IMPLEMENTATION OF TENSOR NETWORK SIMULATION TN-SIM UNDER NWQSIM

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Abstract

- Tensor network methods (MPS) enable efficient simulation of quantum circuits by compressing quantum states and controlling entanglement via SVD truncation.
- We implemented TN-Sim, a new tensor network backend for NWQSim, with support for local and non-local gates, sampling, and fidelity control.
- The simulator was validated against QASMBench circuits and integrated with both iTensor and TAMM backends for scalable performance [1-2].

Motivation

- Quantum circuit simulation scales with the breadth and depth of the circuit..
- For circuits with low or local entanglement, matrix product states can simulate very large circuits.
- Tensor network based simulators are particularly good for simulating circuit cutting, a promising way to distribute quantum computation.

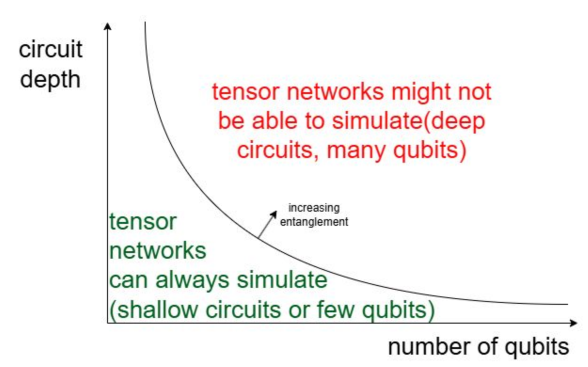


Figure 1

Tensor Network Theory

Quantum circuit simulation traditionally relies on state vector or density matrix methods, both of which suffer from exponential memory growth with the number of qubits. State vectors are efficient for small systems but quickly become infeasible, while density matrices enable noise modeling at even greater computational cost. Tensor network approaches, particularly Matrix Product States (MPS), offer a scalable alternative by compressing quantum states based on their entanglement structure (see Fig. 1).

MPS represents the full quantum state as a chain of smaller tensors connected by bond indices, significantly reducing memory from t, where is the bond dimension (Fig. 2). Gate operations, especially two-qubit gates, are applied via local contractions and followed by SVD to restore the MPS form while controlling accuracy through truncation.
This structure allows dynamic trade-offs between fidelity and performance, enabling simulation of circuits that are otherwise inaccessible to standard methods.

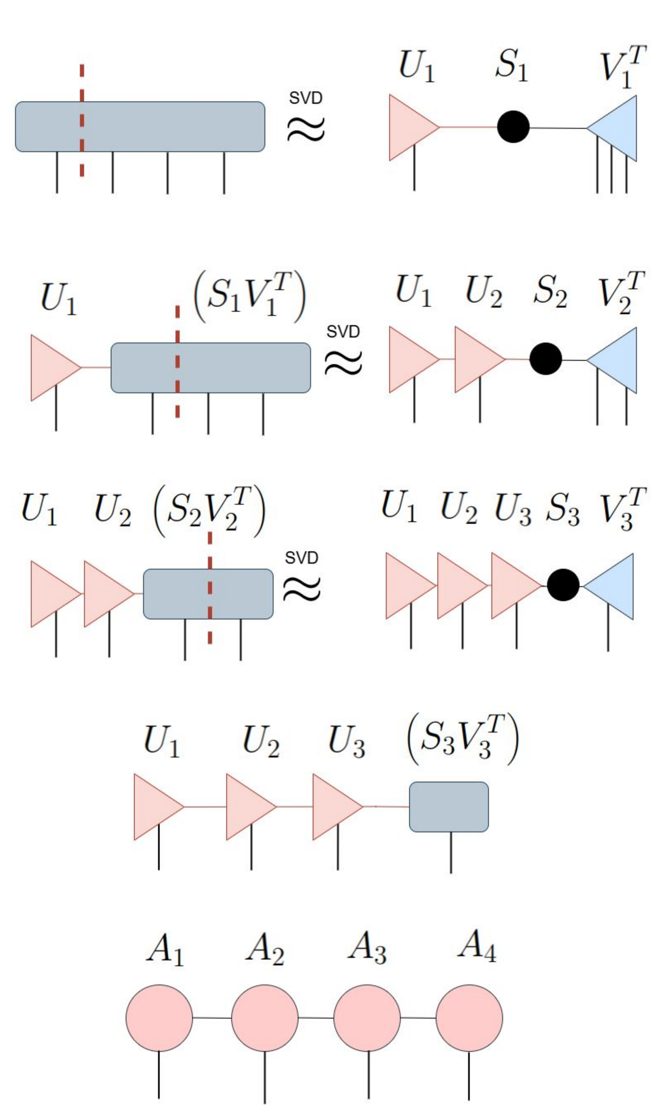
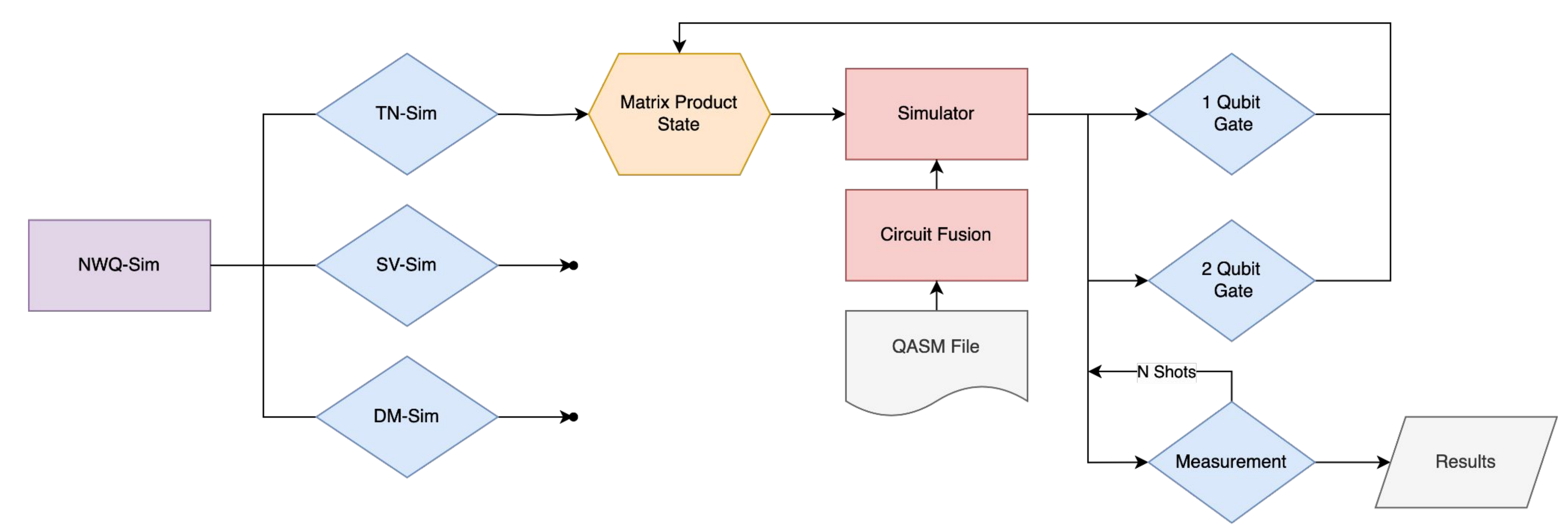


Figure 2

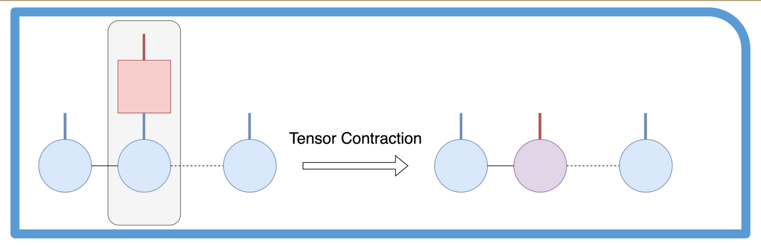
TN Sim

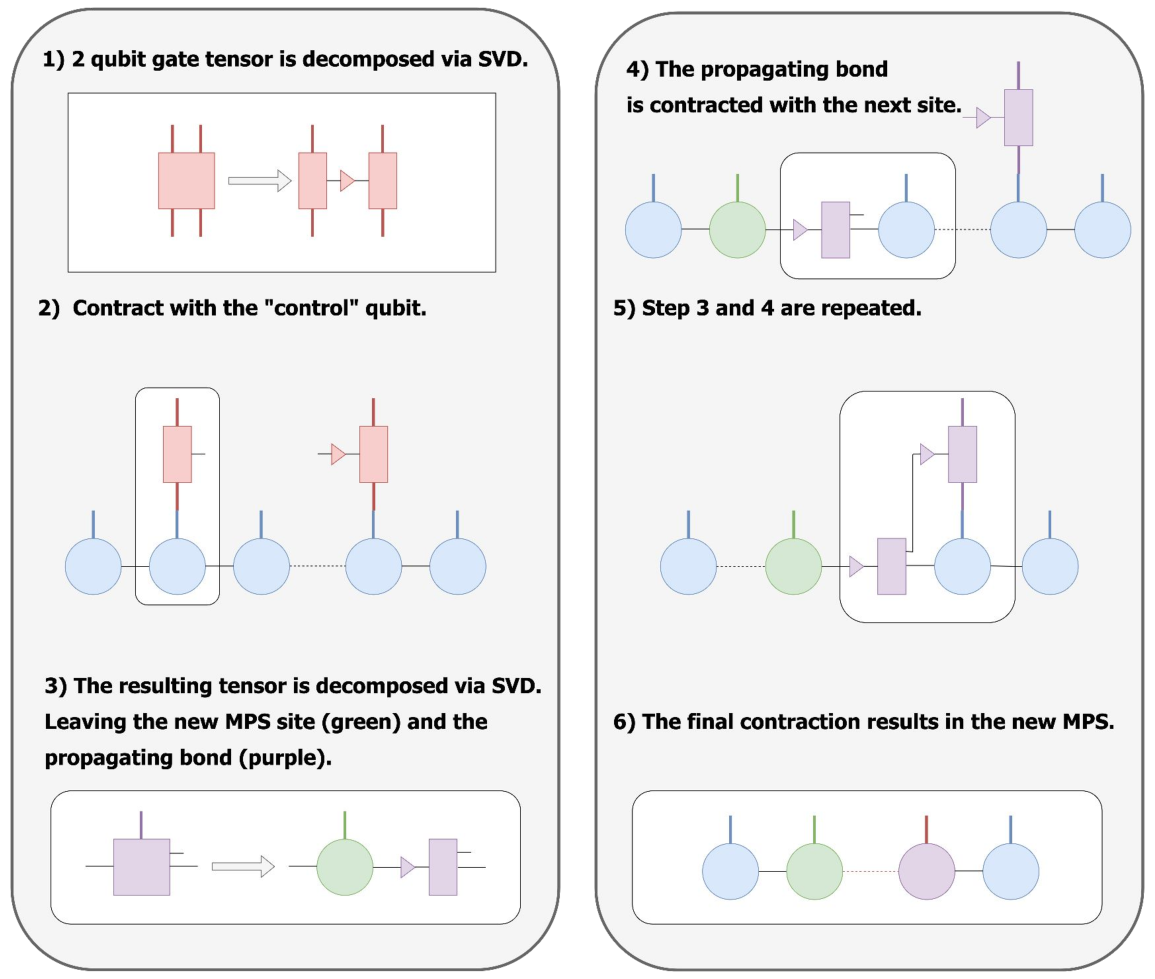


Quantum Gates

One Qubit Gates

- Represented by a matrix.
- The gate is contracted with the MPS site.





Two Qubit Gates

Quantum gates are not limited to one or two qubit gates, however the circuit fusion method converts 3 and higher qubit gates to combinations of 1 and 2.

TN-Sim has implemented local 2 qubit gates and three different algorithms for non-local gates (ones where the distance between qubits is greater than zero).

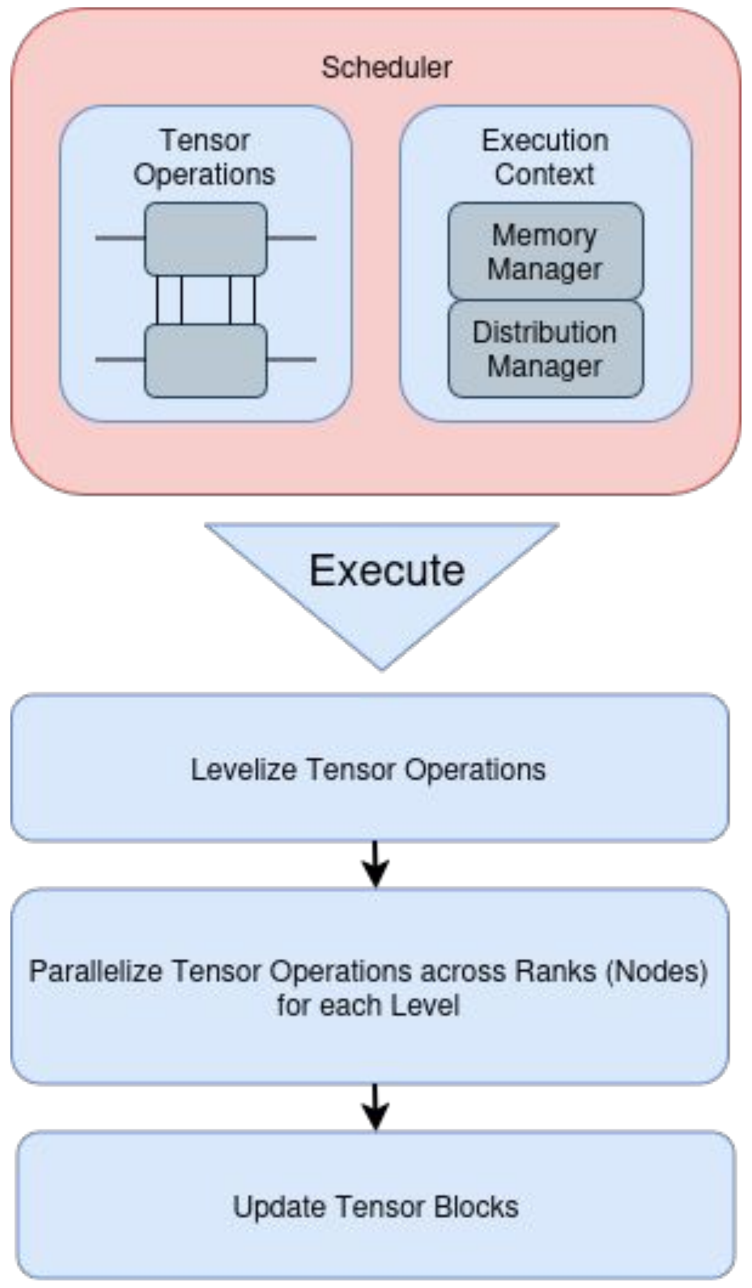
- SWAP Algorithm
- Matrix Product Operator
- Bond Propagation

Measurement

- The amplitudes of the state vector are encoded in the matrix product state. In its fully contracted form the probability of any given state is an entry in the tensor.
- TN Sim uses the "perfect sampling" algorithm to directly probe the state rather than the above.
- Perfect sampling emulates a quantum computer by taking a measurement of the circuit a large number of times, each of which is known as a shot. Each shot then contributes to determining the total state vector.

TAMM Enabled HPC Scaling

We simulate large circuits using the Tensor Algebra for Many-body Methods (TAMM) library from PNNL's NWChemX team, which integrates distributed memory management and MPI routines to scale tensor contractions across multiple compute nodes.



Performance Plots

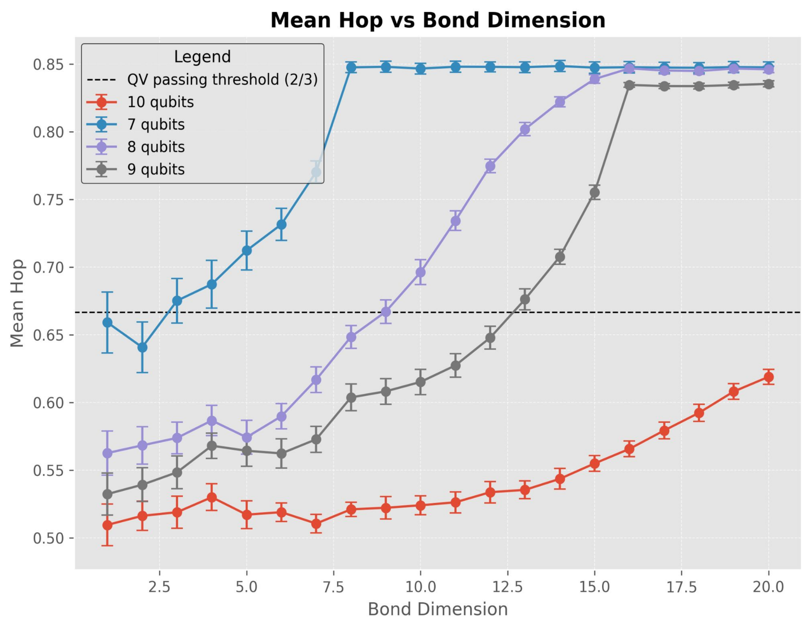


Figure 3: Simulation quality measured by HOP with increasing bond dimension. A HOP greater than ⅔ passes the QV test.

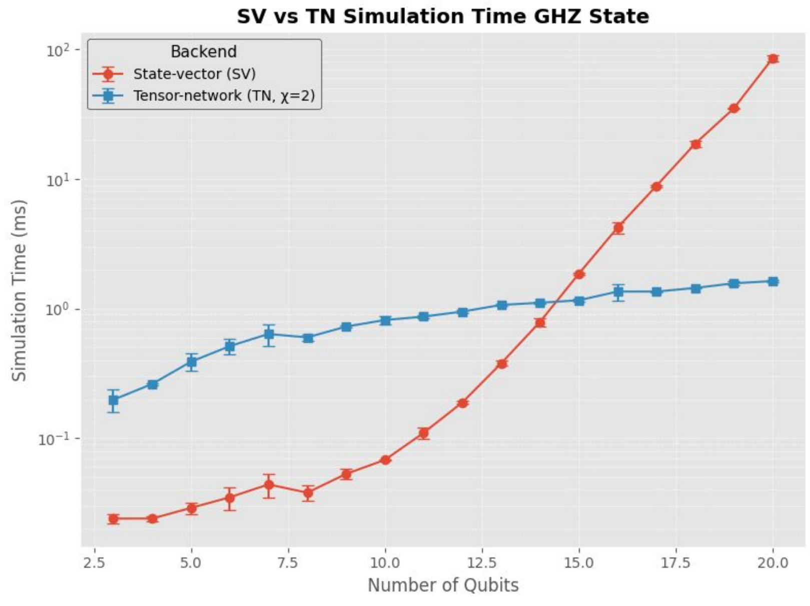


Figure 4: Comparison between TN-Sim and state vector simulation time of a GHZ state with increasing qubit number.

Future Work, References, and Acknowledgments

Future Work: Our tensor network simulator efficiently handles low depth circuits and meets NWQ-Sim benchmarks. Performance may be improved by parallelizing gate contraction, integrating faster SVD routines, and employing alternative tensor topologies such as PEPS for specific problem classes.

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[1]Fishman,M.;White,S.;Stoudenmire,E.M.TheITensorSoftwareLibraryforTensorNetworkCalculations.SciPostPhysicsCodebases2022, 004.https://doi.org/10.21468/SciPostPhysCodeb.4.
[2] E. Mutlu, A. R. Panyala, N. Gawande, A. Bagusetty, J. G. Glabe, J. Kim, K. Kowalski et al., TAMM: Tensor Algebra for Many-body Methods, The Journal of Chemical Physics 159, no. 2:Art.No.02480(2023).PNNL-SA-169718.doi:10.1063/5.014243

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