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

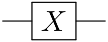
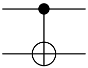
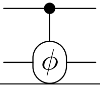
$$|\psi\rangle = \sum_{k=0}^{N-1} c_k |k\rangle, \qquad \sum_{k=0}^{N-1} |c_k|^2 = 1$$

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		$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$
Hadamard		$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$
Controlled NOT		$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$
Controlled phase		$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & e^{i\phi} \end{pmatrix}$

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

Practical implementation of gates

How gates operating on qubits p, q are implemented: "$\leftarrow$" represents assignment and "$\leftrightarrow$" 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**
$H(q)$	$c(..,0_q,..) \leftarrow \frac{1}{\sqrt{2}}\left(c(..,0_q,..) + c(..,1_q,..)\right)$ $c(..,1_q,...) \leftarrow \frac{1}{\sqrt{2}}\left(c(..,0_q,..) - c(..,1_q,..)\right)$
CNOT (p,q)	$c(..,1_p,..,0_q,..) \leftrightarrow c(..,1_p,..,1_q,..)$
CP(p,q)	$c(..,1_p,..,1_q,..) \leftarrow e^{i\pi/2^m} c(..,1_p,..,1_q,..)$
SWAP(p,q)	$c(..,1_p,..,0_q,..) \leftrightarrow c(..,0_p,..,1_q,..)$

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)

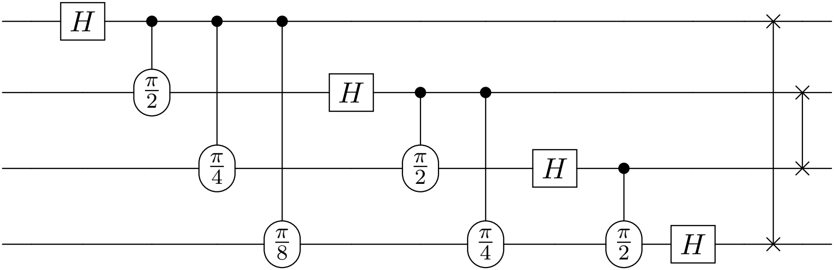
Input:

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

The $N = 2^Q$ output coefficients are the usual FT

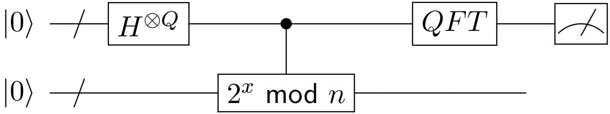
$$|\psi_t\rangle = \sum_{k=0}^{N-1} f_k |k\rangle, \qquad f_k = \frac{1}{\sqrt{N}} \sum_{l=0}^{N-1} c_l e^{2\pi i k l / N}$$

Time complexity $T = O(Q^2)$ versus classical FFT $O(N \log_2 N) = O(Q 2^Q)$



A famous algorithm: Shor's algorithm

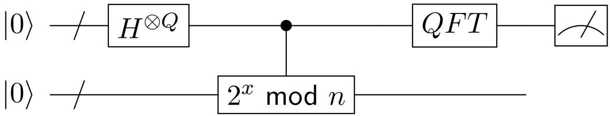
- Problem: factorize $n = p \cdot q$
- Find Q such that $n^2 \leq 2^Q < 2n^2$
- Take into account that the period of the function $f(x) = a^x \bmod n$ divides Euler's totient function $\phi(n) = (p-1)(q-1)$
- Take the FT and measure the position of a peak, then do some math (classical continued fraction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



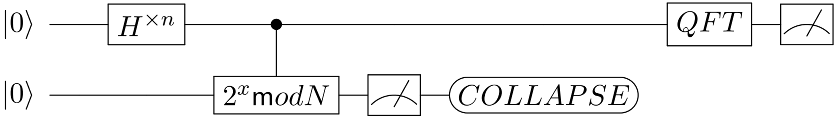
PW Shor, "Polynomial-Time algorithms for prime Factorization and Discrete Logarithms on a Quantum Computer", SIAM J. Comp 1997

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 $f(x) = a^x \bmod n$ 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)
  $|\psi\rangle = \sum_{k=0}^{N-1} c_k |k\rangle \qquad |\psi(t)\rangle = U_G \cdot U_{G-1} ... U_2 \cdot U_1 \cdot |\psi_0\rangle$

  $$T = O(G2^Q)$$
  $$M = O(2^Q)$$

  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

  $$T = O(Q2^{Q-k}(2D)^{k+1})$$
  $$M = O(2^{Q-k} log(D))$$

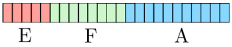
Saving memory with log-polar low precision format

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.



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.

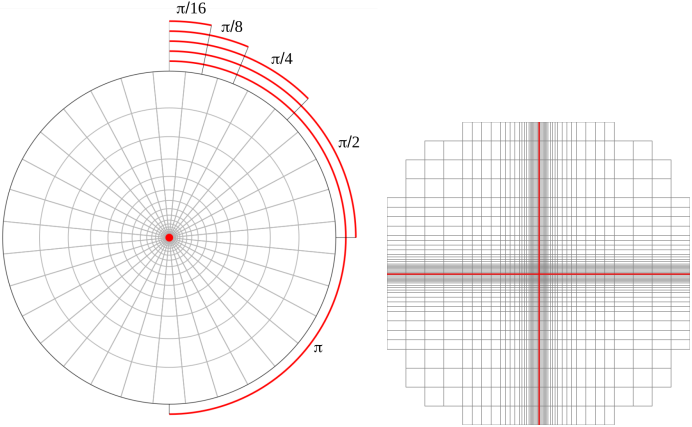


Figure: Very low precision format with $E = 2, F = 2, A = 5$ (9 bits) versus floats with 3 bits of exponent and 2 of mantissa (10 bits). Red are underflows.

Distribution of rounding errors is uniform

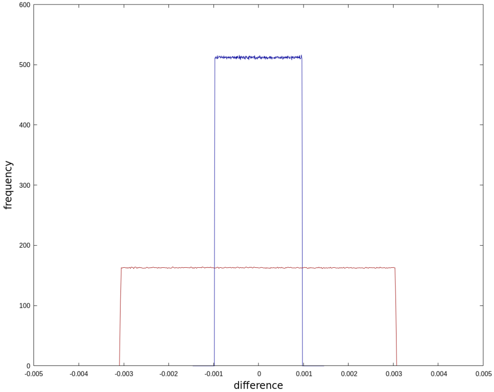


Figure: Empirical histograms of the rounding errors for the logarithm of the modulus (high rectangle) and for the argument of Eq. (1) for $Q = 20$, $E = 5, F = 9$ and $A = 10$. They are uniformly distributed when the real and imaginary parts of the coefficients c_k are random because the rounded binary 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,

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

and assuming the initial condition has maximum entropy,

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

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 $E + F + A = B$.

	$Q = 20$	$Q = 30$	$Q = 40$	$Q = 50$
B	E, F, A	E, F, A	E, F, A	E, F, A
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

$$G = \sum_{g=1}^{n} \beta_g, \tag{2}$$

n is the total number of gates, β_g is the fraction of coefficients affected by gate g,

Gate type	β_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

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

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

using uniform distribution of $-2^{-F}/2 \leq \epsilon_k \leq 2^{-F}/2$ 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 $f(p) \approx N e^{-pN}$

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

$$\Phi = |\langle \psi_G | \psi_{G,exact} \rangle|^2$$

- related to σ^2 as

$$\Phi \geq \left(1 - \sigma^2/2\right)^2$$

- 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

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

- Only counts error-prone gates, many gates are error free.

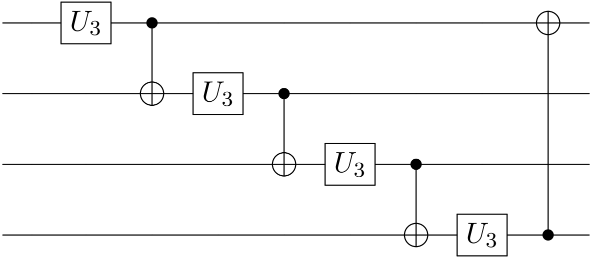
How many gates can be computed with low precision

B	ε_c^2	G_{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 ε_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.



$$U_3(\theta, \lambda, \phi) = \begin{pmatrix} \cos\frac{\theta}{2} & -e^{i\lambda}\sin\frac{\theta}{2} \\ e^{i\phi}\sin\frac{\theta}{2} & e^{i(\lambda+\phi)}\cos\frac{\theta}{2} \end{pmatrix}$$

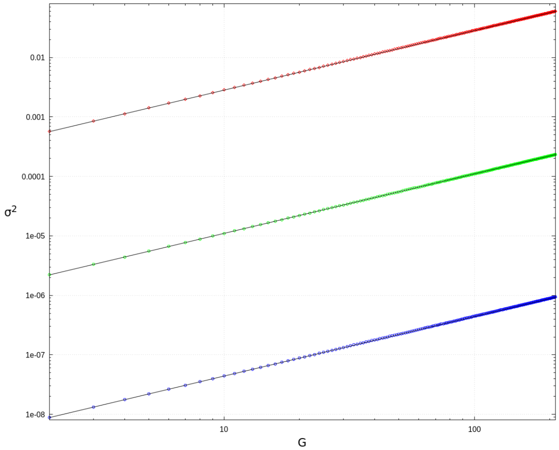


Figure: Growth of the numerical cumulative error (points) for a uniformly distributed, random initial condition, as a function of the number of error prone gates G, compared with the model (lines), with $Q = 30$ for triplets E, F, G: $4, 5, 7$ (top line), $4, 9, 11$ (middle) and $4, 13, 15$ (bottom). 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

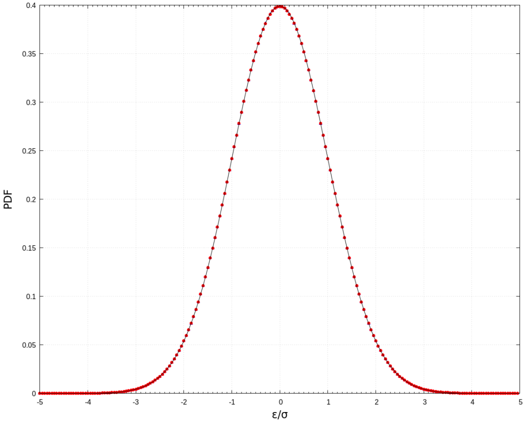


Figure: Starting with a uniform random initial condition we run 7 cycles twice, first with double precision and then with low precision. These are the histograms of the normalized errors of the real part of the coefficients, $\mathrm{Re}(c_{k,double} - c_{k,lowprec})$ for $E = 4, F = 9, A = 11$ (points).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

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
```

Back and forth test

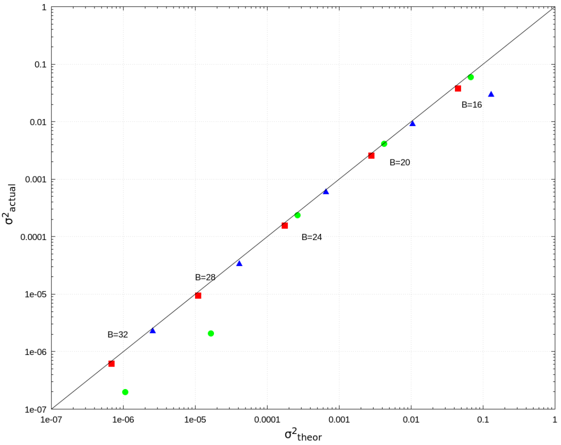


Figure: Random algorithm test, 4 cycles forth and then 4 cycles for the inverse. Comparison of the actual error (y-axis) and the theoretical error (x-axis). Red squares: 20 qubits, brown circles: 30 qubits, blue triangles: 40 qubits. The bits per coefficient are indicated on the labels, with optimal 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 $-2^{-F-1} < \delta_k < 2^{-F-1}$

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

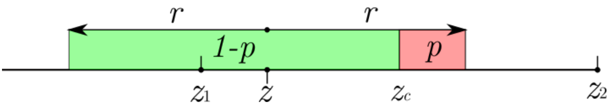
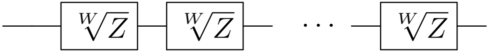


Figure: Let $z = \ln \frac{|c_k|}{\| |\psi\rangle \|}$ and $z_1 < z_2$ be two consecutive discrete logarithms with separation $z_2 - z_1 = 2^{-F} = 2r$ and $z_1 < z < z_2$. We want to round z to the closest of z_1 or z_2. After we add a uniformly distributed random number δ to z, with $-r \leq \delta < r$, 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 $\mathbb{E}(round(z + \delta)) = (1 - p)z_1 + pz_2 = z$.

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



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

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