

# Installation and Execution Guide for Project1(HF and MP2 energy calculation)

## Prerequisites

Before proceeding, ensure the following tools are installed on your system:

- GCC (GNU Compiler Collection)
- Make utility

## Steps to Install and Run the Code

### 1. Download the Repository

Download or clone the Project1 repository to your local system:

```
git clone <repository_url>
```

Navigate into the `project1` directory:

```
cd project3
```

### 2. Understanding the Directory Structure

The repository has the following structure:

- `Makefile`: Contains commands for `make`, `make run`, and `make clean`.
- `src/`: Contains the source files (`mp2.energy`, `utils.c`).
- `data/`: Contains input files and will hold the generated output files.

### 3. Build the Project

Compile the source code using the Makefile:

```
make
```

This will generate the necessary executable files.

## 4. Run the Code

Execute the program using the following command:

```
make run
```

The program will process the input files located in the **data/** directory and generate the output files in the same folder.

## 5. Clean the Project

To remove any compiled files or intermediate build files, use the following command:

```
make clean
```

## Output

The output files will be generated in the **data/** directory after successful execution.

For any issues or troubleshooting, refer to the project documentation or contact the repository maintainer.