Optimization for quantum computer simulation

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Introduction

Quantum circuits, or quantum logic gates, are studied extensively in these decades. Quantum computers have appeared, such as, IBM Q. Useful because it is still limited to obtain large resources of real quantum computer. braket [4], a software and a C++ template library to simulate quantum computers. Propose optimization techniques, a page method and a simple rule of initial permutation of qubits. Report performance of our simulations in the K computer up to 45 qubits.

Using double precision floating point number. Requires 0.5 PB at most.

Quantum gates

A state vector $|\psi\rangle$ is described with $2^N$ complex coefficients $a(n)$.

$$|\psi\rangle = \sum_{n=0}^{2^N-1} a(n) |n\rangle,$$

where $|n\rangle = |n_0\rangle \otimes \cdots \otimes |n_l\rangle$, $n_0 = n_0 \cdots n_l$, and $n_l \in \{0,1\}$.

Quantum gates $\otimes$ unitary operators on $|\psi\rangle$.

Ex.) Hadamard gate $|\psi\rangle = 1/\sqrt{2} (|0\rangle + |1\rangle)$ and controlled phase-shift gate $|\psi\rangle = \alpha |0\rangle \otimes |0\rangle + \beta |1\rangle \otimes |1\rangle$.

$H(a(0)|0\rangle + a(1)|1\rangle) = a(0)|0\rangle - a(1)|1\rangle$.

$$R(\pi/2^n) = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/2^n} \end{pmatrix},$$

$$R(\pi) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$ (3)

Easily parallelized by using OpenMP or any other multithreading libraries.

Permutation of qubits [1, 2]

MPI parallelization is required because we need $2^{N+4}$ bits to keep $a(n)$.

Divide $N$ bits to $M$ global bits and $L = N - M$ local bits:

$$|n\rangle = |n_0\rangle \cdots |n_{M-1}\rangle |n_{M} \cdots n_{N-1}\rangle.$$ (4)

Global bits $\leftrightarrow$ MPI rank $n_0 \cdots n_{M-1}$.

Swap data by using MPI_Sendrecv when operating a global qubit $a(0)$.

$$a(0) \rightarrow a(1) \rightarrow a(0) \cdots a(1) \rightarrow a(0) \cdots a(1) \cdots a(0).$$ (5)

Note that $M = 1$ is assumed in this example.

References


Initial permutation of qubits

Initial permutation of qubits is important to decrease data transfers.

Ex.) Quantum adder of two registers $a_2 a_1 a_0 \rightarrow b_2 b_1 b_0$.

6 data transfers for $(m_0 m_1 m_2 m_3)$. 26 data transfers for $(n_0 n_1 n_2 n_3 n_4 n_5 n_6 n_7 n_8 n_9 n_{10} n_{11} n_{12} n_{13} n_{14} n_{15})$.

Propose a simple method:

Sort by ascending order of the number of gates operating on each qubit.

Ex.) $(m_0 m_1 m_2 m_3)$ for quantum adder $a_2 a_1 a_0 \rightarrow b_2 b_1 b_0$. The proposed method works very well.

Transfer cost

Transfer cost: the number of pages to be transferred in each quantum gate operation.

2 if one global qubit and one local qubit are swapped.

4 if two global qubits and two local qubits are swapped.

Brute-force calculations of transfer costs for quantum adder of two registers.

Transfer costs for the proposed method are much smaller than the averaged ones and close to the best ones in the case of the large number of local qubits $L$.

The proposed method works very well.

Optimized Circuits

Quantum adder of two registers. $|\psi\rangle = |0\rangle |1\rangle |0\rangle |1\rangle |0\rangle |1\rangle |0\rangle |1\rangle |0\rangle |1\rangle |0\rangle |1\rangle |0\rangle |1\rangle |0\rangle |1\rangle |0\rangle |1\rangle |0\rangle |1\rangle |0\rangle |1\rangle |0\rangle |1\rangle |0\rangle |1\rangle |0\rangle |1\rangle |0\rangle |1\rangle |0\rangle |1\rangle $.

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Figure: The elapsed time of simulation of quantum circuits,

(a) the Hadamard gates and (b) the quantum adder (2, 3, and 5 registers). (c) The elapsed time of simulation of the quantum adder for gate operation as a function of the number of qubits.

Elapsed time of simulations

Initial permutation of qubits

Elapsed time of simulations of the quantum adder.

(a) Weak scaling

Solid lines: proposed method

Empty dotted lines: results of initial permutation as a reverse of identity permutation such as $(m_0 m_1 m_2 m_3)$.

(b) Weak scaling

Improved if the number of registers is large.

(c) Strong scaling for two registers simulations and for three registers simulations

Solid lines: proposed method

Empty dotted lines: results of random initial permutation averaged over 100 samples.

Page method

Memory throughput: 64 GB/sec $\Rightarrow$ 0.06-0.09 sec. for each gate operation.

Figure: The elapsed time of simulation of the Hadamard gates.

(a) and (b) decrease intranode data transfer (see left figs.)

$|\psi\rangle = (|0\rangle + |1\rangle) |0\rangle |1\rangle |0\rangle |1\rangle |0\rangle |1\rangle |0\rangle |1\rangle |0\rangle |1\rangle |0\rangle |1\rangle |0\rangle |1\rangle |0\rangle |1\rangle |0\rangle |1\rangle |0\rangle |1\rangle |0\rangle |1\rangle |0\rangle |1\rangle |0\rangle |1\rangle |0\rangle |1\rangle |0\rangle |1\rangle $.

(b) $t_0 \approx t_{intra}$ per gate operation.

Summary

Develop a simulator of quantum computer [4] and test on the K computer.

Simulations of the Hadamard gates and quantum adder up to 45 qubits.

Page method,

Works well if the patterns of MPI intercommunications are irregular.

Initial permutation of qubits.

Proposed simple method works very well.

Future plans

Automatic search of the faster initial permutation by using genetic algorithm.

Reduction of data transfers for some quantum gates represented by diagonal matrices.

Support GPU/FPGA computing.