**Wien 2K Installation Process**

1. If user has recently installed the CentOS and dual boot with Windows.

Install the CentOs with the usb stick and complete the necessary partitions and select the packages and intall. Then reboot

**#\_** If Stuck on yum lock

ps –ef |grep yum

ps aux |grep yum

**#\_** Not showing NTFS partitions

yum install epel-release

yum install ntfs-3g

grub2-mkconfig > dev/null

{if windows partition is showing}

cp /boot/grub2/grub.cfg /boot/grub2/grub.cfg.old

grub2-mkconfig –o /oot/grub2/grub.cfg

#\_ Update All the system packages

yum update

**#\_** install or update the followings

* All the system package
* Kernel package
* Kernel-devel
* Python to version 2.7+
* Gcc to latest version including fortran
* Xpdf, emacs, gnuplot, perl5,

1. Install Intel Fortran Compiler from the site for the ifort and mkl libraries

* Intel Fortran Compiler and MKL Lib are included in their parallel cluster edition so download That.
* After downloading run the install script either in GUI mode or terminal mode.

./install.sh or ./install\_GUI.sh

* Complete the normal 2-3 steps
* At the time of installing the components, customize the components by selecting only the options of fortran compiler and mkl libraries or anything you want to download.
* After that click on the Advanced tab, and configure that.

Give the path of gcc and make to usr/bin/gcc and usr/bin/make.

* Configure the kernel package library or give the path to it
* Start the Install process. It will automatically download and install the process

1. Download any blas-3.\*.\* and gotobals2

* Extract the files after downloading with tar –xvf filename.tar
* Install with either make command or script file according your system like below

$ make

Or $ ./quickinstall.64bit

* If any error occur try with other blas version and files or restart and take a break
* After successful installation

$ make PREFIX=/opt/openblas install

* It will install the file in that directory.
* Configure the ld config file

$ cd /etc/ld.so.conf.d

$ vi randomlibs.conf

In the randomlibs file that open enter the path set to openblas

/usr/local/lib

/opt/openblas/lib

* Configure the .bashrc file by giving the path (explain in the next section)

1. Configure the .bashrc file

Provide the path to the intel fortran compiler and mkl libraries.

source /<path to the compiler> <architecture>

ususally the path is opt/intel/<compiler version>/linux/bin/compilervars.sh

* The bash file will look like this

vi ~/.bashrc

# .bashrc

source /opt/intel/compilers\_and\_libraries\_2017.0.098/linux/bin/compilervars.sh intel64

source /opt/intel/compilers\_and\_libraries\_2017.0.098/linux/mkl/bin/mklvars.sh intel64

export LD\_LIBRARY\_PATH=usr/local/lib

export MKLROOT

* Run the bash again and see if there are no errors in path

$ bash

$ which ifort

1. After Installing WIEN2k\_\_X.X.tar files

**#\_** Extract and expand tar files

tar –xvf WIEN2k\_14.2.tar

gunzip \*.gz

chmod 777 expand\_lapw

./expand\_lapw

#\_ Configure the site

./siteconfig\_lapw

1. Specify the System

If have ifort or mkl select that

Or select gfortran or other according to your system

1. Specify the compiler

Fortran – either ifort or gfortran

C - gcc

1. Compiling options

See if mkl library path is detected, if detected then continue press enter or if not then configure the .bashrc file according the mkl path

1. Set Perl path find it by which perl command
2. Compile the program

It should compile without errors

If not then search for errors on the net, take a break and try again next day by considering all the points and see if the path to all variables are set good or not

#\_ user Configure

./userconfig\_lapw

Editor – emacs

Pdf – xpdf

Wien dir Path – default seems good if not then provide the path

Scratch dir – again provide the path or leave it default

Continue by default

#\_ w2web configure

./w2web

Set admin username and password

Leave all to default

#\_ enjoy