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*The User Manual
of The 3d DFT Program*

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Understanding The Program

This document deals with the technical details of the 3d-dft program. If you have no idea about , what this program does, read my M.Sc project report . The whole program can be used using graphical interface or manually executing the program file.

§0.1 Structure Of The Program

In the 3d-dft directory you will see several files and directories.

- Src : This directory contains the source codes of the programs. Do not change these files unless you know , what you are doing.
- bin : The executable file is kept here after compilation of the source code.
- input: Here the input configuration files are kept.
- info: All output informations while running the program are kept here.
- output: The output charge density , input potentials etc can be found here.
- charge_density_for_vmd : The charge densities are written in the format required by vmd for visualization.
- output_for_vmd: wave functions are written in the format required by vmd for visualization.
- backup: Here the backup of the outputs are created after predefined number of iterations and the backup files can be used to resume a unfinished job.

All other files and directories are required to run the program correctly and are not for your use.

§0.2 Compiling The Program

For compiling the program you need to change the makefile in the *src* directory by hand. You need to give the exact *MKL Library path*. For example if the makefile contains a line *LFLAGS = -L /opt/intel/mkl/9.1.023/lib/32/* where */opt/intel/mkl/9.1.023/lib/32/* is the MKL library path for my system , you need to change the path by your MKL library path. This are very standard practice in program compilations . If you are not familiar with this thing, please contact someone in your lab. You may have to change additional parameters depending upon your system. You need to have fftw3.2 installed and the Library should be in your path. do

```
cd src
```

```
make
```

to compile the program. After successful compilation the executable file *3d_dft.x* will be placed in the *bin* directory.

▣0.2.1 Cleaning after compilation

This is not a necessary step. You can clean by *make clean*. DON'T DELETE ALL THE *.mod FILES BY HAND. THERE ARE SOME ADDITIONAL mod FILES REQUIRED BY THE COMPILATION.

§0.3 RUNNING THE PROGRAM

If you have successfully compiled the program, you can start using the program by executing the *3d_dft.x* file. Several scripts are written to make your work easy. run the *start.sh* for graphical interface. You will need

- zenity Version 2.24.0
- dialog Version 1.1-20080316

for running the scripts properly. The graphical menu is self explanatory. For any help contact 1sandipde@gmail.com.