Vilnius
University

Variational quantum eigensolver algorithm performance analysis on various molecules

Naglis Šuliokas

Supervisor: doc. dr. Linas Petkevičius

Reviewer: lect. Irus Grinius

Vilnius University

Table of contents

Vilnius University

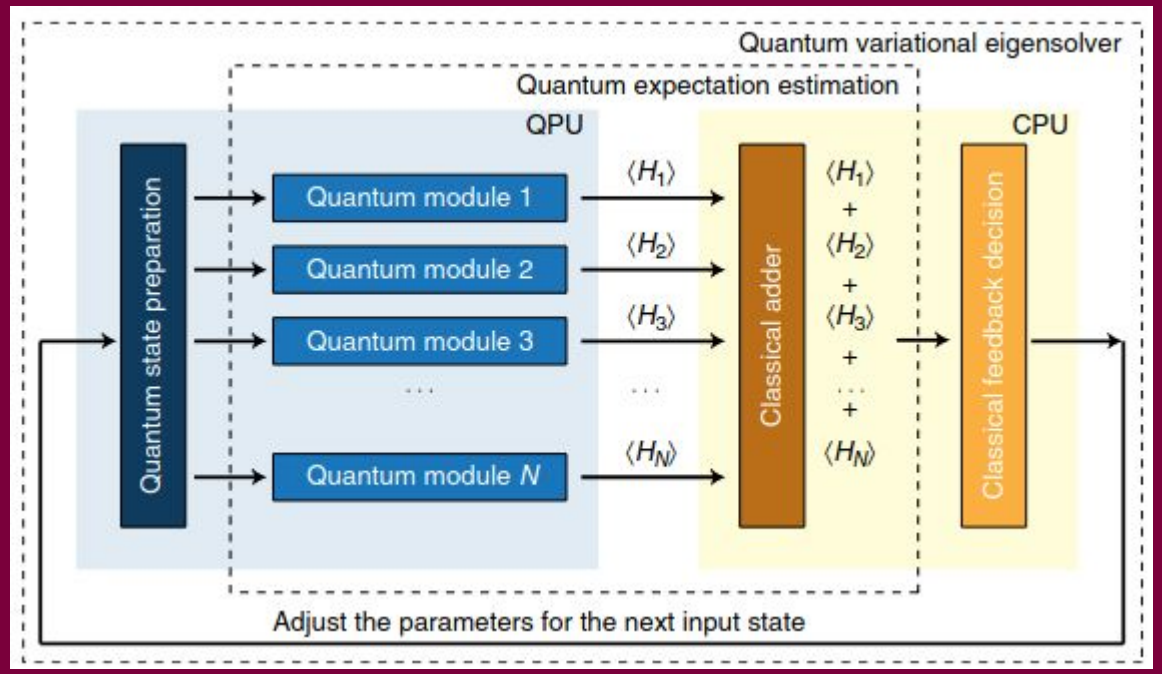
Introduction I

- Quantum computing and NISQ era.
- **Object of the study**:

  Variational quantum eigensolver (Peruzzo et al., 2014).
- **Significance**:

  Material science, medicine.

$$C(\boldsymbol{\theta}) = \langle \psi(\boldsymbol{\theta}) | \hat{H}_{qubit} | \psi(\boldsymbol{\theta}) \rangle$$



Vilnius University

Molecule data H_2

'H .0 .0 .0; H .0 .0 0.735'

Electronic Hamiltonian $\hat{H}_{el}$

$$\hat{H}_{el} = 0.337a_0^\dagger a_0^\dagger a_0 a_0 + 0.332a_0^\dagger a_1^\dagger a_1 a_0 + 0.337a_0^\dagger a_2^\dagger a_2 a_0 + \dots$$

Qubit Hamiltonian $\hat{H}_{\text{qubit}}$

$$\begin{aligned}\hat{H}_{\text{qubit}} = & -1.05237325 \cdot I \otimes I \\ & + 0.39793742 \cdot I \otimes Z \\ & - 0.39793742 \cdot Z \otimes I \\ & - 0.0112801 \cdot Z \otimes Z \\ & + 0.1809312 \cdot X \otimes X\end{aligned}$$

Ansatz $U(\boldsymbol{\theta})$

$$U(\boldsymbol{\theta}) = e^{-i\theta_2(X\otimes Y + Y\otimes X)} \cdot e^{-i\theta_1 Y\otimes I} \cdot e^{-i\theta_0 I\otimes Y}$$

$|\phi_0\rangle = |\phi_{HF}\rangle = |10\rangle$

Ansatz $U(\boldsymbol{\theta})$

$|\psi_n\rangle = U(\boldsymbol{\theta_n})|10\rangle$

$\langle\psi_n|\hat{H}_{qubit}|\psi_n\rangle$

Classical optimizer

$\boldsymbol{\theta_n} \rightarrow \boldsymbol{\theta_{n+1}}$

$$E(\boldsymbol{\theta^*}) = \langle 10|U^\dagger(\boldsymbol{\theta^*})\hat{H}_{qubit}U(\boldsymbol{\theta^*})|10\rangle \approx E_{min}$$

Vilnius University

Introduction II

- **Problem:** finding the ground state energy (many new VQE improvements, few analysis data, tedious implementation).
- **Aim:** analyze, find best VQE method, determine computational limits.
- **Objectives:**
  - literature analysis (Hamiltonian mappings, ansätze, optimizers),
  - benchmarks on simulator and real hardware with H_2, LiH, BeH_2,
  - determine limitations,
  - compare with literature.

Vilnius University

Methodology

- **Devices:** Aer simulator, Madness simulator, ibm_brisbane hardware (127 qubits).
- **Analysis:**
  - Hamiltonian mapping - maximum Pauli weight, depending on qubit count,
  - ansatz - VQE convergence, accuracy,
  - optimizer - accuracy

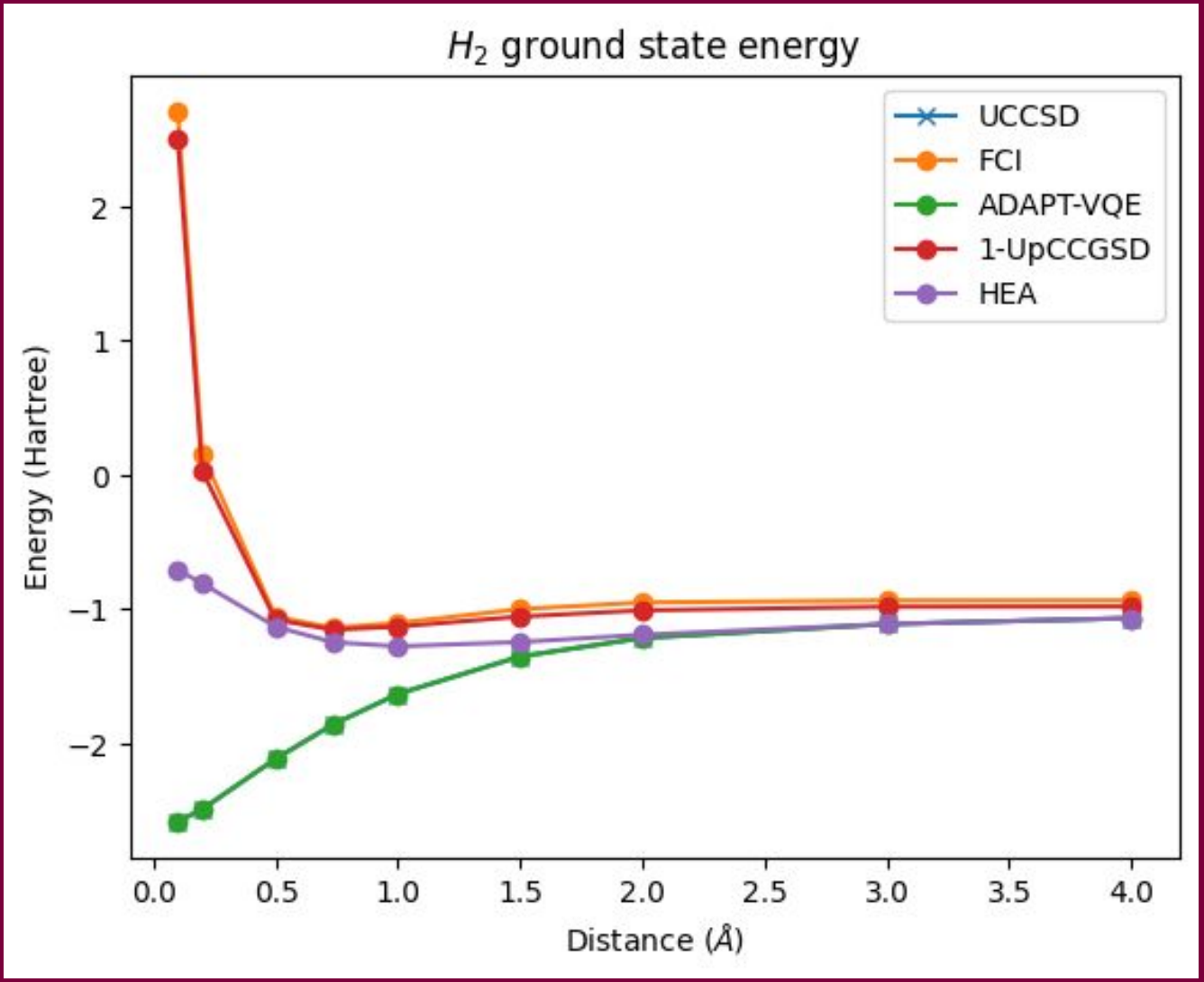
Vilnius University

Experiment structure

- **Hamiltonian mapping**:
  - Jordan-Wigner, Bravyi-Kitaev, parity.
- **Ansatz and VQE variations**:
  - UCCSD, k-UpCCGSD, ADAPT-VQE.
- **Optimizer**:
  - L-BFGS-B, COBYLA.

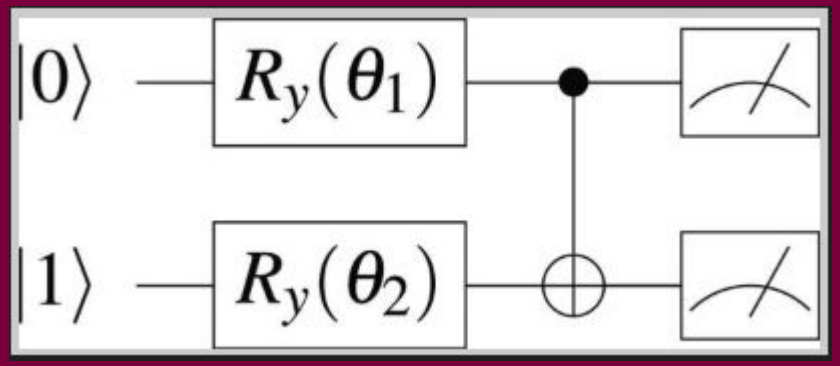
Results I

Vilnius University

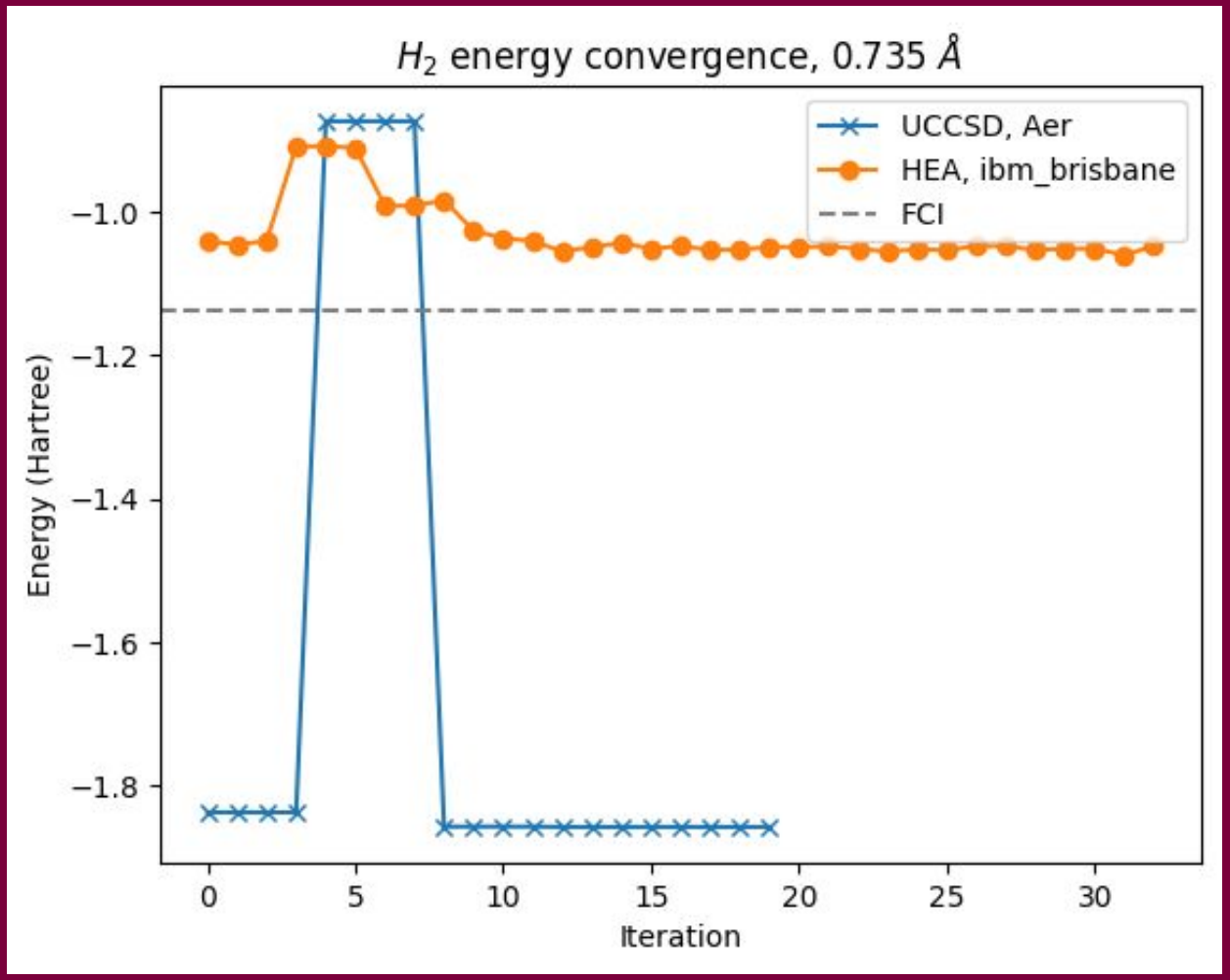


Results II

Vilnius University

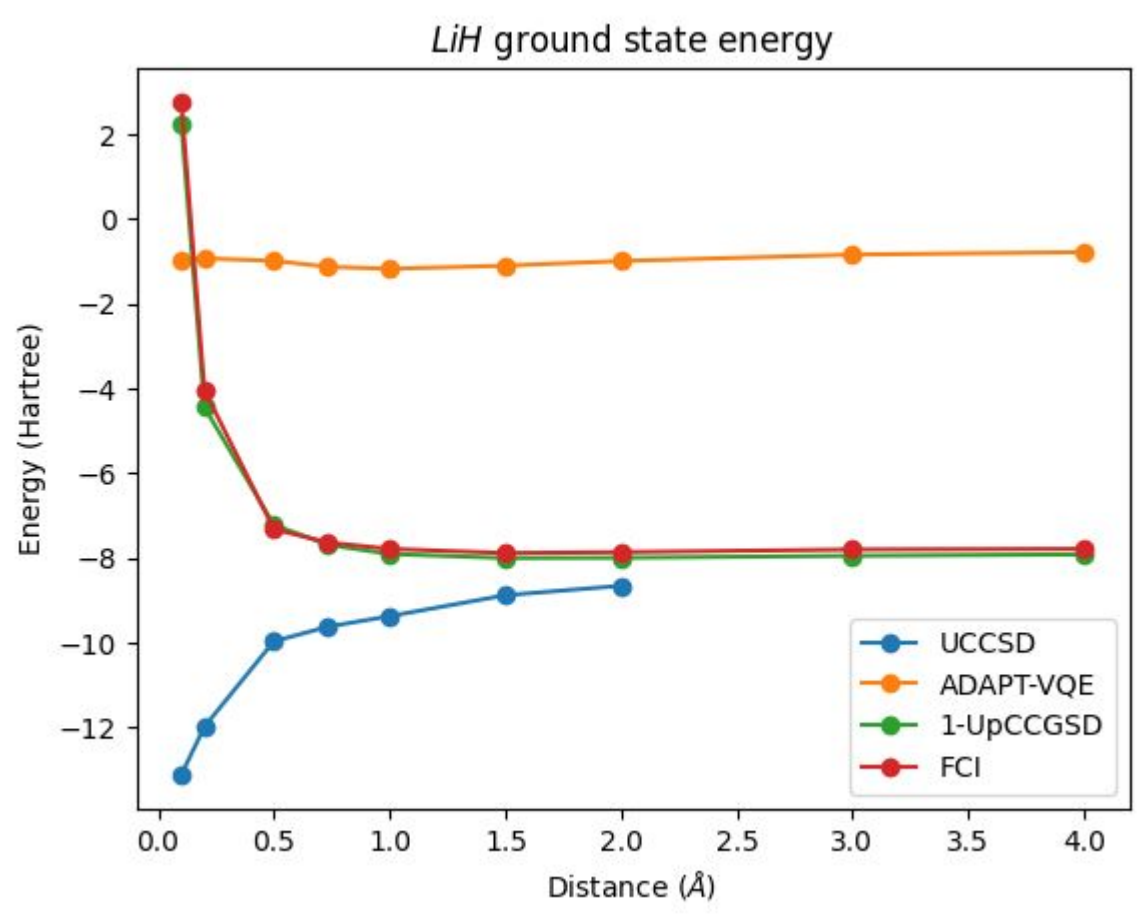


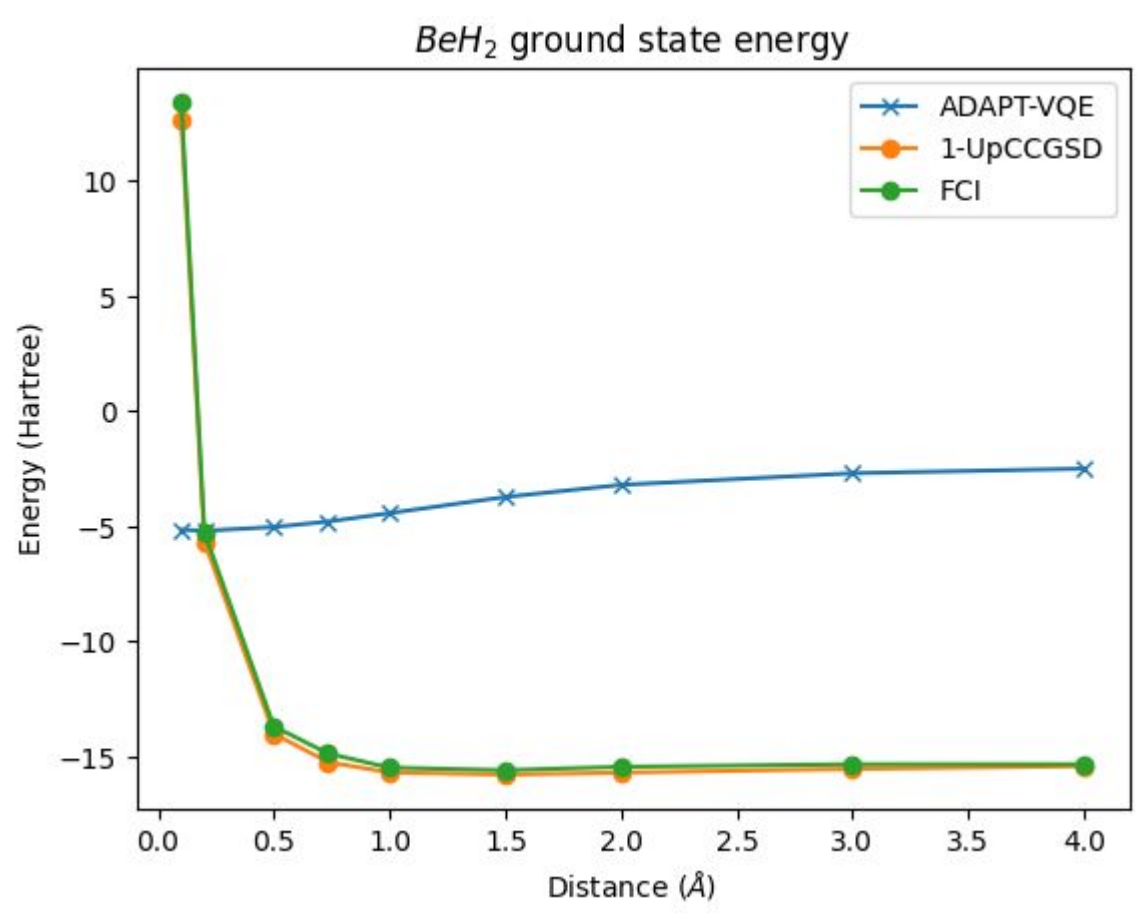
Choy et al. (2023)



Results III

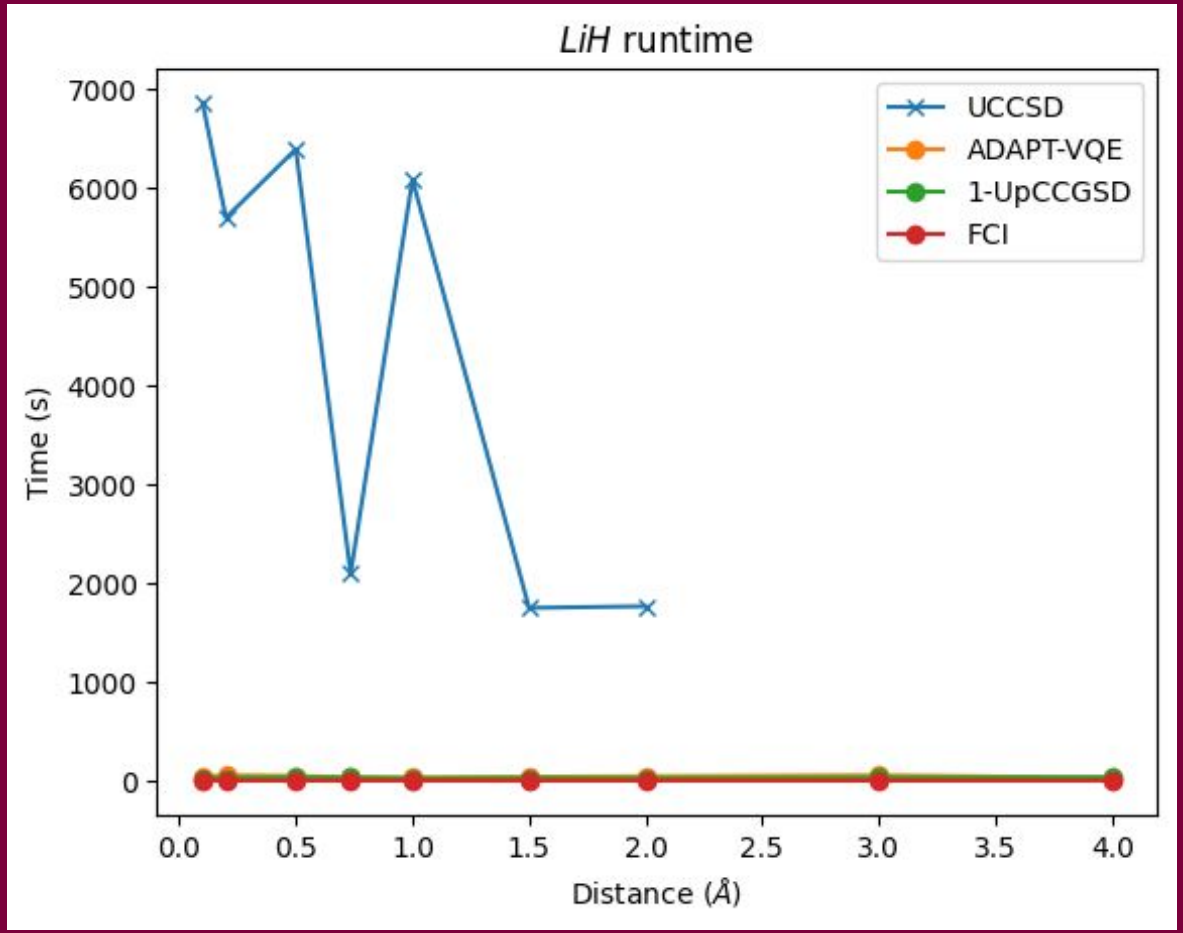
Vilnius University





Results IV

Vilnius University



Vilnius University

Conclusions

- **Comparison**:
  - ADAPT-VQE accuracy contradicted,
  - k-UpCCGSD more accurate than UCCSD (same in literature),
  - Bravyi-Kitaev better than parity, Jordan-Wigner mappings (same in literature),
  - optimizers - no difference for small molecules.
- New data, implementation code.
- **Limitations**:
  - few molecules, few data, broad and shallow algorithm analysis.
- **Future research**:
  - more analysis, more calculations on hardware, adjusting gradient tolerance, robust code implementation for new discoveries.
- **Recommendations**:
  - analysis on chemistry methods related to quantum computation part.

Vilnius University

References

- Peruzzo, A., McClean, J., Shadbolt, P., Yung, M. H., Zhou, X. Q., Love, P. J., ... & O'brien, J. L. (2014). A variational eigenvalue solver on a photonic quantum processor. Nature communications, 5(1), 4213.

- Choy, B., & Wales, D. J. (2023). Molecular energy landscapes of hardware-efficient ansatze in quantum computing. Journal of chemical theory and computation, 19(4), 1197-1206.

Vilnius University

CONTACTS

Naglis Šuliokas
Software engineering bachelor, 4th year
naglis.suliokas@mif.stud.vu.lt
naglis.suliokas@gmail.com