Abstract—Reversible logic has applications in low-power computing and quantum computing. Most reversible logic synthesis methods are tied to particular gate types, and cannot synthesize large functions. This paper extends RMRLS, a reversible logic synthesis tool, to include additional gate types. While classic RMRLS can synthesize functions using NOT, CNOT, and n-bit Toffoli gates, our work details the inclusion of n-bit Fredkin and Peres gates. We find these additional gates reduce the average gate count for three-variable functions from 6.10 to 4.56, and improve the synthesis results of many larger functions, both in terms of gate count and quantum cost.

I. INTRODUCTION

Reversible logic is motivated by its applications in low-power computing. Landauer’s Principle says that some finite amount of energy will be lost for any irreversible computation, but this can be avoided in a fully reversible logic implementation [12]. The challenges of managing power density in modern and future electronics is a strong reason for seeking low-power techniques such as reversible logic [5]. Furthermore, reversible logic has applications in communication [23], optical computing [4], biosynthesis of messenger RNA [3], and particularly quantum computing [2]. In order for such reversible logic technologies to be feasibly implemented, full design flow methodologies, including logic synthesis, must be developed as in the case of conventional irreversible circuits [22].

In [8], Gupta et al. presented an algorithm for reversible logic synthesis using networks of n-bit Toffoli gates. Their algorithm works by searching for candidate factors in the positive polarity Reed-Muller (PPRM) forms of the representative equations that can be substituted to form the operation of a NOT, CNOT, or n-bit Toffoli gates. By traversing a search tree along with practical pruning, their algorithm is capable of synthesizing a wide range of reversible functions with as many as 16 variables.

An n-bit Toffoli gate can be thought of as a controlled XOR operation, and is defined as follows [25]:

\[
y_i = x_i \quad \text{for} \quad 1 \leq i \leq n - 1
\]

\[
y_n = x_n \oplus x_1 x_2 \ldots x_{n-1}
\]

A CNOT gate can be thought of as a two-bit Toffoli gate, and a one-bit Toffoli gate \(y_1 = x_1 \oplus 1\) is the same as a NOT gate. In quantum computing, the NOT, CNOT, and three-bit Toffoli gates are known to have quantum costs of one, one, and five, respectively, while Toffoli gates of four or more bits have even greater quantum costs [2]. Another popular gate is the n-bit Fredkin gate, defined as follows [7]:

\[
y_i = x_i \quad \text{for} \quad 1 \leq i \leq n - 2
\]

\[
y_{n-1} = x_{n-1} x_1 x_2 \ldots x_{n-2} + x_n x_1 x_2 \ldots x_{n-2}
\]

\[
y_n = x_n x_1 x_2 \ldots x_{n-2} + x_{n-1} x_1 x_2 \ldots x_{n-2}
\]

For \(n = 2\), a two-bit Fredkin gate can be thought of as an unconditional SWAP gate (i.e., \(y_1 = x_2\) and \(y_2 = x_1\)). A two-bit SWAP gate has a quantum cost of three and a three-bit Fredkin gate has a cost of five [24], while higher-order Fredkin gates are even more expensive [15]. A third type of gate considered in this paper is the three-bit Peres gate [21]. A Peres gate can simultaneously accomplish the operation of both a CNOT gate and a three-bit Toffoli gate, with an operation defined as follows:

\[
y_1 = x_1 \oplus x_2
\]

\[
y_2 = x_2
\]

\[
y_3 = x_3 \oplus x_1 x_2
\]

Although the definition of Peres gates given in (3) can be extended to include multiple control bits and thus \(n\)-bit Peres gates, this work primarily deals with three-bit Peres gates to remain consistent with the most common definition used by the reversible logic community. The three-bit Peres gate is known to have a quantum cost of four [9].

Because the set of NOT, CNOT, and three-bit Toffoli gates is known to be capable of synthesizing any reversible function, many existing reversible synthesis algorithms do not yet attempt to include “optional” gates such as Fredkin and Peres.

In addition to [8], there have been many recent works on reversible logic synthesis, several of which provide synthesis algorithms that can be practically used, at least for reversible functions of a limited number of variables. Iwama et al. [10] presented a framework for synthesis through repeated local transformations. Shende et al. [23] implemented an algorithm to find optimal circuits and provided their corresponding proofs of constructability, although their method is limited to functions of at most a few variables. Maslov et al. [16] proposed heuristic methods to synthesize reversible functions with the aim of minimizing garbage outputs. They further demonstrated the use of template matching as a heuristic.
technique to take suboptimal circuits and simplify them with a template library [17]. This has even been extended to include Fredkin gates [18]. However, their template-based technique generate less efficient circuits compared to [8], and the addition of new gate types require the generation of an entirely new template library. Miller et al. [20] demonstrated an algorithm to synthesize reversible functions using various bidirectional transformations, although this algorithm often generates quite suboptimal solutions even for functions of as few as three variables.

Our work chooses to build upon RMRLS (Reed-Muller Reversible Logic Synthesizer) [8] because this algorithm has been shown to have speed, success rates, and circuit minimization ability often exceeding those of the above algorithms. We further believe this to be a more robust and extensible platform for parameterizable synthesis options, unlike algorithms requiring pre-derived template libraries, such as those in [18]. This work implements and evaluates extensions to RMRLS for synthesizing circuits with additional gate types. Our specific contributions are as follows:

- We propose and implement extensions to the RMRLS algorithm to include $n$-bit Fredkin gates and Peres gates, and detail our methodology that can be applied to any fundamental reversible logic gate.
- We show that going from the NOT, CNOT, and $n$-bit Toffoli gate (NCT) library to the additional SWAP, Fredkin, and Peres gates (NCTSFP) library reduces the average gate count for three-variable functions from 6.10 to 4.56.
- We synthesize all of the special-purpose reversible functions from [8], in addition to some functions from [15] that could not be synthesized with classic RMRLS, and show that the additional gate types can reduce the gate counts and quantum costs of synthesized circuits.

The rest of the paper is organized as follows. Section II provides motivational examples for including SWAP, $n$-bit Fredkin, or Peres gates in the synthesis algorithm. Section III provides our methodology for extending RMRLS. Section IV details our synthesis of numerous reversible functions and compares these results to those of the existing NCT RMRLS as well as other synthesis algorithms. Section V offers our conclusions.

II. Motivational Examples

This section motivates the need for the support of Fredkin and Peres gates in reversible logic synthesis. We show some simple functions that can benefit from synthesis with the additional gate types, under the suggestion that larger functions are also likely to benefit, as evidenced by the experimental results given later.

The simplest kind of Fredkin gate is a two-bit Fredkin gate, also known as a SWAP gate. For an example of a function that might use this gate in synthesis, consider:

\[
a_{\text{out}} = a \oplus bc \\
b_{\text{out}} = c \\
c_{\text{out}} = b
\]

(4)

This function quite apparently contains a swap between the variables $b$ and $c$. A two-gate realization for this function is shown in Figure 1. Alternatively, when using only Toffoli and CNOT gates, a minimum realization with four gates is shown in Figure 2. Being able to accomplish the swap operation with a single gate has advantages in the synthesis process. In the RMRLS algorithm, for example, performing a swap using three CNOT gates might be a solution that is found only after branching in many other failed directions. An algorithm that can properly identify and move forward on swap opportunities may have a better chance at quickly obtaining a solution.

Our next example presents a function that may be realized with the use of a three-bit Fredkin gate. The Boolean equivalents of the operations of the $n$-bit Fredkin gates may be less obvious when $n > 2$. For example, suppose we need to realize the function:

\[
a_{\text{out}} = a \oplus bc \\
b_{\text{out}} = b \oplus ab \oplus ac \\
c_{\text{out}} = c \oplus ab \oplus ac
\]

(5)

To see how this function could be synthesized using a controlled swap (i.e., a Fredkin gate), it is easiest to look at one such realization, as shown in Figure 3. A four-gate realization without using Fredkin gates is shown in Figure 4. Even for $n$-bit Fredkin gates whose Boolean operations may be less intuitive, identifying the single-gate substitutions may improve the search algorithm’s synthesis ability and also reduce the average gate count.

An additional problem arises when attempting to synthesize the above function using RMRLS. The circuit obtained by classic RMRLS is shown in Figure 5. Although this circuit also consists of four gates, it uses more control bits. If the quantum cost [14] for these circuits is evaluated, the cost of the circuit in Figure 4 is 12 while the cost of the circuit...
III. METHODOLOGY

A. Fredkin Candidate Factors

The synthesis technique in this paper is an extension of RMRLS [8]. RMRLS uses the PPRM expansion of reversible functions and then traverses a search tree to synthesize a circuit through matching candidate factors. These factors refer to common sub-expressions in the Reed-Muller expansions. What ties the original algorithm to Toffoli gates only is that the candidate factors and corresponding substitutions are designed to match the operation of Toffoli gates. In order to extend the algorithm to Fredkin gates, it is necessary to devise a similar scheme to detect Fredkin candidate factors.

In the original NCT-enabled RMRLS, the candidate factors for Toffoli gate transitions must be of the form:

\[ v_{\text{out},i} = v_i \oplus \text{factor} \oplus \ldots \]  

where \( v_i \) refers to a single variable, \( v_{\text{out},i} \) refers to the unique output line labeled by \( v_i \), and \( \text{factor} \) is a term that does not contain \( v_i \). There may also be other terms in the PPRM expression for \( v_{\text{out},i} \).

The corresponding substitution performed if such a candidate factor is found mimics the operation of a Toffoli gate, and thus looks similar to the expression given in (6):

\[ v_i \rightarrow v_i \oplus \text{factor} \]  

In fact, a relaxed rule allows the substitution to be performed even in the case when \( v_i \) does not appear in the original expression. Any sort of relaxed detection schemes are legal, but the substitution itself must be carried out in its entirety as without omitting \( v_i \). For example, even if a Toffoli gate substitution is initiated from just the PPRM expression \( v_{\text{out}} = bc \), the substitution performed would be \( a \rightarrow a \oplus bc \).

Just as Toffoli candidate factors are Boolean expressions revealing the operation of Toffoli gates, the form of a Fredkin candidate factor can be obtained by looking at the definition of the operation of a Fredkin gate. This requires rewriting the definition from (2) in PPRM form. Since the expression must be in positive polarity, there can be no complement operations, and all intermediate operations must be either AND or XOR. Thus, the expressions become:

\[ y_{n-1} = x_{n-1} \oplus x_{n-1}(x_1x_2\ldots x_{n-2}) \oplus x_n(x_1x_2\ldots x_{n-2}) \]
\[ y_{n} = x_n \oplus x_{n-1}(x_1x_2\ldots x_{n-2}) \oplus x_n(x_1x_2\ldots x_{n-2}) \]  

When we represent the common terms as a characteristic \( \text{factor} \), this becomes:

\[ v_{\text{out},i} = v_i \oplus v_i(\text{factor}) \oplus v_j(\text{factor}) \]
\[ v_{\text{out},j} = v_j \oplus v_i(\text{factor}) \oplus v_j(\text{factor}) \]  

This is more restrictive than the candidate factors that give rise to Toffoli substitutions. For one, it requires a total of six matching terms. Second, it requires terms in a PPRM expression for \( v_{\text{out},i} \) to match terms in another PPRM expression for \( v_{\text{out},j} \). As a result, these expressions are not a subset of those with Toffoli candidate factors, but rather a disjoint set.

Just as the Toffoli conditions have a relaxed form, we also opt to use relaxed rules for Fredkin conditions so as to not require all six matching terms. One advantage of a relaxed approach is simplification of the candidate factor detection scheme. Another advantage is that there may still be a benefit from using a Fredkin gate even when not all six terms are
present. If all six terms are present, use of a Fredkin gate can potentially reduce the six terms to only two terms. If one of the six terms is missing, for example, we could likely end up with three terms remaining, whereas the substitution of a Toffoli gate is typically made with the expectation of reducing the complexity by one term. If the result of a substitution turns out to be ineffective, it will automatically be given a low priority in the search tree. The downside of such relaxed conditions is that many of these extra nodes along with their children can pollute the priority queue and slow down the algorithm.

In the end, we chose to use a candidate factor requirement requiring only two matching terms. The requirement is that a PPRM expression for \( v_{out,i} \) must contain terms \( v_i(\text{factor}) \) and \( v_j(\text{factor}) \). This simplifies the search procedure, since such a restriction does not depend on terms in the PPRM expression of \( v_{out,j} \). Under this condition alone, a potential Fredkin branch in the search tree can be created as little as two out of six of the ideal matching terms. Our search procedure mirrors that of the search for Toffoli candidate factors. In the Toffoli case, we would search for terms in \( v_{out,i} \) that do not contain \( v_i \). For the Fredkin case, instead we examine any terms that do contain \( v_i \). Once these are found, we search for any matching subfactor in the same PPRM expression that is identical to the candidate factor, except for replacing \( v_i \) with some other variable \( v_j \). For example, the PPRM expression \( c_{out} = abc \oplus abd \) satisfies this condition, because \( abc \) does contain \( c \) and \( abd \) is the corresponding subfactor with \( c \) replaced by \( d \).

Among special cases, assuming \( \text{factor} \) to be 0 in (9) results in mere pass-through gates, or gates that do nothing. Detecting and substituting in such expressions is useless. When \( \text{factor} = 1 \), however, this is a candidate for a direct SWAP (two-bit Fredkin). This case must be detected differently from typical n-bit Fredkin cases where \( n \geq 3 \). This can be seen by substituting \( \text{factor} = 1 \) into the expressions and seeing that the \( v_i(\text{factor}) \) term cancels out and thus cannot be detected directly. Thus, the two-bit swap is somewhat of an exception in the candidate factor detection scheme. The requirement for a matching candidate factor is that of a term containing only a single variable that is different from \( v_{out,i} \). Again, this is one form of a relaxed rule. A more restrictive requirement would be that \( v_{out,i} \) contains \( v_j \) while \( v_{out,j} \) contains \( v_i \) (for example, \( a_{out} = b \) and \( b_{out} = a \)). However, we opt for the less restrictive case because it gives us the most room for exploration.

### B. Fredkin Substitutions

Appropriate substitutions are performed upon locating suitable candidate factors and their matching subfactors. These substitutions match the operation of a Fredkin gate, as shown earlier, and are specified as follows:

\[
\begin{align*}
v_i & \rightarrow v_i \oplus v_i(\text{factor}) \oplus v_j(\text{factor}) \\
v_j & \rightarrow v_j \oplus v_i(\text{factor}) \oplus v_j(\text{factor})
\end{align*}
\]

(10)

There is one additional complexity in the implementation of complex substitutions, such as the one required for a Fredkin substitution. For the Toffoli substitutions, we have the advantage that \( \text{factor} \) would never contain its corresponding \( v_i \). One convenient effect of this is that when a PPRM expression is represented as a sorted linked list, to perform the substitution the appropriate terms can be added without the worry that they may affect later substitutions. When performing a Fredkin substitution, or even a two-way SWAP, we do not have this luxury since the additional terms will contain instances of \( v_i \) and \( v_j \). In order to work around this, we do not insert new terms into the linked list “in place”. Rather, we create an entirely new linked list of PPRM terms, then destroy the old one. This implementation issue likely adds some overhead, although its runtime is at most linear with respect to the length of the linked list of PPRM terms.

### C. Peres Candidate Factors

The Peres gate presented in Section I must also have its corresponding candidate factors and substitutions in order to be implemented in synthesis. Since a Peres gate is equivalent to a three-bit Toffoli gate followed by a CNOT gate, we in fact use the same candidate factor search mechanism as already implemented. Since we restrict our study to three-bit Peres gates, we add the artificial restriction that the \( \text{factor} \), which does not contain \( v_i \), must consist of exactly two variables.

Unlike Toffoli and Fredkin gates, the Peres gate is not self-reversible. This means that the reverse of the Peres gate [21] is actually a different gate, and we must account for this in our synthesis. The PPRM functional specification of the reverse-Peres gate is shown below:

\[
\begin{align*}
y_1 &= x_1 \oplus x_2 \\
y_2 &= x_2 \\
y_3 &= x_2 \oplus x_3 \oplus x_1 x_2
\end{align*}
\]

(11)

In all, the only difference between this specification and that of the Peres gate is the additional \( x_3 \) term in the PPRM expression for \( y_3 \). Thus, we can use this as the distinguishing choice to decide between whether to apply a Peres or reverse-Peres gate upon encountering the appropriate two-variable candidate factor. Suppose a PPRM contains a Toffoli candidate factor as specified in (6):

\[
v_{out,i} = v_i \oplus \text{factor} \oplus ...
\]

To be considered as a Peres candidate, the \( \text{factor} \) term must contain two variables, say \( a \) and \( b \). If \( a \) also appears in the PPRM expression for \( v_{out,i} \), a search branch is attempted using a reverse-Peres gate with \( a \) as the control bit. If \( b \) also appears in the PPRM expression for \( v_{out,i} \), a search branch is attempted using a reverse-Peres gate with \( b \) as the control bit. If either \( a \) or \( b \) does not appear in the PPRM expression, then branches would be created using a regular Peres gate with \( a \) or \( b \) as the control bit.

As with relaxed candidate factor detection schemes before, the Peres detection schemes do not require \( v_i \) to appear in the PPRM for \( v_{out,i} \). Even if many of these substitutions turn out to be poor choices, the optimistic approach here assumes
that poor substitutions will be properly tagged as such in the search algorithm.

D. Peres Substitutions

The non-self-reversibility of Peres gates brings up another issue when considering the appropriate substitutions to apply upon matching candidate factors. To properly transform the PPRM expressions, we find that the substitutions on applying a Peres gate turn out to be the exact substitutions that define the operation of a reverse-Peres gate. The substitutions applied are as follows:

\[ v_i \rightarrow b \oplus v_i \oplus \text{factor} \]
\[ a \rightarrow a \oplus b \]  

(12)

where factor refers to the two-variable expression, b refers to one of two variables chosen to be the control bit, while a is the other variable. Thus, factor = ab. For the above transformations, it may be tempting to serialize the substitutions as a \( \rightarrow a \oplus b \) followed by \( v_i \rightarrow v_i \oplus \text{factor} \). Although this implementation leads to a correct result while the other possible serialization does not, it is best to reason about and implement all multiple substitution rules as simultaneous substitutions. This is especially important in Fredkin gate substitutions, as no possible serialization for (10) can correctly perform a controlled swap.

Because the substitution required for a reverse-Peres gate reflects the operation of a Peres gate, its expressions are slightly simpler, matching the equations defining the operation of a forward Peres gate given in (3):

\[ v_i \rightarrow v_i \oplus \text{factor} \]
\[ a \rightarrow a \oplus b \]  

(13)

In Section III-F, we provide further intuition for why Peres gate substitutions are defined by the reverse-Peres gate equations, and explain how this duality applies to other gates.

As in the implementation of Fredkin substitutions, the modification of the PPRM linked lists requires creating an entirely new list. The optimization of an “in-place” linked list modification is probably only applicable for the special case of Toffoli gates.

E. Algorithm

The encompassing algorithm framework is still the same as the one used in the original NCT-enabled RMRLS [8]. A priority queue is used for storing partial solutions, and at each iteration a new node is explored. The differences between our algorithm and the original one are two new kinds of candidate factor detection schemes and their corresponding substitutions. A flow chart depicting a high-level view of the algorithm is given in Figure 7. This diagram is in the form of the algorithm given in [1], although it has been extended to include all three kinds of candidate factor detections and their corresponding substitutions.

Our method for adding new gates into the RMRLS framework suggests that synthesis with any other primitive gate types, such as Miller [19] and Margolus [13] gates, could also be developed using the same basic approach. The two primary requirements for enabling synthesis of any arbitrary gate are a candidate factor condition and a procedure for performing the gate’s substitutions. Candidate factor conditions can be obtained by writing the gate’s functional specification in PPRM form. The substitution used for such a branch can be derived by writing the functional specification of the gate’s reverse in PPRM form. The reasons for this slight technicality with non-self-reversible gates is explained in Section III-F.

The flow given in Figure 7 actually only considers the case of an exhaustive search where the algorithm terminates once a solution is found. There are actually other customizable options such as a greedy heuristic search and the ability to continue searching for better solutions after one solution is found.

RMRLS also contains many heuristic parameters to tune its priority queue mechanism and pruning limits. Although we also believe that these heuristics may have potential for dramatically improving the algorithm’s performance and success rate, we opted not to modify these configurations. This way we were able to provide fair comparisons against the NCT results provided in [8].

F. Reversed Substitutions

Because RMRLS synthesizes reversible circuits in the forward direction, it may not be obvious as to why the substitutions for a Peres gate reflect the operation of a reverse-Peres gate. Because NOT, CNOT, and Toffoli gates are self-reversible, this directionality was not an issue in the original RMRLS.

Although RMRLS adds new gates from the beginning to the end of a synthesized circuit, its starting point is the target function and ending point is the identity function. Thus, a reversal effect is achieved while still applying gates in the forward order. This comes about because of a duality between substitution and operation. An operation (for example, \( a_{out} \leftarrow b_{out} \oplus c_{out} \)) sets \( a_{out} \) based on the current PPRM expressions for other output variables. A substitution (for example, \( a \rightarrow b \oplus c \)) modifies any and all PPRM expressions that contain a. An operation has the effect of placing a new gate at the output, while a substitution has the effect of placing a new gate at the input of the currently expressed function.

Because each substitution has the purpose of gradually simplifying the original function toward the identity function, the proper transformations must actually represent the reverse of each applied gate. This technicality does not matter when defining the substitutions for self-reversible gates such as Toffoli and Fredkin gates, but must be upheld with Peres gates. If we were to implement any other non-self-reversible gate, such as the Margolus gate, its substitutions must also take into account this directionality.

G. Synthesis Example

To provide examples of using the various substitutions, we demonstrate the process of synthesizing the specification given
in (5). Because the circuits shown in Figures 3, 5, and 6 can all be synthesized with the extended RMRLS (we will see later in Section IV-D how the circuit in Figure 4 can also be obtained), an exhaustive search would actually encounter all three solutions, as shown in Figure 8. The synthesis example shown depicts various search paths that reach these solutions. A large number of other search nodes, many of which do not lead to solutions, would also be covered in an exhaustive search. For clarity, these have been omitted in the figure.

IV. EXPERIMENTAL RESULTS

We next provide experimental results.

A. Functions of Three Variables

A standard practice for comparing heuristic reversible logic synthesis algorithms is to examine the success at gate minimization for all three-variable reversible functions. We obtain these results by running synthesis on all 40,320 possible three-variable functions. Table I shows our synthesis results in NCTS, NCTSF, and NCTSFP modes, which are formed by enabling the SWAP (S), n-bit Fredkin (F), and Peres (P) gates.

We compare our results against various other heuristic algorithms, as well as the optimal results reported in [23] and [6]. Among heuristic algorithms, RMRLS provides better results than the use of extensive template libraries in [18]. Not shown in the table are the NCTS results for templates [18], which have been shown to be inferior to the NCTS results in [11]. Also not shown are the NCTSF results from [11], which were unable to improve upon the NCTSF template library results in [18]. We have not reported the optimal gate counts for the NCTSFP as we were unable to find such data in the literature. Overall, the extended RMRLS provides better gate counts than all existing heuristic NCTS and NCTSF algorithms, and to the best of our knowledge this is the first algorithm to target the NCTSFP gate library.

B. Other Benchmarks

One of the significant capabilities of the RMRLS algorithm is its ability to synthesize functions of as many as 16 variables [8], whereas some other algorithms may become impractical for such a regime. Since our extensions allow types of gates to be optionally specified by the user, at the very least the modified RMRLS retains all the capabilities of the original algorithm. The question then remains as to whether enabling new gates retains the algorithm’s usability and can further reduce gate counts for large functions.

To answer this question, we use the same benchmark suite as in [8], and synthesize all benchmarks with Fredkin and Peres gates enabled. All of these benchmarks are included in the public releases of the original RMRLS as well as the new version featured in this paper. Each benchmark was attempted in the greedy, exhaustive, and default modes, and the best result was chosen from among these. If given infinite time and memory, the exhaustive mode could theoretically always provide the best results. On our system, however, for several of the larger functions the exhaustive search cannot be completed even in 24 hours. Most results shown were obtainable in the default timeout limit of 180 seconds. The cycle and adder functions, however, have relatively large specifications and
thus took much longer. Some benchmarks, such as these, were given extra time ranging up to one hour.

We compare our results in terms of gate count and quantum cost. Although RMRLS was originally designed to optimize only the gate count, improved quantum cost over results from existing algorithms has sometimes been a side effect [8]. Building upon this, we reasoned that the algorithm can focus on any metric, so we added an option to optimize for quantum cost. We report our gate counts and quantum costs in two categories in Table II. Shown are our best results when optimizing for the minimum number of gates, as well as our best results when optimizing for reduced quantum cost.

In calculating quantum costs, we use the table and rules from [15]. The cost of a Fredkin gate is typically obtained by taking the cost for a Toffoli gate with the same number of inputs, and then adding two to account for two CNOT gates which can combine with a Toffoli gate to form a controlled swap. If all cost calculations were of this form, the best possible quantum cost would not improve with Fredkin gates. There is, however, a known implementation of three-bit Fredkin gates with a quantum cost of five, which is the same as the cost of a three-bit Toffoli gate. When such gates are

![Fig. 8. Various search paths taken in the synthesis of the reversible specification given in (5).](image)

**TABLE I**

**Synthesis results for all three-variable reversible functions. RMRLS improves upon all other heuristic algorithms in both the NCTS and NCTSF categories. The average gate count also reduces significantly with the addition of Peres gates.**

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**Avg.** | **6.18** | **6.01** | **5.44** | **5.87** | **5.63** | **5.13** | **6.10** | **5.75** | **5.25** | **4.56** |
TABLE II
SYNTHESIS RESULTS FOR REVERSIBLE LOGIC BENCHMARKS IN THE NCTSFP MODE COMPARED TO THE BASIC NCT MODE OF THE ORIGINAL RMRLS.

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† Some results in [8] are not repeatable with the publicly available RMRLS due to modified heuristics in the released version. For these, we have compared to our best obtainable NCT results running on the released version.
‡ In only one case, hwb4, did the extended branch heuristic improve the best obtainable quantum cost.

usable, the addition of Fredkin gates can serve to reduce the quantum cost. The Peres gate itself is also a special case, with a quantum cost of four even though an equivalent circuit using Toffoli gates would consist of a three-bit Toffoli alongside a CNOT gate for a total cost of six.

As one example of a synthesized circuit, our minimum cost realization of the majority5 function is as follows: TOF3(a, b; c) TOF2(a; b) RPER(b; d; e) TOF3(b, d; e) TOF2(a; c) TOF3(b, d; c) TOF3(a, c; d) PER(a; d) TOF4(b, d, e; a) PER(c; b; a) FRED4(d, e; a, b) TOF2(c; a) TOF4(a, d, e; c) for a quantum cost of 81 realized with 14 gates. We denote Toffoli gates as TOF#(cb1...cbn−1; tbit) where # denotes the size of the gate, the cbit terms designate zero or more control bits, and tbit designates the target bit. Fredkin gates have a similar notation of FRED#(cb1...cbn−2; tbit1, tbit2) where there are two target bits. Peres gates are denoted as PER(cbit; cb1TOF; cb2CNOT), where tbitTOF signifies the target bit for the output characteristic of a three-bit Toffoli gate and tbitCNOT represents the remaining target bit. Reverse-Peres gates are denoted by RPER with the same format.

Overall, our results show that the addition of Fredkin and Peres gates can always match and often improve the gate count of various benchmarks. When optimizing for quantum cost, we often obtain different circuits possibly with an increased gate count, but always with a quantum cost that matches or improves upon the circuits obtained in [8] or by the heuristic that optimizes the gate count. Furthermore, the addition of Fredkin and Peres gates allowed synthesis of ham7 and hwb5 that (within the constraints of our 4 GB RAM and non-infinite runtime) are not synthesizable in the NCT-only mode.

C. Runtime

In [8], RMRLS was shown to be extremely robust in terms of its ability to find solutions within a practical amount of time. Our extensions for additional gates can be turned off at runtime. Thus, if the goal is to find a solution, even if it is suboptimal, then at the very least a user can obtain this using the NCT mode only.

As expected, using additional gates in the search tree does slow down exhaustive searches. This is because the additional branches at each node can further lead to more branches spawning from them, effectively increasing the exponential growth rate of the search tree. In many cases, we found that exhaustive searches when including Fredkin and Peres gates could take up to four times as long as their corresponding NCT runtimes.
On the other hand, we did not see the same increase in runtime for greedy searches where the purpose was to find any solution. In fact, when asked to find any—not necessarily optimal—solution, for the majority of benchmarks in Table II, we were able to obtain some solution in less than a second. The only benchmarks that took longer than 10 seconds to obtain a solution in the greedy mode were $\text{ham7}$ (67 seconds), $\text{hub5}$ (77 seconds), and $\text{5one245}$ (39 seconds).

All results in this paper were obtained on a platform utilizing an AMD Athlon X2 2.0 GHz processor along with 4 GB of RAM running Fedora Core Linux.

D. Extended Branches Heuristic

The discrepancy between the circuit given in Figure 4 and the equivalent circuit in Figure 5 raises an issue for the original substitution rules of RMRLS. Even in the exhaustive search mode, RMRLS would never come across the solution shown in Figure 4 simply because all of the candidate factors encountered contain at least two variables and thus result in transformations representing only three-bit Toffoli gates. In order to obtain the circuit in Figure 5, which has a reduced quantum cost, the algorithm would have to traverse branches signifying CNOT gates even when a one-variable candidate factor is not available.

An even simpler case that signifies this problem can be found when attempting to synthesize a three-bit Fredkin gate using only Toffoli gates. As revealed in [8], RMRLS cannot synthesize the minimum quantum cost solution for this basic case, even if its solution is minimal in terms of the gate count of three. In general, the observed effect is that lacking any protection against these cases can result in circuits with higher than expected quantum cost. However, we would not necessarily expect much difference in gate count.

To address this problem, we provide the option of additional substitutions. Like the conventional substitutions, these are still based on detected candidate factors. Our special rule, however, is that for any given factor, as depicted in (6), we may substitute a term based on a subset of the variables in factor. For instance, if a substitution of the form $a \rightarrow a \oplus bc$ is suggested by a candidate factor, this substitution would be performed in addition to $a \rightarrow a \oplus b$, $a \rightarrow a \oplus c$, and $a \rightarrow a \oplus 1$. The same expansion is also applied to Fredkin candidates. With this extended branching heuristic, there can quickly arise an intractable number of nodes in the search tree. Thus, at the current time this heuristic is only usable for functions of relatively few variables.

Among all benchmarks, the only one which this heuristic improved upon was $\text{hub4}$, with its quantum cost reduced from 27 to 19.

E. n-bit Peres gates

The bulk of this paper assumes three-bit Peres gates. We chose this because it is the accepted definition used by the reversible logic community, and assuming a system of n-bit Peres gates would exaggerate the gate count reduction for our benchmark results. Nonetheless, it is interesting to consider how our results would change if we assumed n-bit Peres gates as well as n-bit reverse-Peres gates.

In general, any n-bit Peres gate serves as the equivalent of an (n-1)-bit Toffoli gate followed by an (n-1)-bit Toffoli gate, as long as the control bits and target bit of the smaller Toffoli gate form a subset of the control bits of the larger gate. A reverse-Peres gate performs a similar function except the equivalent circuit would have the smaller Toffoli gate placed first.

Because there are no known quantum costs for Peres gates better than their equivalent Toffoli gate-based realizations, it cannot be assumed that use of n-bit Peres gates is expected to reduce the quantum cost, at least under our current cost calculation schemes. n-bit Peres gates would, however, be expected to reduce the gate counts of various reversible benchmarks. If it is later found that n-bit Peres gates also have quantum costs less than their corresponding n-bit Toffoli gates, as in the three-bit case, it will make sense to expect n-bit Peres gates to be a fundamental building block in gate libraries.

Table III shows the subset of benchmarks that can be synthesized with fewer gates using the n-bit Peres gate assumption. Only 10 out of the original 30 benchmarks were able to utilize Peres gates of more than three bits. Regarding quantum cost, with only a pessimistic assumption for higher-ordered Peres gates, these realizations do not reduce the cost under our calculation methods. Thus, we have only listed the number of gates.

As a Peres gate fulfills the function of two Toffoli gates in sequence, the cycle benchmarks benefit by far the most from the n-bit Peres gate assumption. The realizations of cycle functions typically include long chains of Toffoli gates operating on a large set of control bits gradually decreasing in size. Replacing each pair of Toffoli gates with a single Peres gate effectively halves the total number of gates.

While in an ideal situation, the n-bit Peres gate assumption could reduce circuit size by half, this does not explain how the circuit size of cycle28_2 reduced by even more than 50%. Taking this realization and decomposing the larger Peres gates back into their Toffoli equivalents results in a gate count of 59, better than the other realization of 78 gates. This appears to be

<table>
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<th>Gates NCTSP n-bit Peres</th>
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a result of the unpredictable side effects of heuristic pruning under different configurations.

V. CONCLUSIONS

This work builds upon the state-of-the-art reversible logic synthesis algorithm to include Fredkin and Peres gates. We have shown that the process of adding new gates to the algorithm is a generalizable methodology applicable to any arbitrary gate.

For three-variable functions we show that, when including SWAP and Fredkin gates, RMRLS outperforms all other known heuristic methods. Including Peres gates as well reduces the average gate count for three-variable functions to 4.56, notably better than even the optimal case of 5.13 when using Toffoli, SWAP, and n-bit Fredkin gates. For reversible benchmarks, the additional gate types are often able to reduce circuit size in terms of gate count or quantum cost, depending on the option requested by the user.

We have implemented these extensions into RMRLS such that the combination of gate types, limitations on those gates, and choice of whether to optimize for gate count or quantum cost can be chosen by the user at runtime. This new release of RMRLS is freely available for download at http://www.princeton.edu/~cad/.

VI. ACKNOWLEDGMENTS

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REFERENCES
