The limits of quantum circuit simulation with low precision arithmetic

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How to simulate ideal quantum computers and why

The normalized wave function in a circuit of $Q$ qubits is written as

$$|\psi\rangle = \sum_{k=0}^{N-1} c_k |k\rangle,$$

and the output is the result of a series of matrix multiplications,

$$|\psi_t\rangle = U_t \cdot U_{t-1} \cdot \ldots \cdot U_2 \cdot U_1 \cdot |\psi_0\rangle$$

- $N = 2^Q$ is the number of terms. Cannot simulate $Q > 50$ (quantum supremacy)
- $|k\rangle$ are the computational basis states (orthogonal unit vectors).
- $U_i$ are quantum gates, $N \times N$ unitary matrices $U_i^*U_i = I$
- Current quantum computers (IBM Q, Rigetti, Google) very primitive, only way to design and test new quantum algorithms is with simulation
Typical elementary gates (universal)

<table>
<thead>
<tr>
<th>Gate</th>
<th>Circuit</th>
<th>Matrix</th>
</tr>
</thead>
</table>
| NOT                | ![X](image) | \[
\begin{pmatrix}
0 & 1 \\
1 & 0
\end{pmatrix}
\] |
| Hadamard           | ![H](image) | \[
\frac{1}{\sqrt{2}} \begin{pmatrix}
1 & 1 \\
1 & -1
\end{pmatrix}
\] |
| Controlled NOT     | ![controlled NOT](image) | \[
\begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0
\end{pmatrix}
\] |
| Controlled phase   | ![controlled phase](image) | \[
\begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & e^{i\phi}
\end{pmatrix}
\] |

Most useful gates can be represented as tensor products of more elementary gates $U = U_1 \times U_2 \times \ldots \times U_s$ and linear operations
Practical implementation of gates

How gates operating on qubits $p, q$ are implemented: "←" represents assignment and "↔" swapping. Parentheses contain the binary index $k$ of $c_k$ and the dots indicate unaffected bits. $H$ is Hadamard’s gate and CP are the controlled phase gates.

$$|\psi\rangle = c_{00}|00\rangle + c_{01}|01\rangle + c_{10}|10\rangle + c_{11}|11\rangle$$

<table>
<thead>
<tr>
<th>Gate</th>
<th>Operation</th>
</tr>
</thead>
<tbody>
<tr>
<td>$H(q)$</td>
<td>$c(\ldots, 0_q, \ldots) \leftarrow \frac{1}{\sqrt{2}} \left( c(\ldots, 0_q, \ldots) + c(\ldots, 1_q, \ldots) \right)$ $c(\ldots, 1_q, \ldots) \leftarrow \frac{1}{\sqrt{2}} \left( c(\ldots, 0_q, \ldots) - c(\ldots, 1_q, \ldots) \right)$</td>
</tr>
<tr>
<td>CNOT $(p, q)$</td>
<td>$c(\ldots, 1_p, \ldots, 0_q, \ldots) \leftrightarrow c(\ldots, 1_p, \ldots, 1_q, \ldots)$</td>
</tr>
<tr>
<td>CP $(p, q)$</td>
<td>$c(\ldots, 1_p, \ldots, 1_q, \ldots) \leftarrow e^{i\pi/2^m} c(\ldots, 1_p, \ldots, 1_q, \ldots)$</td>
</tr>
<tr>
<td>SWAP $(p, q)$</td>
<td>$c(\ldots, 1_p, \ldots, 0_q, \ldots) \leftrightarrow c(\ldots, 0_p, \ldots, 1_q, \ldots)$</td>
</tr>
</tbody>
</table>

Example circuit: Quantum Fourier Transform (QFT)

Input:

\[ |\psi_0\rangle = \sum_{k=0}^{N-1} c_k |k\rangle \]

The \( N = 2^Q \) output coefficients are the usual FT

\[ |\psi_t\rangle = \sum_{k=0}^{N-1} f_k |k\rangle, \quad f_k = \frac{1}{\sqrt{N}} \sum_{l=0}^{N-1} c_l e^{2\pi i kl/N} \]

Time complexity \( T = O(Q^2) \) versus classical FFT \( O(N \log_2 N) = O(Q2^Q) \)
A famous algorithm: Shor’s algorithm

- Problem: factorize $n = p \cdot q$
- Find $Q$ such that $n^2 \leq 2^Q < 2n^2$
- Take into account that the period of the function $f(x) = a^x \mod n$ divides Euler’s totient function $\phi(n) = (p - 1)(q - 1)$
- Take the FT and measure the position of a peak, then do some math (classical continued fraction expansion) to find the factors.

Quantum simulation benchmark (QuanSimBench)

- Simplify Shor’s algorithm
- Factorize increasing integers until memory exhausted
- Only simulates AQFT: same as QFT but with fewer phases
- Generate data of measured $f(x) = a^x \mod n$ classically.
- Open source https://github.com/datavortex/QuanSimBench

Deferred measurement does not change QFT peaks

Thus result is equivalent to load data after first measurement
Other methods for ideal quantum circuit simulations

G: number of gates, D: depth of circuit, M: memory usage, T: time

- **Schrodinger’s formulation**: full vector states (this work)

  \[ |\psi\rangle = \sum_{k=0}^{N-1} c_k |k\rangle \quad |\psi(t)\rangle = U_G \cdot U_{G-1} \cdots U_2 \cdot U_1 \cdot |\psi_0\rangle \]

  \[ T = O(G2^Q) \]

  \[ M = O(2^Q) \]

  feasible for random states and large depths.

- **Feynman path integration** (very slow)

  \[ T = O(2^G) \]

  \[ M = O(G + Q) \]

- **Tensor contraction family**: time-space tradeoff, good for low entropy states, problematic for large depths and random states

  \[ T = O(Q2^Q-k(2D)^{k+1}) \]

  \[ M = O(2^Q-k log(D)) \]
Saving memory with log-polar low precision format

Encode quantum state

\[ |\psi\rangle = \sum_{k=0}^{N-1} c_k |k\rangle \]

\[
c_k \approx T(c_k) = \exp \left( - \left( e_k + \frac{f_k}{2^F} \right) + 2\pi i \frac{a_k}{2^A} \right), \tag{1}\]

The complex amplitudes are encoded with \( E \) bits for the integer part of the exponent, \( F \) bits for the fraction and \( A \) bits for the argument.

<table>
<thead>
<tr>
<th>E</th>
<th>F</th>
<th>A</th>
</tr>
</thead>
</table>
| bits per coefficient: \( B = E + F + A \)

- Rounding error is uniformly distributed
- Simplifies mathematical analysis
- Some phase gates are exact \( \pi/2^k \), \( k < A \).
- More accurate than pairs of floats for given number of bits.
- Drawback: slower, not native CPU conversions
- Use lookup tables and interpolation to speed up
Log-polar versus pair of floating point numbers

Polar format more regular, simpler error statistics and allows to compute phase gates $P(\pi/2^k)$ without error.

**Figure:** Very low precision format with $E = 2$, $F = 2$, $A = 5$ (9 bits) versus floats with 3 bits of exponent and 2 of mantissa (10 bits). Red are underflows.
Distribution of rounding errors is uniform

Figure: Empirical histograms of the rounding errors for the logarithm of the modulus (high rectangle) and for the argument of Eq. (1) for $Q = 20$, $E = 5$, $F = 9$ and $A = 10$. They are uniformly distributed when the real and imaginary parts of the coefficients $c_k$ are random because the rounded binary digits after the least significant digit are random. This is not true for floating point formats.
Main result: cumulative error after $G$ error-prone gates

Define the cumulative error,

$$\sigma^2 = \| |\psi_G\rangle - |\psi_{G,exact}\rangle \|^2$$

and assuming the initial condition has maximum entropy,

$$\sigma^2(E, F, A, G) \approx \left( \phi + (1 - \phi) \frac{2^{-2F} + 4\pi^2 2^{-2A}}{12} \right) G,$$

where the normalization error due to underflows is

$$\phi = 1 - (N \mu^2 + 1)e^{-N \mu^2}$$

and the smallest representable modulus is

$$\mu = \min |c_k| = \exp(-2^E + 2^{-F})$$

For non-random states, an upper bound for the error (loose bound)

$$\sigma^2 \leq \frac{2^{-2F} + 4\pi^2 2^{-2A}}{4} G^2$$
Optimal triplets $E, F, A$ with respect of the expected value of the conversion error for random states, computed by brute force minimization of the conversion error with the constraint $E + F + A = B$.

<table>
<thead>
<tr>
<th>$B$</th>
<th>$Q = 20$</th>
<th>$Q = 30$</th>
<th>$Q = 40$</th>
<th>$Q = 50$</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>4, 3, 5</td>
<td>4, 3, 5</td>
<td>4, 3, 5</td>
<td>5, 2, 5</td>
</tr>
<tr>
<td>14</td>
<td>4, 4, 6</td>
<td>4, 4, 6</td>
<td>4, 4, 6</td>
<td>5, 3, 6</td>
</tr>
<tr>
<td>16</td>
<td>4, 5, 7</td>
<td>4, 5, 7</td>
<td>4, 5, 7</td>
<td>5, 4, 7</td>
</tr>
<tr>
<td>18</td>
<td>4, 6, 8</td>
<td>4, 6, 8</td>
<td>5, 5, 8</td>
<td>5, 5, 8</td>
</tr>
<tr>
<td>20</td>
<td>4, 7, 9</td>
<td>4, 7, 9</td>
<td>5, 6, 9</td>
<td>5, 6, 9</td>
</tr>
<tr>
<td>22</td>
<td>4, 8, 10</td>
<td>4, 8, 10</td>
<td>5, 7, 10</td>
<td>5, 7, 10</td>
</tr>
<tr>
<td>24</td>
<td>4, 9, 11</td>
<td>4, 9, 11</td>
<td>5, 8, 11</td>
<td>5, 8, 11</td>
</tr>
<tr>
<td>26</td>
<td>4, 10, 12</td>
<td>4, 10, 12</td>
<td>5, 9, 12</td>
<td>5, 9, 12</td>
</tr>
<tr>
<td>28</td>
<td>4, 11, 13</td>
<td>4, 11, 13</td>
<td>5, 10, 13</td>
<td>5, 10, 13</td>
</tr>
<tr>
<td>30</td>
<td>4, 12, 14</td>
<td>4, 12, 14</td>
<td>5, 11, 14</td>
<td>5, 11, 14</td>
</tr>
<tr>
<td>32</td>
<td>4, 13, 15</td>
<td>4, 13, 15</td>
<td>5, 12, 15</td>
<td>5, 12, 15</td>
</tr>
<tr>
<td>34</td>
<td>4, 14, 16</td>
<td>4, 14, 16</td>
<td>5, 13, 16</td>
<td>5, 13, 16</td>
</tr>
<tr>
<td>36</td>
<td>4, 15, 17</td>
<td>4, 15, 17</td>
<td>5, 14, 17</td>
<td>5, 14, 17</td>
</tr>
</tbody>
</table>
Not all gates generate the same errors: effective gates

\[ G = \sum_{g=1}^{n} \beta_g, \quad (2) \]

\( n \) is the total number of gates, \( \beta_g \) is the fraction of coefficients affected by gate \( g \),

<table>
<thead>
<tr>
<th>Gate type</th>
<th>( \beta_g )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( X, Z^{1/k} ) ( k &lt; A ), CNOT, SWAP, TOFF</td>
<td>0</td>
</tr>
<tr>
<td>( Z^{1/k} ) ( k \geq A )</td>
<td>1/2</td>
</tr>
<tr>
<td>( H, X^{1/k}, Y^{1/k} ) ( k &gt; 2 ), ( U_3(\theta, \lambda, \phi) )</td>
<td>1</td>
</tr>
<tr>
<td>Last row with ( k ) controls</td>
<td>( 1/2^k )</td>
</tr>
</tbody>
</table>

Table: Fraction of coefficients affected by rounding error for typical gates.
Compute the expected value of

\[ \varepsilon_c^2 = \| T|\psi\rangle - |\psi\rangle \|^2 = \sum_{k=0}^{N-1} |T(c_k) - c_k|^2 = \]

\[ \sum_{|c_k| < \mu} |c_k|^2 + \sum_{|c_k| \geq \mu} |c_k|^2 \left| e^{\varepsilon_k+i\gamma_k} - 1 \right|^2 \approx \phi + (1 - \phi) \frac{2^{-2F} + 4\pi^2 2^{-2A}}{12} \]

using uniform distribution of \(-2^{-F}/2 \leq \varepsilon_k \leq 2^{-F}/2\) and \(-\pi 2^{-A} \leq \gamma_k \leq \pi 2^{-A}\) and that \(p = |c_k|^2\) are distributed according to Porter-Thomas distribution with PDF \(f(p) \approx Ne^{-pN}\)

For the cumulative error we use unitariness and the recurrence

\[ |\varepsilon_{t+1}\rangle = U_t|\varepsilon_t\rangle + |\tau_t\rangle. \]
How many gates can we compute

- The **fidelity** is defined as

\[ \Phi = |\langle \psi_G | \psi_{G,\text{exact}} \rangle|^2 \]

- related to \( \sigma^2 \) as

\[ \Phi \geq \left(1 - \frac{\sigma^2}{2}\right)^2 \]

- A barely tolerable result has \( \sigma^2 = 1/4 \) represents a fidelity of \( \Phi \geq 0.765 \) (this would be the probability of success of an algorithm if the final state had only one coefficient \( c_k \neq 0 \)).

- Number of error-prone gates we can compute high entropy states

\[ G_{\text{random}} < \frac{12\sigma^2}{2^{-2F} + 4\pi^2 2^{-2A}}. \]

- Only counts error-prone gates, many gates are error free.
How many gates can be computed with low precision

<table>
<thead>
<tr>
<th>$B$</th>
<th>$\varepsilon_c^2$</th>
<th>$G_{random}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>1.35e-01</td>
<td>2</td>
</tr>
<tr>
<td>12</td>
<td>8.42e-03</td>
<td>30</td>
</tr>
<tr>
<td>16</td>
<td>5.26e-04</td>
<td>475</td>
</tr>
<tr>
<td>20</td>
<td>3.29e-05</td>
<td>7600</td>
</tr>
<tr>
<td>24</td>
<td>2.06e-06</td>
<td>121599</td>
</tr>
<tr>
<td>28</td>
<td>1.28e-07</td>
<td>1.94e+06</td>
</tr>
<tr>
<td>32</td>
<td>8.03e-09</td>
<td>3.11e+07</td>
</tr>
<tr>
<td>36</td>
<td>5.02e-10</td>
<td>4.98e+08</td>
</tr>
<tr>
<td>40</td>
<td>3.14e-11</td>
<td>7.96e+09</td>
</tr>
</tbody>
</table>

**Table:** Typical values of one-conversion errors $\varepsilon_c^2$ and maximum number of error prone gates for $\sigma = 1/2$ and $Q = 50$ for random states using the optimal triplets.
Random circuit test: a circuit hard to simulate

- Generates entangled maximum entropy state after $C \approx 7$ cycles
- Test the ability of a simulation (or quantum computer) to ”hold” a maximally entangled state
- Each cycle rotates all qubits in the Bloch sphere with the rotation gate $U_3(\pm \pi/2, \pm \pi/4, \pm \pi/4)$ and random signs.

$$U_3(\theta, \lambda, \phi) = \begin{pmatrix} \cos \frac{\theta}{2} & -e^{i\lambda} \sin \frac{\theta}{2} \\ e^{i\phi} \sin \frac{\theta}{2} & e^{i(\lambda+\phi)} \cos \frac{\theta}{2} \end{pmatrix}$$
Figure: Growth of the numerical cumulative error (points) for a uniformly distributed, random initial condition, as a function of the number of error prone gates $G$, compared with the model (lines), with $Q = 30$ for triplets $E, F, G$: 4, 5, 7 (top line), 4, 9, 11 (middle) and 4, 13, 15 (bottom). The error is computed by comparing the output with low precision $|\psi_G\rangle$ with a computation with double precision as a proxy for the exact solution $|\psi_{ex}\rangle$. 
Resulting coefficients distribution for random circuits

Figure: Starting with a uniform random initial condition we run 7 cycles twice, first with double precision and then with low precision. These are the histograms of the normalized errors of the real part of the coefficients, \( \text{Re}(c_{k,\text{double}} - c_{k,\text{lowprec}}) \) for \( E = 4, F = 9, A = 11 \) (points). The distribution is approximately normal with standard deviation \( \sigma \).
Back and forth test

// CREATE A RANDOM STATE
for i=1,C
    for q=1,Q
        k = Q*i+q
        U3(q, t(k), l(k), p(k) )
        CNOT(q, (q+1)%Q )
    end
end
NORMALIZE

// RUN IN REVERSE ORDER TO RESTORE IC
for i=C,1
    for q=Q,1
        k = Q*i+q
        CNOT(q, (q+1)%Q )
        U3(q, -t(k), -p(k), -l(k) )
    end
end
NORMALIZE
Figure: Random algorithm test, 4 cycles forth and then 4 cycles for the inverse. Comparison of the actual error (y-axis) and the theoretical error (x-axis). Red squares: 20 qubits, brown circles: 30 qubits, blue triangles: 40 qubits. The bits per coefficient are indicated on the labels, with optimal triplets $E, F, A$. 
Reducing errors on amplitudes: normalization

When the normalization deteriorates,

$$\sum_{k=0}^{N-1} |c_k|^2 \neq 1$$

must renormalize each time the total probability departs from unity with random factors $-2^{-F-1} < \delta_k < 2^{-F-1}$

$$c'_k = \frac{c_k}{\|\psi\|} e^{\delta_k},$$

**Figure:** Let $z = \ln \frac{|c_k|}{\|\psi\|}$ and $z_1 < z_2$ be two consecutive discrete logarithms with separation $z_2 - z_1 = 2^{-F} = 2r$ and $z_1 < z < z_2$. We want to round $z$ to the closest of $z_1$ or $z_2$. After we add a uniformly distributed random number $\delta$ to $z$, with $-r \leq \delta < r$, the numbers to the right of $z_c = (z_1 + z_2)/2$ are rounded to $z_2$ with probability $p = (z - z_1)/(2r)$ and the numbers to the left of $z_c$ are rounded to $z_1$ with probability $1 - p$, thus $\mathbb{E}(\text{round}(z + \delta)) = (1 - p)z_1 + pz_2 = z$. 
Reducing rounding errors on phases

Systematic errors accelerates the growth of total error. Below is a potentially failing circuit after $W > 2^A$ applications of the gate. The problem is solved by multiplying the amplitudes with carefully chosen random factors

$$c'_k = c_k \exp(\delta_k + i\gamma_k),$$

(3)

with $-2^{-F-1} < \delta_k < 2^{-F-1}$ and $-\pi 2^{-A} < \gamma_k < \pi 2^{-A}$

In other algorithms normalization may be necessary as well.
Final remarks

Other tests performed
- Quantum Fourier Transform
- Grover’s algorithm
- Simplified Shor’s algorithm (quansimbench)

Open problems
- Is it optimal? (preliminary work says no, but it is close)
- How to speedup?
- Translate to tensor contraction formulations
- Solve partial differential equations of high dimensionality
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● S. Betelu, ”Quansimbench: a benchmark for HPC quantum circuit simulations”, https://github.com/datavortex/QuanSimBench

● S. Betelu, ”C and MPI simulation of quantum circuits with low precision arithmetic”, https://github.com/datavortex/lowprecisionqubits