Documentation and User Guide

Hartree-Fock and MP2 energy calculation program

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1 The program

This program calculates the Hartree-Fock (HF) and Møller–Plesset perturbation theory (MP2) energies from data and integrals stored in HDF5 format. In particular, the number of molecular orbitals, number of spin-up electrons, nuclear repulsion energy, one-electron integrals and two-electron integrals are read from a HDF5 file using the TREXIO library. The program then calculates and outputs the one-electron and two-electron contribution to the Hartree-Fock energy as well as the MP2 energy correction.

2 Installation

2.1 Prerequisites

Ensure you have the following installed on your system.

```
gcc
make
trexio
```

2.2 Installation

1. Clone the repository:

```
git clone https://github.com/pauline-schtt/tccm-homeworks/tree/master/project1
cd project1
```

2. Compile the program using `make`:

```
make
```

3. Then, run the program:

```
./HF_and_MP2 <path_to_the_input_file>
```

Installation instructions can also be found in the `INSTALL.md` file.

3 Usage

To calculate the Hartree-Fock and MP2 energies, provide the full path to the HDF5 file containing the molecular data and integrals as an argument to the program. Important notice: this program works exclusively with the file in HDF5 format, other formats will not produce any results.

Example:

```
./HF_and_MP2 data/h2o.h5
```

If no file is provided, the program is going to ask the user to enter the path to the file on the command line before starting the calculation.

4 Expected output

The expected output from the Hartree-Fock and MP2 energy calculation for water (using the HDF5-file provided in `data/h20.h5`) is pasted below.

```
  ___  ___  ________      _____ ______   ________    _______
|\  \|\  \|\  _____\    |\   _ \  _   \|\   __  \  /  ___  \
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     \|__|\|__|\|__|         \|__|     \|__|\|__|      \|_______|

Welcome to the Hartree-Fock and MP2 energy calculation program.

Calculating the Hartree-Fock energy...
Done!

Calculating the MP2 energy correction...
Done!

################## Energy Summary ##################

Nuclear repulsion energy:             9.194966
One-electron energy:               -123.151186
Two-electron energy:                37.929422
Hartree-Fock energy:               -76.026799
MP2 energy correction:              -0.203960
Total energy (HF + MP2):           -76.230759

################ System Information ################

Number of occupied orbitals:         5
Number of molecular orbitals:        24
Number of two-electron integrals:    13458

################ Timing Information ################
HF calculation time:                 0.000032 seconds
MP2 calculation time:                0.008758 seconds
I/O and setup time:                  0.004182 seconds
Total execution time:                0.012972 seconds

Your calculation is done.
Thank you for using the program!
```

5 Tests

The program was tested on MacOS Sequoia 15.2 and Ubuntu 24.04. To test whether the installation was succesful, you could calculate the Hartree-Fock and MP2 energies on the set of molecules provided in the `data` folder. The reference values are given in the `README.org` file. The expected output for the set of test molecules is provided in the `test` folder.

6 Cleaning up

To clean up the compiled files, run:

```
make clean
```

7 Troubleshooting

If you encounter any issues during the installation, ensure that your versions of the prerequisites meet the required versions mentioned above. In case you're still facing issues, feel free to reach out to any of the contributors or opening an issue on GitHub.

8 License

9 Acknowledgments

This project is based on data and instructions provided by Abdallah Ammar, Yann Damour, Peter Reinhardt and Anthony Scemama, available at https://github.com/scemama/tccm-homeworks.

Appendix

Detailed documentation on the file contents, functions and variables in the code are provided in the documentation as generated using Doxygen (https://www.doxygen.nl/) in the appendix.