

VQEDriver Documentation

v0.0.0

Python3 driver for the Variational Quantum Eigensolver (VQE) algorithm implemented in IBM's Qiskit for the calculation of the ground-state energy of a molecule. The driver reads a structured input file (commonly named `[molecule].inp`) and runs a complete VQE calculation using IBM's Qiskit and PySCF libraries.

Usage of the program from terminal:

```
1 $ vqedriver [INPUTFILE]
```

1. Input File

The input file follows a line by line structure, using keywords for each block and their options. In general, keywords are added in the format:

```
1 %keyword option_keyword1=option option_keyword2=option [...]
```

The input file accepts blank lines and comments beginning with the `#` character. The keywords can be added in any order.

1.1. Geometry

Added using the `%geometry` keyword. Currently, the geometry of the molecule has to be specified using an external XYZ file using the `xyzfile` option keyword.

Optional keywords:

- **charge** (int) – charge of the molecule.

Default: charge=0

- **spin** (int) – $2S$, where S is the total spin angular momentum. Same as the number of unpaired electrons in the molecule.

Default: spin=0

- **units** (str) – length units of the coordinate file.

Available options: **angstrom**, **bohr**

Default: **units=angstrom**

Example:

```
1 %geometry xyzfile=h2.xyz charge=1 spin=1 units=bohr
```

1.2. Basis set

Contains the basis set information for the molecule, added using the keyword **%basis**. Currently, only a single basis set can be added for all the atoms in the molecule using the option keyword **all=[BASIS SET]**. ECPs **are not** available.

Example:

```
1 %basis all=def2-TZVP
```

1.3. Self-Consistent Field (SCF)

Specifies the options for the SCF calculations, added by the **%scf** keyword. By default, the program sets a Restricted Hartree-Fock (RHF) calculation for closed-shell molecules and a Restricted-Open Hartree-Fock (ROHF) for open-shell molecule. Unrestricted Hartree-Fock (UHF) method is also available for open- and close-shell molecules.

Optional keywords:

- **method** (str) – Hartree-Fock method for SCF calculations.

Available options: **rhf**, **rohlf**, **uhf**

Default: **method=rhf** if **spin==0** (closed-shell), **method=rohlf** if **spin!=0** (open-shell)

- **conv** (int) – convergence criteria for the SCF calculations to $10^{-\text{conv}}$ Hartree.

Default: **conv=9**

- **maxcycles** (int) – maximum number of SCF cycles.

Default: **maxcycles=50**

- `maxcore` (int) – maximum memory in MB that PySCF should use.

Default: maxcore=1000

Example:

```
1 %scf method=uhf conv=6 maxcycles=100 maxcore=7500
```

1.4. VQE Settings

1.4.1. Qubit Operator Setup

Contains general settings for the qubit operator setup, built mapping the fermionic operator to the qubit operator. Options are added by the `%qubitop` keyword.

Optional keywords:

- `map` (str) – mapping to convert the fermionic operator to a qubit operator.

Available options: jordan_wigner, parity, bravyi_kitaev Default: map=parity

- `threshold` (int) – threshold for Pauli simplification, eliminate the real and imaginary parts of the weight in each Pauli Operator mapped by $10^{-\text{threshold}}$. If a weight is less than $10^{-\text{threshold}}$, the Pauli is removed from the `WeightedPauliOperator` object.

Default: threshold=8

Example:

```
1 %qubitop map=bksf threshold=9
```

1.4.2. Optimizer Setup

Selects the optimizer for the VQE algorithm using the keyword `%optimizer`.

1.4.3. Variational Form Setup

Available: UCCSD, CHC Keyword: `%ansatz` Opts: method, exctype (s, d, sd) Excitation type election available for both

1.4.4. Backend Setup