Efficient experimental design of high-fidelity three-qubit quantum gates via genetic programming

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Abstract We have designed efficient quantum circuits for the three-qubit Toffoli (controlled–controlled-NOT) and the Fredkin (controlled-SWAP) gate, optimized via genetic programming methods. The gates thus obtained were experimentally implemented on a three-qubit NMR quantum information processor, with a high fidelity. Toffoli and Fredkin gates in conjunction with the single-qubit Hadamard gates form a universal gate set for quantum computing and are an essential component of several quantum algorithms. Genetic algorithms are stochastic search algorithms based on the logic of natural selection and biological genetics and have been widely used for quantum information processing applications. We devised a new selection mechanism within the genetic algorithm framework to select individuals from a population. We call this mechanism the “Luck-Choose” mechanism and were able to achieve faster

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convergence to a solution using this mechanism, as compared to existing selection mechanisms. The optimization was performed under the constraint that the experimentally implemented pulses are of short duration and can be implemented with high fidelity. We demonstrate the advantage of our pulse sequences by comparing our results with existing experimental schemes and other numerical optimization methods.

**Keywords**  NMR quantum computing · Three-qubit gates · Genetic algorithms

### 1 Introduction

Quantum technologies that have been proposed to build quantum computers should be able to achieve a high degree of control over a universal set of quantum gates that form the basic elements of quantum circuits [39]. Any quantum computing circuit can be realized using a universal set of two-qubit gates and a set of local unitaries [2]. However, using this basic set of single- and two-qubit gates to decompose multi-qubit unitary propagators for large qubit registers leads to problems of scalability and decoherence due to long operation times of the circuits [50]. Hence, the idea of multi-level quantum logic was developed which used three- and four-qubit quantum gates to considerably simplify the quantum circuit [34,37].

Three-qubit gates such as the Toffoli gate (which is equivalent to controlled-controlled-NOT operation) and the Fredkin gate (which is equivalent to a controlled-SWAP operation) play an important role in quantum circuits [51], fingerprinting [3], optimal cloning [17] and quantum error correction [7,44]. The Fredkin gate was discussed early on as a useful gate for optical implementations of quantum computing [31, 46]. The Toffoli and the Fredkin gates, in conjunction with the single-qubit Hadamard gate, form a universal set of quantum gates [41,48]. Previous implementations of these universal three-qubit gates relied on their decomposition into sets of single- and two-qubit gates [4,47]. Efficient construction of three- and four-qubit gates using an optimal set of global entangling gates has been recently explored [19], and a machine learning type of algorithm has been used to design high-fidelity single-shot three-qubit gates which do not require prior decomposition into sets of two-qubit gates [58,59].

Three- and four-qubit gates were experimentally realized early on in NMR quantum computing by several groups [9,11,13,60]. The Toffoli gate has been experimentally implemented using trapped ions [35] and circuit QED [54] and superconducting qubits [5,12]. Several studies of the Toffoli gate have focused on its experimental realization using optical setups [24,32,33]. Other implementations of the Toffoli gate include an optimal version using a reduced set of two-qubit gates [27,36]. The Fredkin (controlled-SWAP) gate was recently experimentally realized using photonic qubits [40].

Several optimization techniques have been successfully developed for quantum control such as strongly modulated pulses (SMP) [15], GRAPE optimization [45, 56], sequential convex programming [23] and optimal dynamical discrimination [61]. A novel set of optimization techniques broadly categorized as “Genetic Algorithms (GAs)” have also been proposed as a means to achieve a global minimum for the optimization [18]. GAs borrow their optimization protocol from the basic tenets of
evolutionary biology, wherein the breeding strategy of a population is to increase the fitness levels and offspring-producing capability of individuals by crossing over of genetic information [14]. In quantum information processing, GAs have been used to optimize quantum algorithms [1,16,53] and quantum entanglement [38], for optimal dynamical decoupling [43], and to optimize unitary transformations for a general quantum computation [28,29].

In this work, we explore the efficacy of GAs in optimizing the Toffoli and Fredkin gates along with a set of single-qubit gates, on a three-qubit NMR quantum information processor. We design an implementation of these gates which uses only “hard” (i.e. short duration) rf pulses of arbitrary flip angles and phases, punctuated by intervals of evolution under the system Hamiltonian. We are hence able to substantially avoid the pitfalls associated with “soft” shaped NMR pulses, namely pulse calibration errors and degradation due to decoherence occurring during the long gate times of such pulses. The constraints are put in from practical considerations, whereby we want to design the gate using only a certain kind of short duration rf pulses, and then genetic algorithms are used to optimize the protocol. We compared our experimental results with previous NMR implementations of these three-qubit gates using standard transition-selective shaped pulses. We also compared our results with other numerical optimization methods such as GRAPE [56] and strongly modulating pulses (SMP) [15]. We demonstrate that our scheme is substantially better, with obtained experimental fidelities ≈ 14% higher as compared to the standard implementations and also report a 5–6 times savings in gate implementation time as compared to the standard implementations. The genetic algorithm method is sufficiently general and can be used to generate optimized multi-qubit gates of high fidelity.

The material in this paper is arranged as follows: In Sect. 2 we describe the optimization scheme based on GAs. In Sect. 3 we discuss the implementation of optimized gates on an NMR system of three qubits with Sect. 3.1 containing the details of the NMR system, Sect. 3.2 describing the optimized implementation of a 90° pulse, Sect. 3.3 the implementation of a two-qubit CNOT gate. While Sects. 3.4 and 3.5 describe the implementation of the optimized Fredkin and Toffoli gates, respectively, in Sect. 3.6 we compare our results with standard experimental implementations and other numerical optimization techniques. Section 4 offers some concluding remarks.

2 Numerical optimization of three-qubit gates via genetic programming

Unitary operators corresponding to controlled operations and to quantum gates can be implemented on an NMR quantum information processor by a suitable set of radiofrequency pulses of a specific frequency, amplitude and phase, interspersed with delays which correspond to free evolution under the system Hamiltonian. The problem of numerical optimization of any quantum gate can hence be recast as an optimization problem in genetic programming, wherein the fitness function to be optimized depends on the target unitary operator, with its corresponding set of pulse parameters and delay times. The fitness function which determines the relative distance between two operators is defined in our scenario as [29,52]:

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Fig. 1 Desired unitary propagator is represented by a set of \( N \) pulses of pulse width \( \tau_l \) and phase \( \phi_l \), punctuated by \( N \) delays of interval \( \delta_l \) \((l = 1 \ldots N)\):

\[
\mathcal{F} = \frac{|\text{Tr}(U_{\text{tgt}} U_{\text{opt}}^\dagger)|}{\sqrt{\text{Tr}(U_{\text{tgt}} U_{\text{tgt}}^\dagger) \text{Tr}(U_{\text{opt}} U_{\text{opt}}^\dagger)}}
\]

where \( U_{\text{tgt}} \) is the target unitary operator of the desired gate to be optimized and \( U_{\text{opt}} \) is the actual operator generated by the GA optimization. The fitness function is normalized such that when \( U_{\text{opt}} = U_{\text{tgt}} \), the fitness has the maximum value of unity.

The derived unitary operator of the gate to be optimized, \( U_{\text{opt}} \), is defined as:

\[
U_{\text{opt}} = \prod_{l=1}^{N} \exp[-i(\mathcal{H}_{\text{NMR}} + \Omega I_{\phi_l} k)\tau_l] \exp[-i\mathcal{H}_{\text{NMR}}\delta_l]
\]

\[
I_{\phi_l} = \frac{1}{2}(\sigma_x \cos \phi_l + \sigma_y \sin \phi_l)
\]

where \( \Omega \) denotes the amplitude of the rf pulse, \( \phi_l \) is the phase of the \( l \)th rf pulse, \( k \) labels the qubit which is being controlled, \( \tau_l \) is the pulse length of the \( l \)th pulse, \( \delta_l \) denotes an evolution period under the system Hamiltonian, and \( \sigma_x \) and \( \sigma_y \) are the Pauli \( x \) and \( y \) matrices, respectively. It is to be noted that while the Pauli matrices are \( 2 \times 2 \) matrices and are defined for each qubit, the general three-qubit Hamiltonian has a dimension of \( 8 \times 8 \), and hence in the above equation, the tensor product of the Pauli matrices with unit matrices in the corresponding positions is taken. The first term in the expression for the desired unitary operator \( U_{\text{opt}} \) (Eq. 2) describes the system and RF Hamiltonians, while the second term describes the evolution under only the system Hamiltonian. The system Hamiltonian \( \mathcal{H}_{\text{NMR}} \) in the rotating frame is given by

\[
\mathcal{H}_{\text{NMR}} = -\pi \sum_{i=1}^{n} (v_i - v_{rf}^i) \sigma_z^i + \sum_{i<j=1}^{n} \frac{\pi}{2} J_{ij} \sigma_z^i \sigma_z^j
\]

where \( n \) denotes the number of spins, \( v_i \) and \( v_{rf}^i \) are the chemical shift and the rotating frame frequencies, respectively, \( J_{ij} \) are the scalar coupling constants, and \( \sigma_z \) is the Pauli \( z \) matrix.

We choose to decompose the desired unitary operator \( U_{\text{opt}} \) as a set of \( N \) hard (i.e. high-power, very short duration) rf pulses, each of fixed amplitude \( \Omega \), pulse length \( \tau_l \) and phase \( \phi_l \), and a set of \( N \) delays, each of interval \( \delta_l \) in duration. This set of pulses and delays denotes the basic propagator (Fig. 1). These optimal pulse phase, pulse width and delay values (which together constitute one possible solution...
to the optimization problem) can be encoded in the form of a matrix of order \( N \times 4 \) where the number of rows \( (N) \) specifies the number of operations that the desired unitary operator is decomposed into. By increasing the number of rows, we increase the accuracy and control. The values of the four columns of the matrix are detailed below:

- **Column 1** Represents the width \( (\tau) \) of a hard pulse, which is used to tune the value of the angle of rotation of the pulse \( (\theta \in [0, 2\pi]) \).
- **Column 2 and 3** The phase of rotation of the rf pulse is represented in these two columns. The second column takes the values either 0 or 1, implying a positive or negative phase \( (\phi \in \{0, \pi\} \) or \( \phi \in \{-\pi, 0\}, \) respectively). The third column contains the range of \( \phi \) values from \( \{0, \pi\} \). Hence, these two columns collectively cover a range in the phase of rotation from \( \{0, 2\pi\} \). The total \( 2\pi \) degrees of phase have been represented as two variables, one being 0 or 1 (representing positive or negative phase) and the other being in the range \( \{0, \pi\} \), we allow for two degrees of change in the crossover operation. In the crossover operation, we randomized the number of columns and number of rows to crossover between two matrices (chromosomes). There can in principle be a large change (as a sign change which changes the value of \( \phi \) by 180 degrees), or a small change in degree (which changes the value of \( \phi \) by small amounts). By having a two column representation for \( \phi \) value, we can increase the proliferation of the genetic algorithm in the fitness landscape.
- **Column 4** The values in this column represent the time evolution \( \delta_l \) between hard pulses. The maximum value that an element in this column can assume is relative to the type of gate chosen. A Fredkin gate inherently requires more time than a CNOT gate and hence will be given more freedom in choosing delay lengths.

Due to accuracy constraints imposed by the NMR hardware on which the gates are implemented, we can only obtain a resolution of 0.01 degrees for the phase, and a resolution of 1 \( \mu \)s for the delay. Hence, the values in our results are discretized accordingly. It should also be noted that the power of each hard rf pulse is fixed and is not optimized.

As the first step in the genetic algorithm, an initial population of solutions, i.e. \( n \) “randomly chosen chromosomes,” is created. Considering we run the algorithm using a variable number of rows, we must first decide upon a suitable population size to run the algorithm with. As the number of rows increases, so does the time taken to convert a matrix of rf pulses to a gate matrix. We thus used population sizes ranging from 350 to 750, for rows ranging from 3-20. There are three main operations which form the backbone of the genetic algorithm as described below [18]:

- **Selection** Selecting individuals for crossover and mutation processes is important as it dictates the direction taken by the population in the fitness landscape [18]. We initially use a low selection pressure in order to explore all possible candidate solutions. If a viable solution is recognized, the intensity of the selection pressure is increased, to allow for exploitation of neighbors of the recognized solution. After attempting existing selection mechanisms such as roulette, rank, tournament and stochastic acceptance [20], we devised our own selection mechanism which we call “Luck-Choose.” The Luck-Choose selection mechanism is described below.
– **Luck-Choose** The selection mechanism involves first multiplying pseudo-randomly generated weights to the fitness values of all individuals, and subsequently determining the highest among the output values. By doing so, there is a greater chance of selection for individuals with higher fitness value. Hence, there is higher selection pressure for individuals of higher fitness, and lower selection pressure for those of low fitness. This greatly increases the ability of the genetic algorithm to exploit preferred chromosomes at each generation and hence provides for increased speed in the determination of the most optimal solution. Using our Luck-Choose method, the algorithm converged to a solution much faster.

– **Crossover** The crossover operation in the genetic algorithm method swaps congruent parts of individual members of the population as follows: Two members are chosen from the population using the Luck-Choose selection method. Two numbers are randomly chosen within the maximum number of rows, and two numbers are randomly chosen within the maximum number of columns. The first number of each corresponds to the starting point of the crossover and the second number corresponds to the end point. Using the above four numbers we create a rectangular sub-matrix, which is swapped between both the selected individuals. In addition, we added another operation called *flip* in order to address the problem of non-commutativity of rf pulses. The *flip* operation selects a single member using the Luck-Choose method and swaps its constituent rows.

– **Mutation** This operation depends heavily on the amount of stochastic noise required. Stochastic noise adds a random amount of noise to ensure that the algorithm does not stagnate at any of the local optima. In the initial stages, low stochastic noise is preferred, so the mutation operation may be disabled. However, after the algorithm explores the population landscape through a few generations, the chances of getting stuck in local optima increase. The probability of mutations is then increased in steps up to a threshold value, above which the stochastic noise would only serve to drive candidate solutions away from the global optimum. Mutation takes a single member, selected using the Luck-Choose method, and changes all its data values.

Figure 2 depicts all the steps in the genetic algorithm optimization strategy as a flowchart. We evaluate the fitness after every operation in the algorithm (mutation, flip, crossover), since these three operations have fundamentally different effects on the population. The highest fitness value of any generation is the highest among the fitness values calculated after each operation in that generation. By separating the flip and mutation operations, we can observe the discrete effects that flip and mutation have on the individuals, and correspondingly determine the highest fitness among the three operations. After running the genetic algorithm, outputs are obtained with fidelities in the lower 0.80 range. In order to increase the fidelity, we used the concept of a localized optimizer, which is a GA tool that optimizes only within a very small region of the fitness landscape. This is done by localizing the range of values that constituent chromosomes can take. As the maximum fidelity increases, we increase the selection pressure to further minimize the region of optimization of the algorithm, in the fitness landscape. The chromosomes from the main optimizer, which yield fidelity greater
than 0.8, are then passed through this local optimizer to increase the fidelity. In the general case, we let the local optimizer run for 1000 generations. If the fidelity crossed 0.99, the solution was deemed acceptable. In certain cases, local optimizer runtimes were further increased, to increase the final fidelity. The job of the “Main Optimizer” is to proliferate through the landscape and find regions of high fitness, while the job of the “Local Optimizer” is to exploit these smaller regions of high fitness, to find the individual of highest fitness. When the number of rows is increased, there are increased degrees of freedom. In the “Main Optimizer” this serves to slow down the proliferation as the fitness landscape increases in size exponentially with the number of degrees of freedom. However, in the “Local Optimizer,” since we change all the values of φ and θ simultaneously (simultaneous proliferation in all degrees of freedom) we are able to use these extra degrees of freedom to converge to an optimal solution.
| Row no. | Main optimizer time (s)/GFLOPS | Local optimizer time (s)/GFLOPS | Pulse duration |
|--------|-------------------------------|---------------------------------|---------------|
| 1      | 277.8/901.5                   | NA                              | NA            |
| 2      | 559.1/1814.2                  | NA                              | NA            |
| 3      | 871.3/2827.3                  | 978/3173.6                      | 101.4 µs      |
| 4      | 1183.8/3841.4                 | 46.16/149.8                     | 146.8 µs      |
| 5      | 1435.8/4656.5                 | 59.66/193.6                     | 164.8 µs      |
| 6      | 1751.5/5683.6                 | 28.5/92.5                       | 253.7 µs      |
| 7      | 2005.6/6508.1                 | 23.2/75.3                       | 243.7 µs      |
| 8      | 2176.6/7063.1                 | 19.2/62.3                       | 292.3 µs      |

The optimization time per iteration is shown, along with the corresponding number of FLOPs used for the local optimizer.

The Table 1 gives details of the runtime per iteration in the main and local optimizers, as well as the corresponding count of floating point operations per second (FLOPS), for the optimization of a 90° spin-selective rf pulse. All the rows for which the pulse duration is mentioned in the table have a fidelity greater than 0.99. The genetic algorithm was performed using MATLAB [30]. An iteration of the program running the algorithm for 15 rows and 500 chromosomes took an average time of 3 h using a single core for processing, on an i7-4700MQ processor with 8 GB of RAM. For parallel processing, the Parallel Computing Toolbox was used, enabling us to run six iterations simultaneously on six virtual cores for approximately 4 h. This reduced the average runtime per iteration to approximately 40 m. The local optimizer, however, was run from 10 min to 15 h depending on the final fidelity required and the fidelity of the starting matrix. There are two stopping criteria for the genetic algorithm: the first is when the fitness reaches a value of 0.99 or some pre-decided threshold value, and the second is when the number of generations gets exhausted (i.e. for every rows there are a certain number of iterations which have a fixed number of associated generations and if that gets exhausted, the iteration moves to the next one).

3 Experimental implementation of numerically optimized gates

3.1 Experimental NMR qubits

The three fluorine (19F) spins of the molecule iodotrifluoroethylene were used to encode the three qubits (Fig. 3). The three qubits were initialized into a pseudopure state |110⟩ via the spatial averaging technique [6] with the density operator given by

$$\rho_{110} = \frac{1 - \epsilon}{8} I + \epsilon |110⟩⟨110|$$  \hspace{1cm} (4)
where thermal polarization ($\epsilon$) is approximately $10^{-5}$ and $I$ is a $8 \times 8$ identity matrix. The experimentally created pseudopure state was tomographed with a fidelity of $0.968 \pm 0.008$. All the experimental density matrices were reconstructed using a reduced tomographic protocol [25] and maximum likelihood estimation [49] with the set of operations given by \{III, IIY, IYY, YII, XYX, XXY, XXX\}, where $I$ is the identity operation, $X$ and $Y$ are the single spin angular momentum operators which can be implemented by applying a $\pi/2$ pulse on the corresponding spin. The operators for tomographic protocols were numerically optimized using genetic programming, each having a length of approximately 200 $\mu$s and an average fidelity of $\geq 0.99$. The fidelity of the experimental density matrix was computed by measuring the projection between the theoretically expected and experimentally measured states using the Uhlmann–Jozsa fidelity measure [21, 57]

$$
F = \left( \frac{\text{Tr} \left( \sqrt{\rho_{\text{th}}} \rho_{\text{exp}} \sqrt{\rho_{\text{th}}} \right)}{\text{Tr} \left( \sqrt{\rho_{\text{th}}} \sqrt{\rho_{\text{th}}} \right)} \right)^2
$$

where $\rho_{\text{th}}$ and $\rho_{\text{exp}}$ denote the theoretical and experimental density matrices, respectively. For the implementation of each gate, the experiment was repeated ten times (at a temperature fixed at 294 K) and the average of these ten experimentally reconstructed density matrices was computed. These experimentally reconstructed density matrices were used to compute the mean and standard deviation in the fidelity of each gate implementation (Supporting Information).

Since we used a system of three homonuclear (same spin species) spins, the control on all three spins happens simultaneously and the optimization operator $U_{\text{opt}}$ is modified as:

$$
U_{\text{opt}} = \prod_{l=1}^{N} \exp[-i \left( \mathcal{H}_{\text{NMR}} + \Omega(I_{\phi_l1} + I_{\phi_l2} + I_{\phi_l3}) \right) \tau_l] \exp[-i \mathcal{H}_{\text{NMR}} \delta_l]
$$

The amplitude $\Omega$ of the hard rf pulse was kept fixed at $120.88 \times 10^3$ rad/s, the hard pulse flip angle was taken in the range of $[0, 3\pi/2]$ and the range for length of the pulse $\tau$ was adjusted according to these two factors. The value of the delay between the pulses was chosen depending upon the unitary being optimized. We have used a
Table 2  Table representing the pulse sequence for selective pulse

| l  | τ(μs) | φ_1 (°) | δ_1 (μs) |
|----|-------|---------|-----------|
| 1  | 16    | 87.65   | 21        |
| 2  | 33    | 269.97  | 21        |
| 3  | 16    | 92.29   | 0         |

First column represents the number of propagators. The second, third and fourth columns give the pulse width (τ), phase (φ) and delay (δ) values, respectively.

simple on/off control for gate design as it is more robust as compared to the varying power techniques such as GRAPE and SMP. In the case of varying power algorithms, the errors due to pulse angle miscalibration propagate and accumulate toward the end, which makes them less robust. Whereas in the GA technique we are shutting down the power during the “off” control, which is just a free evolution of the spin system and hence will not contribute to such types of errors. The GA technique can be extended by varying the amplitude of the pulse.

3.2 Implementation of 90° selective rf pulse

To rotate a single spin in a homonuclear system we need a selective excitation pulse. We optimized the pulse sequence via genetic algorithm for a 90° selective pulse on the third qubit along the Y-axis, using only hard pulses and delays. The unitary for the selective pulse is given by,

$$U_{tgt} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \end{bmatrix}$$  (7)

The optimized pulse sequence for this unitary is given in Table 2. The pulse sequence was obtained with a theoretical fidelity of 0.995 with a pulse duration of 107 μs. The numerically optimized pulse sequence was experimentally implemented on an initial thermal equilibrium state, and the result is shown in Fig. 4. There is a substantial advantage in the much shorter duration of the optimized selective pulse which is in μs as compared to the standard pulses which usually take tens of milliseconds, depending on the system interactions. The spectra in Fig. 4 show a clean excitation of the third qubit, with no spillover excitation of the other two qubits.
3.3 Implementation of CNOT gate

Since the interactions in NMR are always “on,” it is most often non-trivial to implement a two-qubit gate in an \( N \) qubit system, while doing nothing on the other \((N - 2)\) qubits in the system, as compared to implementing the same two-qubit gate in a system of two NMR qubits [26]. We hence optimized the two-qubit CNOT gate on our three-qubit system, with the first qubit considered the control qubit, while the second qubit was considered the target qubit. The corresponding unitary matrix is given by

\[
U_{\text{tgt}} = \begin{bmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 \\
\end{bmatrix}
\]  

The optimized pulse sequence for this quantum gate is shown in Table 3 and was obtained with a theoretical fidelity of 0.993 with a pulse duration of 7 ms.

The pulse sequence was experimentally implemented on an initially prepared pseudopure state \(|110\rangle\). The final state was \(|100\rangle\) as expected, with an experimental fidelity of 0.982 ± 0.013. The experimentally tomographed results are shown in Fig. 5.

3.4 Implementation of Fredkin gate

We optimized the three-qubit Fredkin gate (corresponding to a controlled-SWAP operation) in a single shot, i.e. without breaking it down into other unitaries, and using only a set of hard pulses and delays. The first qubit was designated as a control qubit.
Table 3  Table representing the pulse sequence for a two-qubit CNOT gate

| l  | \(\tau_l(\mu s)\) | \(\phi_l\) | \(\delta_l(\mu s)\) |
|----|-----------------|----------|------------------|
| 1  | 30              | 32.181   | 277              |
| 2  | 33              | 320.75   | 69               |
| 3  | 3               | 59.02    | 1                |
| 4  | 39              | 66.28    | 636              |
| 5  | 29              | 306.06   | 292              |
| 6  | 9               | 302.12   | 19               |
| 7  | 39              | 312.81   | 1755             |
| 8  | 11              | 294.12   | 1                |
| 9  | 39              | 296.16   | 636              |
| 10 | 1               | 157.81   | 256              |
| 11 | 4               | 271.97   | 305              |
| 12 | 39              | 329.86   | 1                |
| 13 | 14              | 352.56   | 83               |
| 14 | 24              | 359.89   | 657              |
| 15 | 1               | 2.52     | 1748             |
| 16 | 6               | 55.02    | 69               |
| 17 | 4               | 312.45   | 2                |
| 18 | 37              | 309.7    | 96               |

The first column represents the number of propagators. The second, third and fourth columns represent the pulse width \(\tau\), phase \(\phi\) and delay \(\delta\) values, respectively.

and if the control qubit is 1, then the other two qubits swap their states. The unitary matrix corresponding to the Fredkin gate is given by

\[
U_{tgt} = \begin{bmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1
\end{bmatrix}
\] (9)

The optimized pulse sequence for this gate is shown in Table 4 and was obtained with a fidelity 0.99 and a pulse duration of 51 ms. The pulse sequence was experimentally implemented on an initial state \(|110\rangle\). The output state was \(|101\rangle\) with an experimental fidelity of 0.983 ± 0.012. The experimentally tomographed results are shown in Fig. 6.

3.5 Implementation of Toffoli gate

The first two qubits of this gate were considered as the control qubits, while the third qubit was designated the target qubit. The unitary matrix corresponding to this gate is given by

\[
U_{tgt} = \begin{bmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1
\end{bmatrix}
\]
The numerically optimized sequence for this gate is shown in Table 5 and was obtained with a fidelity of 0.995 and a pulse duration of 27 ms. The pulse sequence was experimentally implemented on an initially prepared pseudopure state $|110\rangle$. The final state was $|111\rangle$ as expected and had an experimental fidelity of $0.968 \pm 0.014$. The experimentally tomographed results are shown in Fig. 7.

In order to compare our GA scheme with existing numerical optimization schemes such as GRAPE and SMP we optimized pulses for these techniques for all the gates as was done with the GA algorithm. We used the basic variants of the GRAPE and SMP optimization schemes without further optimization for robustness, although such
The first column represents the number of propagators. The second, third and fourth columns represent the pulse width ($\tau)$, phase ($\phi$) and delay ($\delta$), respectively.

Robustness optimizations are also possible [22,42]. The total pulse length of the optimized unitary gates which were optimized using the GRAPE and SMP algorithms was divided into equal time steps of 8 $\mu$s for GRAPE and 10 $\mu$s for SMP algorithm, respectively. The numerical optimization using the GRAPE method took up to 2 h and using SMP took up to 2.5 h depending upon the initial guess and the type of unitary being optimized. All the numerical calculations were performed on a single core of an i7-4700MQ processor with 8 GB of RAM. Using the GRAPE scheme, the selective pulse was obtained with a fidelity of 0.995 with a pulse duration of 200 $\mu$s, the two-qubit CNOT was obtained with a fidelity of 0.999 with a pulse duration of 12 ms, the Fredkin gate was obtained with a fidelity of 0.998 with a pulse duration of 50 ms, and for the Toffoli gate the pulses obtained were of fidelity 0.998 with a pulse duration of 30 ms. Similarly, using the SMP scheme the selective pulse was obtained with a fidelity of 0.994 with a pulse duration of 200 $\mu$s, the two-qubit CNOT was obtained with a fidelity of 0.982 with a pulse duration of 13 ms, the pulses for Fredkin gate were obtained with a fidelity of 0.994 with a pulse duration of 50 ms and for the Toffoli gate the pulses obtained were of fidelity 0.995 with a pulse duration of 30 ms.

To check the robustness of the numerically optimized pulse sequences we considered two types of errors: offset errors and flip angle or pulse miscalibration errors. Figure 8 shows the variation of fidelity with the offset frequency (Hz) and flip angle ($^\circ$) for the different gates, optimized using the GA algorithm. We checked the fidelity...
Fig. 6  Real (left) and imaginary (right) parts of the experimental tomographs of a initial $|110\rangle$ state. b After Fredkin gate applied on the $|110\rangle$ state

variation for the range $\pm 20$ for offset and $\pm 14$ for flip errors. The $90^\circ$ selective rf pulse is most robust of all the other gates (as is to be expected since it is a single-qubit gate), the fidelity for this is above 0.90 for the area inside the points $(\pm 12.5, \pm 19.6)$. The two-qubit CNOT gate has fidelity $> 0.9$ for the area inside the points $(-5.2, -20), (1.2, -20), (4.7, 20)$ and $(-1.2, 20)$. For the Fredkin gate, the fidelity is $> 0.9$ for the area which falls under the data points $(0, \pm 7.8)$ and $(\pm 5.3, 0)$ which approximately forms an ellipse. The Toffoli gate has fidelity $> 0.9$ for the area inscribed by points $(-2.8, -13.4), (5.5, 0), (1.4, 12.2)$ and $(-5.5, 0)$. In general, all the gates optimized by the GA method are of high fidelity and are robust against both offset and pulse flip angle errors.

We have plotted the robustness for the numerically optimized pulse sequences obtained via the GRAPE and SMP schemes by considering the same types of error parameters ($x$-axis: flip angles and $y$-axis: offset) as for GA. The results are depicted in Figs. 9 and 10, respectively. The data points for which the area inside them has fidelity greater than 0.90 of the pulses optimized using SMP are the following: for $90^\circ$ selective pulse it is $(\pm 1.4, \pm 20)$, for CNOT it is $(\pm 0.5, 0)$ and $(0, \pm 6)$, for Fredkin it is $(\pm 0.5, 0)$ and $(0, \pm 1.5)$, and for Toffoli gate it is $(\pm 0.2, 0)$ and $(0, \pm 2.5)$. Similarly, the data points for pulses optimized via GRAPE scheme are: for $90^\circ$ selective pulse it is $(\pm 3.5, \pm 20)$, for CNOT it is $(\pm 0.1, 0)$ and $(0, \pm 5)$, for Fredkin it is $(\pm 0.1, 0)$ and
Table 5  Table representing the pulse sequence for the Toffoli gate

|   | \( \tau \) (\( \mu s \)) | \( \phi \) | \( \delta \) (\( \mu s \)) |
|---|------------------|------|------------------|
| 1 | 32               | 243.22 | 539              |
| 2 | 27               | 138.58 | 546              |
| 3 | 39               | 2.47  | 499              |
| 4 | 36               | 320.89 | 3488             |
| 5 | 32               | 352.29 | 2495             |
| 6 | 34               | 355.84 | 536              |
| 7 | 37               | 175.98 | 1938             |
| 8 | 29               | 20.45  | 1957             |
| 9 | 34               | 354.75 | 542              |
| 10| 18               | 297.71 | 564              |
| 11| 15               | 215.55 | 2487             |
| 12| 27               | 308.2  | 550              |
| 13| 32               | 326.82 | 513              |
| 14| 13               | 122.09 | 541              |
| 15| 4                | 332.61 | 2518             |
| 16| 24               | 354.12 | 546              |
| 17| 36               | 310.6  | 3806             |
| 18| 32               | 210.97 | 1971             |
| 19| 30               | 3.74   | 504              |
| 20| 38               | 338.48 | 565              |

The first column represents the number of propagators
The second, third and fourth columns represent the pulse width (\( \tau \)), phase (\( \phi \)) and delay (\( \delta \)), respectively

(0, ±3) and for Toffoli gate it is (± 0.1,0) and (0, ± 3). As can be seen from the figures, the pulses we optimized using GA scheme are much more robust in comparison to the pulses optimized via the SMP and GRAPE schemes. The GRAPE and SMP schemes decompose the unitary operator of the pulse into pulses of continuously varying power, due to which errors in pulse flip angle and rf offset propagate. As already mentioned, we choose an on/off control for our GA method. This leads to a high-power (hard) pulse being implemented during the “on” state which is robust against such errors and during the “off” state only a free evolution occurs, which does not contribute to these types of errors.

The optimization time for methods such as GRAPE and SMP depends heavily on the initial guess and the unitary being optimized, while the accuracy of such algorithms depends on the precision of experimentally obtained parameters [55]. The pulses optimized using the basic variants of the GRAPE and SMP schemes were not robust against the pulse miscalibration errors as is evident from the robustness plots. While the basic schemes can be optimized for robustness, this will obviously increase the optimization time. In contrast, the control protocol we used in GA by default shows an advantage in the robustness against such errors at no additional cost of optimization time and is not dependent upon the precision of the experimental parameters.
We compared the results of our optimization of the Fredkin and the Toffoli gates using GAs, with previous experimental NMR implementations that use transition-selective pulses [10,11,13]. The experimental NMR spectra of this comparison are shown in Figs. 11 and 12 for a Fredkin gate and a Toffoli gate implemented on the $|110\rangle$ pseudopure state, respectively. All spectra were recorded after applying an $I\!X\!X$ operation (i.e. a $90^\circ$ pulse on the third qubit). Since the chemical shifts of the three fluorine qubits in our particular molecule cover a very large frequency bandwidth, we crafted special excitation Gaussian-shaped transition-selective pulses that are frequency modulated [8]. Using transition-selective pulses, the Fredkin gate was experimentally implemented with a fidelity of $0.711 \pm 0.009$ and a pulse length of 242 ms. Using transition-selective pulses, the Toffoli gate was experimentally implemented with a fidelity of $0.851 \pm 0.006$ and a pulse length of 168 ms. The fidelity of both the Fredkin and the Toffoli gates using the pulses crafted using the GA method was $> 0.95$, and the total pulse durations were substantially smaller, being 51 and 27 ms for the Fredkin and the Toffoli gates, respectively. Furthermore, as can be seen from the NMR spectra in Figs. 11 and 12, the standard implementation of these three-qubit gates using transition-selective pulses leads to considerable errors due to decoherence during these
Fig. 8 Robustness of pulse sequences optimized using the genetic algorithm method, corresponding to a 90° selective pulse, b CNOT gate, c Fredkin gate and d Toffoli gate. The x and y axes represent the error in flip angle (°) and the offset (Hz), respectively.

Fig. 9 Robustness of pulse sequences optimized using the GRAPE technique, corresponding to a 90° selective pulse, b CNOT gate, c Fredkin gate and d Toffoli gate. The x and y axes represent the error in flip angle (°) and the offset (Hz), respectively.
Fig. 10 Robustness of pulse sequences optimized by the strongly modulated pulses (SMP) technique, corresponding to (a) 90° selective pulse, (b) CNOT gate, (c) Fredkin gate and (d) Toffoli gate. The x and y axes represent the error in flip angle (°) and the offset (Hz), respectively.

long pulses as well as offset errors. The GA-optimized pulse sequences, on the other hand, have a high fidelity and do not suffer from these errors.

We also compared the results of our genetic algorithm optimization of the Fredkin and the Toffoli gates with those obtained from GRAPE and SMP techniques. The experimental NMR spectra of this comparison are shown in Figs. 11 and 12 for both the gates implemented on an initial pseudopure state $\left| 110 \right>$. All spectra were recorded after applying an IIX operation (i.e. a 90° pulse on the third qubit). Using GRAPE scheme the optimized pulses for Fredkin gate were obtained with a fidelity of 0.998 with a pulse length of 50 ms, and for the Toffoli gate the pulses were obtained with a fidelity of 0.998 with a pulse length of 30 ms. The experimental fidelity obtained using GRAPE scheme for the Fredkin gate is $0.968 \pm 0.008$ and for the Toffoli gate is $0.966 \pm 0.011$. Similarly, using the SMP scheme the optimized pulse for Fredkin gate was obtained with a fidelity of 0.98 with a pulse length of 50 ms and for the Toffoli gate, the optimized pulse were obtained with a fidelity of 0.995 with a pulse length of 30 ms. The experimentally obtained fidelity using SMP scheme for the Fredkin gate is $0.975 \pm 0.013$ and for the Toffoli gate is $0.944 \pm 0.014$.

4 Conclusions

In summary, we have optimally designed and experimentally implemented the universal multi-qubit Toffoli and Fredkin gates on a three-qubit NMR quantum information processor. We used a global optimization method based on genetic algorithms to deter-
Fig. 11 NMR spectra of a pseudopure state \( |110\rangle \); after implementation of a Fredkin gate on the \( |110\rangle \) state, b using transition-selective pulses; c using SMP optimized pulses; d using GRAPE optimized pulses; e using pulses optimized by the genetic algorithm method.

Determine the optimal unitary transformations and generate the corresponding numerically optimized rf pulse profiles. We were able to find optimal constructions for these important three-qubit universal control gates, which are robust against pulse offset errors as well as errors that could arise due to decoherence. We were able to find gate decompositions which are based only on hard (short duration) rf pulses and delays, which take very short times to implement and are of high fidelity. Our gate decompositions are sufficiently general and can be used for other quantum computing hardwares as
Fig. 12  NMR spectra of a pseudopure state $|110\rangle$; after implementation of a Toffoli gate on the $|110\rangle$ state 

- **b** using transition-selective pulses; 
- **c** using SMP optimized pulses; 
- **d** using GRAPE optimized pulses; 
- **e** using pulses optimized by the genetic algorithm method

well. Although some of the optimization protocols took a long time to run, the obvious advantage is that once the optimal pulse sequence for a gate is found, it can be used later without any further optimization as long as one is working on the same quantum computer.

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