# Quantum++ for the impatient

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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 directory<sup>1</sup>, as \$HOME/eigen. You can change the name of the directory, 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 directory 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 next build a simple minimal example to test that the installation was successful. Create a directory called \$HOME/qpp\_examples, and inside it create the file minimal.cpp, with the content listed in the listing below. A verbatim copy of the above program is also available at \$HOME/qpp/examples/minimal.cpp.

```
// Minimal example
// Source: ./examples/minimal.cpp
#include <qpp.h>

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

Next compile the file using a C++11 compliant compiler such as g++ version 4.8 or later. From inside the directory \$HOME/qpp\_examples, type

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

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 minimal in the directory \$HOME/qpp\_examples. To run it, type ./minimal from inside the directory \$HOME/qpp\_examples. The output should look like

```
>>> Starting Quantum++...
>>> Thu Dec 4 17:10:25 2014

Hello Quantum++!

>>> Exiting Quantum++...
>>> Thu Dec 4 17:10:25 2014
```

In line 3 of the program we include the main header file of the library, qpp.h. This file includes all other necessary Quantum++ header files, as well as the following C++ standard library files

```
<algorithm>
<chrono>
<cmath>
<complex>
<cstdlib>
<cstring>
<ctime>
<exception>
```

 $<sup>^{1}</sup>$ I implicitly assume from now on that you use a UNIX-based system, although everything should translate into Windows as well, with slight modifications

```
<fstream>
<functional>
<initializer_list>
<iomanip>
<iostream>
<iterator>
<limits>
<numeric>
<ostream>
<random>
<sstream>
<stdexcept>
<string>
<tuple>
<type_traits>
<utility>
<vector>
and Eigen header files
<Eigen/Dense>
<Eigen/SVD>
```

Most of the time, you should be fine including only the header qpp.h in your main project, except when you want to use the MATLAB input/output interface support, in which case you have to explicitly include the header file MATLAB/matlab.h.

## 3 Data types, constants and global objects

All header files of Quantum++ are located inside the include directory. All functions, classes and global objects defined by the library belong to the namespace qpp. To avoid additional typing, I will omit the prefix qpp:: in the rest of this document. I recommend to use

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

#### 3.1 Data types

The most important data types are defined via typedefs in the header file types.h. We list them in Table 1.

#### 3.2 Constants

The important constants are defined in the header file constants.h and are listed in Table 2.

#### 3.3 Global singleton classes and instances

Some useful classes are defined as singletons, are globally available, and are initialized at runtime in the header file qpp.h, before the starting of main(), as listed in Table 3.

cplx	Complex number, alias for std::complex <double></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></scalar>	Dynamic matrix template alias over the field Scalar, alias for		
	Eigen::Matrix <scalar, eigen::dynamic="" eigen::dynamic,=""></scalar,>		
dyn_col_vect <scalar></scalar>	Dynamic column vector template alias over the field Scalar, alias for		
	Eigen::Matrix <scalar, 1="" eigen::dynamic,=""></scalar,>		
dyn_row_vect <scalar></scalar>	Dynamic row vector template alias over the field Scalar, alias for		
	Eigen::Matrix <scalar, 1,="" eigen::dynamic=""></scalar,>		

Table 1: User-defined data types

<pre>constexpr double pi = 3.1415;</pre>	$\pi$
constexpr double ee = 2.7182;	e, base of natural logarithms
constexpr idx infty = -1;	Infinity
<pre>constexpr idx maxn = 64;</pre>	Maximum number of allowed qu(d)its (subsystems)
constexpr double eps = 1e-12;	Used in comparing floating point values to zero
<pre>constexpr double chop = 1e-10;</pre>	Used in display manipulators to set numbers to zero
constexpr cplx operator""_i	User-defined literal for the imaginary number $i := \sqrt{-1}$
(unsigned long long int x)	
constexpr cplx operator""_i	User-defined literal for the imaginary number $i := \sqrt{-1}$
(unsigned long double int x)	
cplx omega(idx D)	D-th root of unity $e^{2\pi i/D}$

Table 2: User-defined constants

<pre>const Init&amp; init = Init::get_instance();</pre>	Library initialization
<pre>const Codes&amp; codes = Codes::get_instance();</pre>	Quantum error correcting codes
<pre>const Gates&amp; gt = Gates::get_instance();</pre>	Quantum gates
<pre>const States&amp; st = States::get_instance();</pre>	Quantum states
RandomDevices& rdevs =	Random number generator engines
<pre>RandomDevices::get_instance()</pre>	

Table 3: Global singleton classes and instances

## 4 Simple examples

All examples of this section are copied verbatim from the directory ./examples and compiled successfully. For convenience, the location of the source file is also displayed in the first line of each example, as a C++ comment.

The examples are simple and demonstrate the main feature of Quantum++. They cover only a small part of library functions, but enough to get the interested user started. For extensive about all library functions, including various overloads, the user should consult the complete reference located at ./doc/refman.pdf. A more comprehensive (but also more complicated) example, that consists of a collection of quantum information processing routines, is located at ./examples/example.cpp.

#### 4.1 Gates and states

We introduce the main objects used by Quantum++: gates, states and basic operations. Consider the code in the listing below

```
// Gates and states
   // Source: ./examples/gates_states.cpp
   #include <qpp.h>
   using namespace qpp;
   int main()
   {
       ket psi = st.z0; // |0> state
        cmat U = gt.X;
9
       ket result = U * psi;
        std::cout << "The result of applying the bit-flip gate X on |0> is:\n";
12
        std::cout << disp(result) << std::endl;</pre>
13
       psi = mket({1, 0}); // |10> state
15
       U = gt.CNOT; // Controlled-NOT
       result = U * psi;
17
       std::cout << "The result of applying the gate CNOT on |10> is:\n";
19
       std::cout << disp(result) << std::endl;</pre>
20
21
       U = randU(2);
22
        std::cout << "Generating a random one-qubit gate U:\n";</pre>
        std::cout << disp(U) << std::endl;</pre>
24
       result = applyCTRL(psi, U, {0}, {1});
26
       std::cout << "The result of applying the Controlled-U gate on |10> is:\n";
        std::cout << disp(result) << std::endl;</pre>
28
   }
29
   which may output
   >>> Starting Quantum++...
   >>> Thu Dec 4 17:10:25 2014
   The result of applying the bit-flip gate X on |0> is:
   1.0000
6
   The result of applying the gate CNOT on |10> is:
         0
         0
         0
10
   1.0000
11
   Generating a random one-qubit gate U:
   -0.6904 + 0.1545i -0.2261 + 0.6696i
   -0.3688 - 0.6029i
                        0.7074 - 0.0023i
   The result of applying the Controlled-U gate on |10> is:
```

```
16 0

17 0

18 -0.6904 + 0.1545i

19 -0.3688 - 0.6029i

20 21 >>> Exiting Quantum++...

22 >>> Thu Dec 4 17:10:25 2014
```

In line 4, we bring the namespace qpp into the global namespace.

In line 8 we use the States singleton st to declare psi as the zero eigenvector  $|0\rangle$  of the Z Pauli operator. In line 9 we use the Gates singleton gt and assign to U the bit flip gate gt.X. In line 10 we compute the result of the operation  $X|0\rangle$ , and display the result  $|1\rangle$  in lines 12 and 13. In line 13 we use the format manipulator 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.

In line 15 we reassign to psi the state  $|10\rangle$  via the function mket(). We could have also used the Eigen insertion operator

```
ket psi(4); // must specify the dimension before insertion of elements via << psi << 0, 0, 1, 0;
```

however the mket() function is more concise. In line 16 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 17 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 19 and 20.

Next, in line 22 we generate a random unitary gate via the function randU(), then in line 26 apply the Controlled-U, with control as the first qubit and target as the second qubit, to the state psi. Finally, we display the result in lines 27 and 28.

#### 4.2 Measurements

Let us now complicate things a bit and introduce measurements. Consider the example in the listing below

```
// Measurements
   // Source: ./examples/measurements.cpp
   #include <qpp.h>
   using namespace qpp;
5
   int main()
   {
       ket psi = mket({0, 0});
        cmat U = gt.CNOT * kron(gt.H, gt.Id2);
q
       ket result = U * psi; // we have the Bell state (|00>+|11>)/sqrt(2)
10
        std::cout << "We just produced the Bell state:\n";
12
        std::cout << disp(result) << std::endl;</pre>
13
14
        // apply a bit flip on the second qubit
        result = apply(result, gt.X, {1}); // we produced (|01>+|10>)/sqrt(2)
16
        std::cout << "We produced the Bell state:\n";</pre>
        std::cout << disp(result) << std::endl;</pre>
18
```

```
19
        // measure the first qubit in the X basis
20
        auto m = measure(result, gt.H, {0});
21
        std::cout << "Measurement result: " << std::get<0>(m);
        std::cout << std::endl << "Probabilities: ";</pre>
23
        std::cout << disp(std::get<1>(m), ", ") << std::endl;
        std::cout << "Resulting states: " << std::endl;</pre>
        for (auto && elem : std::get<2>(m))
            std::cout << disp(elem) << std::endl << std::endl;</pre>
27
   }
28
   which outputs
   >>> Starting Quantum++...
   >>> Thu Dec 4 17:10:25 2014
   We just produced the Bell state:
   0.7071
5
         0
         0
   0.7071
   We produced the Bell state:
10
   0.7071
   0.7071
12
13
   Measurement result: 1
14
   Probabilities: [0.5000, 0.5000]
   Resulting states:
16
   0.5000
             0.5000
   0.5000
             0.5000
18
    0.5000
              -0.5000
20
   -0.5000
               0.5000
22
23
   >>> Exiting Quantum++...
24
   >>> Thu Dec 4 17:10:25 2014
25
```

In line 9, 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, then we left-multiply it by the Controlled-NOT gate. In line 10 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 12 and 13.

In line 16 we use the function apply() to apply the gate X on the second qubit<sup>2</sup> 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 17 and 18 we display the newly created Bell state.

In line 21 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

<sup>&</sup>lt;sup>2</sup>Quantum++ uses the C/C++ numbering convention, with indexes starting from zero.

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 22-27 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.

#### 4.3 Quantum operations

In the listing below we introduce quantum operations: quantum channels, as well as the partial trace and partial transpose operations.

```
// Quantum operations
   // Source: ./examples/quantum_operations.cpp
   #include <qpp.h>
   using namespace qpp;
   int main()
6
   {
7
        cmat rho = st.pb00; // projector onto the Bell state (|00>+|11>)/sqrt(2)
        std::cout << "Initial state:\n";</pre>
9
        std::cout << disp(rho) << std::endl;</pre>
10
        // partial transpose of first subsystem
12
        cmat rhoTA = ptranspose(rho, {0});
13
        std::cout << "Eigenvalues of the partial transpose of Bell-0 state are:\n";
14
        std::cout << disp(transpose(hevals(rhoTA))) << std::endl;</pre>
15
16
        std::cout << "Measurement channel with 2 Kraus operators:\n";</pre>
17
        std::vector<cmat> Ks {st.pz0, st.pz1}; // 2 Kraus operators
        std::cout << disp(Ks[0]) << "\n
                                              and \n" << disp(Ks[1]) << std::endl;</pre>
19
20
        std::cout << "Superoperator matrix of the channel:\n";</pre>
21
        std::cout << disp(super(Ks)) << std::endl;</pre>
22
        std::cout << "Choi matrix of the channel:\n";</pre>
24
        std::cout << disp(choi(Ks)) << std::endl;</pre>
26
        // apply the channel onto the first subsystem
        cmat rhoOut = apply(rho, Ks, {0});
28
        std::cout << "After applying the measurement channel on the first qubit:\n";</pre>
        std::cout << disp(rhoOut) << std::endl;</pre>
30
        // take the partial trace over the second subsystem
32
        cmat rhoA = ptrace(rhoOut, {1});
33
        std::cout << "After partially tracing down the second subsystem:\n";
        std::cout << disp(rhoA) << std::endl;</pre>
36
```

```
// compute the von-Neumann entropy
37
        double ent = entropy(rhoA);
38
        std::cout << "Entropy: " << ent << std::endl;</pre>
39
   }
   The output of this program is
   >>> Starting Quantum++...
   >>> Thu Dec 4 17:10:25 2014
   Initial state:
   0.5000
             0
                  0
                      0.5000
             0
                  0
                            0
         0
         0
             0
                  0
                            0
   0.5000
             0
                  0
                      0.5000
   Eigenvalues of the partial transpose of Bell-O state are:
   -0.5000
              0.5000
                        0.5000
                                   0.5000
   Measurement channel with 2 Kraus operators:
11
   1.0000
             0
         0
13
        and
   0
15
        1.0000
16
   Superoperator matrix of the channel:
17
   1.0000
             0
                  0
                            0
18
         0
             0
                  0
                            0
19
         0
             0
                  0
                            0
20
         0
             0
                  0
                      1.0000
21
   Choi matrix of the channel:
22
   1.0000
             0
                  0
23
              0
                  0
                            0
24
         0
             0
                  0
                            0
             0
                  0
                      1.0000
26
   After applying the measurement channel on the first qubit:
   0.5000
                            0
28
                            0
         0
             0
                  0
         0
             0
                  0
                            0
30
             0
                  0
                      0.5000
   After partially tracing down the second subsystem:
32
   0.5000
33
             0.5000
         0
34
   Entropy: 1.0000
35
   >>> Exiting Quantum++...
37
   >>> Thu Dec
                  4 17:10:25 2014
```

The example should by now be self-explanatory.

In line 8 we define the input state **rho** as the projector onto the Bell state  $(|00\rangle + |11\rangle)/\sqrt{2}$ , then display it in lines 9 and 10.

In lines 13–15 we partially transpose the first qubit, then display the eigenvalues of the resulting matrix rhoTA.

In lines 17–19 we define a quantum channel Ks consisting of two Kraus operators:  $|0\rangle\langle 0|$  and  $|1\rangle\langle 1|$ , then display the latter. Note that Quantum++ uses the std::vector<cmat> container to store the Kraus operators and define a quantum channel.

In lines 21–25 we display the superoperator matrix as well as the Choi matrix of the channel Ks.

Next, in lines 28-30 we apply the channel Ks to the first qubit of the input state rho, then display the output state rhoOut.

In lines 33–35 we take the partial trace of the output state rhoOut, then display the resulting state rhoA. Finally, in lines 38 and 39 we compute the von-Neumann entropy of the resulting state and display it.

#### 4.4 Timing

To facilitate simple timing tasks, Quantum++ provides a Timer class that uses internally a std::steady\_clock. The following program demonstrate its usage.

```
// Timing
   // Source: ./examples/timing.cpp
   #include <qpp.h>
   using namespace qpp;
   int main()
   {
       std::cout << std::setprecision(8); // increase the default output precision
       // get the first codeword from Shor's [[9,1,3]] code
10
       ket c0 = codes.codeword(Codes::Type::NINE_QUBIT_SHOR, 0);
12
       Timer t; // declare and start a timer
       std::vector<idx> perm = randperm(9); // declare a random permutation
14
       ket cOperm = syspermute(cO, perm); // permute the system
       t.toc(); // stops the timer
16
       std::cout << "Permuting subsystems according to " << disp(perm, ", ");</pre>
       std::cout << "\nIt took " << t << " seconds to permute the subsytems.\n";
18
19
       t.tic(); // restart the timer
20
       std::cout << "Inverse permutation: ";</pre>
21
       std::cout << disp(invperm(perm), ", ") << std::endl;</pre>
22
       ket c0invperm = syspermute(c0perm, invperm(perm)); // permute again
23
       std::cout << "It took " << t.toc();
       std::cout << " seconds to un-permute the subsystems.\n";</pre>
25
        std::cout << "Norm difference: " << norm(cOinvperm - cO) << std::endl;
27
   }
   A possible output of this program is
   >>> Starting Quantum++...
   >>> Thu Dec 4 17:10:25 2014
   Permuting subsystems according to [6, 8, 2, 4, 0, 3, 5, 1, 7]
   It took 0.00010900 seconds to permute the subsytems.
   Inverse permutation: [4, 7, 2, 5, 3, 6, 0, 8, 1]
   It took 0.00009500 seconds to un-permute the subsystems.
```

```
8 Norm difference: 0.00000000
9
10 >>> Exiting Quantum++...
11 >>> Thu Dec 4 17:10:25 2014
```

In line 8, we change the default output precision from 4 to 8 decimals after the delimiter.

In line 11, we use the Codes singleton codes to retrieve in c0 the first codeword of the Shor's [[9,1,3]] quantum error correcting code.

In line 13 we declare an instance timer of the class Timer. In line 14 we declare a random permutation perm via the function randperm(). In line 15 we permute the codeword according to the permutation perm using the function syspermute() and store the result. In line 16 we stop the timer. In line 17 we display the permutation, using an overloaded form of the disp() manipulator for C++ standard library containers. The latter takes a std::string as its second parameter to specify the delimiter between the elements of the container. In line 18 we display the elapsed time using the ostream operator<<() operator overload for Timer objects.

Next, in line 20 we reset the timer, then display the inverse permutation of perm in lines 21 and 22. In line 23 we permute the already permuted state coperm according to the inverse permutation of perm, and store the result in coinvperm. In lines 24 and 25 we display the elapsed time. Note that in line 24 we used directly t.toc() in the stream insertion operator, since, for convenience, the member function Timer::toc() returns a const Timer&.

Finally, in line 27, we verify that by permuting and permuting again using the inverse permutation we recover the initial codeword, i.e. the norm difference has to be zero.

#### 4.5 Input/output

We now introduce the input/output functions of Quantum++, as well as the input/output interfacing with MATLAB. The program below saves a matrix in both Quantum++ internal format as well as in MATLAB format, then loads it back and tests that the norm difference between the saved/loaded matrix is zero.

```
// Input/output
   // Source: ./examples/input_output.cpp
   #include <qpp.h>
   #include <MATLAB/matlab.h> // must be explicitly included
   using namespace qpp;
   int main()
8
       // Quantum++ native input/output
9
       cmat rho = randrho(256); // an 8 qubit density operator
10
       save(rho, "rho.dat"); // save it
        cmat loaded_rho = load<cmat>("rho.dat"); // load it back
12
       // display the difference in norm, should be 0
       std::cout << "Norm difference load/save: ";</pre>
14
       std::cout << norm(loaded_rho - rho) << std::endl;</pre>
16
       // interfacing with MATLAB
       saveMATLABmatrix(rho, "rho.mat", "rho", "w");
18
       loaded_rho = loadMATLABmatrix<cmat>("rho.mat", "rho");
19
       // display the difference in norm, should be 0
20
       std::cout << "Norm difference MATLAB load/save: ";</pre>
       std::cout << norm(loaded_rho - rho) << std::endl;</pre>
22
   }
23
```

```
1  >>> Starting Quantum++...
2  >>> Thu Dec   4 17:10:25 2014
3
4   Norm difference load/save: 0.0000
5   Norm difference MATLAB load/save: 0.0000
6
7  >>> Exiting Quantum++...
8  >>> Thu Dec   4 17:10:25 2014
```

Note that in order to use the MATLAB input/output interface support, you need to explicitly include the header file MATLAB/matlab.h, and you also need to have MATLAB or MATLAB compiler installed, otherwise the program fails to compile. See the file README.md from the root directory of Quantum++ for more details about how to compile with MATLAB support.

## 5 Brief description of Quantum++ file structure

A brief description of the Quantum++ file structure is presented below. The directories and their brief descriptions are emphasized using **bold fonts**. The main header file **qpp.h** is emphasized in **red fonts**.

```
doc/ ...... Documentation
html/ ...... HTML documentation
_ex*.cpp ......Example source files
_{
m include}/ ....... Header files
MATLAB/ ...... MATLAB support
 _matlab.h ...... Input/output interfacing with MATLAB
_exception.h ..... Exceptions
 experimental/ ..... Experimental/test functions/classes, do not use or modify
__test.h ..... Experimental/test functions/classes
internal / ...... Internal implementation details, do not use/modify
 classes/ ...... Internal class definitions
  entanglement.h . . . . . . . . . . . . Entanglement functions
entropies.h ..... Entropy functions
```

## 6 Advanced topics

The output of this program is

#### 6.1 Exceptions

Exceptions...

```
// Exceptions
   // Source: ./examples/exceptions.cpp
   #include <qpp.h>
   using namespace qpp;
   int main()
        cmat rho = randrho(16); // 4 qubits (subsystems)
       try
        {
10
            double mInfo = qmutualinfo(rho, {0}, {4}); // throws qpp::Exception
            std::cout << "Mutual information between first and last subsystem: ";</pre>
12
            std::cout << mInfo << std::endl;</pre>
        }
14
        catch (const std::exception& e)
16
            std::cout << "Exception caught: " << e.what() << std::endl;</pre>
        }
18
   }
```

```
>>> Starting Quantum++...

>>> Thu Dec 4 17:10:25 2014

Exception caught: IN qpp::qmutualinfo(): Subsystems mismatch dimensions!

>>> Exiting Quantum++...

>>> Thu Dec 4 17:10:25 2014
```

- 6.2 Aliasing
- 6.3 Optimizations
- 6.4 Extending Quantum++