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

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

\[
\sum_{k=0}^{N-1} |c_k|^2 = 1
\]

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)

| Gate                      | Circuit | Matrix                  |
|---------------------------|---------|-------------------------|
| **NOT**                   | ![X gate](image) | $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ |
| **Hadamard**              | ![H gate](image) | $\frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$ |
| **Controlled NOT**        | ![Controlled NOT gate](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 gate](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.

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

| Gate       | Operation                                                                 |
|------------|---------------------------------------------------------------------------|
| $H(q)$     | $c(\ldots, 0_q, \ldots) \leftarrow \frac{1}{\sqrt{2}} (c(\ldots, 0_q, \ldots) + c(\ldots, 1_q, \ldots))$ |
|            | $c(\ldots, 1_q, \ldots) \leftarrow \frac{1}{\sqrt{2}} (c(\ldots, 0_q, \ldots) - c(\ldots, 1_q, \ldots))$ |
| CNOT $(p, q)$ | $c(\ldots, 1_p, \ldots, 0_q, \ldots) \leftrightarrow c(\ldots, 1_p, \ldots, 1_q, \ldots)$ |
| CP $(p, q)$ | $c(\ldots, 1_p, \ldots, 1_q, \ldots) \leftarrow e^{i\pi/2^m} c(\ldots, 1_p, \ldots, 1_q, \ldots)$ |
| SWAP $(p, q)$ | $c(\ldots, 1_p, \ldots, 0_q, \ldots) \leftrightarrow c(\ldots, 0_p, \ldots, 1_q, \ldots)$ |

K. De Raedt, K. Michielsen, H. De Raedt, B. Trieu, G. Arnold, M. Richter, Th. Lippert, H. Watanabe, N.Ito, "Massively parallel quantum computer simulator", Computer Physics Communications, 176, 2, (2007)
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 \( O(N \log_2 N) = O(Q^2) \)
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.

\[
\begin{align*}
|0\rangle & \xrightarrow{H \otimes Q} \quad |0\rangle \xrightarrow{2^x \mod n} \\
& \quad \xrightarrow{QFT} \quad \text{PW Shor, “Polynomial-Time algorithms for prime Factorization and Discrete Logarithms on a Quantum Computer”, SIAM J. Comp 1997}
\end{align*}
\]
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

\[ |0\rangle \xrightarrow{H \otimes Q} |0\rangle / 2^{x \mod n} \]

Deferred measurement does not change QFT peaks

\[ |0\rangle \xrightarrow{H \times n} |0\rangle / 2^x \mod N \]

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
  \[
  T = O(Q2^{Q-k}(2D)^{k+1}) \\
  M = O(2^{Q-k}log(D))
  \]
Encode quantum state

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

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

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.

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,

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

and assuming the initial condition has maximum entropy,

$$\sigma^2(E, F, A, G) \approx \left(\phi + (1 - \phi)\frac{2^{-2F} + 4\pi^22^{-2A}}{12}\right) G,$$

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)

$$\sigma^2 \leq \frac{2^{-2F} + 4\pi^22^{-2A}}{4} G^2$$
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 $E + F + A = B$.

| $B$ | $Q = 20$ | $Q = 30$ | $Q = 40$ | $Q = 50$ |
|-----|----------|----------|----------|----------|
| 12  | 4, 3, 5  | 4, 3, 5  | 4, 3, 5  | 5, 2, 5  |
| 14  | 4, 4, 6  | 4, 4, 6  | 4, 4, 6  | 5, 3, 6  |
| 16  | 4, 5, 7  | 4, 5, 7  | 4, 5, 7  | 5, 4, 7  |
| 18  | 4, 6, 8  | 4, 6, 8  | 5, 5, 8  | 5, 5, 8  |
| 20  | 4, 7, 9  | 4, 7, 9  | 5, 6, 9  | 5, 6, 9  |
| 22  | 4, 8, 10 | 4, 8, 10 | 5, 7, 10 | 5, 7, 10 |
| 24  | 4, 9, 11 | 4, 9, 11 | 5, 8, 11 | 5, 8, 11 |
| 26  | 4, 10, 12| 4, 10, 12| 5, 9, 12 | 5, 9, 12 |
| 28  | 4, 11, 13| 4, 11, 13| 5, 10, 13| 5, 10, 13|
| 30  | 4, 12, 14| 4, 12, 14| 5, 11, 14| 5, 11, 14|
| 32  | 4, 13, 15| 4, 13, 15| 5, 12, 15| 5, 12, 15|
| 34  | 4, 14, 16| 4, 14, 16| 5, 13, 16| 5, 13, 16|
| 36  | 4, 15, 17| 4, 15, 17| 5, 14, 17| 5, 14, 17|
Not all gates generate the same errors: effective gates

\[ G = \sum_{g=1}^{n} \beta_g, \]  

(2)

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

| Gate type                                      | \( \beta_g \) |
|-----------------------------------------------|----------------|
| \( X, Z^1/k \) (\( k < A \)), CNOT, SWAP, TOFF | 0              |
| \( Z^1/k \) (\( k \geq A \))                  | 1/2            |
| \( H, X^1/k, Y^1/k \) (\( k > 2 \)), \( U_3(\theta, \lambda, \phi) \) | 1              |
| Last row with \( k \) controls               | \( 1/2^k \)    |

**Table:** Fraction of coefficients affected by rounding error for typical gates.
Sketch of derivation

Compute the expected value of $$\varepsilon_c^2 = \| T|\psi\rangle - |\psi\rangle \|^2 = \sum_{k=0}^{N-1} |T(c_k) - c_k|^2 =$$

$$\sum_{|c_k|<\mu} |c_k|^2 + \sum_{|c_k|\geq\mu} |c_k|^2 |e^{\epsilon_k+i\gamma_k} - 1|^2 \approx \phi + (1 - \phi) 2^{-2F} + 4\pi^2 2^{-2A}$$

using uniform distribution of $$-2^{-F}/2 \leq \epsilon_k \leq 2^{-F}/2$$ 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
  \[ \Phi \geq (1 - \sigma^2/2)^2 \]

- 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

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

**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 $|\psi_{ex}\rangle$. 
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

$$c'_k = c_k \exp(\delta_k + i\gamma_k), \quad (3)$$

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