Title: Towards scalable quantum simulation

Abstract:

Quantum Computing is a new topic in computer engineering and aims to solve complex problems in a small fraction of the time it would take on a classical computer. Quantum is based on quantum bits or qubits, and it is still far from a reliable physical implementation. Nevertheless, quantum computations can be simulated with the aim of studying algorithms that will be able to run on quantum computers. Due to the huge amount of memory required to store the information of the possible states of the qubits, the only possible approach to simulate a reasonable-sized quantum circuit is recurring to a distributed and parallel approach.

The mathematical representation of quantum operations is expressed as tensor operations, that result in matrix representations of the quantum gates and matrix operations to compute their outputs. There is some open-source matrix-based simulators, but such approach suffers mainly of high memory consumption, limiting the number of gates that can be used in a simulation.

Another approach, followed in this work, is the state-based method of simulating qubits, using arithmetic operations, which reduces exponentially the memory usage compared to the matrix-based simulation. Even though, a simulation with 34 qubits requires 500GB to 1TB of total system memory, and the target in this research, is to be able to simulate circuits with up to 50 qubits.

This limitation can be overcome with a parallel machine by distributing the data structure of the state representation among different machines and processes, and the use of MPI. The experiments with the current version of the distributed data structure were successful, and they were run in the Juelich HPC center. Using its high count of available system memory, we were able to test the limits of our implementation and find the current limitations that impedes us to simulate a larger number of qubits.

The current state of our work is in overcoming the memory addressing limitations. Currently, the main obstacle is in tracking the position of the distributed quantum states across the various machines executing the simulator. The values to address such positions are exceeding the maximum value representable in an integer in C++ (uint64_t) when simulating a larger number of qubits. This limitation can only be found when simulating 34 qubits.

We are considering and analyzing several solutions to solve the addressing problem, in order to overcome the 64-bit address limitation. Functions to map addresses to processes are under development and testing.

The results of the work will allow to further advance in the study of quantum algorithms that require much more qubits than current simulators can support.