

Towards Distributed Quantum Algorithms

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Abstract

Quantum computers are capable of efficiently executing computations that are intractable on classical computers. This difference in computational power is achieved by exploiting some properties of quantum mechanics. However, these same properties impose tough challenges on the development of large scale quantum computers. Small quantum computers have already been built, and some experts have proposed a distributed grid of small quantum computers as an alternative to large scale monolithic architectures.

Currently the literature offers no support for the design of distributed quantum programs. This thesis aims to cover this gap, presenting an algorithm that automatically distributes any input quantum circuit. The algorithm proceeds by reducing the problem of efficiently distributing a quantum circuit to the problem of hypergraph partitioning. Two extensions of our algorithm are proposed. The algorithm is evaluated by distributing a collection of benchmark circuits drawn from the literature.

Informal Summary

Quantum computers are more powerful than the computers we use nowadays. Quantum computers could be used to perform calculations that our current computers can not possibly solve in a reasonable amount of time. Small quantum computers have already been built, but for a quantum computer to be useful, it should be at least ten times larger than the ones we can currently build. However, building large quantum computers is extremely challenging, and there is still a long way until we develop the technology that would be needed.

There is an alternative to building a single large quantum computer, and it is to create a spider web of smaller ones that cooperate to perform calculations. This approach is commonly known as *distributed computing*, and in this thesis we aim to make it more accessible to quantum computer scientists. We propose an automated translator that adapts calculations meant to be solved by a single quantum computer so it can be performed by a group of smaller quantum computers. In order to give a better intuition of the problem at hand, let's temporarily deviate from quantum matters and describe a situation we might encounter in real life, which is fairly similar to our problem:

Imagine you are the human resources manager of a company that has just made a contract with a client. The contracted project is so demanding that all the employees of the company must work on it. The company has a large number of employees and you have to assign each of them to one of the multiple office buildings. The employees must work in groups, which are very interconnected, as each employee may work in multiple groups – in mathematics, we call a network of interconnections such as this a *hypergraph*. Now, the problem is that whenever you allocate to different buildings employees that work in the same group, you will need to hire an additional employee that communicates messages between the buildings. Clearly, you want to minimise the number of messengers you need to hire, but doing so requires a bit of planning. In fact, this is a difficult problem, known by computer scientists as the *hypergraph partitioning* problem.

We can draw an analogy between the human resource problem and the problem of efficiently distributing a quantum program: Employees are *qubits* – the basic working unit of a quantum computer –, each building is one of the small quantum computers, and the messengers are a special kind of qubits. The company is the spider web of quantum computers itself, the client is the user, and the project contracted is the calculation the user wishes our computers to solve. What we propose in this thesis is

an automated method for the resource manager to figure out what is the best way of allocating each qubit to the different computers so the least amount of messengers are required.

To do so, we make use of an already existent hypergraph partitioning solver. The subtlety here is that we do not know beforehand how the qubits have to work together to perform a given calculation; we do not know the hypergraph. The main contribution of this thesis is the automated generation of such hypergraph out of the description of the calculation given by the user. We give formal proof that an optimal partition of the hypergraph gives an optimal solution of how to distribute the qubits. Additionally, we propose two extensions that improve how good such a solution can be.

We used our method to distribute some programs scientists would be interested to execute on a quantum computer. The results were quite satisfying: Our method manages to make an efficient use of messengers, assigning each of them to multiple communications.

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Declaration

I declare that this thesis was composed by myself, that the work contained herein is my own except where explicitly stated otherwise in the text, and that this work has not been submitted for any other degree or professional qualification except as specified.

(Pablo Andres-Martinez)

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Chapter 1

Introduction

In this thesis, we propose an algorithm for the automated translation of programs from monolithic quantum computers to distributed grids of quantum computers. The reader is not required to have any prior knowledge of quantum computing, as we will introduce the concepts needed in an incremental manner. In some occasions, we will use analogies from classical computer science – ranging from distributed architectures to compilers – that should help understand the key concepts of distributed quantum computing. Our main contribution consists in reducing the problem of efficiently distributing a quantum circuit to the problem of hypergraph partitioning, which is a problem thoroughly studied in the literature of classical computer science.

Quantum computing aims to take advantage of quantum mechanics to speed-up computations. There are many examples of problems that, although being solvable by a classical computer, would take an unreasonable amount of time to compute regardless how large or fast your classical computer is. Some of these *intractable problems* can be solved efficiently on a quantum computer. Well-known examples of such problems are:

- *Factorisation of large numbers*: In classical computers, all known factorisation algorithms take exponential time with respect to the input size. It is strongly believed that there is no way a classical computer can solve the problem efficiently – in fact, we are so confident about it that most widely used encryption systems, like RSA, rely on this. However, quantum computers are capable of solving this problem in polynomial time (i.e. making it tractable), using Shor’s algorithm (Shor, 1999).
- *Unstructured search*: The aim is to perform a brute-force search (i.e. requiring

no prior knowledge about the search space) over N data-points. Classical computers have no other option than testing each data-point, so the time they take to perform the search is proportional to N . With a quantum computer, using Grover's algorithm (Grover, 1996), the search is finished in time proportional to \sqrt{N} .

Besides, a recent result by Raz and Tal (2018) gives formal proof of the existence of a large family of problems that a classical computer may never solve in polynomial time, but are solvable in polynomial time on a quantum computer. Nevertheless, all of these results are theoretical in nature, and giving experimental evidence of this gap in computational power is a highly active area of research, known as *quantum supremacy*.

Quantum computing would be very valuable in many areas of research that deal with problems that are intractable on classical computers. Some of the main applications that have been discussed in the literature are:

- *Chemistry, medicine and material sciences*: Calculating molecular properties on complex systems is extremely demanding for classical computers. However, polynomial algorithms for this kind of problems are known for quantum computers (Lanyon et al., 2010).
- *Machine learning*: Finding patterns in a large pool of data is the essence of machine learning. Multiple quantum algorithms have been shown to be able to detect patterns that are believed not to be efficiently attainable classically (Biamonte et al., 2017).
- *Engineering*: Optimisation and search problems are common in almost every area of engineering. Quantum computers are particularly well suited for these tasks, with Grover's algorithm (unstructured search) being an obvious example.

For any of these applications we will require large scale quantum computers. Due to the obstacles in the way of building a large quantum computer, some experts have advocated the alternative of building a *quantum multicomputer*: a grid of small quantum computers that cooperate to perform an overall computation (Van Meter et al., 2010). Small quantum computers have already been built, and the technology needed to connect them in a grid is known. Thus, it is possible that large scale grids of quantum computers become available before large monolithic quantum computers do. Even if this were not the case, distributed quantum computing would still be a desirable asset,

for similar reasons it is in classical computing: a cluster of small computers may be cheaper than a large mainframe, and a multicomputer is intrinsically modular, so we may easily adjust the amount of resources we dedicate to a computation.

Unfortunately, there is virtually no support for developing programs to be run on distributed quantum architectures. The literature on quantum algorithms and quantum programming languages focuses almost exclusively on a single model of quantum computation – the circuit model –, meant to be run on a monolithic computer. In this thesis, we intend to make a first step towards the spread of distributed quantum algorithms, providing an automated method for distributing any input circuit across an arbitrary number of quantum computers.

1.1 Outline of the chapters

Chapters 2 and 3 correspond to the literature review relevant to this thesis, and they identify the problem we intend to solve. Chapter 2 introduces the key concepts of quantum computer science that will be required throughout this thesis. Most importantly, §2.1 explains the principles of quantum computing, and gives an intuition behind the speed-up it achieves; while §2.2 discusses the scalability challenges of quantum computers, and presents the main model of quantum computing – the circuit model. Chapter 3 gives an introduction to distributed quantum computing: In §3.1 we explain how quantum information may be communicated across QPUs, §3.2 reviews the main paper our thesis is built upon (Yimsiriwattana and Lomonaco Jr, 2004), and §3.3 describes an abstract distributed quantum architecture.

Our contributions are presented in Chapter 4. First, in §4.1 we propose two extensions of the work by Yimsiriwattana and Lomonaco Jr (2004). §4.2 is the core of the thesis, where we describe our algorithm for automated distribution of quantum circuits. We present our first version of the algorithm, then we describe its two extensions, corresponding to the ones we proposed in §4.1. §4.3 outlines a third potential extension that we propose as further work.

Finally, in Chapter 5, we present the results of using our algorithm to distribute different benchmark circuits drawn from the literature. We discuss these results and study the effect of both extensions of our algorithm. Chapter 6 ends the thesis by drawing some conclusions and suggesting further work.

Chapter 2

Quantum Computing: A brief overview

2.1 The principles of quantum computing

The advantages of using quantum mechanics to perform computations come down to the following three principles:

- *Superposition*: In classical computing, the unit of information is the *bit*, which may take one of two values: 0 or 1. In quantum computing, the *bit*'s counterpart is the *qubit*, whose value may be *any linear combination* of the 0 state and the 1 state, known as a *superposition*, and usually written as:

$$|qubit\rangle = \alpha|0\rangle + \beta|1\rangle$$

where α and β are complex numbers that must satisfy: $\alpha^2 + \beta^2 = 1$.

A popular analogy of a qubit's superposition is a coin spinning¹: the classical states (0 and 1) are *heads* and *tails*, but when the coin is spinning, its state is neither of them. If we knew exactly how the coin was spinning, we would be able to describe the probability of seeing heads or tails when it stops; these would be our α^2 and β^2 values. Besides, we may *measure* a qubit, and doing so corresponds in our analogy to abruptly stopping the coin, then checking if it is *heads* or *tails*. Through certain operations – that would correspond to altering the axis of spin of the coin –, we may change the coefficients α and β of the superposition.

In most quantum programs, we encode input and read output (after measurement) as standard classical binary strings. Therefore, for input/output we use as

¹Note this is just an analogy, and while a coin spinning can be perfectly described using classical physics, a qubit can not.

many qubits as bits would be required. Superposition allows us to maintain – during mid-computation – a superposition of all potential solutions to the problem, and update all of them simultaneously with a single operation to the qubits. In some sense, superposition allows us to explore multiple choices/paths of the computation, using only the resources required to explore a single one of those paths. And the number of paths we can explore simultaneously can be up to exponential, as a collection of N qubits may be in a state of superposition of all the possible 2^N classical states.

- *Interference*: As we just discussed, superposition gives us the ability to simultaneously explore different paths to solve a problem. However, in the end we will need to measure the qubits – stop the coins – and the result will be intrinsically random. For quantum computing to be any better than a probabilistic classical computer, we require the ability to prune the paths that have led to a result we do not want. This is precisely what *interference* provides: some operations on the qubits may make different classical states in the superposition cancel each other out. Interference is at the core of any speed-up achieved by a quantum algorithm, and taking advantage of it is the main challenge when designing quantum algorithms.
- *Entanglement*: Quantum mechanics allows the possibility of having a pair of qubits a and b in a superposition such as:

$$|a, b\rangle = \frac{1}{\sqrt{2}}|0, 0\rangle + \frac{1}{\sqrt{2}}|1, 1\rangle$$

This implies that, when we measure the qubits, we may either read $a = 0, b = 0$ or $a = 1, b = 1$ as outcome, never $a \neq b$ (the coefficients for $|0, 1\rangle$ and $|1, 0\rangle$ are both 0). Then, what happens if we only measure a ? In this particular case, we would also know b 's outcome, without measuring it. In short, acting on one qubit has an instantaneous effect on the other. Whenever a group of qubits exhibits this property, we say they are *entangled*. Entanglement holds regardless how far apart a is from b ; for instance, they could be on two different quantum processing units of a distributed grid. Indeed, entanglement will be key in our discussion of distributed quantum algorithms, and we explain how to use it to perform non-local operations in §3.2.

2.2 Building quantum computers

Physicists have come up with different ways of realising qubits in labs. The key idea is to find a physical system that displays non-classical behaviour, and put it under the appropriate circumstances so we can manage its quantum properties. At the same time, we must ensure that noise from the environment does not interfere with our quantum information. Van Meter and Devitt (2016) give an excellent survey of the state of the art of quantum architectures. Among these, the three most developed are:

- *Quantum optics*: The state of a qubit is represented in the properties of photons, for instance, their polarisation (Kok et al., 2007). A great advantage of this technology is that photons can be easily sent over long distances, while preserving their quantum state. Thus, protocols in quantum information that heavily rely on communication, such as Quantum Key Distribution (Shor and Preskill, 2000), are usually discussed and experimented with using quantum optics. The downside of this technology is that it is very difficult to make photons interact, which is required for universal computation.
- *Ion-traps*: Each qubit is embodied as an ion, confined inside a chamber by means of an electric or magnetic fields. The qubit is acted upon by hitting the ion with electromagnetic pulses (e.g. laser light or microwave radiation). Groups of experimentalists have proposed how to scale up the technology (Weidt et al., 2016), and are currently building prototypes.
- *Superconductors*: Small circuits, similar to classical electrical circuits, are cooled down to near absolute zero so the quantum interactions of electrons are not obscured by other perturbations. Different parts of the circuit encode different qubits, which can be acted upon by applying electric potentials. One of the main advantages of this approach is that the technology required for building the chips is fairly similar to the one for classical computer chips. This technology is the most experimentally developed. In fact, using it, both IBM and Intel have already built small generic-purpose quantum computers with up to 50 qubits, and Google claims to own a 72 qubit machine.

However, for quantum computers to be useful in real world applications, their qubit count should be larger than that. And, unfortunately, increasing the amount of qubits in a quantum computer is particularly difficult, due to some challenges we will now discuss.

2.2.1 Scalability challenges

There are two main challenges to overcome in order to build large scale quantum computers:

- *Decoherence*: In §2.1 we discussed the importance of having superposition in quantum computing, and we compared a qubit in superposition with a coin spinning. For similar reasons why a coin spinning will eventually stop, a qubit in superposition will eventually degenerate into a classical state (i.e. either $|0\rangle$ or $|1\rangle$). This phenomenon is known as *decoherence*. Experimentalists attempt to increase the time it takes for the state of the qubit to degenerate². Decoherence is the main constraint to scalability for quantum computers, as it limits the lifespan of qubits, limiting the number of operations that can be applied in a single program.

Certainly, the state of bits also degenerates in classical computers. However, in their case this is easier to account for: we can monitor the bits, and make sure to correct any unwanted change. This is not so simple in quantum computers, as monitoring a qubit would require *measuring* it, which destroys any quantum superposition. Nevertheless, it is still to some extent possible to protect our quantum state from errors – either due to decoherence or imperfect hardware – through specialised quantum error correction routines (Knill et al., 2000). This is a very active area of research, and it will be essential for the implementation of reliable large scale quantum computers.

- *Connectivity*: In order to run any computation on qubits, we will need to be able to apply multi-qubit operations on any subset of the computer's qubits. However, it is not realistic to expect that quantum computers will have fast connectivity between all qubits, for instance due to spatial separation of these in the hardware. In classical systems, the same problem is solved by a memory hierarchy, with a ceaseless flow of data going up and down of it, from main memory to registers (where computation is performed) and back. The memory hierarchy model works because data can stay idly in main memory while computation on the registers is carried out. However, in quantum computers we must avoid qubits

²A fundamentally different approach, *anyonic* (a.k.a. topological) quantum computing, has been proposed to avoid the problem of decoherence altogether. It would use physical systems that, theoretically, can be completely protected against decoherence (Nayak et al., 2008). Although promising, currently this proposal has little experimental underpinning, and it is not regarded as attainable in the near future.

being idle, as decoherence prevents the existence of long-lasting memory. An alternative found in classical computers is to distribute the computation across different processing units each having its own local memory, which they use intensively. In these distributed systems, communication across computers is the main bottleneck, and it should be performed as little as possible.

2.2.2 Models of computation

In this section, we give a brief introduction to some models of quantum computation relevant to this thesis.

Circuit model. Any operation on n qubits – as long as measurement (i.e. destruction of information) is not involved – can be represented as a square matrix of complex numbers, of dimension 2^n . These matrices must be unitary, which means that a matrix U satisfies $UU^\dagger = I = U^\dagger U$, where I is the identity matrix and U^\dagger is the conjugate transpose of U . Essentially, unitarity ensures that any operation on qubits can be reversed (i.e. undone), reason why this model is sometimes called the reversible model. Multiplying matrices AB corresponds to applying the operation described by B first, then A , on the same qubits. Application of two operations on disjoint sets of qubits corresponds to the Kronecker product of the matrices, $A \otimes B$. Given that any of these matrices can be represented as a product of other unitary matrices, we may decompose any operation into smaller building blocks: quantum gates.

In this model, qubits are pictured as wires to which quantum gates are applied, similarly to a classical digital circuit. The set of quantum gates used is determined by the hardware. There is an (uncountable) infinite amount of different quantum operations, but a small finite set of them is enough to approximate any operation up to a desired error factor. The most common choice of such a universal gate-set is *Clifford+T*, which contains six one-qubit gates, and a single two-qubit gate. The depiction of the gates from the Clifford+T set, and some of their most important properties are shown in Figures 2.1 and 2.2. All the properties from Figure 2.2 can be easily checked by calculating the matrix representing each of the circuits³. Circuits are read from left to right.

The CNOT gate is particularly interesting. The qubit where the filled dot is (see Figure 2.1) acts as the ‘control’, and the qubit with \oplus acts as the ‘target’. Whenever the control is $|0\rangle$, no change is made in either of the qubits; but if it is $|1\rangle$, an X gate is

³Overall factors of norm 1 are irrelevant to the computation, so they are ignored in the circuit representation. E.g., algebraically: $iXZ = Y = -iZX$, but the i and $-i$ factors are ignored in Figure 2.2.

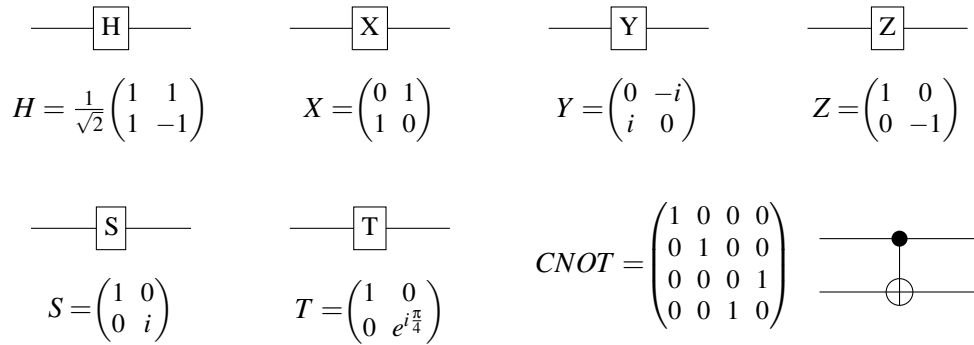


Figure 2.1: The Clifford+T gate set. Both their matrix and circuit representation are given.

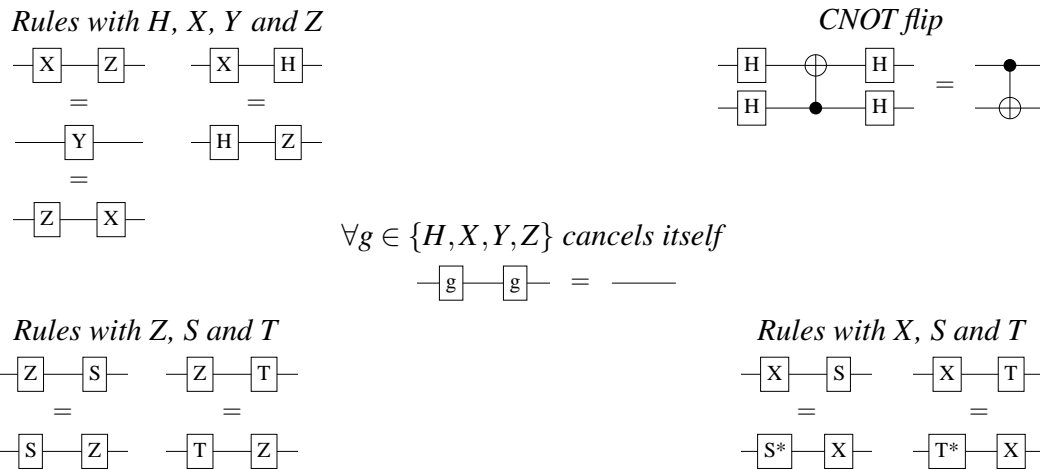


Figure 2.2: Some basic properties of the gates in the Clifford+T set. Here, S^* and T^* represent the inverse gates of S and T , i.e. their conjugate transpose, usually written as S^\dagger and T^\dagger .

applied to the target, flipping the state of the qubit. This works in any superposition, so given an arbitrary two-qubit state

$$|c, t\rangle = \alpha|0, 0\rangle + \beta|0, 1\rangle + \gamma|1, 0\rangle + \delta|1, 1\rangle$$

if the CNOT were to act in $|c\rangle$ as control and in $|t\rangle$ as target, the outcome would be:

$$CNOT \cdot |c, t\rangle = \alpha|0, 0\rangle + \beta|0, 1\rangle + \gamma|1, 1\rangle + \delta|1, 0\rangle$$

MBQC model. The acronym stand for Measurement Based Quantum Computing. Unlike the circuit model, where measurements are done at the very end of the circuit, MBQC carries out computations by means of repeatedly measuring an initially entangled resource. The process can be thought of as sculpting a rock. The rock would be the initial resource, which is a collection of entangled qubits forming certain lattice structure. By measuring some qubits in the lattice – hitting the rock with a chisel – we remove some of the excess qubits, changing the overall state in the process. The outcome of measurements is probabilistic so, in order to provide deterministic computation, we must apply corrections on the neighbouring qubits whenever the measurement outcome deviated from the desired result. After multiple iterations of measurements and corrections, we end up with a set of qubits encoding the result. In this model, the input is incorporated into the lattice at the beginning of the process.

In this way, any computation may be performed by applying 1-qubit measurements and 1-qubit correcting gates (controlled by classical signals). The initial resource state contains all the entanglement that is required, which may be prepared experimentally through multi-qubit interactions, such as Ising interactions (Raussendorf and Briegel, 2001), which are within our experimental capabilities. This model deals with the connectivity problem by applying a single operation involving *all* the qubits at the beginning of the process, then only requiring cheap single qubit operations for the rest of the computation. The main drawback of MBQC is the large amount of qubits that are required for even the simplest of operations. The MBQC model was proposed for the first time by Raussendorf and Briegel (2001) under the name of *one-way quantum computer*, which highlights its main difference with the circuit (reversible) approach.

Distributed model. We may find a balance between the circuit model and MBQC. In it, multiple small quantum processing units (QPUs) would run fragments of the overall circuit. Communication is achieved through a shared entangled resource, reminiscent of the MBQC approach. This model has been discussed in detail in the literature (Van Meter et al., 2010) and it is at the core of the main project from the

Networked Quantum Information Technologies Hub (NQIT)⁴. In §3.3, we discuss an abstract distributed quantum architecture in detail.

2.3 Programming on quantum computers

As of today, most quantum programming languages are merely high level circuit descriptors, providing the means to define circuits gate by gate, or build them up from combinations of smaller circuits. All of the well-known languages belong to this category, such as *QCL* (Ömer, 2003) (imperative paradigm, and one of the first quantum programming languages ever implemented), *Q#* (Svore et al., 2018) (imperative, designed by Microsoft), and *Quipper* (Green et al., 2013) (functional, built on top of Haskell).

Besides, there are attempts at designing quantum programming languages that are completely hardware agnostic, meaning they aim to describe the computation, rather than a particular circuit that implements it. Examples of these are the different attempts at defining a quantum lambda calculus, for instance the ones by Van Tonder (2004) or Díaz-Caro (2017). However, these are not particularly programmer friendly, as they are generally quite verbose.

Most of the literature on quantum algorithms describes them by explicitly giving a circuit that implements the algorithm. Fortunately, there is a constructive procedure, given by the Solovay-Kitaev theorem – of which Dawson and Nielsen (2005) give a good introductory review –, that takes any circuit and a choice of universal gate-set and outputs an equivalent circuit using only those gates. In particular, for the case of the Clifford+T gate set, Ross and Selinger (2014) gave an algorithm that outputs the optimal implementation of some quantum operations on this gate set. Hence, programmers do not need to worry about the gates they are using when describing their circuits.

Unfortunately, the fact that algorithms are almost exclusively defined in the circuit model implies that other models of quantum computing are disregarded by a large portion of the community. In order to make other models of computation accessible, we need to provide automated procedures for transforming algorithms from the circuit model to the rest (and vice versa). Work has been done on the transformation from circuit to MBQC and backwards, the latter being the most challenging (Duncan and Perdrix, 2010). However, there is little amount of literature describing how to go from

⁴A project supported by the UK National Quantum Technology program, aiming to provide scalable quantum computing.

the circuit model to the distributed model. In §3.2 we give an overview of the existent work on that aspect, and identify the gap on the literature we aim to cover in this thesis.

Remark 2.1. Here are the key concepts to keep in mind while reading the rest of this thesis:

- Quantum computers provide a computing power well beyond the capabilities of classical computers, which would be exploitable in many areas of science.
- Small quantum computers are already available.
- Scaling up is a challenging problem due to: *decoherence*, which may be overcome by the joint effort of the error-correction, physics and engineering communities; and *connectivity*, which may be solved using distributed architectures.
- There is practically no programming support for distributed architectures.

Chapter 3

Distributed Quantum Computing

As we discussed in §2.2, there are different approaches on how to build quantum computers. Now that many of these have been experimentally demonstrated, the question of how to scale up is increasingly relevant. This has led to the proposal of distributed architectures (Van Meter and Devitt, 2016).

In classical computing, an standard example of a distributed computer is the Non-Uniform Memory Access (NUMA) architecture: A system of independent computing nodes, each having its own local memory. In order to collaborate to perform an overall computation, the different nodes will need to communicate. In NUMA, they do so by accessing each other's memory. While nodes can manage their own local memory efficiently, accessing another node's memory is slow. Hence, we always attempt to minimise the amount of communication between nodes. A distributed quantum computer would follow the same principles, where each quantum processing unit (QPU) would own a collection of qubits (its local memory) and may access another QPU's qubits at the cost of some overhead, using entanglement.

3.1 Communication through entanglement

For a QPU to be able to access another's qubit, we must provide them with some sort of communication channel. Simply using a classical channel (sending bits) is not helpful: the whole point of representing the state of the computation in qubits is that they may be in a superposition of classical states, which would take up to an exponential amount of space and processing on bits. We could consider physically moving the system that encodes the qubit from one QPU to another, and while that is certainly possible with photons, in general it is not feasible to have a channel that is both fast and protects well

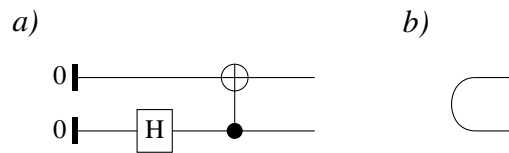


Figure 3.1: Generation of the Bell state $|\Phi^+\rangle = \frac{1}{\sqrt{2}}|0,0\rangle + \frac{1}{\sqrt{2}}|1,1\rangle$ shown in *a*). Its shorthand circuit notation is given in *b*).

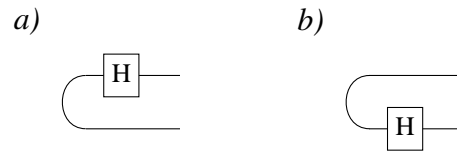


Figure 3.2: Applying a gate on a Bell state. The circuits shown in *a*) and *b*) are equivalent.

against information loss due to decoherence.

In §2.1, we explained it was possible to affect a distant qubit by acting on another qubit with which it was entangled. We wish to exploit this property in order to allow a QPU to query another’s QPU qubits. There are different degrees of how strong a pair of qubits is entangled – intuitively, how much they affect each other. This is often formalised as the correlation between the qubits measurement outcomes; for instance, the pair of qubits $\frac{1}{\sqrt{2}}|0,0\rangle + \frac{1}{\sqrt{2}}|1,1\rangle$ is said to be *maximally entangled*¹, as measuring both of these qubits in the same basis will always yield matching outputs: either (0,0) or (1,1). Naturally, the most efficient communication channel will take advantage of entanglement in its strongest form, and so we will make use pairs of qubits entangled in this particular maximally entangled state. This qubit pair configuration is generally known as a Bell state, and Figure 3.1 shows how to prepare it.

An interesting property of the Bell state is shown in Figure 3.2: if a quantum gate, whose matrix representation is symmetric, is applied to one of the qubits, it is the same as if the gate was applied to the other qubit. In some sense, the gate can ‘slide’ through the entanglement, like beads on a string; as if the entangled state were a curved wire, connecting the pair of qubits. Hopefully, this serves as a first intuition of how Bell states are a natural choice for implementing quantum communication.

¹Meaning that the outcome of measuring one of the qubits in any basis will determine, with hundred percent certainty, the result of a later measurement on the other one (in the same basis).

3.1.1 Entanglement distillation

So far, we have explained how to generate a Bell state $|\Phi^+\rangle = \frac{1}{\sqrt{2}}|0,0\rangle + \frac{1}{\sqrt{2}}|1,1\rangle$ inside a QPU (as in Figure 3.1). However, what we aim for is that two different QPUs each own one of the qubits from $|\Phi^+\rangle$. The challenge is then to send one of the qubits to another QPU, while preserving the state. The problem of sharing a Bell state between two parties is solved by the *entanglement distillation* protocol (Bennett et al., 1996), which ensures the shared pair of qubits are in the Bell state, up to some small error factor. In this section, we will give a brief explanation of how this protocol works.

In practice, there are no perfect communication channels. This means that it is impossible to send a quantum state without potentially altering it, introducing errors. And, as we mentioned earlier in §2.2.1, detecting and correcting errors in quantum information is particularly challenging. Fortunately, in our case there is an easy way around it. We can create multiple $|\Phi^+\rangle$ states in the first QPU, and send one of the qubits of each of these pairs to the second QPU, through a noisy channel. Then, we would have shared multiple imperfect $|\Phi^+\rangle$ pairs, whose fidelity we can improve by making them interact with each other, destroying some of the pairs in the process. Before going into details on how we perform these interactions, we need some definitions:

- *Werner state*: It is the result of sending one of the qubits from $|\Phi^+\rangle$ through a noisy channel characterised by a constant $F \in [0, 1]$. F determines the *fidelity* of the channel, i.e. the probability that the qubit is sent without altering its state. Rather than an actual quantum state, the Werner state is a probability distribution of quantum states, known in the literature as a *mixed state*. In particular, it is the probability distribution of actually having $|\Phi^+\rangle$, with probability F , or having $|\Phi^+\rangle$ with an X gate mistakenly applied to the sent qubit, having $|\Phi^+\rangle$ with a Z gate on it or having $|\Phi^+\rangle$ with both X and Z errors, each of these three cases² occurring with equal probability $\frac{1-F}{3}$.
- *Bilateral XOR (BXOR)*: Simply, two CNOT gates applied inside two different QPUs. Its intended use is to be applied to two Werner states; one QPU should have one of the qubits of each Werner state, and apply a CNOT on them, while

²Although a channel will rarely introduce each of these errors with equal $\frac{1-F}{3}$ probability, it is always possible to apply some local operations on each of the qubits so the probability distribution converges to that of the Werner state. Moreover, there may be channels that introduce errors other than X and Z ; however the resulting state after sharing $|\Phi^+\rangle$ through any of these will always be some Werner state with some particular F .

the other should do the same on the other two qubits. Thus, one of the Werner states acts as control of both CNOTs, and the other as their target.

The entanglement distillation protocol takes a collection of Werner states and repeats the following three steps multiple times, until the fidelity of the Werner states is the one desired:

1. Make pairs of two Werner states, and apply a BXOR to each pair. The new probability distribution (mixed state) on each of these four qubits is given in Table 3.1.
2. For each pair of Werner states, measure the qubits corresponding to the Werner state that acted as the target of the BXOR – this will require one measurement in each QPU. The outcome of the two measurements will match precisely in the cases where the fifth column of Table 3.1 shows no X error. Examining the table, we can calculate the probability of that event:

$$T(F) = F^2 + \frac{2}{3}F(1-F) + \frac{5}{9}(1-F)^2$$

which, for $F > \frac{1}{2}$, is always over a half.

3. If the outcome of both measurements matched, keep the other two qubits (i.e. the control Werner state). Otherwise, discard them, not to be used again. Among the eight cases when we keep the Werner state, in two of them (greyed rows in Table 3.1) the state we keep has no errors. This happens with probability:

$$P(F) = \frac{F^2 + 1/9(1-F)^2}{T(F)}$$

Thus, the kept qubit pairs are all Werner states with fidelity $P(F)$ which, as shown in Figure 3.3, is greater than F whenever $F > \frac{1}{2}$.

Figure 3.3 implies that we may use a communication channel as noisy as to introduce errors slightly less than half of the times, and still generate a Werner state whose fidelity is arbitrarily close to one. Naturally, the more fidelity we wish to attain, and the worse the fidelity we start with is, more iterations of the protocol will be required. This would increase the amount of time and resources – number of initial Werner states – we must pay in order to obtain a single entangled qubit pair.

Often in distributed quantum computing literature, a Bell state shared by two QPUs is known as an *ebit* (entangled-bit) which, put another way, is just a Werner state with a fidelity close to one. Thus, this protocol produces ebits, which is the fundamental resource for quantum communication in distributed circuits. During the rest of this thesis, we use the term *ebit half* to refer to any of the two qubits that comprise an ebit.

Table 3.1: Probability distribution defining a pair of Werner states, and the errors present in each case, before and after the BXOR is applied.

| Probability | Errors before | | Errors after | | Kept? |
|----------------------|---------------|--------|--------------|--------|-------|
| | Source | Target | Source | Target | |
| F^2 | – | – | – | – | ✓ |
| $\frac{1}{3}F(1-F)$ | – | Z | Z | Z | ✓ |
| $\frac{1}{3}F(1-F)$ | – | X | – | X | |
| $\frac{1}{3}F(1-F)$ | – | X,Z | Z | X,Z | |
| $\frac{1}{3}F(1-F)$ | Z | – | Z | – | ✓ |
| $\frac{1}{9}(1-F)^2$ | Z | Z | – | Z | ✓ |
| $\frac{1}{9}(1-F)^2$ | Z | X | Z | X | |
| $\frac{1}{9}(1-F)^2$ | Z | X,Z | – | X,Z | |

| Probability | Errors before | | Errors after | | Kept? |
|----------------------|---------------|--------|--------------|--------|-------|
| | Source | Target | Source | Target | |
| $\frac{1}{3}F(1-F)$ | X | – | X | X | |
| $\frac{1}{9}(1-F)^2$ | X | Z | X,Z | X,Z | |
| $\frac{1}{9}(1-F)^2$ | X | X | X | – | ✓ |
| $\frac{1}{9}(1-F)^2$ | X | X,Z | X,Z | Z | ✓ |
| $\frac{1}{3}F(1-F)$ | X,Z | – | X,Z | X | |
| $\frac{1}{9}(1-F)^2$ | X,Z | Z | X | X,Z | |
| $\frac{1}{9}(1-F)^2$ | X,Z | X | X,Z | – | ✓ |
| $\frac{1}{9}(1-F)^2$ | X,Z | X,Z | X | Z | ✓ |

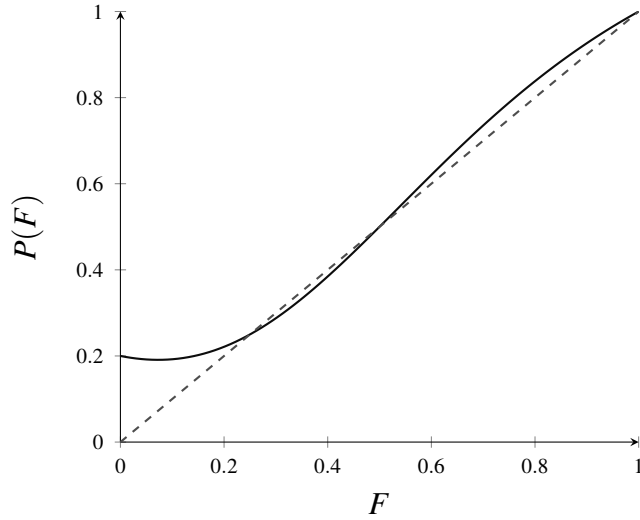


Figure 3.3: Fidelity after a single iteration of the distillation protocol, versus the original fidelity. The figure shows that $F > \frac{1}{2} \Rightarrow P(F) > F$.

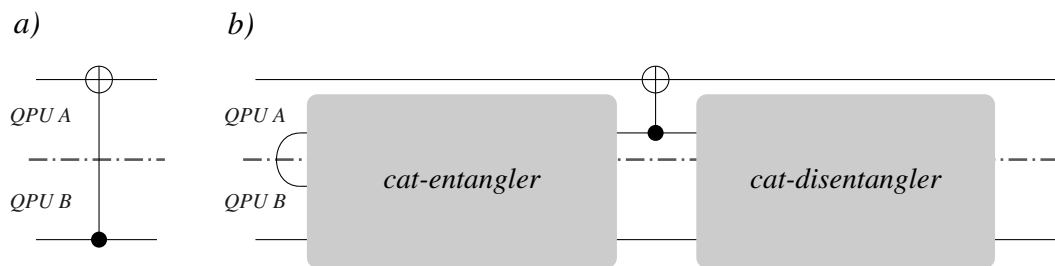


Figure 3.4: A non-local CNOT, shown in *a*). The dashed line indicates how the circuit is separated into two QPUs. The implementation scheme is given in *b*).

3.2 Distributing circuits

We now explain how ebits are used to allow a QPU to peek into another’s qubits. Here, we will introduce the proposal of Yimsiriwattana and Lomonaco Jr (2004). Later on, in §4.1, we will extend this work with our own contributions.

We aim to split a given circuit and distribute the fragments across multiple QPUs. The gates that should operate over qubits on different QPUs are known as *non-local* gates. As we previously mentioned in §2.2.2, any circuit can be converted to Clifford+T circuit. In Clifford+T, the only gate that operates on more than one qubit is the CNOT. Hence, we only need to understand how CNOTs can be implemented non-locally.

The construction we will use is a slight variation of what was proposed by Yimsiriwattana and Lomonaco Jr (2004), and its scheme is shown in Figure 3.4. The dashed grey line in the figure represents the *boundary* where QPU A ends and QPU B starts. This is the convention we will use on the figures throughout this thesis. All of the wires (qubits) and quantum gates above the dashed line should be implemented on one QPU, and the ones below it on another. Any line crossing the boundary represents communication across QPUs, which for a valid distributed circuit is only allowed if it is an ebit – a curved wire – or it represents classical communication – as in Figure 3.5. We will call the QPU that holds the target qubit (the one with a \oplus) the ‘target QPU’ and similarly for the control qubit.

The implementation of a non-local CNOT gate has three steps. First, we must apply what the authors refer to as the *cat-entangler* (shown in Figure 3.5), which creates a local ‘copy’³ of the control qubit inside the target QPU. In the process, the ebit

³Note that there is no such thing as copying a quantum state (due to the non-cloning theorem). What we mean here by ‘copying’ is generating, from $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$, the state $|\psi'\rangle = \alpha|0,0\rangle + \beta|1,1\rangle$ where each of the classical states is duplicated. This is fundamentally different from an actual copy: $|\psi\rangle \otimes |\psi\rangle = \alpha^2|0,0\rangle + \alpha\beta|0,1\rangle + \alpha\beta|1,0\rangle + \beta^2|1,1\rangle$.

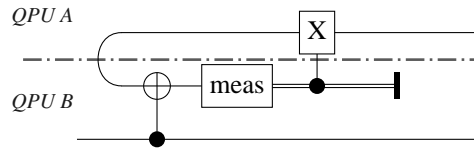


Figure 3.5: Implementation of the cat-entangler. An ebit is used to make the information in QPU *B*'s wire available to QPU *A*. A doubled line indicates the wire holds classical information. Hence, the *X* gate is classically controlled, and the line that crosses the boundary represents classical communication. For any input state $\alpha|0\rangle + \beta|1\rangle$, the output is $\alpha|0,0\rangle + \beta|1,1\rangle$.

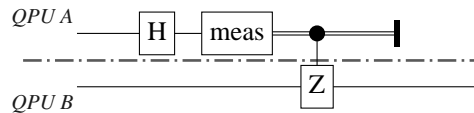


Figure 3.6: Implementation of the cat-disentangler. Essentially, it destroys the ebit half (top wire) that the cat-entangler coupled with QPU *B*'s wire. A doubled line indicates the wire holds classical information (a bit). For any input state $\alpha|0,0\rangle + \beta|1,1\rangle$, the output is $\alpha|0\rangle + \beta|1\rangle$.

half in the control QPU is measured (and thus destroyed), and the outcome is used to correct the other half, in the same spirit as in the MBQC model. These corrections are done via *classically controlled gates*; devices that either apply a transformation to the qubit or none, depending on the value of a classical bit. Notice that the only information physically crossing the boundary between blocks is the *classical* outcome of the measurement (a bit, either 0 or 1).

Then, the CNOT gate is applied *locally* inside the target QPU, between its ebit half and the target qubit. At the end, the *cat-disentangler* must be applied (shown in Figure 3.6), which simply destroys – with a measurement – the remaining ebit half and then corrects the control qubit. Once again, only classical information crosses the boundary.

In this way, we have implemented a non-local CNOT gate using one ebit and two classical bit messages between QPUs. However, the true advantage of this approach is gained when multiple non-local CNOTs are implemented using a single ebit: Once the cat-entangler is applied, any number of CNOTs that are controlled by the same wire and whose target QPU is the same, may all be implemented using the same ebit half as control, as shown in Figure 3.7.

Now, depending of how we choose to partition the circuit, there will be different groups of CNOTs that we may be able to implement using a single ebit. We will then

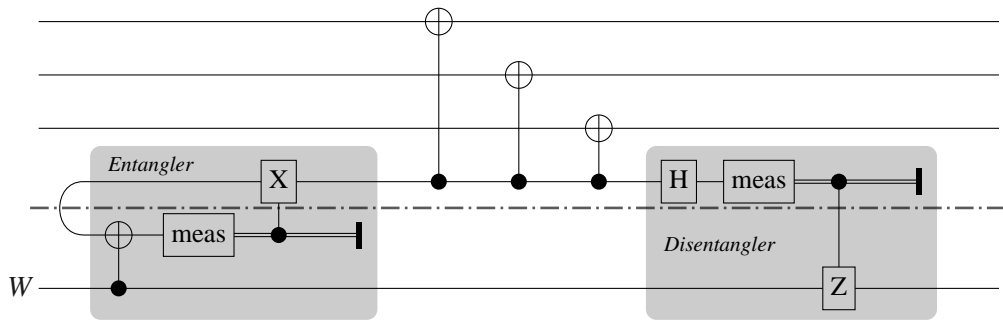


Figure 3.7: Implementing three non-local CNOTs using a single ebit. Wire W acts as control for the three of them. Only classical information crosses the boundary between QPUs, apart from the previously shared ebit.

wish to find the partition that requires the fewest ebits to implement all of its CNOT gates. This optimisation problem is not discussed in the original paper, nor in any other work, as far as we know. It will be our main contribution in this thesis, along with an extension of the results just explained, both found in Chapter 4.

3.3 Distributed quantum architectures

In this section we propose an abstract distributed quantum architecture. We claim that any distributed quantum computing technology will be characterised by the following features:

- *Multiple quantum processing units (QPUs):* Each of the QPUs should be able to perform universal quantum computation on its collection of ‘workspace’ qubits. It should be possible to prepare these qubits to hold the input data of a program, and read output from them (measurement). It should also be possible to apply classically controlled gates on the qubits.
- *Specialised space for ebits:* Each QPU should have some extra qubits meant to be used as ebit halves. These should be specialised so the operations necessary for ebit generation can be applied on them fast and reliably. The QPU should support the application of CNOTs (or some other suitable 2-qubit gate) between these specialised qubits and the ones in its workspace.
- *Ebit generation hardware:* This includes the (noisy) quantum communication channel itself and the ability to perform the distilling process. The generation

of ebits may be done either in a centralised manner, with a separated device that creates Bell states and sends them to the different QPUs, or decentralised, each QPU having their own hardware for creating and sharing ebits. Depending on the technology used, entanglement distillation may be more or less essential; for instance, if the step of sharing Bell states is done using quantum optics (photons), the quantum channel is likely to be fairly reliable, so it would only require a few iterations of the distilling process.

- *Classical communication network*: Which will be required in the process of entanglement distillation, as well as to perform cat-entanglers and cat-disentanglers. The QPUs will send signals through the network when they measure their qubits, and read from it to apply corrections.

As we discussed in §3.1.1, there is a compromise between the quality of the ebits and the effort put into preparing them. Fortunately, Cirac et al. (1999) showed that efficient distributed quantum computation using noisy ebits is feasible. Nevertheless, ebit generation will always be the main bottleneck of any distributed quantum architecture, as it is by far more expensive than classical communication and any local operation (in fact, multiple local operations are required in order to generate and use an ebit). Therefore, we will want to minimise the number of ebits required to implement any given algorithm.

Van Meter et al. (2010) have proposed an experimental distributed quantum architecture. They explain how each of the features listed above may be implemented, particularly focusing on how entanglement across QPUs is achieved (ebit generation). Their proposal is to use cavities (traps) where the particles encoding the qubits are kept, and use laser pulses (photons) to entangle cavities of different QPUs together.

Chapter 4

Automated Distribution of Quantum Algorithms

4.1 Implementing non-local CNOT gates

In §3.2, we explained the proposal by Yimsiriwattana and Lomonaco Jr (2004) of how to implement a non-local gate. In their work, a single ebit could be used to implement multiple CNOTs only if they shared a common control wire, and no operation was applied on it between the CNOTs. We will now extend their results.

Our first extension comes from the fact that some of the 1-qubit gates from the Clifford+T set commute with the CNOT gate. This means that, if there are operations in between CNOTs, we may transform the circuit to an equivalent version where the CNOT gates are brought together. All of the relevant circuit transformations are shown in Figure 4.1. As also shown in Figure 4.1, some gates do not commute with CNOT, but we can still interchange them if we add an extra 1-qubit gate.

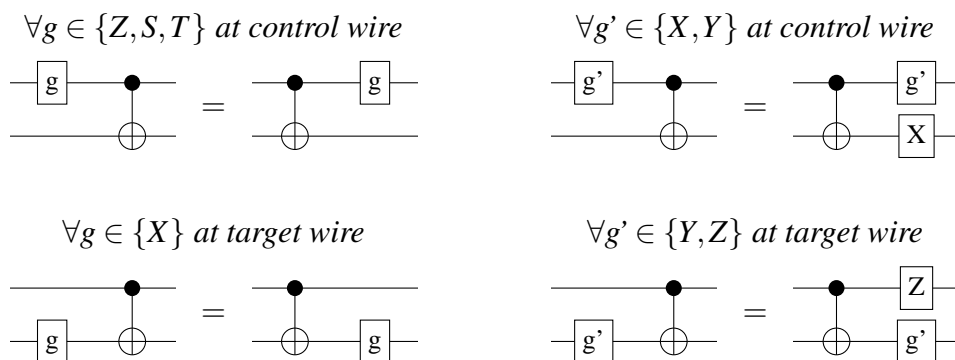


Figure 4.1: Different cases when a 1-qubit gate can be pushed through a CNOT gate.

The second improvement comes by realising that the method used to implement multiple CNOT gates controlled by the same wire can also be applied if multiple CNOTs have a common target qubit instead. We will refer to the former method as the *remote-control* method, and to the latter as the *remote-target* method. The derivation of the remote-target method is shown in Figure 4.2, which uses some of the properties listed in Figure 2.2.

4.2 Finding an efficient distribution

In this section we explain how we search for an efficient distribution of the circuit. First, we establish what we mean by a distributed circuit to be efficient. This notion is based on our discussion about the essential characteristics of distributed quantum architectures (see §3.3). We say that a distributed circuit is efficient when there is:

- *Minimal amount of quantum communication* between the QPUs, meaning it requires as little number of ebits as possible. In comparison, message passing of classical bits is considered negligible and it is not taken into account.
- *Load-balance across the QPUs*, up to a tolerance margin. Our notion of load-balance is that the different QPUs should have a similar number of qubits assigned to them. Uniform depth of the local circuits (i.e. length of the circuits) would also be desirable. However, none of our distribution techniques change the depth in a significant way. Hence, we will not optimise circuit depth when distributing a circuit, and instead assume that methods for depth reduction, such as the one described by da Silva et al. (2013), have already been applied on the input circuit, and may be applied again to each QPU's local circuit. As we do not take into account circuit depth, we consider the cost of local gates negligible.

The problem at hand is similar to the (k, ϵ) -*graph partitioning* problem. In it, a graph partition in k subgraphs has to be found, minimising the number of *cut edges*: edges that reach vertices in different subgraphs. Additionally, the partition must satisfy that the number of vertices in each subgraph is less than $(1 + \epsilon)\frac{N}{k}$, where N is the total number of vertices in the graph. In Table 4.1 we list the correspondences between the graph partitioning problem and the efficient distribution of quantum circuits.

But there is a caveat. If we use graph partitioning we will not be exploiting the fact that multiple CNOT gates may be implemented using a single ebit. As shown

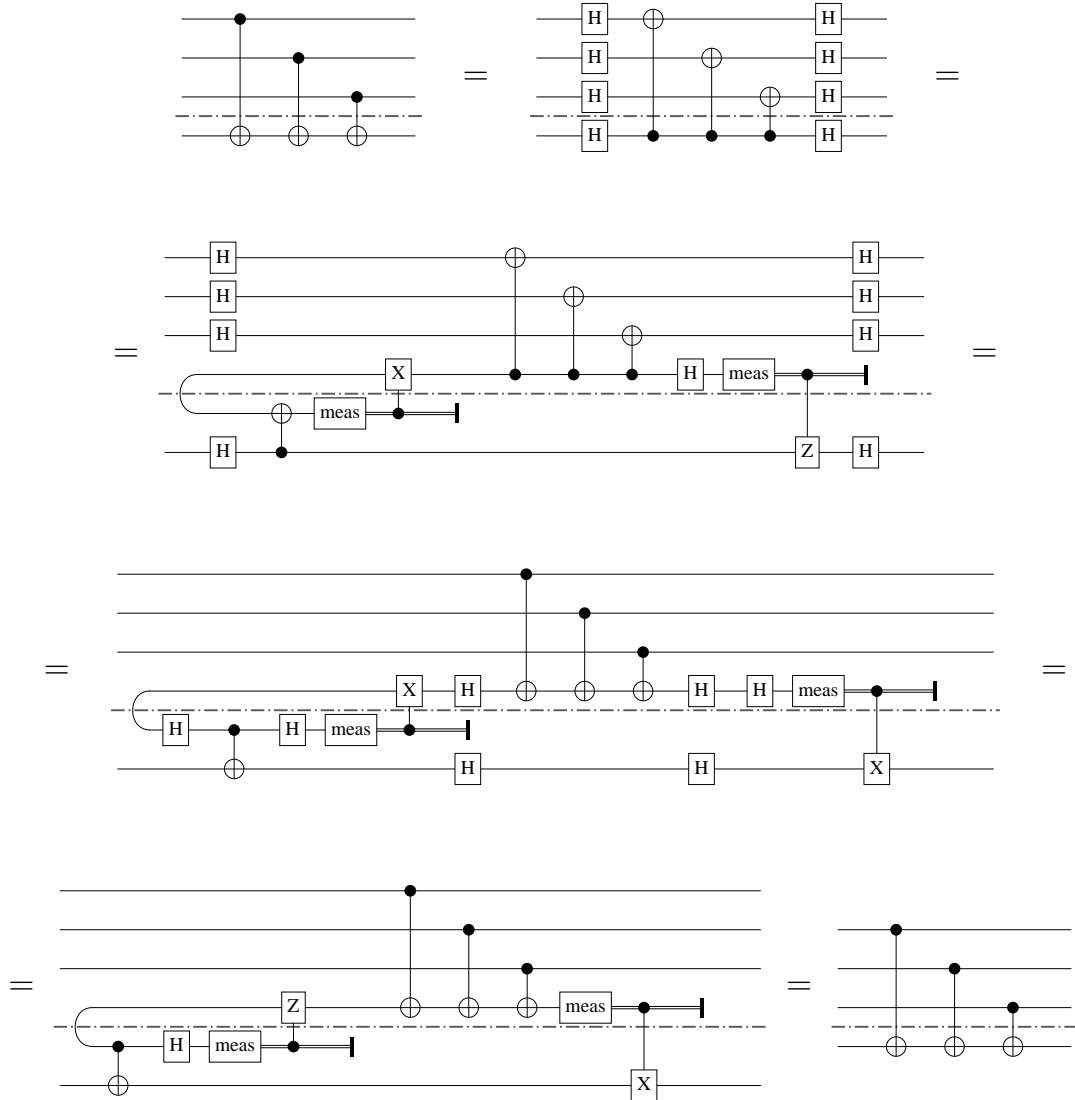


Figure 4.2: Proof of the remote-target method: implementation of multiple non-local CNOT gates that share a common target, using a single ebit. The proof uses properties given in Figures 2.2, 3.2 and 3.7. The distributed circuit is similar to the one for the remote-control method (Figure 3.7). Both cat-entangler and cat-disentangler slightly differ.

Table 4.1: Correspondence between the graph partitioning problem and the efficient distribution of quantum circuits.

| <i>Graph partitioning</i> | <i>Efficient distribution</i> |
|---------------------------|-------------------------------|
| Vertices | Circuit wires (qubits) |
| Edges | CNOT gates |
| Partitioned graph | Distributed circuit |
| Subgraph | QPU |
| Min. cut edges | Min. non-local gates |
| Uniform subgraph size | Load-balance |

in Table 4.1, the graph partitioner would minimise the number of non-local CNOTs, instead of the number of ebits. In what follows, we will explain how to make use of *hypergraph* partitioning to minimise the ebit count. A more detailed review of the hypergraph partition problem is given in Appendix A, here we summarise the key concepts:

- Hypergraphs extend graphs to accommodate edges that may reach more than two vertices. More formally, a hypergraph is a pair (V, H) , where V is the set of vertices and $H \subseteq 2^V$ is the collection¹ of hyperedges. Each hyperedge is defined as the subset of vertices from V it connects. We will not consider any notion of directionality.
- Hypergraph partitioning follows the same premise as graph partitioning. The user provides a hypergraph and two parameters (k, ϵ) , which have the exact same meaning as before. What the problem now attempts to minimise is a metric known as $\lambda-1$, which is defined as follows: Given a partition of the hypergraph, the function $\lambda: H \rightarrow \mathbb{N}$ maps each hyperedge to the number of different *blocks*² its vertices are in. Then, $\lambda-1 = \sum_{h \in H} \lambda(h) - 1$ provides a measure of not only how many hyperedges are cut but also how many blocks they are connecting.

In the following subsections, we explain how hypergraph partitioning can be used to find the most efficient distribution of a circuit. First, we only use the implementation of non-local gates described by Yimsiriwattana and Lomonaco Jr (2004), reviewed in

¹We will allow the existence of multiple identical hyperedges, in the same way as multigraphs allow multiple edges across a pair of edges.

²The term *block* is often used to refer to each of the sub-hypergraphs the hypergraph is partitioned into. It is the term we will use throughout this thesis.

Algorithm 4.1: Builds the hypergraph of a given circuit. H may contain multiple hyperedges connecting the same vertices. This algorithm runs in time $O(g)$, where g is the number of gates in the input circuit.

```

1  input: circuit
2  output: (V,H)
3  begin
4    V  $\leftarrow$   $\emptyset$ 
5    H  $\leftarrow$   $\emptyset$ 
6    hedge  $\leftarrow$   $\emptyset$ 
7    foreach wire in circuit do
8      V  $\leftarrow$  V  $\cup$  {wire}
9      hedge  $\leftarrow$  {wire}
10     foreach gate in wire do
11       if gate == CNOT and controlOf(gate) == wire then
12         hedge  $\leftarrow$  hedge  $\cup$  {targetOf(gate)}
13       else
14         H  $\leftarrow$  H + {hedge}
15         hedge  $\leftarrow$  {wire}
16     H  $\leftarrow$  H + {hedge}
17  end

```

§3.2. Later on, we extend the algorithm to include the improvements we have proposed in §4.1.

4.2.1 Vanilla algorithm

The main challenge is how to use hyperedges to represent a collection of CNOT gates that could be implemented using a single ebit. In this first version of the algorithm, we will group CNOTs together only if they share a common control wire and there are no other gates in between their connections to that wire. For every such a collection of CNOT gates, we will create *a single hyperedge*. The hyperedge's vertices will correspond to the controlling wire and each of the different wires the CNOTs target. Algorithm 4.1 receives a circuit as input and builds its hypergraph in this way.

We then solve the hypergraph partitioning problem (see Appendix A) on the resulting hypergraph. Once a partition of the hypergraph is obtained, we map the partition back to the circuit, distributing it. The way the vertices are assigned to the blocks determines how the corresponding wires are allocated to the different QPUs. The $\lambda - 1$

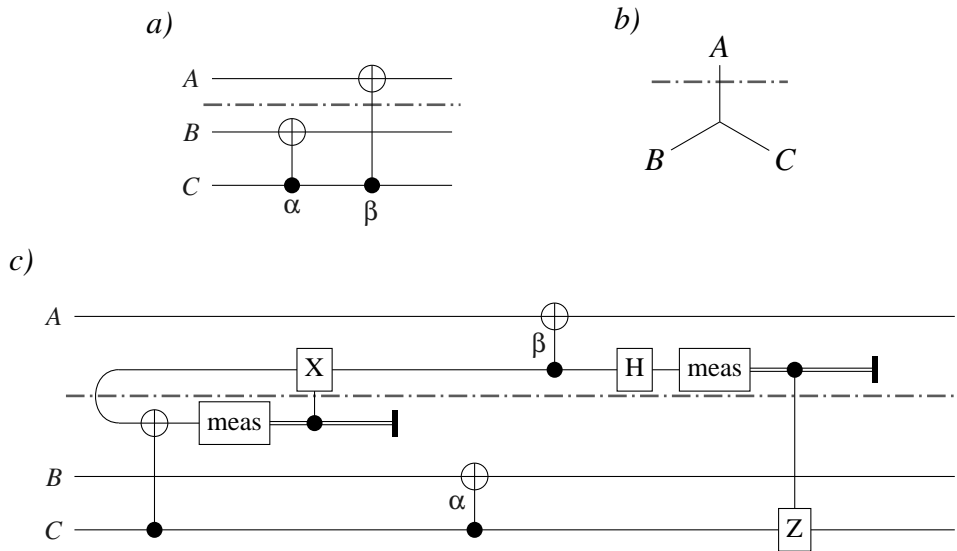


Figure 4.3: The CNOTs in circuit *a*), labelled α and β , are adjacent at their control wire. Therefore, a single hyperedge is used to represent both in *b*). The proposed cut makes only one of the CNOTs non-local, which is implemented in *c*) using one ebit.

metric of the partition indicates the number of ebits that will be necessary to implement all the non-local CNOT gates. The problem of finding the optimal partition for a hypergraph built by Algorithm 4.1, and the problem of efficiently³ distributing a circuit are equivalent – given any solution to one of them, we can compute a solution for the other. We formalise this fact in the Theorem 4.1.

Figures 4.3, 4.4 and 4.5 provide simple examples of the one-to-one correspondence discussed in Theorem 4.1. In these figures, and in all of the figures throughout this thesis, hypergraphs are represented using the following convention: Letters are vertices, and each hyperedge is represented as a collection of line segments that reach each of the hyperedge’s vertices, while the other end of the segments meet at the same point. A hypergraph partition is represented in a similar way as a partition of circuits; a dashed grey line splits the hypergraph, determining which vertices go to each block.

Theorem 4.1. *Given any circuit C , and its hypergraph \mathcal{H} generated by Algorithm 4.1, there is a bijection between partitions of \mathcal{H} with λ_c cuts and vanilla⁴ distributions of C that use λ_e ebits; satisfying $\lambda_c = \lambda_e$.*

Proof. We define this bijection inductively. First, we provide the bijection between the

³Where efficiency is assessed as discussed in the beginning of this section.

⁴Meaning that non-local CNOT gates may only be implemented using the remote-control method from Figure 3.7.

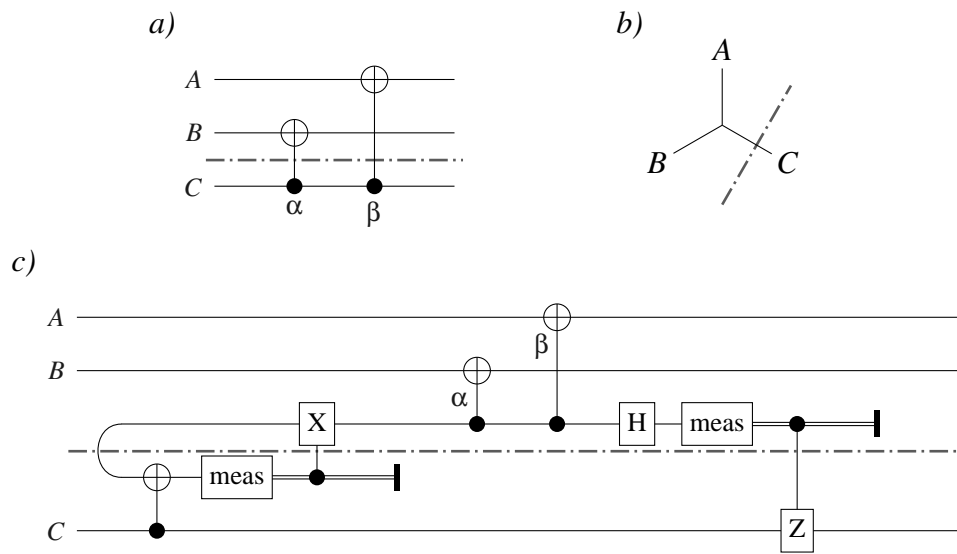


Figure 4.4: Same as in Figure 4.3, but now the cut makes both CNOTs non-local. Still, only one ebit is required, as implied by hypergraph *b*).

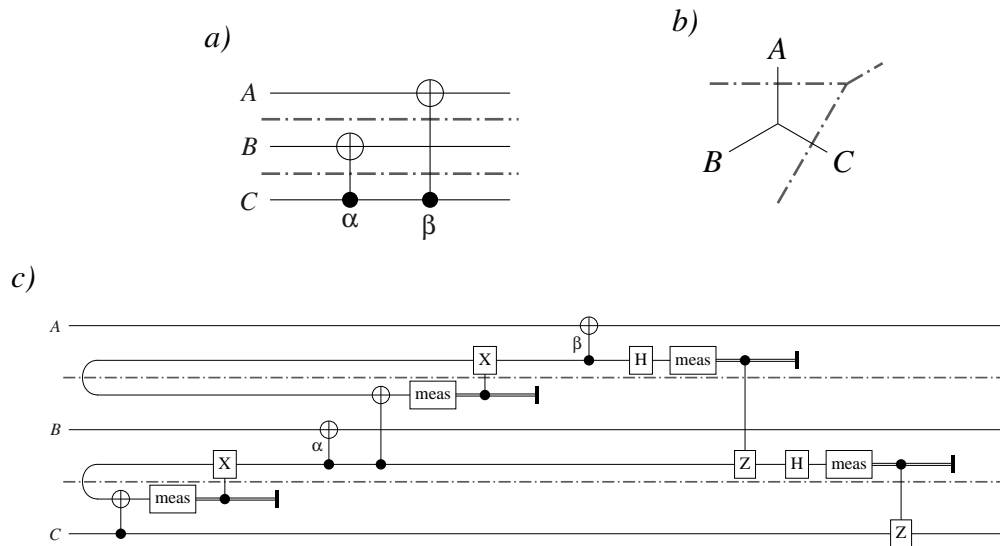


Figure 4.5: Same as in Figure 4.3, but now there are two cuts, distributing the circuit across three QPUs. Hence, two ebits are required.

trivial configurations:

- The partition of \mathcal{H} where all vertices are in the same block corresponds one-to-one to
- the whole circuit \mathcal{C} being executed in a single QPU.

Then, we define a *primitive transformation* for both problems, which allows us to move vertices/wires around. To do so, we use the one-to-one correspondence between vertices and wires that Algorithm 4.1 imposes. We additionally require to have an indexed set of hypergraph blocks and QPUs.

- Given a partition of \mathcal{H} , moving vertex x from block i to block j corresponds one-to-one to
- picking wire x – which is guaranteed to be in QPU i – and allocating it in QPU j .

Using this primitive, any partition/distribution can be reached, so we indeed have a bijection. Notice that wire x is guaranteed to be in QPU i thanks to our inductive definition of the bijection itself: all vertices/wires start in the same block (trivial configuration), while the primitive moves any x vertex/wire respectively to a block or a QPU, both indexed by the same j . It remains to prove that the given bijection preserves $\lambda_c = \lambda_e$. We give a proof by induction over the sequence of primitives that, starting from the trivial configuration, generates the partition/distribution.

- The trivial configuration of both problems has $\lambda_c = 0 = \lambda_e$.
- Given a sequence of $n + 1$ primitives, we assume that $\lambda_c = \lambda_e$ holds after the n -th primitive was applied (our induction hypothesis). We must prove that it still holds after the $(n + 1)$ -th primitive is applied. When a vertex is reallocated, all of its hyperedges are affected, which may create/remove multiple cuts. We will consider the contribution of each of these hyperedges separately, then add them up to obtain the overall effect. Besides, reallocating vertex x from block i to block j , as determined by the $(n + 1)$ -th primitive, may affect each hyperedge h differently whether x corresponds to the control wire shared by all the CNOTs represented in h , or it corresponds to a target wire. If x corresponds to a target wire, applying the primitive may:

- a). *Increase λ_c .* λ_c increases (by one) iff a new cut is added to the hyperedge h . This happens iff the block/QPU j did not already contain a vertex/wire from h . In that case, x becomes an isolated target wire, and to implement its CNOT it will be necessary and sufficient to create an extra ebit, increasing λ_e (by one). Therefore, λ_e will increase iff λ_c does so, both by the same amount.
- b). *Decrease λ_c .* In the same spirit, λ_c decreases (by one) iff a previously isolated target vertex/wire is allocated where some fellow vertices/wires are. When and only when this happens, one less ebit will be required, as the previously isolated target wire x will no longer need its own ebit: it will either use an existent one or be allocated to the same QPU as the control wire. Therefore, λ_e will decrease iff λ_c does so, both by the same amount.

If x is the control wire of the CNOTs in h , we analyse the reallocation of x from i to j as a multiple step process. First, we move all of the other vertices of hyperedge h from their current block to i . All of those vertices are target vertices, and thus both λ_c and λ_e are decreased equally, as discussed above. Then, we reallocate all of the vertices of h from i to j , which has no effects on the cuts of hyperedge h (which currently has zero cuts) or in the number of ebits (as all qubits are in the same QPU). Finally, we reallocate each of the other (target) vertices of h back to their respective blocks, increasing both λ_c and λ_e equally, as discussed above. Notice that all target vertices/wires end up where they began, so the only effect on the partition/distribution has been to move the control vertex/wire x from i to j .

Until this point, we have studied how the application of a primitive affects a single hyperedge. However, a vertex may take part in multiple hyperedges. For each one of the hyperedges, we may follow the method above, and arrive to the conclusion that $\lambda_c = \lambda_e$ is preserved in each case. Therefore, starting from $\lambda_c = \lambda_e = 0$, applying the whole sequence of primitives one by one, maintains $\lambda_c = \lambda_e$.

□

Remark 4.2. In Figure 4.5, the second cat-entangler ‘copies’ the information held by the local ebit half previously entangled with wire C , instead of being directly coupled with C . The latter option would also be correct⁵. Either of these ways is represented by the same hypergraph partition, so in order to maintain our one-to-one correspondence, we should rather say there is a bijection between hypergraph partitions

⁵However, in that case, wires B and C should interchange places in the circuit representation if we want to visualise in 2D that only ebits and classical information crosses the boundary between QPUs.

and equivalence classes⁶ of circuit distributions. Although for our algorithm all of the solutions in one such equivalence class are indistinguishable, some of the solutions will offer a more decentralised network of ebits than others. Optimisations taking this fact into account could be performed as post-processing of our proposed algorithm.

A closer look at the bijection proposed in Theorem 4.1 reveals that we can transform back and forth between hypergraph partition and circuit distribution in polynomial time: To go from partition to distribution, we just need to read where each of the vertices are assigned, and apply the primitive to move each wire to its QPU – which affects all the CNOTs on that wire. The opposite direction works the same way. Hence, the time complexity of the transformation in either direction is $O(n \cdot m)$, where n is the number of vertices/wires and m the number of hyperedges/CNOTs. This leads us to two results, one per direction of the bijection:

Corollary 4.3. *The best vanilla distribution of a circuit can be efficiently derived from an optimal partition of the hypergraph built by Algorithm 4.1.*

Proof. We know it will be the best distribution thanks to Theorem 4.1: The optimal partition will have the lowest possible λ_c , and given that at any point $\lambda_c = \lambda_e$, the corresponding circuit distribution will also have the lowest λ_e possible.

We say the circuit distribution is efficiently derived because the required transformations – Algorithm 4.1 and the translation from hypergraph partition to circuit distribution – both run in polynomial time.

□

Corollary 4.4. *The quantum circuit distribution problem is an NP-complete problem.*

Proof. To prove NP-completeness we first need to show that the problem is in the NP class, then show it is NP-hard. The problem is in NP, as allocating each of the $|V|$ wires to a QPU takes $O(|V|)$ time (and checking how many ebits are required takes $O(|H|)$), so a non-deterministic oracle would be able to output the solution in polynomial time.

To prove NP-hardness we simply need to show that, in case the quantum circuit distribution problem could be solved in polynomial time (on a deterministic machine), we would be able to solve an NP-complete problem in polynomial time too. The hypergraph partitioning problem happens to be NP-complete (Lyudet, 2010), and Theorem 4.1 allows us to take the solution for the efficient circuit distribution problem and

⁶Families of circuit distributions that are equivalent in the sense that their wires are allocated to the same way, and that the number of ebits required also matches.

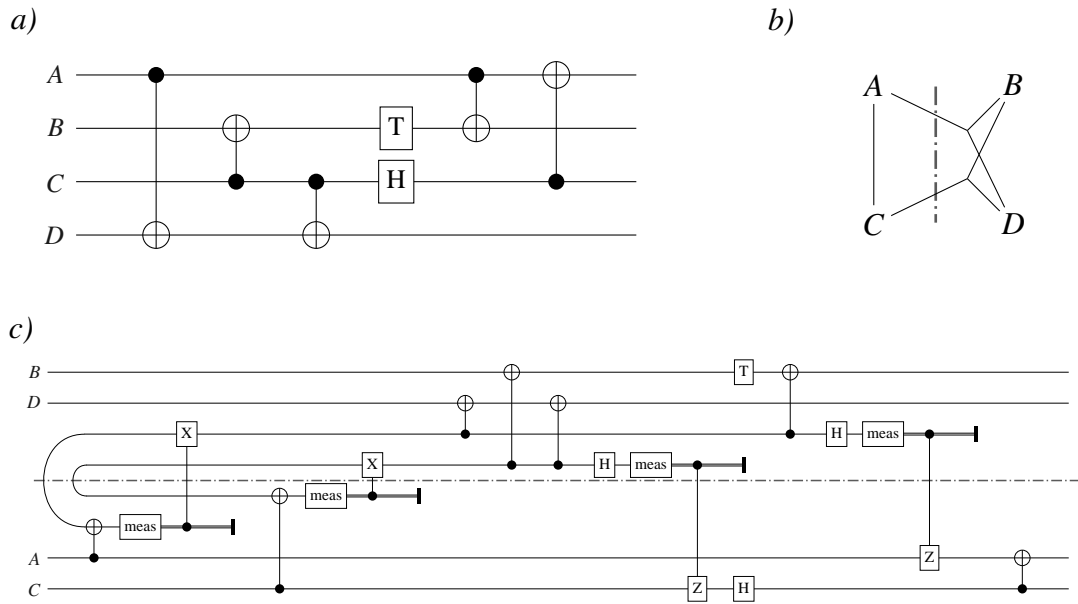


Figure 4.6: The circuit is distributed using only 2 ebits. The other two possible distributions: $\{\{A, B\}, \{C, D\}\}$ and $\{\{A, D\}, \{B, C\}\}$ both require 3 ebits to be implemented. The wires in the distributed version of the circuit have been rearranged, in order to make it possible to visualise in 2D that no quantum information crosses the boundary⁷.

provide the optimal partition of its hypergraph. The only caveat is that we need to be able to do this for any hypergraph \mathcal{H} , so we must be able to build a non-distributed circuit \mathcal{C} that is represented by an arbitrary \mathcal{H} – the opposite direction of what Algorithm 4.1 does. There will be multiple such circuits; building one of these in polynomial time is possible, and the details are straight-forward.

□

On the pessimistic side, Corollary 4.4 means that unless $P = NP$, finding the best distribution of an arbitrary quantum circuit takes exponential time. On the optimistic side, many problems that compilers from classical computer science deal with are also NP-complete. In order to implement fast compilers that prepare quantum algorithms to be run in distributed architectures, we will not need to design better algorithms to solve our particular problem: we may use the already rich research on fast algorithms for hypergraph partitioning (Akhremtsev et al., 2017), as the polynomial overhead of transforming back and forth between problems will be negligible.

A simple circuit, its optimally partitioned hypergraph and the resulting distributed circuit are shown in Figure 4.6. Each of the QPUs can be set to implement its own local

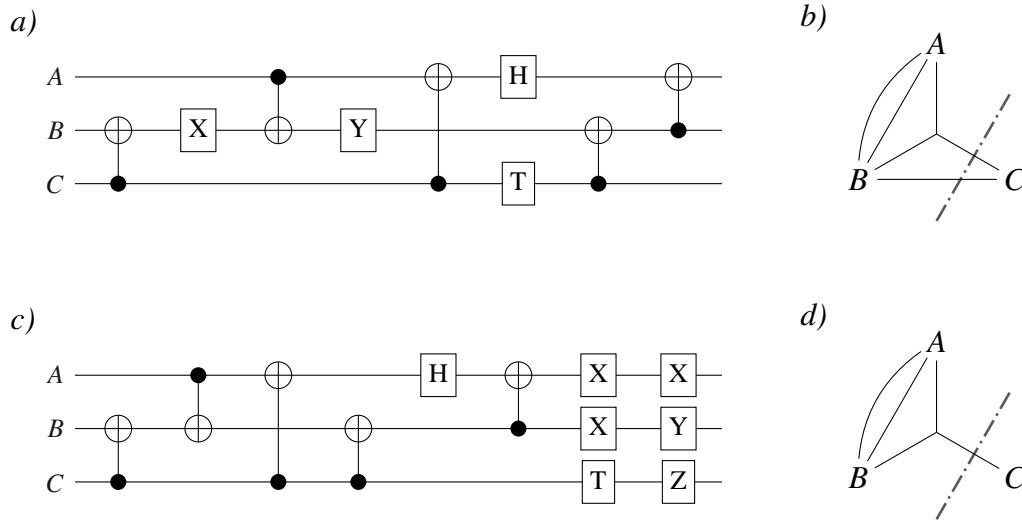


Figure 4.7: Example where an ebit can be saved by sliding CNOTs closer together. This figure shows the original circuit *a)*, its optimally partitioned hypergraph *b)*, the pre-processed circuit *c)*, and its optimally partitioned hypergraph *d)*, which has one less cut hyperedge.

circuit, distilling ebits and using them along classical communication when indicated.

4.2.2 SlideCNOTs: Bringing CNOT gates together

In Figure 4.1 we showed that any 1-qubit gate in the Clifford+T set acting on the control wire of a CNOT gate, with the exception of the H gate, can commute with the CNOT up to some byproduct. Here we use this fact, applying some pre-processing on the input circuit that brings together nearby CNOT gates, allowing us to implement more non-local CNOTs using a single ebit. Figure 4.7 gives an example of how these transformations – listed in Figure 4.1 – can lead to a more efficient distribution of the circuit. We will refer to the pre-processing described in this subsection as SlideCNOTs.

The procedure is fairly straight-forward: Exploring the circuit from left to right, whenever a CNOT gate is found, use the transformations listed in Figure 4.1 to move it as early in the circuit as possible. The procedure introduces some additional X and Z gates. Fortunately, X and Z are their own inverse (i.e. $XX = I$ and $ZZ = I$) and every 1-qubit gate in Clifford+T can be interchanged with X and Z in a simple way (as shown in Figure 2.2). Hence, we should expect no significant increase in the depth

⁷Even though in a distributed circuit no quantum information crosses the QPU boundary (apart from the shared ebits), not every distributed circuit can be visualised in 2D in a way that no CNOT crosses it. In graph theory this is known as the *planarity* problem.

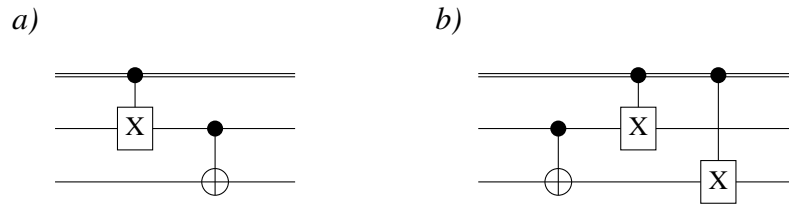


Figure 4.8: Pushing a classically controlled gate through a CNOT. The same rule as in Figure 4.1 is applied, while making sure any new gate is also controlled. Here, only the case for X gate is shown, but this works for any of the transformations in Figure 4.1.

(i.e. length) of the circuit, as most byproduct gates will cancel each other out.

So far we have been talking about standard 1-qubit gates, but in practical circuits we are likely to find 1-qubit gates that are *classically controlled*, meaning that a classical signal (a bit, either 0 or 1) decides whether the gate is applied or not. These gates are commonly used to perform corrections on qubits after a measurement is done during the computation. These classically controlled gates are no issue for the distribution of the circuit, as the classical control may only require classical communication between QPUs. Concerning the pre-processing we just described, classically controlled 1-qubit gates can commute with CNOT under the exact same circumstances as their uncontrolled version. The only difference is that, whenever a byproduct gate is created, we must make sure it is controlled by the same classical signal that controlled the original gate, as shown in Figure 4.8.

The same procedure can be used to commute 1-qubit gates (except H , S and T) across the target wire of the CNOT gates. This additional pre-processing would have no effect at all on the vanilla version of the algorithm, but it will be advantageous after we apply our next extension (`EitherRemote`), which benefits from CNOT gates to be adjacent on the target wire.

Remark 4.5. *Using `SlideCNOTs` will never increase the minimal ebit count required to implement a distributed circuit.*

This pre-processing simply moves the CNOTs along their wires. The same CNOTs that were non-local before `SlideCNOTs` was applied will still be non-local. On the worst case, these non-local CNOTs could be implemented in the exact same way as they were before, so the ebit count would remain the same.

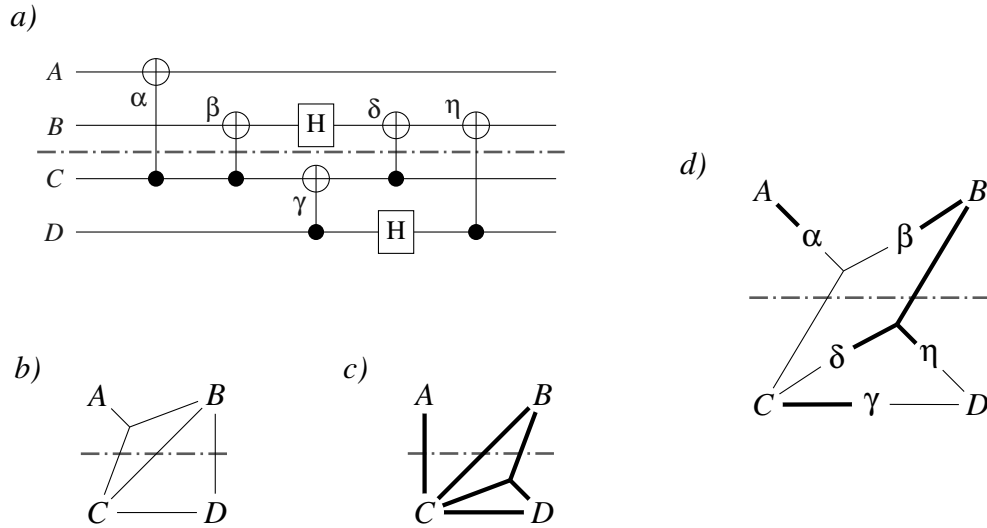


Figure 4.9: A circuit *a*) and its hypergraph *b*) as built by Algorithm 4.1. Hypergraph *c*) is the result of running the same algorithm but grouping CNOTs in the same hyperedge if and only if they share the same target (instead of control). Hypergraph *d*) is the one built by Algorithm 4.2. Any (vertex balanced) partition of *b*) or *c*) cuts three hyperedges; a partition of *d*) cuts two.

4.2.3 EitherRemote: Including the remote-target method

In §4.1 we showed that the trick for implementing multiple CNOT gates using a single ebit also works if they share a common target wire (instead of a control wire). This makes our optimisation problem more intricate: Now, when the CNOTs are to be implemented non-locally, we can choose to implement them using the remote-control or remote-target method. For explanation purposes, we will use two different kinds of hyperedges in this subsection's figures, depending on whether their CNOTs are controlled by the same wire, or act on the same target (thicker line). We will refer to the extension we propose in this subsection as `EitherRemote`.

Figure 4.9 shows an example where using both the remote-control and remote-target methods in the same circuit is advantageous: CNOTs α and β can be implemented using a single ebit if the remote-control method is used. CNOT γ is local, and CNOTs δ and η can be implemented using a single ebit if the remote-target method is used. Therefore, we could distribute the circuit using only two ebits. However hypergraph *b*), built by Algorithm 4.1, can only be partitioned cutting at least three hyperedges. This is because, in hypergraph *b*), CNOTs are only grouped by common control, in 'control-hyperedges' (thin lines). Hence, δ and η appear as two distinct hyperedges: $\{B, C\}$ and $\{B, D\}$ respectively. Hypergraph *c*) is the counterpart of *b*) where

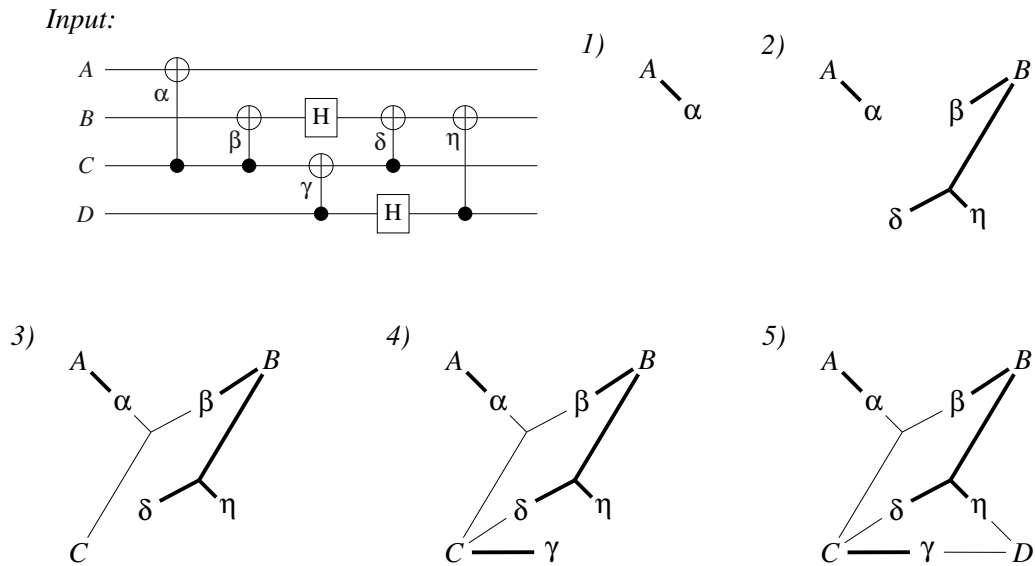


Figure 4.10: Step by step execution of Algorithm 4.2.

‘target-hyperedges’ (thick lines) are used instead (i.e. CNOTs are grouped by common target). In this case, the minimum number of cuts is also three, as now it is α and β the CNOTs that are not grouped together. Hypergraph *d*) is a hybrid between the previous two, that can be partitioned cutting only two hyperedges. This is the hypergraph representation we will develop and use for the `EitherRemote` extension.

If we want to guarantee that a hypergraph partitioner can always find the most efficient circuit distribution, our hypergraph representation must have the following requirements:

1. Both options of how to implement each non-local CNOT (remote-control and remote-target) are represented.
2. A partition of the hypergraph must determine, for each non-local CNOT, which method should be used to implement it.
3. The $\lambda-1$ metric of a partition – the number of cuts – should accurately determine how many ebits are required to implement the circuit distribution it describes.

Algorithm 4.2 builds, for any circuit, a hypergraph that satisfies these requirements. Figure 4.10 shows how the hypergraph from Figure 4.9*d*) is built step by step. The three requirements above are satisfied: First, we include all of the control-hyperedges (those from Figure 4.9*b*)) and target-hyperedges (those from Figure 4.9*c*)). For the second requirement, we give additional structure to the hypergraph, adding vertices

Algorithm 4.2: Builds the hypergraph of a given circuit, without choosing whether non-local CNOTs are implemented using the remote-control or the remote-target method. This algorithm runs in time $O(g)$, where g is the number of gates in the input circuit.

```

1  input: circuit
2  output: (V,H)
3  begin
4    V  $\leftarrow$   $\emptyset$ 
5    H  $\leftarrow$   $\emptyset$ 
6    hedge  $\leftarrow$   $\emptyset$ 
7    foreach wire in circuit do
8      V  $\leftarrow$  V  $\cup$  {wire}
9      hedge  $\leftarrow$  {wire}
10     hType  $\leftarrow$  unknown
11     foreach gate in wire do
12       if gate == CNOT then
13         V  $\leftarrow$  V  $\cup$  {labelOf(gate)}
14         if controlOf(gate) == wire then
15           if hType == target then
16             H  $\leftarrow$  H + {hedge}
17             hedge  $\leftarrow$  {wire}
18             hType  $\leftarrow$  control
19           if targetOf(gate) == wire then
20             if hType == control then
21               H  $\leftarrow$  H + {hedge}
22               hedge  $\leftarrow$  {wire}
23             hType  $\leftarrow$  target
24         hedge  $\leftarrow$  hedge  $\cup$  {labelOf(gate)}
25       else
26         H  $\leftarrow$  H + {hedge}
27         hedge  $\leftarrow$  {wire}
28         hType  $\leftarrow$  unknown
29     H  $\leftarrow$  H + {hedge}
30 end

```

that represent CNOT gates. The way a CNOT is implemented will be determined by the block its CNOT-vertex is assigned to. The third requirement is the most subtle one. Intuitively, we satisfy it by imposing that each CNOT-vertex participates in only two hyperedges; one connecting it to its control wire-vertex, the other to its target. A more detailed account of how this third requirement holds is given in the proof of Theorem 4.6. Corollary 4.7 confirms that the optimal partition of our hypergraph determines the most efficient circuit distribution.

Theorem 4.6. *Given any circuit C , and its hypergraph \mathcal{H} generated by Algorithm 4.2, there is a bijection between partitions of \mathcal{H} with λ_c cuts and distributions of C that use λ_e ebits; satisfying $\lambda_c = \lambda_e$.*

Proof. We define the same trivial configuration from Theorem 4.1. In the case of the vanilla algorithm (§4.2.1), the CNOT operation itself was always applied in the same QPU as its target, regardless of the CNOT being local or not (see Figure 3.7). Thus, the primitive from Theorem 4.1 for reallocating a wire-vertex x is defined here with the extra constraint that all CNOT-vertices connected by a target-hyperedge to x must move with it to the same block/QPU x does. In this way, the primitive has on our new hypergraph representation the exact same meaning it had in the original.

We need to add another primitive that allows us to move a CNOT-vertex x independently from its wire-vertices; otherwise not every hypergraph partition would be reachable. Conversely, in order to reach any arbitrary circuit distribution, we need a primitive that changes the QPU where a CNOT gate x is implemented, which determines the method used to implement the CNOT. This pair of primitives is defined to correspond one-to-one to each other. Let's consider the four distinct cases of how x may be allocated regarding its two neighbour wire-vertices, which act as x 's control c_x and its target t_x :

- *Local:* The three vertices x , c_x and t_x are in the same block i . In this case, x 's allocation causes *no cut* to either its control-hyperedge or its target-hyperedge. The CNOT gate is implemented locally in QPU i , so *no ebit* is required to implement it.
- *Remote-control:* Both x and t_x are in a block i , while c_x is in a different block j . In this case, x 's allocation causes its control-hyperedge to be cut. The cut will be already present if there are other vertices from the hyperedge allocated to i ; otherwise *one cut* will be added. On the other hand, an ebit is required to

implement CNOT x . If there are other CNOTs in i controlled by the same c_x wire – they are in the same control-hyperedge –, the ebit they require can be used to implement x ; otherwise *one ebit* will be added.

- *Remote-target*: Both x and c_x are in a block i , while t_x is in a different block j . In this case, x 's allocation causes its target-hyperedge to be cut. Again, the cut will be already present if there are other vertices from the hyperedge allocated to i ; otherwise *one cut* will be added. On the other hand, an ebit is required to implement CNOT x . If there are other CNOTs in i that target the same t_x wire – they are in the same target-hyperedge –, the ebit they require can be used to implement x ; otherwise *one ebit* will be added.
- *External*: The three vertices are in different blocks, with x in some block i . An example of this situation is shown in Figure 4.11. In this case, x 's allocation contributes to *two cuts*, one on its control-hyperedge and another on its target-hyperedge. In this case, *two ebits* are required; the one used to access c_x may be shared with other CNOT gates in i that have c_x as control, while the ebit used to access t_x may be shared with CNOTs in i that have t_x as target.

The proof by induction discussed in Theorem 4.1 holds here too if we manage to show that any application of the new CNOT-vertex reallocation primitive still preserves $\lambda_c = \lambda_e$. Changing the allocation of a CNOT-vertex x may change its situation among the four cases above. As we detailed, in each case x 's allocation contributes to the same amount of cuts as ebits the CNOT x requires. Hence, changing the allocation of x always preserves $\lambda_c = \lambda_e$.

□

The procedure for distributing the circuit following a given hypergraph partition is very similar to that in the vanilla version of the algorithm, now taking into account the new primitive defined in Theorem 4.6. The time complexity of the procedure still is $O(n \cdot m)$, where n is the total number of vertices and m is the number of hyperedges. Also, notice that the cat-entangler and the cat-disentangler are slightly different whether the CNOTs are implemented through remote-control or remote-target (see Figure 4.11).

Corollary 4.7. *The best distribution of a circuit can be efficiently derived from an optimal partition of the hypergraph built by Algorithm 4.2.*

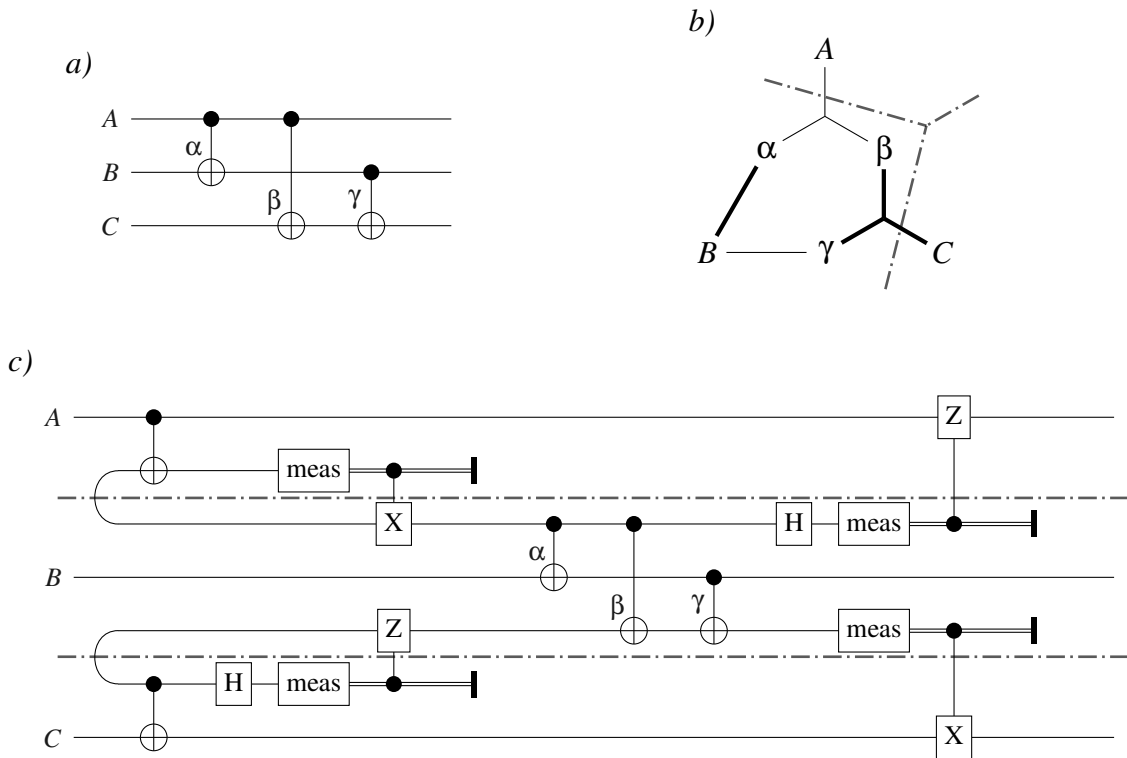


Figure 4.11: Distribution of circuit *a)* when each wire is in a different QPU. Gate β is implemented as an ‘external’ CNOT, i.e. both its control and target are in a remote QPU. The three non-local CNOTs only need two ebits in total, as α and γ can use the ebits β requires.

Proof. Follows directly from Theorem 4.6, by the same argument given for Corollary 4.3. □

Corollary 4.8. *The distributed circuit we obtain using the vanilla algorithm (from §4.2.1) is the same as the one obtained if we restrict the approach in this subsection so either:*

- a). No CNOT is implemented using the remote-target method.*
- b). Our hypergraph partitioner never cuts target-hyperedges.*
- c). The CNOT operation is always executed in the CNOT’s target QPU.*

All of these restrictions are equivalent.

Proof. Follows directly from the proof of Theorem 4.6. □

The hypergraph built by Algorithm 4.2 has one caveat: When discussing load-balancing in §4.2, we explained that we were interested in allocating a uniform number of wires to each QPU. Previously, the hypergraph partitioner took care of this, as it tried to assign a uniform number of vertices to each block. But now, the hypergraph partitioner has no way of distinguishing between ‘wire’ vertices and ‘CNOT’ vertices, the latter being an artificial gadget that should not count towards load-balancing. The solution is simple, instead of the standard hypergraph partition problem, we apply a version of it where vertices can have a weight assigned (see Appendix A). Then, each wire-vertex is given weight 1, and each CNOT-vertex is given weight 0, effectively ignoring them for the load-balancing aspect.

Remark 4.9. *Enabling `EitherRemote` will never increase the minimal ebit count required to implement a distributed circuit.*

This extension simply changes how each non-local CNOT is implemented, while the number of non-local CNOTs remains the same. On the worst case, these non-local CNOTs could be implemented in the exact same way as they were before, so the ebit count would remain the same.

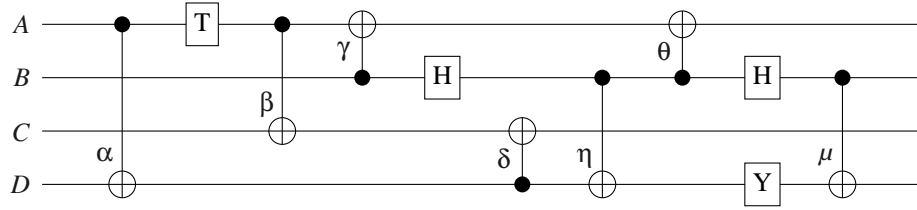
As a wrap up for this section, Figure 4.12 shows the same circuit being distributed in four different ways: with or without `SlideCNOTs` and with or without `EitherRemote`. This provides a simple example where both extensions are shown to reduce the number of ebits required to distribute a circuit.

4.2.4 Communication bottlenecks

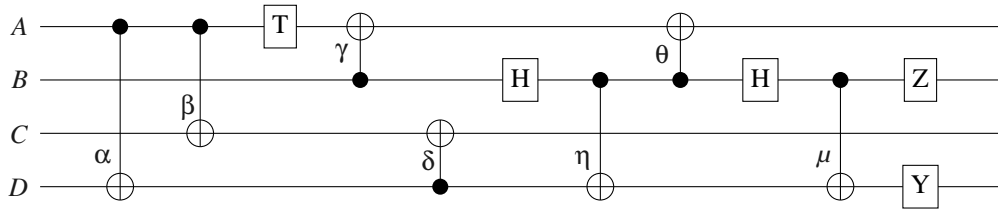
The case illustrated in Figure 4.11 can be seen intuitively as passing a message through a middle-man. Sometimes, using communication through an already available middle-man is better than putting up a full blown connection just for a single message. The hypergraph partitioner acting on the hypergraph built by Algorithm 4.2 will automatically use this strategy whenever it reduces the number of ebits required. However, some criticism is relevant here: if we put no constraint on the exploitation of ‘middle-men’ QPUs, it may happen that communication across many of the QPUs all use the same middle-man QPU to deliver their messages, potentially creating a bottleneck. We see two solutions:

1. Specialise the hardware to be efficiently managed as a centralised communication network, where the middle-man QPU has a similar role to a classical server.

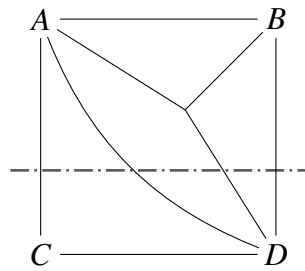
Input:



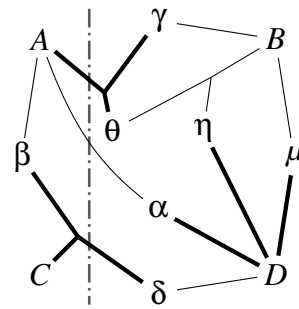
After preprocessing (*SlideCNOTs extension*):



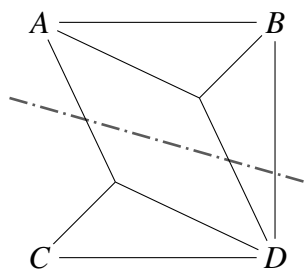
a)



b)



c)



d)

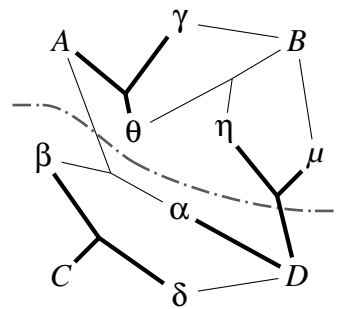


Figure 4.12: Different hypergraphs representing the input circuit. *a)* corresponds to no extensions active. *c)* and *d)* use *SlideCNOTs*. *b)* and *d)* use *EitherRemote*. For each hypergraph, the optimal $k = 2$ partition (into two QPUs) is shown. The number of ebits required in each case is: *a)* 4, *b)* 3, *c)* 3, *d)* 2.

The server should be capable of managing a large number of ebits fast and reliably. This is the natural option if the algorithms we wish to run have an intrinsically centralised behaviour – for instance, if all the gates are controlled by the same wire.

2. In case we wish to have a decentralised network, we will need to find a way to ensure the hypergraph partition we get has some kind of load-balancing of the usage of ebits. Fortunately, there is a simple way to do this: instead of giving CNOT vertices weight 0 as we previously discussed, we may give them some weight $\mu > 0$ that indicates how relevant communication load-balancing is in comparison to the load-balancing of wire allocation across QPUs. Alternatively, we could use a custom version of the hypergraph partitioning problem where we provide three parameters instead of two, (k, ε, η) , where now ε acts only as the tolerance for imbalance of wire-vertices, while η is a separate tolerance for imbalance of CNOT-vertices, both tolerances being enforced at any partition.

The best choice between either of the options above, and the selection of a suitable value for μ or η , will be dependent on the algorithms we intend to run. However, users may not know beforehand which configuration is best for their algorithms. This problem also exists in classical computer science, as the effectiveness of many compiler optimisations depend on the choice of the parameter configuration. In those cases, compiler writers tend to follow one of two solutions: One option is to include a decision algorithm in the compiler’s code, that looks at particular characteristics of the input and chooses a suitable parameter configuration for its compilation. Another option is to provide a default configuration that does a reasonable job in most cases, and leave the task of fine-tuning to the user, who should compile the program multiple times with different configurations until the best one is found. Making a decision on which approach to use requires a thorough study of the effects of each parameter on a diverse benchmark. We include this study in our list of suggestions for further work (see §6.1).

4.3 Interchanging CNOT gates

In this section we discuss a potential third extension to our algorithm. We focus on explaining the challenges it implies, and we outline an approach to tackle them. Overall, this section should be understood as a draft idea for future work.

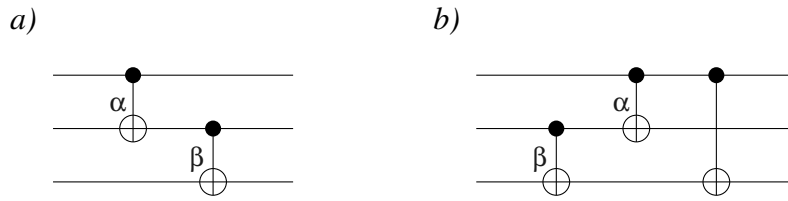


Figure 4.13: Equivalent circuits with the two gates in *a)* being interchanged in *b)*. A byproduct CNOT gate is created in the process.

When applied to disjoint sets of wires, CNOT gates commute trivially. If one of the wires is in common, and it has the same role for both CNOTs (control or target), we can implement both gates with a single ebit (using the remote-control and remote-target methods respectively). If both wires are in common and have the same role, the CNOTs cancel each other out. But what happens if two CNOTs act on the same wire with different roles? In that case, we can still interchange the gates as in Figure 4.13, but this creates an additional CNOT.

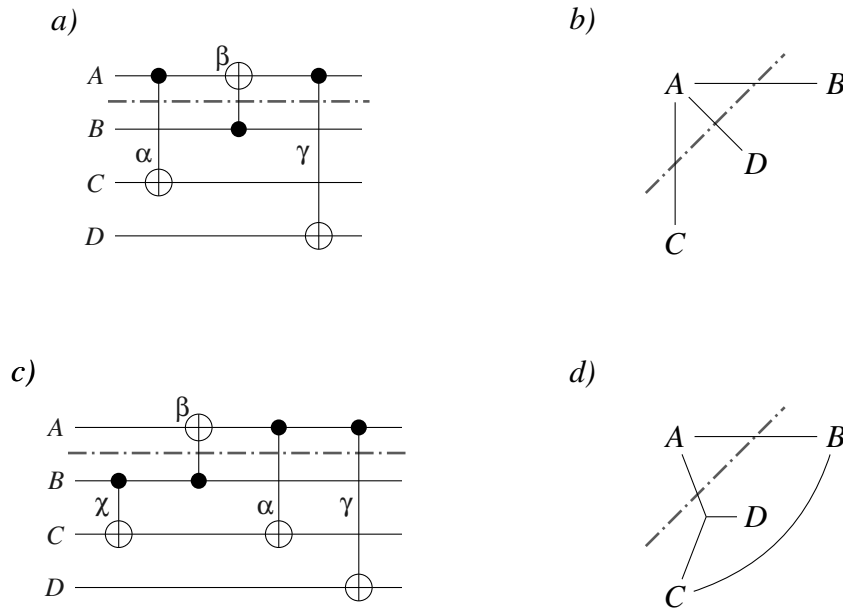


Figure 4.14: Example of a circuit *a)* where interchanging CNOTs α and β saves an ebit. The byproduct gate χ in circuit *c)* will be implemented locally, so its addition has no impact. CNOTs α and γ can be implemented using a single ebit after the interchange. Hypergraph *b)* corresponds to the circuit *a)*. Hypergraph *d)* corresponds to *c)*, and it has one less cut.

It may seem like pre-processing the circuit so it has the minimum possible number

of CNOT gates would always be the best option. However, it does not guarantee the optimal solution, as shown in Figure 4.14. In some cases interchanging CNOTs may unlock a more efficient distribution of the circuit, even though it creates additional CNOTs. To account for this, the effect of CNOT interchange should also be encoded in our hypergraph representation. However, encoding that information in a hypergraph is not natural, due to the following reasons:

- *The way CNOT gates are ordered in the circuit is important.* This is something we omit in the hypergraphs built by Algorithms 4.1 and 4.2. Looking at the hypergraphs from Figure 4.14, we can not tell whether α goes before or after β . However, this information is key when interchanging, as it will determine which are the new neighbours of the interchanged CNOTs.
- *Interchanging CNOT gates adds new CNOTs.* The CNOT interchange problem is substantially different from the one we discussed and solved in §4.2.3. The essence of our solution was to represent all of the potential choices in a single hypergraph. However, if we were to interchange a pair of CNOTs, new choices would become available: Is it worth interchanging the CNOTs again with their new neighbours? Should the byproduct CNOT be itself interchanged further? Although the number of options to take into account is finite, it increases considerably fast. Furthermore, each choice would not be independent from the rest – as some interchanges are only available if others have been done before – so the structure of the hypergraph would have to be quite complex in order to accommodate this information.

Instead of representing these CNOT interchanges within the hypergraph partitioning problem, we may abandon the idea of guaranteeing the optimal solution, and approach this problem through pre-processing and post-processing. We suggest that a reasonable approach in that case would be to:

1. Apply a pre-processing phase that finds an equivalent circuit whose CNOT count is minimal.
2. Apply our algorithm, as described in §4.2, which decides how to partition the circuit.
3. Apply a post-processing phase that exhaustively explores each possible interchange of CNOTs. Those that reduce the number of ebits required to implement the partition are used.

Even in this situation, finding the best ordering of CNOTs is difficult. The first option that may come to mind is to use a dynamic programming approach. To do so we need to identify some structure in the problem, so the solution can be built recursively. Unfortunately, the most natural way of doing it – finding the best ordering for the first N CNOTs, then recursively extending the solution one CNOT at a time – fails to display the properties we would wish to have on a typical dynamic programming strategy: We found no guarantee that we can reject an inefficient ordering for the first N CNOTs without the risk of discarding the best overall ordering. Put another way, we did not find a way to recursively narrow down the search space without the risk of losing the best solution in the process. We do not claim, however, that such a strategy does not exist; but if it does, it is likely to be quite subtle, and we suggest to look for it during future work (see §6.1).

In case no good strategy is found, there are other – less elegant – options, whose impact is difficult to predict. We suggest to implement each of these ideas and test (e.g. with the benchmark circuits from §5.2) which combination of them is the most advantageous. The alternatives we propose are:

- Identifying CNOT interchanges whose byproduct CNOT can be implemented locally (as it is the case of χ from Figure 4.14). These interchanges are simpler to manage, as the byproduct CNOT does not affect the ebit count, so we do not need to consider interchanging it further. Then, we may find the combination of these kind of interchanges that yields the lowest number of ebits.
- Identifying the ebits that are used by the least amount of CNOTs. For instance, those ebits that are used to implement a single gate. We may try to interchange one of this ebit's CNOTs with others, so they can make use of a different ebit. This is the case of CNOT α from Figure 4.14, which required an ebit that was used by no other gate. After interchanging α with β , the former shares the ebit γ uses, so the one that was originally required to implement α is no longer needed.
- Performing an exhaustive search over the possible CNOT orderings, but giving some constraint to the size of the search space, so we may maintain the execution inside a reasonable time frame. One option is to impose that no CNOT can be interchanged with more than p other CNOTs. Another option could be to split the circuit into fragments containing m CNOTs each, then find the best ordering inside each of these blocks separately.

Chapter 5

Evaluation

In the previous chapter we proposed an algorithm that finds an efficient distribution of any given quantum circuit. Additionally, we have given two extensions that allow the algorithm to apply some extra optimisations. In this chapter, we will evaluate the distributed circuits our algorithm generates. The quantum programs we distribute are examples drawn from the literature of what we may want to run on quantum computers.

The code of our algorithm’s implementation can be found at <https://github.com/PabloAndresMartinez/Distributed>, along with the generated executables and all the data discussed in this chapter.

5.1 Implementation details

The algorithm described in §4.2.1 and its two extensions (`SlideCNOTs` §4.2.2 and `EitherRemote` §4.2.3) have been implemented in Haskell. `Quipper`, a quantum circuit description language, is embedded on Haskell. The quantum programs we use in our evaluation (see §5.2) are all available as part of the `Quipper` system, so by using Haskell we could easily manage them. The hypergraph partitioning problem is solved by a specialised third-party software, `KaHyPar` (Akhremtsev et al., 2017), that is called by our program when needed. A brief overview of `KaHyPar` is given in Appendix A.

The main contributions of this thesis were described in Chapter 4. Our implementation is only meant as a demonstration of our algorithm, and it is intended for evaluation purposes only. Thus, efficiency was not a main concern. Nevertheless, the implementation is efficient enough to manage circuits with up to 50,000 CNOT gates within a reasonable amount of resources (see §5.3).

Our implementation receives a circuit described in `Quipper`’s internal data structure

and outputs its distributed version, also in Quipper’s format. Thus, it can be integrated inside any Quipper program. However, along the process the circuit is managed as a list of gates, rather than using Quipper’s internal data structure. This is the main cause of inefficiencies in our code. Quipper is presented to its users as a language to define circuits, rather than a language to define circuit transformations. Therefore, there are not enough functionalities available at user-level to comfortably implement our algorithm within Quipper. If we intended to achieve better efficiency, we would likely need to extend the internal workings – the back-end – of Quipper, which is beyond the scope of this thesis.

Once our input circuit is converted¹ from Quipper’s data structure to a list of gates, implementing our algorithm is straight-forward. Depending on two input flags, the extensions `SlideCNOTs` and `EitherRemote` are applied or not; and the parameters (k, ϵ) – number of QPUs and load-imbalance tolerance – are also given as input. Throughout this chapter we use a small load-imbalance tolerance, chosen arbitrarily to be $\epsilon = 0.03$. The hypergraph generated by Algorithm 4.1 (or Algorithm 4.2) is written in a file using `KaHyPar`’s format, and the resulting partition is read from `KaHyPar`’s output file and used to create the distributed circuit as described in §4.2.1.

5.2 Test suite

The quantum programs whose circuits we will input to our algorithm are available as part of the Quipper system. At the time of writing this thesis, the Quipper system provides seven quantum programs, each with their own default configuration parameters. We use four of these seven examples, with their default configuration unless stated otherwise. The three programs we omit in our evaluation either lack an explicit (gate by gate) implementation of some fragment of their circuits, or their size is beyond the capabilities of our implementation (see §5.3). Detailed information about each of these quantum programs can be found in Quipper’s online documentation². The four programs we consider are the following:

- *Boolean Formula (BF)*: Ambainis et al. (2007) showed that the problem of evaluating a boolean formula over N variables could be solved in time \sqrt{N} on a quantum computer. We consider the circuit implementing the main part of the algorithm – the quantum walk. Implemented on Quipper by A. Green.

¹This conversion and its backwards counterpart are provided by Quipper.

²Quipper’s documentation: <https://www.mathstat.dal.ca/~selinger/quipper/doc/>.

- *Binary Welded Tree (BWT)*: Childs et al. (2002) proposed the problem of finding a path between two nodes in a particular kind of graph (a binary welded tree), and gave a quantum program that solves it exponentially faster than any known classical algorithm. We consider the circuit implementing the overall algorithm, making the tree height twice as large as the default input. Implemented on Quipper by P. Selinger and B. Valiron.
- *Ground State Estimation (GSE)*: Whitfield et al. (2011) proposed how to efficiently calculate the energy of a molecular system's ground state, which is relevant in chemistry. We consider the circuit implementing the overall algorithm. We doubled the default number of basis functions and the number of occupied orbitals. Implemented on Quipper by A. Green et al.
- *Unique Shortest Vector (USV)*: Regev (2004) proposed a problem where some characteristic vector of an input lattice must be found. This problem requires a large amount of resources, so we only consider a part of it, labelled 'R' in Quipper's library. We reduced the default dimension of the lattice from 5 to 2. Implemented on Quipper by N. Ross.

Apart from these four programs, we will include in our test suite the circuit for the *Quantum Fourier Transform (QFT)*. The QFT is a key component in many quantum algorithms, such as Shor's factorisation algorithm. Its implementation is also provided in Quipper's libraries. We will consider multiple QFT circuits of different sizes, referring to the one that uses $N+1$ qubits as QFT- N .

5.3 Results

Our code was compiled using GHC version 8.0.2, with the optimisation flag `-O2`. The tests we discuss in this section were run each on a single core of a i7-4710HQ processor, with 8GB of available RAM, on an Ubuntu 16.04 machine. The time it takes to distribute a given circuit mainly depends on the number of CNOT gates it has. Table 5.1 shows the number of CNOTs of each circuit and how long it takes to run our algorithm on them. Beyond a circuit size of around 50,000 CNOTs, our implementation takes quite long to run. This is because our code was not implemented with scalability as a concern, and it is not a characteristic of the algorithm itself.

Figure 5.1 shows, for different circuits, the proportion of CNOTs that become non-local once the circuit is partitioned. We also display the proportion of ebits the circuit

Table 5.1: CNOT count and the CPU time it takes to distribute each of the circuits discussed in this section. The data shown corresponds to executions with both extensions `pullCNOTs` and `EitherRemote` enabled and using distribution parameters $k=5$, $\epsilon=0.03$.

| <i>Circuit</i> | <i>CNOTs</i> | <i>Time (s)</i> |
|----------------|--------------|-----------------|
| BF | 25,590 | 64 |
| BWT | 13,824 | 15 |
| GSE | 70,158 | 675 |
| USV | 101,806 | 1,273 |

| <i>Circuit</i> | <i>CNOTs</i> | <i>Time (s)</i> |
|----------------|--------------|-----------------|
| QFT-10 | 450 | 0.6 |
| QFT-25 | 3,000 | 3 |
| QFT-50 | 12,250 | 17 |
| QFT-100 | 49,500 | 255 |
| QFT-200 | 199,000 | 5,253 |

requires. The key idea behind our algorithm is to take advantage of the remote-control and/or remote-target methods to implement multiple CNOTs using a single ebit. A naive approach would require one ebit per non-local CNOT instead. Therefore, the larger the difference between the two proportions shown in Figure 5.1 is, the more successful our approach has been in reducing the ebit count.

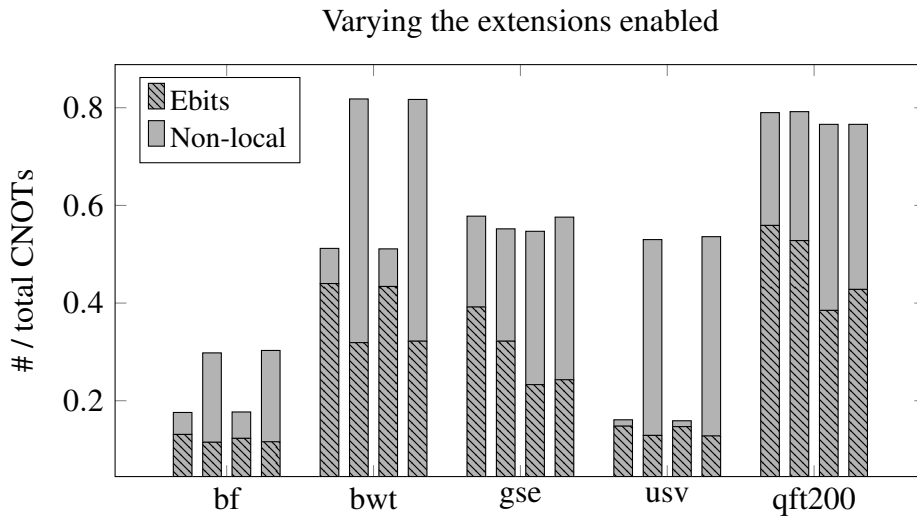


Figure 5.1: For each circuit, the bars correspond from left to right to: the vanilla algorithm, only `SlideCNOTs` enabled, only `EitherRemote` enabled and both extensions enabled. Each bar shows the number of non-local CNOTs and ebits required, normalised over the total number of CNOTs the original circuit had. The partition parameters are: $k=5$, $\epsilon=0.03$.

Each of the four bars shown for every circuit corresponds to a different configuration of active extensions (from left to right): the vanilla algorithm, only `SlideCNOTs` enabled, only `EitherRemote` enabled and both extensions enabled. Among the four

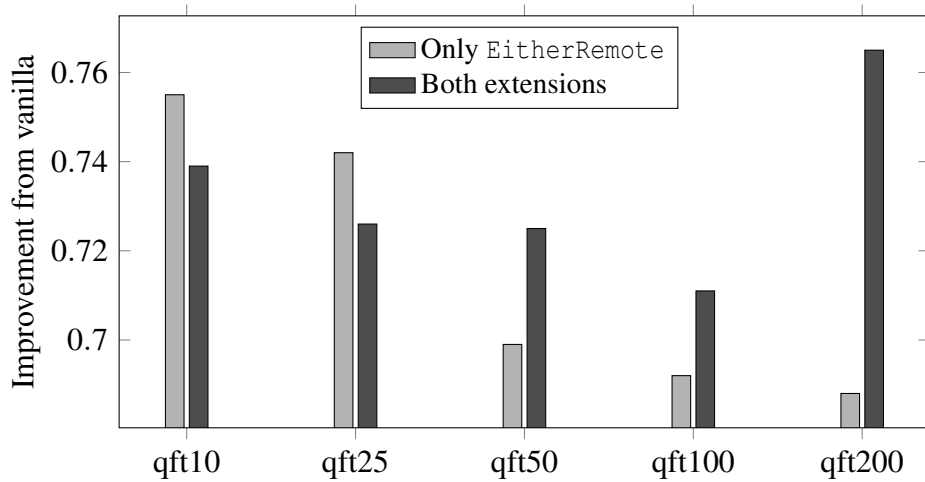


Figure 5.2: Improvement of the ebit count with respect to the vanilla algorithm, when using only `EitherRemote` or both extensions. The circuits considered are QFT with different dimensions. Each circuit is distributed across five QPUs with a tight load-balance ($k = 5$, $\epsilon = 0.03$).

configurations, the best one is that whose proportion of ebits is the lowest³. Interestingly, in cases such as BWT when `SlideCNOTs` is enabled, the algorithm finds a more efficient solution by partitioning the circuit in a way that increases the amount of non-local CNOTs, but ultimately reduces the number of ebits.

As discussed in Remarks 4.5 and 4.9, in theory, enabling extensions should never increase the ebit count. However, Figure 5.1 proves it otherwise in practice, most notably for QFT-200. This is because we were assuming that the optimal solution to the hypergraph partitioning problem was always found, but this is not the case in practice. Considering the hypergraph partitioning problem is NP-complete, a partitioner that ensures that the optimal solution is found can not possibly be efficient (unless $P = NP$). Thus, most hypergraph partitioners instead try to return a near optimal solution in a short amount of time. Whenever an extension is enabled, partitioning the hypergraph becomes a more complex task: `SlideCNOTs` increases the number of vertices reached by each hyperedge, while `EitherRemote` creates a hypergraph at least twice as large. The problem in cases such as QFT-200 is that one of the extensions (`EitherRemote` in this case) does exceptionally well, while the other has little impact. Then, when both are enabled, the latter extension essentially makes the partitioner’s job more difficult while contributing barely anything. When the hypergraph is large enough, this results in the partitioner yielding a worse solution. Figure 5.2 makes this evident, as for QFT with dimension 25 and lower, enabling both extensions is best, but beyond 50 it is not.

³Notice that for a given circuit, the number of CNOTs is independent of the extensions enabled. Thus, the number of ebits is normalised by the same value for each of the four configurations.

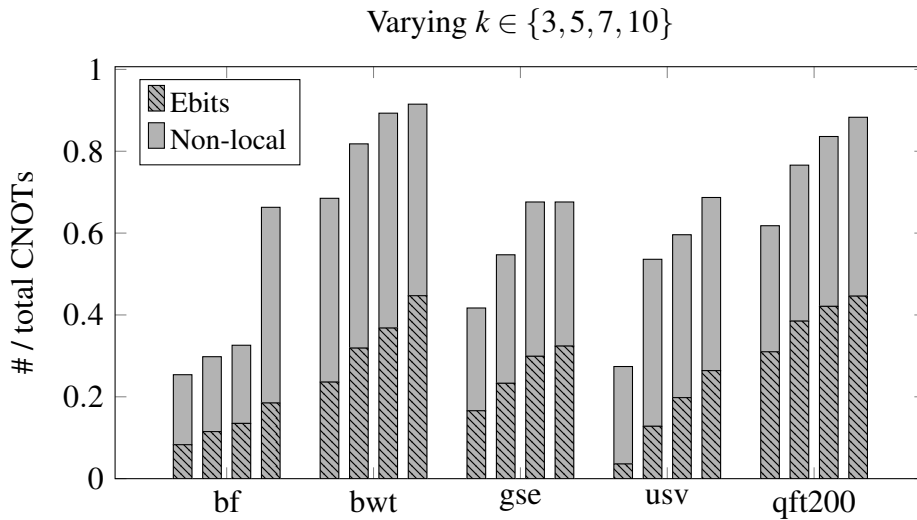


Figure 5.3: For each circuit, the bars correspond from left to right to a value of k equal to: 3, 5, 7 and 10. Each bar shows the number of non-local CNOTs and ebits required, normalised over the total number of CNOTs the original circuit had. The results shown are for the best combination of active extensions in each case.

Still, in all of our tests, enabling any combination of extensions was always better than running the algorithm with none. In practice, we would distribute the circuit with different extensions enabled, and choose the best combination. Considering that, in all of our tests, enabling both extensions was always in the top two best configurations, we would propose it as the default configuration to use. This is similar to how classical compilers provide a default set of optimisation flags (e.g. `-O2`), but you may obtain a more efficient object code if you enable/disable some of the fine-grained compilation flags manually.

Figure 5.3 follows the same format as in Figure 5.1, but now the different bars correspond to different values of the parameter k – the number of QPUs the circuits are distributed across. For each circuit, its best combination of extensions is used. As we would expect, distributing the circuit across more QPUs makes more CNOTs non-local and, correspondingly, the ebit count also increases. However, we can see how this increase is not necessarily uniform: When distributing the GSE circuit, the number of non-local gates and ebits required to distribute it across 10 QPUs is almost the same as if we distribute across 7 QPUs. The opposite situation happens for the BF circuit, as it seems to have a natural way of being partitioned across up to 7 QPUs – possibly because the qubits form groups that, for the most part, work isolated from other groups –, but, beyond 10 QPUs, wires that communicate intensively have to be separated – as a single QPU can not hold all of the qubits from a group. Still, in this particular case

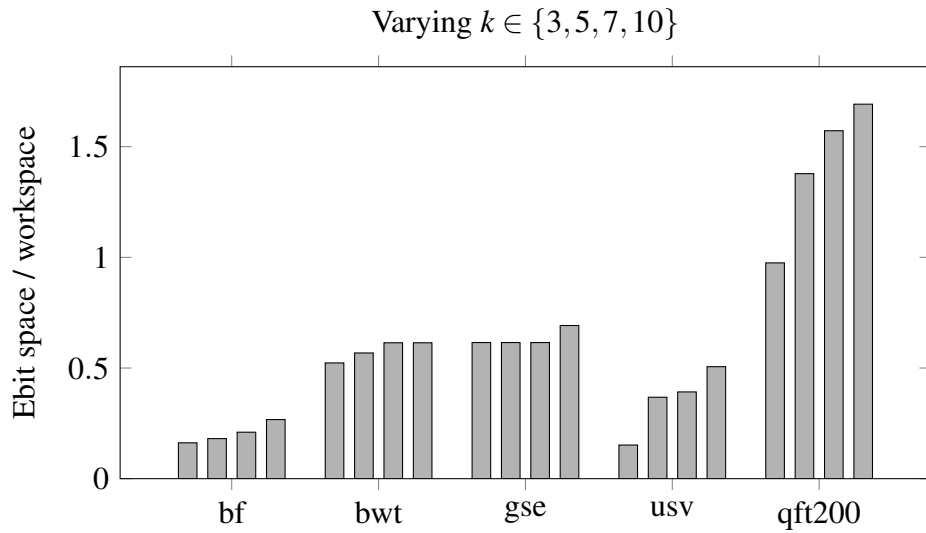


Figure 5.4: For each circuit, the bars correspond from left to right to a value of k equal to: 3, 5, 7 and 10. Each bar shows the ratio between the space that must be dedicated to communication (i.e. managing ebit halves) and the space dedicated to the computation itself. The results shown are for the best combination of active extensions in each case.

our algorithm manages to maintain a comparatively low ebit count.

Finally, Figure 5.4 shows the ratio between QPU space dedicated to communication (ebit space) versus space dedicated to computation (workspace qubits). A lower ratio is desirable, as we want as much computation space as possible. Naturally, the ratio is worse as we increase the number of QPUs we distribute across, because the workspace required stays the same, while more ebits are needed (as we just saw in Figure 5.3). Therefore, there is a tension here: we would like to use as many QPUs as possible, but we want them to manage a small space each. Figure 5.4 shows that this tension is different for each circuit: In cases such as BWT and GSE, the ratio barely changes, so if we decide to distribute them, we should use a relatively large amount of QPUs. On the other hand, circuits such as QFT-200 are not good candidates for distribution, as using only 3 QPUs already doubles the amount of space needed, and the ratio keeps increasing for larger k .

Chapter 6

Conclusions

In this work, we have proposed an algorithm that distributes any quantum circuit across a given number of QPUs. As far as we know, this is a novel contribution, as no other procedure for the automated distribution of quantum circuits can be found in the literature. Our algorithm minimises the ebit count, meaning that it yields minimal quantum communication across QPUs.

We make use of the work by Yimsiriwattana and Lomonaco Jr (2004), where groups of non-local CNOTs are implemented using a single ebit. We refer to their approach as the remote-control method. In §4.1 we gave two extensions of their work. First, we argued that in order to be in the same group, CNOTs are not required to be contiguous in the input circuit, as we may interchange CNOTs with other gates from Clifford+T to bring them together. Second, we showed that a construction dual to the remote-control method was also possible. Our main contribution was described in §4.2, where we proposed the vanilla version of our algorithm – that uses the results from the previous paper – and two extensions of it, corresponding to the two extensions we previously introduced.

Our algorithm reduces the problem of efficiently distributing a quantum circuit to the problem of hypergraph partitioning. As we discussed at the beginning of §4.2, hyperedges allow us to represent groups of CNOTs that share a wire in common. Using standard graph partitioning instead would correspond to the naive approach of creating an edge per individual CNOT. In that case, we would require an ebit per non-local CNOT. Using our approach, the number of ebits is in many cases considerably smaller than the number of non-local CNOTs, as shown in the figures from Chapter 5.

In Chapter 5 we analysed how well our algorithm distributed some benchmark quantum circuits. Figure 5.1 showed that enabling both of our algorithm extensions is

not always the best option in practice. We argued that this is due to the hardness of our problem (which is NP-complete, as discussed in Corollary 4.4), as the hypergraph partitioner does not manage to find the optimal partition of large/complex graphs. Nevertheless, enabling at least one of the extensions is always better than using none; and in our tests, enabling both extensions was always at least the second best option, so we propose it as the default configuration. Besides, discussing Figure 5.4 we concluded that not every quantum circuit is susceptible to being efficiently distributed, as in cases such as the Quantum Fourier Transform (QFT), the number of ebits required is larger than the number of qubits used in the actual computation.

This thesis may be seen as the first few steps towards compilers that adapt quantum programs to be run in distributed architectures. The implementation of our algorithm – although just a prototype – was integrated within the Quipper system, a quantum programming language with its own compiler. Further work should be dedicated to refining our implementation, so it is as efficient and scalable as it would be needed for practical use.

What we achieve in this thesis is a fine-grained distribution of the circuit, in the sense that our algorithm decides where each qubit – the smallest unit of information – is allocated. However, we know from classical computer science that it is often better to have a coarse-grained distribution, where the user explicitly indicates blocks of operations that should be executed locally. Our approach could be easily extended to accommodate this idea, as described in the first point of the following section.

6.1 Further work

In this section we suggest functionalities and other improvements that would be worthwhile working on in the future:

- *Coarse-grained distribution*: We may allow the user to assert that a group of qubits should be allocated to the same QPU. The user would use this functionality whenever the selected qubits had to interact intensively (e.g. a group of qubits participating on the circuit implementing an oracle). The user could convey this information using the comment command provided by Quipper (as if it were a compiler pragma). Our algorithm would read these comments and group the corresponding wires in a single vertex of the hypergraph, so they would always be allocated together. This would simplify the work of the hypergraph partitioner,

potentially allowing it to find a better partition of the rest of the circuit.

- *CNOT interchange optimisation*: We discussed this problem in §4.3, arguing it would be a natural extension to our algorithm. However, we were unable to find a procedure that guaranteed some degree of optimality. Still, there might be a subtle strategy to do so, involving dynamic programming. If no strategy can be found, we could still implement the different approaches we propose at the end of section §4.3, then test which combination of them yields the best results.
- *Choice of parameters*: Apart from k – the number of QPUs we wish to distribute across – there is an extra parameter, ϵ (load-imbalance tolerance), whose impact we have not tested. Additionally, we may have some extra parameters to fix depending on how we decide to control communication bottlenecks (see §4.2.4) or how we choose to manage the CNOT interchange problem (see §4.3). We should test different configurations of these parameters and decide on a default value for them. Besides, if we studied the effect of each parameter in detail, we may be able to come up with a decision algorithm that chooses the appropriate values to use depending on some characteristics of the input.
- *Non-uniform partition*: Throughout the thesis we assumed that the user would wish to distribute the circuit across multiple identical QPUs. However, it may happen that the QPUs available to the user have different numbers of qubits. Our algorithm can be easily adapted to manage this problem by asking the hypergraph partitioner to split the hypergraph into non-uniform blocks (i.e. with different number of vertices, decided beforehand). `KaHyPar`, the hypergraph partitioner we use, does give this option, so adding this functionality is straightforward.
- *Refined implementation*: As we discussed in §5.1, our implementation makes use of a simple list data structure, which is the main cause of inefficiencies in our code. `Quipper` has an internal data structure meant to manage circuits in an efficient and scalable manner. We should adapt our implementation to make use of their data structure, which is likely to improve efficiency considerably.

Appendix A

Hypergraph Partitioning

In this appendix we review the hypergraph partitioning problem and give a brief explanation of how `KaHyPar` (Akhremtsev et al., 2017) solves it. The version of `KaHyPar` we used can be found at: <https://github.com/SebastianSchlag/kahypar>.

A hypergraph is defined as a pair (V, H) , where V is some arbitrary set, known as the set of vertices, and $H \subseteq 2^V$ is the subset of hyperedges. Thus, each hyperedge is defined as a subset of vertices, which we refer to as the vertices reached by the hyperedge. The hypergraph partitioning problem has as input a hypergraph (V, H) and two parameters (k, ϵ) , where k is the number of blocks – sub-hypergraphs – we wish to partition the hypergraph into, and ϵ is known as the load-imbalance tolerance. The output is an assignment $f: V \rightarrow \{1, 2, \dots, k\}$ of vertices to blocks, satisfying¹:

- *Load-balance*: $\forall i \in \{1, 2, \dots, k\}: \|\{v \in V \mid f(v) = i\}\| < (1 + \epsilon) \frac{\|V\|}{k}$.
- *Minimal number of cuts*: Given a procedure for calculating a score metric $\chi_g \in \mathbb{N}$ of an assignment $g: V \rightarrow \{1, 2, \dots, k\}$, ensure that for each of the possible assignments f' , it holds that $f \neq f' \Rightarrow \chi_f < \chi_{f'}$. The metric χ_g may be calculated in multiple ways, each of them corresponding to a different variation of the hypergraph partitioning problem. Two commonly used metrics are:

a). The *cut* metric, defined as

$$\chi_g := \|\{h \in H \mid \exists v, u \in h: g(v) \neq g(u)\}\|$$

which corresponds to the number of hyperedges that reach vertices assigned to different blocks. Such hyperedges are said to be cut.

¹In the following mathematical definitions we use $\|A\|$ to refer to the cardinal of set A (i.e. the number of elements in it).

b). The $\lambda-1$ metric, defined as $\chi_g := \sum_{h \in H} \lambda_g(h) - 1$ where

$$\lambda_g(h) = \|\{i \in \mathbb{N} \mid \exists v \in h: g(v) = i\}\|$$

This metric is the one we use in the thesis. It not only takes into account the number of cut hyperedges, but also how many different blocks they reach.

The hypergraph partitioning problem is an NP-complete problem (Lyaudet, 2010). Therefore, fast algorithms to solve it can not guarantee that the solution they give is optimal, as to do so would require exponential time (unless $P = NP$). `KaHyPar` is a state-of-art hypergraph partitioner, which has been shown to perform better than the rest of its competitors (Akhremtsev et al., 2017). `KaHyPar` is comprised by three consecutive phases:

1. *Coarsening*: Groups of highly connected vertices are identified, and each of these groups is temporarily substituted by a single vertex. All of the hyperedges that reached a vertex in one of these groups now reach the vertex that substituted the group. This phase allows us to reduce the size of the hypergraph, and it ensures that highly connected vertices are not assigned to different blocks during the second phase of the algorithm.
2. *Initial partition*: The hypergraph is partitioned into k blocks. To do so, the hypergraph is first split in two blocks with equal number of vertices each, trying to minimise the chosen metric χ_g . Then, each block is recursively split further, until k blocks are obtained.
3. *Local search optimisation*: In this final phase, each of the groups of vertices substituted in the coarsening phase are restored. A local search is performed over the blocks, moving some of their vertices to neighbouring blocks whenever the reallocation yields a smaller value of the chosen metric χ_g . This reallocation must not violate the load-balance condition.

In §4.2.3 we make use of a variation of the hypergraph partitioning problem where vertices have a weight assigned to them. Adjusting the above algorithm to account for this variation is straight-forward; we just need to change the checks of the load-balance condition to be dependent on the sum of the weights from each block, instead of on the number of vertices. `KaHyPar` provides this variation of the problem among its options.

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