QUANTUM CHEMISTRY CALCULATIONS WITH QUNATUM COMPUTER PERFORMANCE STUDY

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In photosynthesis the energy of light is being absorbed by the LH2 complexes where bacteria-chlorophyll and carotenoid systems are responsible for this phenomena. β-Carotene molecule is the typical model used for researching carotenoid properties, which systems contains polyene chains [1, 2]. Thus, various quantum chemistry methods are required in order to model carotenoids. All carotenoid molecule calculations are very long and complex even for modern HPC (supercomputers). Quantum computers are expected to have a breakthrough in this field but its possibilities are not yet understood. There is a possibility to access the IBM quantum computers and various quantum computer simulators. The simulators can be run on supercomputers which creates a good development environment for quantum type algorithms. The new breakthrough is expected in Couple Cluster (CC) class quantum chemistry calculation where the problem complexity grows exponentially when increasing molecular calculation size. CC methods are based on Hartree-Fock (HF) calculations. Specialized calculation libraries, such as "Qiskit Aqua Chemistry" are being developed for the IBM quantum computer and the quantum simulators [3]. There are already demonstrated quantum algorithm applications for the small molecules [4]. The library use mixed calculations by combining quantum algorithms with well know packages such as PSI4, PySCF, PyQuante, which are based on objective oriented Python programming.

In order to perform quantum computer simulations it is necessary to have the needed Python libraries and supercomputing facilities. The one used is the "HPC Saulėtekis" supercomputer Fizika2000 (www.supercomputing.ff.vu.lt). The results must be compared with the traditional computing algorithms which are in the PySCF package. The main research object is the β-Carotene molecule and different length polyene chains. However, in order to perform such task there is a need to do quantum computing simulator performance study with various qubits and its parameters. Thus the primary molecule was used H_2 molecule for initial performance analysis.

There were successfully installed Qiskit aqua chemistry libraries and the PySCF package into supercomputer "Fizika 2000". The ground state energy of the H_2 molecule was calculated with the quantum simulators using two different algorithms: Quantum Phase Estimation (QPE) and Variational Quantum Eigensolver (VQE). The QPE algorithm has a limited number of the changeable parameters, but enough for it to be sophisticated. The changed variable parameters were ancillary qubits (*num_ancillae*), the number of time slices (*num_time_slices)* and expansion mode (*expansion_mode*). There were several hundred runs of various modifications of the H_2 molecule ground state energy problem changing all the available parameters in order to find the optimal energy value and the execution time we have sorted out the results (see some examples in Table 1).

Table 1. Example of H_2 problem results (expansion mode: suzuki, number of time slices: 50, variable: ancillary qubits)

num	time, s	Energy, Hartrees
1	4.890022755	-1.320490405
2	6.591337919	-1.320490405
3	8.608515263	-0.810375555
4	11.24328351	-1.320490405
5	13.53698087	-1.192961693
6	16.06198859	-1.129197336
7	18.35524225	-1.129197336
8	20.9236033	-1.097315158
9	23.63072705	-1.15310897
10	28.32836843	-1.11724152
11	31.93432903	1.133182609
12	38.39482903	-1.134178927

The QPE algorithm give out randomized results no matter how the parameters are changed. The VQE algorithm has more added variable parameters which is essential to our work in finding out the optimal parameters to run the problem with consistent results. The VQE algorithm is better predictable and comparable with classical algorithms.

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