# LIMDD: Unifying Decision Diagrams and the Stabilizer Formalism

**Lieuwe Vinkhuijzen[†,1], Tim Coopmans[†,1,2], David Elkouss[2,3], Vedran Dunjko[1], Alfons Laarman[1],**
[1] Leiden University, [2] Delft University of Technology, [3] Okinawa Institute of Science and Technology,
{l.t.vinkhuijzen, t.j.coopmans,v.dunjko, a.w.laarman}@liacs.leidenuniv.nl, d.elkousscoronas@tudelft.nl

## Abstract

Efficient methods for representing and transforming quantum states and operations are crucial for optimizing real-world quantum circuits beyond tolerable error levels. Conversely, quantum computing has forced us to re-examine existing knowledge representation techniques and improve upon their limitations. In this work, we investigate and bridge the gap between one such technique, decision diagrams (DDs) —originally used for representing boolean functions—, and the stabilizer formalism, an important tool for simulating quantum circuits in the tractable regime. We first show that, although DDs were suggested to represent important quantum states succinctly, they actually require exponential space for certain stabilizer states. To remedy this, we introduce a more powerful decision diagram variant, called Local Invertible Map-DD (LIMDD). We prove that the set of quantum states represented by poly-sized LIMDDs strictly contains the union of stabilizer states and other decision diagram variants. Finally, there exist circuits which LIMDDs can efficiently simulate, while their output states cannot be succinctly represented by two state-of-the-art simulation paradigms: the stabilizer decomposition techniques for Clifford + $T$ circuits and Matrix-Product States. By uniting two successful approaches, LIMDDs thus pave the way for fundamentally more powerful solutions for simulation and analysis of quantum circuits and provide a prime example of the cross-fertilization between quantum computing and traditional knowledge representation techniques.

## Context: cross-fertilization between knowledge representation and quantum

In the context of quantum computing, knowledge compilation deals with the design of classical data structures for efficiently representing and transforming quantum information such as quantum states and circuits. Such data structures are crucial for circuit design, studying noise resilience in the era of Noisy Intermediate-Scale Quantum (NISQ) computers, and identifying scenarios in which a quantum computational advantage cannot be obtained. A multitude of classical knowledge representation methods have been applied to quantum computing, with great impact on knowledge representation, as the following examples show:

- Decision diagrams (DDs) for representing pseudo-Boolean functions have evolved to support complex numbers for representing quantum states, e.g., Algebraic Decision Diagram evolved into QuiDD and Edge-Valued DD (EVDD) into Quantum Multi-Valued DD (QMDD).
- Model counting has been used for quantum circuit simulation and equivalence checking, showing that quantum circuit compilation involves #P problems that have been handled by this community for decades, but with a twist: negative weights representing destructive interference.
- Tensor networks and matrix product states (MPS), where one stores the quantum state or gate (a large matrix) as product of many smaller matrices, have been used by quantum physicists for decades in order to solve questions in, e.g., many-body physics. Tensor networks are applied in much the same way as DDs: representing and manipulating relations (operations) and states.
- The stabilizer formalism efficiently simulates quantum circuits containing only Clifford gates (a non-universal quantum gate set) , which produce so-called 'stabilizer states.' It plays a fundamental role throughout quantum information, e.g., in quantum error correction and measurement-based quantum computation.

Many applications in quantum computing and physics thus require the (classical) representation of quantum information. The cross-fertilization observed above is therefore a very natural one, with many future opportunities. However, for optimal results and to avoid re-inventing the wheel, this process should be guided by firm insights from knowledge representation and compilation.

In this work, we follow this approach by showing that QMDD (and hence its predecessor Algebraic-DD) cannot represent the crucial set of stabilizer states, prompting the development of a new data structure, LIMDD (Vinkhuijzen et al. 2023a), which combines the best of both worlds between DDs and the stabilizer formalism. We also map its succinctness and tractability characteristics, showing that LIMDD is always more succinct than other DDs, with only polynomial runtime overhead. Finally, we show that QMDD is subsumed by MPS in both succinctness and tractability, but LIMDD is not.

**Decision diagrams.** A DD is a directed acyclic graph (DAG) in which each path represents an amplitude (note

[*] These authors contributed equally.

there can be exponentially many paths even in a DAG of bounded degree). A succinct version of DDs are QMDDs, which represent an $n$-qubit state $|\phi\rangle = \alpha_1|0\rangle \otimes |\phi_0\rangle + \alpha_1|1\rangle \otimes |\phi_1\rangle$ as a node with two outgoing edges: a *low* edge to the node for the $(n-1)$-qubit (sub)state $|\phi_0\rangle$ with label $\alpha_0$, and a *high* edge to the node for the (sub)state $|\phi_1\rangle$ with label $\alpha_1$. By enforcing canonicity, i.e., that there exists only a single unique node for each possible substate (up to a complex factor), frequently-occurring substates only need to be stored once. Various manipulation operations for DDs exist which implement any quantum operation in polytime in the DD size, enabling strong quantum-circuit simulation. Indeed, DD-based simulation was empirically shown to be competitive with state-of-the-art simulators; one highlight is the QMDD-based 37-qubit simulation of Shor's factoring algorithm.

## Contribution 1: The first decision diagram that is succinct for stabilizer states and beyond

We first focus on the capabilities of DDs to statically store quantum states. We prove that QMDDs representing certain stabilizer states, called cluster states, necessarily consist of exponentially many nodes. This exponential separation implies that QMDDs and the stabilizer formalism are qualitatively distinct in their simulation capabilities.

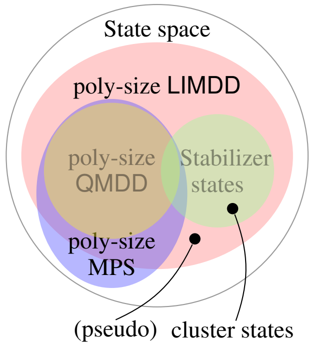


Figure 1: The set of stabilizer states and states representable as poly-sized: (Pauli-)LIMDDs (this work), QMDDs and MPS. Here, a (pseudo) cluster state is a specific family of stabilizer states (with a non-stabilizer-state attached).

Next, in order to unite the strengths of these two, we propose LIMDD: a new DD for quantum computing using local invertible maps (LIMs), i.e., tensor products of single-qubit invertible operations. Specifically: while QMDDs represent substates that are equal up to a constant factor only once, LIMDDs eliminate the need to store multiple *locally-equivalent* (LIM-equivalent) states. Consequently, LIMDDs are exponentially more succinct than QMDDs: we prove that each $n$-qubit stabilizer state is represented by a LIMDD on $O(n)$ nodes. A separation between LIMDDs and the stabilizer formalism is evident since QMDDs and hence LIMDDs can store states which are not stabilizer states. In separate work we also demonstrated that MPS is as succinct as QMDD (Vinkhuijzen, Coopmans, and Laarman 2024). The separations are summarized in Figure 1.

## Contribution 2: separations by LIMDDs in simulation with other state-of-the-art methods

Next, we turn our attention to simulating quantum circuits with LIMDDs. We focus on Pauli-LIMDDs, i.e. where the LIMs are local Pauli operations. We prove that stabilizer-state simulation can be done efficiently *within* Pauli-LIMDDs by providing efficient algorithms (i.e. polytime in the LIMDD's size) for computational-basis measurement and the gates which generate the Clifford group: Hadamard, phase gate, and CNOT. Furthermore, our algorithms also apply to poly-size Pauli-LIMDDs which do not represent a stabilizer state, where efficiency is retained for measurement, phase gate and CNOT (in some cases, also for Hadamard). We also present an algorithm for updating the Pauli-LIMDD after a general multi-qubit gate, which has worst-case exponential runtime. The workhorse behind LIMDDs is a novel algorithm which merges two DD nodes when they are equivalent up to local Pauli operations.

By construction, LIMDDs are never slower slower than QMDDs (up to overhead which scales polynomially in the number of qubits) and in fact are sometimes exponentially faster, as QMDDs cannot efficiently simulate Clifford circuits (stabilizer states). We empirically observed this performance gain in our open-source implementation (separate, published work (Vinkhuijzen et al. 2023b)) too: For example, for simulating the Quantum Fourier Transform, a key subroutine in algorithms with a strong quantum advantage (e.g. Shor's algorithm), LIMDDs outperform QMDDs for more than $n \approx 19$ qubits. Since, like QMDD, MPS cannot succinctly represent all stabilizer states, LIMDDs also have an exponential separation with MPS for simulation.

Finally, we compare LIMDDs with the extended stabilizer formalism for arbitrary-circuit simulation with the Clifford+$T$ universal gate set, whose runtime is (exponentially) fixed-parameter tractable in the number of $T$ gates. We achieve a (conditional) exponential separation as LIMDDs can prepare all $n$-qubit Dicke states in poly($n$) time and space, while Dicke-state circuits generally require linearly many $T$ gates (under the exponential time hypothesis).

In summary, LIMDDs strictly combine QMDD and stabilizer formalism for quantum-circuit simulation, and have separations with other state-of-the-art techniques. Thus, LIMDDs not only are promising candidates for extending the limits of the quantum-circuit analysis, but also a prime example of the cross-fertilization between quantum computing and traditional knowledge representation approaches.

## References

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