# Reviewer's report on the minimal thesis of MSc. Yury Chernyak

**Title**: *Resource Efficient Non-Gradient Optimization Methods for Variational Quantum Eigensolvers*
**Author**: MSc. Yury Chernyak
**Supervisor**: Doc. RNDr. Martin Plesch, PhD.
**Reviewer**: Mgr. Martin Friák, Ph.D.

The minimal thesis of MSc. Yury Chernyak is very well written (in English) and has numerous neatly prepared figures and illustrations. The thesis consists of 6 chapters, followed by LiH Hamiltonian and the list of 27 literature sources (the total length is 74 numbered pages).

The thesis focuses on (i) performance testing of several optimization methods used in hybrid quantum-classical computational approaches as well as (ii) the development of new methods. This is a very timely topic that deserves much attention due to the growing number of applications of quantum computers, e.g. in computational chemistry, which is represented in the current thesis by calculations of lithium hydride. However, this is also a very challenging topic due to the interdisciplinary nature of computational quantum informatics.

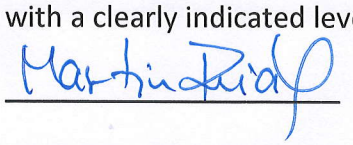
The author summarizes several mathematical (linear-algebra) prerequisites in the first chapter, then follows by explaining the variational quantum eigensolver (VQE) methods in the second chapter and continues with the description of the particle swarm optimization (PSO) gradient-free method in the third chapter. Most importantly, a new and improved PSO method called Harmonic-Oscillator PSO (abbreviated as HOPSO), the development of which the author of the thesis has significantly contributed into, is introduced in the fourth chapter. The fifth chapter then contains results of an extensive performance testing of the PSO and the new HOPSO method in comparison with (i) one classical local gradient-free method (Constrained Optimization by Linear Approximation - COBYLA) and (ii) one global gradient-free method (Differential Evolution - DE). The last (sixth) chapter contains conclusions and outlook.

The thesis aims to compare the performance of the newly developed HOPSO method with other gradient-free methods. The testing was performed for several analytic functions as well as the quantum-computer calculations of the ground-state energy of lithium hydride. The author has achieved a wealth of very interesting results that warrant future publication(s) in impact-factor journal(s).

**Final evaluation: passed**

**(in Czech, *Celkové hodnocení práce: prospěl*).**

My question for the student: can the figures with results on pages 46 – 58 be presented with a logarithmic vertical scale (in order to see the box plots that collapsed into a single line) and with a clearly indicated level of the searched minimum (e.g., by a horizontal red line)?



Mgr. Martin Friák, Ph.D.

In Brno on the 12th of September 2024