Exploring quantum algorithms and their simulation on HPC systems

Presentation of Summer Internship research

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Alternative Title:
“What I did on my summer holidays”

Research Objectives

- What are the efficient algorithms to run on Noisy Intermediate Scale Quantum (NISQ) machines coming down the line?
  - How can they be optimized?
- Testing the software currently being created for quantum machines
- What potential do HPC systems have for simulating these quantum machines?
  - What optimisations can we make?

State of the Art

- IBM is now offering machines for use with 27 qubits and a Quantum Volume of 64
  - https://newsroom.ibm.com/2020-08-20-IBM-Delivers-Its-Highest-Quantum-Volume-to-Date-Expanding-the-Computational-Power-of-its-IBM-Cloud-Accessible-Quantum-Computers
- Google this summer ran it's most complex simulation yet, modelling energy levels of Hydrogen chains with VQE & Hartree-Fock methods
  - https://ai.googleblog.com/2020/08/scaling-up-fundamental-quantum.html
- The US Department of Energy has pledged $125m in five QC centres over the next five years
  - www.sciencemag.org/news/2020/08/united-states-establishes-dozen-ai-and-quantum-information-science-research-centers

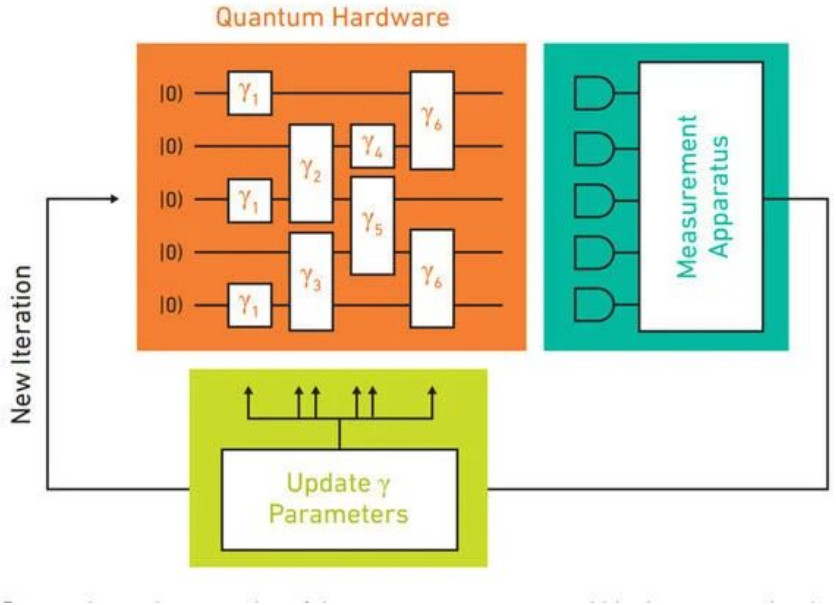
Qiskit and other software used

Qiskit

- A major part of this project was spent testing IBM's Qiskit software. Qiskit is an open-source all-in-one package for Quantum Computing in Python
  - Contains the tools for constructing circuits, performing chemistry calculations, appyling quantum algorithms and error correction, and running the circuits as a simulator or on IBM's quantum computers
  - Qiskit's strengths are its ease of use, accessibility, it's broad set of tools, and the strong community and collection of accompanying resources
- OpenFermion was used for the molecular calculations detailed later. Qiskit does not integrate itself easily with other frameworks

Variational Quantum Eigensolver (VQE) algorithm

- Classical-Quantum hybrid algorithm for solves for the eigenstates of an operator
- Takes an initial state ψ . Starting with a trial set of variables γ, it applies it repeatedly, after each run classically computing a more optimal set of values for γ
- The effectiveness of the algorithm is highly dependent on the quality of our trial ansatz ψ, in our case the Hartree Fock-calculated eigenstate



VQE & Chemical Modelling

- The VQE is one of the most promising algorithms in QC for NISQ machines
- It has the potential to be of great use, particularly for its potential for chemical modeling
- Possible use in developing medicines and fertilizers

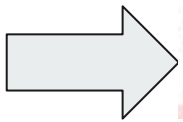
Final project:
Reducing the computational and gate demands of a chemical simulation

Reduction Methods

Some methods are standard and often built into software packages

- Spin Merging: Treating the up and down spin orbitals as single orbitals of double “weight”
  - This is as simple as adding corresponding terms to collapse the 1-dim Reduced Density Matrix
  - Below is the 1-RDM of H2

```
['0.987334', '0.00000', '-0.000000', '0.00000']
['0.00000', '0.987334', '0.00000', '-0.000000']
['-0.000000', '0.00000', '0.012666', '0.00000']
['0.00000', '-0.000000', '0.00000', '0.012666']
```



```
['1.974668', '-0.000000']
['-0.000000', '0.025332']
```

A word on mapping options

- Standard is Jordan-Wigner
- The Bravyi Kitaev transformation reduces simulation cost from O(n) to O(log n), used here
    - The Bravyi Kitaev ‘Superfast’ Method exists, promising even more efficient calculations. It was not tested during this project

Seeley, Jacob T., Martin J. Richard, and Peter J. Love. “The Bravyi-Kitaev Transformation for Quantum Computation of Electronic Structure.” The Journal of Chemical Physics 137.22 (2012): 224109..

Orbital Elimination

- Under the STO-3g basis, the basis is comprised of Slater-type orbital. We can simplify this by eliminating orbitals by their Natural Orbital Occupation Number, it's entry in the 1-RDM after diagonalization
- If the NOON is approximately 0, we can assume the orbital is always empty and remove it from calculations
- If the NOON is approximately 2 (filled in the spin up and a spin down forms), we take it as always full, remove it and two electrons from calculations

McArdle, Sam et al. "Quantum Computational Chemistry." Reviews of Modern Physics 92.1 (2020)

Orbital Elimination Example

$$\begin{pmatrix} \mathbf{1.99992} & 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.00000 \\ 0.00000 & \mathbf{1.96206} & 0.00000 & 0.00000 & 0.00000 & 0.00000 \\ 0.00000 & 0.00000 & \mathbf{0.03454} & 0.00000 & 0.00000 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & \mathbf{0.00005} & 0.00000 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.00000 & \mathbf{0.00171} & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.00000 & \mathbf{0.00171} \end{pmatrix}.$$

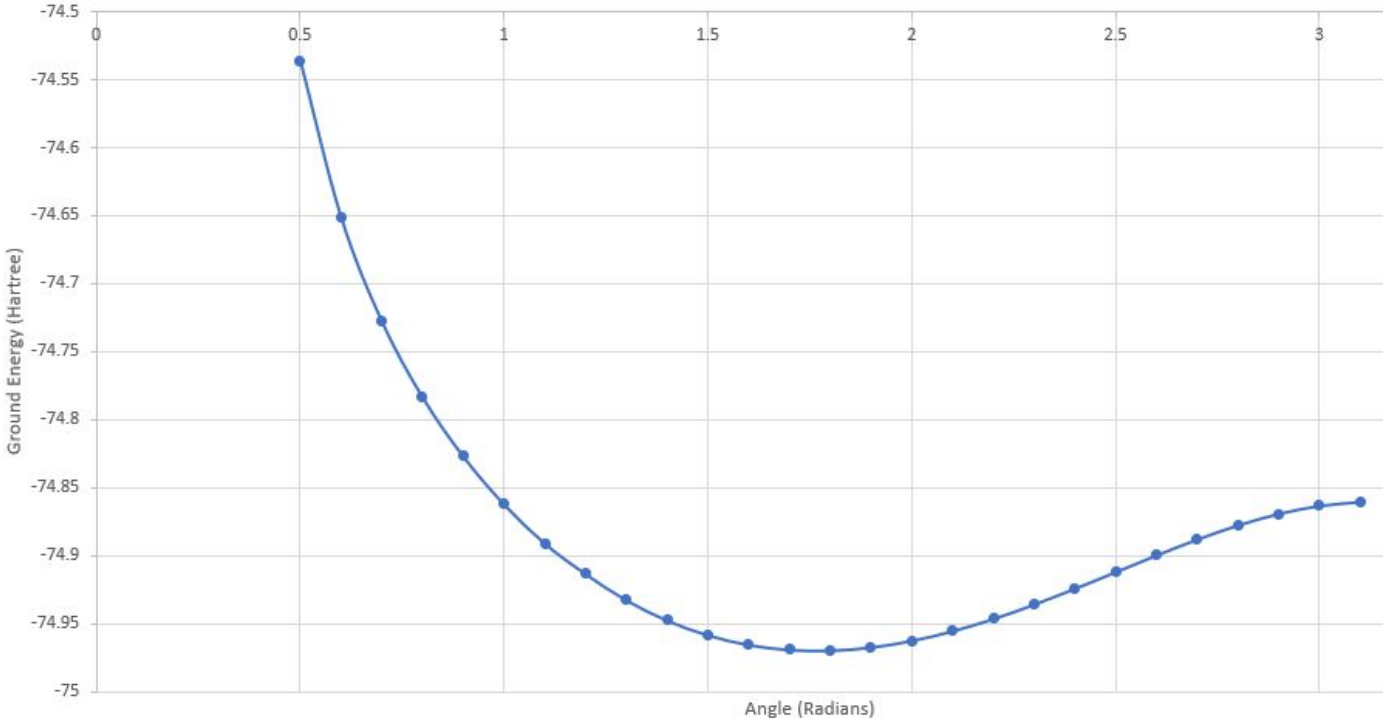
The 1-RDM of LiH

- Here we see that the 1st orbital is effectively 2, and the 4th is effectively zero. These can be removed, leaving a 8 orbital problem
- This was achieved in OpenFermion, calculating the 1-RDM integrals in the CISD basis with Psi4

Z2 & other symmetries

- This is just a snapshot of some reductions that can be done to reduce these problems
- One also performed here was the Z2 Symmetry reduction, which had a function in-built into Qiskit
- As Quantum Simulations proceeds to model larger and larger molecules, our options of symmetries to exploit will increase. There will be a future need for more algorithms that identify these symmetries and use them to reduce computational complexities

Result: Ground Energy of H2O vs. mol. angle

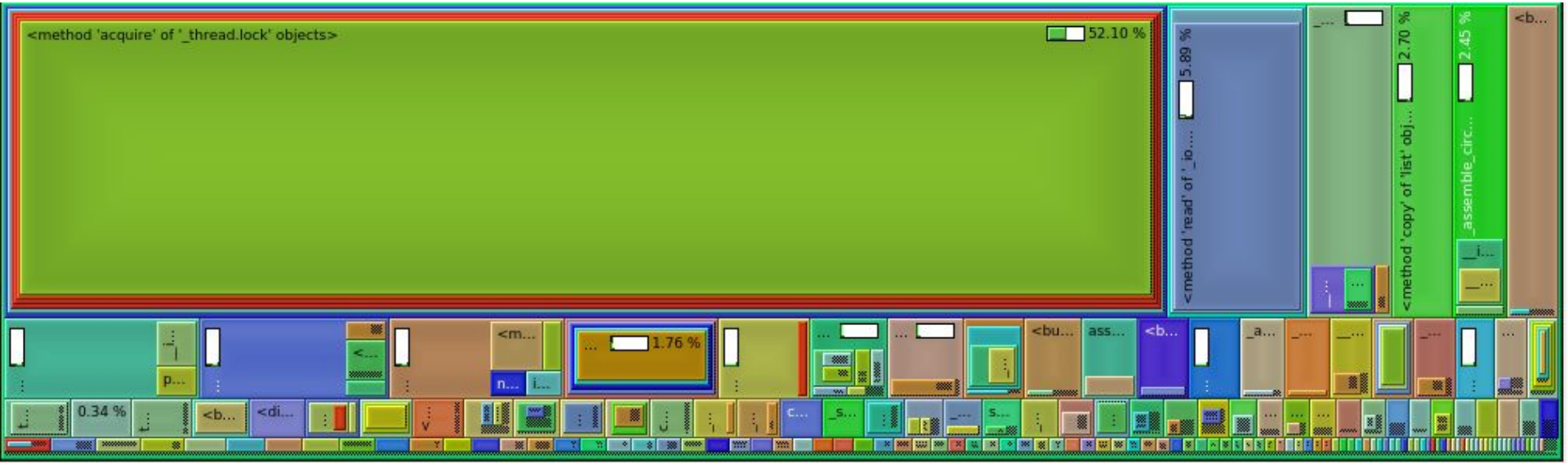


We plot the ground state energy as found by the VQE simulation as a function of the molecular angle,

The minimum is at the 1.82 radians that is the correct angle

Each simulation result took under 7 min to calculate

cProfile Analysis of the program



The majority of the calls made the profile is calls inherent to Python. It seems if one wanted to create an optimally efficient simulator, Python and Qiskit would not be the tools of choice

Closing Statements

- Quantum Computation Simulations run on machines such as Kay can be a great asset in creating future quantum algorithms for the NISQ era
- Qiskit is an accessible and versatile tool, but other options may offer greater efficiency and flexibility to integrate with other frameworks
- A significant amount of productive work exist to produce further methods for reducing quantum problems

Thank you.

Questions?