The University of Edinburgh
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# Quantum Computing Project: Report

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Edinburgh, 24th of March 2015

# Contents

# 1 Introduction

This report is an accumulation of knowledge and results from the course 'Quantum Computing Project' at the University of Edinburgh and is meant to be comprehensible to 3rd year undergraduate students of physical science (especially informatics and physics).

The report will begin by describing the aims of the project and providing a background for the topic of Quantum Computing. That is followed by a chapter about the theory needed for the underlying mathematics of the program which is purposely not intended to be exhaustive (see references for further information).

After that we will describe the implementation of the project including how we organised the programming, which development environment we used, how we structured the program, etc.

We finish with a chapter about the results followed by a discussion of these results and what we would do differently if we were to recreate the programme.

## 1.1 Aims

The aims of the project:

- **Comprehend quantum computing**
  One goal is to get familiar with quantum computing as a generalisation of conventional computing.
- **Programming**
  The main goal is to simulate a quantum computer on a conventional classical computer. This includes programming basic concepts like qubits, quantum registers and quantum gates. Finally it should be possible to run quantum algorithms like Grover's algorithm (optional: Shor's algorithm).
- **Presenting results**
  This includes not only this report and a verbal presentation but also proper documentation of the programming code to make it comprehensive to other programmers.
- **Teamwork and organisation**
  A project like this needs organisation and division of tasks but also successful communication between all group members. It is a further goal to encourage teamwork and organisation skills.

## 1.2 Background

The history of computers reaches back to the middle of the 19th century when a design for an Analytical Engine was proposed by Charles Babbage, one of the early pioneers of computation. However, for almost 100 years this branch stayed as an interesting but rather conceptional one until the invention of the transistor in 1925. The transistor was the core of classical computers as it provided a physical mechanism for reliably storing a bit of information that could be easily adjusted between two possible states. The first working computers were built in the 1940s and up to today computers work principally the same way.

Quantum computation on the other hand is a quite recent research field which emerged from the physics of quantum mechanics (1920s). In 1982 Richard Feynman theorised that there seemed to be essential difficulties in simulating quantum mechanical system on classical computers and suggested that a quantum computer would solve these issues.[5] At its core a quantum computer would not be limited to two states for each unit during computation but could theoretically be in any superposition of the units in it's circuit (see quantum register).

The increased flexibility of a quantum computation led to remarkable theoretical breakthroughs in the 1990s, when Peter **Shor** demonstrated that essential problems – like factorising integers –

could be solved far more efficiently on quantum computers than on conventional, classical computers. Besides Shor's algorithm Lov **Grover** proposed another algorithm in 1995 (only one year later) showing that the problem of conducting a search through some unstructured search space is as well more efficient on quantum computers.

The practical challenges for building a quantum computer are high and therefore the realisation of real quantum computers is still in it's infancy. However, in 2001 the first real quantum computer was able to factorise 15 into its prime numbers (3 and 5) by using a 7-qubit system.[7] Since then experimental progress is booming but the state-of-the-art is still a fair way off from practical (and even less daily-life) usage.

# 2 Theory

In this chapter we introduce the basic concepts of quantum computation, starting off with definitions of **qubits**, **quantum registers** and the presentation of several **quantum gates**. Afterwards we will talk about two **quantum algorithms** that we implemented in our virtual quantum computer. The last chapter will briefly talk about the challenges of **building a real quantum computer**.

## 2.1 Qubits

### 2.1.1 Generalised bits

A qubit (from *qu*antum *bit*) is the smallest unit in a quantum computer and therefore the quantum mechanical **generalisation of a classical bit**, as it is used in computers nowadays. A classical bit has one and only one of the two possible states

$$|0\rangle \quad \text{or} \quad |1\rangle \tag{1}$$

at the same time, whereas a qubit is able to be in a state $|\Psi\rangle$ which is a superposition of these two classical states:

$$|\Psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle\,, \quad \text{where } |\alpha|^2 + |\beta|^2 = 1 \tag{2}$$

One can depict the states via matrices with basis $(|0\rangle\,, |1\rangle)$:

$$|0\rangle = \begin{pmatrix}1\\0\end{pmatrix}, \qquad |1\rangle = \begin{pmatrix}0\\1\end{pmatrix}, \qquad |\Psi\rangle = \begin{pmatrix}\alpha\\\beta\end{pmatrix} \tag{3}$$

### 2.1.2 Measurement

The superposition of states leads to a new understanding of measurement. There are two things to consider:

1. **Probabilities** $P$
   Given a classical state ($|\Psi\rangle$ either $|0\rangle$ or $|1\rangle$) the result of a measurement is certain (and trivial). That's no longer true for the quantum state: Given the state $|\Psi\rangle$ in Eq. 2, it is solely possible to calculate the **probabilities** $P_\Psi$ of the outcome:

$$P_\Psi(0) = |\langle 0|\Psi\rangle|^2 = \left|\alpha \underbrace{\langle 0|0\rangle}_{=1} + \beta \underbrace{\langle 0|1\rangle}_{=0}\right|^2 = |\alpha|^2 \tag{4}$$

$$P_\Psi(1) = |\langle 1|\Psi\rangle|^2 = \left|\alpha \underbrace{\langle 1|0\rangle}_{=0} + \beta \underbrace{\langle 1|1\rangle}_{=1}\right|^2 = |\beta|^2 \tag{5}$$

2. **Collapse of $|\Psi\rangle$**
   In classical measurements it is fair to say that the measurement itself has no (noticeable) influence on the result. This is no longer true in quantum mechanics: The wave function $|\Psi\rangle_i$ **collapses after a measurement** to a projection onto the measured eigenstate and therefore becomes a different state $|\Psi\rangle_f$:

$$|\Psi\rangle_i = \alpha\,|0\rangle + \beta\,|1\rangle \quad \xrightarrow{\text{Measurement: Value } m} \quad |\Psi\rangle_f = \begin{cases} |0\rangle\,, \text{ if } m = 0 \\ |1\rangle\,, \text{ if } m = 1 \end{cases} \tag{6}$$

## 2.2 Quantum Register

A quantum register of size $n$ is a **collection of $n$ qubits**. Therefore we get $N \equiv 2^n$ basic states:

$$|b_{n-1}\rangle \otimes |b_{n-2}\rangle \otimes ... \otimes |b_1\rangle \otimes |b_0\rangle \tag{7}$$

where $b_i \in \{0, 1\}$. One can interpret this chain of zeros and ones as binary code, able to store numbers in the range of $[0, 1, ..., N-1]$. For example for a 3-qubit system we get:

$$\begin{aligned} |0\rangle \otimes |0\rangle \otimes |0\rangle &\equiv |000\rangle \equiv |0\rangle & \qquad |1\rangle \otimes |0\rangle \otimes |0\rangle &\equiv |100\rangle \equiv |4\rangle \\ |0\rangle \otimes |0\rangle \otimes |1\rangle &\equiv |001\rangle \equiv |1\rangle & \qquad |1\rangle \otimes |0\rangle \otimes |1\rangle &\equiv |101\rangle \equiv |5\rangle \\ |0\rangle \otimes |1\rangle \otimes |0\rangle &\equiv |010\rangle \equiv |2\rangle & \qquad |1\rangle \otimes |1\rangle \otimes |0\rangle &\equiv |110\rangle \equiv |6\rangle \\ |0\rangle \otimes |1\rangle \otimes |1\rangle &\equiv |011\rangle \equiv |3\rangle & \qquad |1\rangle \otimes |1\rangle \otimes |1\rangle &\equiv |111\rangle \equiv |7\rangle \end{aligned}$$

We call this collection the **computational basis** of our register.

However, in contrast to a classical system, a quantum register is able to be in a **state of superposition** which turns out to be the fundamental advantage for quantum computation. If for example the second qubit is set to a superposition $|\Psi_{b_1}\rangle = \frac{1}{\sqrt{2}}\binom{+1}{-1}$ the total state of the register will be:

$$\begin{aligned} \left|\Psi^{\text{tot}}\right\rangle &= |\Psi_{b_2}\rangle \otimes |\Psi_{b_1}\rangle \otimes |\Psi_{b_0}\rangle & (8) \\ &= |0\rangle \otimes \left[\tfrac{1}{\sqrt{2}}\left(|0\rangle - |1\rangle\right)\right] \otimes |1\rangle & (9) \\ &= \tfrac{1}{\sqrt{2}}\left[|001\rangle - |011\rangle\right] & (10) \\ &\equiv \tfrac{1}{\sqrt{2}}\left[|1\rangle - |3\rangle\right] & (11) \end{aligned}$$

Eq. 11 is always reducible to a (tensor) product of three single states, as Eq. 8 suggests. This is not always the case. Consider the 2-qubit system where

$$\left|\Psi^{\text{ent}}\right\rangle = \tfrac{1}{\sqrt{2}}\left[|00\rangle + |11\rangle\right]. \tag{12}$$

There is no way to separate this wave function into a (tensor) product of two states $\{|\Psi_{b_1}\rangle\,, |\Psi_{b_0}\rangle\}$. Thus, the state $|\Psi^{\text{ent}}\rangle$ is called **entangled**.

## 2.3 Quantum Gates

After defining the quantum register, we now want to process it through a number of so-called quantum gates. These are **unitary operations** applied to our register in order to change its total state $|\Psi^{\text{tot}}\rangle$. Since we work in the Hilbert space, all our operations are **linear**, therefore we can represent any gate working on a $n$-qubit register by a $N \times N$ matrix.

In the following subsections we will first introduce the most important gates used in our project, and then speak about generalisations of these gates for bigger registers.

### 2.3.1 Pauli-X Gate

The first example for a simple 1-qubit gate is the Pauli-X gate. It simply maps the state $|0\rangle \rightarrow |1\rangle$ and vice versa and is therefore equivalent to the logic NOT. The representing matrix in the computational basis $\{|0\rangle, |1\rangle\}$ is:

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{13}$$

$$X|0\rangle = |1\rangle \tag{14}$$

$$X|1\rangle = |0\rangle \tag{15}$$

$$\tag{16}$$

$$|b\rangle \; -\boxed{X}- \quad |1-b\rangle$$

### 2.3.2 Hadamard Gate

A common gate in quantum computation is the Hadamard gate. It performs the Hadamard transformation on a single qubit system in the following way:

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \tag{17}$$

$$H|0\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}} \tag{18}$$

$$H|1\rangle = \frac{|0\rangle - |1\rangle}{\sqrt{2}} \tag{19}$$

$$|b\rangle \; -\boxed{H}- \quad \frac{1}{\sqrt{2}}\left[(-1)^b |b\rangle + |1-b\rangle\right]$$

The Hadamard gate is a 'real' quantum gate since it is able to set the state to a superposition of basic states.

For a $n$-qubit system it is necessary to define on which qubit a gate is acting. In the following we will use the subscript to depict this: The gate $G_k$ is acting on the $k$-th qubit.

Note that a combination of Hadamard gates acting on every single qubit in a $n$-qubit register with initial state $|\Psi\rangle = |00...0\rangle$ will lead to an **uniform superposition** of all basic states:

$$\left(\prod_{k=0}^{n-1} H_k\right)|\Psi\rangle = H_{n-1}\underbrace{|b_{n-1}\rangle}_{=|0\rangle} \otimes ... \otimes H_0 \underbrace{|b_0\rangle}_{=|0\rangle} \tag{20}$$

$$= \frac{|0\rangle + |1\rangle}{\sqrt{2}} \otimes ... \otimes \frac{|0\rangle + |1\rangle}{\sqrt{2}} \tag{21}$$

$$= 2^{-\frac{n}{2}} \sum_{k=0}^{N-1} |k\rangle \tag{22}$$

### 2.3.3 Phase Gate

The Hadamard gate already uses special properties of quantum computation, but all operations are part of the real subspace of the Hilbert space. In general the gates and quantum register can operate on a complex vector space. The phase gate is such a gate which is defined for a single qubit system as:

$$R_\phi = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{pmatrix} \tag{23}$$

$$R_\phi|0\rangle = |0\rangle \tag{24}$$

$$R_\phi|1\rangle = e^{i\phi}|1\rangle \tag{25}$$

$$|b\rangle \; -\boxed{R_\phi}- \quad e^{ib\phi}\,|b\rangle$$

### 2.3.4 Control Gates

Apart from single qubit gates, there are also control gates. The gate

### 2.3.5 Extension to bigger registers

As roughly mentioned before, any single qubit gate can by applied to the $k$th qubit of a $n$-qubit register. The challenge now is how to construct a matrix representation of a single qubit gate is when it is applied to a register with multiple qubits. Mathematically, this involves taking the tensor product of the matrix representing the gate on the desired target qubit with the identity on others. Consider the example of applying a single qubit gate $G$ on the left qubit in a 2-qubit system. The resulting matrix $G_{\text{tot}}$ is:

$$G_{\text{tot}} = G_1 \otimes \underbrace{G_0}_{=\mathbb{I}_2} \tag{26}$$

$$= \begin{pmatrix} g_{00} & g_{01} \\ g_{10} & g_{11} \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{27}$$

$$= \begin{pmatrix} g_{00}\left(\begin{smallmatrix} 1 & 0 \\ 0 & 1 \end{smallmatrix}\right) & g_{01}\left(\begin{smallmatrix} 1 & 0 \\ 0 & 1 \end{smallmatrix}\right) \\ g_{10}\left(\begin{smallmatrix} 1 & 0 \\ 0 & 1 \end{smallmatrix}\right) & g_{11}\left(\begin{smallmatrix} 1 & 0 \\ 0 & 1 \end{smallmatrix}\right) \end{pmatrix} \tag{28}$$

$$= \begin{pmatrix} g_{00} & 0 & g_{01} & 0 \\ 0 & g_{00} & 0 & g_{01} \\ g_{10} & 0 & g_{11} & 0 \\ 0 & g_{10} & 0 & g_{11} \end{pmatrix} \tag{29}$$

The general expression for $n$-qubit systems is analogous:

$$G_{\text{tot}} = G_{n-1} \otimes \ldots \otimes G_k \otimes \ldots \otimes G_0 \tag{30}$$

$$= \mathbb{I}_2 \otimes \ldots \otimes \left(\begin{smallmatrix} g_{00} & g_{01} \\ g_{10} & g_{11} \end{smallmatrix}\right) \otimes \ldots \otimes \mathbb{I}_2 \tag{31}$$

Instead of carrying out this tensor product explicitly, which is likely to be computationally expensive and inefficient, we notice that the linear operation serves as an active transformation of the state vector. From linear algebra, we know the columns within the matrix that describes such a transformation are the basis vectors of the transformed basis (or the new basis) expressed in terms of the old basis. Therefore, we can construct the matrix for this transformation easily if we know how each basis state in the new basis is described by the old basis.

This turns out to be a simple task to do on a classical computer using bitwise operations, provided that we know how the gate operates on a single qubit. Consider a $n$-qubit system and we wish to apply an arbitrary gate $G$ on the $k$th qubit. Suppose $G$ has the following effect on the states $|0\rangle$ and $|1\rangle$ of a single qubit:

$$G\,|0\rangle = \alpha_0\,|0\rangle + \beta_0\,|1\rangle \tag{32}$$

$$G\,|1\rangle = \alpha_1\,|0\rangle + \beta_1\,|1\rangle \tag{33}$$

We can write this more compactly as

$$G\,|y\rangle = \alpha(y)\,|0\rangle + \beta(y)\,|1\rangle\,, \tag{34}$$

where we let $\alpha(0) = \alpha_0$, $\alpha(1) = \alpha_1$ and similarly for $\beta$. We wish to find the relationship between the new basis $|x\rangle'$ and the old basis $|x\rangle$ such that $|x\rangle' = G\,|x\rangle$. For this discussion, it would be most convenient to write each basis state in terms of the computational basis, which is $|x\rangle \equiv$

$|x_{n-1}x_{n-2}\cdots x_0\rangle$ where $x = x_{n-1}2^{n-1}+x_{n-2}2^{n-2}+\cdots+x_0 2^0$. The new basis state $|x\rangle'$ is therefore given by:

$$|x\rangle' = G\,|x\rangle = G\left(|x_{n-1}\rangle\,|x_{n-2}\rangle\cdots|x_k\rangle\cdots|x_0\rangle\right) \tag{35}$$
$$= |x_{n-1}\rangle \otimes |x_{n-2}\rangle \otimes \cdots \otimes G\,|x_k\rangle \otimes \cdots \otimes |x_0\rangle \tag{36}$$

where we used the fact that $G$ only operates on the $k$th qubit. Using equation 34, we can see that every new basis state can be described by two, and only two, basis vectors from the old basis:

$$|x\rangle' = |x_{n-1}\rangle \otimes |x_{n-2}\rangle \otimes \cdots \otimes \left(\alpha(x_k)\,|0\rangle + \beta(x_k)\,|1\rangle\right) \otimes \cdots \otimes |x_0\rangle \tag{37}$$
$$= \alpha(x_k)\,|x_{n-1}x_{n-2}\cdots 0\cdots x_0\rangle + \beta(x_k)\,|x_{n-1}x_{n-2}\cdots 1\cdots x_0\rangle \tag{38}$$

This means that there would only be two elements in each column within the matrix $G$. Let $G(i,j) \equiv G_{ij}$ and since $G_{ij} = \langle i|\,G\,|j\rangle$, the two elements in column $x$ of $G$ are:

$$G(x_{n-1}x_{n-2}\cdots 0\cdots x_0,\, x_{n-1}x_{n-2}\cdots x_k\cdots x_0) = \alpha(x_k) \tag{39}$$
$$G(x_{n-1}x_{n-2}\cdots 1\cdots x_0,\, x_{n-1}x_{n-2}\cdots x_k\cdots x_0) = \beta(x_k) \tag{40}$$

Therefore, we can find all elements of the matrix by iterating over the column index $x$, $x \in [0, N-1]$. We notice the value of the element depends on $x_k$, or whether the $k$th bit is 0 or 1. This can be found by performing the bitwise AND operation between $x$ and a *mask* with value $2^{k-1}$. If the result is zero, $x_k = 0$; otherwise, $x_k = 1$. We can also toggle the $k$th bit in $x$ to find the row index of the two elements by performing an XOR operation between $x$ and the mask.

The matrix representation of a control gate can also be found using the same procedure. From the previous section, we know the operation in a control gate is only performed if the control qubits are all 1. Consider the gate $G$ that is controlled by $m$ qubits with values $c_1, c_2, \ldots, c_m$, $c_i \in \{0, 1\}$. The new basis is related to the old basis by:

$$|x\rangle' = G^{c_1 c_2 \cdots c_m}\,|x\rangle = \begin{cases} G\,|x\rangle & \text{if} \quad c_1 = c_2 = \ldots = c_m = 1 \\ \mathbb{I}\,|x\rangle & \text{otherwise} \end{cases} \tag{41}$$

Hence, we can still iterate over the column index $x$ to find the elements, except we need to check whether each of the control bits $\{c_i\}$ in $x$ is 1 using the AND operation as described above. If the bits are all 1, we would obtain the two elements as stated in equation 39 and 40; otherwise, the new basis state would be the same as the old basis state, so the only non-zero element in column $x$ would be $G(x, x) = 1$.

### 2.3.6 Gate representations

The resulting matrix $G_{\text{tot}}$ is in general a $N \times N$-matrix with two and only two non-zero entries in every row and column. That means that only $2 \cdot 2^n$ of $2^{n^2}$ entries are non-zero. The ratio is $2^{1-n}$ which rapidly goes towards zero for big $n$. Thus, most entries of the gate matrices will be zero.

This leads to the consideration of the following three possible representations:

1. **Dense matrix representation**
   A dense matrix representation is the standard representation, storing every single entry of a matrix. This leads to two major disadvantages in our special case:

   (a) *Memory*
   A classical computer reserves a certain amount of memory for every entry of a conventional matrix, no matter if the value is zero or non-zero. Therefore using dense matrices for big quantum registers might cause a serious lack of working memory.

(b) *Calculation*
We get a lot of trivial (and unnecessary) calculations using the standard matrix multiplication rule.

The quantum register, however, has mostly non-zero entries for most of the steps of the usual algorithms.

2. **Sparse matrix representation**
A sparse matrix representation only stores non-zero elements of a matrix in a list. Therefore every non-zero element requires a positioning index and the number itself to store. This representation is particularly useful in representing the gates because there are a only two non-zero elements in each column of a gate matrix. Therefore on an N-qubit register a Sparse matrix representation will only require roughly $4N$ storage elements (the index and value of each non zero element in N columns). This is significantly smaller than the $N^2$ required elements in a dense matrix both speeds up computation and decrease memory pressure for higher values of N.

3. **Functional representation**
Another representation of the gates that deviates slightly from the underlying maths representation is to use a functional representation of the gates. The key difference between a matrix and functional representations is that a functional representation doesn't generate a final gate matrix to multiply to the register. Instead the elements for each column are calculated iteratively and then applied to the necessary elements of the register. This significantly decreases memory pressure as the program no longer has to create a matrix for each gate in the circuit. However, the increased computational complexity can make the program run more slowly in some cases. (See Results )

## 2.4 Quantum algorithms

After defining quantum gates it is now simple to predict the next step: A so-called quantum algorithm defines in what manner a quantum register is applied to a sequence of quantum gates in order to achieve a certain computation result. Two very important algorithms are Grover's algorithm and Shor's algorithm which we are going to introduce next.

### 2.4.1 Grover's Algorithm

Grover's algorithm is also known as the quantum search algorithm. On a classical computer, searching through a non-ordered list with $N$ entries would require $O(N)$ operations. This can be reduced remarkably to $O(\sqrt{N})$ operations using a quantum circuit that implements Grover's algorithm.

Different from most search operations, this algorithm searches through the *index* of the elements (which ranges from 0 to $N-1$) rather than the elements themselves. Each index corresponds to a basis state in the register. In addition, the algorithm requires a quantum 'black box' (also known as an *oracle*) which can *recognise* the states associated with the solutions, or the solution states, without *knowing* them explicitly. Using the oracle, the algorithm finds a solution to the search problem by repeatedly performing a certain set of transformations on the register to maximise the probability of measuring the solution states.

**The Oracle**

Suppose we want to search through a list of $N$ elements, and there are $M$ solutions to the search, where $1 \leq M \leq N$. For simplicity, let $N = 2^n$ such that the index of the elements can be exactly represented by $n$ qubits in the register. As mentioned above, the oracle has the ability to recognise the solution states. This is signalled by the state change of a qubit $|q\rangle$ in the oracle (i.e.

$|0\rangle \to |1\rangle$ or $|1\rangle \to |0\rangle$). In other words, if we let $|x\rangle$ to be a basis state of the register associated with a particular element such that $f(x) = 1$ if $|x\rangle$ is a solution and $f(x) = 0$ if it is not, the oracle performs the following unitary operation (denoted as $O$):

$$|x\rangle |q\rangle \xrightarrow{O} |x\rangle |q \oplus f(x)\rangle \tag{42}$$

where $\oplus$ denotes the addition modulus 2 (i.e. $(q + f(x))$ mod 2). As the equation suggests, $|q\rangle$ would only change its state if $f(x) = 1$, which is when the oracle has recognised a solution. For convenience, we can prepare the qubit in the oracle to be $|q\rangle = (|0\rangle - |1\rangle)/\sqrt{2}$ such that the signal for recognising a solution is reflected on the basis state of the register:

$$|x\rangle \left(\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right) \xrightarrow{O} (-1)^{f(x)} |x\rangle \left(\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right) \tag{43}$$

As $|q\rangle$ remains unchanged in the process, we can ignore it along with the internal workspace of the oracle completely for the rest of this discussion. We can simply think that the oracle marks the solution states by applying a phase shift of -1 to them:

$$|x\rangle \xrightarrow{O} (-1)^{f(x)} |x\rangle \tag{44}$$

**Procedure of the Algorithm**

The algorithm begins with setting the register to a uniform superposition state:

$$|\psi\rangle = \frac{1}{\sqrt{N}} \sum_{x=0}^{N-1} |x\rangle \tag{45}$$

To maximise the probability of the solution states, the algorithm repeatedly applies the following set of operations on the register, which, as a whole, is known as the Grover's iteration (denoted as $G$):

1. Apply the oracle $O$
2. Apply the Hadamard operation on all qubits $H^{\otimes n}$
3. Perform a phase shift of -1 on every basis state of the register apart from $|0\rangle$:

$$|x\rangle \;\to\; -(-1)^{\delta_{x0}} |x\rangle \tag{46}$$

   It is easy to check that $2|0\rangle\langle 0| - \mathbb{I}$ would perform this transformation.

4. Apply the Hadamard operation on all qubits again $H^{\otimes n}$

Step 2 to step 4 is also known as the *inversion about mean* operation. It can be written as:

$$H^{\otimes n}(2|0\rangle\langle 0| - \mathbb{I})H^{\otimes n} = 2|\psi\rangle\langle\psi| - \mathbb{I} \tag{47}$$

So the operations in each iteration can be expressed compactly as:

$$G = (2|\psi\rangle\langle\psi| - \mathbb{I})\, O. \tag{48}$$

Geometrically, the iteration performs a rotation of the state vector $|\psi\rangle$ towards the vector representing a uniform superposition of the solution states on the plane spanned by the

$$|\alpha\rangle \equiv \frac{1}{\sqrt{N-M}} \sum_{\text{solutions}} |x\rangle \tag{49}$$

$$|\beta\rangle \equiv \frac{1}{\sqrt{M}} \sum_{\text{non solutions}} |x\rangle \tag{50}$$

Substituting these to the state vector gives:

$$|\Psi\rangle = \sqrt{\frac{N-M}{N}} |\alpha\rangle + \sqrt{\frac{M}{N}} |\beta\rangle \tag{51}$$

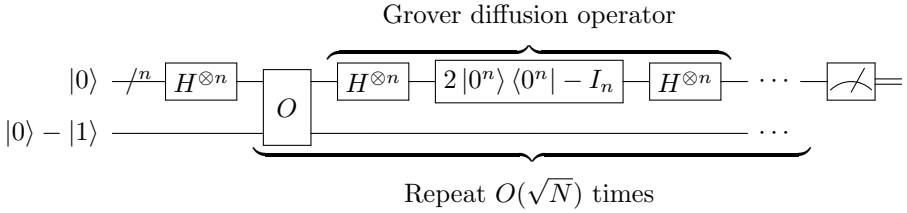



**Figure 1:** Circuit of Grover's Algorithm[1]

Fig. 1 shows a schematic circuit diagram for Grover's algorithm.

**Limitations of Grover's Algorithm**

### 2.4.2 Shor's Algorithm

Shor's algorithm was published 1994 by Peter Shor and proposes an procedure for factorising integers who's factors are coprime. It is able to find non-trivial divisors in polynomial time and space (the number of gates required), whereas naïve classical algorithms run in exponential time. The best classical factoring algorithm, the general number field sieve, is able to factorise integers in sub-exponential time but it has so far been impossible to devise a classical algorithm which runs in polynomial time.

This could have vast impacts on modern cryptography: Many encryption systems (like RSA) rely on the fact, that it is impossible to factorise integers in a reasonable amount time. Shor's algorithm showed that it is (theoretically) possible for quantum computers to achieve this goal, however the practical difficulties of building a real quantum computer are still preventing Shor's algorithm from undermining modern cryptography.

Shor's algorithm is able to reduce the factoring problem to an on order finding one. (p. 233 in the big book of knowledge) The order finding problem itself is simply the phase estimation algorithm applied to the unitary operator (§5.36 in the book). The proof of this is provided in "Quantum computation and quantum information" The most interesting part of all of these algorithms must be the Quantum Fourier Transform. Mathematically it performs the same function as the Classical Fourier Transform, except that it acts on a quantum register instead of a vector.

As seen in figure xx, Shor's algorithm requires the use of two registers. The first is the one the QFT acts on but it is first prepared by the second. The second register has the unitary operator mentioned above applied to it. The states of the two registers are then entangles and when the second register is measured it causes a partial collapse in the first. This leaves only the states which satisfy the equation $x^j \mathrm{mod} N = 1$. By then applying the QFT, the period of the function can be very easily determined.

Fig. 2 shows a schematic circuit diagram for Shor's algorithm.

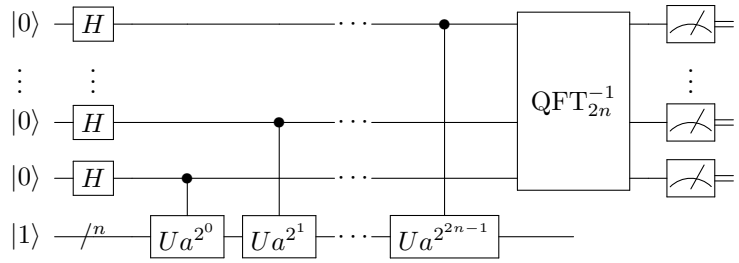



**Figure 2:** Circuit of Shor's Algorithm[3]

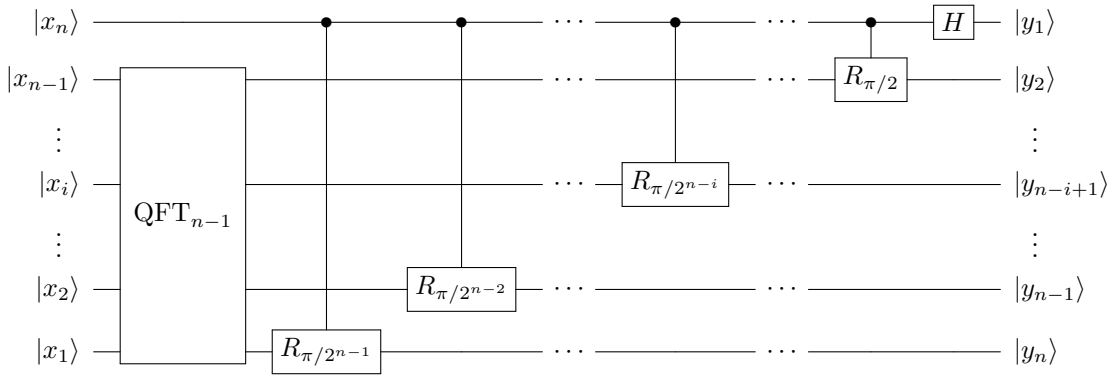



**Figure 3:** Circuit of Quantum Fourier Transforms[2]

# 3 Implementation

In this section we go over the approach we used to tackle the task of simulating the aforementioned concepts on a classical computer. The problem of representing many different concepts, which both built on and used one another, naturally led to a large object-oriented programme. Aside from modeling the quantum concepts that ultimately formed a simulation of a basic quantum computer this project also required the creation of the matrix libraries used in the underlying mathematics and a user interface to test and interact with the simulated computer. Thus the implementation of the program can be understood by understanding each of these three major components and how they interact. This section will begin by a discussion of what software development tools were leveraged in order to organise the project between the group members and create the simulator. Following that is a more in depth discussion of how each component of the program is designed. (For even more detailed documentation of our project see the Javadoc documentation provided with the submission.)

## 3.1 Project organisation

Prior to implementing the program an overall architecture was formed in order to define the interfaces by which each of the various parts of the program would communicate with one another. A simplified view of this architecture is provided below. The full design includes the interfaces

used to communicate between these components, including the method names expected inputs and expected outputs.

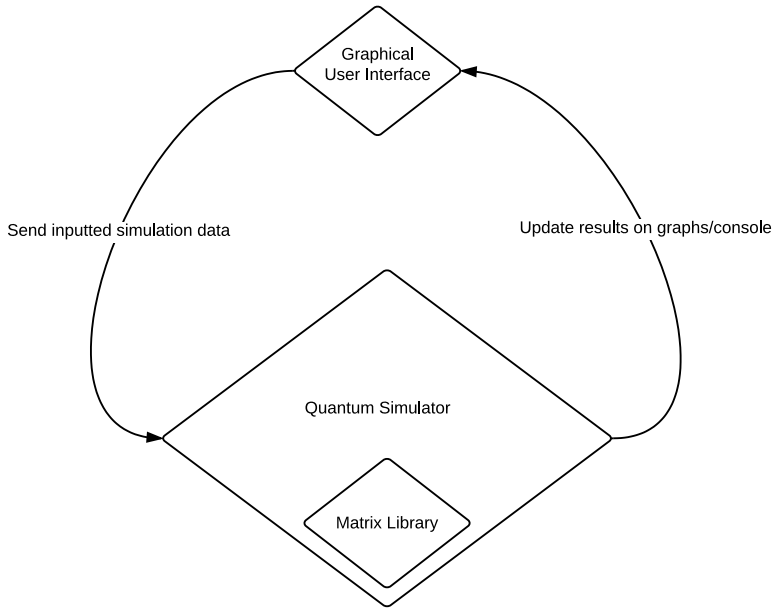



**Figure 4:** An high level overview of how the three main components of the program interact

### 3.1.1 Java

There were many viable programming languages that could be used to implement this simulator. The primary considerations in choosing the appropriate language were the following.

1. The language should readily support large object oriented design implementations
2. The program should be able to efficiently simulate as large of a quantum register as possible
3. The resulting program should run on as many platforms as possible
4. All members of the group should be comfortable with the language

The two primary languages that were ultimately considered were Java and C++. Java was chosen for two primary reasons: it provided an operating system agnostic, well-documented library for Graphical User Interface creation and more of our group members were familiar with the language. It is worth noting that a 'lower level' programming language such as C++ would have allowed for more efficient memory management and optimisations but at the cost of increased code complexity. Since we only had limited time to complete our task we decided that we would forgo the speed benefits of C++ for the robustness and ease of Java.

### 3.1.2 Git

Once an architecture and programming language were decided, the next task was to implement the program as a team. The primary challenge involved in this is allowing each group member to work on the project simultaneously without interfering with each another's progress. The primary tool used in this project to solve this problem is Git source control. Git allows many contributors to simultaneously add changes to a working code base remotely by storing the iterations of the project

on both a central server and also on each contributor's local device. In addition it provides many tools to assist in simultaneous development such as previous version recovery, conflict resolution (when multiple contributors change the same lines of code in a file), and branch creation (which allows a developer to work in their own version of a project without seeing changes made by other contributors).

## 3.2 Development environment

Two primary software solutions were used in order to implement our project. The first was Github, which was used to host the Git repository and also functioned as a communication tool. The second was Eclipse and Integrated Development Environment (IDE), which was the primary text editor and compiler used to create and test the program. Eclipse also contained a built in unit-testing environment called JUnit. This was we used in data collection because it allowed testing that bypassed the GUI to speed up how quickly the results were obtained.

### 3.2.1 Github

As mentioned earlier Github was not only a means of hosting the git repository of our project but also one of the primary means of communication between the group members. The primary feature of the software that was leveraged for this was the issue tracker, which was used as a forum, to-do list, and bug reporting platform. The primary advantage of having this platform is that it allowed the group members to work remotely from one another and still have consistent communication about changes and problems that arose during development.

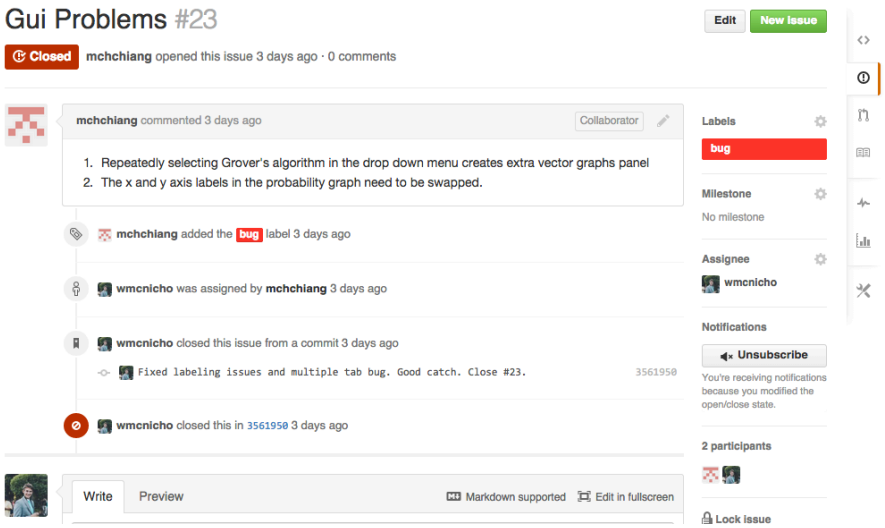



**Figure 5:** A sample issue tracked on Github with communication between members

## 3.3 Programme structure

### 3.3.1 Overview

As mentioned previously, the architecture for this simulator contains three major components.

1. The quantum computer
2. The underlying matrix library

3. The graphical user interface for testing the computer

This section will presented some overall design considerations and then will go in-depth in describing the design and implementations of each of the components.

The design of the quantum computer simulator requires a careful consideration as it is the backbone for running various quantum algorithms. An effective, well-structured design allows one to implement any algorithm easily and compare the performance of the programme under different representations. Our group has identified the following key specifications for the programme:

1. It should be consistent with a circuit-model quantum computer.
2. It should be capable to work with different representations of the computer components (e.g. matrix and functional representation of the quantum gates).
3. It should be extendible and compatible. One should be able to implement another representation of the components that would work with the current code.
4. It should maximise code reusability.
5. It should be stable and user friendly.

The first point is fundamental as the project brief specifically asks us to create a simulator of a circuit-model quantum computer. We therefore design the programme based on the physical objects that exist in such computer. This includes the register, which is an array storing n qubits, the quantum gates, and the circuits, which consist of a series of gates that perform more complex operations on the register, such as the quantum search algorithm. These form the three main groups of classes for the computer part of the programme.

To achieve the remaining specifications, we created an interface for each type of object in the program and adhered to common object oriented design patterns. Each interface describes the fundamental behaviours of the corresponding object that are independent of the representation. This allows objects to interact without having to be concerned about each other's representation. It thus separates the task of representing an object and using it to build circuits for implementing the algorithms, which is key for maximising code reusability and making the programme extendible. The use of commonly used design architectures (such as the Factory Pattern and MVVM) allow for other developers to quickly understand the design and usage of the parts of the program.

### 3.3.2 The Computer

The computer is at the heart of our programme for simulating the quantum algorithms. Figure 6 shows the overall structure of this part of the programme. As discussed above, we designed the programme based on the components of the computer, which are the register, the gates, and the circuits. We developed an interface for each of these components, and they are `QRegister`, `QGate`, and `QCircuit` respectively. Below we describe in detail the programme structure and design choices we made for each component.

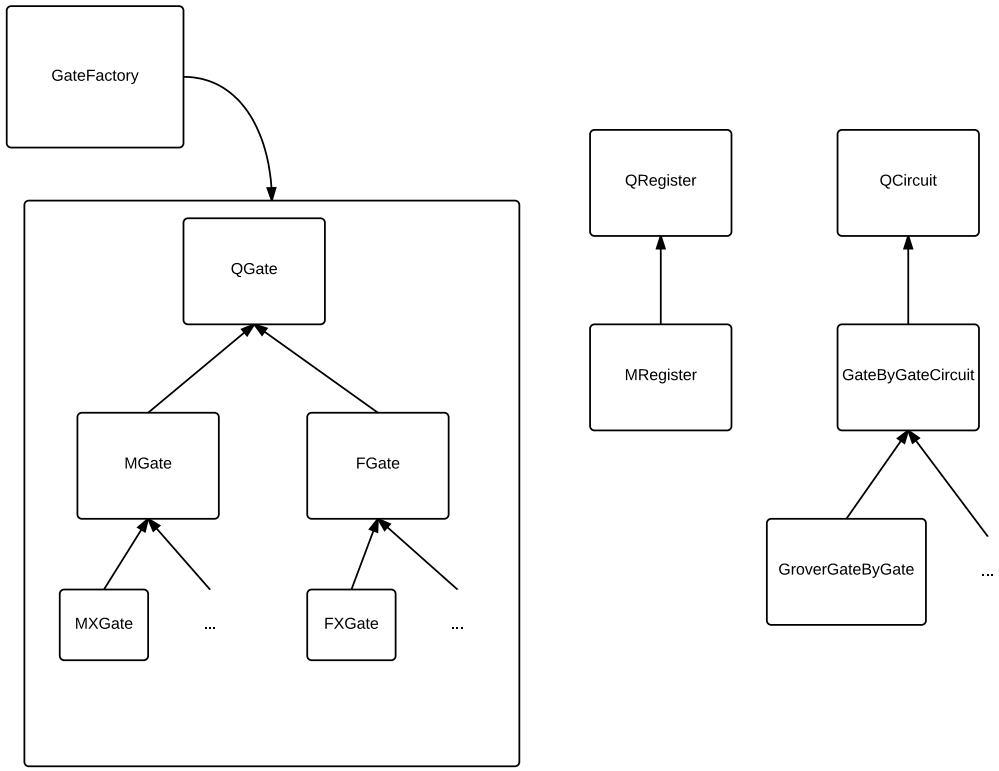



**Figure 6:** A diagram of the class relationships for the quantum computer model

1. **Register**
   The register consists of an array of $n$ qubits that would be manipulated by the gates. From an object-oriented perspective, one might be tempted to create a qubit object with the register storing an array of these objects. This, however, is unphysical as qubits can be entangled and may not be separable as shown in equation 12. Hence, we decided to treat the $n$ qubits as a single system, and the register should store an array of the complex amplitudes of the basis states formed by the qubits (i.e. from $|0\rangle$ to $|2^n - 1\rangle$).

   We developed the `QRegister` interface with the above concept in mind. It requires the classes representing the register to have accessor methods for setting and getting the amplitudes of the basis states. It also requires these classes to provide a method for measuring the register, as such operation is required to obtain physical results after applying a circuit to the register. We created a concrete class called `MRegister` that complies with the interface. It stores the amplitudes of the basis state as a column vector. Since the amplitudes of most of the states would generally not be non-zero, we decided to use a regular dense matrix representation for the vector.

2. **Gates**
   As discussed in section 2.3, there are many single qubit gates and their associated operations on the register can be represented as a matrix or a function. To maximise code reusability, we developed an inheritance structure for modelling the gates. We first constructed an interface called `QGate` to describe a general quantum gate. The interface requires any gate classes to implement the method called `applyGate(QReigster reg)`, as each gate must perform an operation on the register. We then created an abstract class for each representation of the gate: `MGate` for matrix representation and `FGate` for functional representation. These

classes handle the generic behaviours associated with the corresponding gate representation. Finally, we constructed a set of concrete classes that inherit from these abstract classes to model the specific single qubit gates (e.g. Hadamard, Pauli-X gate, etc.).

In matrix representation, the `MGate` class has a method called `initGate(...)` which can create the matrix for any single qubit gate using the procedure described in section 2.3.5. The class also implements the `applyGate(...)` method from `QGate` to perform the matrix multiplication of the gate matrix with register's state vector. A set of classes were extended from `MGate` to model specific single qubit gates. They provide the necessary information, such as the target qubit and how the gate operates on a single qubit (i.e. $\alpha$ and $\beta$ in equation (34)), to `MGate` for it to generate an appropriate matrix for the gate.

A similar design is used in functional representation. The `FGate` class implements the `applyGate(...)` method to perform the functional procedure for applying a single qubit gate on the register as mentioned in section 2.3.6. To do so, it needs to know how that particular gate operates on a single qubit. This is supplied by the set of concrete classes which inherit `FGate` to represent a specific qubit gate.

| Gate | Matrix Rep. Class | Functional Rep. Class |
|---|---|---|
| $H$ | `MHGate` | `FHGate` |
| $X$ | `MXGate` | `FXGate` |
| $Y$ | `MYGate` | `FYGate` |
| $Z$ | `MZGate` | `FZGate` |
| $S$ | `MSGate` | `FSGate` |
| $T$ | `MTGate` | `FTGate` |
| $R_\phi$ | `MPhaseGate` | `FPhaseGate` |

**Table 1:** A complete list of gates implemented in the programme.

We know the representation of the gate would depend on the qubit that it is applied to (i.e. the target qubit) and the control qubits associated with gate. This leads to two options for designing the gates:

(a) Construct a general form of the gate that would require one to specify the target qubit and the set of control qubits as parameters when the gate is applied to the register.

(b) Construct a specific form of the gate that would only work for a specific target qubit and set of control qubits

Although the first option keeps the gate class generic and more flexible, it requires the representation to be recalculated every time the gate is used. This may lead to a significant increase in computation time, hindering the programme performance. The latter option does not have such problem, as the gates are instantiated for a specific target qubit and set of control qubits. However, this has the side effect of consuming more memory, as we need to store multiple versions of the same gate for different targets and controls. We decided to design our gates based on the second option, as we believed such usage of memory is tolerable, and we would like to obtain results within a reasonable amount of time. In addition, it simplifies the task for building a quantum circuit. As each gate is pre-programmed to operate on a specific target with a specific set of controls, we would only need to create a list of gates to be applied for building the circuit. We would not need store an extra, complicated set of instruction telling the gate which qubit it should operate on and the control qubits it has.

3. **Circuits**
   The design structure for the circuits is similar to that for the gates. We created an interface called `QCircuit` that describes a general quantum circuit. The interface requires classes representing a quantum circuit to implement the `applyCircuit(QRegister reg)` method, as each circuit is expected to perform some operations on the register. We designed a general circuit class called `GateByGateCircuit` which allows the user to construct a circuit by assembling gates together, regardless of their representation. Furthermore, we take advantage of the universality of this circuit class by extending it to build the various circuits required for the quantum algorithms studied in this project. This includes the quantum Fourier transform circuits (`ForwardQFTCircuit` and `BackwardQFTCircuit`) and the circuit for Grover's algorithm (`GroverGateByGate`).

4. **Implementation of the Quantum Algorithms**

   (a) **Grover's Algorithm**

   (b) **Shor's Algorithm**
   When implementing Shor's algorithm, the most important step was creating a functioning quantum Fourier transform. We had several options when deciding how to implement this as there are several different algorithms available. As we were on a rather tight deadline we decided to implement the easiest version of the algorithm. This ease of implementation came at the cost of higher computational complexity. The main benefit we got from implementing this version of the algorithm was that it only used gates which had already been implemented, so it became a simple task of applying the gates in the right order.

   In an actual quantum computer there would be two registers active in every run of the algorithm. As we are limited on the number of qubits we are able to represent and store in a classical computer (due to memory limitations), we decided to implement a classical equivalent to the second register. The second register simply defines the amplitudes of the different states of the first register. Using a classical modular exponentiation algorithm and some random number generation the same results are achieved as using two registers, except that we had much more memory available for our QFT.

   The classical parts of the algorithm were easy to implement as most of them are very well known algorithms in computer science. We required algorithms to find the highest common factor of two numbers, find the convergents of a continued fraction and do modular exponentiation of numbers. As the continued fraction algorithm was the most complex of them all we wrote a separate class for this. The other two algorithm were simply methods in our Shor's algorithm class.

   To ensure the algorithm only runs when it is required we added checks to the number being factorised. We check if it is even or if it has a factor in the form $a^b$ as these can be easily checked for in polynomial time. We also check if the input is prime. This ensures only numbers which two co-prime factors ever reach the quantum parts of the Shor's algorithm code as these are the most computationally expensive.

   To factorise numbers which do not factorise into two primes, the user would have to run the code several times, each time factorising the factors returned by the previous run if they are not themselves prime.

### 3.3.3 Matrix

After deciding that we wanted to implement a variety of gate implementations. We decided that for our code to be as user friendly as possible we should be able to switch between our two different

matrix representations by only changing a single argument that is passed to the Matrix package. The package should hide the representation from the user and deal with all of the messiness internally.

To achieve this we created an abstract class `Matrix` which is then implemented by all of our concrete matrix representations. The user only ever has to deal with this abstract class. This presented some challenges in implementing this design. The first challenge we encountered was how to call the constructors for the different implementations from a single method call, where one of the arguments decided the type of the Matrix. To solve this problem we employed a simple factory design pattern. Our `MatrixFactory` contains a static method, `MatrixFactory.create(int i, int j, String type)` which returns a matrix of the type specified in the by the string passed in the method.

The `Matrix` class contains methods for all of the matrix manipulations we require in our project. This is mainly involves getting and setting elements and multiplication of matrices. Each of the concrete implementations of Matrix override the get and set methods in Matrix as they need to be written specifically for the data structure which each implementation used.

The two main types of matrices we implemented were dense and sparse matrices. The dense matrix itself comes in two different types: real and complex. These two share some common features such as the fact that each element is explicitly stored even if it is a zero. This contrasts with the sparse matrix as only non-zero elements and their indices are stored.

We made several choices in our data structures which are related to the performance of the dense matrices. Firstly we decided that the overhead created by 2 dimensional arrays is too much as it results in more memory lookups and more cache misses. This can be reduced by using a single array to store all the matrix entries. It then requires some trivial arithmetic to retrieve the array indices (element read and writes are still $O(1)$ as with multi-dimensional arrays). The cost of calculating these indices is lower than the time wasted on cache misses. The next optimisation we implemented was not storing complex numbers in a complex object as it would again introduce a non-negligible amount of overhead, both in terms of object allocation and a general memory overhead associated with every Java object.

Our sparse matrix implementation contains both a general sparse matrix class as well as a specially optimised class designed for gates. In section 666.666 we saw that each gate can be represented by a matrix containing two elements in each column. This allowed us to design a data structure specifically tailored towards this problem.

The `SparseGateMatrix` class only stores the non-zero entries in the matrix. As we know each column only contains 2 entries, it is enough to store the value and the row index of the element. As long as the entries for each column are stored in order, the true index can be easily recovered with trivial arithmetic in $O(1)$ operations.

The matrix multiplication is dealt with in a separate helper class called `MatrixMultiply`. It contains a very general and naïve implementation of a matrix multiplication algorithm. It then contains further methods which are optimised towards each of our implementations, the most important of these being the multiplication of a complex matrix by a sparse matrix representing a gate. This method is where almost of the computational resources are spent when applying our circuits to the register. It turns out that it is possible to write a more efficient sparse-dense multiplication algorithm if we consider $|\psi\rangle$* operator rather than operator * $\langle\psi|$. This is because in this case we know that there are only 2 elements in reach row of the sparse matrix which are very quick to access as they will be located next to each other in the system memory. It is then only required to find the 2 corresponding elements in the register to be able to calculate the corresponding element in the answer. While this approach incurs a small overhead due to having to convert from $\langle\psi|$ to $|\psi\rangle$ and back again at the end, this can be minimised very easily and the final code runs faster than if this approach was not used.

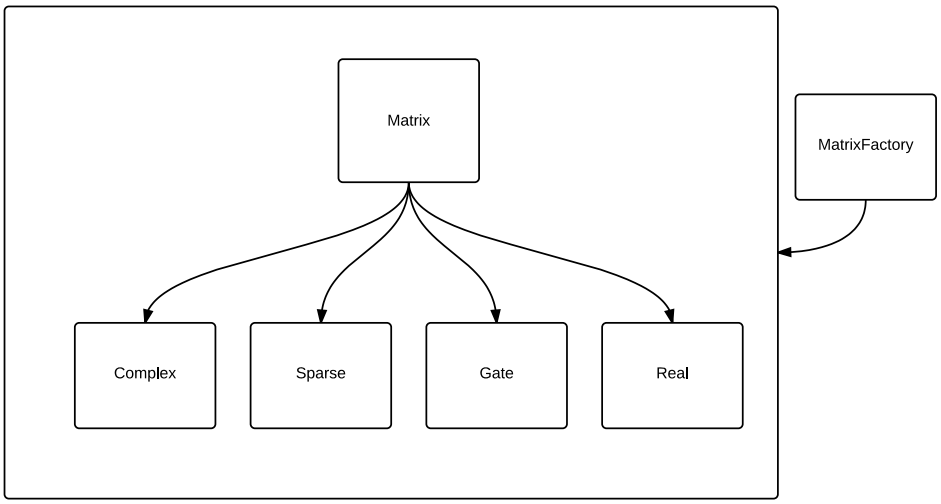



**Figure 7:** A diagram of the class relationships of the Matrix library

### 3.3.4 Graphics User Interface

The Graphics User Interface (GUI) for this program is constructed through the use of the Java swing library and one external, open source library for graphing called JFreeChart. In designing the GUI there were a couple of goals in mind.

1. Make it easy to use
2. Have it display as much of the potential of the simulator as possible
3. Ensure its usage does not significantly slow down the simulation process

To accomplish the first goal the entire interface is limited to a small selection of buttons and drop down menus that requires the user to do very little to start a simulation. The GUI also dynamically changes itself in an attempt to instruct the end-user on how to use the programme. The programme also has a built in help window with instructions on how to perform the various simulations.

To accomplish the second and third goals, a variation of the Model-View-ViewModel interface was implemented. In this architecture, the Model (i.e. the quantum simulator) would communicate relevant data changes to the ViewModel (`QViewModel`) through static methods. The ViewModel would then perform any necessary conversion or reinterpretation of the data and then would instruct the view (i.e. the animations and console window) to update what it is displaying. This accomplished the goal of not slowing down the program because the simulation code does not need to wait for the GUI to render to continue its simulation. It achieves the second goal because it provides a simple interface for the people working on the model code to use in order to make changes to the GUI and facilitates communication between the View and Model programmers.

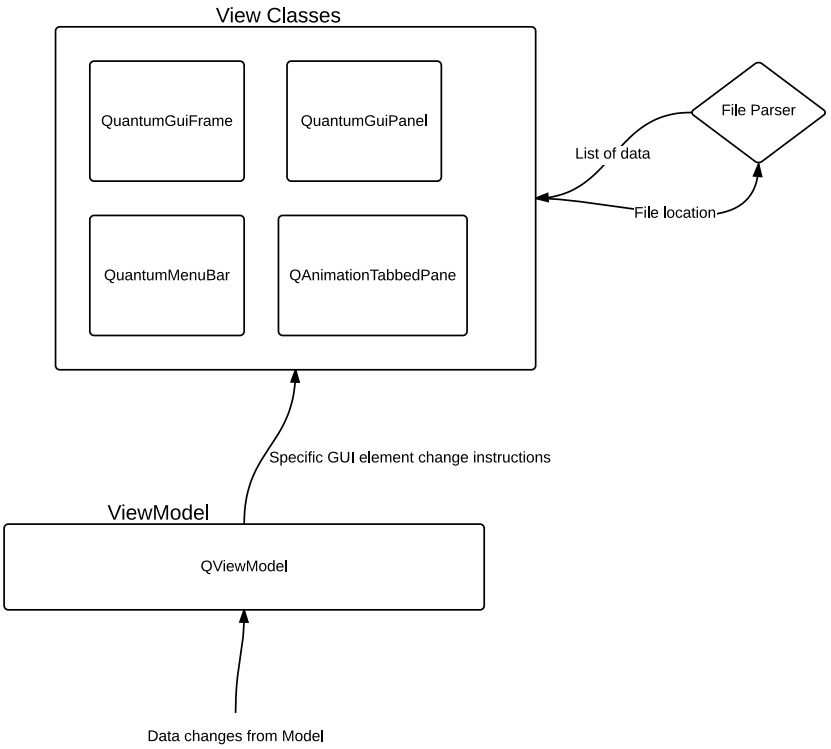



**Figure 8:** A diagram of the classes used in the GUI code and how they communicate with other components

The GUI window is composed entirely out of four Java swing components. The class `QuantumGuiFrame` contains all of the other created classes that ultimately form the overall GUI. These include `QuantumMenuBar` and `QuantumGuiPanel` (which contains a `QAnimationTabbedPane`). Note that `QAnimationTabbedPane` uses the JFreeChart open source library to create the graphs and animations in the program and it's code was not written by us.

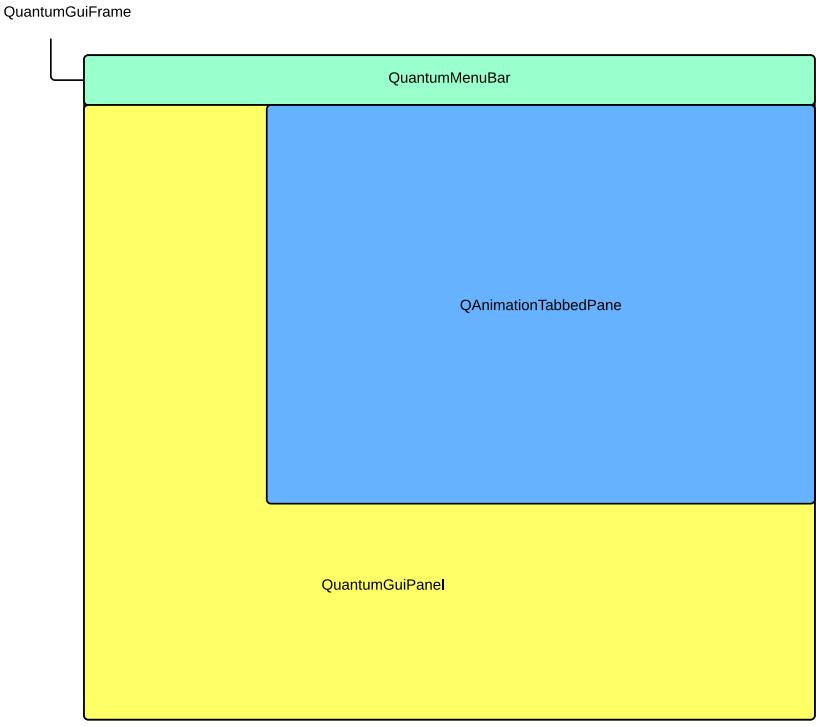



**Figure 9:** A graphical representation of the GUI classes corresponding to where they lie in the running program.

## 3.4 Programme execution

The execution flow of the program is a two threaded system but could be expanded to many more threads in the event this program is extended to have multi-core or GPU support. When the program is started the main function in `QuantumGuiFrame` creates the GUI and waits for user input. Once the user has selected the type of simulation and the associated data they will then press the start button which will create a `QProcess` object. This object will launch a new thread in its constructor that will create a quantum circuit based off of the specifications that the user provided and run that circuit on the inputted data. The GUI thread and the simulation thread will then run in parallel until the simulation is complete. As the simulation runs it updates the GUI informing the user of the progress through various animation elements and a console window. Upon completion of the simulation, the simulation thread ends and the GUI thread waits for the user to input new data and start a new simulation. Theoretically the programme's architecture could be extended to support multiple threads in a simulation or even multiple parallel simulations with minor changes to the ViewModel code to handle multiple sources of view update requests.

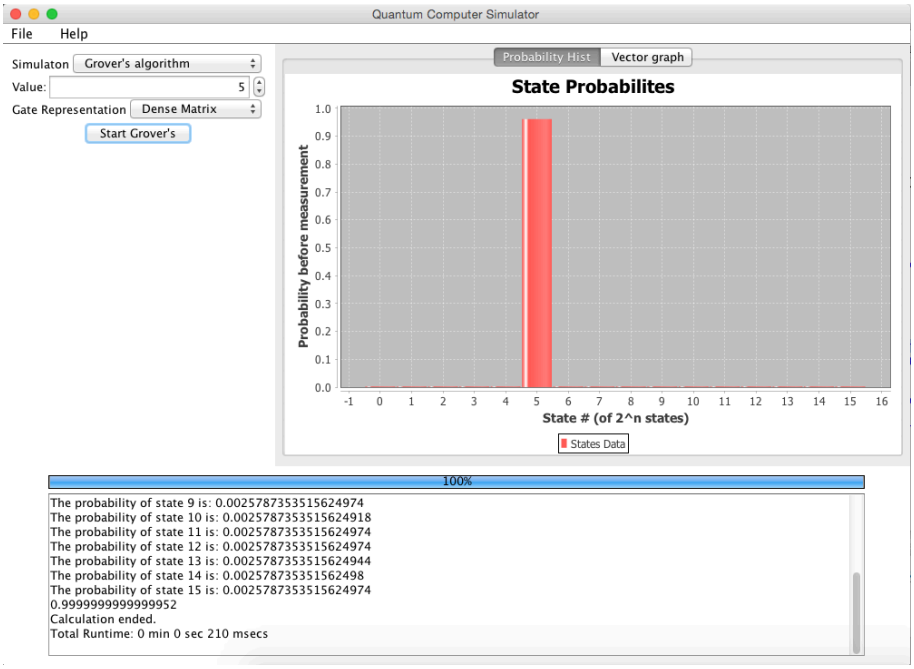


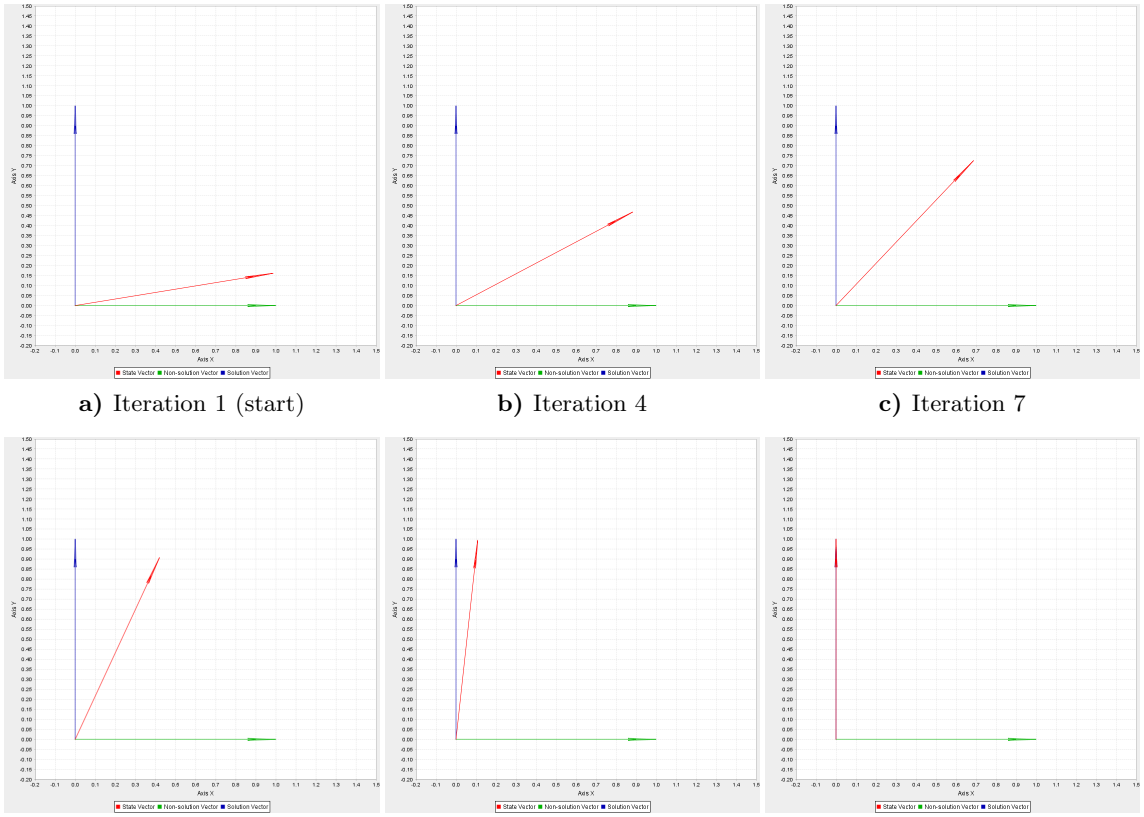

**Figure 10:** A screen shot of the program after running a sample simulation of Grover's algorithm

# 4 Results

## 4.1 Grover's Algorithm

### 4.1.1 Rotation of the state vector

Basically, Grover's Algorithm can be depicted as a rotation in a two dimensional plane by projecting the current state vector. This is depicted in Fig. 11. After each iteration of the loop in Grover's Algorithm (see Fig. 1) the state vector approaches the solution state.



**a)** Iteration 1 (start) **b)** Iteration 4 **c)** Iteration 7

**d)** Iteration 10 **e)** Iteration 13 **f)** Iteration 14 (end)

**Figure 11:** Depiction of Grover's Algorithm: The green vector depicts the non-solution vector, the blue vector depicts the vector of the solution. The red vector is the projection of the current state. With every consecutive iteration the state vector rotates towards the solution state.

### 4.1.2 Computational time

Fig. 12 shows the computational time of Grover's algorithm. All the measurements were executed on the same computer by varying the number of qubits $n$ for the three different representations.

We note the following observations:

- **Dense representation at a disadvantage**
  One can see that the dense representation is the slowest one since for already $n \geq 10$ first noticeable computation times occur whereas the algorithm using functional and spare representation is still immediately executed. However, when they start to show noticeable computational times, the dense representation already takes a unbearable amount of time.

- **Spare vs. functional representation**
  Considering computational time the sparse representation is superior to the functional representation. It appears to be roughly a factor 2, but since we don't have data for bigger registers, this quantitative observation is quite vague.

- **Exponential behaviour**
  All three representations show an exponential behaviour. To illustrate the point we plotted the same data in a log-plot (Fig. 14) and got a linear relation.

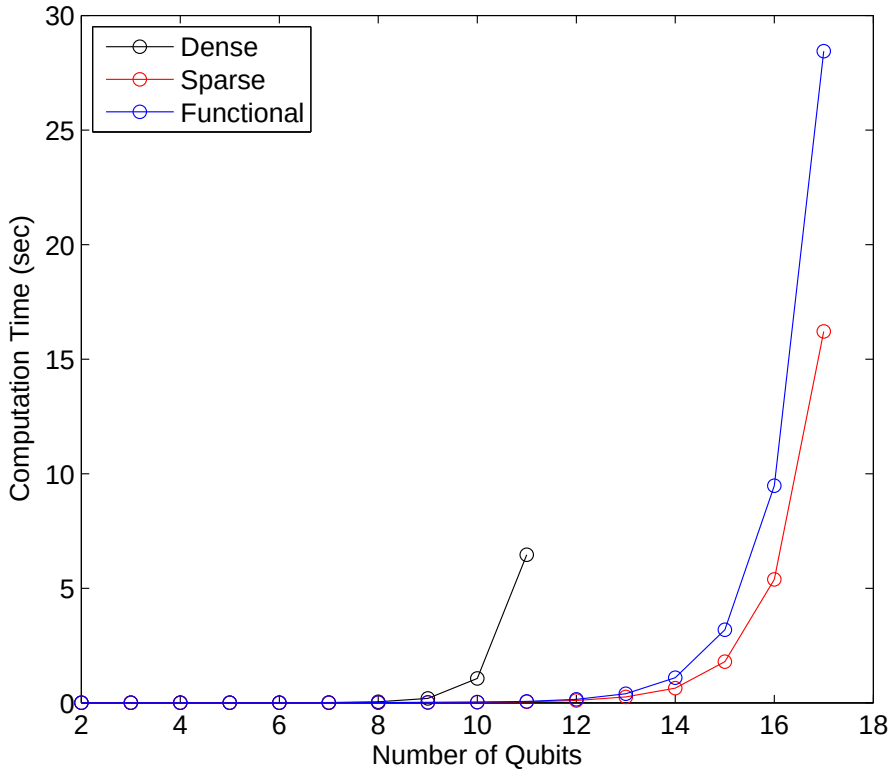



**Figure 12:** Computational time of Grover's Algorithm in nanoseconds as a function of the quantum register size for the three different forms of representation (dense, sparse, functional).

### 4.1.3 Memory Usage

Fig. 13 shows the memory usage of Grover's algorithm. All the measurements were executed on the same computer by varying the number of qubits $n$ for the three different representations.

We note the following observations:

- **Dense representation at a disadvantage**
  The memory usage of dense matrices is enormous. For only 11 qubits the execution requires working memory of 750 megabytes. It is impossible to run the algorithm for 12 qubits since this already exceeds the working memory of a normal computer ( 4 gigabyte).

- **Spare vs. functional representation**
  In terms of computational time the sparse representation was slightly faster than the functional representation. Measuring the memory usage, however, the functional representation uses almost no working memory (even for 17 qubits!), whereas the sparse representation, since it stores matrices in a compact way, has to increase dramatically at a certain number of qubits. In our case the working memory would be exceeded (using sparse representation) for less than 25 qubits.

- **Exponential behaviour**
  The dense and sparse representation show an exponential behaviour. To illustrate the point we plotted the same data in a log-plot (Fig. 15) and got a linear relation. The functional representation, however, shows no tendency for the range we investigated.

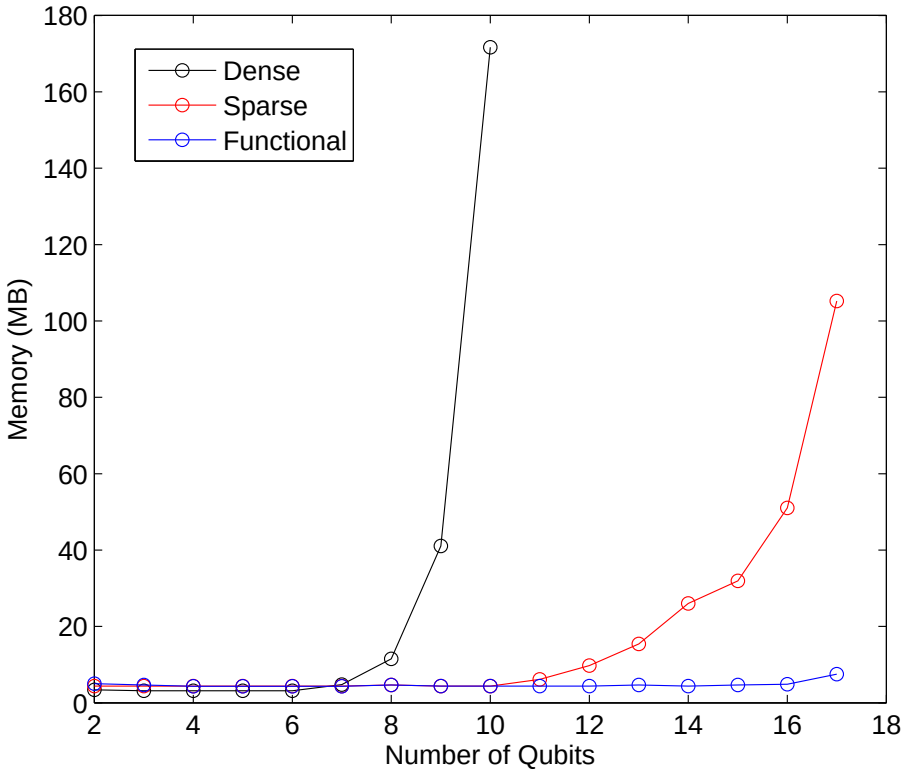



**Figure 13:** Memory Usage of Grover's Algorithm (in megabyte) as a function the quantum register size $n$ for the three different representations (dense, sparse, functional).

### 4.2 Shor's Algorithm

## 5 Discussion

### 5.1 Matrix or functional representation

In section 4.1 we've shown the results for the three different

As we have seen in the **dense matrix representation** is at a disadvantage in every sense.

### 5.2 Improvements and further steps

#### 5.2.1 What we did not have time to do

The program we were able to write during this project covers the criteria we set out at the beginning and it is able to do everything we want it to. This does not mean that we would not want to add more features if we had more time.

A major feature we would have liked to add, is providing a full API which would allow anyone to create their own quantum circuits and run them. This would include functionality for creating an arbitrary circuit and running it. While this should currently be possible by extending the basic classes we created for gates and extending `GateByGateCircuit`. We feel like by slightly restructuring some of our code we would be able to provide a more robust framework for creating new circuits. This idea could then also be extended to the GUI, where a user could create their

own circuits in real time. This could either involve a drag and drop interface where a user could select from a set of existing gates or our own scripting language where the user could write code which calls all of the gates. This would then be parsed into our program and it would deal with it all internally.

Another major feature we would like to implement is some level of parallelisation. This could involve multithreading support for the matrix multiplications or the creation of the gates as they are both very well suited to parallelisation. Another option would be to use a GPGPU library, such as openCL, to offload the matrix multiplications to a GPU for even greater parallelisation.

There are also some minor points we would like to improve upon. These are mainly small fixes for areas of the current program which we are not entirely happy with. Firstly, we would like some kind of way to combine gates as it would allow for less matrix multiplications overall if the gate is used many times. It may also make some of the syntax clearer when adding gates to a circuit as only one would have to be added instead a collection which do the same job.

# 6 Conclusion

# 7 Appendix

## 7.1 Grover's Algorithm

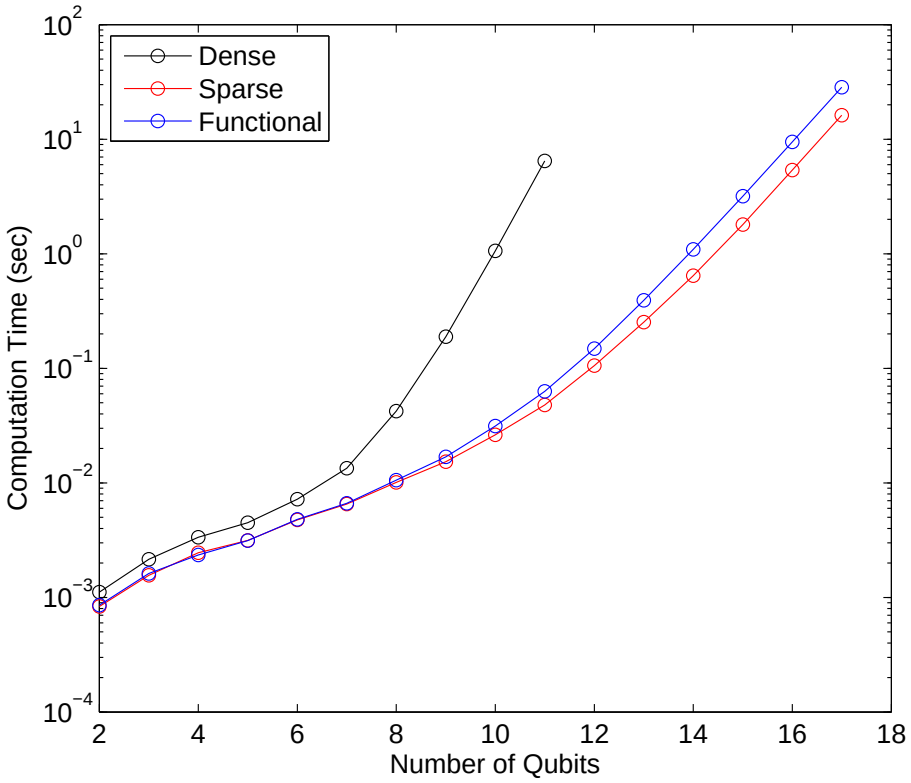



**Figure 14:** Computational time (log-scale) of Grover's Algorithm in nanoseconds as a function of the quantum register size for the three different forms of representation (dense, sparse, functional). Note that only the behaviour for bigger registers is meaningful (linear).

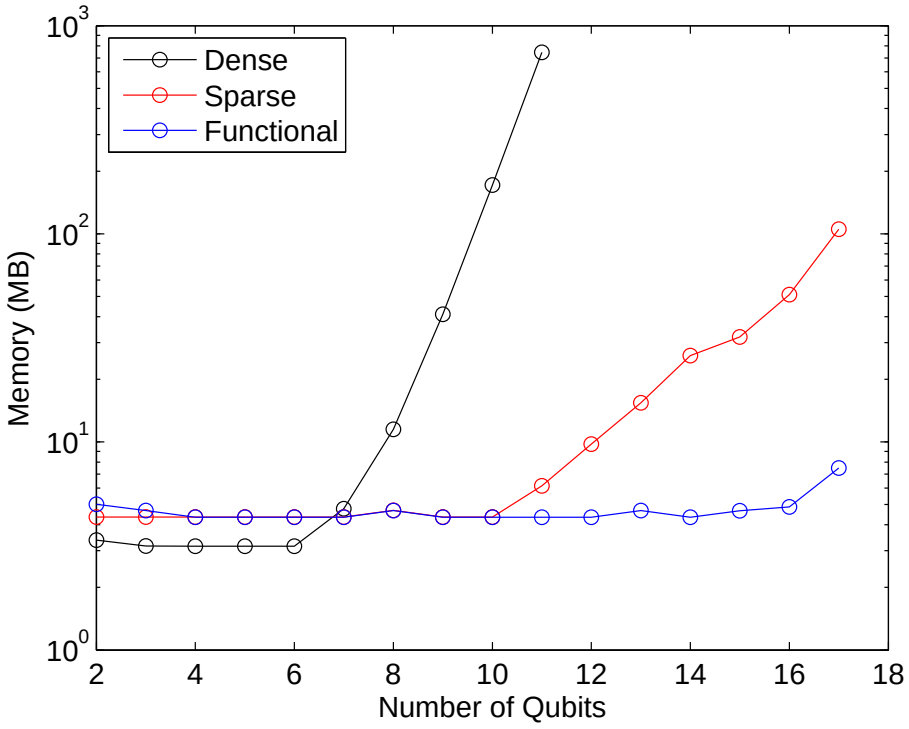



**Figure 15:** Memory Usage of Grover's Algorithm (in megabyte, logarithmic) as a function the quantum register size $n$ for the three different representations (dense, sparse, functional).

## 7.2 Details

The data for the computational time (Fig. 12 and Fig. 14) was collected on a:

Intel i5 3570@3.4 GHz 2x4 GB 1600 Mhz Ram Windows 7

# References

[1] *Grover's algorithm.* http://commons.wikimedia.org/wiki/File%3AGrovers_algorithm.svg, . – [Online; last accessed on 06.03.2015]

[2] *Quantum Fourier transform.* http://commons.wikimedia.org/wiki/File:Quantum_Fourier_transform_on_n_qubits.svg, . – [Online; last accessed on 19.03.2015]

[3] *Shor's algorithm.* http://commons.wikimedia.org/wiki/File:Shor%27s_algorithm.svg, . – [Online; last accessed on 06.03.2015]

[4] Ekert, Artur ; Hayden, Patrick ; Inamori, Hitoshi: *Basic concepts in quantum computation*, 2008

[5] Nielsen, Michael A. ; Chuang, Isaac L.: *Quantum Computation and Quantum Information - 10th Anniversary Edition.* Cambridge : Cambridge University Press, 2010. – ISBN 978–1–139–49548–6

[6] Perry, Riley T.: *Quantum Computing from the Ground Up.* Singapur : World Scientific, 2012. – ISBN 978–9–814–41211–7

[7] Vandersypen, Lieven M. K.: *Experimental realization of Shor's quantum factoring algorithm using nuclear magnetic resonance.* – [Online; last accessed on 13.03.2015]