Quantum++ for the impatient

Author: Vlad Gheorghiu vgheorgh@gmail.com

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1 Introduction

Quantum++ is a C++11 general purpose quantum computing simulator, composed solely of of header files, and uses the Eigen linear algebra library. The simulator defines a large collection of (template) quantum computing related functions and few useful classes. The main data types are complex vectors and complex matrices, as I will describe below. Most functions operate on such vectors/matrices, and always return the result by value. Collection of objects are implemented via the standard library container std::vector<>, specialized accordingly. Ease of use and performance were among the most important design factors.

2 Installation

To get started with Quantum++, first download the Eigen library from http://eigen.tuxfamily.org and unzip it into the home folder¹, as \$HOME/eigen. You can change the name of the folder, but in the current document I will use \$HOME/eigen as the location of Eigen library. Next, download the Quantum++ library from http://vsoftco.github.io/qpp/ and unzip it into the home folder as \$HOME/qpp. Finally, make sure that your compiler supports C++11 and preferably OpenMP. I recommend g++, version 4.8 or later. You are now ready to go!

We now build a simple minimal example to test that the installation was successful. Create a folder called \$HOME/example, and inside it create the file example.cpp, with the content listed in the Listing 1. Next compile the file using a C++11 compliant compiler such as g++ version 4.8 or later. From inside the

```
#include "qpp.h"

int main()
{
    std::cout << "Hello Quantum++" << std::endl;
}</pre>
```

Listing 1: Minimal example

folder \$HOME/example, type

```
g++ -std=c++11 -isystem $HOME/eigen -I $HOME/qpp/include example.cpp -o example
```

Your compile command may differ from the above, depending on the name of your C++ compiler and operating system. If everything went fine, then the above command builds the executable example in the current folder. To run it, type ./example from inside the \$HOME/example folder. The output should look like

```
>>> Starting Quantum++...
>>> Thu Nov 20 12:00:26 2014

Hello Quantum++
>>> Exiting Quantum++...
>>> Thu Nov 20 12:00:26 2014
```

Congratulations, everything seems to work fine!

3 Basic usage

All functions, classes and global objects defined by the library lie inside the namespace qpp. To avoid additional typing, I will omit the prefix qpp:: in the rest of this document. I recommend the using directive

```
using namespace qpp; in your main .cpp file.
```

¹I implicitly assume from now on that you use a UNIX-based system, although everything should translate into Windows as well, with slight modifications

3.1 Data types

The most important data types are defined via typedefs in types.h² (inside the include folder of the Quantum++ source distribution). We list them below.

- cplx Complex number, alias for std::complex<double>
- idx Index (non-negative integer), alias for std::size_t
- cmat Complex dynamic matrices, alias for Eigen::MatrixXcd
- dmat Double dynamic matrices, alias for Eigen::MatrixXd
- ket Complex dynamic column vector, alias for Eigen::VectorXcd
- bra Complex dynamic row vector, alias for Eigen::RowVectorXcd
- dyn_mat<Scalar> Dynamic matrix template alias over the field Scalar, alias for Eigen::Matrix<Scalar, Eigen::Dynamic, Eigen::Dynamic>
- dyn_col_vect<Scalar> Dynamic column vector template alias over the field Scalar, alias for Eigen::Matrix<Scalar, Eigen::Dynamic, 1>
- dyn_row_vect<Scalar> Dynamic row vector template alias over the field Scalar, alias for Eigen::Matrix<Scalar, 1, Eigen::Dynamic>

3.2 Constants

The important constants are defined in the file constants.h as follows.

- constexpr double pi = 3.1415...; $-\pi$
- constexpr double ee = 2.7182...; e, base of natural logarithms
- constexpr idx infty = -1; Infinity
- constexpr idx maxn = 64; Maximum number of allowed qu(d)its (subsystems)
- constexpr double eps = 1e-12; Used in comparing floating point values to zero
- constexpr double chop = 1e-10; Used in display manipulators to set to zero numbers which are in absolute values smaller than chop
- constexpr cplx operator""_i(unsigned long long int x) - User-defined literal for the imaginary number $i := \sqrt{-1}$
- constexpr cplx operator""_i(unsigned long double int x) User-defined literal for the imaginary number $i := \sqrt{-1}$
- cplx omega(idx D) D-th root of unity

²All necessary Quantum++ header files, together with other important system headers, such as <iostream>, <cmath> etc., are automatically included in qpp.h, hence most of the time you should only include qpp.h in the main .cpp file.

3.3 Global singleton classes

Some useful classes are defined as singletons, are globally available, and are initialized at runtime in the file qpp.h, before the starting of int main(), as follows.

- const Init& init = Init::get_instance(); Library initialization (displayed messages etc.)
 const Codes& codes = Codes::get_instance(); Quantum error correcting codes
 const Gates& gt = Gates::get_instance(); Quantum gates
- const States& st = States::get_instance(); Quantum states
- RandomDevices& rdevs = RandomDevices::get_instance() Random number generator engines

3.4 Simple examples

3.4.1 Gates and states

We are now ready for a more sophisticated example that actually does something useful. Consider the code in Listing 2.

```
#include "qpp.h"
   using namespace qpp;
   int main()
   {
5
       ket psi = mket({1,0});
        cmat U = gt.CNOTab;
       ket result = U * psi;
        std::cout << "The result of applying the Controlled-NOT gate CNOTab on |10> is:\n";
10
        std::cout << disp(result) << std::endl;</pre>
11
12
       ket phi = st.z0;
13
        U = gt.X;
14
       result = U * phi;
15
16
        std::cout << "The result of applying the bit-flip gate X on |0> is:\n";
17
        std::cout << disp(result) << std::endl;</pre>
18
```

Listing 2: Gates and states

The result of applying the bit-flip gate X on |0> is:

```
0
1.0000
>>> Exiting Quantum++...
>>> Thu Nov 20 13:30:09 2014
```

In line 2, we bring the namespace qpp into the global namespace. In line 6 we declare a state vector, and assign to it the value $|10\rangle$ via the function mket(). We could have also used an Eigen-like equivalent syntax leat $|10\rangle$ via the dimension before insertion of elements via (6).

```
ket psi(2); // must specify the dimension before insertion of elements via <<
psi << 0, 0, 1, 0;</pre>
```

however the mket() function is more convenient. In line 7 we declare a gate U as the Controlled-NOT with control as the first subsystem, and target as the last, using the global singleton gt. In line 8 we declare the ket result as the result of applying the Controlled-NOT gate to the state $|10\rangle$, i.e. $|11\rangle$.

We then display the result of the computation in lines 10 and 11. In line 11 we use the format manipulator $\mathtt{disp}()$, which is especially useful when displaying complex matrices, as it displays the entries of the latter in the form a+bi, in contrast to the form (a,b) used by the C++ standard library. The manipulator also accepts additional parameters that allows e.g. setting to zero numbers smaller than some given value (useful to chop small values), and it is in addition overloaded for standard containers, iterators and C-style arrays.

Next, in line 13 we use the singleton st to declare phi as the zero eigenvector $|0\rangle$ of the Z Pauli operator. In line 14 we assign to the gate U the bit flip gate gt.X, compute the result of the operation $X|0\rangle$ in line 15, and finally display the result $|1\rangle$ in lines 17 and 18.

3.4.2 Measurements

Let us now complicate things a bit and introduce measurements. Consider the example in Listing 3. A possible output of this program is

```
>>> Starting Quantum++...
>>> Thu Nov 20 15:39:17 2014
We produced the Bell state:
0.7071
     0
     0
0.7071
We produced the Bell state:
0.7071
0.7071
Measurement result: 1
Probabilities: [0.5000, 0.5000]
Resulting states:
0.5000
         0.5000
0.5000
         0.5000
0.5000
          -0.5000
-0.5000
           0.5000
>>> Exiting Quantum++...
>>> Thu Nov 20 15:39:17 2014
```

```
#include "qpp.h"
   using namespace qpp;
2
   int main()
5
        ket psi = mket({0,0});
6
        cmat U = gt.CNOTab * kron(gt.H, gt.Id2);
        ket result = U * psi; // we have the Bell state (|00>+|11>)/sqrt(2)
        std::cout << "We just produced the Bell state:\n";</pre>
10
        std::cout << disp(result) << std::endl;</pre>
11
12
        // apply a bit flip on the second qubit
13
        result = apply(result, gt.X, \{1\}); // we produced (|01\rangle+|10\rangle)/sqrt(2)
14
        std::cout << "We produced the Bell state:\n";</pre>
15
        std::cout << disp(result) << std::endl;</pre>
17
        // measure the first qubit in the X basis
18
        auto m = measure(result, gt.H, {0});
19
        std::cout << "Measurement result: " << std::get<0>(m);
20
        std::cout << std::endl << "Probabilities: ";</pre>
21
        std::cout << disp(std::get<1>(m),", ") << std::endl;
22
        std::cout << "Resulting states: " << std::endl;</pre>
23
        for(auto&& elem: std::get<2>(m))
24
                 std::cout << disp(elem) << std::endl << std::endl;</pre>
25
   }
26
```

Listing 3: Measurements

In line 7, we use the function kron() to create the tensor product (Kronecker product) of the Hadamard gate on the first qubit and identity on the second qubit. In line 8 we compute the result of the operation $CNOT_{ab}(H \otimes I)|00\rangle$, which is the Bell state $(|00\rangle + |11\rangle)/\sqrt{2}$. We display it in lines 10 and 11.

In line 14 we use the function apply() to apply the gate X on the second qubit³ of the previously produced Bell state. The function apply() takes as its third parameter a list of subsystems, and in our case {1} denotes the *second* subsystem, not the first. The function apply(), as well as many other functions that we will encounter, have a variety of useful overloads, see doc/refman.pdf for a detailed library reference. In lines 15 and 16 we display the newly created Bell state.

In line 19 we use the function measure() to perform a measurement of the first qubit (subsystem {0}) in the X basis. You may be confused by the apparition of gt.H, however this overload of the function measure() takes as its second parameter the measurement basis, specified as the columns of a complex matrix. In our case, the eigenvectors of the X operator are just the columns of the Hadamard matrix. As mentioned before, as all other library functions, measure() returns by value, hence it does not modify its argument. The return of measure is a tuple consisting of the measurement result, the outcome probabilities, and the possible output states. Technically measure() returns a

```
std::tuple<std::size_t, std::vector<double>, std::vector<cmat>>
```

Instead of using this long type definition, we use the new C++11 auto keyword to define the type of the result m of measure(). In lines 20-25 we use the standard std::get<> function to retrieve each element of the tuple, then display the measurement result, the probabilities and the resulting output states.

³Quantum++ uses the C/C++ numbering convention, with indexes starting from zero.

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