

Simulation cost of classically simulable quantum evolutions

Su Yeon Chang,¹ Supanut Thanasilp,² Zoë Holmes,³ and M. Cerezo¹

¹*Los Alamos National Laboratory, Los Alamos, NM 87545, USA*

²*Chulalongkorn University, Bangkok 10330, Thailand*

³*Ecole Polytechnique Fédérale de Lausanne (EPFL), Lausanne 1015, Switzerland*

Introduction. Over the past years, researchers have found that certain quantum evolutions can be classically simulated—provided they are paired with the right initial state and set of observables [1–12]. Here, by classical simulability we mean that, despite the fact that the dimension of the underlying Hilbert space scales exponentially with the system size, there exist classical algorithms that reproduce the relevant quantum outcomes using time and memory resources that scale only polynomially with the system size. Beyond mere curiosities, these examples of classically simulable quantum processes have had deep impact in quantum information sciences, as they can be used to benchmark quantum computers, have helped us better trace the border between classical and quantum dynamics, identify the resources needed for universal quantum computation [1–12], and have also flagged models for variational quantum algorithms (VQAs) and quantum machine learning (QML) that cannot achieve an exponential quantum advantages over their classical counterparts [5]. However, just because something can be “efficiently” classically simulated does not meet that it is always efficient to do so, as even modest polynomial scaling can be prohibitively expensive in practice. Thus, a natural question arises: *Is it more (time/memory) efficient to classical simulate such evolutions versus directly deploy them on quantum hardware?*

To address this, we compare the efficiency of *Quantum Simulation* (i.e., deploy in quantum hardware) and *(Quantum-Enhanced) Classical Simulation* [5] (i.e., classically simulate the evolution using simple measurements we get from a quantum computer), illustrated in Figure 1. We quantify the resources required by both approaches using three metrics: (i) quantum sample complexity $N_{Q.S.}$ (number of quantum measurements), (ii) classical time complexity $N_{C.T}$ (number of classical operations), and (iii) quantum time complexity $N_{Q.T}$ (circuit depth).

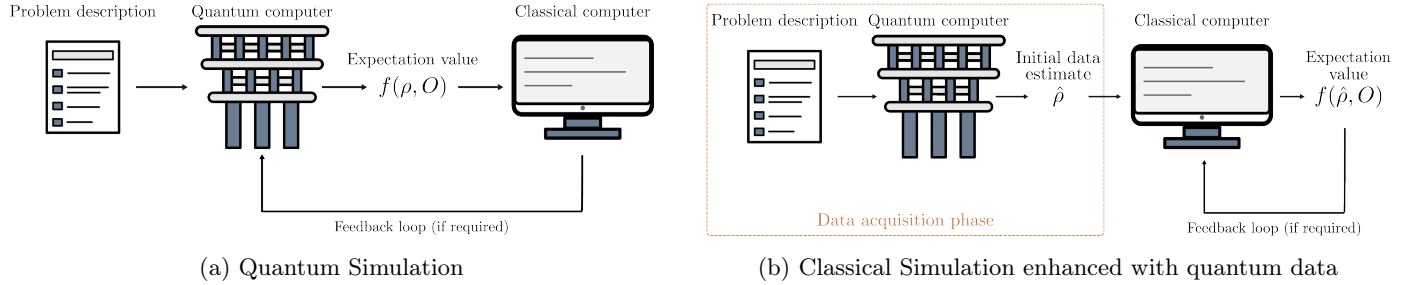


Figure 1. **Schematic description comparing Quantum and Classical Simulations.**

Framework. We consider an input state ρ on the Hilbert space $\mathcal{H}$ and a quantum circuit of the form $U = \prod_{\ell=1}^L U_{\ell} = \prod_{\ell=1}^L e^{-i\mathbf{w}_{\ell} H_{\ell}}$, where $\mathcal{G} = \{H_{\ell}\}_{\ell=1}^L$ is a Hermitian generator set and $\mathbf{w} \in \mathbb{R}^L$. The interpretation of $\mathbf{w}$ depends on the application: in VQAs or QML $\mathbf{w}$ correspond to trainable parameters, while in quantum dynamics simulations, they represent discrete time steps. The observable is expanded into M orthonormal basis operators as $O = \sum_{\alpha} c_{\alpha} P_{\alpha}$, where $P_{\alpha} \in \mathcal{P}_n = \{\mathbf{1}, X, Y, Z\}^{\otimes n}$ are the Pauli strings, and $\mathbf{c} \in \mathbb{R}^M$. The objective is to estimate the expectation values $f(\rho, O) = \text{Tr}[U^{\dagger} \rho U O]$, either in the Schrodinger picture by evolving ρ , or in the Heisenberg picture by backpropagating O .

The quantum sample complexity is determined by direct circuit measurements. We adopt a weighted measurement strategy in which the number of measurements assigned to each (non-commuting) Pauli string P_{α} is proportional to $|c_{\alpha}|$ as $N_{\alpha} = N|c_{\alpha}|(\sum_{\alpha} |c_{\alpha}|)^{-1}$, with the total number of measurements N . Under this strategy, Quantum Simulation requires $N_{Q.S.} \in \mathcal{O}(MT \log(M/\delta) \epsilon^{-2} \|\mathbf{c}\|_1^2)$ samples to estimate $f(\rho, O)$ with an additive error ϵ and success probability $1 - \delta$. Here, T depends on the application: in variational setting, it denotes the total number of expectation values determined by the gradient calculation method [13], whereas in digitized adiabatic quantum computing, it corresponds to either a single final measurement, or the number of measured time steps.

On the other hand, the classical time complexity of the simulation depends on the required classical processing and is therefore application-dependent. For example, in VQA/QML setting, it is dominated by the parameter updates, which scale linearly with the number of the parameters and iterations. Unless additional classical pre- or post-processing steps are required, this cost is negligible.

Problem	Simulation Methods	Quantum Sample	Quantum Time	Classical Time
General QNN	Quantum Simulation	$\mathcal{O}(\frac{MT}{\epsilon^2} \log(\frac{M}{\delta}) \ \mathbf{c}\ _2^2)$	$\mathcal{O}(L)$	$\mathcal{O}(TL)$
Clifford circuit	$\text{Sp}(2n, \mathbb{F}_2)$ matrix	$\mathcal{O}(\frac{MT}{\epsilon^2} \log(\frac{M}{\delta}) \ \mathbf{c}\ _2^2)$	$\mathcal{O}(1)$	$\mathcal{O}(Mn^2)$
Shallow HEA	Reduced U	$\mathcal{O}(\frac{16^k n^4}{\epsilon^2} \log(\frac{MT}{\delta}) \ \mathbf{c}\ _1^2)$	$\mathcal{O}(1)$	$\mathcal{O}(MTn^{2\omega})$
Matchgate	$\mathbf{g}$ -sim [10]	$\mathcal{O}(\frac{n^{3\kappa/2} \kappa^{3/2}}{\epsilon^2} \log(\frac{n}{\delta}) \ \mathbf{c}\ _2^2)$	$\mathcal{O}(1)$	$\mathcal{O}(Ln^{3\kappa} + TLn^{2\kappa})$
S_n -equivariant	Block-diagonalized U [14]	$\mathcal{O}(\frac{n^2}{\epsilon^2} \log(\frac{MT}{\delta}) \ \mathbf{c}\ _1^2)$	$\mathcal{O}(n \text{ poly}(\epsilon_{\text{QST}}^{-1}))$	$\mathcal{O}(Ln^3 + TLn^{\omega+1})$
$U(1)$ -equivariant	Givens rotation [15]	$\mathcal{O}(\frac{n^{3h}}{\epsilon^2} \log(\frac{n}{\delta}) \ \mathbf{c}\ _1^2)$	$\mathcal{O}(1)$	$\mathcal{O}(Ln^h)$
QCNN	Pauli Propagation* [16]	$\mathcal{O}(\frac{n^{3\tau}}{\epsilon^2} \log(\frac{n}{\delta}) \ \mathbf{c}\ _1^2)$	$\mathcal{O}(1)$	$\mathcal{O}(Tn^{2\tau})$
ADAPT VQE	Majorana Propagation* [17]	$\mathcal{O}(1)$	$\mathcal{O}(1)$	$\mathcal{O}((L \mathcal{A} + T_{\text{VQE}})n^\tau)$

Table I. **Classical simulation methods and their computational costs for provably classically simulable problems.** All methods estimate $f(\rho, O)$ with failure probability δ and error ϵ and approximate methods are marked with *. Here, ω is the matrix multiplication exponent [18]; k and κ the Pauli and fermionic locality of O ; h the Hamming weight of ρ ; τ the Pauli propagation truncation threshold; ϵ_{QST} the the Schur-transform error; and $\|\mathbf{c}\|_1$ and $\|\mathbf{c}\|_2$ the ℓ_1 - and ℓ_2 - norms of the coefficient vectors. In all cases, the classical-shadow post-processing cost is negligible.

Efficiency of Classical simulation of quantum circuits. Our first contribution is a thorough analysis and compilation of classically simulable quantum algorithms and their corresponding Classical Simulation methods, together with their computational complexity. While the quantum sample complexity of Quantum Simulation is completely agnostic to the specific circuit architecture, for Classical Simulations, *there is no single classical surrogate model to rule them all*. Table I summarizes the resource and time complexity for various classically simulable quantum algorithms. Below, we outline a few representative examples to give the readers insight into how we derived the computational complexity.

A Shallow Hardware Efficient Ansatz (HEA) with depth $L \in \mathcal{O}(\log(n))$ followed by a k -local observable is classically simulable via a light-cone argument. The locality of quantum circuit and observable restricts the light-cone to $\mathcal{O}(\log(n))$ qubits, enabling efficient classical simulation with reduced unitary matrix multiplication and local Pauli shadows [19]. This yields a classical time complexity $N_{\text{C.T}} \in \mathcal{O}(MTn^{2\omega})$ and a quantum sample complexity $N_{\text{Q.S.}} \in \mathcal{O}(\log(MT\delta^{-1}) 16^k n^4 \epsilon^{-2} \|\mathbf{c}\|_1^2)$. The scaling n^4 arising from randomized Pauli measurements represents the worst-case upper bound. However, this equation provides a sufficient condition and in practice, the required number of measurements is often significantly lower than this upper bound, as demonstrated in Ref. [19].

Matchgate circuits describe the evolution of non-interacting fermionic Hamiltonian [3, 20], described by $2n$ Majorana operators $\gamma_1, \dots, \gamma_{2n}$ for n -qubit system. The κ -local Majorana strings $\gamma_\mu = \gamma_{\mu_1} \cdots \gamma_{\mu_\kappa}$, $\mu \in \mathcal{C}_{2n, \kappa}$, with $\mathcal{C}_{2n, \kappa}$ the set of ordered index vectors, span the invariant submodule $\mathcal{B}_\kappa = \text{span}\{(-i)^\kappa \gamma_\mu\}_{\mu \in \mathcal{C}_{2n, \kappa}}$ of dimension $\binom{2n}{\kappa}$. A matchgate Hamiltonian is quadratic in Majorana strings, $H_Q = \frac{i}{2} \sum_{\nu_1 < \nu_2} h_{\nu_1 \nu_2} \gamma_{\nu_1} \gamma_{\nu_2}$, where h is a real antisymmetric matrix and $Q = e^{2h} \in \text{SO}(2n)$. The corresponding circuit $U_Q = e^{-iH_Q}$ preserves $\mathcal{B}_\kappa$ through the adjoint action $U_Q^\dagger \gamma_\mu U_Q = \sum_{\nu \in \mathcal{C}_{2n, \kappa}} \det(Q_{\mu\nu}) \gamma_\nu$ where $Q_{\mu\nu}$ is the $\kappa \times \kappa$ submatrix of Q . Among different methods, we employ Matchgate $\mathbf{g}$ -sim [10], which computes the adjoint action of U_Q on $O \in \mathcal{B}_\kappa$. Moreover, as γ_μ are highly nonlocal in the Pauli basis, we reconstruct the initial state using Matchgate shadows [21–23], based on fermionic Gaussian unitaries, rather than randomized Pauli shadows. These contributions yield the classical time complexity $N_{\text{C.T.}} \in \mathcal{O}(Ln^{3\kappa} + TLn^{2\kappa})$ and the quantum sample complexity $N_{\text{Q.S.}} \in \mathcal{O}(n^{\frac{3\kappa}{2}} \kappa^{\frac{3}{2}} \epsilon^{-2} \log(n\delta^{-1}) \|\mathbf{c}\|_2^2)$. Note that the classical shadow post-processing cost scales as $\mathcal{O}(N_{\text{Q.S.}} \cdot n)$ which is negligible compared to the other contributions.

S_n -equivariant circuits can be efficiently simulated using the representation-theoretic structure of the S_n -equivariant operators. In the Schur basis, which implements the isotypic decomposition of the S_n representation, an S_n -equivariant circuit and observable decompose as $U \cong \bigoplus_\lambda (\mathbb{1}_{m_\lambda} \otimes U_\lambda)$ and $O \cong \bigoplus_\lambda (\mathbb{1}_{m_\lambda} \otimes O_\lambda)$ where U_λ and O_λ are $d_\lambda \times d_\lambda$ matrices associated with the irrep λ of multiplicity m_λ [24]. Then, the expectation value decomposes into a sum over all irreps as $f(\rho, O) = \sum_\lambda \text{Tr}[\rho_\lambda U_\lambda^\dagger O_\lambda U_\lambda]$, where ρ_λ is the projection of ρ onto the corresponding irrep subspace, summed over all m_λ . Note that ρ need not to be S_n -equivariant.

As a result, the simulation reduces to independent multiplication of the irrep blocks, with ρ reconstructed using the Symmetric Classical Shadows [25]. This yields the classical time complexity $N_{\text{C.T}} \in \mathcal{O}(Ln^3 + TLn^{\omega+1})$, from one-time irrep-block diagonalization and subsequent matrix multiplications, respectively, and the quantum sample

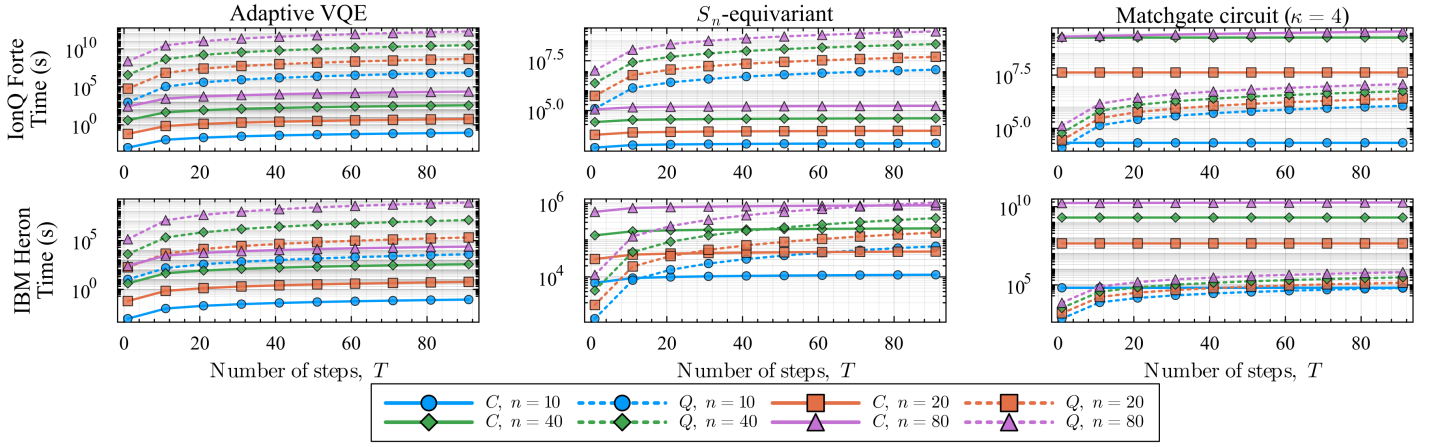


Figure 2. **Estimated wall-clock between Quantum and Classical Simulation for IonQ Forte (trapped-ion) and IBM Heron (superconducting).** Results are analytical estimates based on publicly available hardware specifications [32–35], rather than direct runtime measurements, with constant factors neglected. For IBM Heron, we include the SWAP-gate overhead arising from heavy-hex connectivity, and two-qubit gates acting on disjoint qubits are assumed to be fully parallelizable on both platforms. Results beyond 36 qubits for IonQ Forte assume unchanged hardware specifications.

complexity $N_{Q.S.} \in \mathcal{O}(n^2 \epsilon^{-2} \log(MT \delta^{-1}) \|c\|_1^2)$ [14]. Furthermore, the quantum time complexity of the classical shadow scales as $N_{Q.T} \in \mathcal{O}(n \text{ poly}(\epsilon_{QST}^{-1}))$ where ϵ_{QST} is the error of quantum Schur transform.

The **Adaptive Variational Quantum Eigensolver (ADAPT-VQE)** [26–28] minimizes the energy $f(|\psi_0\rangle, H) = \langle \psi_0 | U^\dagger(\mathbf{w}) H U(\mathbf{w}) | \psi_0 \rangle$, with $|\psi_0\rangle$ typically chosen as the Hartree-Fock state [29–31]. At each iteration, ADAPT-VQE constructs $U(\mathbf{w})$ iteratively by selecting circuit generator $A^* \in \mathcal{A}$ with the largest energy gradient, followed by repotimization of all parameters. Here, we consider $\mathcal{A}$ which consists of Majorana strings with low κ and employ Majorana propagation [17], which evolves a fermionic observable $O = \sum_{\mu} c_{\mu} \gamma_{\mu}$, in the Heisenberg picture, leading to $U^\dagger(\mathbf{w}) O U(\mathbf{w}) = \sum_{\mu} c_{\mu}(\mathbf{w}) \gamma_{\mu}$, where $c(\mathbf{w})$ are the backpropagated coefficients. We then truncate propagation paths either by discarding terms with high κ , or with small coefficients $c_{\mu}(\mathbf{w})$, to approximate the expectation value. As the Hartree-Fock state admits an analytical expression in terms of γ_{μ} , no quantum hardware is required for initial data acquisition. This yields a quantum sample complexity of $N_{Q.S.} \in \mathcal{O}(1)$ and a classical time complexity of $N_{C.T} \in \mathcal{O}(L|\mathcal{A}|n^{\tau} + T_{VQE}n^{\tau})$ with τ the truncation threshold of Majorana propagation. The first term corresponds to constructing the classical surrogate, while the second term to reoptimizing $\mathbf{w}$. This is the worst-case bound: in practice, the circuit reevaluation cost is in general negligible compared to the surrogate construction.

Classical versus Quantum simulation times. Here we arrive at the central question: *which approach—Quantum or Classical—is computationally more efficient?* To answer this, we compare the estimated wall-clock time of Quantum Simulation and its corresponding Classical Simulation.

Based on Figure 2, quantum algorithms can be broadly classified into three regimes. First, where no quantum data acquisition is required (e.g., VQE with an analytically known ρ), classical simulation incurs no sampling overhead and is consistently more efficient than repeated quantum execution. Second, when Classical Simulation requires only a moderate number of quantum measurements, while Quantum Simulation involves a sufficiently deep circuit (e.g., $N_{Q.S.} \in \mathcal{O}(n^2)$ for S_n -equivariant circuits with $L \in \mathcal{O}(n^2)$), the relative efficiency depends on hardware and T . Superconducting hardware with short gate time (~ 90 ns) exhibits a crossover when T increases, whereas the longer gate (~ 900 μ s) of trapped-ion hardware generally favors Classical Simulation making gate time the dominant cost. Finally, when Classical Simulation requires large $N_{Q.S.}$ for initial data acquisition while Quantum Simulation needs a moderate circuit depth (e.g., $N_{Q.S.} \in \mathcal{O}(n^6)$ for matchgate circuits with $\kappa = 4$ and circuit depth $L \in \mathcal{O}(n)$), the data acquisition cost dominates the computational savings of the classical surrogate, making Classical Simulation more expensive. These results suggest that, even for classically simulable problems, Quantum Simulation can be more resource-efficient than Classical Simulation depending on the quantum hardware and circuit architectures.

As a final remark, we emphasize that these results are only rough estimates intended to provide qualitative insight. Actual performance depends on additional factors, including circuit optimization techniques [36], the classical hardware and degree of parallelization, and in fault-tolerant regimes, the overhead of quantum error correction cycles. Therefore, the actual runtime may differ substantially, making direct comparisons more challenging.

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