Orbitals - Speeding up Chemistry Simulations

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Our Project Background

- BioDac - Improving the simulation of the spectra of different photons. Used for a röntgen detector (for now with simulated radiation.)
  - Starting with calculating the ground state energy of Hydrogen as a proof of concept

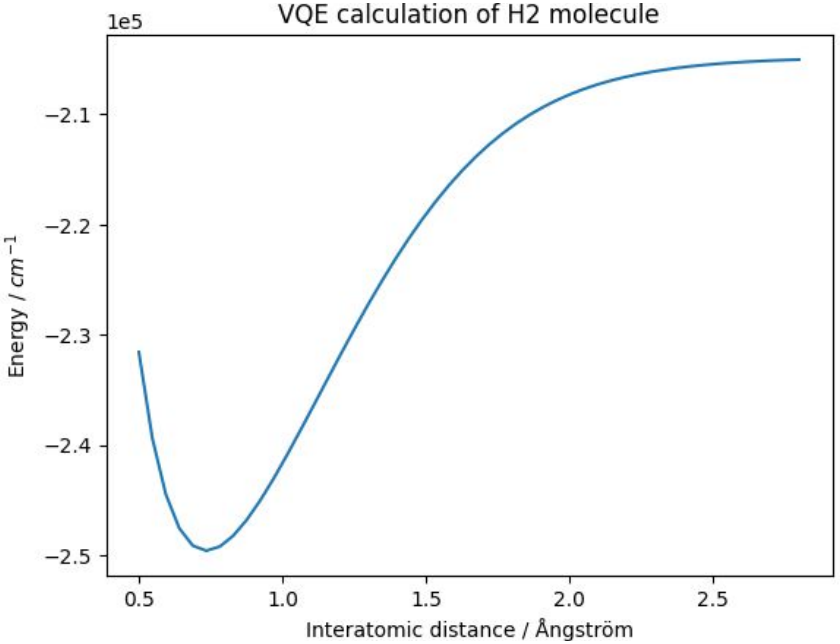
- Using multiple simulations to find the ground state energy in Qiskit and Julia, comparing the results.
  - Accuracy ➜ Efficiency
  - Suitability

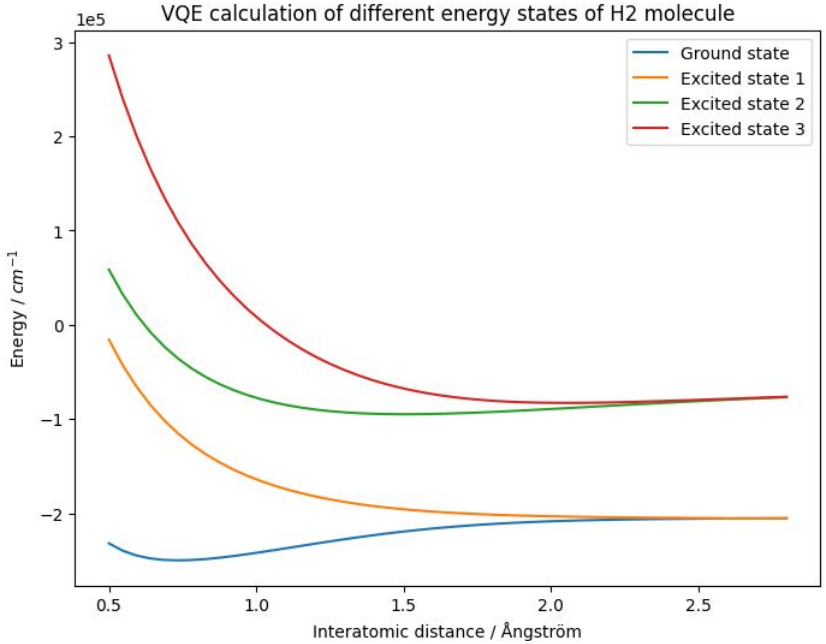
- Using a real quantum computer in this process.
  - Quantum Inspire

Variational Quantum Eigensolver

- Finding the ground state (Lowest energy state) of a given hamiltonian.
  - Using existing hamiltonian creation libraries: OpenFermion & Qiskit Nature

- With a classically updated parameterized ansatz you can find the solution.
  - Golden-Section Search


VQE calculation of H2 molecule
1e5
−2.1
−2.2
−2.3
−2.4
−2.5
Energy / cm^{-1}
0.5
1.0
1.5
2.0
2.5
Interatomic distance / Ångström


VQE calculation of different energy states of H2 molecule
1e5
3
2
1
0
−1
−2
Energy / cm^{-1}
Ground state
Excited state 1
Excited state 2
Excited state 3
0.5
1.0
1.5
2.0
2.5
Interatomic distance / Ångström

Results (simulated)

- Qiskit Nature (in ± 6 sec):

Inter atomic distance: 0.7348613106 Angstrom

Energy: -1.137306051164 Hartree

- Julia (in ± 5 sec):

Inter atomic distance: 0.734851576192 Angstrom

Energy: -1.13730604836 Hartree

- Exact (Numpy eigensolver):

Exact Inter atomic distance: 0.734865291339 Angstrom

Exact Energy: -1.13730605122 Hartree

Results

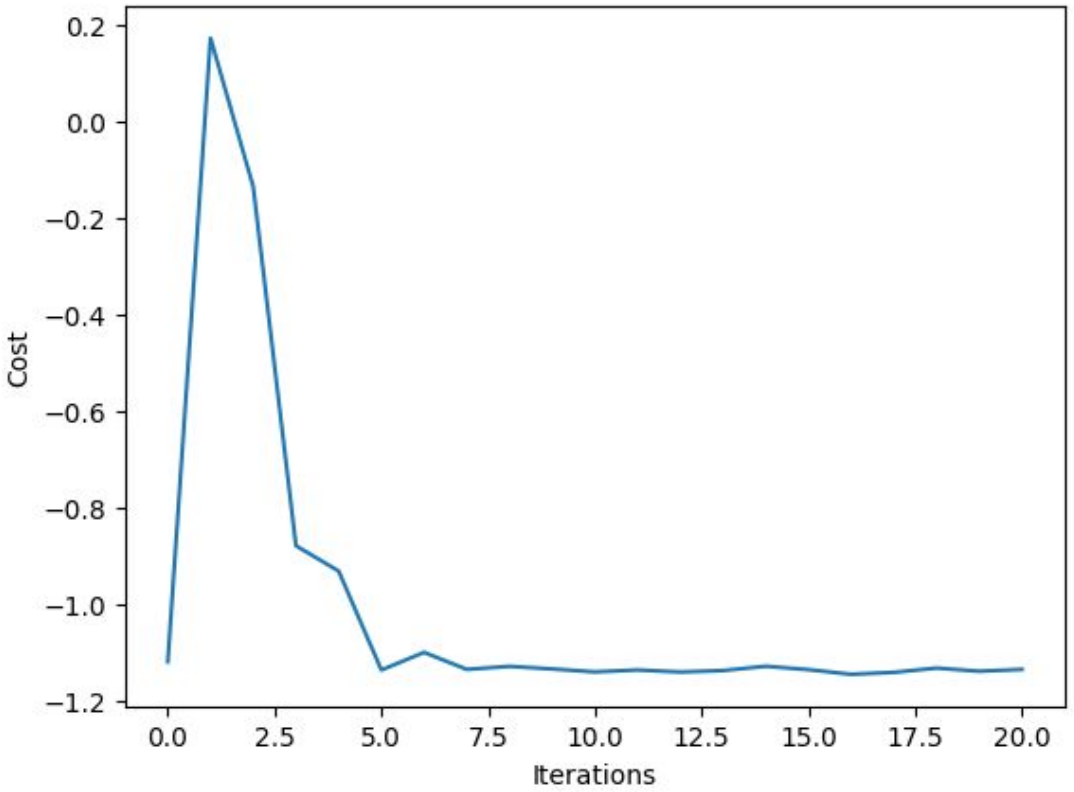
- Qiskit Nature:

Largest deviation from exact result (distance): 8.397245523372732e-07
Largest deviation from exact result (energy): 5.749023479495463e-11

- Julia:

Largest deviation from exact result (distance): 1.37151469836e-05
Largest deviation from exact result (energy): 2.85392998123e-9

Quantum Inspire



Quantum Inspire

Simulated

```
message: Optimization terminated successfully.
success: True
 status: 1
    fun: -1.1351385328823618
      x: [-1.562e-01]
   nfev: 20
  maxcv: 0.0
```

Quantum Inspire

```
message: Optimization terminated successfully.
success: True
 status: 1
    fun: -1.130809069534584
      x: [-1.427e-01]
   nfev: 20
  maxcv: 0.0
```

Simulations using Julia

Julia

- Using Yao
- Finding the ground state energy
  - Python: OpenFermion
- Demo

Qiskit Nature & Quantum Inspire

Future steps and recommendations

- Qiskit has more comprehensive documentation and a larger community.
  - More options
  - More accurate
- Yao has a slightly better circuit simulation run performance but lacks in any ways to implement on real hardware.
  - Python vs Julia

- Qiskit is the way to go, but Yao looks promising in the future.
  - Not possible to use all Qiskit Nature features on real hardware

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