Quantum Gate Calculator

The Quantum Gate Calculator (QGC) is a package for calculating the action of a series of quantum gates on the initial state of a set of qubits.

Installation

The package has been tested on MacOS 10.13.5 (High Sierra) with Apple LLVM version 10.0.0 (clang-1000.10.44.4), but it should compile for most UNIX-like operating systems with current GCC compilers. To compile the package:

- Download files to the directory where you wish the executable to be installed;
- run the shell script `Install.sh`;
- add the path to that directory to the file `$HOME/.bash_profile`;
- run the command `source .bash_profile` from your `$HOME` directory.

Running QGC

To run QGC, use the command

```
qgc <filename_qubits> <filename_gates> <iterations>,
```

the program takes two input files, as discussed in the following section, followed by the number of iterations of the calculation to be performed.

Input Files

QGC takes two input files. The file `<filename_qubits>` contains the initial states for all qubits in the system and the file `<filename_gates>` contains the sequence of gates to be applied to this state.

<filename_qubits>

The state of a single qubit can be described by a point on the Bloch sphere. In the file that specifies the initial states of all qubits, this point is specified using 3 numbers: the amplitude of the $|0\rangle$ state, the amplitude of the $|1\rangle$ state, and the phase shift between the two states, separated by spaces. The state of each qubit is specified on a separate line. For example, the file with the following contents:

```
1.0 0.0 0.0
1.0 0.0 0.0
1.0 0.0 0.0
```

specifies a system of 3 qubits, each initially in state $|0\rangle$. The sum of squares of the amplitudes of states $|0\rangle$ and $|1\rangle$ must add up to 1.

<filename_gates>

This file specifies the gates that are applied to the initial state of the system. Each line contains specification of a single gate, with the gate specifier and any required parameters for the gate separated by spaces. The file may also include separate comment lines that start with the hashtag symbol ("#") with no preceding spaces. See the following section for the description of available gates.

Gates

The following **single-qubit gates** are available:

Name	Single-qubit matrix	Command	Parameters
Identity	$\begin{bmatrix}1 & 0\\0 & 1\end{bmatrix}$	`I`	Qubit number
Hadamard	$\frac{1}{\sqrt{2}}\begin{bmatrix}1 & 1\\1 & -1\end{bmatrix}$	`HAD`	Qubit number
Pauli X (NOT)	$\begin{bmatrix}0 & 1\\1 & 0\end{bmatrix}$	`PX`	Qubit number
Pauli Y	$\begin{bmatrix}0 & -i\\i & 0\end{bmatrix}$	`PY`	Qubit number
Pauli Z	$\begin{bmatrix}1 & 0\\0 & -1\end{bmatrix}$	`PZ`	Qubit number

X rotation	$\begin{bmatrix} \cos\left(\frac{\theta}{2}\right) & -i\sin\left(\frac{\theta}{2}\right) \\ -i\sin\left(\frac{\theta}{2}\right) & \cos\left(\frac{\theta}{2}\right) \end{bmatrix}$	`RX`	Qubit number, rotation angle θ
Y rotation	$\begin{bmatrix} \cos\left(\frac{\theta}{2}\right) & -\sin\left(\frac{\theta}{2}\right) \\ \sin\left(\frac{\theta}{2}\right) & \cos\left(\frac{\theta}{2}\right) \end{bmatrix}$	`RY`	Qubit number, rotation angle θ
Z rotation	$\begin{bmatrix} \exp\left(-i\frac{\theta}{2}\right) & 0 \\ 0 & \exp\left(i\frac{\theta}{2}\right) \end{bmatrix}$	`RZ`	Qubit number, rotation angle θ
T	$\begin{bmatrix} 1 & 0 \\ 0 & \exp\left(i\frac{\pi}{4}\right) \end{bmatrix}$	`T`	Qubit number, `false` (“no dagger”)
T†	$\begin{bmatrix} 1 & 0 \\ 0 & \exp\left(-i\frac{\pi}{4}\right) \end{bmatrix}$	`T`	Qubit number, `true` (“dagger”)
S	$\begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}$	`S`	Qubit number, `false` (“no dagger”)
S†	$\begin{bmatrix} 1 & 0 \\ 0 & -i \end{bmatrix}$	`S`	Qubit number, `true` (“dagger”)
Projection onto state $\vert 0\rangle$	$\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$	`P0`	Qubit number
Projection onto state $\vert 1\rangle$	$\begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$	`P1`	Qubit number

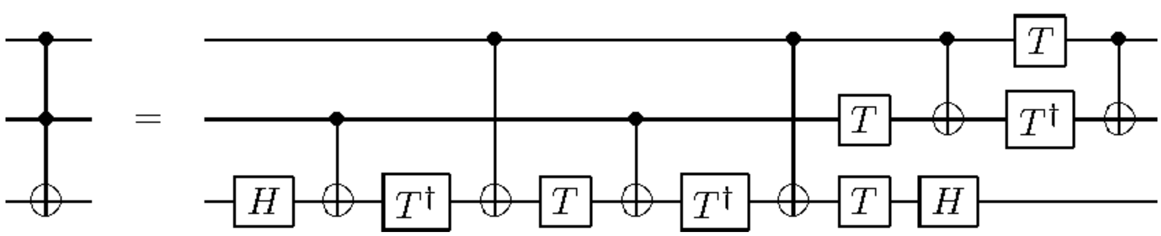
In addition, there is a **single-qubit measurement operation** available. It samples a random number between 0 and 1, then, if the generated number is less than the probability of the measured qubit being in state $|0\rangle$, then that qubit is collapsed to state $|0\rangle$, and otherwise that qubit is collapsed to state $|1\rangle$. The resulting N-qubit system states with non-zero probability are then renormalized. The measurement operation is called using the **command** `M` with the **number of the qubit to be measured as the only parameter**.

The following **two-qubit gates** are available (a is the number of the qubit that the gates acts on and c is the number of the control qubit; *note that the parameters must be specified in this order*):

Name	Definition	Command	Parameters
CNOT	$\bigotimes_{n=1}^{N}\left[(1-\delta_{nc})I_n+\delta_{nc}P_c^{(0)}\right]+$ $+\bigotimes_{n=1}^{N}\left[(1-\delta_{nc}-\delta_{na})I_n+\delta_{nc}P_c^{(1)}+\delta_{na}X_a\right]$	`CX`	Qubit number, control qubit number
CPHASE	$\bigotimes_{n=1}^{N} I_n-$ $-\bigotimes_{n=1}^{N}\left[(1-\delta_{nc}-\delta_{na})I_n+\delta_{nc}P_c^{(1)}+\delta_{na}P_a^{(1)}\right]$	`CZ`	Qubit number, control qubit number
SWAP	$\mathrm{CNOT}_{ca}\mathrm{CNOT}_{ac}\mathrm{CNOT}_{ca}$	`SW`	Qubit number, control qubit number

Finally, two **three-qubit gates** are available: the Toffoli and Fredkin gates.

The **Toffoli (CCNOT) gate** is decomposed into the subsequent application of the following gates:



The Toffoli gate is called using the **command** `TF` with **three parameters**: number of the qubit acted on, number of the control qubit, and the number of the control-control qubit, in this order.

The **Fredkin (CSWAP) gate** is decomposed into the subsequent application of three Toffoli gates: CSWAP_{abc} = CNOT_{abc} CNOT_{bac} CNOT_{abc}, where a and b are the numbers of the qubits being swapped and c is the number of the control qubit. The Fredkin gate is called using the **command** `FR` with **three parameters**: the numbers of the two qubits acted on and the number of the control qubit, in this order.

Output

The output of a calculation contains the initial state of the N-qubit system, as well as its state after the application of each gate (for each iteration). The gate applied in each step is identified by its sequential number (as well as a one-letter internal code that corresponds to its type: I – identity; H – Hadamard; X, Y, Z – Pauli X, Y, Z; x, y, z – x, y, z rotations; t – T; d – $T^\dagger$; s – S; a - $S^\dagger$; 0, 1 – qubit projections onto $|0\rangle$ or $|1\rangle$ states; C – CNOT; c – CPHASE; S – SWAP; T – Toffoli; F – Fredkin; M – measurement).

The following data is provided:

- the *binary representation* of each N-qubit basis state (the single-qubit states, 0 or 1, for qubits 1 through N are listed from left to right);
- the *decimal encoding* of each N-qubit basis state (corresponding to the binary representation, read from right to left);
- the *real part* of the complex coefficient that represents the contribution of each N-qubit basis state to the state of the system;
- the *imaginary part* of the complex coefficient that represents the contribution of each N-qubit basis state to the state of the system;
- the *absolute value* of the complex coefficient that represents the contribution of each N-qubit basis state to the state of the system.

To save space, only the data for N-qubit basis states with a non-negligible contribution to the system state are printed out (the cutoff for the absolute value of the complex coefficient in order for the state to be printed out is set to 10^{-4}).

For single-qubit measurement operations, the probability of the measured qubit collapsing to state $|0\rangle$ and the random number sampled are also printed out. (If the random number is below the probability of the measured qubit collapsing to state $|0\rangle$, that qubit collapses to state $|0\rangle$, otherwise, it collapses to state $|1\rangle$.)

Example: Preparing and Measuring a Bell State

Input files:

Qubits.in	Gates.in
1.000 0.000 0.000 1.000 0.000 0.000	HAD 1 CX 2 1 M 1 M 2

Run (for 3 iterations)*:* `qgc Qubits.in Gates.in 3`

Output:

```
2 qubits.
Number of qubits is 2, number of states is 4.

Iteration 1.

Initial state:
00      0   1.000   0.000  1.000

Gate 1: H
State after gate 1:
00      0   0.707   0.000  0.500
01      2   0.707   0.000  0.500

Gate 2: C
State after gate 2:
00      0   0.707   0.000  0.500
11      3   0.707   0.000  0.500

Prob0 = 0.50000000, random = 0.69474253
Gate 3: M
State after gate 3:
11      3   1.000   0.000  1.000

Prob0 = 0.00000000, random = 0.53767001
Gate 4: M
State after gate 4:
11      3   1.000   0.000  1.000
```

```
Iteration 2.

...

Iteration 3.

Initial state:
00      0   1.000   0.000  1.000

Gate 1: H
State after gate 1:
00      0   0.707   0.000  0.500
01      2   0.707   0.000  0.500

Gate 2: C
State after gate 2:
00      0   0.707   0.000  0.500
11      3   0.707   0.000  0.500

Prob0 = 0.50000000, random = 0.00865508
Gate 3: M
State after gate 3:
00      0   1.000   0.000  1.000

Prob0 = 1.00000000, random = 0.46586880
Gate 4: M
State after gate 4:
00      0   1.000   0.000  1.000
```

Discussion

Each of the two qubits in the system is initially in state $|0\rangle$ (in the file `Qubits.in`, the amplitudes are 1.000 for state $|0\rangle$ and 0.000 for state $|1\rangle$ and the phase shift is 0.000 for both qubits). This corresponds to the 2-qubit system initially being in state $|0\rangle_1 \otimes |0\rangle_2$, where the subscripts indicate the qubit number, with a probability of 1. Thus, this is the only basis state that contributes to the state of the system. In the output, this state is denoted as 00 (decimal encoding 0); the real part of the complex coefficient for this basis state is 1.000, the imaginary part is 0.000, and the absolute value is 1.000.

When the Hadamard gate is applied to the first qubit, its state becomes

$$\frac{1}{\sqrt{2}}(|0\rangle_1 + |1\rangle_1),$$

and the state of the 2-qubit system, thus, becomes

$$\frac{1}{\sqrt{2}}(|0\rangle_1 + |1\rangle_1) \otimes |0\rangle_2 = \frac{1}{\sqrt{2}}\left(|0\rangle_1 \otimes |0\rangle_2 + |1\rangle_1 \otimes |0\rangle_2\right)$$

In the output, the two 2-qubit basis states that contribute to the system state are 00 (decimal encoding 0) and 01 (decimal encoding 2 – we are reading the binary number from right to left, that is, from qubits with higher numbers to qubits with lower numbers). For both states, the real part of the complex coefficient is 0.707 ($\frac{1}{\sqrt{2}}$), the imaginary part is 0.000, and the absolute value is 0.500.

When the CNOT gate controlled by the first qubit is applied to the second qubit, the second qubit either remains in its initial state $|0\rangle_2$ (if the first qubit is in state $|0\rangle_1$) or goes to state $|1\rangle_2$ (if the first qubit is in state $|1\rangle_1$). Therefore, the state of the 2-qubit system now becomes

$$\frac{1}{\sqrt{2}}\left(|0\rangle_1 \otimes |0\rangle_2 + |1\rangle_1 \otimes |1\rangle_2\right),$$

a maximally entangled state (Bell state). In the output, the two 2-qubit basis states that contribute to the system state are 00 (decimal encoding 0) and 11 (decimal encoding 3). For both states, the real part of the complex coefficient is 0.707 ($\frac{1}{\sqrt{2}}$), the imaginary part is 0.000, and the absolute value is 0.500.

The application of each preceding step corresponds to a unitary transformation and is the same for all iterations. In the following steps, the two qubits are measured. Before the measurements, the probabilities of the first qubit being in states $|0\rangle_1$ and $|1\rangle_1$ are the same, 0.5 (they correspond to the 2-qubit system states $|0\rangle_1 \otimes |0\rangle_2$ and $|1\rangle_1 \otimes |1\rangle_2$, respectively).

In the first iteration, a random value of 0.69474253 > 0.5 is generated, therefore, the first qubit is measured to be in state $|1\rangle_1$, meaning that the 2-qubit system after the measurement is in state $|1\rangle_1 \otimes |1\rangle_2$. In the output, the only basis state that contributes to the state of the 2-qubit system is denoted as 11 (decimal encoding 3); the real part of the complex coefficient for this basis state is 1.000, the imaginary part is 0.000, and the absolute value is 1.000. Now, when the second qubit is measured, the probability of it being in state $|0\rangle_2$ is 0, because the system is already known to be in state $|1\rangle_1 \otimes |1\rangle_2$. Therefore, *regardless of the random number that is generated* (in the first iteration that number is 0.53767001), the second qubit will be measured to be in state $|1\rangle_2$. The state of the system does not change as a result of this measurement. In the output, the only basis state that contributes to the final state of the 2-qubit system is denoted as 11 (decimal encoding 3); the real part of the complex coefficient for this basis state is 1.000, the imaginary part is 0.000, and the absolute value is 1.000.

In the third iteration, a random value of $0.00865508 < 0.5$ is generated when the first qubit is measured. Therefore, the first qubit is measured to be in state $|0\rangle_1$, meaning that the 2-qubit system after the measurement is in state $|0\rangle_1 \otimes |0\rangle_2$. In the output, the only basis state that contributes to the state of the 2-qubit system is denoted as 00 (decimal encoding 0); the real part of the complex coefficient for this basis state is 1.000, the imaginary part is 0.000, and the absolute value is 1.000. Now, when the second qubit is measured, the probability of it being in state $|0\rangle_2$ is 1, because the system is already known to be in state $|0\rangle_1 \otimes |0\rangle_2$. Therefore, *regardless of the random number that is generated* (in the third iteration that number is 0.46586880), the second qubit will be measured to be in state $|0\rangle_2$. The state of the system does not change as a result of this measurement. In the output, the only basis state that contributes to the final state of the 2-qubit system is denoted as 00 (decimal encoding 0); the real part of the complex coefficient for this basis state is 1.000, the imaginary part is 0.000, and the absolute value is 1.000.