG
Institute for Advanced Studies

Quantum Computing Applications

- Factorization
 - Shor [25] $\mathcal{O}(\log N^3)$ vs. GNFS [20]
 $\mathcal{O}(\exp \sqrt{\frac{64}{9}} \log N^{\frac{1}{3}} \log \log N^{\frac{2}{3}})$
- Unstructured search
 - Grover [9] $\mathcal{O}(\sqrt{N})$ vs. linear search [14] $\mathcal{O}(N)$
- Simulation of quantum systems
 - Molecular interaction [1]
- Quantum artificial intelligence
 - Perovskite structure prediction [19]
 - Climate modelling [29]

⇒ Near exponential speedup for certain applications



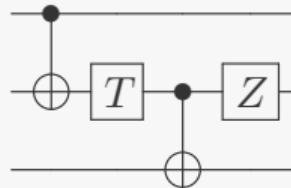
Quantum Computing Applications

- Factorization
 - Shor [25] $\mathcal{O}(\log N^3)$ vs. GNFS [20]
 $\mathcal{O}(\exp \sqrt{\frac{64}{9}} \log N^{\frac{1}{3}} \log \log N^{\frac{2}{3}})$
- Unstructured search
 - Grover [9] $\mathcal{O}(\sqrt{N})$ vs. linear search [14] $\mathcal{O}(N)$
- Simulation of quantum systems
 - Molecular interaction [1]
- Quantum artificial intelligence
 - Perovskite structure prediction [19]
 - Climate modelling [29]

⇒ Near exponential speedup for certain applications

Quantum Circuits [21]

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



Quantum Computing Applications

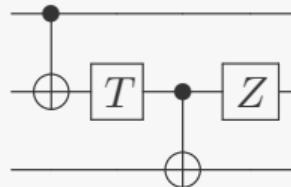
- Factorization
 - Shor [25] $\mathcal{O}(\log N^3)$ vs. GNFS [20]
 $\mathcal{O}(\exp \sqrt{\frac{64}{9}} \log N^{\frac{1}{3}} \log \log N^{\frac{2}{3}})$
- Unstructured search
 - Grover [9] $\mathcal{O}(\sqrt{N})$ vs. linear search [14] $\mathcal{O}(N)$
- Simulation of quantum systems
 - Molecular interactions [21]
- Quantum artificial intelligence
 - Perovskite structure prediction [19]
 - Climate modelling [29]

⇒ Near exponential speedup for certain applications

Quantum Circuits [21]

- Analogous to classical logic gates
- But **reversible**
- Input is reconstructable from output
- CNOT gate is unitary operator
- All gates have classical counter part (eg. Hadamard)

What is the catch?



Quantum Computing

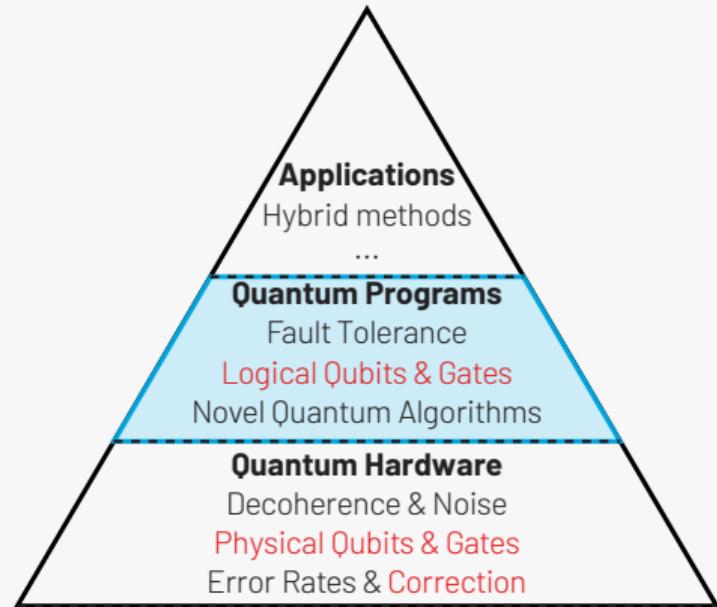
- **Ressource restrictions:**

- 127 logical qubits [6]
- up to ≈ 5000 logical gates
- short coherence time ($80[\mu\text{s}]$ to $1[\text{ms}]$) [26]

- **Error correction:**

- noise drives gate error rate [28]
- limits the number of usable gates
- overhead varies by an order of magnitude for different gates [24]

- **Quantum computing limited to artificial problems**



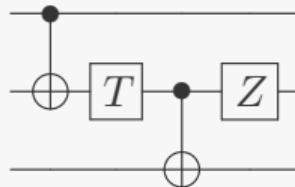
⇒ **Architecture-independent QC optimization**

Quantum Computing

Current Challenges in Quantum Computing

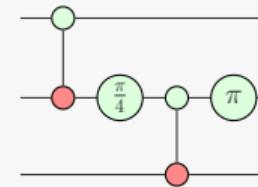
QC Optimization

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



ZX Calculus [2, 3]

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

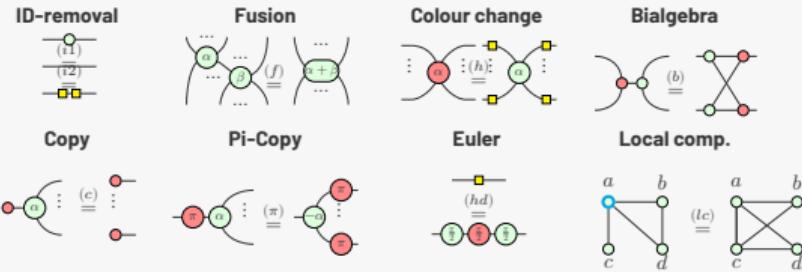


⇒ State-space for combinatorial optimization is (infinitely) large

ZX calculus

Diagrammatic Reasoning Framework

- Every QC can be expressed as a ZX diagram [30]
- **Semantic preserving rewriting rules**
- Circuit extraction is # P-hard [4]
- Applied for QC optimization and verification

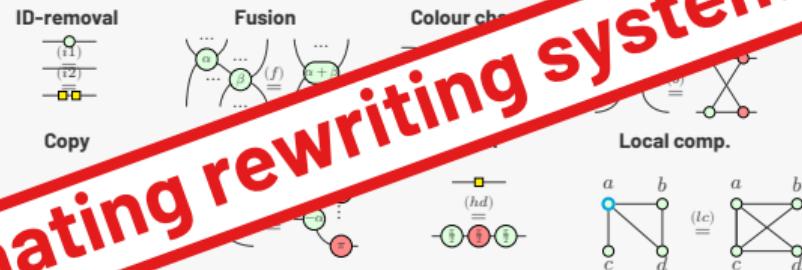


| ID | Z | Z-Phase | T | X | X-Phase | H | CNOT |
|-------------|--|---|--|--|---|-------------|--|
| \boxed{I} | \boxed{Z} | $\boxed{R_z(\alpha)}$ | \boxed{T} | \boxed{X} | $\boxed{R_x(\alpha)}$ | \boxed{H} | \bullet |
| — | $\circlearrowleft \pi \circlearrowright$ | $\circlearrowleft \alpha \circlearrowright$ | $\circlearrowleft \frac{\pi}{4} \circlearrowright$ | $\circlearrowleft \pi \circlearrowright$ | $\circlearrowleft \alpha \circlearrowright$ | \square | $\begin{array}{c} \bullet \\ \oplus \\ \circlearrowleft \bullet \circlearrowright \end{array}$ |

ZX calculus

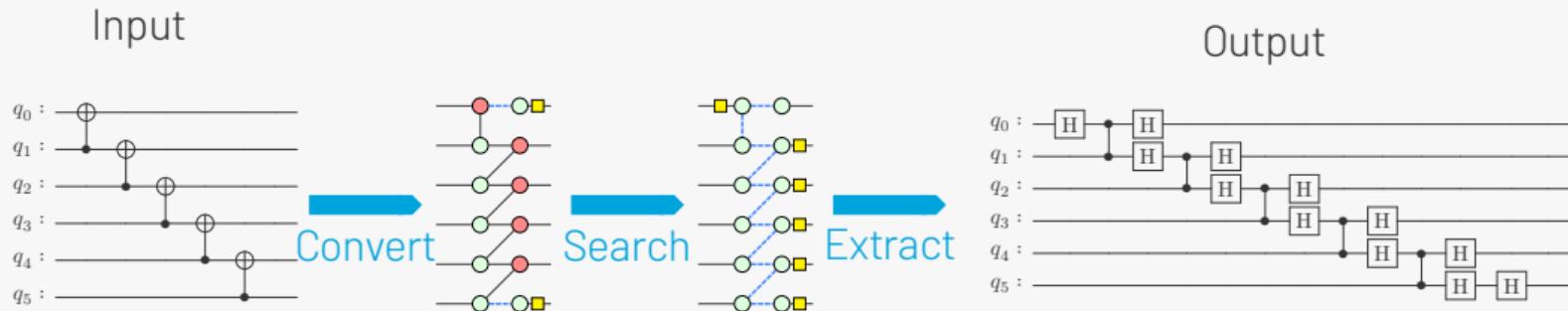
Diagrammatic Reasoning Framework

- Every QC can be expressed as a ZX diagram [30]
- **Semantic preserving rewriting rules**
- Circuit extraction is # P-hard [4]
- Applied for QC optimization and verification



| ID | Z | Z-Phase | X | X-Phase | H | CNOT |
|-----|-----------|----------|-----------------|---------|---------------|------|
| I | \square | | T | X | $R_x(\alpha)$ | H |
| | π | α | $\frac{\pi}{4}$ | π | α | |
| | | | | | \square | |
| | | | | | | |

Optimization Pipeline



Search

Extract

Output

Experimental Setup

Challenges

- Non-termination → select efficient pruning conditions
- Failed circuit extraction → compute metrics on ZX diagram; ensure graph-likeness
- High-memory requirement → 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

DFS

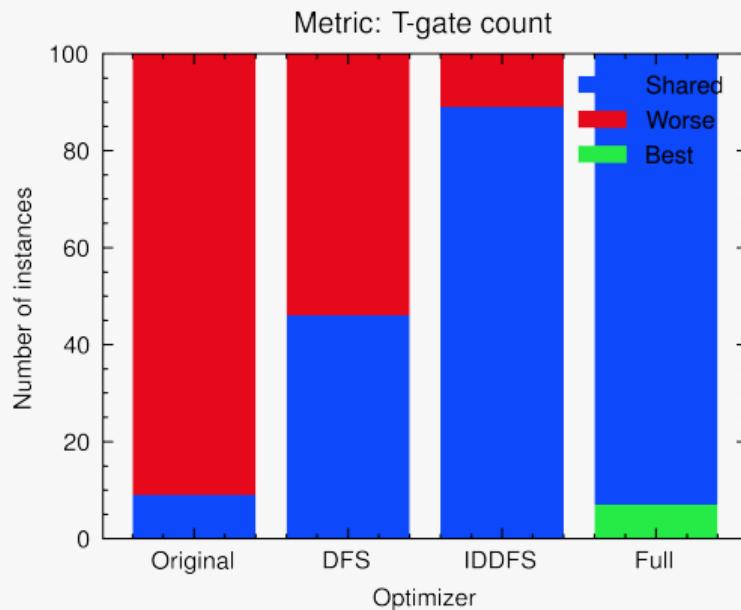
- reduces T-gate count by $\approx 10\%$
- equates Full reduce on 46% of the instances

IDDFS

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

Full reduce [13]

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



Results

T-gate reduction

DFS

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

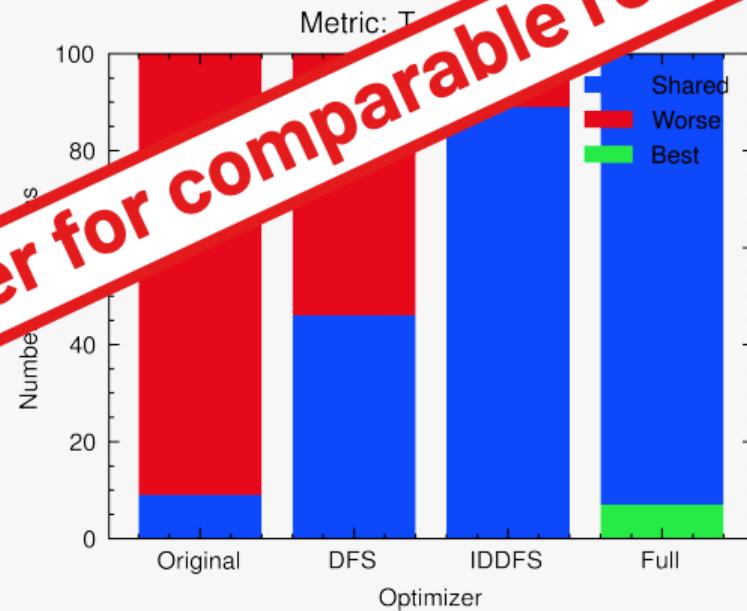
IDDFS

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

Full reduce [13]

- reduces T-gate count by $\approx 27\%$

• leads to the best result



Results

Edge count reduction

DFS

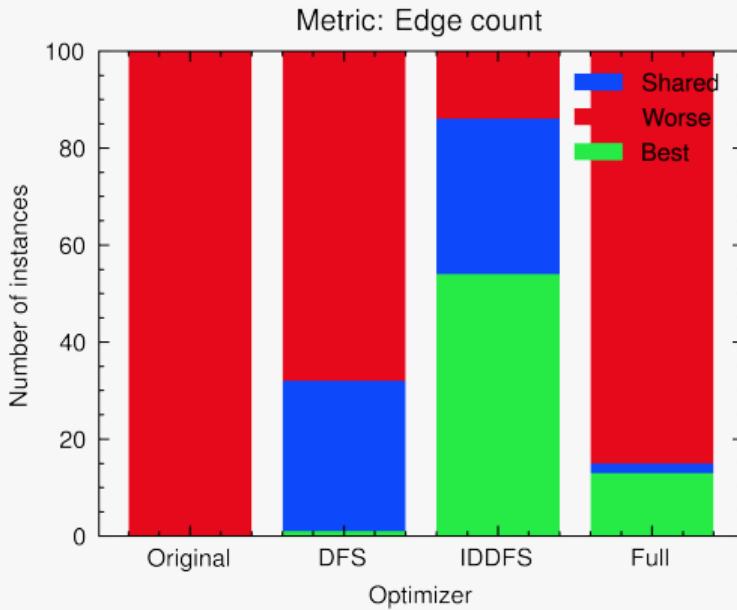
- reduces Edge count by $\approx 11\%$
- best solution on 32% of the instances

IDDFS

- reduces Edge count by $\approx 22\%$
- best solution on 86% of the instances
- comparable to SOTA algorithms that target Edge count (29% reduction) [27]

Full reduce

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



Results

Edge count reduction

DFS

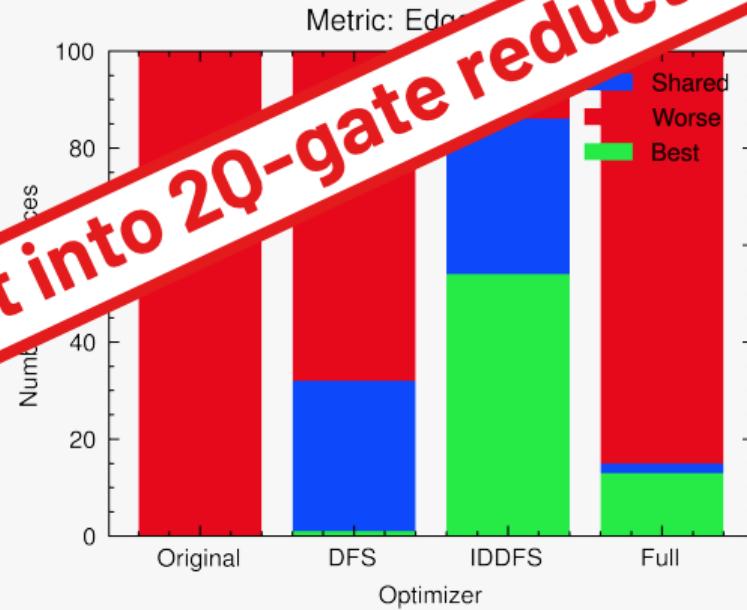
- reduces Edge count by $\approx 11\%$
- best solution on 32% of the instances

IDDFS

- reduces Edge count by $\approx 22\%$
- best solution on 86% of the instances
- comparable to SOTA algorithm target Edge count (200) [27]

Full reduce

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



How to translate Edge count into 2Q-gate reduction?

Challenges

- Non-termination → select efficient pruning conditions
- Failed circuit extraction → compute gflow or cflow
- High-memory requirement → open question
- Slow → Improve heuristic
- Improved results → consider all rules; allow temporary worse metrics
- Balanced circuits → Multiobjective optimization



Improved Heuristic

- No rule has a vanishing probability → Limited-Discrepancy Search inefficient
- Restrict worsening of metrics by $x\%$ (new pruning condition) [27, 10]
- Compute flow properties instead of circuit extraction
- Allow rule reversal [27, 22, 17]
 1. verify cflow (computationally cheap)
 2. verify gflow only if cflow not present (computationally expensive)
- Order rules by:
 1. spider degree \deg
 2. edge count N_e
 3. spider count N_{spiders}

$$h : \{\mathbf{ZX}, r \in \mathbf{R}\} \Rightarrow \{(x_i, v \in \mathbf{ZX}), (x_{i+1}, w \in \mathbf{ZX}) \dots \| x, i \in \mathbb{N}\}$$

$$x_i = \deg \cdot (\Delta N_e + \Delta N_{\text{spiders}})$$



Composite Score

$$S = \sum_i w_i \cdot \frac{m_i^{\text{current}}}{m_i^{\text{input}}}$$

- w_i : weight for metric i and $\sum_i w_i = 1$
- m_i : value of metric i

$$S = S_{\text{indep}}^{\text{ZX}} + S_{\text{arch}}^{\text{ZX}} + S_{\text{indep}}^{\text{QC}} + S_{\text{arch}}^{\text{QC}}$$

⇒ There is not one metric that defines a good ZX diagram or QC

Composite Score

ZX

N_e

N_{he}

N_{spiders}

N_{phases}

N_T

ZX

deg_{avg}

Architecture-independent

Number of diagram edges

Number of Hadamard edges

Spider count

Number of non-zero phase spiders

Number of spiders with phase $\pi/4$

Architecture-dependent

Average degree of spiders

QC

G_{2Q}

G_{1Q}

T

T_d

D

Q

C

QC

G_{CS}

D_{phys}

Q_{phys}

E_{total}

F_{expected}

Architecture-independent

Number of two-qubit gates

Number of one-qubit gates

T-count

T-depth

Logical circuit depth

Number of logical qubits

Clifford count

Architecture-dependent

Number of SWAP added

Physical circuit depth

Physical qubits

Estimated total gate error

Circuit fidelity

Multiobjective optimization

SOTA

- Lexiographic optimization of T-gates (full reduce) followed by two-qubit gates or two-qubit depth → same starting point
- Tree search allows temporary worsening of a metric for better results in the future [27, 10]
- Genetic algorithm that targets two-qubit gates and circuit depth, but only approximately [7]
- Combination of tree search with reinforcement learning is effective and scales well for larger circuits (future work?) [17]

Simulated Annealing

- adjust probability by rule order heuristic
- IDDFS for tree exploration
- keep metric score and rule order heuristic in memory
- prune solutions that worsen the composite metric by more than $x\%$

Proposed Roadmap

- implement improved rule selection heuristic
- new pruning condition for worse circuits based on composite metric
- select suitable parameters for composite metric
- balance computational requirement of metric with quality of solution
- use multiobjective optimization techniques such as simulated annealing to improve speed

Bibliography I

-  Alberto Baiardi, Matthias Christandl, and Markus Reiher. **Quantum Computing for Molecular Biology.** *ChemBioChem*, 24(13):e202300120, 2023. ISSN: 1439-7633. DOI: 10.1002/cbic.202300120. (Visited on 11/30/2024).
-  Bob Coecke and Ross Duncan. **Interacting Quantum Observables.** In Luca Aceto, Ivan Damgård, Leslie Ann Goldberg, Magnús M. Halldórsson, Anna Ingólfssdóttir, and Igor Walukiewicz, editors, *Automata, Languages and Programming*, pages 298–310, Berlin, Heidelberg. Springer, 2008. ISBN: 978-3-540-70583-3. DOI: 10.1007/978-3-540-70583-3_25.
-  Bob Coecke and Ross Duncan. **Interacting quantum observables: categorical algebra and diagrammatics.** *New Journal of Physics*, 13(4):043016, April 2011. ISSN: 1367-2630. DOI: 10.1088/1367-2630/13/4/043016. (Visited on 11/30/2024).

Bibliography II

-  Niel de Beaudrap, Aleks Kissinger, and John van de Wetering. **Circuit Extraction for ZX-diagrams can be #P-hard.** 19 pages, 927080 bytes, 2022. ISSN: 1868-8969. DOI: [10.4230/LIPIcs.ICALP.2022.119](https://doi.org/10.4230/LIPIcs.ICALP.2022.119). arXiv: [2202.09194 \[quant-ph\]](https://arxiv.org/abs/2202.09194). (Visited on 04/19/2024).
-  Ross Duncan, Aleks Kissinger, Simon Perdrix, and John van de Wetering. **Graph-theoretic Simplification of Quantum Circuits with the ZX-calculus.** *Quantum*, 4:279, June 2020. DOI: [10.22331/q-2020-06-04-279](https://doi.org/10.22331/q-2020-06-04-279). (Visited on 11/30/2024).
-  **Eagle's quantum performance progress | IBM Quantum Computing Blog.** <https://www.ibm.com/quantum/blog/eagle-quantum-processor-performance>. (Visited on 11/30/2024).
-  Tom Ewen, Ivica Turkalj, Patrick Holzer, and Mark-Oliver Wolf. **Application of zx-calculus to quantum architecture search.** *Quantum Machine Intelligence*, 7(1), March 2025. ISSN: 2524-4914. DOI: [10.1007/s42484-025-00264-6](https://doi.org/10.1007/s42484-025-00264-6). URL: <http://dx.doi.org/10.1007/s42484-025-00264-6>.

Bibliography III

-  Stefano Gogioso and Richie Yeung. **Annealing Optimisation of Mixed ZX Phase Circuits.** In *Electronic Proceedings in Theoretical Computer Science*, volume 394, pages 415–431, November 2023. doi: [10.4204/EPTCS.394.20](https://doi.org/10.4204/EPTCS.394.20). (Visited on 12/01/2024).
-  Lov K. Grover. **A fast quantum mechanical algorithm for database search.** In *Proceedings of the Twenty-Eighth Annual ACM Symposium on Theory of Computing*, STOC '96, pages 212–219, New York, NY, USA. Association for Computing Machinery, July 1996. ISBN: 978-0-89791-785-8. doi: [10.1145/237814.237866](https://doi.org/10.1145/237814.237866). (Visited on 11/30/2024).
-  Calum Holker. **Causal flow preserving optimisation of quantum circuits in the ZX-calculus.** January 2024. doi: [10.48550/arXiv.2312.02793](https://doi.org/10.48550/arXiv.2312.02793). arXiv: [2312.02793](https://arxiv.org/abs/2312.02793) [quant-ph]. (Visited on 02/23/2024).
-  Calum Holker. **Causal flow preserving optimisation of quantum circuits in the ZX-calculus.** January 2024. doi: [10.48550/arXiv.2312.02793](https://doi.org/10.48550/arXiv.2312.02793). arXiv: [2312.02793](https://arxiv.org/abs/2312.02793). (Visited on 11/30/2024).

Bibliography IV

-  Aravind Joshi, Akshara Kairali, Renju Raju, Adithya Athreya, Reena Monica P, Sanjay Vishwakarma, and Srinjoy Ganguly. **Quantum Circuit Optimization of Arithmetic circuits using ZX Calculus.** June 2023. DOI: [10.48550/arXiv.2306.02264](https://doi.org/10.48550/arXiv.2306.02264). arXiv: 2306.02264. (Visited on 12/01/2024).
-  Aleks Kissinger and John van de Wetering. **Reducing T-count with the ZX-calculus.** January 2020. DOI: [10.48550/arXiv.1903.10477](https://doi.org/10.48550/arXiv.1903.10477). arXiv: 1903.10477. (Visited on 11/30/2024).
-  Donald E. Knuth. **The Art of Computer Programming, Volume 3: (2nd Ed.) Sorting and Searching.** Addison Wesley Longman Publishing Co., Inc., USA, 1998. ISBN: 978-0-201-89685-5.
-  Richard E. Korf. **Depth-first iterative-deepening: An optimal admissible tree search.** *Artificial Intelligence*, 27(1):97–109, September 1985. ISSN: 0004-3702. DOI: [10.1016/0004-3702\(85\)90084-0](https://doi.org/10.1016/0004-3702(85)90084-0). (Visited on 12/01/2024).

Bibliography V

-  Dexter C. Kozen. **Depth-First and Breadth-First Search.** In Dexter C. Kozen, editor, *The Design and Analysis of Algorithms*, pages 19–24. Springer, New York, NY, 1992. ISBN: 978-1-4612-4400-4. DOI: [10.1007/978-1-4612-4400-4_4](https://doi.org/10.1007/978-1-4612-4400-4_4). (Visited on 12/01/2024).
-  Alexander Mattick, Maniraman Periyasamy, Christian Utrecht, Abhishek Y. Dubey, Christopher Mutschler, Axel Plinge, and Daniel D. Scherer. **Optimizing quantum circuits via zx diagrams using reinforcement learning and graph neural networks.** 2025. arXiv: 2504.03429 [cs.LG]. URL: <https://arxiv.org/abs/2504.03429>.
-  Maximilian Nägele and Florian Marquardt. **Optimizing ZX-Diagrams with Deep Reinforcement Learning.** September 2024. DOI: [10.48550/arXiv.2311.18588](https://doi.org/10.48550/arXiv.2311.18588). arXiv: 2311.18588. (Visited on 11/30/2024).
-  Mosayeb Naseri, Sergey Gusarov, and D. R. Salahub. **Quantum Machine Learning in Materials Prediction: A Case Study on ABO₃ Perovskite Structures.** *The Journal of Physical Chemistry Letters*, 14(31):6940–6947, August 2023. DOI: [10.1021/acs.jpclett.3c01703](https://doi.org/10.1021/acs.jpclett.3c01703). (Visited on 11/30/2024).

Bibliography VI

-  Carl Pomerance. **A Tale of Two Sieves.** In Arthur Benjamin and Ezra Brown, editors, *Biscuits of Number Theory*, pages 85–104. American Mathematical Society, Providence, Rhode Island, 2009. ISBN: 978-0-88385-340-5 978-1-4704-5843-0. DOI: [10.1090/do1/034/15](https://doi.org/10.1090/do1/034/15). (Visited on 11/30/2024).
-  Robert Raussendorf and Hans J. Briegel. **A One-Way Quantum Computer.** *Physical Review Letters*, 86(22):5188–5191, May 2001. DOI: [10.1103/PhysRevLett.86.5188](https://doi.org/10.1103/PhysRevLett.86.5188). (Visited on 10/27/2024).
-  Jordi Riu, Jan Nogué, Gerard Vilaplana, Artur Garcia-Saez, and Marta P. Estarellas. **Reinforcement Learning Based Quantum Circuit Optimization via ZX-Calculus.** December 2023. arXiv: 2312.11597 [quant-ph]. (Visited on 03/04/2024).
-  Jordi Riu, Jan Nogué, Gerard Vilaplana, Artur Garcia-Saez, and Marta P. Estarellas. **Reinforcement Learning Based Quantum Circuit Optimization via ZX-Calculus.** June 2024. DOI: [10.48550/arXiv.2312.11597](https://doi.org/10.48550/arXiv.2312.11597). arXiv: 2312.11597. (Visited on 11/30/2024).

Bibliography VII

-  Joschka Roffe. **Quantum Error Correction: An Introductory Guide.** July 2019. DOI: [10.48550/arXiv.1907.11157](https://doi.org/10.48550/arXiv.1907.11157). arXiv: [1907.11157](https://arxiv.org/abs/1907.11157). (Visited on 11/30/2024).
-  P.W. Shor. **Algorithms for quantum computation: discrete logarithms and factoring.** In *Proceedings 35th Annual Symposium on Foundations of Computer Science*, pages 124–134, November 1994. DOI: [10.1109/SFCS.1994.365700](https://doi.org/10.1109/SFCS.1994.365700). (Visited on 11/30/2024).
-  Aaron Somoroff, Quentin Ficheux, Raymond A. Mencia, Haonan Xiong, Roman Kuzmin, and Vladimir E. Manucharyan. **Millisecond Coherence in a Superconducting Qubit.** *Physical Review Letters*, 130(26):267001, June 2023. ISSN: 0031-9007, 1079-7114. DOI: [10.1103/PhysRevLett.130.267001](https://doi.org/10.1103/PhysRevLett.130.267001). (Visited on 11/30/2024).
-  Korbinian Staudacher, Tobias Guggemos, Sophia Grundner-Culemann, and Wolfgang Gehrke. **Reducing 2-Qubit Gate Count for ZX-Calculus based Quantum Circuit Optimization.** November 2023. DOI: [10.48550/arXiv.2311.08881](https://doi.org/10.48550/arXiv.2311.08881). arXiv: [2311.08881](https://arxiv.org/abs/2311.08881). (Visited on 11/30/2024).

Bibliography VIII

-  Andrew M. Steane. **Overhead and noise threshold of fault-tolerant quantum error correction.** *Physical Review A*, 68(4):042322, October 2003. DOI: [10.1103/PhysRevA.68.042322](https://doi.org/10.1103/PhysRevA.68.042322). (Visited on 11/30/2024).
-  F. Tennie and T. N. Palmer. **Quantum Computers for Weather and Climate Prediction: The Good, the Bad, and the Noisy.** *Bulletin of the American Meteorological Society*, 104(2):E488–E500, February 2023. ISSN: 0003-0007, 1520-0477. DOI: [10.1175/BAMS-D-22-0031.1](https://doi.org/10.1175/BAMS-D-22-0031.1). (Visited on 11/30/2024).
-  J. V. D. Wetering. **ZX-calculus for the working quantum computer scientist.** In December 2020. (Visited on 02/20/2024).
-  David Winderl, Qunsheng Huang, and Christian B. Mendl. **A recursively partitioned approach to architecture-aware ZX Polynomial synthesis and optimization.** March 2023. DOI: [10.48550/arXiv.2303.17366](https://doi.org/10.48550/arXiv.2303.17366). arXiv: 2303.17366. (Visited on 12/01/2024).