Extending scientific computing system with structural quantum programming capabilities

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November 12, 2009

Abstract—We present a basic high-level structures used for developing quantum programming languages. The presented structures are commonly used in many existing quantum programming languages and we use quantum pseudo-code based on QCL quantum programming language to describe them.

We also present the implementation of introduced structures in GNU Octave language for scientific computing. Procedures used in the implementation are available as a package quantum-octave, providing a library of functions, which facilitates the simulation of quantum computing. This package allows also to incorporate high-level programming concepts into the simulation in GNU Octave and Matlab. As such it connects features unique for high-level quantum programming languages, with the full palette of efficient computational routines commonly available in modern scientific computing systems.

To present the major features of the described package we provide the implementation of selected quantum algorithms. We also show how quantum errors can be taken into account during the simulation of quantum algorithms using quantum-octave package. This is possible thanks to the ability to operate on density matrices.

Index Terms—quantum information, quantum programming, models of quantum computation

I. INTRODUCTION

Quantum information theory aims to harness the quantum nature of information carriers in order to develop more efficient algorithms and more secure communication protocols [1]. Unfortunately, counterintuitive laws of quantum mechanics make the development of new quantum information processing procedures highly non-trivial task. This can be seen as one of the reasons why only few truly quantum algorithms were proposed [5].

The laws of quantum mechanics are in many cases very different from those we know from the classical world. That is why one needs to seek for the novel methods for describing information processing which involves quantum elements. To this day several formal models were proposed for the description of quantum computation process [7].

The most popular of them is the quantum circuit model [7], which is tightly connected to the physical operations implemented in a laboratory. It allows to operate with the basic ingredients of quantum information processing – namely qubits, unitary evolution operators and measurements. However, it does not provide too much flexibility concerning operations on more sophisticated elements required to develop scalable algorithms and protocols e.g. quantum registers or classical controlling operations.

Another model widely used in the study of theoretical aspects of quantum information processing is the quantum Turing machine [7]. This model is mainly used in the analysis of quantum complexity problems [11]. Its main advantage it that it provides method of comparing efficiency of classical and quantum algorithms. Unfortunately quantum Turing machine, in analogy to its classical counterpart, operates on very basic data and thus it cannot be easily used to construct quantum algorithms.

Both quantum circuit model and quantum Turing machine share some serious drawbacks concerning lack of support for high-level programming and very limited flexibility. These problems were addressed in the recent research in the area of quantum programming languages [15].

Quantum programming languages are based on the Quantum Random Access Machine (QRAM) model. QRAM is equivalent, with respect to its computational power, to the quantum circuit model or quantum Turing machine. However, it has strictly distinguished two parts: quantum and classical. The quantum part is responsible for performing parts of an algorithm which cannot be computed efficiently by a classical machine. The classical part is used to control quantum computation. This model is used as a basis for most quantum programming languages [14].

Among high-level programming languages designed for quantum computers we can distinguish imperative
and functional languages. The later are seen by many researchers as a means of providing robust and scalable methods for developing quantum algorithms [17]. We, however, focus on the imperative paradigm as it provides more straightforward way of implementing high-level quantum programming concepts.

This paper is organized as follows. In Section II we briefly describe the QRAM model of quantum computer and introduce the quantum pseudocode, which was designed to describe this model. In Section III we introduce high-level programming structures used in quantum programming languages. These structure are based on the QRAM model of quantum computer. In Section IV the implementation of presented concepts is described and quantum-octave package is presented. In Section V implementation of quantum algorithms using quantum-octave package is presented. Also the analysis of quantum errors is provided in the case of quantum search algorithm. Finally Section VI summarize the presented work and provides reader with some concluding remarks.

II. QRAM MODEL OF QUANTUM COMPUTATION

Quantum random access machine is interesting for us since it provides convenient model for developing quantum programming languages. However, these languages and basic concepts used to develop them are our main area of interest. For this reason here we provide only the very basic introduction to the QRAM model. Detailed description of this model is given in [18] and [19] together with the description of hybrid architecture used in quantum programming.

A. Classical RAM model

As in many situations in quantum information science, the QRAM models is based on the concepts developed to describe classical computational process – in this case on the Random Access Machine (RAM) model. The classical model of random access machine (RAM) is the example of more general register machines [20], [21], [22].

The Random Access Machine consists of an unbounded sequence of memory registers and finite number of arithmetic registers. Each register may hold an arbitrary integer number. The programme for the RAM is a finite sequence of instructions \( \Pi = (\pi_1, \ldots, \pi_n) \). At each step of execution register \( i \) holds an integer \( r_i \) and the machine executes instruction \( \pi_\kappa \), where \( \kappa \) is the value of the programme counter. Arithmetic operations are allowed to compute the address of a memory register.

Despite the difference in the construction between Turing machine and RAM, it can be easily shown that Turing machine can simulate any RAM machine with polynomial slow-down only [21]. The main advantage of the RAM models is its resemblance with the real-world computers.

B. Quantum RAM model and quantum pseudocode

Quantum Random Access Machine (QRAM) model is build as an extension of the classical RAM model. Its main goal is to provide the ability to exploit quantum resources. Moreover, it can be used to perform any kind of classical computation. The QRAM allows us to control operations performed on quantum registers and provides the set of instructions for defining them. Schematic presentation of such architecture is provided in Figure 1.

Fig. 1. The model of classically controlled quantum machine [19].

Classical computer is responsible for performing unitary operations on quantum memory. The results of quantum computation are received in the form of measurement results.

The quantum part of QRAM model is used to generate probability distribution. This is achieved by performing measurement on quantum registers. The obtained probability distribution has to be analysed using a classical computer.

Quantum algorithms are, in most of the cases, described using the mixture of quantum gates, mathematical formulas and classical algorithms. The first attempt to provide a uniform method of describing quantum algorithms was made in [23], where the author introduces a high-level notation based on the notation known from computer science textbooks [24], [25].

In [18] Knill introduced the first formalized language for description of quantum algorithms. Moreover, it was tightly connected with the model of Quantum Random Access Machine.

Quantum pseudocode proposed by Knill [18] is based on conventions for classical pseudocode proposed in [24] Chapter I. Classical pseudocode was designed to be readable by professional programmers, as well as people who had done a little programming. Quantum pseudocode introduces operations on quantum registers. It also allows to distinguish between classical and quantum registers. In quantum pseudocode quantum registers are distinguished with an underline. They can be introduced by applying quantum operations to classical registers or by calling
a subroutine which returns a quantum state. In order to convert a quantum register into a classical register measurement operation has to be performed.

The example of quantum pseudocode is presented in Listing 1. It shows the main advantage of QRAM model over quantum circuits model – the ability to incorporate classical control into the description of quantum algorithm.

\[
\begin{align*}
|q_0\rangle & \quad H \quad S \quad T \\
|q_1\rangle & \quad H \quad S \\
|q_2\rangle & \quad H
\end{align*}
\]

Fig. 2. Quantum circuit representing quantum Fourier transform for three qubits. Elementary gates used in this circuit are described in [1].

Procedure: FOURIER(q, \(d\))
Input: A quantum register \(q\) with \(d\) qubits. Qubits are numbered form 0 to \(d - 1\).
Output: The amplitudes of \(q\) are Fourier transformed over \(Z_{2^d}\).

C: assign value to classical variable
\(\omega \leftarrow e^{i2\pi/2^d}\)

C: perform sequence of gates
for \(i = d - 1\) to \(i = 0\)
for \(j = d - 1\) to \(j = i + 1\)
if \(q_j\) then \(R_{2^{d-i}+j}(q_i)\)
C: number of loops executing phase depends on \(c\), the required accuracy of the procedure \(H(q_i)\)
C: change the order of qubits
for \(j = 0\) to \(j = \frac{d}{2} - 1\)
SWAP \((q_j, q_{d-j})\)

Listing 1. Quantum pseudocode for quantum Fourier transform on \(d\) qubits. Quantum circuit for this operation with \(d = 3\) is presented in Figure 2.

Operation \(H(q_i)\) executes a quantum Hadamard gate on a quantum register \(q_i\) and \(SWAP(q_i, q_j)\) performs SWAP gate between \(q_i\) and \(q_j\). Operation \(R_\phi(q_i)\) executes a quantum gate \(R_\phi\) defined as
\[
R_\phi = \begin{pmatrix}
1 & 0 \\
0 & e^{i\phi}
\end{pmatrix},
\]
on the quantum register \(q_i\). Using conditional construction
if \(q_j\) then \(R_\phi(q_i)\)
it is easy to define controlled phase shift gate. Similar construction exists in QCL quantum programming language [19]. In Section IV we describe implementation of this construction in quantum-octave.

The measurement of a quantum register can be indicated using an assignment \(a_j \leftarrow q_j\).

C. Requirements for quantum programming language
Taking into account QRAM model we can formulate basic requirements which have to be fulfilled by any quantum programming language [9], [26], [15].

- Completeness: Language must allow to express any quantum circuit and thus enable the programmer to code every valid quantum programme written as a quantum circuit.
- Extensibility: Language must include, as its subset, the language implementing some high level classical computing paradigm. This is important since some parts of quantum algorithms (for example Shor’s algorithm) require non-trivial classical computation.
- Separability: Quantum and classical parts of the language should be separated. This allows to execute any classical computation on purely classical machine without using any quantum resources.
- Expressivity: Language has to provide high level elements for facilitating the quantum algorithms coding.
- Independence: The language must be independent from any particular physical implementation of a quantum machine. It should be possible to compile a given programme for different architectures without introducing any changes in its source code.

III. HIGH-LEVEL PROGRAMMING STRUCTURES

A. Quantum memory
Quantum memory is a set of qubits indexed by integer numbers. Quantum register is a set of indices pointing to distinct qubits. We will denote those registers as \(r_1, r_2, \ldots\) or in case of single qubits as \(q_1, q_2, \ldots\). The state of a quantum memory is a quantum state of size equal to the number of qubits. In the case of quantum-octave we operate on density matrices (although some operations on state vectors are allowed). We will denote the state of the quantum memory by \(\rho\).

Following operations on quantum memory are allowed:
- Allocation of new register of size \(n\):
\[
\rho_{t+1} = \rho_t \otimes |0\ldots0\rangle \langle 0\ldots0|,
\]
where \(\otimes\) denotes tensor product, \(|\cdot\rangle\) the column vector and \(\langle\cdot|\) the dual vector.
- Deallocation of a register indexed by register \(r\):
\[
\rho_{t+1} = Tr_r \rho_t,
\]
where \(Tr_r(\rho)\) denotes partial trace of \(\rho\) with regard to the subsystem indexed by \(r\).
- Unitary evolution \(U\) of the quantum memory:
\[
\rho_{t+1} = U\rho_t U^\dagger.
\]
• Application of quantum channel $K_i$ on the quantum memory:
\begin{equation}
\rho_{t+1} = \sum_i K_i \rho_t K_i^\dagger.
\end{equation}

• Measurement in the computational basis:
\begin{equation}
\rho_{t+1} = \sum_i |i\rangle\langle i| \rho_t |i\rangle\langle i|,
\end{equation}
\begin{equation}
P(i) = \text{Tr} \left( |i\rangle\langle i| \rho_t \right),
\end{equation}
where $i$ enumerates the states of computational basis.

For a solid introduction to quantum computation the reader may refer to book by Nielsen and Chuang [1], where all the needed notions are explained in detail.

In quantum computation, construction of the unitary gate is the essential part of quantum algorithm. For a given control register $r_c$, target register $r_t$ and two quantum gates $G_1$ and $G_2$, we may define quantum condition in the more general way, namely
\begin{equation}
IF_{r_c}(G_1 r_t)ELSE(G_2 r_t) = \prod_{i \in P(r_c) \setminus \emptyset} \left( \text{Not}_{r_c} G_{2 r_t[r_c]} \text{Not}_{r_t} G_{1 r_t[r_c]} \right)
\end{equation}
where $P(\cdot)$ denotes the power set.

2) Condition on mixture of classical and quantum variables: One may consider the relation between the state of quantum register and the value of the classical variable. By $\lbrack x \rbrack_r$ we will denote a numerical value of ordered (ascending order) elements of the register $x$ in regard to register $r$, for example the value of $\lbrack \{4, 9\} \rbrack_{\{2, 4, 7, 9\}}$ is 10. By $\lbrack x \rbrack_r$ we will denote the value of the register in order to use it as argument for arithmetic comparison. For example $\lbrack r \rbrack_r < 4$ means: “all those values of $r$ that are less than four.”

Code and circuit in Figure 3 show the idea and the implementation of conditional operation controlled by expression ‘less than’ operating on classical constant and quantum register.

- B. Composed and controlled gates

1) Composed gate: Given one-qubit unitary gate $G$, quantum register $r$, and size of the gate $s$ we can construct composed gate $U^s_r$ according to the formula:
\begin{equation}
U^s_r = \bigotimes_{i=1}^s X_i ,
\end{equation}
where $X_i = \begin{cases} G & \text{if } i \in r, \\ 1 & \text{if } i \notin r \end{cases}$.

2) Controlled gate with multiple controls: Given one-qubit unitary gate $G$, quantum register $r_c$, we call control, and quantum register $r_t$ we call target, and size of the gate $s$ we can construct controlled gate $U^s_{r_t[r_c]}$ according to the formula:
\begin{equation}
U^s_{r_t[r_c]} = \bigotimes_{i=1}^s X_i + \bigotimes_{i=1}^s Y_i,
\end{equation}
where $X_i = \begin{cases} |0\rangle \langle 0| & \text{if } i \in r_c, \\ \text{I} & \text{if } i \notin r_c \end{cases}$,
$Y_i = \begin{cases} |1\rangle \langle 1| & \text{if } i \in r_t, \\ \text{I} & \text{if } i \notin r_t \cup r_c \end{cases}$.

We assume that $r_t \cap r_c = \emptyset$. Sometimes we will omit the size parameter $s$.

C. Conditionals

One of high-level technique used in quantum programming are quantum conditions [27]. The main idea behind quantum conditions is construction of quantum gates controlled by predicates on control registers.

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![Example of quantum conditional operation with inequality.](image-url)
In the general case, gate implementing any relation (marked as ⊕) can be constructed in the following way:

\[ IF_{r_c} \oplus N(G_1 r_1) ELSE(G_2 r_1) = \prod_{i \in F} (Not_i G_{2 r_1} \oplus Not_i) \prod_{i \in T} (Not_i G_{1 r_1} \oplus Not_i) , \]

where sets \( T \) and \( F \) are defined as follows:

\( T = \mathcal{P}(r_c) \setminus \{ x | x \in \mathcal{P}(r_c) \land [x]_{r_c} \oplus N \} \), \hspace{1cm} (13)
\( F = \mathcal{P}(r_c) \setminus \{ x | x \in \mathcal{P}(r_c) \land \neg ([x]_{r_c} \oplus N) \} \). \hspace{1cm} (14)

Note that \( T \cup F = \mathcal{P}(r_c) \).

In quantum-octave standard arithmetic relations \( =, \neq, <, >, \leq, \geq \) are implemented.

**D. Expressions**

We may consider more complicated expression on quantum registers. For example logical operators and quantum pointers. Logical operators allow to apply an controlled operation to the target register only if a given logical expression on control registers is true. A quantum pointer allows to apply controlled gate on the target register selected by the state of the control register.

1) **Logical expressions on quantum variables**: The gate that implements logical expression (denoted here by \( \odot \)) is constructed according to the following equation:

\[ IF_{r_c} \odot \oplus \otimes N(G_1 r_1) ELSE(G_2 r_1) = \prod_{i \in F} (Not_i G_{2 r_1} \odot \otimes Not_i) \prod_{i \in T} (Not_i G_{1 r_1} \odot \otimes Not_i) , \]

where sets \( T \) and \( F \) are defined as follows:

\( T = \mathcal{P}(r_c) \setminus \{ x_1 \cup x_2 | x_1 \subseteq r_c, x_2 \subseteq r_c \} \lambda (\{ [x_1]_{r_c} \odot \otimes N_1 \oplus [x_2]_{r_c} \odot \otimes N_2 \} \), \hspace{1cm} (16)
\( F = \mathcal{P}(r_c) \setminus \{ x_1 \cup x_2 | x_1 \subseteq r_c, x_2 \subseteq r_c \} \lambda \neg (\{ [x_1]_{r_c} \odot \otimes N_1 \oplus [x_2]_{r_c} \odot \otimes N_2 \} \)

and \( r_c = r_c \cup r_c \).

An example of quantum conditional gate controlled by logical expression defined on quantum registers is presented in Figures 5 and 6.

2) **Quantum pointers**: In analogy to the concept of pointers and indirect addressing in classical programming, one may introduce quantum pointers. The idea is to use control register to control on which of the target registers an operation should be applied.

Let us assume that one has the \( n \)-bit control register and a set of \( 2^n \)-bit target registers. The control register stores the address of target register to which given unitary operation shall be applied. In order to visualise the use of a quantum pointer an example is shown in Figure 7.

**IV. PACKAGE ** **QUANTUM-OCTAVE**

Package quantum-octave [29], [30], [31] provides a quantum programming, simulation and analysis language implemented as a library of functions for GNU Octave [32].

GNU Octave is computer algebra system (CAS) and high level programming language designed primarily to perform numerical calculations. The basic data
structure in Octave is a matrix (integer, real or complex), therefore it is a natural choice as a basis for the implementation of quantum programming language.

GNU Octave supports sparse matrices and distributed computing in shared and distributed memory models. GNU Octave is a very flexible and easily extendible tool. It is also free software and it can be used in a wide range of operating systems.

A. Design choices

The main goal of the design of quantum-octave is to provide a flexible and useful tool for simulation of quantum information processing. Therefore it is based on GNU Octave a high-level scientific programming language. This allows for a seamless integration of very efficient matrix operations and numerical procedures with the library of specialized functions provided by quantum-octave. As GNU Octave is to large extent compatible with Matlab, provided functions can be also used to simulate and analyse quantum algorithms in Matlab.

One of the unique features of quantum-octave is its ability to operate on pure and mixed quantum states. It allows to perform unitary as well as non-unitary evolution represented by quantum channels.

Quantum gates can be constructed by the user in various ways: by calling provided subroutines, by building their own subroutines, by using quantum control structures. Additionally the user can build and use quantum channels or use those already provided. Most of the quantum-octave functions operate on quantum registers and therefore the quantum operations build with their use are re-allocatable.

A good illustration of those features is presented in the following listing that contains the implementation of Quantum Fourier transform in quantum-octave.

It can be compared to pseudo code version of the same procedure listed in Listing 1.

```
function ret = dft (gatesize)
    n = gatesize;
    cir = id(n);
    for i = [1:n]
        for j = [1:i-1]
            cir = circuit (cir, cphase (pi/(2 ^ (i-j))), j, i, gatesize);
        endfor
    cir = circuit (cir, productgate (h, i, gatesize));
    endfor
    ret = cir = circuit (cir, flip(n));
endfunction
```

Listing 2. Quantum Fourier transform in quantum-octave

Package quantum-octave can operate on sparse and full matrices depending on users choice. Sparse matrices need much less memory to store but operations on them may be slower. Full matrices tend to consume huge memory space, but operations on them are generally faster. In case of full matrices it should be possible to operate on states of size up to ten qubits on a contemporary workstation. Sparse matrices should allow to simulate the quantum systems of up to 20 qubits.

Although quantum-octave is not, strictly speaking, a programming language ready to program real quantum devices, with some effort it can be transformed in such a way that it would be able to compile a high level programs to some sort of quantum assembler. One should note that broad range of functions allowing the analysis of states is implemented in the package. Those function are described in the following section.

B. Description

Package quantum-octave is designed to allow the user to operate on different levels of abstraction. User can prepare complex gates and quantum channels from basic primitives such as single qubit rotations, controlled gates, single qubit channels. Most of the functions that form this library operate on quantum registers, which makes the preparation of quantum gates and channels very "natural". The library is implemented in such a way that depending of user's choice it may operate on full or sparse matrices.

quantum-octave can work in two modes: as a library or as a programming language/simulator. Library mode is the default. To switch to language/simulator mode one has call quantum_octave_init() function. In case of the second mode quantum-octave allocates and manages an internal quantum state and maintains the quantum registers. Such functions as evolve(), applychannel(),
measurecompbasis() operate directly on the internal state. Listings of Deutsch’s \[3\] and Grover’s \[4\] algorithms show use of language/simulation mode.

1) *Convention:* Following conventions are used in quantum-octave.

- **Quantum register** is horizontal integer vector containing indices of qubits starting from one.
- **Ket** is vertical complex vector.
- **Bra** is horizontal complex vector.
- **Density matrix** is complex square matrix always of dimension \(n\)-th power of two by \(n\)-th power of two.
- **Binary string** is 0,1-horizontal vector, that encodes a binary number. Order of bits is from MSB to LSB.
- **Size** of the gate or channel is always given in terms of a number of qubits it acts on. If size is written in square brackets it means that it can be omitted if the gate or channel acts on the whole system and quantum-octave was initialised.

2) **Quantum gates:** Package quantum-octave supplies set of elementary gates known in quantum computation.

- **sx, sy, sz** – returns one-qubit Pauli operators \(sx\), \(sy\), \(sz\).
- **id(n)** – returns identity matrix: \(I_n\).
- **roty(a), rotz(a)** – return rotation matrix by angle \(a\) around appropriate axis.
- **qft(n)** – returns quantum Fourier transform on \(n\) qubits.
- **swap(size, qubits)** – returns swap gate of a given size that swaps qubits given as two-element vector.
- **qubitpermutation(permutation)** – returns unitary gate that performs given permutation.
- **h** – returns one-qubit Hadamard gate.
- **phase(p0, p1)** – returns one-qubit phase gate, with \(p0, p1\) phase parameters.

3) **Basic functions:** Following functions are essential to prepare a quantum state and to implement a quantum algorithm, protocol or game.

- **ket(binvec)** – returns ket for given binary string.
- **ketn(int, size)** – returns a ket of size \(2^{\text{size}}\) for given integer number.
- **state(pure_state)** – returns density matrix for a given ket.
- **mixstates(a1, mixed_statel, [a2, mixed_statel, ...])** – returns convex combination of density matrices with coefficients \(a1, a2, ...\).
- **productgate(gate, targetreg[, size])** – returns a controlled gate of a given size that applies given gate on target register. See \[Eq. 8\]
- **controlledgate(gate, controlreg, targetreg[, size])** – returns a controlled gate of given size that applies gate on specified target register and is controlled by control register. See \[Eq. 9\]

4) **Quantum conditional operations:** The functions listed below implement quantum conditional operations, quantum expressions and pointers. They are useful to simplify the implementation.

- **qif(expression, ifpart, elsepart, size)** – returns quantum gate of given size, controlled by expression that applies ifpart if expression is true and elsepart if expression is false. ifpart and elsepart are cellarrays in the form: \{gate, target_register\}. See \[Eq. 11\]
- **qreq(register, integer)** – returns expression: [register] equals integer. See \[Eq. 12\]
- **qrne(register, integer)** – returns expression: [register] not equal integer.
- **qrge(register, integer)** – returns expression: [register] is greater or equal to integer.
- **qrle(register, integer)** – returns expression: [register] is lesser or equal to integer.
- **qrlt(register, integer)** – returns expression: [register] is lesser than integer.
- **qrgt(register, integer)** – returns expression: [register] is greater than integer.
- **qror(expr1, expr2)** – returns logical or on expressions expr1 and expr2. See \[Eq. 15\]
- **qrand(expr1, expr2)** – returns logical and on expressions expr1 and expr2.
- **qpointer(gate, contreg, targetregister[, size])** – returns quantum gate of given size, controlled by control register that applies gate on target register. See \[Eq. 18\]

5) **Evolution, channels and measurement:** The following group of functions allows to control the evolution of quantum states and introduces the application of channels and measurement.

- **evolve(evolution[, state])** – applies unitary evolution to the state, returns the result of the evolution. See \[Eq. 2\]
- **channel(name, p)** – returns Kraus operators acting on one qubit, parametrised by \(p\) allowed names are: "depolarizing", "amplitudedamping", "amplituderotatigdamping", "bitflip", "phasedamping" and
Some of the states commonly used in quantum algorithms are implemented in the quantum-octave library as separate functions.

- `localchannel(kraus, targetreg[, chsize])` – returns a channel being the extension of defined by kraus operators channel, acting on target register.
- `applychannel(elements[, state])` – applies on the state non unitary evolution defined by set of Kraus operators (elements), returns the result of the evolution. See Eq. 5
- `ptrace(state, targetreg)` – returns reduced density matrix for the state with target register traced out. See Eq. 3
- `circuit(gate[, gate])` – returns circuit composed of the sequence of gates.
- `measurecompbasis([state])` – returns the internal quantum state.
- `clearregister(regid)` – removes regid register from quantum heap. Traces out appropriate qubits from the internal state.
- `qureg(regid)` – returns quantum register to which regid points.
- `getstate()` – returns the internal quantum state.

**6) Computation and control:** Following functions allows to control the quantum heap and configure the behaviour of the library.

- `quantum_octave_init()` – initialises the simulated system, creates quantum state with zero qubits allocated and empty list of registers.
- `set_quantum_octave_sparse([true | false])` – switches on or off use of sparse matrices by all quantum-octave functions.
- `newregister(size)` – creates new register of given size, allocates qubits on quantum heap, returns register id.
- `clearregister(regid)` – removes regid register from quantum heap. Traces out appropriate qubits from the internal state.
- `qureg(regid)` – returns quantum register to which regid points.
- `getstate()` – returns the internal quantum state.

**7) Well known states:** Some of the states commonly used in quantum algorithms are implemented in the library as separate functions.

- `ghz(n)` – returns Greenberger-Horne-Zeilinger state for n qubits: \(\frac{1}{\sqrt{2}}|0\rangle^n \otimes |1\rangle^n\).
- `phip` – returns Bell \([\Phi^+]\) state: \(\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)\).
- `phim` – returns Bell \([\Phi^-]\) state: \(\frac{1}{\sqrt{2}}(|00\rangle - |11\rangle)\).
- `psip` – returns Bell \([\Psi^+]\) state: \(\frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)\).
- `psim` – returns Bell \([\Psi^-]\) state: \(\frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)\).
- `maximallymixed(n)` – returns density matrix maximally mixed state: \(\frac{1}{n}I_n\).
- `wernersinglet(a)` – returns 2-qubit Werner state: \(a(|00\rangle - |11\rangle)(|01\rangle + |10\rangle) + (1 - a)\frac{1}{2}I_2\).

**8) Analysis:** Package quantum-octave provides standard functions for analysis of quantum states, widely used in quantum information literature. Among them the most important are:

- `negativity(state, qubits)` – computes negativity of the state in respect to qubits.
- `entropy(state)` – computes Von Neuman entropy of the state.
- `concurrence(state)` – computes concurrence of the state.
- `fidelity(rho, sigma)` – computes fidelity between density matrices rho and sigma.
- `fidelitypuremixed(psi, rho)` – computes fidelity between ket psi and density matrix sigma.
- `partialtranspose(state, targetreg)` – returns matrix being partial transposition of state matrix in regard to target register.

The next section presents the applications of quantum-octave and various programming techniques for solutions of quantum programming problems.

**V. EXAMPLES AND APPLICATIONS**

In what follows the applications of quantum-octave and various high-level programming techniques are discussed. It is shown how quantum processes, such as algorithms may be implemented, simulated and analysed with this tool.

**A. Deutsch’s problem**

One of the simplest quantum algorithms is Deutsch’s algorithm. Although it may seem trivial, this algorithm shows two very important features of quantum computation. The first one is that by taking the advantage of a superposition one can compute any binary function for all its arguments in one step. The second features is that it is only possible to retrieve information about property of a function and not on its values.

Let us assume that we have a black box that is usually called the oracle. This box computes a function \(f : \{0, 1\} \rightarrow \{0, 1\}\). We do not know if that function is constant \(f(0) = f(1)\) or injective \(f(0) \neq f(1)\). In classical case we have to ask the oracle twice to check which kind the function \(f\) is. But in quantum case it is possible to solve this problem asking the oracle only once.

The algorithm goes as follows:

1) Prepare the state: \(|\Psi\rangle = |0\rangle \otimes |1\rangle\).
2) Apply the Hadamard $H^{\otimes 2}$ gate on the state $|\Psi\rangle$, you will get
\[
|\Psi_1\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}} \otimes \frac{|0\rangle - |1\rangle}{\sqrt{2}}.
\] (19)

3) Apply the gate $U_f : |x\rangle \otimes |y\rangle \rightarrow |x\rangle \otimes |f(x) + y\rangle$ on the state $|\Psi_1\rangle$; you will get:
\[
|\Psi_2\rangle = \begin{cases} 
\frac{|0\rangle + |1\rangle}{\sqrt{2}} \otimes \frac{|0\rangle - |1\rangle}{\sqrt{2}} & \text{for constant } f, \\
\frac{|0\rangle - |1\rangle}{\sqrt{2}} \otimes \frac{|0\rangle + |1\rangle}{\sqrt{2}} & \text{for injective } f.
\end{cases}
\] (20)

4) Apply $H \otimes I$ on the state $|\Psi_2\rangle$; you will get:
\[
|\Psi_3\rangle = \begin{cases} 
\frac{|0\rangle - |1\rangle}{\sqrt{2}} \otimes |0\rangle & \text{for constant } f, \\
\frac{|1\rangle + |0\rangle}{\sqrt{2}} \otimes |0\rangle & \text{for injective } f.
\end{cases}
\] (21)

5) Measure state of the first qubit, you will get $|0\rangle$ in case of constant function, $|1\rangle$ for injective function.

Quantum circuit representation of Deutsch’s algorithm is presented in Figure 8. The $U_f$ gate provide a reversible implementation of function $f$ and the symbol $\oplus$ denotes a measurement.

Fig. 8. Deutsch’s algorithm

The implementation of Deutsch’s algorithm presented in listing 3 is an introductory example of application of quantum-octave for simulation of a quantum algorithm with all basic steps of computation: initialization of the quantum computer, unitary evolution and measurement.

Below we describe simulation steps (compare with circuit in Figure 8). Numbers on the left refer to the line numbers in Listing 3.

```quantum-octave
# declare and allocate registers
7 r1=newregister(1);
9 r2=newregister(1);
# declare functions
11 f(1)=identity(2);
13 f(2)=productgate(sx,qureg(r2));
14 f(3)=qif(qureg(r1),1,...)
15 f(4)=qif(qureg(r1),0,...)
17 (sx,qureg(r2))... (id,qureg(r2)));
# do the algorithm
19 evolve(productgate(sx,qureg(r2)));
20 evolve(productgate(h,[qureg(r1),qureg(r2)]));
21 evolve(f(num));
23 # throw away second register
clearregister(qureg(r2));
25 # return the outcome
ret=measurecompbasis();
27 endfunction
Listing 3. Deutsch algorithm in quantum-octave
```

B. Grover’s algorithm

To illustrate more advanced usage of the presented concepts we use the quantum algorithm for searching a unordered database. The algorithms was proposed by Grover [33, 34, 35] and its detailed description and analysis can be found in [36, 37]. Here we present the implementation of Grover’s algorithm which presents the features of quantum-octave related to the observation of quantum errors. We show the propagation of initial errors during the execution of the algorithm.

Grover’s search algorithm is one of the most important quantum algorithms. This is especially true since many algorithmic problems can be reduced to exhaustive search. However, like in the case of any quantum procedure, the efficiency of the algorithm depends on the ability to avoid errors during the procedure. Thus, it is important how quantum errors affect the executions of the algorithm.

1) Statement of the problem: Let $X$ be a set and let $f : X \rightarrow \{0, 1\}$, such that
\[
f(x) = \begin{cases} 
1 & x = x_0, x \in X, \\
0 & x \neq x_0, x \in X,
\end{cases}
\] (22)

for some marked $x_0 \in X$.

For the simplicity we assume that $X$ is a set of binary strings of length $n$. Therefore $|X| = 2^n$ and $f : \{0, 1\}^n \rightarrow \{0, 1\}$.

We can map the set $X$ to the set of states over $\mathcal{H}^{\otimes n}$ in the natural way as
\[
x \leftrightarrow |x\rangle.
\] (23)

The goal of the algorithm is to find the marked element. This is achieved by the amplification of the appropriate amplitude [38, 39].

2) The algorithm: The Grover’s algorithm is composed of two main procedures: the oracle and the diffusion.
a) Oracle: By oracle we understand a function that marks one defined element. In the case of this algorithm, the marking of the element is done by negation of the amplitude of the state that we search for.

With the use of elementary quantum gates the oracle can be constructed using an ancilla |q⟩ in the following way:

$$O|x⟩|q⟩ = |x⟩|q ⊗ f(x)⟩.$$  \hfill (24)

If the register |q⟩ is prepared in the state:

$$|q⟩ = H|1⟩ = \frac{|0⟩ - |1⟩}{\sqrt{2}}.$$  \hfill (25)

then by substitution, equation 24 is re-transformed to:

$$O|x⟩\frac{|0⟩ - |1⟩}{\sqrt{2}} = (-1)^{f(x)}\frac{|0⟩ - |1⟩}{\sqrt{2}},$$  \hfill (26)

and by tracing out the ancilla we get:

$$O|x⟩ = -(-1)^{f(x)}|x⟩.$$  \hfill (27)

Thus the oracle marks a given state by inverting its amplitude.

b) Diffusion: The operator D rotates any state around the state

$$|ψ⟩ = \frac{1}{\sqrt{2^n}} \sum_{x=0}^{2^n-1} |x⟩,$$  \hfill (28)

D may be written in the following form:

$$D = -H ⊗ n (2|0⟩⟨0| - I) H ⊗ n = 2|ψ⟩⟨ψ| - I.$$  \hfill (29)

c) Grover iteration: The first step of the algorithm is to apply Hadamard gate H ⊗ n on all the qubits. Then we apply gate G = DO several times.

d) Number of iterations: Application of diffusion operator on the base state |n⟩ gives

$$-H ⊗ n I_0 H ⊗ n |n⟩ = -|x₀⟩ + \frac{2}{N} \sum_y |y⟩.$$  \hfill (30)

Application of this operator on any state gives

$$D|x⟩ = \sum_x α_x (-|x⟩ + \frac{2}{N} \sum_y |y⟩)$$

$$= \sum_x (-α_x + 2s)|x⟩,$$

where

$$s = \frac{1}{N} \sum_x α_x$$  \hfill (31)

is arithmetic mean of coefficients αx, x = 0, ..., 2n - 1.

k-fold application of Grover’s iteration G on initial state |s⟩ leads to [36]:

$$G^k|s⟩ = \alpha_k ∑_{x≠x₀} |x⟩ + \beta_k|x₀⟩,$$  \hfill (32)

with real coefficients:

$$\alpha_k = \frac{1}{\sqrt{N-1}} \cos (2k + 1) \theta, \quad \beta_k = \sin (2k + 1) \theta,$$  \hfill (33)

where θ is an angle that fulfills the relation:

$$\sin(\theta) = \frac{1}{\sqrt{N}}.$$  \hfill (34)

Therefore the coefficients αk, βk are periodic functions of k. After several iterations amplitude of βk rises and others drop. The influence of the marked state |x₀⟩ on the state of the register is that the initial state |s⟩ evolves towards the marked state.

The βk attains its maximum after approximately \(\frac{\pi}{4} \sqrt{N}\) steps. Then it begins to fall. Thus, the number of steps needed to transfer the initial state towards the marked state is of \(O(\sqrt{N})\). In the classical case the number of steps is of \(O(n)\).

e) Measurement: The last step of the Grover’s algorithm is the measurement. Probability of obtaining of the proper result is \(|β_k|^2\).

Fig. 9. The circuit for Grover’s algorithm.

3) Graphical interpretation: There exists very nice graphical interpretation of Grover’s algorithm.

Let |α⟩ denotes the sum of states orthogonal to the state we are searching for |x₀⟩.

$$|α⟩ = \frac{1}{\sqrt{2^n-1}} ∑_{x≠x₀} |x⟩,$$  \hfill (35)

and for consistence we will write \(|β⟩ = |x₀⟩\). Then, on the plane spanned by |α⟩ and |β⟩, we can observe of evolution of the state vector.

By putting values from equation 33 into equation 32 we get following relation:

$$G^k|s⟩ = \cos((2k + 1)θ)|α⟩ + \sin((2k + 1)θ)|β⟩.$$  \hfill (36)

Exemplar behaviour of this equation for 2³ states is presented in Figure 10.

4) Implementation: Listing 4 presents the implementation of function grover. We will apply quantum noise at the end of each Grover iteration and observe its influence on its efficiency.

To simulate this behaviour we will insert the code from Listing 5 after line 21 of the implementation.

10
Fig. 10. Visualisation of Grover’s algorithm. Projection on plane spanned by $|\alpha\rangle$ and $|\beta\rangle$. Vector $|\psi\rangle$ is flat superposition of all the possible states.

Listing 4. Grover’s algorithm in quantum-octave

```octave
# function implementing Grover’s algorithm
# input: number we are looking for, size of the system
# output: probability distribution after execution of the algorithm
function ret = grover(n, S)
    quantum_octave_init();
    # allocate register
    rl = new_register(S);
    # number of elements
    N = 2^length(rl);
    # calculate number of iterations
    k = floor((pi/4)*sqrt(N));
    # prepare the system in flat superposition of base states
    evolve(productgate(h, qureg(rl))); # Grover iterations
    for i = 1:k
        # ask the oracle
        evolve(oracle(n, qureg(rl))); # diffuse
        evolve(diffuse(qureg(rl)));
    endfor
    # return probability distribution of base states
    ret = measurecompbasis();
endfunction
```

Listing 5. Adding noise to Grover’s algorithm

```octave
# function implementing oracle
# input: number to mark, size of the system
# output: gate implementing oracle of the size 2^n
function ret = oracle(n, register)
    l = length(register);
    ret = id(l);
    ret(n+1, n+1) = -1;
endfunction
```

```octave
# function implementing diffusion
# input: register in which implement diffusion
# output: diffusion gate of the size 2^n
function ret = diffuse(register)
    l = length(register);
    ret = circuit(...
        productgate(h, register, 1) ...
    );
endfunction
```

Fig. 11. Influence of depolarizing channel parametrized by single real number $\alpha$ on probability of successful finding of sought element in Grover’s algorithm implemented with 3, 4, 5 and 6 qubits.

VI. SUMMARY

We have introduced an original solution to the problem of simulation of quantum processes. This solution is provided by quantum-octave, a library that is build upon GNU Octave high level programming language, which provides high-level quantum programming structures.

Although strictly speaking, quantum-octave is not a programming language but a library, together with GNU Octave, it is very convenient and flexible tool. Programs written in quantum programming languages, such as QCL, can be easily rewritten using this library, thanks to the use of quantum memory,
registers and routines. Scalable programs can be easily implemented in quantum-octave, so the programmer does not have to think about details of the implementation.

ACKNOWLEDGEMENTS

We acknowledge the financial support by the Polish Ministry of Science and Higher Education under the grant number N519 012 31/1957 and by the Polish research network LFPII. The numerical calculations presented in this work were performed on the Leming server of The Institute of Theoretical and Applied Informatics of the Polish Academy of Sciences.

Package quantum-octave is distributed as free software and it can be downloaded from the project web-page \cite{quantum-octave}.

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