Acceleration of Classical Simulation of Hamiltonian Dynamics by Simultaneous Diagonalization with Clifford Transformation

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Recently, the controlled quantum dynamics of a wide range of physical systems has become experimentally accessible. For quantum simulation, Hamiltonian dynamics of many-body quantum systems exhibits non-trivial phenomena such as many-body localization, scrambling, and discrete time crystal. For quantum computing, Hamiltonian dynamics takes an important rule in quantum algorithms such as quantum phase estimation and adiabatic quantum computing. Classical simulation of them is vital to numerically verify these phenomena or the performance of quantum algorithms prior to the experiments. However, classical simulation of quantum many-body dynamics is hard in general, because of the exponentially increasing dimensions of the quantum systems. For a system with over 25 qubits an exact diagonalization would be intractable if there is no symmetry to reduce the dimensions. Without the exact diagonalization, we have to update the state vector step by step with Trotter decomposition of the Hamiltonian dynamics, which increases the number of operations substantially. The amount of memory required to store the state vector exponentially increases in the number of qubits. Such a massive memory access makes a reliable classical simulation of quantum dynamics over 25 qubits challenging.

In this work, we propose a method to reduce a computational complexity and memory accesses to accelerate classical simulation of Hamiltonian dynamics using GPU (graphics processing unit). Specifically, we assume a Hamiltonian is written as a sum of Pauli products. We partition the terms in a Hamiltonian into mutually commuting groups, i.e., each group forms a stabilizer group. The same technique is also employed to reduce the number of measurements in variational quantum eigensolver [3]. Then, the mutually commuting terms are made diagonal, that is products of Pauli Z operators, by a Clifford transformation. To find such a Clifford transformation, we use an efficient representation of the stabilizer operators with a binary tableau [1], where an n-qubit Pauli operator is represented as $2n+1$ bit binary valuable, for example $XYZI \to [1100|0110|0]$. Recently, in Ref. [2], the authors use the binary tableau to reduce the circuit complexity of digital quantum simulations. However, this optimization is intended to reducing CNOT counts on a quantum circuit implemented on a quantum computer. Here we use a similar method to reduce the number of the memory access to accelerate classical simulation of Hamiltonian dynamics.

We consider each term in a Hamiltonian as a vertex and construct a graph, where if two terms are mutually commuting, corresponding two vertices are connected by an edge. Then, partitioning the Hamiltonian into mutually commuting terms is equivalent to find cliques in the corresponding graph. We find a large clique, i.e., a large group of commuting terms, by a greedy strategy. Then the commuting terms are diagonalized by using a sequence of H-CNOT-CZ-S-H gates, where H, CNOT, CZ, and S indicate the Hadamard, controlled-NOT, controlled-Z, and phase gates, respectively. While the Clifford transformation is inserted additionally, the diagonalized rotations can be implemented with a single update of the state vector, which reduces the total number of memory accesses substantially. Regarding the Clifford transformation, we provide the fast implementation of multiple S, CNOT, and CZ gates.

We perform numerical experiments for Hamiltonian dynamics of the fully connected transverse Ising model and Majorana fermions with the SYK model. In this simulation, we use one of the fastest simulator "qulacs"[4] as a baseline. We further implement an efficient implementation of updating a quantum state by Clifford transformations and diagonal operations. It is confirmed that the execution time of simulation with our method is about 10 times faster than that without the diagonalization on both CPU and GPU. For example, the simulating 100 trotter steps of the fully connected transverse Ising model with 30 qubits, which has 465 terms, can be executed in 55 minutes by CPU and 4.2 minutes by GPU, while a naive implementation of Hamiltonian dynamics using qulacs takes 7.9 hours on CPU. Since the Ising dynamics has been frequently employed in quantum algorithms such as quantum approximation optimization algorithm [6] and quantum machine learning [5, 7], and quantum annealing [8], this acceleration would helpful to analyse and improve the performance of quantum algorithms on the near-term quantum computers.

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