Supplementary Materials of Estimating the randomness of quantum circuit ensembles up to 50 qubits

Minzhao Liu[1,2*], Junyu Liu[3,4,5,6*], Yuri Alexeev[2,4] and Liang Jiang[3,4]

[1]Department of Physics, University of Chicago, Chicago, IL 60637, USA.
[2]Computational Science Division, Argonne National Laboratory, Lemont, IL 60439, USA.
[3]Pritzker School of Molecular Engineering, University of Chicago, Chicago, IL 60637, USA.
[4]Chicago Quantum Exchange, Chicago, IL 60637, USA.
[5]Kadanoff Center for Theoretical Physics, University of Chicago, Chicago, IL 60637, USA.
[6]qBraid Co., Harper Court 5235, Chicago, IL 60615, USA.

*Corresponding author(s). E-mail(s): mliu6@uchicago.edu; junyuliu@uchicago.edu;
Contributing authors: yuri@anl.gov; liangjiang@uchicago.edu;

1 Supplementary Methods

1.1 Determination of sample sizes

Since the simulation of large circuits is expensive, we adaptively terminate sampling simulations based on the estimated standard error in the frame potential according to various rules we implement. For example, the simulation stops if the frame potential is larger than the Haar value by a few standard errors or takes too long. If the estimated frame potential is less than the Haar value or smaller than that of a lower depth circuit, the simulation would run longer to steer away from unphysical results.

1.2 Bootstrapping for uncertainty quantification

As discussed in the main manuscript, we use bootstrapping to analyze the uncertainties in the data. This is because of the highly asymmetric nature of the error due the highly skewed distribution of $|\mathrm{Tr}\left(U^\dagger V\right)|^k$ (rare cases where U and V collide, making the quantity is very large, and the skewedness worsens for larger ks). Performing naive error propagation using the standard error without taking asymmetry into account after curve fitting and solving for intersection is therefore unreliable.

Bootstrapping is a good method for uncertainty quantification because it does not assume the distribution of the estimator. Given a set S of N samples obtained from population P, we are interested in the estimator value E and its uncertainty. Bootstrapping resamples N samples with replacement from S to form S_i, and calculates E_i multiple times to form a set of bootstrap samples $\{E_i\}$. This means each S_i must repeat and omit some samples from S. Assuming S is a good representation of the population P, it is as if each E_i is sampled from P. Therefore, the distribution of E_i should approximate the actual distribution of E.

In our analysis, P is the trace distributed over the ansätze measure, E can be the frame potential, layers needed to reach ϵ, etc. We use 300 bootstrap samples in our analysis.

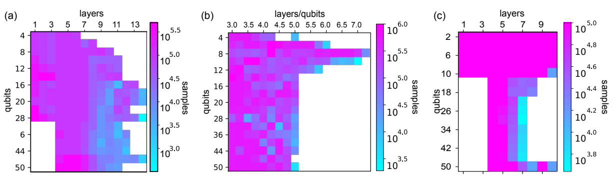
1.3 Choice of curve fitting region

Assuming exponential scaling of $\mathcal{F}$ in l, we can fit an exponential curve. As can be seen from Supplementary Figure 1, 4, 6, and 8 of the main manuscript, $\log \mathcal{F}$ does not scale linearly until large l or small $\mathcal{F}$. Therefore, we choose layers that has $\frac{\mathcal{F}_{\mathcal{E}}^{(k)} - \mathcal{F}_{\text{Haar}}^{(k)}}{\mathcal{F}_{\text{Haar}}^{(k)}} < 5$, which by eye roughly corresponds to the exponential scaling regimes as shown in Supplementary Figure 4, 6, and 8 of the main manuscript.

2 Supplementary Figures

2.1 Sample sizes

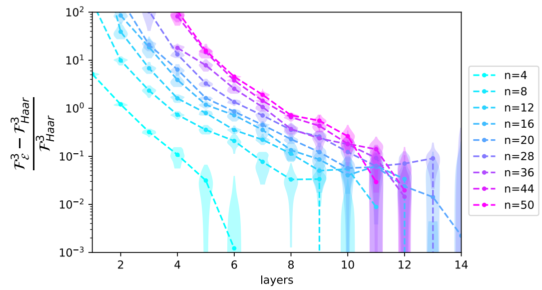
We show in Supplementary Figure 1 the number of independently sampled circuits used to obtain the frame potential for a single data point. We compute and store the individual trace values $\text{Tr}(U^\dagger V)$ for each sampled circuit, and use the same trace values to compute frame potentials with different k values. Therefore, the number of samples has only qubit and layer dependence. As we can see, most data points are obtained with at least 1000 samples.



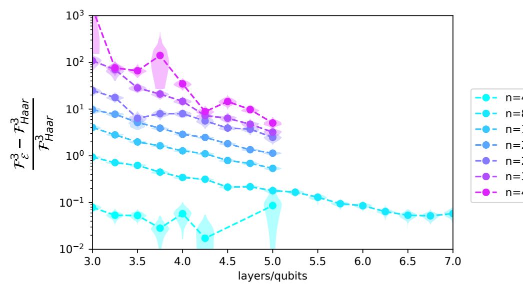
Supplementary Figure 1 Number of circuit samples used for estimating the frame potential for each circuit configuration. (a) Parallel random unitary. (b) Local random unitary. (c) Hardware-efficient ansätze.

2.2 Detailed uncertainties obtained from bootstrapping

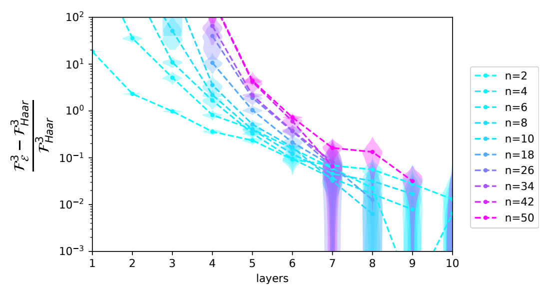
The main manuscript does not show uncertainties obtained from bootstrapping for the percentage deviation of the frame potential. This is because we want to prioritize illustrating traces of all qubit counts on the same plot, and bootstrapping errors can obfuscate the graphs. Supplementary Figure 2, 3, 4 are violin plots that shows the bootstrap distributions of the frame potential percentage deviations as shadows around data points. To avoid cluttering the plots, we only show traces for half of the qubit counts.



Supplementary Figure 2 Percentage deviation of the $k = 3$ frame potential from the Haar value as a function of layers for the parallel random unitary ansätze.



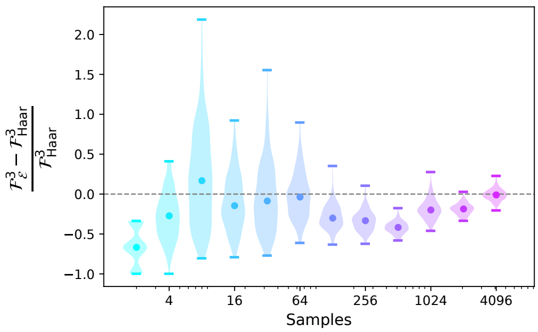
Supplementary Figure 3 Percentage deviation of the $k = 3$ frame potential for the local random unitary ansätze.



Supplementary Figure 4 Percentage deviation of the $k = 3$ frame potential from the Haar value for the CNOT hardware efficient ansätze.

2.3 Validation of calculated frame potentials

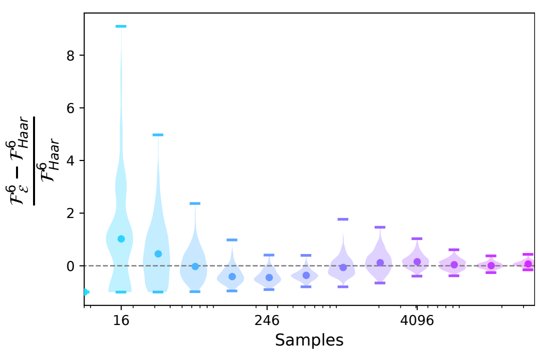
To show the convergence process, we take the parallel random unitary as an example, showing specifically the $n = 50, l = 11$ case, which is the largest number of qubits we simulated, and the largest number of layers simulated for this qubit count. We choose this as a weak data point since it is hard to simulate and obtain good statistics. Supplementary Figure 5 shows the decrease in uncertainties as the number of samples increases. In this particular instance, the ansätze is close to a 3-design.



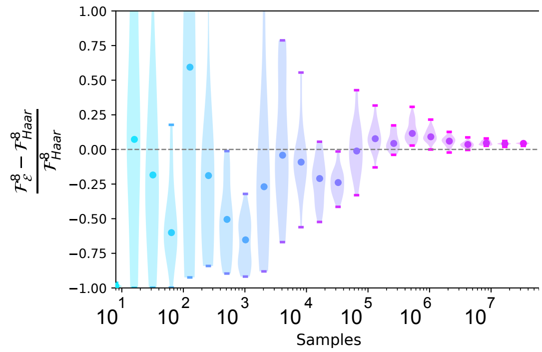
Supplementary Figure 5 Convergence process of the estimated frame potential as the number of samples increases. The plot shows the data for the parallel random unitaries with 50 qubits and 11 layers. Error analysis is similarly performed using bootstrapping. Solid points are medians of the bootstrap sample, and the vertical shadows represent the sample distribution where the width corresponds to the density. Horizontal bars show the extrema in the bootstrap samples.

2.4 Validation of sampling Haar random two-qubit unitaries

Parallel and local random unitaries require random two-qubit unitaries sampled from the Haar measure. The decomposition approach we use indeed satisfy this criterion. We observe for $n = 2$ and $l = 1$, which is a single random unitary gate, that the frame potential agrees with the Haar value $k!$ even at high k values, verifying that it is sampling the Haar measure. Specifically, we show the convergence process for $k = 6$ and $k = 8$ in Supplementary Figure 6, 7.



Supplementary Figure 6 Convergence of $\mathcal{F}$ for the two-qubit random gate to the Haar measure.



Supplementary Figure 7 Convergence for $k = 8$.

3 Supplementary Discussion

3.1 Missing data points

Increasing k or n leads to an increase in the frame potential percentage deviation from the Haar value, which means that the valid exponential regime starts later in l for large k and n. Further, due to the simulation difficulty of large n circuits, we may not be able to simulate large l and have to terminate the curves of $\frac{\mathcal{F}_{\mathcal{E}}^{(k)} - \mathcal{F}_{\text{Haar}}^{(k)}}{\mathcal{F}_{\text{Haar}}^{(k)}}$ v.s. l early. This means that curves at large k and n are shorter in the exponential regime. Together with the larger uncertainties at large k and n, there may not be enough data points for proper fitting, which is the reason why data points in the layer scaling plots (Figure 5, 7, and 9 of the main manuscript) are missing for large k and n. One or more bootstrap samples for the missing data points fail to converge during the fit.

3.2 Weak spurious correlation

Since frame potentials of different ks are computed from the same set of $\mathrm{Tr}\left(U^\dagger V\right)$, there is a correlation between different k's. For example, the layer scaling for in Figure 5 and 9 of the main manuscript shows some weakly correlated fluctuations for both $k = 2$ and $k = 3$. However, if we split the data into three equal partitions and plot three curves, such fluctuations are no longer correlated, therefore do not represent genuine patterns.