

BCNTLS ^4He DFT Codebase — Quickstart Guide

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An Internet connection and the ‘git’-program is required on the machine where the Git commands are going to be executed ! This should already be installed in most cases.

1 Obtaining the code

To obtain the code only one command in a terminal window is required. Change to the directory where you want the top level directory of the code to reside and execute

```
$ git clone <GitHub URL>
```

where <GitHub URL> needs to be substituted by one of

1. <https://github.com/bcntls2016/4hedft.git>
2. <https://github.com/bcntls2016/4hedft-vortex.git>
3. <https://github.com/bcntls2016/4hetddft-isotropic.git>
4. <https://github.com/bcntls2016/4hetddft-anisotropic.git>

These repositories contain, respectively,

1. Static ^4He DFT
2. Static ^4He DFT with vortex support
3. Time Dependent ^4He DFT for impurities in an isotropic electronic state (e.g. s-states)
4. Time Dependent ^4He DFT for impurities in an anisotropic electronic state (e.g. p-states)

2 Compiling the code

After git has downloaded the repository from the Internet, change to the repository directory which should be named after the last part of the URL without the .git part. Then execute

```
$ git checkout -b work
```

This will create a new git 'branch' called work where we can work in while not contaminating the 'master' branch.

You need to create a makefile to tailor it to your machines architecture. You can use one of the templates named `makefile.<machine>` if you want and save it as `makefile`. After you have created your own makefile and saved it as `makefile` execute

```
$ make
```

After there are no errors one of {BCN4HeDFT, `scalarimp_absor_new`, `vectorimp_absor`} executables should be ready to use, unless you changed the name in your makefile.

Make sure that the makefile's file name is `makefile` otherwise your own customizations could be overwritten after an update !