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Exploring Quantum Computation Through the Lens of Classical Simulation

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I, Padraic Calpin, confirm that the work presented in this thesis is my own. Where information has been derived from other sources, I confirm that this has been indicated in the thesis.

Signature

June 28, 2019

Date

Abstract

My research is about stuff.

It begins with a study of some stuff, and then some other stuff and things.

There is a 300-word limit on your abstract.

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Acknowledgements

Acknowledge all the things!

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Methods for Simulating Stabilizer Circuits

2.1 Introduction

In the previous chapter (INSERT SECTION REFERENCE LATER), we briefly introduced the notion of stabilizer circuits as a class of efficiently simulable quantum computations. In this chapter, we revisit stabilizer circuits in detail, with a focus on different classical data structures for encoding stabilizer states and the corresponding algorithms for simulations.

Several informal definitions of stabilizer circuits have been used in the quantum computing literature [1, 2, 3, 4]. However, what each definition has in common is that the operations $\mathcal{E}$ acting on an abelian subgroup $\mathcal{S} \subseteq \mathcal{P}_n$ generate a new subgroup $\mathcal{S}' \subseteq \mathcal{P}_n$. These groups $\mathcal{S}$ are also called a stabilizer groups.

In this thesis, we focus exclusively on stabilizer circuits acting on pure states $|\phi\rangle$ called stabilizer states. These can be entirely characterized by their associated stabilizer group as

$$s\,|\phi\rangle = |\phi\rangle \;\forall s \in \mathcal{S} \tag{2.1}$$

For an n-qubit state, the group $\mathcal{S}$ has 2^n elements [1]. As $\mathcal{S}$ is also abelian, this means it can be described by a generating set with n elements,

$$\mathcal{S} = \langle g_1, g_2, \ldots, g_n\rangle \;: g_i \in \mathcal{S}, \tag{2.2}$$

which are commonly referred to as the 'stabilizers' of the state $|\phi\rangle$. We also note that this definition allows us to write

$$|\phi\rangle\langle\phi| = \frac{1}{2^n}\sum_{s\in\mathcal{S}} s = \frac{1}{2^n}\prod_{i=1}^{n}(\mathbb{I}+g_i) \tag{2.3}$$

Given that these circuits map stabilizer states to other stabilizer states, this means they must be built up of unitary operations U which map Pauli operators to other Pauli operators under conjugation. This set is commonly denoted as $\mathcal{C}_2$, or the 'second level of the Clifford hierarchy'

$$\mathcal{C}_2 \equiv \{U : UPU^\dagger \in \mathcal{P}_n \;\forall P \in \mathcal{P}_n\} \tag{2.4}$$

$$\mathcal{C}_j \equiv \{U : UPU^\dagger \in \mathcal{C}_{j-1} \;\forall P \in \mathcal{P}_n\} \tag{2.5}$$

where in Eq. 2.5 we have also introduced the (recursive) definition for level j of the Clifford hierarchy. From this definition

$$V\mathcal{S}V^\dagger = \langle Vg_iV^\dagger\rangle = \langle g_i'\rangle = \mathcal{S}' \tag{2.6}$$

We also allow stabilizer circuits to contain measurements in the Pauli basis [1].

Simulating stabilizer circuits

From the above definitions, we can see that simulating a stabilizer circuit on n qubits corresponds to updating the n stabilizer generators for each unitary and measurement we apply. As the number of generators grows linearly in the number of qubits, if these group updates can be computed in time $O(\text{poly}(n))$ then it follows the circuits can be efficiently simulated clasically.

The first proof of this was given by Gottesman in [1], by showing through examples that stabilizer updates can be quickly computed for the CNOT, H and S gates, and for single qubit Pauli measurements. This is significant as the n qubit Clifford group can be entirely generated from these gates.

$$\mathcal{C}_2 = \langle CNOT_{i,j}, H_i, S_i : i,j \in \mathbb{Z}_n\rangle. \tag{2.7}$$

This result is typically referred to as the 'Gottesman-Knill' theorem.

A more formal proof follows from the work of Dehaene & de-Moor, who showed that the action of Clifford unitaries on Pauli operators corresponds to multiplication of $(2n+1)\times(2n+1)$ symplectic binary matrices with $(2n+1)$-bit binary vectors [5]. The dimension of these elements also grows just linearly in the number of qubits, and as matrix multiplication requires time $O(n^{2.37})$ it follows that we can update the stabilizers in $O(mn^{2.73})$ for m Clifford gates.

This work was then extended by Aaronson & Gottesman, who introduced an efficient data structure for stabilizer groups, and algorithms for their updates under Clifford gates and Pauli measurement [2]. This method avoids the need for matrix multiplications, instead providing direct update rules allowing stabilizer circuits to be simulated in $O(n^2)$.

Since 2004, there have been several papers looking at different data structures and algorithms for simulating stabilizer circuits of the type we consider here. For example, a method based on encoding stabilizer states as graphs [6], refinements of the Aaronson & Gottesman encoding [7], and an encoding using affine spaces and phase polynomials [3, 8].

In the rest of this section, we will discuss different aspects of simulating stabilizer circuits, focusing on updating stabilizer states under gates and measurements, computing stabilizer inner products, and the connections between stabilizer circuits and states.

2.1.1 Tableau Encodings of Stabilizer States

The method in [2] is based on a classical data structure they call the ‘stabilizer tableau’, a collection of Pauli matrices that define the stabilizer group, encoded using the binary symplectic representation of [5]

$$P = i^{\delta} - 1^{\epsilon} \bigotimes_{i=1}^{n} x_i z_i \tag{2.8}$$

where the Pauli matrix at qubit i is defined by two binary bits such that

$$x_i z_i = \begin{cases} I & x_i = z_i = 0 \\ X & x_i = 1, z_i = 0 \\ Z & x_i = 0, z_i = 1 \\ Y & x_i = z_i = 1 \end{cases} \tag{2.9}$$

Together with the δ and ϵ phases, a generic Pauli operator can be encoded in $2n+2$ bits; two bits to encode the phase, and two n-bit binary strings $\tilde{x}, \tilde{z} \in \mathbb{Z}_2^n$ to encode the Pauli acting on each qubit, commonly referred to as 'x-bits' and 'z-bits' respectively. In this picture, multiplication of Pauli operators corresponds to addition of x and z bits modulo 2, with some additional, efficiently computable function for correcting the phase [5]

$$PQ = i^{\delta_{pq}} - 1^{\epsilon_{pq}} \bigotimes_{i=1}^{n} x'_i z'_i \tag{2.10}$$

$$x'_i = x_{pi} \oplus x_{qi} \tag{2.11}$$

$$z'_i = z_{pi} \oplus x_{qi} \tag{2.12}$$

where $\delta_{pq} = \delta_p \oplus \delta_q$, $\epsilon_{qr} = f(\tilde{x}_p, \tilde{z}_p, \tilde{x}_q, \tilde{z}_q)$.

In stabilizer groups, we can restrict ourselves to considering Pauli operators with only real phase. This is because if $iP \in \mathcal{S}$, then $(iP)^2 = -I \in \mathcal{S}$. But, this implies that $-I\,|\phi\rangle = |\phi\rangle$, which is a contradiction.

While only n generators S_i are needed to characterize the stabilizer group $\mathcal{S}$, the tableau also includes an additional $2n$ operators called 'destabilizers' $D_i \in \mathcal{P}_n$. Together, these $2n$ operators generate all 4^n elements of $\mathcal{P}_n$.

There are many possible choices of destabilizer, but the tableau chooses operators such that [2]

$$
\begin{aligned}
[D_i, D_j] &= 0 \, \forall i, j \in \{1, \dots, n\} \\
[D_i, S_j] &= 0 \iff i \neq j \\
\{D_i, S_i\} &= 0
\end{aligned}
$$

Altogether, the full tableau has spatial complexity $4n^2 + 2n$. These are sometimes referred to as 'Aaronson-Gottesman 'tableaux or 'CHP' tableaux, after the software implementation by Aaronson [9].

$$
\begin{array}{c|ccc|ccc|c}
\mathcal{D}_1 & x_{1,1} & \cdots & x_{1,n} & z_{1,n} & \cdots & z_{1,n} & r_1 \\
\vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots \\
\mathcal{D}_n & x_{n,1} & \cdots & x_{n,n} & z_{n,1} & \cdots & z_{n,n} & r_n \\
\hline
\mathcal{S}_1 & x_{n+1,n} & \cdots & x_{n+1,n} & z_{n+1,1} & \cdots & z_{n+1,n} & r_{n+1} \\
\vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots \\
\mathcal{S}_n & x_{2n,1} & \cdots & x_{2n,n} & z_{2n,1} & \cdots & z_{2n,n} & r_{2n}
\end{array}
\qquad (2.13)
$$

Figure 2.1: Example of a 'CHP' tableau, where the first n rows are the Destabilizers and the next n rows are the stabilizers. The $2n+1$th column gives that phase -1^{r_i} for each operator.

Simulating Gates

Gate updates for each individual operator in the tableau can be computed constant time. For example, the Hadamard transforms single qubit Pauli matrices under conjugation as

$$
HPH^\dagger = \begin{cases} I & P = I \\ Z & P = X \\ X & P = Z \\ -Y & P = Y \end{cases} \qquad (2.14)
$$

In the symplectic form, we then have to update the ith Pauli operator as

$$
x_i' z_i' = (x_i \oplus p)(z_i \oplus p) \, : \, p = x_i \oplus z_i \qquad (2.15)
$$

and the phase as

$$
\delta' = \delta \oplus (x_i \wedge z_i) \qquad (2.16)
$$

Similar update rules exist for the CNOT and S gates, which together generate the n qubit Clifford group. As there are $O(n)$ operators in the tableau, and each update is constant time, gate updates overall take $O(2n)$ [2]. This is in contrast to the $O(n^{2.37})$ complexity of [5]

Simulating Measurements

The addition of the destabilizer information is used to speed up the simulation of Pauli measurements on Stabilizer states. Measuring some operator P on a stabilizer state will always produce either a deterministic outcome, or an equiprobable random outcome [1].

If the outcome is deterministic, then $\pm P$ is in the stabilizer group, and the outcome is $+1$ or -1 respectively. Using the stabilizer genereators, this allows us to write

$$[P, S_i] = 0 \,\forall S_i \in \mathcal{S} \implies \prod_i c_i S_i = \pm P. \tag{2.17}$$

for binary coefficients c_i.

Checking if the outcome is deterministic takes $O(n^2)$ time in general, using the symplectic inner product to check the commutation relations [5]. However, checking which measurement outcome occurs involves computing the coefficients c_i. In the symplectic form, thiscan be rewritten as

$$Ac = P$$

where c is a binary vector, A is a matrix with each stabilizer as a column vector, P is the operator to measure, and we have dropped the phase. Solving this would require inverting the matrix A, and take time $O(n^3)$.

Aaronson & Gottesman show that for single qubit mesurements, including destabilizer information instead allows us to compute the c_i and the resulting measurement outcome in $O(n^2)$. As this is a single qubit measurement, they also show that the commutivity relation requries checking only individual bits of the stabilizer vectors, also reducing that step to $O(n)$ time.

For random measurements, from Eq. 2.17, $\exists S_i : \{S_i, P\} = 0$, and it suffices to replace this stabilizer with P, and update the other elements of the group as $S'_j = PS_j$ iff $\{S_j, P\} = 0$ [1, 2].

'Canonical' Tableaux

There are multiple possible choices of generators for each stabilizer group/state. For example, for the Bell state $|\phi^+\rangle = \frac{1}{2}(|00\rangle + |11\rangle)$

$$\mathcal{S} = \{II, XX, -YY, ZZ\} = \langle XX, -YY\rangle = \langle XX, ZZ\rangle = \langle -YY, ZZ\rangle. \tag{2.18}$$

In simulation, tableau are fixed by choice of a convention. For example, it is possible to arrive at a 'canonical' set of stabilizer generators using an algorithm which strongly resembles Gaussian elimination [7]. This method rearranges the stabilizer rows of the tableau by multiplying and swapping generators, such that the overall stabilizer group is left unchanged. Computing this canonical form requires time $O(n^3)$ [7].

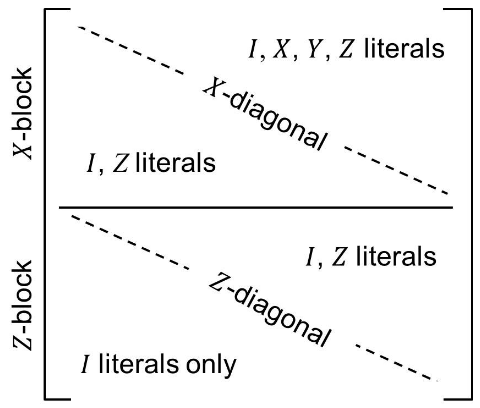


Figure 2.2: Representation of the canonical or 'row-reduced' set of stabilizer generators. Figure taken from [7].

These tableau can then be updated using the same methods as in [2], though this will in general not preserve the canonical form. Each Clifford gate will change one or two columns of the tableau, and thus an additional $O(n)$ row multiplications are required to restore it to canonical form, taking total time $O(n^2)$ per gate [10]. Importantly this canonical tableau can also be used to compute deterministic measurement outcomes in time $O(n)$, and so this method can simulate measurement outcomes more efficiently at the cost of more expensive gate updates [10].

In contrast, Aaronson & Gottesman fix the stabilizer tableau through an initial state, $|0\rangle^{\otimes n}$. The full tableau for this state looks like the identity matrix, with an additional zero-column for the phases. The tableau of a given state $|\phi\rangle$ is then built-up gate by gate using a stabilizer circuit $V : |\phi\rangle = V\,|0^{\otimes n}\rangle$.

2.1.2 Connecting Stabilizer States and Circuits

The convetion for 'CHP' stabilizer tableaux mentioned above, and the definition of stabilizer circuits given in Section 2.1, show that stabilizer states can also be defined by a stabilizer circuit and an initial state.

In [2], the authors derive examples of these 'canonical circuits', and show that its possible for any stabilizer state to be synthesised by a unique circuit acting on the $|0^{\otimes n}\rangle$ state

$$|\phi\rangle = V\,|0\rangle = H\,C\,S\,C\,S\,C\,H\,S\,C\,S\,|0^{\otimes n}\rangle \tag{2.19}$$

where each letter denotes a layer made up of only Hadamard (H), CNOT (C) or S gates. The proof is based on a sequence of operations reducing an arbitrary tableau to the identity matrix, each step of which corresponds to applying layers of a given Clifford gate [2]. As a corollary, the total number of gates in the canonical circuit for an n-qubit stabilizer state scales as $O(n\log(n))$ [2], based on previous work on synthesising $CNOT$ circuits with the $O(n\log(n))$ gates [11], and that each H and P layer can act on at most n-qubits.

A slightly simpler canonical form was derived in 2008, which allows a stabilizer circuit to be written as

$$|\phi\rangle = S\,CZ\,X\,C\,H\,|0^{\otimes n}\rangle \tag{2.20}$$

where the CZ and X layers are made up of Controlled-Z gates and Pauli X gates, respectively [3]. This circuit follows from the work of [5], who showed that any stabilizer state can be written as

$$|\phi\rangle = \frac{1}{\sqrt{2^k}} \sum_{x\in\mathcal{K}} i^{f(x)}\,|x\rangle\,. \tag{2.21}$$

In this equation, $\mathcal{K} \subseteq \mathbb{Z}_2^n$ is an affine subspace of dimension k, and $f(x)$ is a binary function evaluated $\mod 4$. Thus, a stabilizer state is always a uniform superposition of computational basis strings, with individual phases ±i, ±1. The affine space $\mathcal{K}$ has the form

$$\mathcal{K} = \{Gu + h\}$$

for k-bit binary vectors u, an $n \times k$ binary matrix G, and an n-bit binary 'shift-vector' h.

Van den Nest notes that this representation can be directly translated into a stabilizer circuit; we begin by applying H to the first k qubits to initialize the state $\sum_u |u\rangle \otimes \left|0^{\otimes n-k}\right\rangle$. We then apply CNOTs to prepare $\sum_u |Gu\rangle$, and finally Pauli Xs to preapre $\sum_u |Gu \oplus h\rangle$ [3].

The phases can be further decomposed into two linear and quadratic binary functions $l, q : \mathbb{Z}_2^n \to \mathbb{Z}_2$, such that $i^{q(x)} = i^{l(x)}(-1)^{q(x)}$. The linear terms correpsond to single qubit phase gates, which can be generated by the S gate, and the quadratic terms to two-qubit phase gates, generated by the CZ [3]. Thus,

$$|\phi\rangle = \sum_{x \in \mathcal{K}} i^{l(x)}(-1)^{q(x)} |x\rangle = S\ CZ\ X\ C\ H\ |0\rangle \tag{2.22}$$

While [3] showed that these simpler canonical circuits exist, an algorithm to compute them first introduced in 2012 [7]. This method allowed such a circuit to be read off from the 'canonical' set of stabilizer generators introduced in Section 2.1.1.

2.1.3 Computing Inner Products

The final task we might consider in simulating stabilizer circuits is the problem of computing probability amplitudes $P(x) = |\langle x|\phi\rangle|^2$. As computational states are also stabilizer states, this corresponds more broadly to computing inner products between stabilizer states.

From the affine space form in Eq. 2.21, we can see that

$$\langle \varphi|\phi\rangle = \frac{1}{\sqrt{2^{k+k'}}} \sum_{x \in \mathcal{K} \cap \mathcal{K}'} i^{f(x) - f'(x)} \tag{2.23}$$

and the problem of computing the inner product corresponds to computing the magnitude of an 'exponential sum' of phase differences (±i, ±1) for each string x in the intersection of the two affine spaces [8]. From inspection, we can see that

$$|\sum_x i^{f(x)-f'(x)}| = \begin{cases} 0 \\ 2^{s/2} : s \in \{0, 1, \ldots, n\} \end{cases}$$

This sum can be solved in $O(n^3)$ time, using an algorithm developed by Sergey Bravyi [8, 12, 13]. An algorithm for computing this intersection was also described in [8], which we discuss further in Section 2.2.3.

Alternatively, the inner product can also be computed using the stabilizer generators directly. Consider two states $|\phi\rangle, |\varphi\rangle$ with respective generators G_i, H_i. If $\exists i, j : G_i = -H_j$, the states are orthogonal and the inner product is 0. Otherwise, the inner product is given by 2^{-s}, where s the number of generators $G_i \notin \{H_i\}$.

While there are multiple choices of stabilizer generators, we note that inner products are invariant under unitary operations U as

$$\langle\varphi|\phi\rangle = \langle\varphi|U^\dagger U|\phi\rangle .$$

Thus, given the canonical circuit $V : |\varphi\rangle = V |0^{\otimes n}\rangle$

$$\langle\varphi|\phi\rangle = \langle\varphi|V^\dagger V|\phi\rangle = \langle 0^{\otimes n}|V|\phi\rangle .$$

Each stabilizer G'_i of $|0^{\otimes n}\rangle$ has a single Pauli Z operator acting on qubit i. By simplifying the stabilizer H'_i of $V|\phi\rangle$ using Gaussian elimination, then we have

$$|\langle 0^{\otimes n}|V|\phi\rangle| = \begin{cases} 0 & \exists H'_i = \bigotimes_i Z_i \\ 2^{-s} & \exists H'_i : \{H'_i, G'_i\} = 0 \end{cases} \tag{2.24}$$

where s is the number of stabilizers that anticommute with the corresponding stabilizer G'_i [2]. The second case arises as if $\{H'_i, G'_i\} = 0$, then H'_i acts as either Pauli X or Y on qubit i. Thus, the qubit is in state $|\pm 1\rangle$ or $|\pm \mathrm{i}\rangle$, and $\langle 0|\pm i, 1\rangle = \frac{1}{\sqrt{2}}$. Because this method involves computing the canonical circuit and then applying gaussian elimination, it runs in time $O(n^3)$.

The first implementation of this algorithm was given in [7], where the authors first use their canonical form to construct a 'basis circuit' $B : |\varphi\rangle = B\,|b\rangle$ for some computational state $|b\rangle$, and then compute $\langle b|B|\phi\rangle$ using the same method outlined above [7].

2.2 Results

The main result of this chapter is to introduce two new classical representations of stabilizer states developed in collaboration with Sergey Bravyi [12]. We will discuss their algorithmic complexity, and implementation in software. We will also briefly discuss the implementation of a classical datastructure based on affine spaces, introduced in [8].

Finally, we present data evaluating the performance of all three methods. For the affine space representation, we benchmark against existing implementations in MATLAB [8]. For the two novel representations, we present data comparing their performance to two pieces of existing stabilizer circuit simulation software [2, 6].

2.2.1 Novel Representations of Stabilizer States

Existing classical simulators have two important limitations. One is that they focus only on implementations of single qubit Pauli measurements made in the Z basis. Multi-qubit measurements, or measurements in different bases, need to be built up in sequence, or involve applying additional basis changes gates like H and S, respectively.

These simulators also do not track global phase information. For the case of simulating individual stabilizer circuits, this is sufficient as global phase does not affect measurement outcomes. However, if we wish to extend our methods to simulating superpositions of stabilizer states, then phase differences between terms in the decomposition must also be recorded [10].

Here, we present two data structures, which we call the 'DCH' and 'CH' forms.

Definition 2.1. DCH Representation:

Any stabilizer state $|\phi\rangle$ can be written as

$$|\phi\rangle = \omega^e U_D U_{CNOT} U_H |s\rangle \tag{2.25}$$

where U_D is a diagonal Clifford unitary such that

$$U_D |x\rangle = i^{f(x)} |x\rangle ,$$

U_{CNOT} is a layer of $CNOT$ gates, U_H is a layer of Hadamard gates, acting on a computational state $|s\rangle$, and with a global phase factor w^e where $\omega = \sqrt{\text{i}}$ and $e \in \mathbb{Z}_8$.

Any diagonal Clifford matrix of the form U_D is described by its 'weighted polynomial' $f(x)$, evaluated mod 4, which can be expanded into linear and quadratic terms as

$$f(x) = \sum_i a_i x_i + 2 \sum_{c,t} x_j x_k \mod 4 = L(x) + 2Q(x)$$

where the coefficients $a_i \in \mathbb{X}_4$ [3, 14]. This was also the expansion used in the definition of the affine space representation in Eq. 2.22.

We observe that the linear terms can be entirely generated by the S, Z and $S^\dagger$ gates acting on single qubits, and the quadratic terms by CZ gates acting on pairs of qubits [14]. Thus, any unitary U_D can be built up of these gates. As a corollary, we note that these 'DCH' circuits can be obtained from the 7-stage circuits given in Eq. 2.20, by commuting the X layer through to the beginning of the circuit and acting it on the $|0^{\otimes n}\rangle$ initial state. [3].

The computational string s can be encoded as an n-bit binary row-vector. This is also true of the Hadamard layer, which can be expanded in terms of a binary vector h as

$$U_H = \bigotimes_{i=1}^{n} H^{h_i}. \tag{2.26}$$

A $CNOT$ gate controlled on qubit c and targeting qubit t transforms the computational basis states as

$$CNOT_{c,t}\,|x\rangle = CNOT_{c,t}\bigotimes_{i=1}^{n}|x_i\rangle = \bigotimes_{i=1}^{n}|x_i \oplus \delta_{i,t}x_c\rangle$$

i.e. it adds the value of bit c to bit t, modulo 2. Thus, we can encode the action of U_{CNOT} as an $n \times n$ binary matrix E which is equal to the identity matrix, with an additional one at $E_{c,t}$, such that

$$CNOT_{c,t}\,|x\rangle = |xE\rangle \;:\; E_{i,j} = \begin{cases} 1 & i = j \\ 1 & i = c, j = t \\ 0 & otherwise \end{cases} \tag{2.27}$$

We can then build up U_{CNOT} from successicve CNOT gates as

$$U_{CNOT}\,|x\rangle = |xE_1E2E_3\ldots E_m\rangle \equiv |xW\rangle \tag{2.28}$$

where $W = E_1E_2\cdots E_n$ is the matrix representing the full circuit, obtained by successive right multiplication of the matrices encoding a single CNOT.

Finally, we need to encode the action of U_D. The phase resulting from a single qubit diagonal Clifford is conditional on the qubits being in the $|1\rangle$ state. Thus, we can write the linear part of the weighted polynomial as Lx^T for some row-vector L of integers mod 4, which we call the linear phase vector. Each value in L can be stored using just 2 bits.

Each gate $CZ_{i,j}$ between qubits i and j also contributes a factor of 2 to the overall phase, conditioned on the ith and jth qubits being in the $|1\rangle$ state. For a given computational string x, the overall phase from the CZ gates is thus $2\sum_{i,j:CZ_{i,j}} x_ix_j$.

We can encode the action of the CZ gates using an $n \times n$ symmetic binary matrix Q where $Q_{i,j} = Q_{j,i} = 1$ if we apply $CZ_{i,j}$, and zero otherwise, which we call the quadratic phase matrix. We can then compute the phase from the CZ gates as

$$\begin{aligned}
xMx^t &= \sum_p x_p \left(Qx^T\right) \\
&= \sum_p x_p \left(\sum_q Q_{p,q} x_q\right) \\
&= \sum_{p,q} x_p x_q Q_{p,q} \\
&= 2 \sum_p \sum_{q>p} x_p x_q Q_{p,q} \\
&= 2 \sum_{i,j: CZ_{i,j} \in U_D} x_i x_j
\end{aligned}$$

where the last line follows from the definition of the matrix Q. Altogether, this allows us to write [8]

$$U_D \left|x\right\rangle = i^{f(x)} \left|x\right\rangle = i^{Lx^T + xQx^T} \left|x\right\rangle = i^{xBx^T} \left|x\right\rangle \tag{2.29}$$

where B is a matrix such that $B_{ii} = L_i$, $B_{i,j} = Q_{i,j}$, as by definition Q has zero diagonal. We refer to B as simply the phase matrix, with diagonal elements stored mod 4 and off-diagonal elements stored mod 2.

Finally, we include the global phase factor, an integer modulo 8 and stored using just three bits, meaning overall the DCH representation is specified by the tuple (e, s, h, B, W). The spatial complexity is thus $\Theta(n^2)$. In order to optimize certain subroutines, which we discuss later in this section, we also store a copy of W^{-1}, the inverse of the CNOT matrix, and W^T, the transpose of the CNOT matrix. We further introduce two variables $p \in \{0, 1, \ldots, n\}$, $\epsilon = 0, 1$, which are used to ensure normalisation of the DCH state under certain operations. Together with the phase e, they define a coefficient we denote $c = 2^{-p/2}\epsilon\omega^e$. We store p as an unsigned integer, and ϵ as a single binary bit. Overall, then, the DCH form requires roughly $4n^2 + 4n + 36$ bits of memory.

Definition 2.2. CH Representation:

Any stabilizer state $\left|\phi\right\rangle$ can be written as

$$\left|\phi\right\rangle = \omega^e U_C U_H \left|s\right\rangle \tag{2.30}$$

where U_C is a Clifford operator such that

$$U_C \left|0^{\otimes n}\right\rangle = \left|0^{\otimes n}\right\rangle, \tag{2.31}$$

U_H is a layer of H gates, $|s\rangle$ is a computational basis state, and with global phase factor ω^e where $\omega = \sqrt{i}$ and $e \in \mathbb{Z}_8$.

The CH representation is based on a notion of a 'control-type' Clifford operator, which stabilizes the all zero computational basis state. Examples of control-type Clifford gates include the S, CZ and $CNOT$ gates. A control type operator U_C can be obtained from the DCH form, for example, by concatenating U_D and U_{CNOT} layers. Thus, we can see that any stabilizer state can be generated by a CH-type circuit.

Similarly to above, we encode the initial computational basis state s and the Hadamard layer U_H as n-bit binary row-vectors. The control-type layer we then encode using a stabilizer tableau, made up of $2n$ Pauli operators $U_C^\dagger X_i U_C$ and $U_C^\dagger Z_i U_C$. This tableau resembles a CHP-type tableau for the state $U_C \left|0^{\otimes n}\right\rangle$, where the Pauli X entries are the destabilizers and the Pauli Z entries are the stabilizers. Alternatively, we can see this as characterising the operator U_C by its action on the generators of the Pauli group.

Using a normal CHP-tableau, each Pauli would require $2n+1$ bits to encode. However, from the definition of the control-type operators, $U_C^\dagger Z_i U_C$ will never result in a Pauli X or Y operator, as otherwise $U_C \left|0^{\otimes n}\right\rangle \neq \left|0^{\otimes n}\right\rangle$. Thus, we can ignore the n 'x-bits' and phasebits of each of the Pauli Z rows. Specifically, we write

$$U_C^\dagger Z_j U_C = \bigotimes_{k=1}^{n} Z^{G_{j,k}} \tag{2.32}$$

$$U_C^\dagger X_j U_C = i^{\gamma_j} \bigotimes_{k=1}^{n} X^{F_{j,k}} Z^{M_{j,k}} \tag{2.33}$$

for binary matrices G, F, M, and a phase vector $\gamma : \gamma_i \in \mathbb{Z}_4$, as $Y = -\mathrm{i}XZ$. Note that this differs from the CHP method, where the string 11 encodes Pauli Y directly, without tracking a separate complex phase.

Finally, we again require three further bits to encode the global phase, and the CH representation is thus given by the tuple (e,s,h,G,M,F). Overall, the CH form also has spatial complexity $\theta(n^2)$. In order to optimize some subroutines, we additionally store copies of M^T and F^T, and again include the variables p and ϵ, requiring a total of $5n^2+4n+36$ bits of memory.

2.2.2 Simulating circuits with the DCH and CH Representations

In this section, we will outline how to update the DCH and CH representations under different stabilizer circuit operations, and how to compute the inner product. For both methods, gate updates can be split into two types: control-type operators, and Hadamard gates. The technique for treating the Hadamard also shares some aspects with applying Pauli projectors to the states, and deciding measurement outcomes. Some of the techniques employed will be common to both representations, differing only in their implementation on the underlying datastrucutre.

Gate updates: The DCH Representation

In the DCH picture, the complexity of a gate depends on whether it is a $CNOT$, or a diagonal Clifford operator S, Z, $S^\dagger$ or CZ. Diagonal gates can be simulated in constant time $O(1)$ by simply updating the linear or quadratic part of the diagonal layer. Single qubit gates applyed to qubit i update the ith element of the linear phase vector D, as they contribute only to the linear part of the weighted polynomial. Thus, we have

$$S_i\left|\phi\right\rangle \implies B_{i,i} \leftarrow B_{i,i}+1 \mod 4 \tag{2.34}$$

$$Z_i\left|\phi\right\rangle = S^2\left|\phi\right\rangle \implies B_{i,i} \leftarrow B_{i,i}+2 \mod 4 \tag{2.35}$$

$$S_i^\dagger = s^3\left|\phi\right\rangle \implies B_{i,i} \leftarrow B_{i,i}+3 \mod 4. \tag{2.36}$$

Similarly, a CZ gate applied to qubits i and j will change entries $B_{i,j}$ and $B_{j,i}$ of the quadratic phase matrix as

$$B'_{i,j} \leftarrow B_{i,j} \oplus 1, \tag{2.37}$$

and equivalently for $B_{j,i}$.

For $CNOT$ gates, we first need to commute them past the diagonal layer before updating U_{CNOT}. The overall effect on the DCH form is then

$$\begin{aligned}CNOT_{c,t}\left|\phi\right\rangle &= i^e\, CNOT_{c,t}U_D U_{CNOT} U_H \left|s\right\rangle \\ &= i^e\, CNOT_{c,t}U_D CNOT^{\dagger}_{c,t} U'_{CNOT} U_H \left|s\right\rangle \\ &= i^e\, U'_D U'_{CNOT} U_H \left|s\right\rangle \end{aligned} \tag{2.38}$$

updating U_{CNOT} using matrix multiplication as in Eq. 2.28, and where the last line relies on the following Lemma:

Lemma 1 *For any CNOT circuit U_{CNOT} and any diagonal Clifford circuit U_D, $U^{\dagger}_{CNOT}U_D U_{CNOT}$ is also a diagonal Clifford circuit U'_D with corresponding phase matrix $B' = WBW^T$.*

Proof of Lemma 1. Consider the case of a single CNOT gate on qubits c and t. We have

$$\begin{aligned}CNOT^{\dagger}_{c,t}U_D CNOT_{c,t}\left|x\right\rangle &= CNOT_{c,t}U_D CNOT_{c,t} \\ &= CNOT_{c,t}U_D \left|x + x_j e_k \mod 2\right\rangle \\ &= \mathrm{i}^{f(x+x_je_k)} CNOT_{c,t}\left|x + x_j e_k \mod 2\right\rangle \\ &= \mathrm{i}^{f(x+x_je_k)} \left|x + 2x_j e_k \mod 2\right\rangle \\ &= \mathrm{i}^{f(x+x_je_k)} \left|x\right\rangle \end{aligned} \tag{2.39}$$

where we have used the fact that a single CNOT gate is self-inverse. Thus, $CNOT^{\dagger}_{c,t}U_D CNOT_{c,t}$ acts as a diagonal Clifford gate. As any CNOT circuit is a sequence of individual CNOT gates, $U^{\dagger}_C U_D U_C$ is also a diagonal Cliford circuit.

Using the matrix representation of the action of U_C, it is easy to show that

$$\begin{aligned}U^{\dagger}_C U_D U_C &= U_{C^{\dagger}} U_D \left|xW\right\rangle \\ &= \mathrm{i}^{(xW)B(xW)^T} U^{\dagger}_C \left|xW\right\rangle \\ &= \mathrm{i}^{(xW)B(xW)^T} \left|xWW^{-1}\right\rangle \\ &= \mathrm{i}^{xWBW^Tx^t} \left|x\right\rangle, \end{aligned} \tag{2.40}$$

completing the proof. □

In general, computing the updated form of $U^{\dagger}_{CNOT}U_DU_{CNOT}$ would require time $O(n^2)$. However, for the case of a single gate $CNOT_{c,t}$, recall that the matrix E differs from the identity matrix at a single element, $E_{c,t} = 1$. This allows us to simplify the updates as

$$\left[E_{c,t}BE^T_{c,t}\right]_{i,j} = \sum_{k,l} E_{i,k}E_{j,l}B_{k,l} = \begin{cases} B_{i,j} & i,j \neq c \\ B_{c,j} + B_{t,j} & i = c,\, j \neq c \\ B_{i,c} + B_{i,t} & i \neq c,\, j = c \\ B_{c,c} + B_{t,t} + B_{c,t} + B_{t,c} & i = j = c \end{cases} \tag{2.41}$$

Additionally, we need to update W and W^{-1}. The inverse of U_C is the same sequence of CNOT gates, applied in reverse order. Thus, we have $W^{-1} = E_mE_{m-1}\cdots E_1$, and we update W^{-1} by left multiplication with the CNOT matrix. Using the definition of the CNOT matrix,

$$[WF]_{ij} = \quad \textstyle\sum_k W_{i,k}F_{k,j} = \quad \begin{cases} W_{i,j} & j \neq t \\ W_{i,c} + W_{i,t} & j = t \end{cases}$$

$$[FW^{-1}]_{i,j} = \quad \textstyle\sum_k F_{i,k}W^{-1}_{k,j} = \quad \begin{cases} W^{-1}_{i,k} & i \neq c \\ W^{-1}_{c,j} + W^{-1}_{t,j} & i = c \end{cases}$$

updating just the target column and the control row of W and W^{-1}, respectively.

Putting together these two pieces, we thus have

$$\begin{aligned} CNOT_{c,t}\,|\phi\rangle \implies & \mathrm{row}_c(B) \leftarrow \mathrm{row}_c(B) + \mathrm{row}_t(B) \\ & \mathrm{col}_c(B) \leftarrow \mathrm{col}_c(B) + \mathrm{col}_t(B) \\ & \mathrm{col}_t(W) \leftarrow \mathrm{col}_t(W) + \mathrm{col}_c(W) \\ & \mathrm{row}_c(W^{-1}) \leftarrow \mathrm{row}_c(W^{-1}) + \mathrm{row}_t(W^{-1}) \end{aligned} \tag{2.42}$$

These updates take $O(n)$ time, as we update a constant number of rows and columns.

Gate Updates: The CH Representaiton

For the CH representation, whenver we apply a new control-type operator C we need to update the stabilizer tableau by conjugating each element $U_C^\dagger X_i$, $Z_i U_C$ with the matrix C. This can be implemented using the usual rules for updating Pauli operators under Clifford operations, with the additional note that we have to adjust the updates to correctly track the phases of the Pauli X terms, and that we are conjugating as $U_C^{-1} P U_C$, rather than $U_C P U_C^{-1}$.

The control-type circuit is built out of individal operations $U_C = C_m C_{m-1} \dots C_1$. We we update U_C with some new operator C_{m+1}, change the tableau as

$$(C_{m+1}U_C)^\dagger P C_{m+1} U_C = U_C^\dagger \left(C_{m+1}^\dagger P C_{m+1} \right) U_C. \tag{2.43}$$

Because C_{m+1} is a Clifford operator, the term $C_{m+1}^\dagger P C_{m+1}$ is also a Pauli operator $P' = i^\alpha \prod_{i=1}^n X_i^{x_i} Z_i^{z_i}$ for some phase α and bit strings x and z. This allows us to write

$$\begin{aligned} U_C^\dagger C_{m+1}^\dagger P C_{m+1} U_C &= i^\alpha U_C^\dagger \left(\prod_{i=1}^n X_i^{x_i} Z_i^{z_i} \right) U_C \\ &= i^\alpha \prod_{i=1}^n U_C^\dagger X_i^{x_i} Z_i^{z_i} U_C \\ &= i^\alpha \prod_{i=1}^n U_C^\dagger X_i^{x_i} U_C U_C^\dagger Z_i^{z_i} U_C \\ &= i^\alpha \prod_{i=1}^n \left(i^{\gamma_i} \prod_{j=1}^n X_i^{F_{i,j}} Z_i^{M_{i,j}} \right)^{x_i} \left(\prod_{i=1}^n Z_i^{G_{i,j}} \right)^{z_i} \end{aligned} \tag{2.44}$$

where the last line is a product of terms from the tableau of U_C.

As an example, consider the action of the S gate. For each term, we have

$$S^\dagger P S = \begin{cases} I & \rightarrow & I \\ X & \rightarrow & -\mathrm{i} XZ \\ Z & \rightarrow & Z \end{cases}$$

The Z stabilizers are unchanged, and the X/Y stabilizers flip from $\mathrm{i}^\alpha X^a Z^b$ to $\mathrm{i}^{\alpha+3} X^a Z^{b \oplus 1}$. On the tableau, acting an S gate on qubit q will only act non-trivially on the term $U_C^\dagger X_q U_C$, and thus

$$U_C^\dagger S^\dagger X_q S_q U_C = i^3 U_C^\dagger X_q U_C U_C^\dagger Z_q U_C \implies \begin{cases} \text{row}_q(M) & \leftarrow & \text{row}_q(M) + \text{row}_q(G) \\ \gamma_q & \leftarrow & \gamma_q + 3 \mod 4 \end{cases}$$

We can compute the updates for CZ and CX in the same way, giving overall gate update rules

$$\begin{aligned} S &\begin{cases} \text{row}_q(M) & \leftarrow & \text{row}_q(M) + \text{row}_q(G) \\ \gamma_q & \leftarrow & \gamma_q + 3 \mod 4 \end{cases} \\ CZ_{q,p} &\begin{cases} \text{row}_q(M) & \leftarrow & \text{row}_q(M) + \text{row}_p(G) \\ \text{row}_p(M) & \leftarrow & \text{row}_p(M) + \text{row}_q(G) \end{cases} \\ CNOT_{q,p} &\begin{cases} \text{row}_p(G) & \leftarrow & \text{row}_p(G) + \text{row}_q(G) \\ \text{row}_q(F) & \leftarrow & \text{row}_q(F) + \text{row}_p(G) \\ \text{row}_q(M) & \leftarrow & \text{row}_q(M) + \text{row}_p(M) \\ \gamma_q & \leftarrow & \gamma_q + \gamma_p + 2\sum_i M_{q,i} F_{p,i} \mod 4 \end{cases} \end{aligned} \tag{2.45}$$

Where on the final line, we apply an extra phase correction that results from re-ordering the Pauli operators in the CNOT updates. This arises as, expanding out the action on the X stabilizers,

$$\begin{aligned} U_C^\dagger CNOT_{q,p} X_q CNOT_{q,p} U_C &= U_C^\dagger X_q X_p U_C \\ &= U_C^\dagger X_q U_C U_C^\dagger X_p U_C \\ &= i^{\gamma_q + \gamma_p} \prod_{i=1}^{n} X_i^{F_{q,i}} Z_i^{M_{q,i}} X_i^{F_{p,i}} Z_i^{M_{p,i}} \end{aligned}$$

and we pick up an extra phase of -1 each time $M_{q,i} = F_{p,i} = 1$ as $ZX = -XZ$. All of these updates take time $O(n)$, as we are updating the n-element rows of $n \times n$ matrices.

Hadamard gates and Pauli Measurements

Simulating Hadamard gates and arbitrary Pauli measurements is done using an algorithm with the same general structure in the DCH and CH representation. These routines employ an algorithm developed by Sergey Bravyi for application to the CH method, which can also be applied to the DCH case.

Hadamard gates and Pauli projectors can both be written as $\frac{1}{\sqrt{2}}(P_1+P_2)$ for some Pauli operators P_1, P_2. In the Hadamard case, we have $P_1 = X_i, P_2 = Z_i$, and in the projector case $P_1 = I, P_2 = P$. Given this structure, we then commute these operators through to the comutational basis state

$$\begin{aligned}\epsilon 2^{-p/2} i^e \frac{1}{\sqrt{2}}(P_1+P_2) U_C U_H |s\rangle &= \epsilon 2^{-(p+1)/2} i^e U_C U_H (P_1'+P_2') |s\rangle \\ &= \epsilon 2^{-(p+1)/2} i^{e'} U_C U_H \Big(|t\rangle + i^\beta |u\rangle\Big)\end{aligned}$$

where $P_{1,2}'$ can be efficiently computed as the circuit $U_C U_H$ is Clifford, $\beta \in Z_4$, and t and u are two new computational basis states obtained from the action of $P_{1,2}$ on s. Note that we are writing U_C here as a shorthand, as the circuit $U_D U_{CNOT}$ in the DCH represntation is also a control-type unitary.

Once in this form, we employ the following proposition, called Proposition 4 in [12]:

Proposition 1 *Given a stabilizer state $U_H\Big(|t\rangle + i^\beta |u\rangle\Big)$, we can construct a circuit W_C built out of $CNOT$, CZ and S gates, and a new Hadamard circuit U_H', such that we can write*

$$U_H\Big(|t\rangle + i^\beta |u\rangle\Big) = i^{\beta'} W_C U_H' |s'\rangle .$$

As a means of proving this proposition, we will go through and construct W_C and U_H'.

Proof of Proposition 1. Firstly, consider the case $t = u$. Then we have $s' = t$, and the result depends on the phase β. If $\beta = 0$, then the state is unchaged. If $\beta = 1, 3$, then we have

$$\frac{1}{\sqrt{2}} U_H \Big(1 + i^\beta\Big) |s'\rangle = \frac{(1 \pm \mathrm{i})}{\sqrt{2}} U_H |s'\rangle$$

and it suffices to update the global phase term

$$\begin{aligned}\beta = 1 \quad &\Longrightarrow \quad e \leftarrow e+1 \mod 8 \\ \beta = 3 \quad &\Longrightarrow \quad e \leftarrow e+7 \mod 8\end{aligned}$$

Finally, if $\beta = 2$, we have $|s'\rangle - |s'\rangle$ and the state is cancelled out. We denote this by setting $\epsilon \leftarrow 0$. This only arises in the case of applying a Pauli projector that is orthogonal to the state.

If $t \neq u$, then we instead note that we can always define some sequence of $CNOT$ gates V_C such that

$$|t\rangle = V_C |y\rangle \quad |u\rangle = V_C |z\rangle$$

where y, z are two n-bit binary strings such that $y_i = z_i$ everywhere except bit q where $z_q = y_q + 1$. We can assume without loss of generality that $\exists q : t_q = 0, u_q = 1$, else we swap the two strings and update the phase accordingly. Then

$$V_C = \prod_{i: i \neq q,\, t_i \neq u_i} CNOT_{q,i}$$

and we can commute this circuit past U_H to obtain a new circuit V'_C. We can always freely pick $q : v_q = 0$, unless $v_i = 1 \forall i$, and thus V'_C is given by:

$$V'_C = \begin{cases} \prod_{i \neq q,\, v_i=0} CNOT_{q,i} \prod_{i \neq q,\, v_i=1} CZ_{q,i} & v_q = 0 \\ \prod_{i \neq q} CNOT_{i,q} & v_i = 1 \forall i \end{cases}$$

We complete the proof by considering the action of U_H on the new strings $|y\rangle + \mathrm{i}^{\beta} |z\rangle$. Again, fixing $y_q = 0, z_q = 1$, we can write

$$U_H \left(|y\rangle + i^{\beta} |z\rangle \right) = H^{v_q} S^{\beta} |+\rangle = \omega^a S_q^b H_q^c |d\rangle$$

for some bits $a, b, c, d \in \{0, 1\}$ that can be computed exactly from the values of β and v_q.

This completes the proof of Proposition 1, where $W_C = V'_C S_q^b$, $U'_H = U_H H_q^{v_q + c}$, and $s' = y \oplus d e_q$, where e_q is an indicator vector that is 1 at position q and zero elsewhere. $\square$

Computing the circuits W_C and U'_H given the two strings t, u takes time $O(n)$, as it involves inspecting the $n - bit$ strings t, u and v. Given this proposition, we now need to show how to commute a Pauli operator through the stabilizer circuit in both representations, and then how to update the layers $U_D U_{CNOT}$ and U_C by right multiplication with the circuit W_C. This can be rewritten in terms of binary vector-matrix multiplication, and we introduce the following notation:

$$\prod_{i=1}^{n} X_i^{x_i} \equiv X(x) \quad \prod_i Z_i^{z_i} \equiv Z(z)$$

for binary strings x and z.

Applying Proposition 1 to DCH States

When commuting a Pauli operator P through a Clifford circuit, it is important to fix the ordering of the X and Z terms, as Pauli operators can be expanded out as $P = i^a X(x)Z(z) = i^a(-1)^{x\cdot z}Z(z)X(x)$, as $XZ = -ZX$, and where we use $x\cdot z$ to denote the binary inner product

$$x\cdot z = \sum_i x_i z_i \mod 2.$$

In the DCH case, we fix $P = i^a Z(z)X(z)$, as this simplifies the phase terms when commuting past the U_D layer.

Pauli Z terms are unchanged by the DCH layer as they commute with diagonal Clifford oeprtors. To commute the X terms past the U_D layer, we use $X(x)U_D = U_D\left(U_D^\dagger X(x)U_D\right)$, and compute the new Pauli $U_D^\dagger P' U_D = i^{a'}Z(z')X(x)$.

The diagonal entries of the phase matrix B contribute as

$$(S^{B_{ii}})^\dagger X_i^{x_i} S^{B_{ii}} = \begin{cases} S^\dagger X^{x-i} S & \rightarrow & i(ZX)^{x_i} \\ ZXZ & \rightarrow & -X^{x_i} \\ SXS^\dagger & \rightarrow & -i(ZX)^{x_i} \end{cases} = i^{B_{ii}} X^{x_i} Z^{x_i B_{ii} \pmod 2}$$

We also have that $CZ(X\otimes I)CZ = XZ$, $CZ(I\otimes X)CZ = ZX$, i.e. a CZ conjugated with a Pauli X on the control (target) qubit adds a Pauli Z on the target (control) qubit. Qubit i picks up a Z operator each time there is a CZ between qubits i and j, and an X acting on qubit j. Using the off-diaognal entries of the phase matrix, we can write

$$Z_i^{z_i'} : z' = \sum_{j\neq i} x_j B_{j,i} \mod 2$$

Combining this with the fact we also pick up a Pauli Z from the diagonal if $B_{ii} = 1,3$, we can write $z_i = aB \mod 2$. Finally, we need to consider the extra -1 phase contributions for each $i : x_i z'_i = 1$, as a result of preserving the ordering of P'. Together with the diagonal phases, this can be simplified to

$$\sum_i x_i B_{ii} + 2\sum_i x_i \sum_{j\neq i} x_j B_{j,i} = xBx^T \mod 4$$

Overall then, we have

$$U_D^\dagger X(x) U_D = i^{xMx^T} Z(xM)X(x) \tag{2.46}$$

A similar result applies to commuting a Pauli operator through the U_{CNOT} layer. $CNOT$ has the property that it maps $I_c Z_t \to Z_c Z_t$ and $X_c I_t \to X_c X_t$ under conjugation. Thus, we can compute the new strings x', z' by applying an appropriate CNOT matrix.

For the X bits, we can simply apply $x' = xW^{-1}$, where we use the inverse matrix as we are computing $U_{CNOT}^\dagger X U_{CNOT}$ and thus the binary string is subject to the inverse sequence of CNOT gates.

For the string z, we need to apply a CNOT matrix with the controls and targets swapped. From the definition given in Eq. 2.27, we can see that if the binary matrix E encodes $CNOT_{c,t}$, then $CNOT_{t,c}$ is encoded by E^T. We then update the strign z under the sequence $E_m^t E_{m-1}^t \dots E_1^t = W^T$. This gives

$$U_{CNOT}^\dagger i^a Z(z)X(x)U_{CNOT} = i^a Z(zW^T)X(xW^{-1}). \tag{2.47}$$

As mentioned, we store copies of W^{-1} and W^T with the DCH representation. This helps to avoid the $O(n^3)$ computational cost associated with inverting W, and the $O(n^2)$ cost of transposing W. We can thus compute this update in time $O(n^2)$.

Finally, to commute a Pauli operator past the U_H layer, we note that the Hadamard acts as

$$\begin{aligned} HXH &\to Z \\ HZH &\to X \\ HZXH &\to -ZX \end{aligned}$$

The x and z bits are only changed for those bits where $v_i = 1$, and so we can write

$$z_i' = z_i(1-v_i) + x_i v_i$$

and vice-versa for the x bits. In terms of boolean operations, this can also be written as $z_i' = z_i \wedge \neg v_i \oplus x_i \wedge v_i$. Finally, we have the phase correction whenere $x_i = z_i = z_i = 1$. Thus, overall, we can write

$$U_H^\dagger i^a Z(z) X(z) U_H = i^{a+v\cdot(x\wedge z)} Z(z \wedge \neg v \oplus x \wedge v) X(x \wedge v) \tag{2.48}$$

and this update takes time $O(n)$ to compute.

To complete the application of Propositon 1, we also need to be able to update $U_D U_{CNOT}$ by right multiplication with W_C. We can split $W_C = W_{CNOT} W_D$, where W_D is made up of CZ gates and the single S gate.

The U_{CNOT} layer updates as $U_{CNOT}' = U_{CNOT} W_{CNOT}$. Because of the ordering of the circuits, we here update the matrix W by left multiplication, and update $W^\dagger$ by right multiplication. Thus, for each $CNOT$ gate in W_{CNOT}, we update the columns of W^{-1} and the rows of W using the rules given in Eq. 2.47.

We then need to commute the diagonal layer W_D past U_{CNOT}'. We can do this by adapting Eq. 2.40 to instead compute $U_{CNOT} W_D U_{CNOT}^\dagger$, giving a new phase matrix $C' = W^{-1} C W^{-1}$ where C encodes the action of W_D. This computation again benefits from storing W^{-1} in the DCH information, and can be further optimized by noting that many entries of C are zero. Finally, we can combine the two phase matrices by simplying adding all the elements, keeping the diagonal entries $\bmod 4$ and the off-diagonal entries $\bmod 2$. All together, including the Pauli updates, applying Proposition 1 takes time $O(n^2)$.

Applying Proposition 1 to CH States

Commuting a Pauli operator through the layers of the CH circuit can be done using methods already introduced in previous sections. Distinctly from the DCH case, here we fix $P = i^a X(x) Z(z)$.

To commute a Pauli past the U_C layer, we need to compute $U_C^\dagger P U_C$, and this can be expanded out in a similar manner to Eq. 2.44. This gives

$$\begin{array}{ll} U_C^\dagger X(x) U_C = & \prod_{i:x_i=1} U_C^\dagger X_i U_C \\ U_C^\dagger Z(z) U_C & \prod_{i:z_i=1} U_C^\dagger Z_i U_C \end{array}$$

We can thus build up P' term by term as

$$\begin{aligned} U_C^\dagger P U_C &= \prod_{j=1}^{n} x_j \left(\mathrm{i}^{\gamma_j} X(\mathrm{row}_j(F)) Z(\mathrm{row}_j(M))\right) \prod_{j=1}^{n} z_i \left(Z(\mathrm{row}_j(G))\right) \\ &= \mathrm{i}^{\sum_{j=1}^{n} x_j\gamma_j + 2\sum_{j=1}^{n}\sum_{k>j} x_j x_k (\mathrm{row}_j(F)\cdot \mathrm{row}_j(M))} X(xF) Z(xM+zG) \\ &= \mathrm{i}^{xJx^T} X(xF) Z(xM+zG). \end{aligned} \tag{2.49}$$

The extra factor of 2 in the phase arises from having to commute the Pauli Z terms in $U_C^\dagger X_j U_C$ past the following Pauli X terms. We can encode these commutation relations as a binary matrix

$$MF^T : \left[MF^T\right]_{i,j} = \mathrm{row}_i(M)\cdot \mathrm{row}_j(F),$$

which is additionally symmetric as

$$\left[U_C^\dagger X_j U_C, U_C^\dagger X_k U_C\right] = [X_j, X_k] = 0.$$

Similiar to the way we encode the phase polynomial in the DCH form, we can then simplify the overall phase calculation as

$$aJa^T : [J]_{i,j} = \begin{cases} \gamma_i & i = j \\ MF^T_{i,j} & i \neq j \end{cases}$$

where we pick up the correct factor of 2 from the symmetric nature of MF^T. Computing each of the matrix-vector multiplications to commute past $U_C$takes $O(n^2)$ time. We can then use the same update rule as for the DCH form to commute the Pauli operator past the U_H layer.

Finally, to finish applying Proposition 1, we need to update the tableau of U_C to

$U_C W_C$. We have

$$(U_C W_C)^\dagger X_i, Z_i (U_C W_C) = W_C^\dagger \left(U_C^\dagger X_i, Z_i U_C \right) W_C$$

an thus we need to update the Paulis in the tableau by conjugtion with $CNOT$, CZ and S gates. These rules for updating U_C by right-multiplication with a control type unitary are the same as for the CHP tableau, with some additional corrections for phase.

$$\begin{aligned}
&S \begin{cases} \mathrm{col}_q(M) & \leftarrow \quad \mathrm{col}_q(M) + \mathrm{col}_q(G) \\ \gamma & \leftarrow \quad \gamma - \mathrm{col}_q(F) \bmod 4 \end{cases} \\
&CZ_{q,p} \begin{cases} \mathrm{col}_q(M) & \leftarrow \quad \mathrm{col}_q(M) + \mathrm{col}_p(F) \\ \mathrm{col}_p(M) & \leftarrow \quad \mathrm{col}_p(M) + \mathrm{col}_q(F) \\ \gamma & \leftarrow \quad \gamma + \mathrm{col}_p(F) \cdot \mathrm{col}_q(F) \end{cases} \\
&CNOT_{q,p} \begin{cases} \mathrm{col}_q(G) & \leftarrow \quad \mathrm{col}_q(G) + \mathrm{col}_p(G) \\ \mathrm{col}_p(F) & \leftarrow \quad \mathrm{col}_p(F) + \mathrm{col}_q(F) \\ \mathrm{col}_q(M) & \leftarrow \quad \mathrm{col}_q(M) + \mathrm{col}_p(M) \end{cases}
\end{aligned} \tag{2.50}$$

There are $O(n)$ row and column updates to perform, and thus this final step runs in time $O(n^2)$. Overall, then, the complexity of applying Proposition 1 to the CH form is $O(n^2)$, arising from computing $U_C^\dagger P U_C$ and then updating the tableau under W_C.

Sampling Pauli Measurements with Proposition 1

Proposition 1 can also be extended to apply to sampling measurements of arbitrary Pauli operators. Measuring a Pauli operator P is closely related to applying a projector $\Pi_{\pm P} = \frac{1}{\sqrt{2}}(I \; \pm P)$. As mentioned previously, there are three possible outcomes for a Pauli measurement

$$\begin{aligned}
\Pi_{+P} \left|\phi\right\rangle = \left|\phi\right\rangle \quad & P\left|\phi\right\rangle = \left|\phi\right\rangle \quad \text{Deterministic Outcome } +1 \\
\Pi_{+P} \left|\phi\right\rangle = 0 \quad & P\left|\phi\right\rangle = -\left|\phi\right\rangle \quad \text{Determinitic Outcome } -1 \\
\Pi{+}P \left|\phi\right\rangle = \left|\phi\right\rangle + \left|\varphi\right\rangle \quad & P\left|\phi\right\rangle = \left|\varphi\right\rangle \quad \text{Random Outome}
\end{aligned}$$

In terms of measuring an operator P, then we can begin by commuting the projector $I + P$ through the Clifford circuit as described in the previous sections. Dropping the normalisation, we have

$$\begin{aligned}(I+P)V|s\rangle &= V\left(I+V^{\dagger}PV\right)|s\rangle\\ &= V\left(|s\rangle + P'|s\rangle\right) = V\left(|s\rangle + i^{\beta}|s'\rangle\right)\end{aligned}$$

which is the equivalent to the statement of Proposition 1, with $t=s$ and $u=s'$.

If $s=s'$, then the measurement outcome is deterministic. As we have used the projector Π_{+P}, the measurement outcome is $+1$ unless $\beta=2$, in which case the outcome is -1. Otherwise, if $s\neq s'$, the measurement outcome is random and equiprobable. We can sample the ±1 outcome using random number generation techniques, and then apply the corresponding projector $(I\pm P)$. As computing P' takes in general $O(n^2)$ time, deciding on the measurement outcome also takes $O(n^2)$ time. However, compare to other stabilizer simulators, we note that this algorithm works for arbitrary Pauli operators P as opposed to just single-qubit Pauli Z measurements.

Computational Amplitudes and Sampling Output Strings

Commuting Pauli operators through the layers of control type operators can also be used to compute the probability of a given computational basis state. Recall that a control-type Clifford circuit U_C is defined such that $U_C|0^{\otimes n}\rangle = |0^{\otimes n}\rangle$. Recall also that for the DCH representation, U_D and U_{CNOT} are also a control-type operators. Thus,

$$\begin{aligned}\langle 0^{\otimes n}|\phi\rangle &= w^e\langle 0^{\otimes n}|U_C U_H|s\rangle\\ &= w^e\left(\langle 0^{\otimes n}|U_C\right)U_H|s\rangle\\ &= w^e\langle 0^{\otimes n}|U_H|s\rangle .\end{aligned}$$

This trick, using the definition of a control-type operator to simplify the inner product, can be extended to any comptuational basis state. Writing $|t\rangle = X(t)|0^{\otimes n}\rangle$, we can then commute the X operators past the control-type layer (s) to obtain

$$\begin{aligned}\langle t|U_C U_H|s\rangle &= \langle 0^{\otimes n}|P'U_H|s\rangle\\ &= \langle 0^{\otimes n}|i^{\mu}Z(z')X(x')U_H|s\rangle = \langle x'|U_H|s\rangle \end{aligned}\tag{2.51}$$

where we have used the 'ZX' convention in the definition of the Pauli operator. If instead we use the 'XZ' convention, then we pick up an additional phase factor of $-1^{x'\cdot z'}$.

The action of the Hadamard layer on a computational basis state can be expanded out as

$$U_H \left|s\right\rangle = 2^{-|v|/2} (-1)^{s\cdot v} \sum_{x \leq v} (-1)^{s\cdot x} \left|s \oplus x\right\rangle \tag{2.52}$$

where $x \leq v$ denotes the binary strings $x : x_i = v_i \iff v_i = 0$ and $|v|$ is the Hamming weight of the string v. Thus, we have overall that

$$\langle t|\phi|=\rangle\, 2^{-|v|/2} i^{\mu} \prod_{j:v_j=1} (-1)^{x'_j s_j} \prod_{j:v_j=0} \left\langle x'_j \middle| s \right\rangle, \tag{2.53}$$

which equals 0 if any $u_j \neq s_j$ for $v_j = 0$, and is propostional to $2^{-|v|/2}$ otherwise. As this requires commuting a Pauli operator through the C/DC layer (s), computing these amplitudes takes time $O(n^2)$.

This result can also be extened to sample strings from the probability distriution $P(x) = |\langle t|V|s\rangle|^2$, where V_C is a Clifford circuit such that $V_C = U_C U_H \equiv U_D U_{CNOT} U_H$. From the above, we know that any string with a non-zero amplitude occurs with equal probability. This, it is sufficient to start with a binary string

$$w : w_j = \begin{cases} s_j & v_j = 0 \\ 0 & \text{otherwise} \end{cases}$$

and then pick each of the remaining $|v|$ bits at random with equal probability.

Computing Inner Products

The computational basis are a special case of stabilizer state inner products. Here, we present a general method for computing inner products $\langle \varphi|\phi\rangle$ using the DCH and CH forms. Both methods proceed by combining the two control-type layers, and then breaking down the computation into a sum of different computational basis state amplitudes

$$\begin{aligned}\langle\varphi|\phi\rangle &= \langle t|V_H V_C^\dagger U_C U_H|s\rangle \\ &= \langle t|V_H|\Phi\rangle : |\Phi\rangle = V_C^\dagger\,|\phi\rangle\,.\end{aligned}$$

Proposition 2 *Given a stabilizer inner product of the form*

$$\langle t|V_H|\Phi\rangle$$

where $|\Phi\rangle$ is encoded in DCH or CH form, we can compute the inner product by computing the computational state ampliude $\langle t|\Phi'\rangle$ where $|\Phi'\rangle = V_H\,|\Phi\rangle$, in time $O(n^3)$.

Proof of Proposition 2. In both the DCH and CH form, we can simulate the action of a single Hadamard gate in time $O(n^2)$. The Hadamard circuit V_H contains at most n Hadamard gates, and so we can compute $V_H\,|\Phi\rangle$ in time $O(n^3)$. The amplitude then reduces to computing the amplitude $\langle t|\Phi'\rangle$, which takes time $O(n^2)$. The overall worst-case complexity is thus $O(n^3)$. □

This method bares a strong resemblence to the 'basis circuit' method described in [7], with the advantage that the 'basis circuit' is explicity stored in the DCH and CH datastructures, rather than needing to be computed froma tableau. In the following sections, we will show how to compute $|\Phi\rangle$ from the DCH/CH data of $|\varphi\rangle$ and $|\phi\rangle$.

The DCH Case

In this representation, we need to compute $U_D' U_{CNOT}' = V_{CNOT}^\dagger V_D^\dagger U_D U_{CNOT}$. We begin by combining the two phase layers, noting that

$$U_D^\dagger\,|x\rangle = \mathrm{i}^{-xBx^t}\,|x\rangle$$

and thus given the two phase matrices A, B, the phase matrix encoding the combined circuit is

$$V_D^\dagger U_D\,|x\rangle = \mathrm{i}^{x(A-B)x^T}\,|x\rangle$$

where, as per the definition, the subtraction is $\bmod 2$ on the off-diagonal entries and $\bmod 4$ on the diagonal entries.

We then need to commute $V^{\dagger}_{CNOT}$ past the new U'_D layer, and combine it with U_{CNOT}. As this circuit is an inverse, it is characterised by the binary matrix Q^{-1}, and its inverse is Q. Thus

$$\begin{aligned} B' &\leftarrow Q^{-1}B'Q \\ W &\leftarrow WQ^{-1} \\ W^{-1} &\leftarrow QW^{-1} \end{aligned} \tag{2.54}$$

Altogether then, the updated DCH information of $|\Phi\rangle$ can be computed in time $O(n^2)$.

The CH Case

Given two tableau describing control-type unitaries V_C and U_C, we can combine them using Eq. 2.49, as

$$\begin{aligned} (V_C U_C)^{\dagger} X_j V_C U_C &= U_C^{\dagger}\left(V_C^{\dagger} X_j V_C\right) U_C \\ &= \mathrm{i}^{\gamma'_j} U_C^{\dagger} P U_C \\ &= \mathrm{i}^{\gamma'_j + \mathrm{row}_j(F') J \mathrm{row}_j(F')^T} X(\mathrm{row}_j(F')F) Z(\mathrm{row}_j(M')M), \end{aligned}$$

and similarly for the Z_j entries. Combining two tableau in this way will require time $O(n^3)$, as there are $2n$ entries and each update takes time $O(n^2)$. However, to compute the tableau of $|\Phi\rangle$, we will require the following Lemma:

Lemma 2 *Given the tableau of a control type operator U_C, specified by the binary matrices F, M and G, then the inverse tableau has matrices G', F' and M' such that*

$$\begin{aligned} G' &\equiv G^{-1} \\ F' &\equiv G^T \\ M' &\equiv M^T. \end{aligned} \tag{2.55}$$

Proof of Lemma 2. The entries of the tableau for $U_C^\dagger$ have the property

$$U_C\left(U_C^\dagger X_j, Z_j U_C\right)U_C^\dagger = U_C^\dagger\left(U_C X_j, Z_j U_C^\dagger\right)U_C = X_j, Z_j$$

Consider first the Pauli Z terms. Using Eq. 2.49, can see that

$$U_C\left(U_C^\dagger Z_j U_C\right)U_C^\dagger = Z(\text{row}_j(G)G') = Z_j$$

for all $j \in \{1, 2, \ldots, n\}$. Expanding out this requirement, we can see that $\text{row}_j(G)\cdot\text{col}_k(G') = \delta_{jk}\forall\, j,k$. If we change the order of the multiplications, we obtain the additional constraint $\text{row}_j(G')\cdot\text{col}_k(G) = \delta_{jk}$. We thus require that

$$GG' = G'G = I \tag{2.56}$$

and thus, $G' = G^{-1}$.

A feature of CHP tableaux is that the jth stabilizer and destabilizer anticommute. Here, similarly

$$U_C^\dagger X_j U_C\, U_C^\dagger Z_k U_C = (-1)^{\delta_{jk}}\, U_C^\dagger Z_k U_C\, U_C^\dagger X_j U_C$$

where the extra phase arises from the commutation relations of Pauli operators. In terms of the entries of the tableau, this tells us that

$$\text{row}_j(F)\cdot\text{row}_k(G) = \delta_{jk}\forall j,k \implies FG^T = I.$$

This also holds for the tableau of $U_C^\dagger$. From this, we can concldue that $F = \left(G^{-1}\right)^T$, and similarly $F' = G^T$.

Finally, consider the X_j entries. Again applying Eq. 2.49, we have

$$U_C\left(U_C^\dagger X_j U_C\right)U_C^\dagger = X(\text{row}_j(F)F')Z(\text{row}_j(F)M' + \text{row}_j(M)G') = X_j.$$

As the Pauli Z terms cancel, we have

$$\begin{aligned}\mathrm{row}_j(F)\cdot\mathrm{col}_k(M')+\mathrm{row}_j(M)\cdot\mathrm{col}_k(G') = 0\ \forall j,k \\ \implies \mathrm{row}_j(F)\cdot\mathrm{col}_k(M') = \mathrm{row}_j(M)\cdot\mathrm{col}_k(G')\ \forall j,k.\end{aligned}$$

Using $F^T = (G^{-1})$, and Eq. 2.56, we thus have

$$\mathrm{row}_j(F)\cdot\mathrm{col}_k(M') = \mathrm{row}_j(M)\cdot\mathrm{row}_k(F)\ \forall j,k \implies M_{j,k} = M'_{k,j} \tag{2.57}$$

completing the proof. □

Specialization for 'Equatorial' Stabilizer States

A specialisation exists for computing the inner product when the state $|\varphi\rangle$ is of the form

$$|\varphi\rangle = \sum_{x\in\mathbb{Z}_2^n} i^{xAx^T}|x\rangle$$

a superposition of all 2^n computational basis states with relative phases. We call these 'equatorial' stabilizer states, as they are like n-qubit generalisations of single qubit states $|0\rangle + \mathrm{e}^{i\theta}|1\rangle$ which lie on the equator of the Bloch sphere.

Claim 1 *If $|\varphi\rangle$ is an equatorial state, we can write the inner product as*

$$\langle\phi|\varphi\rangle = 2^{-(n+|v|)/2}\mathrm{i}^{sKs^T+2s\cdot v}\sum_{x\in\mathbb{Z}_2^{|v|}}\mathrm{i}^{xK(1,1)x^T+2x[s+sK](1)^T} \tag{2.58}$$

where $s(1)$ denotes the elements of a vector $s_j : v_j = 1$, and $K(1,1)$ is the submatrix with rows i and columns j such that $v_i, v_j = 1$.

Proof of Claim 1. Let us assume that, given a control-type unitary $U_C \equiv U_D U_{CNOT}$, we can write $U_C^\dagger|\varphi\rangle = \sum_{x\in\mathbb{Z}_2^n} i^{xKx^T}|x\rangle$ for an appropriate phase matrix K. We will show in the following section how to construct this matrix K given the CH and DCH representation of a state $|\phi\rangle$. Given this form then, we have

$$\begin{aligned}\langle\varphi|\phi\rangle &= (\langle\phi|\varphi\rangle)^* \\ &= 2^{-n/2}\left(\sum_{x\in\mathbb{Z}_2^n} \mathrm{i}^{xKx^T}\langle s|U_H|x\rangle\right)^*\end{aligned}$$

Using Eq. 2.52 to expand out the left hand side of this expression, we obtain a sum over terms

$$\sum_{x\in\mathbb{Z}_2^n} \mathrm{i}^{xKx^T}\langle s|U_H|x\rangle = 2^{-|v|/2}(-1)^{s\cdot v}\sum_{y<v}(-1)^{s\cdot y}\sum_{x\in\mathbb{Z}_2^n}\mathrm{i}^{xKx^T}\langle s\oplus y|x\rangle$$

From the orthogonality of computational basis states, we can set $x = s\oplus y$ and drop all other terms in the sum. Doing so changes the phase calculation to

$$(s\oplus y)K(s\oplus y)^T = sKs^T + yKy^T + yKs^T + sKy^T = sKs^T + yKy^T + 2yKs^T$$

where the final equality follows from the symmetric nature of K. From the the definition of $y \le v$, $y_j = 0 \iff v_j = 0$. Thus, we can take the global phase of sKs^T out and reduce the sum to the sum over strings $y \in \mathbb{Z}_2^{|v|}$, as in Claim 1.

To complete the proof, we need to show how to obtain K in both cases. In the DCH form, we have

$$\langle\phi|\varphi\rangle = \langle s|U_H U_{CNOT}^{-1} U_D^{-1}|\varphi\rangle .$$

Using the definition of an equatorial stabilizer state, we can write $|\varphi\rangle = V_D\left|+^{\otimes n}\right\rangle$, and simply compute $|\varphi'\rangle = U_D^{-1}V_D\left|+^{\otimes n}\right\rangle$ by combining the two phase layers to obtain a new phase matrix $(A-B)$.

Another feature of the state $\left|+^{\otimes n}\right\rangle$ is that it is invariant under $CNOT$ circuits, as it is a superposition of all computational basis states and subsequently invariant under their permutation. Applying Lemma 1, we can commute the circuit U_{CNOT}^{-1} past $U_D' = U_D^{-1}V_D$ and eliminate it. This gives a new phase

Property	CH	DCH	CHP	Canonical	Graph States [6]
Memory	$O(n^2)$	$O(n^2)$	$O(n^2)$	$O(n^2)$	$O(nd)$
Z	$O(n)$	$O(1)$	$O(n)$	$O(n^2)$	$O(1)$
X	$O(n)$	$O(n)$	$O(n)$	$O(n^2)$	$O(1)$
S	$O(n)$	$O(1)$	$O(n)$	$O(n^2)$	$O(1)$
H	$O(n^2)$	$O(n^2)$	$O(n)$	$O(n^2)$	$O(1)$
CZ	$O(n)$	$O(1)$	$O(n)$	$O(n^2)$	$O(d^2)$
CX	$O(n)$	$O(n)$	$O(n)$	$O(n^2)$	$O(d^2)$
Measurement	$O(n^2)$	$O(n^2)$	$O(n^2)$	$O(n^2)$	$O(d^2)$
Inner Product	$O(n^3)$	$O(n^3)$	$O(n^3)$	$O(n^3)$	N/A

Table 2.1: Comparison of the asymptotic complexity of different stabilizer circuit simulators, including common operations and their memory footprint. We include the graph based representation of Anders & Briegel, discussed later in this section, and omit the 'Affine Space' simulator as it has no current implemention for gate updates.
Here, d is the degree of the graph used as an internal representation, which varies from $\log n$ to n [6]. We further note that, while all algorithms for measurement are in principle extensible beyond single qubit measurements, only the DCH and CH simulators currently implement arbtirary Pauli measurements.

matrix $K = G(A-B)G^T$.

In the CH case, using Eq. 2.49, we can write

$$U_C^{-1}|x\rangle = U_C^{-1}X(x)U_C\left|0^{\otimes n}\right\rangle = \mathrm{i}^{xJx^T}|xF\rangle$$

Applying this to $|\varphi\rangle$ thus gives

$$U_C^{-1}\sum_{x\in\mathbb{Z}_2^n}\mathrm{i}^{xAx^T}|x\rangle = \sum_{x\in\mathbb{Z}_2^n}\mathrm{i}^{x(A+J)x^T}|xF\rangle.$$

Using $FG^T = I$, as introduced in the previous section, and setting $x = yG^T$, we have

$$\sum_{y\in\mathbb{Z}_2^n}\mathrm{i}^{yG^T(A+J)Gy^T}|y\rangle = \sum_{y\in\mathbb{Z}_2^n}\mathrm{i}^{yKy^T}|y\rangle$$

as required where $K = G^T(A+J)G$. $\square$

Once the calculaton is in this form, we can compute the inner product in time $O(|v|^3)$ using the algorithm for exponential sums developed by Sergey Brayyi [12]. Computing the phase matrix K takes time $O(n^2)$ in both cases, and thus as $|v| \leq n$ we have a general performance $O(n^3)$.

2.2.3 Implementations in Software

The DCH and CH data structures and most routines were implemented in `C++`, to produce a stabilizer circuit simulator. The one expection was the arbitrary stabilizer state inner product, which was derived but left unimplemented due to time constraints. In this section, we will review some of the optimizations employed, and present data comparing their performance with existing software implementations.

The resulting simulators were also validated through the use of testing random circuits. The CH representation was validated by comparison to a `MATLAB` version of the simulator develoepd independently by David Gosset. The DCH representation was then validated against this successfully tested CH representation, using random circuits and conversion to state-vectors through 2^n calls of the computational amplitude routine.

Efficient Binary Operations

The datastructures and subroutines underpinning the CH and DCH representations are built out of arithmetic performed modulo 2 and 4, depending on the context. This allows us to efficiently store the representations using binary bits as opposed to integers, and then use boolean operations as part of the simulation routines.

Addition and subtraction modulo 2, such as is required in the U_C updates of the CH representation and the U_D updates in the DCH representation, is equivalent to the boolen 'XOR' operation, defined as

a	b	$a \oplus b$	$a+b \pmod 2$	$a-b \pmod 2$
0	0	0	0	0
0	1	1	1	1
1	0	1	1	1
1	1	0	0	0

For addition modulo 4, we encode each number using two binary bits a and b as $2*a+b$. In this context, a is typically referred to as the '2s' bit and b as the '1s' bit. Addition can be done for the 1s and 2s terms separetly, with an additional carry correction

$$x+y \pmod 4 = 2*(a_x \oplus a_y \oplus (b_x \wedge b_y)) + (b_x \oplus b_y)\,.$$

In the case of subtraction modulo 4, we note that adding and subtracting 2 can be achieved using just the *xor* operation, as only the two bit is changed. Otherwise, we note that

a	$a-3 \pmod 4$	$a-1 \pmod 4$
0	1	3
1	2	0
2	3	1
3	0	2

i.e. $a-3=a+1$, and $a-1=a+3$, where the addition is again modulo 4. This trick allows us to simplify $a-b \pmod 4$ by setting $b_2 \leftarrow b_2 \oplus b_1$, and then using addition.

Vector and matrix multiplcations modulo 2 can also be reduced to a set of binary operations. Each element $[aM]_i]$, $[LM]_{i,j}$ can be written as a binary inner product, respectively $a \cdot \mathrm{col}_i(M)$ and $\mathrm{row}_i(KL) \cdot \mathrm{col}_j(M)$. Computing the binary inner product can then be expanded out in terms of boolean operations as

$$x \cdot y = (x_1 \wedge y_1) \oplus (x_2 \wedge y_2) \cdots \oplus (x_n \wedge y_n)\,.$$

Typically, we are applying the same operation to entire vectors, rows or columns of a binary matrix. Thus, we can employ a technique called 'bit-packing' to efficiently store and update these binary values. In `C++`, integers can by stored using 8, 16, 32 or 64 binary bits (1, 2, 3 and 4 bytes, respectively). The builtin in `bool` datatype is also typically stored using 1 byte, as this is the smallest unit of memory addressable by a processsor [15].

Bitpacking instead stores up to 64 binary bits in a single variable, manipulating them through the use of 'bitwise' oeprators [16]. Bitpacking typically achievs an 8-fold reduction in the memory footprint. Additionally, a bitwise operation between two variables acts on all bits simulatenously in a single timestep. For example, considering the XOR between two binary vectors, we can write

$$x \oplus y = [x_1 \oplus y_1, \cdots x_n \oplus y_n] \iff \texttt{uint64\_t z = x \^{} y //bitwise XOR}$$

We can also make use of so called 'intrinsic' functions to optimise computing the binary inner product, and sums of terms modulo 4. Intrinsic functions allow certain special processor instructions to be called directly. Specifically, we use two intrinsics for calculating the hamming weight and the parity of a binary string, each of which are computed in a single time step. Using these operations, we can write the binary inner product as

$$\sum_i x_i y_i = |x \wedge y| \bmod 2 \iff \texttt{parity(x \& y)}$$

and a sum of integers modulo 4 as

$$2 * \sum_i a_i + \sum_i b_i \iff \texttt{(2*parity(2bits)+hamming\_weight(1bits))\%4}$$

where `%` is the `C++` modulo operator.

Using these operations allows us to reduce the effective complexity of many common subroutines by a factor of n, as long as the number of variables n is less than 64. For example, instead of $O(n)$ time, computing the binary inner product now requires just two operations: a bitwise logical AND, and the parity intrinsic. However, above 64 bits, we need to pack the bits across multiple variables, and so the number of calls to intrinsic functions will again asymptotically as $O(n)$. Specifically, the number of operations required will go as $n/64$.

Case study: Stabilizer simulations with Affine Spaces

As an example of the use of bitpacking to optimize stabilizer simulators, we developed a `C++` implementation of the stabilizer state simulator introduced in Appendices B, C and E of [8]. While not a full simulator, they provide explicit algorithms for performing Pauli measurements and computing stabilizer inner products. These methods were implemented by the authors in `MATLAB`, using matrices of integers and reprated calls to the `mod` function in MATLAB.

In particular, in their encoding a stabilizer state is based on Eq. 2.21, described by a tuple

$$|\phi\rangle = \Big(n, k, h, G, G^{-1}, Q, D, J\Big)$$

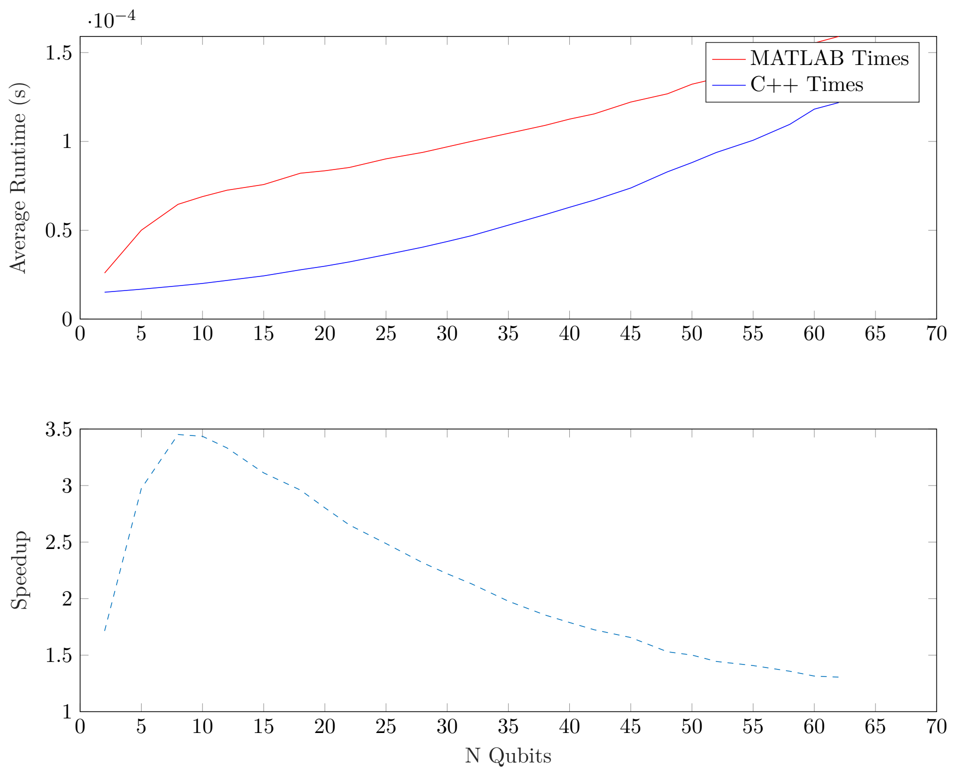
where n is the number of qubits, k is dimension of the the affine space $\mathcal{K}$, generated by the first k columns of the $n \times n$ binary matrix G and an n-bit binary vector h. The inverse matrix G^{-1} is also stored. The phase terms are encoded in a quadratic form using a constant offset $Q \in \mathbb{Z}_4$, a vector D of elements $\bmod 4$, and a symmetric $n \times n$ binary matrix J.

The `C++` simulator makes use of bitpacking to efficiently store h, G, G^{-1} and J. Additionally, we store the elements of D using two binary variables, separating the 1s and 2s bits. The routines were verified and benchmarked against the existing `MATLAB` implementation using the `MATLAB` EXternal languages (MEX) interface, which allows compiled code to be called from within `MATLAB` applications [17].

The results of the benchmark are shown in Figure 2.3. We include two core subroutines specific to the affine space simulator, called `Shrink` and `Extend`, which are called as part of computing stabilizer inner products and simulating Pauli measurements respectively, as well as results for arbitrary n qubit Pauli mesaurements and computing the inner product between stabilizer states.

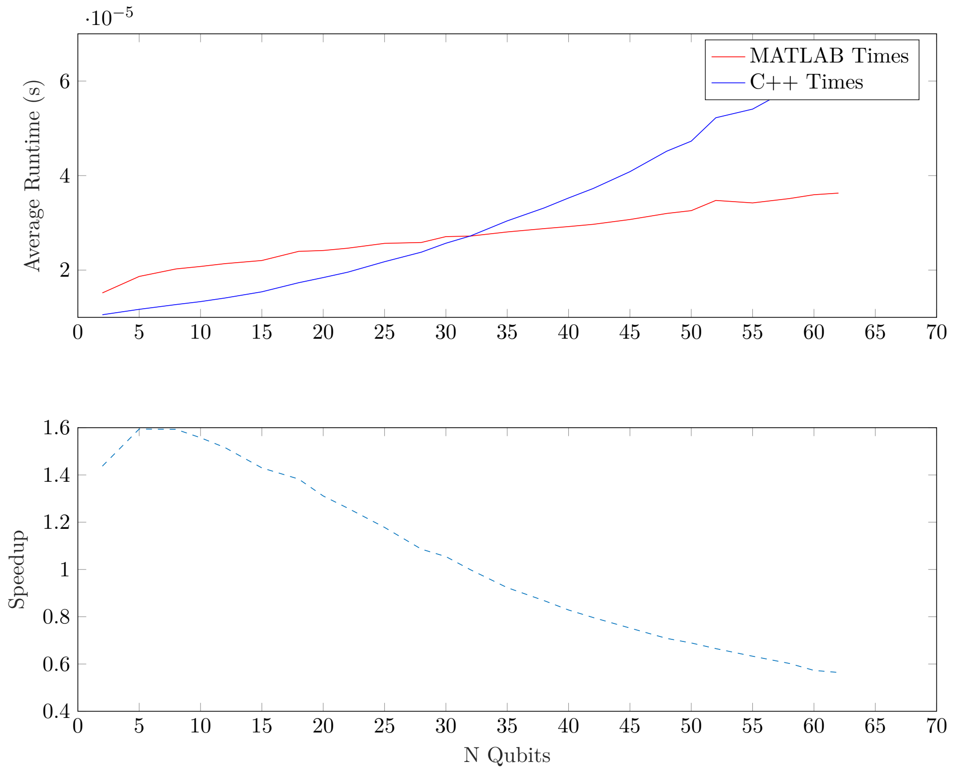
The obsereved differences in runtime are relatively consistent across each routine. In general, the `C++` implementation has a significant advantage in the 5–15 qubit range, with a speedup of anywhere from 1.6 to 10 times. This advantage then drops off as the number of qubits increases, tending to a constant speedup of between 1.5 to 3 times. The notable exception to this is in the

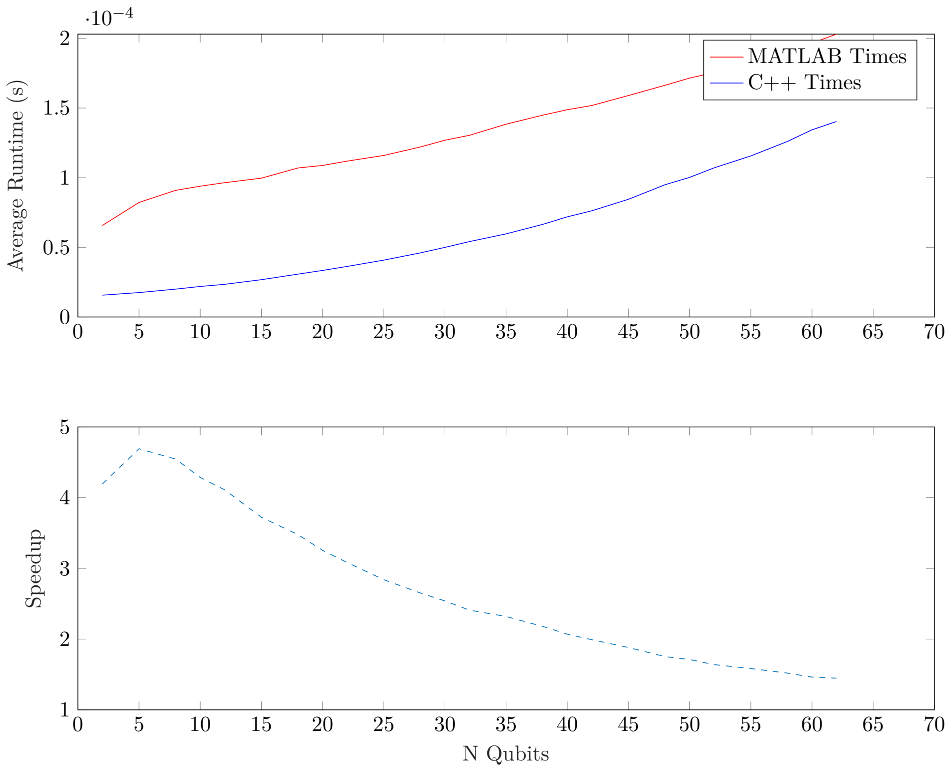
Figure 2.3: Figures showing the perforamnce of the `MATLAB` and `C++` implementations of a stabilize simulator based on Affine Spaces.



(a) Average runtime and resulting speedup of the `Shrink` routine.

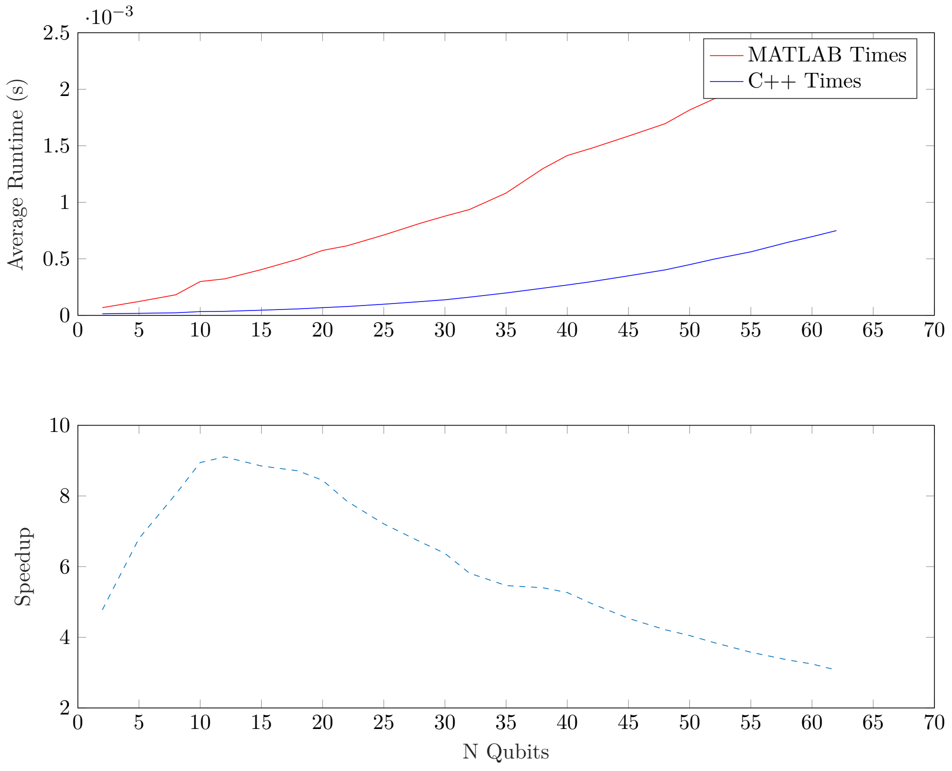
(b) Average runtime and resulting speedup of the `Extend` routine.





(c) Average runtime and resulting speedup of Pauli measurements.

(d) Average runtime and resulting speedup of stabilizer inner products.



`Extent` routine, which actually performs worse than the `MATLAB` version above 35 qubits. All benchmarks have a cutoff below 64 qubits, which is enforced by the use of 64 bit integers for bitpacking in the `C++` simulator.

Specific Optimizations for the CH and DCH Forms

We make use of bitpacking to efficiently store the CH and DCH forms. As many subroutines require computing vector-matrix multiplcations of the form aM, we store the matrices in 'column format' where each bitpacked variable stores one column of the binary matrix. This allows us to make use of intrinsic functions to speedup these multiplcations.

Transposed matrices are computed using 'lazy evaluation'. When the transposed matrix is required, we compute it and store it. We then additionally store a flag to indicate if the transposed matrix is up to date. If later function calls change the values of the transposed matrix, the flag is set to false and the tranpose will be recomputed only when required.

Whenever the result of a calculation is expected to be symmetric, we an halve the number of operations by copying values across. This gives a constant factor speedup in, for example, computing the phase matrices K as part of inner product calculations. We can also make use of this symmetic structure to avoid tranposing a matrix when accessing a row.

Typically, phase matrices are stored as binary matrices with 0 diagonal, and then a separate pair of bitpacked variables storing the diagonal entries which are modulo 4. When required, we update the diagonals separately using an explicit expansion of the matrix multiplcations.

Some updates for the DCH form are further optimised by using explicit expansions of the matrix multiplications. For example, when commuting a Pauli Z through the CNOT layer as in Eq. 2.47, we avoid a call to the transpose

W^T by noting that

$$[zW^T]_i = \sum_j z_j W^T_{j,i} = \sum_j z_j W_{i,j}$$

i.e. each entry $[zW^T]_i$ is a sum of some entries in row i. We can thus build up the new vector $z' = zW^T$ by repeatedly doing $z' \leftarrow z' \oplus \mathrm{col}_j(W)$ for each $j : z_j = 1$.

2.2.4 Performance Benchmarks

To establish the performance of the DCH and CH implementations, we benchmark them against two existing stabilizer circuit simulators, which are available publicly online. The first is the `C` implementation of the CHP method, developed by Scott Aaronson [9]. This uses a variant of bitpacking based on 32-bit integers. The second method is a radically different representation of stabilizer states, based on the fact that any stabilizer state can be generated by a local Clifford circuit (single qubit Clifford gates), acting on a special class of stabilize state called a graph state [18, 19].

Graph states are named as their structure is described by a mathematical graph of vertices V and endges E, where each qubit is a vertex. From this grpah, a graph-state is then built-up as

$$|(V,E)\rangle = \left(\prod_{i,j\in E} CZ_{i,j}\right)\left|+^{\otimes n}\right\rangle,$$

by performing a CZ gate between every pair of qubits connected by an edge of the graph [19].

The so called 'Anders & Briegel' simulator describes a stabilizer state by its corresponding graph, and by sequences of local Clifford operators acting at each vertex. A `C++` implementation of this simulator also exists, called `GraphSim` [20]. This stores a graph as a list of vertices, each with local information about the vertices connected to it.

The expected runtime of different routines using the Anders & Briegel method are also given in Table 2.1. Importantly, in their analysis, routines are quoted with a runtime that scales as d, the maximum 'degree' or number of edges involving a given vertex. By definition, $d \leq n$, the number of vertices in the graph, and thus the simulator has a worst case performance comparable to the DCH, CH and tableau methods. However, this analysis makes explicit a feature of stabilizer circuit simulators; their runtime in practice depends on the state/circuit being considered.

This phenomenon was first described in [2], who observed that the runtime for Pauli measurements seemingly varied between linear and quadratic scaling in the number of qubits, despite the expected asymptotic quadratic scaling. In particular, the algorithm for computing a given measurement in the CHP representation requires between 1 and n calls to a subroutine which takes $O(n)$ to evaluate, and the exact number is determined by the sparsity of the X-bits of the stabilizers, which is in turn related to the number of entangling gates in the circuit.

Similar results hold in detailed analysis of the CH and DCH representations, where the exact number of calcuations required will depend on the sparisty of the matrices/vectors encoding different features of the stabilizer circuits. Consider for example the inner product algorithm of Proposition 2, where we need to apply $|v|$ H gates at a cost of $O(n^2)$ each.

As a result, Aaronson & Gottesman introduced a heuristic for evaluating stabilizer circuit simulators. We begin by applying a random stabilizer circuit to the state, choosing H, S and $CNOT$ gates at random, before applying the operation we are benchmarking and recording the runtime. Using an argument based on message passing, the authors claim that in general we need $O(n \log n)$ gates in the circuit to observe this transition between easier and harder instances of stabilizer circuit simulation, and so we apply $\beta n \log n$ gates where β is a parameter that varies between 0.5 and 1.2. This heuristic is also employed by Garcia et al. in their paper presenting an algorithm for computing stabilizer inner products, where they observe a transition between quadratic and cubic scaling with varying β [7].

Here we present results comparing the performance of different operations between the DCH, CH, CHP and GraphSim methods, for different values of the paramter β. All runtimes are averages taken over 100000 repetitions, where we first apply a random stabilizer circuit of $\beta n \log n$ gates, and then record the time taken by the particular operation.

We also present data for routines specific to the DCH and CH routines. In particular, we present data demonstrating the runtime of arbitrary n-qubit Pauli measurements, and for the specialised 'equatorial' inner product defined in Claim 1. We also consider the effect of weight on the complexity of Pauli measurements.

2.3 Discussion

In this chapter, we have introduced two new representations for simulating stabilizer circuits, including their implementation in software, and presented data evaluating their performance against previous methods.

In particular, we make use of bitpacking techniques to try and further improve their runtime. Figure 2.3 introduced results comparing a bitpacked simulator with a prior `MATLAB` implementation. In general, we see a broad speedup over the `MATLAB` version across the full parameter range, though the exact degree of this speedup decreases with increasing n. The main exception is the `Extend` routine, where we observe the `C++` implementation scaling roughly quadratically with the input size, whereas the `MATLAB` version exhibits a closer to linear scaling.

One possible explanation for this effect is an unfortunate side-effect of the use of MEX files, namely that the `C++` version additionally needs to convert the MATLAB data into a C++ data-structure. This adds an additional $O(n^2)$ overhead to the runtime of the `C++` simulator. Otherwise as coded, the `Extend` algorithm has only $O(n)$ steps. In more complex functions like measurement, `Shrink` and inner products, which have runtimes $10-100$ times longer than

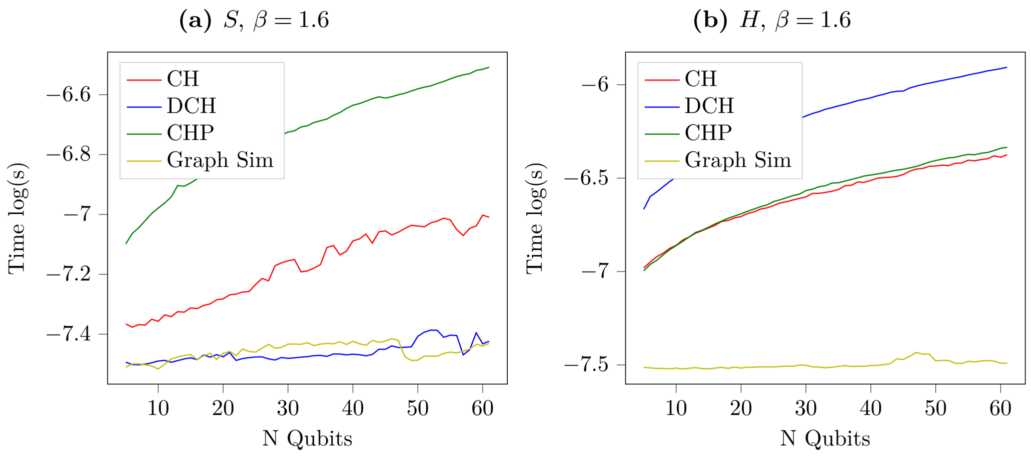


Figure 2.4: Average runtime of the single qubit H and S gates as a function of the number of qubits across different stabilizer simulators. Single qubit gates show no dependence on length of the preceeding circuit, encoded as the β parameter.

Figure 2.5: Average runtime of entangling $CNOT$ and CZ gates as a function of the number of qubits for different stabilizer simulators, for extremal values of β. The Anders & Briegel method shows a signficant dependence on circuit length.

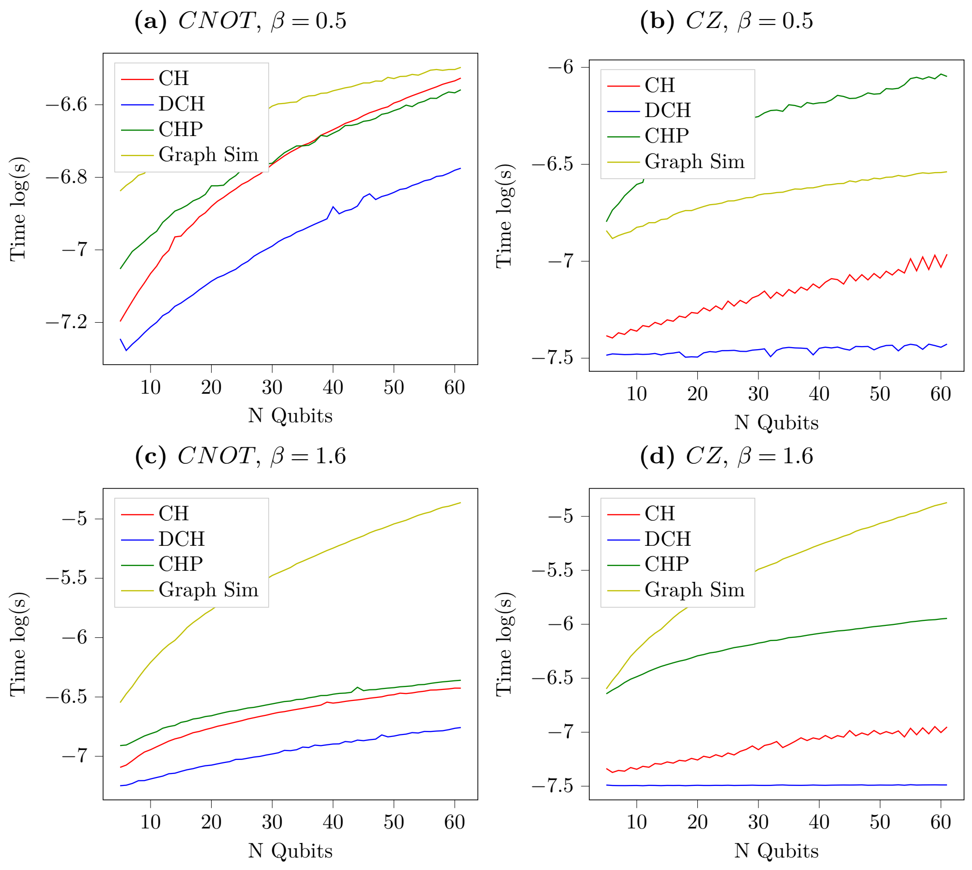
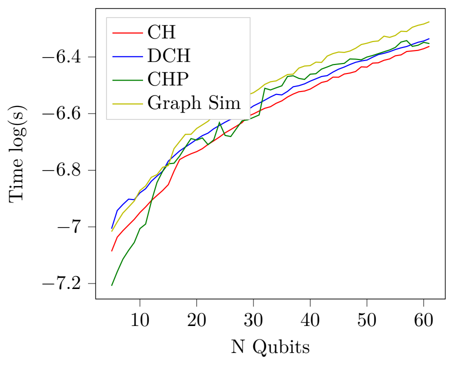
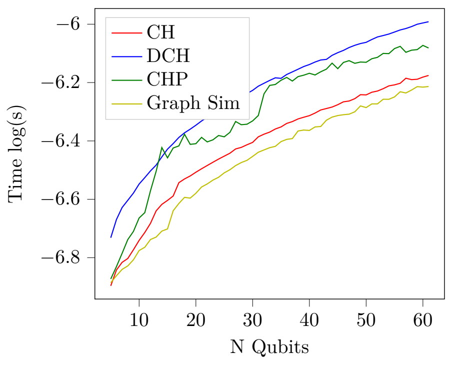


Figure 2.6: Average runtime of single qubit measurements in the X and Z basis, as a funciton of the number of qubits and the length of the preceeding stabilizer circuit, for 4 stabilizer simulators.

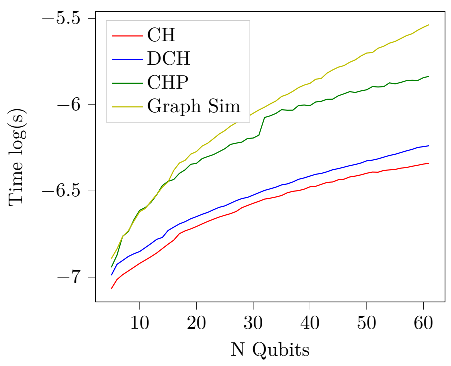
(a) Z measurement, $\beta = 0.5$



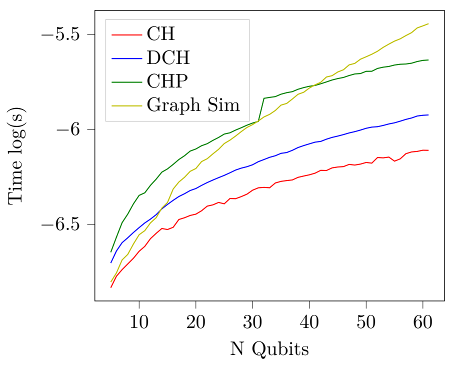
(b) X measurement, $\beta = 0.5$



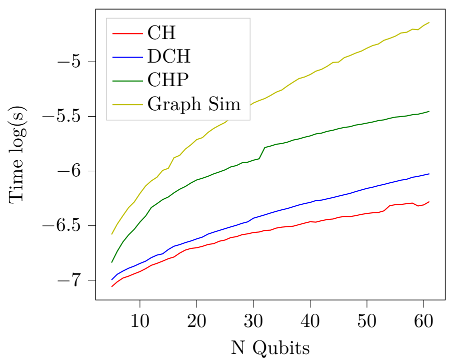
(c) Z measurement, $\beta = 0.8$



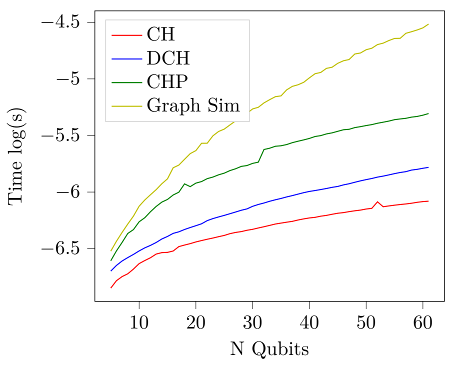
(d) X measurement, $\beta = 0.8$



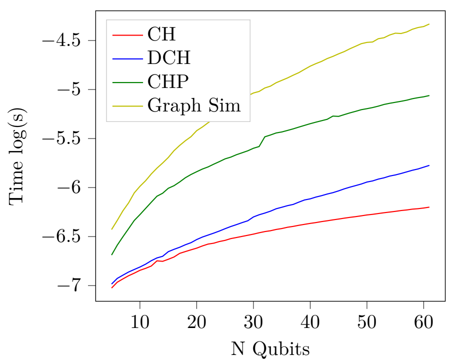
(e) Z measurement, $\beta = 1.2$



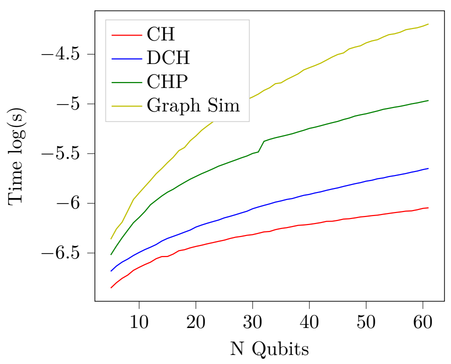
(f) X measurement, $\beta = 1.2$



(g) Z measurement, $\beta = 1.6$



(h) X measurement, $\beta = 1.6$



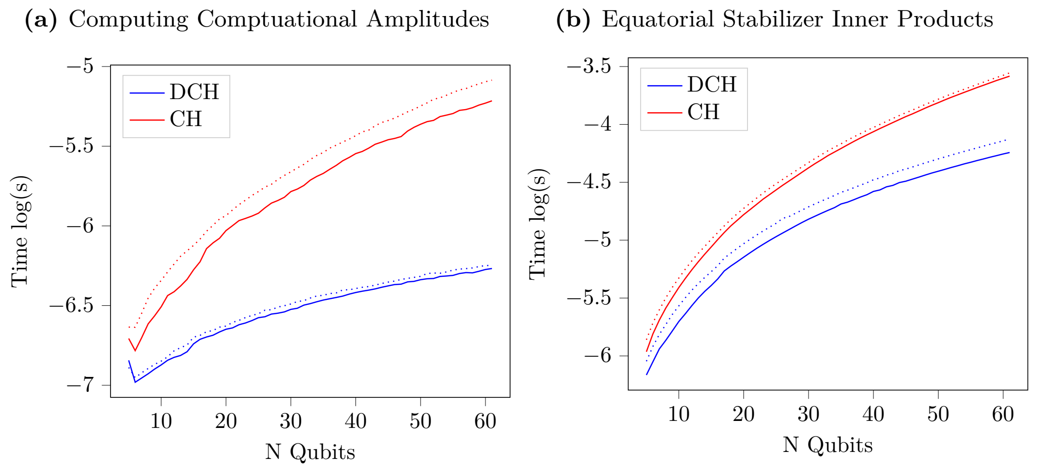
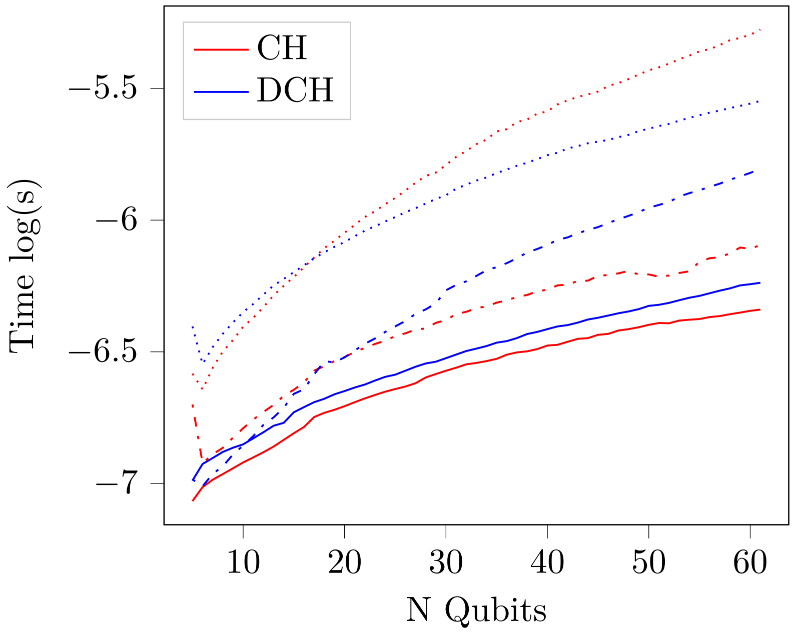


Figure 2.7: Average runtime of two routines specific to the DHC and CH routines, as a function of the number of qubits. Solid lines are for $\beta = 0.5$, and dash lines for $\beta = 1.6$. A slight dependence on circuit length is observed.

Figure 2.8: Average runtime of Pauli measurements for the CH and DCH simulators. A solid line represnets a single Pauli Z measurement. The dashed lines repesenent n-qubit Pauli Z measurements, and the dotted line random n-qubit Paulis.



`Extend`, this effect is less significant, but nonetheless likely contributes to the steeper gradient of the `C++` scalings.

The difference in performance is most significant for the inner product routine, which has an overall complexity that scales as $O(n^3)$ resulting from up to n calls to the `Shrink` routine, and a call to Sergey Bravyi's Exponential Sum routine which also has runtime $O(n^3)$. In this case, the effect of the additional data-copying is suppressed by the overall runtime of the algorithm.

It is important to note that the `MATLAB` implementations also benefit from a degree of parallelization, through a combination of multithreading, and so called 'Single Instruction stream Multiple Data stream' (SIMD) operations [21]. Matrix and vector multiplications are intrinsically parallelisable, as each element in the result is computed from a unique set of multiplication and addition operations. One option for optimising parallel code is to make multiple 'threads' available to the program, which each tackle a different part of the computation. However, as we are frequently performing lots of identical operations over different inputs, they can also benefit from SIMD CPU instructions. These are optimizations which speedup computations by loading multiple values into a special shared binary registers, applying a common operation to the entire register, and then reading the result back out [22]. `MATLAB` is built atop the long established `LAPACK` and `BLAS` libraries for linear algebra, which implement these types of optimization [23, 24, 25].

The effect of these optimizations becomes apparent when we try to extend a bitpacked simulation beyond 64 qubits. In this case, we need to use an array of integer values to encode each binary vector, and each operation now incurs the overhead of looping over these arrays. As an example, Figure 2.9 shows the runtime of the Exponential Sum algorithm of [12], extended up to 150 qubits. We choose Exponential Sum for this benchmark as it has a complexity that scales as $O(n^3)$, reducing the impact of the MEX interface on performance. As before, the speedup shown by the `C++` impelmentation continually decreases with increasing n. Given that some measure of performance improvement is

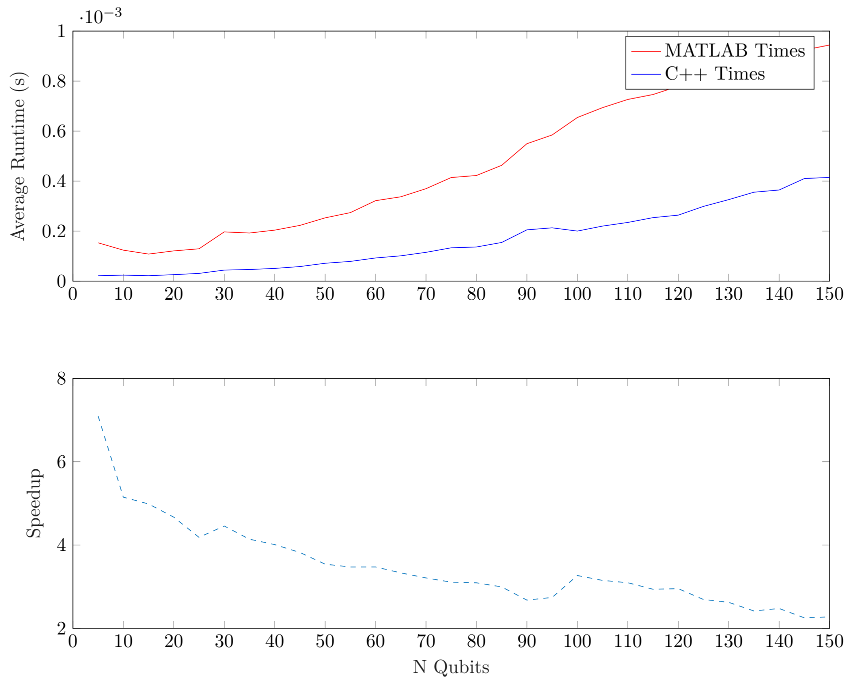


Figure 2.9: Figure comparing the runtime of the `C++` and `MATLAB` implementations of Sergey Bravyi's Exponential Sum routine, up to 150 qubits.

expected by virtue of using a compiled language, compared with the dynamic langauge `MATLAB`, we can see that the bitpacking method is no longer providing significant speedup.

It would also be possible to further optimize the implementation developed here with the addition of SIMD operations. Instead of looping over each integer variable used to encode large bitpacked vectors, the variables could instead be loaded into SIMD registers. THis would significantly optimize the computations up to 512 qubits, as 512 bits is the largest register currently supported [22]. An SIMD implementation is outside the scope of this thesis, but would be a significant performance upgrade to the CH and DCH simulators.

CH and DCH Performance

Comparisons between the DCH and CH forms and previous stabilizer simulators are shown in Figures 2.4, 2.5 and 2.6. Broadly, we see that the DCH and CH representations are competetive with previous techniques, in spite of tracking additional phase information and offering additional 'functionality'.

Specifically, for single qubit Clifford gates, we see that the Graph Sim method has the best overall performance. Because applying a single qubit operator in this picutre only requires updating 'local' information, it can be implemented using a lookup table and thus has constant complexity. This is a significant advantage over the other methods.

However, as mentioned in Table 2.1, the graph based datastructure employed by Anders & Breigel has a runtime that scales as the maximum degree d of the graph for entangling gates, as they alter this underlying graph. This effect becomes clear with increasing β, where the complexity of graph and subsequently the runtime of entangling gates significantly increases. At the largest tested value, 61 qubits, the runtime of an entangling gate grew from $\approx 3\text{x}10^{-7}$ at $\beta = 0.5$, to $\approx 1\text{x}1-^{-5}$ at $\beta = 1.6$. In contrast, we note that the CHP, CH and DCH methods also show no apparent dependence on β. This would be expected from the update algorithms, which rely on binary operations that are independent of the sparsity of the data structures.

The DCH also benefits from a constant time complexity for all phase gates, leading to its improved performance for the 'CZ' gate. The CH representation has no constant time operations, but is broadly competitive in terms of single qubit gate performance. Thois is especially true in the case of the Hadamard cade, inspite of the theoretical $O(n^2)$ complexity of thisoperation. However, the DCH representation shows a significantly increased overhead in simulating Hadamard gates. This suggests the simulator is a poor choice for circuits involving many basis changes.

The origin of this increased overhead can potentially be explained by comparing the performance of Pauli measurements, where the CH simulator also out-performs the DCH method. This suggests that the additional overhead is incurred when commuting Pauli operators through the cicuit layers. We might also expect that applying the circuit correction of Proposition 1 is slower for the DCH form, as it involves explicit matrix operations. In contrast, the CH form here requires only column updates, which take a single time-step as we store binary matrices ias bitpacked column matrices.

The effect of commuting Paulis can be clarified by also considering Figure 2.8. We see that the CH method has a significant advantage for both single and n qubit Z-rotations, but that the DCH method shows slightly better performance for arbitrary Pauli operators. This likely follows from the need to compute a transpose of the F and M matrices, whereas the DCH method is optimized to avoid then need for transposition.

Transposition is also likely the cause of the increased overhead incurred by the CH representation in computing the equatorial inner products, and in computing computational state amplitudes, shown in Figure 2.7. Importantly, as discussed before, transposed matrices are stored 'lazily', computed only when required and then cached until outdated. Thus, in computing multiple anplitudes or inner products as is likely in a practical simulation, this performance gap between the two representations would likely decrease.

An interesting feature of computing computational basis state amplitudes and equatorial inner produts is that they do not show only a small dependence on the length of the preceeding stabilizer circuit. This is in contrast to the results of [7], which observed a transition from quadratic to cubic scaling in the number of qubits when computing stabilizer inner products, even for computational state amplitudes. This would be expected from the implementation of both routines, making use of intrinsic functions. These allow us to avoid inspecting matrices and vectors elementwise, instead operating on rows and columns at a time, and thus makes us less sensitive to the sparsity of the DCH/CH encoding.

Finally, if we consider simulating of Pauli measurements, we again observe that as implemented the DCH and CH forms have little apparent dependence on the sparisty of the underlying datastructures. At low values of β, each method shows a similar performance for Pauli X and Z measurements, with a slight advantage for the CH and GraphSim methods when simulating X measurements. However, as previously mentioned, Pauli measurements in the CHP method have a scaling that increases with the number of non-zero entries in the tableau. The measurement routine of the GraphSim method, like the entangling gates, also depends on the maximal degree of the underlying graph. Thus, both routines see a significant increase in runtime as β increases. The GraphSim method in particular sees an almost 100 times increase in runtime between the smallest and largest values of β at $n = 60$.

Again, likely as a result of the bitpacked implementation, the DCH and CH methods are mostly unaffected by increasing β, with their runtime growing by a factor of $1.33 - 2$ between the extremeal values. This small shift can be attributed to an increase in the number of non-zero entries, and thus the number of operations required in commuting a Pauli through the circuit and applying Proposition 1.

If we were to extend the CH and DCH methods above 64 qubits, we might expect this effect to become slightly more pronounced, as we would also incur the overhead of checking multiple binary variables. This effect can in fact be observed in the CHP data, which employs a version of bitpacking based on 32-bit integers. Above 32 qubits, we see a sharp jump in the runtime, which arises from the need to employ two integers for each bitpacked variable. In conclusion then, we have developed two novel stabilizer simulators which are performant, and offer improved 'functionality' over previous methods. To further develop these tools, it would be important to extend them beyond the current 64 qubit limit, and to finish the implementation of arbitrary stabilizer inner products. With the addition of these routines, this software would form a very versatile toolset for simulating different aspects of stabilizer circuits.

Chapter 3

Stabilizer decompositions of Gates and Unitaries

Chapter 4

Simulating Quantum Circuits with the Stabilizer Rank Method

4.1 Introduction

4.2 Results

4.2.1 Methods for Manipulating Stabilizer Decompositions

Building Decompositions

Output Variables

Implementation and Parallelization

Integration with `Qiskit-Aer`

4.2.2 Simulations of Quantum Circuits

Hidden Shift Circuits

QAOA

Random Circuit Models

4.3 Discussion

4.3.1 Simulating NISQ Circuits

4.3.2 Simulating Random Circuits

4.3.3 Incorporating Noise

Chapter 5

General Conclusions

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