Symbolic Quantum Circuit Simulation

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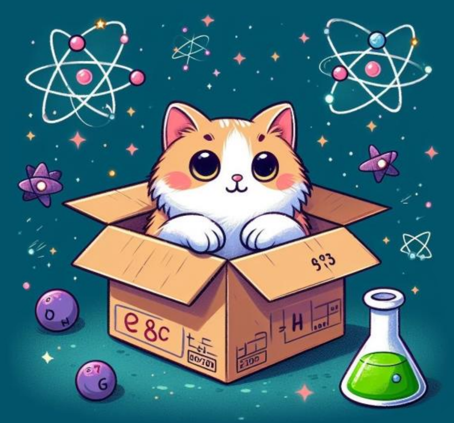

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Motivation

- Even though the history of quantum computing dates to the 1980s, the availability of quantum HW remains limited due to technical challenges and the price associated with it.
- Observing the state of a qubit in a real system requires a measurement of this qubit, which irreversibly collapses its state (i.e., the direct examination of probability amplitudes is possible only in simulation).
- Simulation on classical computers is not a trivial task due to the size difference of the state space of a classical bit and a qubit.

MTBDD-based Quantum Circuit Simulation

- MTBDDs (***Multi-terminal binary decision diagrams***) encode functions $f(v_0, \dots, v_{n-1})\colon \{0,1\}^n \to \mathbb{D}$. They are a generalised variant of ROBDDs (Reduced ordered binary decision diagram), usually simply called BDDs, where terminals can have an arbitrary value.
- We view the system's state as a function $f\colon \{0,1\}^n \to \mathbb{C}$ and represent it with a single MTBDD.

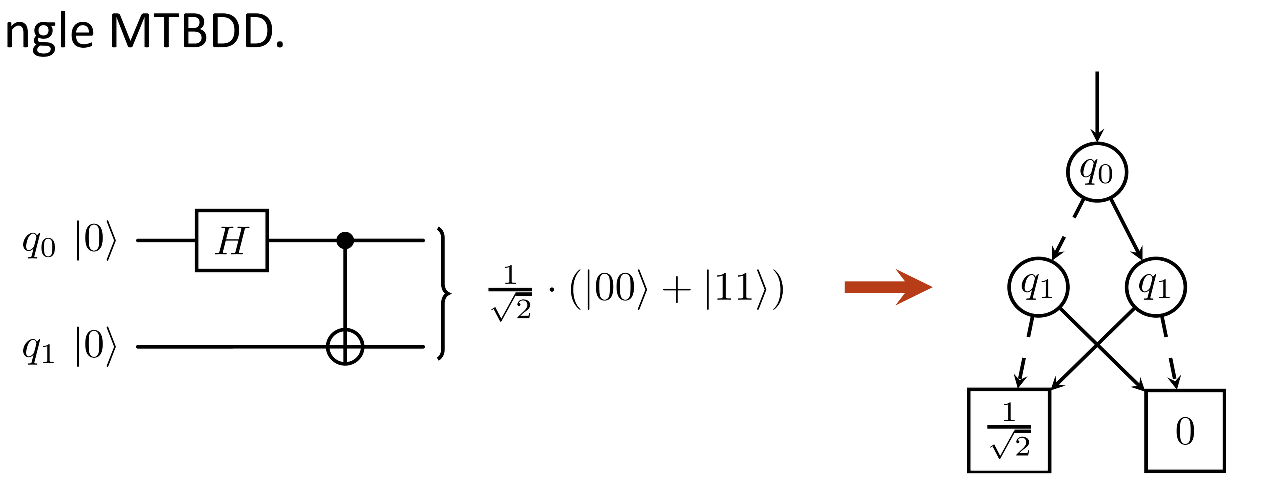


Figure 2: One of the Bell states represented with an MTBDD

- We use exact algebraic representation of complex numbers $z \in \mathbb{C}$

$$z = \left(\frac{1}{\sqrt{2}}\right)^k \cdot (a + b\omega + c\omega^2 + d\omega^3)\,, \qquad (1)$$

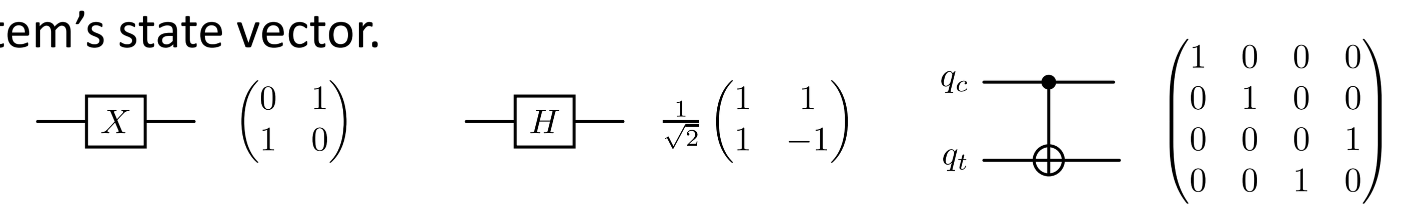
  where $a, b, c, d, k \in \mathbb{Z}$ and $\omega = e^{\frac{i\pi}{4}}$ [2]. The subset of $\mathbb{C}$ representable in this way is sufficient for quantum circuit simulation w.l.o.g.
- Gate application is executed as a single custom *Apply* if possible (single qubit gates and controlled phase gates), else as a sequence of operations over the MTBDD using the standard *Apply* procedure.

Quantum Circuit Basics

- A qubit's ***quantum state*** $|\psi\rangle$ can be in a superposition of the computational basis states $|0\rangle$ and $|1\rangle$

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle\,,$$

  where $\alpha, \beta \in \mathbb{C}$ are the ***probability amplitudes*** for the respective basis states. I.e., it is a two-dimensional unit complex vector representing the probabilities that upon measurement the qubits value will be $|0\rangle$ or $|1\rangle$.
- ***Quantum gates*** are used to perform operations on qubits. They can be represented as unitary matrices, then the update of the system's quantum state is carried out as a matrix multiplication of the gate matrix with the system's state vector.



(a) Pauli-X gate (a NOT gate equivalent) (b) Hadamard gate (c) Controlled-NOT (CNOT) gate

Figure 1: Some example gates and their matrix representation

Adding Symbolic Execution

- Symbolic simulation allows us to compute the ***big-step semantics of loops*** in the quantum circuit (often a key element of the algorithm) leading to significant acceleration of the calculation (no need to re-evaluate gates).
- Symbolic simulation is performed with a ***pair of symbolic MTBDDs*** - one maps the original MTBDD leaves to variables and the other holds values of the variables (linear expressions with these variables).

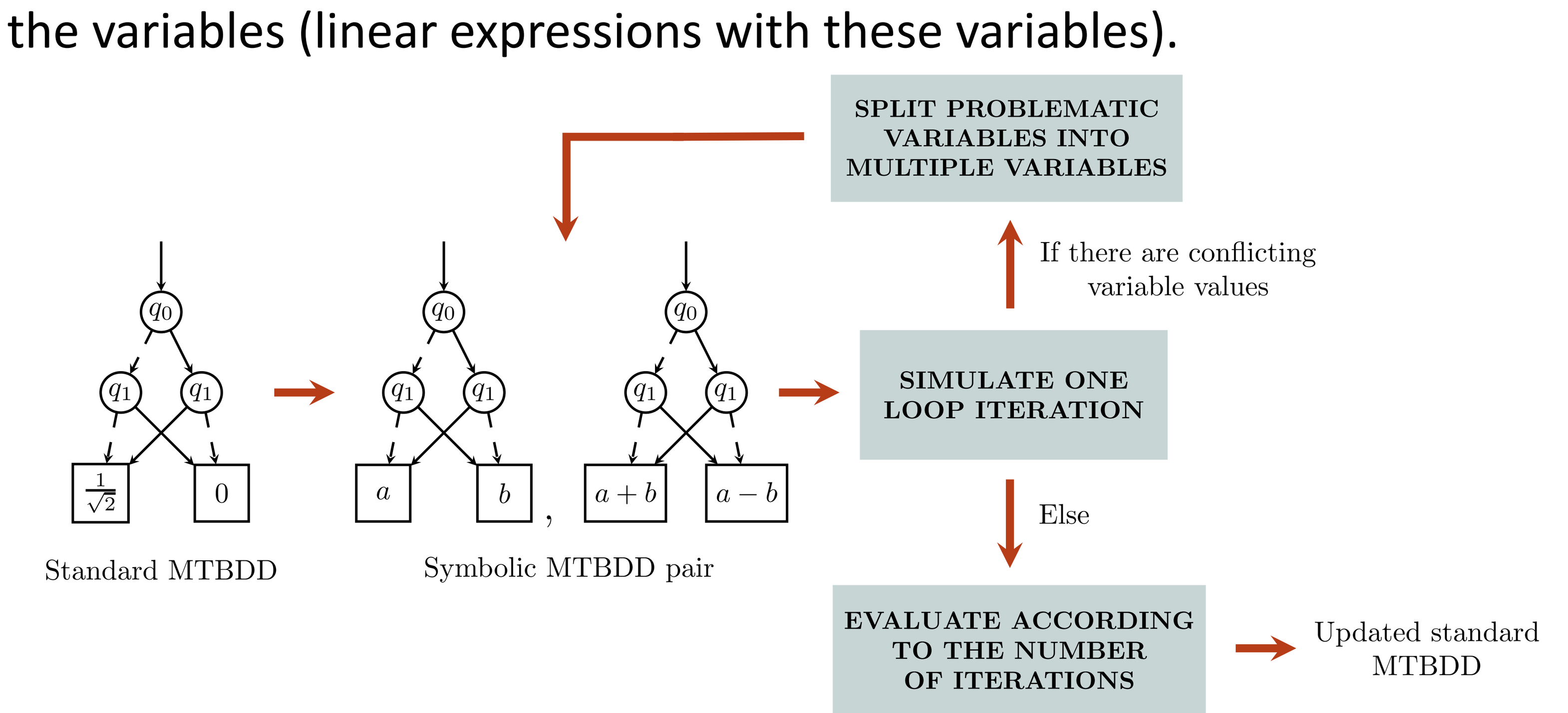


Figure 3: Process of symbolic execution

Experimental Results

- Comparison of the implemented quantum simulator MEDUSA to the current state-of-the-art simulators SliQSim [4], Quasimodo [3], MQT DDSIM [5], and Quokka# [1] by measuring their respective runtimes and memory usage for various quantum circuits. The time-out limit was 1 hour.

Table 1: Benchmark results for some Grover's search algorithm circuits (only shows the best Quasimodo backend)

Qubits	MEDUSA symb.		MEDUSA		SliQSim		DDSIM		Quasimodo (WBDDs)		Quokka#	
	t (s)	Mem (MB)	t (s)	Mem (MB)	t (s)	Mem (MB)	t (s)	Mem (MB)	t (s)	Mem (MB)	t (s)	Mem (MB)
10	0.0541	27.94	0.0195	30.35	0.0129	11.99	0.0031	28.87	0.0064	441.8	TO	TO
40	0.195	39.04	31.3	387	3176	25.36	12.44	118.5	72.6	768.8	TO	TO
46	0.567	39.07	146	1733	TO	TO	TO	TO	1750	1708	TO	TO
48	0.917	38.99	699	3670	TO	TO	TO	TO	TO	TO	TO	TO

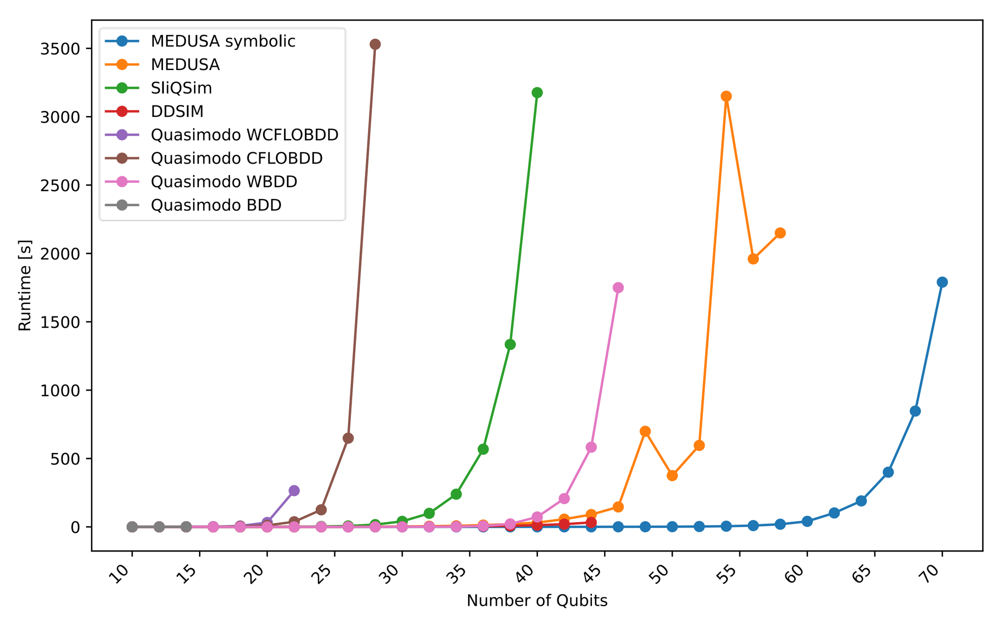


Figure 4: Results for Grover's search algorithm

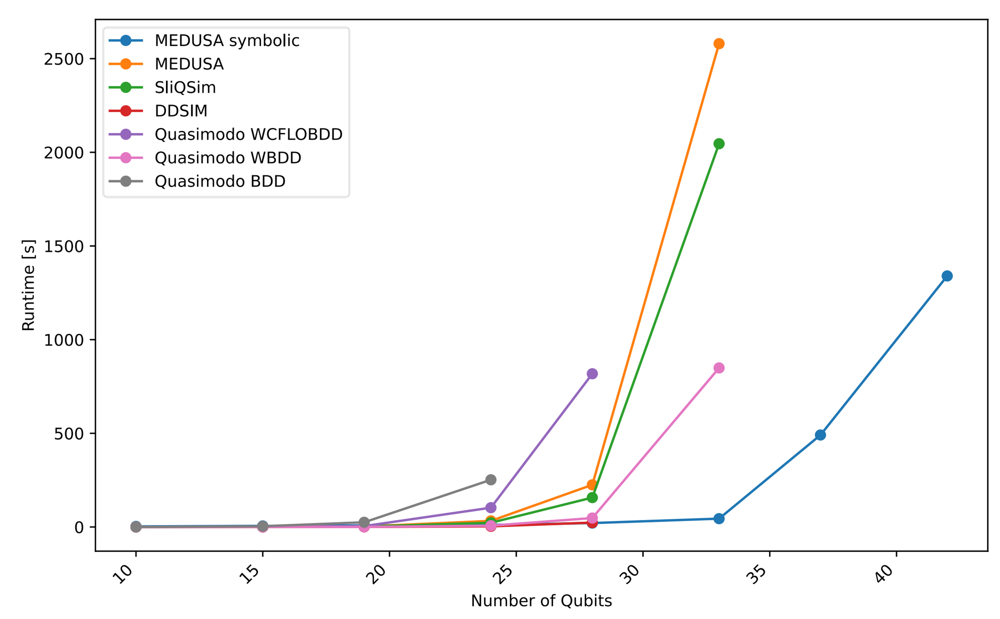


Figure 5: Results for period finding (w/o inverse QFT)

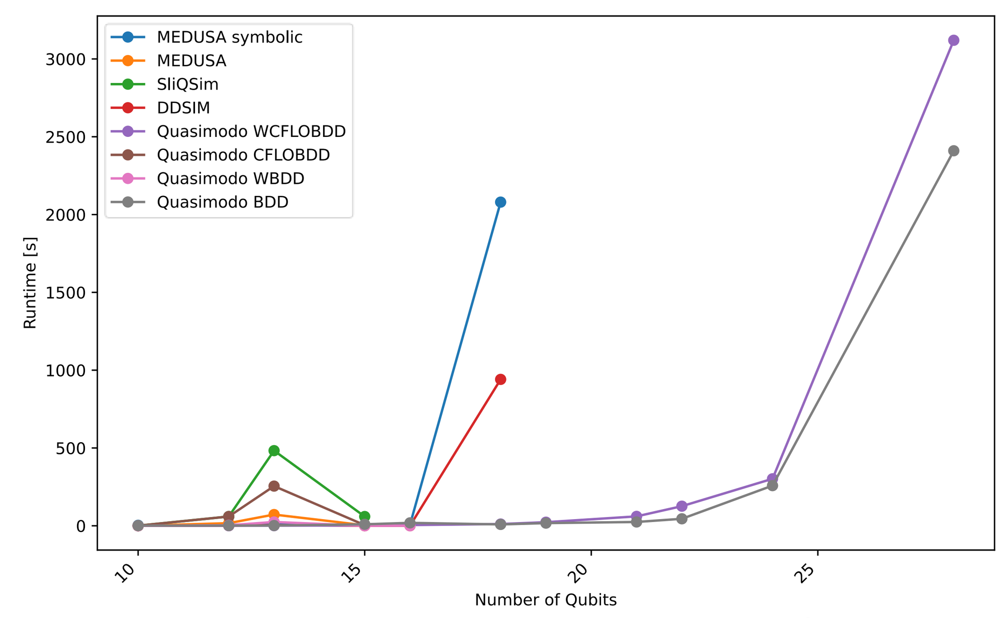


Figure 6: Results for quantum counting (w/o inverse QFT)

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[2] Niemann, P., Zulehner, A., Drechsler, R. and Wille, R. Overcoming the Tradeoff Between Accuracy and Compactness in Decision Diagrams for Quantum Computation. IEEE Trans. Comput. Aided Des. Integr. Circuits Syst. 2020, vol. 39, no. 12, p. 4657–4668. DOI: 10.1109/TCAD.2020.2977603.

[3] Sistla, M., Chaudhuri, S. and Reps, T. W. Symbolic Quantum Simulation with Quasimodo. In: Enea, C. and Lal, A., ed. Computer Aided Verification - 35th International Conference, CAV 2023, Paris, France, July 17-22, 2023, Proceedings, Part III. Springer, 2023, vol. 13966, p. 213–225. Lecture Notes in Computer Science. DOI: 10.1007/978-3-031-37709-9_11.

[4] Tsai, Y.-H., Jiang, J.-H. R. and Jhang, C.-S. Bit-Slicing the Hilbert Space: Scaling Up Accurate Quantum Circuit Simulation. In: 2021 58th ACM/IEEE Design Automation Conference (DAC). 2021, p. 439–444. DOI: 10.1109/DAC18074.2021.9586191.

[5] Zulehner, A. and Wille, R. Advanced Simulation of Quantum Computations. Trans. on CAD of Integrated Circuits and Systems. 2019, vol. 38, no. 5, p. 848–859. DOI: 10.1109/TCAD.2018.2834427.