2 Installation

2.1 Download

To download the code go to the `GitHub` site, `https://github.com/AMDKIIT/amdkiit` and download the `tar or zip` file in your system. For source compilation, extract the archive using the usual command:

`tar -xzvf amdkiit-main.tar.gz` (for tar file)
or
`unzip amdkiit-main.zip` (for zip file)

The additional packages require to compile the code can be downloaded from different sites as mentioned in the next section.

2.2 Prerequisite

To install AMDKIIT software:

- User should have a minimal unix environment. Installation using the source code requires **Fortran** compiler (GNU or Intel). For parallel environment user should use MPI libraries and parallel compiler.
- Install `cmake` (**version 3.22 or higher**) to compile the code.

2.3 Installation

Two approaches are available for installing AMDKIIT:

1. **Automated Installation**: This method involves a script being run, which automatically downloads and installs all the required libraries, eliminating the need for manual intervention.
2. **Manual Installation**: In this approach, the necessary libraries are individually installed, and their paths are then manually specified in the CMakeLists.txt file.

These methods offer flexibility based on whether an automated setup is preferred or greater control over the installation process is desired.

2.3.1 Automated Installation:

In the automated process, the CMakeLists.txt file manages the downloading, configuration, and installation of all required libraries. To build the executable, run the following commands within the source directory:

```
$ mkdir build
$ cd build
$ cmake -DUSE_INTEL=ON ..    [for INTEL compiler],
or,
$ cmake -DUSE_GNU=ON ..    [for GNU compiler],
$ make
```

2.3.2 Manual Installation:

Install the libraries from the individual sites:

- FFTW: Download and intstall from `http://www.fftw.org`
- BLAS and LAPACK: Download and install from `https://netlib.org/lapack`
- LIBXC: For exchange-correlation functional, download the latest library from `https://libxc.gitlab.io/`

User should edit, the line in the `CMakeLists.txt` file inside `source` directory that sets the MANUAL_INSTALL variable. Modify that line to turn the manual installation option on by changing OFF to ON

- `set(MANUAL_INSTALL ON)`

Edit the path for lapack, fftw3 and libxc library in the `CMakeLists.txt` file inside `source` directory.

- `set(MATH_ROOT "path to the lapack library")`
- `set(FFTW_ROOT "path to the fftw directory")`
- `set(LIBXC_ROOT "path to the libxc directory")`

To `make` the executable, execute the following command within the source directory:

```
$ mkdir build
$ cd build
$ cmake -DUSE_INTEL=ON ..    [for INTEL compiler],
or,
$ cmake -DUSE_GNU=ON ..    [for GNU compiler],
$ make
```

This will generate the executable file `amdkiit.x` inside the `build` directory.

Note: When compiling and linking libraries and "AMDKIIT" software, it is crucial to ensure that all components are built using the same version of the compiler, whether it's Intel or GNU.