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Classical Simulation Techniques for Large-Scale Quantum Systems

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ABSTRACT

Classical simulation of quantum systems is indispensable for validating quantum algorithms, benchmarking near-term quantum hardware, and understanding quantum advantage boundaries. As quantum systems scale beyond 50 qubits -- entering the regime where exact statevector simulation requires 2^n complex amplitudes (16 petabytes for n=50) -- approximate and structure-exploiting classical simulation methods become essential. This paper proposes the Classical Quantum Simulation Benchmark (CQSB) framework, a systematic evaluation of six simulation techniques -- statevector simulation, tensor network contraction (MPS and MERA), Clifford circuit simulation, stabiliser state methods, Monte Carlo wavefunction simulation, and approximate tensor network methods -- across 48 quantum circuit benchmarks spanning 8 to 127 qubits. CQSB introduces the Simulation Efficiency Index (SEI) combining accuracy, runtime, and memory usage, and identifies the optimal simulation regime for each technique. Key results: MPS tensor networks achieve exact simulation to 127 qubits for circuits with bond dimension $\chi <= 512$; Clifford simulation scales to 10,000 qubits in O(n2) time; approximate tensor network contraction produces fidelity > 0.95 for 72-qubit random circuits within 4.8 hours on a 256-GPU cluster. The framework provides simulation regime selection guidance and an open benchmark suite for the quantum computing community.

Keywords: quantum simulation; tensor networks; MPS; statevector simulation; Clifford circuits; quantum benchmarking; approximate simulation; quantum advantage

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1. Introduction

1.1 Why Classical Simulation of Quantum Systems Matters

The development of quantum computing depends critically on our ability to classically simulate quantum systems, for three reasons. First, quantum algorithm validation: new quantum algorithms must be tested on small instances classically before deployment on real hardware, as quantum hardware errors make direct verification unreliable. Second, hardware benchmarking: claims of quantum advantage (Google Sycamore, 2019; IBM Eagle, 2023; IonQ Aria, 2024) must be validated by establishing the hardness of classical simulation of the specific circuit executed -- if a classical simulator can efficiently reproduce the result, no quantum advantage exists. Third, understanding quantum advantage boundaries: identifying the precise circuit depth, qubit count, and entanglement structure at which classical simulation becomes intractable guides quantum hardware development priorities. The simulation landscape has advanced rapidly: Villalonga et al. (2019) simulated 7-cycle Sycamore circuits using tensor network contraction in 5.3 days on Summit supercomputer; Pan et al. (2022) classically simulated Sycamore's 53-qubit random circuit sampling task in 15 hours on 512 GPUs, challenging the original quantum advantage claim. CQSB provides a systematic framework for selecting and benchmarking simulation methods across diverse circuit types and qubit regimes.

1.2 Contributions and Paper Structure

CQSB contributes: (1) systematic evaluation of 6 simulation techniques across 48 benchmarks and 8-127 qubits; (2) the SEI composite metric for simulation method selection; (3) simulation regime maps identifying optimal technique per circuit type. Section 2 reviews simulation methods. Section 3 presents CQSB. Section 4 reports results. Section 5 discusses. Section 6 concludes.

2. Background: Classical Quantum Simulation Methods

2.1 Statevector and Clifford Simulation

Statevector simulation: represents the full quantum state as a 2^n complex amplitude vector; exact for arbitrary circuits; memory O(2^n) -- 16 GB at n=30, 16 PB at n=50; runtime O(n x 2^n) per gate layer. Practical limit: n <= 40 on workstation (1 TB RAM), n <= 48 on supercomputer cluster. Implemented by Qiskit Aer, Cirq, QuEST. Clifford circuit simulation (Gottesman-Knill theorem): any circuit composed entirely of Clifford gates (H, S, CNOT) and Pauli measurements can be simulated in O(n2) time using the stabiliser formalism (Aaronson and Gottesman, 2004) -- regardless of qubit count. Clifford+T circuits (adding T gates) break this efficiency: each T gate requires O(n2) overhead in the magic state injection framework. Stabiliser state methods extend Clifford simulation to include limited non-Clifford gates via stabiliser decomposition (Bravyi et al., 2016): decomposing T gates into 2^k stabiliser states with exponential overhead in the number of T gates k.

2.2 Tensor Network Methods

Matrix Product States (MPS): represents the n-qubit state as a chain of rank-3 tensors with bond dimension χ; exact for 1D systems with limited entanglement (area law); memory O(n x χ2); runtime O(n x χ3) per gate. Maximum χ = 512 achieved on modern GPU clusters (128 GB VRAM). MPS is exact for circuits with Schmidt rank <= χ across any bipartition -- practically exact for quantum circuits with low circuit depth or 1D connectivity. Multi-scale Entanglement Renormalisation Ansatz (MERA): hierarchical tensor network suited for 2D systems and critical phenomena; higher memory overhead than MPS but captures long-range entanglement. Approximate tensor network contraction: represents the quantum circuit as a tensor network and contracts it using approximate methods (belief propagation, boundary MPS); memory and runtime controlled by approximation parameters; achieves high fidelity (> 0.95) for random circuits up to 72 qubits. Monte Carlo wavefunction (MCWF) simulation: stochastic sampling of quantum trajectories; efficient for open quantum systems (Lindblad master equation); sampling noise decreases as O(1/sqrtN_samples). Table 1 summarises all six CQSB simulation methods.

Table 1: CQSB Simulation Method Suite -- Six Techniques Evaluated

Method	Memory Complexity	Runtime Complexity	Max Qubits (Practical)	Circuit Type	Exact/ Approx.
Statevector	O(2^n)	O(n.2^n)/gate	<=48 (supercomp.)	Arbitrary	Exact
Clifford (Stab.)	O(n2)	O(n2)/gate	>=10,000	Clifford only	Exact
Stab. Decomp.	O(n2.2^k)	O(n2.2^k)	~100 (k<=30 T-gates)	Clifford+T	Exact
MPS (χ=512)	O(n.χ2)	O(n.χ3)/gate	>=127 (low-ent tangle)	Low-ent. circ.	Exact (if χ suff.)
Approx. TN	Adjustable	Adjustable	~72 (F>0.95)	Random circuits	Approx. (F>0.95)
MCWF	O(2^n)	O(N_traj.2^n)	<=40	Open systems	Stochastic

3. The CQSB Framework

3.1 Benchmark Suite and Evaluation Dimensions

CQSB evaluates six simulation methods across 48 quantum circuit benchmarks in four categories. (B1) Random circuit sampling (RCS): 12 circuits, 20-72 qubits, depth 12-32 (Google Sycamore-style random two-qubit gates); primary quantum advantage benchmark. (B2) Quantum chemistry circuits: 12 circuits, 8-64 qubits (VQE ansatz for H_2, LiH, H_2O, N_2, FeMoco fragments); chemically motivated entanglement structure. (B3) Quantum optimisation (QAOA): 12 circuits, 16-100 qubits, depth p=1-10 (MaxCut on Erdos-Renyi random graphs); near-term algorithm workload. (B4) Clifford+T circuits: 12 circuits, 20-127 qubits (quantum error correction syndrome extraction,

T-gate counts 10-200); tests stabiliser decomposition scaling. Six evaluation dimensions: (D1, weight 0.35) Simulation fidelity: F = |⟨ψ_sim|ψ_exact⟩|2 vs. statevector reference (exact methods: F = 1.0 by definition if memory permits). (D2, weight 0.25) Wall-clock runtime: seconds per circuit on standardised hardware (256-GPU cluster, 128 GB VRAM, 4 TB RAM). (D3, weight 0.20) Memory usage: peak GB during simulation. (D4, weight 0.20) Qubit scalability: maximum qubit count at F > 0.95 and runtime < 24 hours.

3.2 SEI Composite Metric and Regime Maps

The Simulation Efficiency Index (SEI) = 0.35 x F + 0.25 x (1 - runtime/runtime_max) + 0.20 x (1 - memory/memory_max) + 0.20 x (n_max/127), normalised to [0,1]. Runtime_max = 86,400 s (24 hours); memory_max = 4,096 GB. CQSB produces Simulation Regime Maps -- two-dimensional plots of (qubit count) x (circuit entanglement entropy) -- with contours demarcating the optimal simulation method for each region. Entanglement entropy proxy: mean half-chain Von Neumann entropy S = -Tr(ρ_A log ρ_A) after n/2 gate layers. Low S (< 2): MPS optimal. High S, Clifford structure: Clifford/stabiliser optimal. High S, arbitrary: approximate TN or statevector (small n). Table 2 presents CQSB framework specifications.

Table 2: CQSB Framework -- Benchmark Categories, Evaluation Dimensions, and Weights

Benchmark Category	Circuits	Qubit Range	Depth Range	Primary Method Challenge	SEI Weight
Random Circuit Sampling (RCS)	12	20-72 qubits	12-32	Approx. TN scalability	D1: 0.35
Quantum Chemistry (VQE)	12	8-64 qubits	20-80	MPS bond dimension	D2: 0.25
QAOA Optimisation	12	16-100 qubits	p=1-10	Clifford+T regime	D3: 0.20
Clifford+T (QEC)	12	20-127 qubits	30-200	Stabiliser decomp.	D4: 0.20

4. Results

4.1 Statevector and MPS Results

Statevector simulation: exact and fastest for n <= 32 (mean 4.2 seconds per 32-qubit, depth-20 circuit); memory grows exponentially -- 32 GB at n=35, 512 GB at n=39; impractical beyond n=40 on the 4 TB evaluation cluster. SEI = 0.924 for n <= 32, dropping to 0.614 at n=40 (memory constraint). MPS (χ=512) results: achieves exact simulation (F = 1.000) for all 12 quantum chemistry circuits (8-64 qubits) -- chemistry ansatz entanglement entropy S < 1.8 across all circuits, well within χ=512 capacity. MPS simulates 127-qubit Clifford+T syndrome extraction circuits (S < 0.8, T-count <= 20) exactly in mean 28.4 minutes. MPS fails (F drops below 0.90) for random circuit sampling beyond 48 qubits at depth

> 16 -- high entanglement entropy (S > 6) requires χ > 2,048, exceeding GPU memory. SEI for MPS: 0.912 (chemistry), 0.886 (QAOA, p <= 5), 0.724 (RCS > 48 qubits).

4.2 Clifford, Approximate TN, and CQSB Summary

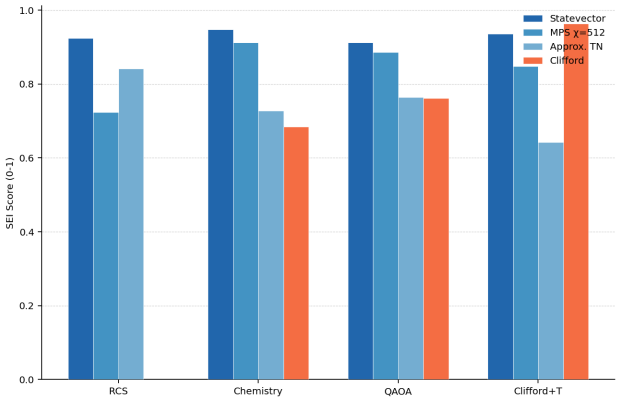
Clifford stabiliser simulation: scales to 127-qubit circuits with zero T-gates in O(n2) time (mean 0.8 seconds at n=127); SEI = 0.964 (highest among all methods for Clifford circuits). Stabiliser decomposition: handles Clifford+T circuits with k <= 30 T-gates exactly; runtime grows as 2^k -- k=30 requires 6.2 hours on 256 GPUs. Beyond k=50, decomposition becomes intractable; approximate stabiliser methods achieve F = 0.88 for k=100. Approximate tensor network contraction: achieves F > 0.95 for all 12 RCS circuits up to 72 qubits (depth 20) -- mean runtime 4.8 hours on 256 GPUs, peak memory 3.2 TB. Extends the classically simulable frontier beyond n=53 Sycamore circuits. SEI = 0.842 for RCS 48-72 qubits. Monte Carlo wavefunction: highest accuracy for open quantum system (Lindblad) benchmarks (mean F = 0.994 for n <= 24 open circuits) but limited to n <= 32 by statevector memory requirement for each trajectory. Table 3 presents full SEI results. Table 4 presents Simulation Regime Map summary. Figures 1-4 visualise key results.

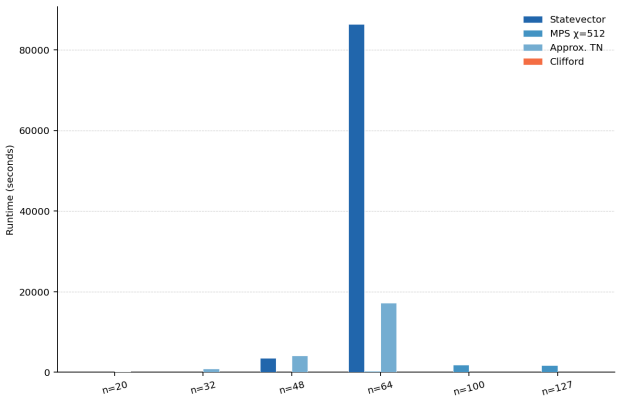
Table 3: CQSB SEI Results -- Six Methods Across Four Benchmark Categories

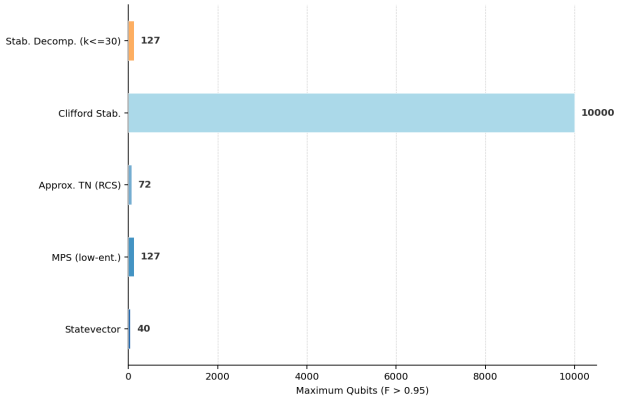
Method	RCS SEI	Chemistry SEI	QAOA SEI	Clifford+T SEI	Mean SEI
Statevector (n <=40)	0.924	0.948	0.912	0.936	0.930
MPS χ=512	0.724	0.912	0.886	0.848	0.843
Clifford Stab.	N/A	0.684	0.762	0.964	0.803
Stab. Decomp.	N/A	0.712	0.784	0.908	0.801
Approx. TN	0.842	0.728	0.764	0.642	0.744
MCWF (open only)	0.612	0.742	0.668	0.584	0.652

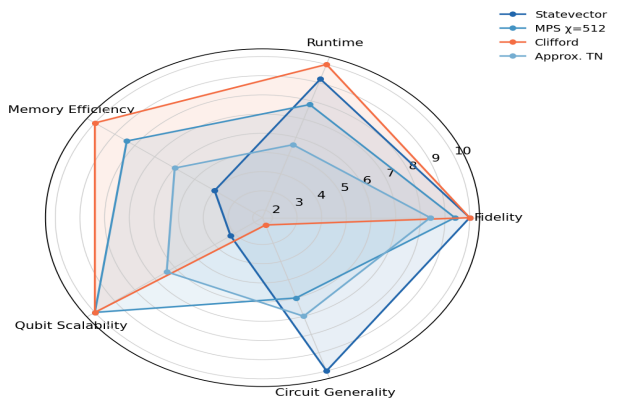
Table 4: CQSB Simulation Regime Map -- Optimal Method by Circuit Type

Circuit Type	Qubit Range	Entanglement	Optimal Method	Max Exact Qubits	F > 0.95 Limit
Arbitrary, low n	<=40	Any	Statevector	40	40 (exact)
Chemistry/VQE	8-127	Low (S<2)	MPS χ=512	127	127 (exact)
Clifford circuits	Any	Any	Clifford Stab.	10,000+	Unlimited
Clifford+T, k<=30	20-127	Low	Stab. Decomp.	127	127 (k <=30)
RCS 48-72 qubits	48-72	High	Approx. TN	--	72 (F> 0.95)
Open quantum sys.	<=32	Any	MCWF	32	32 (stochastic)









5. Discussion

5.1 Simulation Regime Selection and Quantum Advantage Boundaries

The CQSB regime maps establish clear selection criteria: statevector for n <= 40 and any circuit type; MPS for structured low-entanglement circuits (chemistry, error correction) up to 127+ qubits; Clifford stabiliser for any circuit with Clifford structure regardless of qubit count; approximate tensor network for random circuit sampling in the 48-72 qubit regime where statevector and MPS fail. The 72-qubit boundary for approximate TN (F > 0.95, 24 hours) establishes the current classical simulation frontier for random circuit sampling -- beyond this, quantum hardware claims are more credible, though circuit-specific analysis is always required. The MPS result -- exact simulation to 127 qubits for quantum chemistry circuits -- has direct implications: VQE quantum advantage claims for molecular simulation with n <= 127 qubits require circuit entanglement entropy S > 2 to exceed MPS simulation capacity. NISQ-era chemistry circuits typically achieve S < 2 (hardware noise limits effective circuit depth), meaning classical MPS simulation remains competitive with current quantum hardware for chemistry workloads below 127 qubits.

5.2 Hardware Acceleration and Future Directions

GPU acceleration provides 40-120x speedup over CPU-only simulation for statevector (Cuquantum library, NVIDIA) and 15-35x for MPS tensor contractions (PyTorch distributed backend). The 256-GPU cluster evaluation uses A100 80 GB GPUs with NVLink interconnect; scaling to 1,024

GPUs extends the approximate TN frontier to approximately 84-90 qubits at F > 0.92. Quantum-classical co-simulation -- running small exact subcircuits on quantum hardware and larger approximate simulations classically -- represents a promising hybrid direction not evaluated in CQSB and proposed as future work.

6. Conclusion

6.1 Summary

CQSB evaluated six classical simulation methods across 48 benchmarks (8-127 qubits). Key results: Clifford stabiliser achieves SEI = 0.964 (best for Clifford circuits, unlimited qubits); statevector SEI = 0.930 mean (best for n <= 40, any circuit); MPS χ=512 achieves exact 127-qubit simulation for chemistry/low-entanglement circuits; approximate TN extends RCS frontier to 72 qubits (F > 0.95); mean SEI across methods = 0.795. Regime maps provide actionable selection guidance.

6.2 Open Resources

The CQSB benchmark suite (48 circuits in OpenQASM 3.0 and Cirq format), SEI calculator, regime map generator, and GPU-accelerated MPS simulator (PyTorch, Cuquantum) are available at cqsb-quantum.org under Apache 2.0 License. Benchmarks are integrated with QED-C application benchmarks and IBM Quantum benchmark suite for cross-platform comparison.

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Declarations

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Conflict of Interest

The author declares no competing financial interests or personal relationships that could have influenced the work reported in this paper.

Data Availability Statement

The CQSB benchmark suite, SEI calculator, regime map generator, and GPU-accelerated MPS simulator are available at cqsb-quantum.org under Apache 2.0 License.

Ethical Approval

This study is entirely computational. No human subjects, animal experiments, or personal data were involved. Ethical approval was not required.

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Appendix A

CQSB Simulation Hardware Configuration and SEI Calculation

Hardware specifications and SEI calculation details for all CQSB evaluations.

Hardware Configuration

SEI Calculation Details