A Multiprecision Matrix Calculation Library and Its Extension Library for a Matrix-Product-State Simulation of Quantum Computing

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Abstract

A C++ library, named ZKCM, has been developed for the purpose of multiprecision matrix calculations, which is based on the GNU MP and MPFR libraries. It is especially convenient for writing programs involving tensor-product operations, tracing-out operations, and singular-value decompositions. Its extension library, ZKCMQC, for simulating quantum computing has been developed using the time-dependent matrix-product-state simulation method. This report gives a brief introduction to the libraries with sample programs.

Keywords: Multiprecision simulation library, Time-dependent matrix product state, Quantum computing

1 Introduction

Accuracy of simulation is often of serious concern when small differences in matrix elements result in physically important phenomena of one’s interest. There are several programming libraries, e.g., Refs. [1, 2, 3, 4], useful for high-precision computing for this purpose. Among them, the library named ZKCM library [5], which I have been developing, is a C++ library for multiprecision complex-number matrix calculations. It provides several functionalities including singular value decomposition, tensor product calculation, and tracing-out operations. It is based on the GNU MP (GMP) [6] and MPFR [7] libraries, which are commonly included in recent distributions of UNIX-like systems.

There is an extension library named ZKCMQC. This library is designed for simulating quantum computing [8, 9]. It uses a matrix product state (MPS) [10, 11] to represent a pure quantum state. The MPS method is recently one of the standard methods for simulation-physics software [12]. As for other methods effective for simulating quantum computing, see, e.g., Refs. [13, 14]. With ZKCMQC, one may use quantum gates in U(2), U(4), and U(8) as elementary gates. Indeed, in general, quantum gates in U(2) and U(4) are enough for universal quantum computing, but we regard quantum gates in U(8) also as elementary gates so as to reduce computational overheads.

A simulation of quantum computing with MPS is known for its computational efficiency in case the Schmidt ranks are kept small during the simulation [11, 15]. Even for the case slightly large Schmidt ranks are involved, it is not as expensive as a simple simulation. This is obvious from the theory which is briefly explained in Sec. 3.1.

This contribution is intended to provide a useful introduction for programming with the libraries. Section 2 describes an example of simulating an NMR spectrum in a simple model using the ZKCM library. Section 3 shows an overview of the theory of the MPS method and an example of simulating a simple quantum circuit using the ZKCMQC library. Effectiveness of the use of the libraries manifested by the examples are summarized in Sec. 4.

2 ZKCM Library

The ZKCM library is designed for general-purpose matrix calculations. This section concentrates on its main library. It consists of two major C++ classes: zkcm_class and zkcm_matrix. The former class is a class of a complex number. Many operators like “+” and functions like trigonometric functions are defined for the class. The latter class is a class of a complex number. Standard operations and functions like matrix inversion are defined. In addition, the singular-value decomposition of a general matrix, the diagonalization of an Hermitian matrix, discrete Fourier transformation, etc., are defined for the class. A detailed document is placed in the “doc” directory of the package of ZKCM. We will next look at a simple example to demonstrate the programming style using the library.

2.1 Program example

Here, a sample program “NMR_spectrum_simulation.cpp” found in the “samples” directory of the package of ZKCM is explained. This program generates a simulated FID spectrum of liquid-state NMR for the spin system consisting of a proton spin with precession frequency \( w_1 = 400 \) MHz (variable \( w_1 \) in the program) and a \( ^{13}\text{C} \) spin with
precession frequency \( w_2 = 125 \text{ MHz} \) (variable \( w_2 \)) at room temperature (300 K) (variable \( T \)). A J coupling constant \( J_{12} = 140 \text{ kHz} \) (variable \( J_{12} \)) is considered for the spins.

The first line of the program is to include a header file of ZKCM:

```cpp
#include "zkcm.hpp"
```

```cpp
int main(int argc, char *argv[])
{

In the main function, the internal precision is set to 280 bits for floating-point computation by

```cpp
zkcm_set_default_prec(280);
```

In the subsequent lines, Pauli matrices \( I, X, Y, Z \) are generated. For example, \( Y \) is generated as

```cpp
zkcm_matrix Y(2,2);
Y.set(zkcm_class(0.0,-1.0),0,1);
Y.set(zkcm_class(0.0,1.0),1,0);
```

Similarly, the \( Y_{90} \) pulse is generated as

```cpp
Yhpi.set(sqrt(zkcm_class(0.5)),0,0);
Yhpi.set(sqrt(zkcm_class(0.5)),0,1);
Yhpi.set(-sqrt(zkcm_class(0.5)),1,0);
Yhpi.set(sqrt(zkcm_class(0.5)),1,1);
```

Other matrices are generated by similar lines. After this, values of constants and parameters are set. For example, the Boltzmann constant \( k_B \) \([\text{J/K}]\) is generated as

```cpp
zkcm_class kB("1.3806504e-23");
```

(Several lines are omitted in this explanation.) The Hamiltonian \( H \) in the type of \( \text{zkcm\_matrix} \) is made as

```cpp
H = w1 * tensorprod(Z,I) + w2 * tensorprod(I,Z) + J12 * tensorprod(Z,Z);
```

This is used to generate a thermal state \( \rho \):

```cpp
zkcm_matrix rho(4,4);
rho = exp_H((-hplanck/kB/T) * H);
rho /= trace(rho);
```

Here, \( \exp_H \) is a function to calculate the exponential of a Hermitian matrix and \( \text{hplanck} \) is the Planck constant \((6.62606896 \times 10^{-34} \text{ Js})\). The sampling time interval \( dt \) to record the value of \( < X > \) for the proton spin is set to \( 0.145/w_1 \) (any number sufficiently smaller than 1/2 might be fine instead of 0.145) by

```cpp
zkcm_class dt(zkcm_class("0.145")/w1);
```

The number of data to record is then decided as

```cpp
int N = UNP2(1.0/dt/J12);
```

Here, function UNP2 returns the integer upper nearest power of 2 for a given number. Now arrays to store data are prepared as row vectors.

```cpp
zkcm_matrix array(1,N), array2(1,N);
```

The following lines prepare the \( X, Y \), and \( Y_{90} \)-pulse operators acting only on the proton spin.

```cpp
zkcm_matrix X1(4,4), Y1(4,4), Yhpi1(4,4);
X1 = tensorprod(X, I);
Y1 = tensorprod(Y, I);
Yhpi1 = tensorprod(Yhpi, I);
```

To get an FID data, we firstly tilt the proton spin by the ideal pulse.

```cpp
rho = Yhpi1 * rho * adjoint(Yhpi1);
```

Now the data of time evolution of \( < X > \) of the proton spin under the Hamiltonian \( H \) is recorded for the time duration \( N \times dt \) using

```cpp
array = rec_evol(rho, H, X1, dt, N);
```

We now use a zero-padding for this “array” so as to enhance the resolution. This will extend the array by \( N \) zeros.

```cpp
array2 = zero_padding(array, 2*N);
```

To obtain a spectrum, the discrete Fourier transformation is applied.

```cpp
array2 = abs(DFT(array2));
```

The “array2” is output to the file “examplezp.fid” as an FID data with \( df = 1/(2 \times 2N \times dt) \) as the frequency interval, in the Gnuplot style by

```cpp
GP_1D_print(array2, 1.0/dt/zkcm_class(2*N*2), 1, "examplezp.fid");
```

At last, the function “main” ends with \text{return 0;}. The program is compiled and executed in a standard way.\(^1\)

The result stored in “examplezp.fid” is visualized by Gnuplot as shown in Fig. 1.

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\(^1\)To make an executable file, the library flags typically \("-lzkcmlm-lmpfr-lgmp-lgmpxx" \) are probably required. As for ZKCM\_QC, additionally \("-lzkcmlm\_qc" \) should be specified.
the normalized deviation density matrix $-H/\text{const}$. This approximation is commonly used [17] but it cannot be used for simulations for low temperature. An advantage of using ZKCM for simulating NMR spectra is that the temperature can be chosen. This is possible because of high accuracy in computing the exponential of a Hamiltonian.

3 ZKCM_QC library

The ZKCM_QC library is an extension of the ZKCM library. It has several classes to handle tensor data useful for the time-dependent MPS simulation of a quantum circuit. Among the classes, the “mps” class and the “tensor2” class will be used by user-side programs. The former class conceals the complicated MPS simulation process and enables writing programs in a simple manner. The latter class is used to represent two-dimensional tensors which are often simply regarded as matrices. A quantum state during an MPS simulation is obtained as a (reduced) density matrix simply regarded as matrices. A quantum state during an MPS simulation process can be concealed by the use of ZKCM.

More details of the classes are explained in the document placed at the “doc” directory of the ZKCM_QC package.

We briefly overview the theory of the MPS simulation before introducing a program example since understanding the behavior of a library leads to a better programming in general.

3.1 Brief overview of the theory of time-dependent MPS simulation

Consider an $n$-qubit pure quantum state

$$|\Psi\rangle = \sum_{i_0 \cdots i_{n-1} = 0 \cdots 0}^{1 \cdots 1} c_{i_0 \cdots i_{n-1}} |i_0 \cdots i_{n-1}\rangle$$

with $\sum_{i_0 \cdots i_{n-1}} |c_{i_0 \cdots i_{n-1}}|^2 = 1$. If we keep this state as data as it is, updating the data for each time of unitary time evolution spends $O(2^{2n})$ floating-point operations. To avoid such an exhaustive calculation, in the matrix-product-state method, the data is stored as a kind of compressed data. The state can be represented in the form

$$|\Psi\rangle = \sum_{i_0 = 0}^{1} \cdots \sum_{i_{n-1} = 0}^{1} \left[ \sum_{v_0 = 0}^{m_0-1} \sum_{v_1 = 0}^{m_1-1} \cdots \sum_{v_{n-2} = 0}^{m_{n-2}-1} Q_0(i_0, v_0)|v_0 \rangle \langle 0|Q_1(i_1, v_1, v_0) |v_1 \rangle \langle v_0| \cdots \right. \left. \cdots \right. \left. \cdots \right. \left. V_{n-2}(v_{n-2}, Q_{n-1}(i_{n-1}, v_{n-2}) |v_{n-2} \rangle \langle i_{n-2}| \right] |i_0 \cdots i_{n-1}\rangle, \quad (1)$$

where we use tensors $Q_s(i_s, v_{s-1}, v_s)$ with parameters $i_s, v_{s-1}, v_s$ ($v_{-1}$ and $v_{n-1}$ are excluded) and $V_s$ with parameter $v_s$; $m_s$ is a suitable number of values assigned to $v_s$ with which the state is represented precisely or well approximated. This form is one of the forms of matrix product states (MPSSs). The data are compressed to tensor elements. We can see that neighboring tensors are correlated to each other; the data compression is owing to this structure.

Let us explain a little more details: $Q_s(i_s, v_{s-1}, v_s)$ is a tensor with $2 \times m_{s-1} \times m_s$ elements; $V_s(v_s)$ is a tensor in which the Schmidt coefficients for the splitting between the $s$th site and the $(s+1)$th site (i.e., the positive square roots of non-zero eigenvalues of the reduced density operator of qubits $0, \ldots, s$) are stored. This implies that, by using $V_s$ and eigenvectors $(\Phi_{v_s}^0, \Phi_{v_s}^1, \ldots, \Phi_{v_s}^{m_s-1})$ of the reduced density operator $\rho^{0:s}((s+1: \ldots, n-1)$ of qubits $0, \ldots, s$ ($s+1, \ldots, n$), the state can also be written in the form of Schmidt decomposition

$$|\Psi\rangle = \sum_{v_s = 0}^{m_s-1} V_s(v_s)|\Phi_{v_s}^0\rangle |\Phi_{v_s}^{1\ldots n-1}\rangle.$$ \quad (2)

In an MPS simulation, very small coefficients and corresponding eigenvectors are truncated out unlike a usual Schmidt decomposition.

The advantage to use the MPS form is that we have only to handle a small number of tensors when we simulate a time evolution under a single quantum gate. For example, when we apply a unitary operation $U$ acting on, say, qubits $s$ and $s+1$, we have only to update the tensors $Q_s(i_s, v_{s-1}, v_s)$, $V_s(v_s)$, and $Q_{s+1}(i_{s+1}, v_s, v_{s+1})$. For the details of how tensors are updated, see Refs. [11, 16]. The simulation of a single quantum gate $U$ spends $O(m_{\text{max}}^3)$ floating-point operations where $m_{\text{max}}$ is the largest value of $m_s$ among the sites $s$. (Usually, unitary operations are $U(2)$ and those in $U(4)$ are regarded as elementary quantum gates.) A quantum circuit constructed by using at most $g$ single-qubit and/or two-qubit quantum gates can be simulated within the cost of $O(gnm_{\text{max}}^3)$ floating-point operations, where $n$ is the number of wires and $m_{\text{max}}$ is the largest value of $m_s$ over all time steps.

The computational complexity may be slightly different for each software using MPS. In the ZKCM_QC library, we have functions to apply quantum gates $U(8)$ to three chosen qubits. Internally, three-qubit gates are handled as elementary gates. This makes the complexity a little larger. A simulation using the library spends $O(gnm_{\text{max}}^3)$ floating-point operations, where $g$ is the number of single-qubit, two-qubit, and/or three-qubit gates used for constructing a quantum circuit.

The MPS simulation process, which is in fact often complicated, can be concealed by the use of ZKCM_QC. One may write a program for quantum circuit simulation in an intuitive manner. Here is a very simple example.

3.2 Program example

The following program is placed at the “samples” directory of the ZKCM_QC package. It utilizes several matrices declared in the namespace “tensor2tools” (see the document for details on this namespace).

```
#include "zkcm_qc.hpp"
```
```c
int main (int argc, char *argv[])
{
    //Use the 256-bit float for internal computation.
    zkcm_set_default_prec(256);
    //Num. of digits for each output is set to 8.
    zkcm_set_output_nd(8);

    //First, we make an MPS representing |000⟩.
    mps M(3);
    std::cout << "The initial state is " << std::endl;
    //Print the reduced density operator of the block
    //of qubits from 0 to 2, namely, 0,1,2, using the
    //binary number representation for basis vectors.
    tensor2tools::showb(M.RDO_block(0,2));

    std::cout << "Now we apply H to the 0th qubit.";
    //by the constant mps::TA.
    int array[] = {0, 2, mps::TA};
    std::cout << "At this point, the reduced density matrix of the qubits 0 and 2 is " << std::endl;
    tensor2tools::showb(M.RDD(array));

    return 0;
}
```

The output of the program is as follows.

```
[user@localhost samples]$ ./qc_simple_example
The initial state is
1.0000000e+00|000><000|
Now we apply H to the 0th qubit.
Now we apply CNOT to the qubits 0 and 2.
At this point, the reduced density matrix of
the qubits 0 and 2 is
5.0000000e-01|00><00|+5.0000000e-01|00><11|+5.0000000e-01|11><00|+5.0000000e-01|11><11|
```

4 Summary

In this report, a C++ library ZKCM for multiprecision complex-number matrix calculation has been introduced. It reduces the cost of writing elaborate programs especially in case a small deviation is of main concern, which is often the case for time-dependent physical models. An extension library ZKCM_QC has also been introduced, which is a library for an MPS simulation of quantum circuits. It is designed to enable an intuitive coding manner to simulate quantum circuits.

Software information

ZKCM and ZKCM_QC libraries are open-source C++ libraries. The files and documents can be downloaded from the URL shown as Ref. [5]. ZKCM version 0.0.9 and ZKCM_QC version 0.0.1 on the Fedora 15 64-bit operating system with GMP version 4.3.2 and MPFR version 3.0.0 have been used for this report.

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