WIEN2k 23.2 Install with OneAPI (ifort)

June 25, 2023

Linux Operating System Version (lsb_release -a): Ubuntu 22.04.2 LTS
Fortran Compiler Version (ifort -v): ifort version 2021.9.0
WIEN2k Version (cat $WIENROOT/WIEN2k_VERSION): 23.2 (Release 9/3/2022)

The Ubuntu 22.04.2 LTS was already installed, but if that is needed it should be available at:

https://ubuntu.com/download/desktop

Operating system packages that were needed were installed before proceeding with step 1 given below. If that hasn't been done, then install them:

```
username@computername:~$ sudo apt update
…
username@computername:~ $ sudo apt upgrade
…
username@computername:~ $ sudo apt install tcsh make autoconf libtool git
…
username@computername:~ $ sudo apt install gnuplot gnuplot-x11 libgd-dev
…
username@computername:~$ sudo apt install libquadmath0 libglu1-mesa-dev
…
username@computername:~$ sudo apt install libtogl-dev tcl-dev tk-dev libfftw3-dev libxmu-dev
…
```

Note: If prompted with "Do you want to continue [Y/n]", enter: Y.

The XCrySDen 1.6.2 was installed using:

```
username@computername:~ $ sudo apt install xcrysden
```

```
username@computername:~ $ gedit ~/.bashrc
...
XCRYSDEN_TOPDIR=/usr/bin
XCRYSDEN_LIB_BINDIR=/usr/lib
export XCRYSDEN_TOPDIR XCRYSDEN_LIB_BINDER
```

```
username@computername:~ $ source ~/.bashrc
```

Of note, for xcrysden to work, you may need to set Wayland to X as described at:

https://askubuntu.com/questions/1410256/how-do-i-use-x-instead-of-wayland-on-22-04

Installed OneAPI [https://www.intel.com/content/www/us/en/docs/oneapi/installation-guide-linux/2023-0/apt.html#apt] using:

```
username@computername:~$ wget -O- https://apt.repos.intel.com/intel-gpg-keys/GPG-PUB-KEY-INTEL-SW-PRODUCTS.PUB \
| gpg --dearmor | sudo tee /usr/share/keyrings/oneapi-archive-keyring.gpg > /dev/null
...
username@computername:~$ echo "deb [signed-by=/usr/share/keyrings/oneapi-archive-keyring.gpg] https://apt.repos.intel.com/oneapi all main" | sudo tee /etc/apt/sources.list.d/oneAPI.list
...
username@computername:~$ sudo apt-get update
...
username@computername:~$ sudo apt install intel-hpckit
...
Do you want to continue? [Y/n] Y
...
done.
Setting up intel-oneapi-mpi-devel-2021.9.0 (2021.9.0-43482) ...
Setting up intel-oneapi-tbb-common-2021.9.0 (2021.9.0-43484) ...
Setting up intel-oneapi-ipp-common-2021.8.0 (2021.8.0-46345) ...
Setting up intel-oneapi-dpcpp-debugger-2023.1.0 (2023.1.0-43513) ...
Setting up intel-oneapi-inspector (2023.1.0-43486) ...
Setting up intel-oneapi-compiler-dpcpp-eclipse-cfg (2023.1.0-46305) ...
Setting up intel-oneapi-compiler-shared-common-2023.1.0 (2023.1.0-46305) ...
Setting up intel-oneapi-openmp-2023.1.0 (2023.1.0-46305) ...
Setting up intel-oneapi-mpi-devel (2021.9.0-43482) ...
Setting up intel-oneapi-tbb-common-devel-2021.9.0 (2021.9.0-43484) ...
Setting up intel-oneapi-dev-utilities-eclipse-cfg (2021.9.0-44447) ...
Setting up intel-oneapi-dal-common-devel-2023.1.0 (2023.1.0-46349) ...
Setting up intel-oneapi-mkl-common-2023.1.0 (2023.1.0-46342) ...
Setting up intel-oneapi-ippcp-common-devel-2021.7.0 (2021.7.0-43492) ...
Setting up intel-oneapi-tbb-2021.9.0 (2021.9.0-43484) ...
Setting up intel-oneapi-ipp-2021.8.0 (2021.8.0-46345) ...
Setting up intel-oneapi-libdpstd-devel (2022.1.0-43490) ...
Setting up intel-oneapi-ippcp-devel-2021.7.0 (2021.7.0-43492) ...
Setting up intel-oneapi-diagnostics-utility (2022.3.0-43897) ...
Setting up intel-oneapi-clck-2021.7.3 (2021.7.3-45658) ...
Setting up intel-oneapi-mkl-common-devel-2023.1.0 (2023.1.0-46342) ...
Setting up intel-oneapi-itac-2021.9.0 (2021.9.0-43491) ...
Setting up intel-oneapi-ipp-common-devel-2021.8.0 (2021.8.0-46345) ...
Setting up intel-oneapi-dpcpp-ct-eclipse-cfg (2023.1.0-44450) ...
Setting up intel-oneapi-ccl-2021.9.0 (2021.9.0-43543) ...
Setting up intel-oneapi-compiler-shared-runtime-2023.1.0 (2023.1.0-46305) ...
Setting up intel-oneapi-compiler-dpcpp-cpp-common-2023.1.0 (2023.1.0-46305) ...
Setting up intel-oneapi-ippcp-devel (2021.7.0-43492) ...
```

```
Setting up intel-oneapi-compiler-dpcpp-cpp-and-cpp-classic-common-2023.1.0 (2023
.1.0-46305) ...
Setting up intel-oneapi-ccl-devel-2021.9.0 (2021.9.0-43543) ...
Setting up intel-oneapi-dpcpp-debugger (2023.1.0-43513) ...
Setting up intel-oneapi-compiler-fortran-common-2023.1.0 (2023.1.0-46305) ...
Setting up intel-oneapi-ccl-devel (2021.9.0-43543) ...
Setting up intel-oneapi-dpcpp-ct-2023.1.0 (2023.1.0-44450) ...
Setting up intel-oneapi-ipp-devel-2021.8.0 (2021.8.0-46345) ...
Setting up intel-oneapi-dpcpp-ct (2023.1.0-44450) ...
Setting up intel-oneapi-tbb-devel-2021.9.0 (2021.9.0-43484) ...
Setting up intel-oneapi-dev-utilities-2021.9.0 (2021.9.0-44447) ...
Setting up intel-oneapi-itac (2021.9.0-43491) ...
Setting up intel-oneapi-clck (2021.7.3-45658) ...
Setting up intel-oneapi-tbb-devel (2021.9.0-43484) ...
Setting up intel-oneapi-compiler-dpcpp-cpp-classic-fortran-shared-runtime-2023.1
.0 (2023.1.0-46305) ...
Setting up intel-oneapi-compiler-shared-2023.1.0 (2023.1.0-46305) ...
Setting up intel-oneapi-compiler-dpcpp-cpp-runtime-2023.1.0 (2023.1.0-46305) ...
Setting up intel-oneapi-dev-utilities (2021.9.0-44447) ...
Setting up intel-oneapi-dal-2023.1.0 (2023.1.0-46349) ...
Setting up intel-oneapi-ipp-devel (2021.8.0-46345) ...
Setting up intel-oneapi-compiler-dpcpp-cpp-and-cpp-classic-runtime-2023.1.0 (202
3.1.0-46305) ...
Setting up intel-oneapi-dal-devel-2023.1.0 (2023.1.0-46349) ...
Setting up intel-oneapi-dal-devel (2023.1.0-46349) ...
Setting up intel-oneapi-dpcpp-cpp-2023.1.0 (2023.1.0-46305) ...
Setting up intel-oneapi-compiler-fortran-runtime-2023.1.0 (2023.1.0-46305) ...
Setting up intel-oneapi-compiler-fortran-2023.1.0 (2023.1.0-46305) ...
Setting up intel-oneapi-dnnl (2023.1.0-46343) ...
Setting up intel-oneapi-mkl-2023.1.0 (2023.1.0-46342) ...
Setting up intel-oneapi-compiler-fortran (2023.1.0-46305) ...
Setting up intel-oneapi-compiler-dpcpp-cpp-2023.1.0 (2023.1.0-46305) ...
Setting up intel-oneapi-compiler-dpcpp-cpp-and-cpp-classic-2023.1.0 (2023.1.0-46
305) ...
Setting up intel-oneapi-compiler-dpcpp-cpp (2023.1.0-46305) ...
Setting up intel-oneapi-dnnl-devel (2023.1.0-46343) ...
Setting up intel-oneapi-mkl-devel-2023.1.0 (2023.1.0-46342) ...
Setting up intel-oneapi-compiler-dpcpp-cpp-and-cpp-classic (2023.1.0-46305) ...
Setting up intel-oneapi-mkl-devel (2023.1.0-46342) ...
Setting up intel-basekit (2023.1.0-46401) ...
Setting up intel-hpckit (2023.1.0-46346) ...
...
username@computername:~$ echo "source /opt/intel/oneapi/setvars.sh intel64" >> .bashrc
username@computername:~$ grep oneapi ~/.bashrc
source /opt/intel/oneapi/setvars.sh intel64
username@computername:~$ source ~/.bashrc
```

:: initializing oneAPI environment ...
bash: BASH_VERSION = 5.1.16(1)-release
args: Using "$@" for setvars.sh arguments: intel64
:: advisor -- latest
:: ccl -- latest
:: clck -- latest
:: compiler -- latest
:: dal -- latest
:: debugger -- latest
:: dev-utilities -- latest
:: dnnl -- latest
:: dpcpp-ct -- latest
:: dpl -- latest
:: inspector -- latest
:: ipp -- latest
:: ippcp -- latest
:: ipp -- latest
:: itac -- latest
:: mkl -- latest
:: mpi -- latest
:: tbb -- latest
:: vtune -- latest
:: oneAPI environment initialized ::

username@computername:~$ ifort -v
ifort version 2021.9.0
username@computername:~$ icc -v
icc: remark #10441: The Intel(R) C++ Compiler Classic (ICC) is deprecated and will be removed from product release in the second half of 2023. The Intel(R) oneAPI DPC++/C++ Compiler (ICX) is the recommended compiler moving forward. Please transition to use this compiler. Use '-diag-disable=10441' to disable this message.
icc version 2021.9.0 (gcc version 11.3.0 compatibility)
username@computername:~$ mpiifort -v
mpiifort for the Intel(R) MPI Library 2021.9 for Linux*
Copyright Intel Corporation.
ifort version 2021.9.0

1. The following was entered into the terminal to install libxc:

   username@computername:~$ cd ~
   username@computername:~$ wget http://www.tddft.org/programs/libxc/down.php?file=6.2.2/libxc-6.2.2.tar.gz
   ...
   username@computername:~$ tar xvf down.php\?file\=6.2.2%2Flibxc-6.2.2.tar.gz
   ...

username@computername:~$ cd libxc-6.2.2/
username@computername:~/libxc-6.2.2$ autoreconf -i --force
...
username@computername:~/libxc-6.2.2$ ./configure FC=ifort CC=icc --prefix=$HOME/libxc-6.2.2
...
username@computername:~/libxc-6.2.2$ make
...
username@computername:~/libxc-6.2.2$ make check
...
PASS: xc-run_testsuite
==========
Testsuite summary for libxc 6.2.2
==========
TOTAL: 1
PASS: 1
SKIP: 0
XFAIL: 0
FAIL: 0
XPASS: 0
ERROR: 0
==========
...
username@computername:~/libxc-6.2.2$ make install
...
username@computername:~/libxc-6.2.2$ ls ~/libxc-6.2.2/lib
libxc.a libxcf03.a libxcf03.la libxcf90.a libxcf90.la libxc.la pkgconfig

2. The following was entered into the terminal to install fftw:

username@computername:~/libxc-6.2.2$ cd ~
username@computername:~$ wget https://www.fftw.org/fftw-3.3.10.tar.gz
...
username@computername:~$ tar xvf fftw-3.3.10.tar.gz
...
username@computername:~$ cd fftw-3.3.10/
username@computername:~/fftw-3.3.10$ ./configure FCC=ifort CC=icc MPICC=mpiicc CFLAGS="-gcc-sys" --enable-mpi --prefix=$HOME/fftw-3.3.10
...
username@computername:~/fftw-3.3.10$ make
...
username@computername:~/fftw-3.3.10$ make install
...

```
username@computername:~/fftw-3.3.10$ ls ~/fftw-3.3.10/include/ ~/fftw-3.3.10/lib
/home/username/fftw-3.3.10/include/:
fftw3.f    fftw3.h     fftw3l-mpi.f03  fftw3-mpi.h
fftw3.f03  fftw3l.f03  fftw3-mpi.f03   fftw3q.f03

/home/username/fftw-3.3.10/lib:
cmake  libfftw3.a  libfftw3.la  libfftw3_mpi.a  libfftw3_mpi.la  pkgconfig
```

3. Go to:
   http://www.wien2k.at/reg_user/index.html

4. Click "Code download (after registration)"

5. Enter your username and password that you were given when you purchased WIEN2k.

6. Click the link "here" in "You can download the complete source code (about 160 MB) from here" to download "WIEN2k_23.2.tar". You should now have the source code package for WIEN2k 23.2.

7. If you have the folder "WIEN2k" in your Linux operating system home directory (for example at /home/username/WIEN2k, where username is replaced by your user name). You can rename it something else, such as "WIEN2k23.1".

8. The following was entered into the terminal to install WIEN2k 23.2:

```
username@computername:~/fftw-3.3.10$ cd ~
username@computername:~$ mkdir WIEN2k
username@computername:~$ cd WIEN2k
username@computername:~/WIEN2k$ ls
WIEN2k_23.2.tar
username@computername:~/WIEN2k$ tar xvf WIEN2k_23.2.tar
...
username@computername:~/WIEN2k$ gunzip *.gz
username@computername:~/WIEN2k$ chmod +x ./expand_lapw
username@computername:~/WIEN2k$ export LC_NUMERIC=en_US.UTF-8
username@computername:~/WIEN2k$ ./expand_lapw
...
continue (y/n)
y
...
username@computername:~/WIEN2k$ ./siteconfig
...
    Press RETURN to continue
...
  Selection: LI
...
    Press RETURN to continue
```

...
    Your compiler: ifort
...
    Your compiler: icc
...
    Press RETURN to continue
...
Hit Enter to continue
...
 Would you like to use LIBXC (needed ONLY for self-consistent gKS mGGA calculations, for the stress tensor and experts who want to play with different DFT options. It must have been installed before)? (y,N):
y
...
 Do you want to automatically search for LIBXC installations? (Y,n):
Y
 Please specify a comma separated list of directories to search! (If no list is entered, /usr/lib64, /usr/local and /opt will be searched as default):
/home/username/libxc-6.2.2
...
 More than one libxc was found in the specified directory(ies).
 Pick one of the following (enter the number of the line of your choice or 0 to manually specify a path)!:
/home/username/libxc-6.2.2/lib/libxc.a
/home/username/libxc-6.2.2/src/.libs/libxc.a
1
...
    Press RETURN to continue
...
 Do you want to automatically search for FFTW installations? (Y,n):
Y
 Please specify a comma separated list of directories to search! (If no list is entered,
 /usr/lib64, /usr/local and /opt will be searched as default):
/home/username/fftw-3.3.10
...
Do you want to use a FFTW version from the list above? (Y,n):
Y
 Please enter the line number of the chosen version or enter 0 to manually specify your choice!:
1
...
 Please specify the target achitecture of your FFTW library (e.g. lib64) or accept present choice (enter): lib
...
 Please specify the name of your FFTW library or accept present choice (enter): fftw3
...
  Is this correct? (Y,n): Y

```
...
Current settings:
  M   OpenMP switch:           -qopenmp
  O   Compiler options:        -O -FR -mp1 -w -prec_div -pc80 -pad -ip -DINTEL_VML -
traceback -assume buffered_io -I$(MKLROOT)/include
  L   Linker Flags:            $(FOPT) -L$(MKLROOT)/lib/$(MKL_TARGET_ARCH) -lpthread -
lm -ldl -liomp5
  P   Preprocessor flags       '-DParallel'
  R   R_LIBS (LAPACK+BLAS):    -lmkl_intel_lp64 -lmkl_intel_thread -lmkl_core
  F   FFTW options:            -DFFTW3 -I/home/username/fftw-3.3.10/include
      FFTW-LIBS:               -L/home/username/fftw-3.3.10/lib -lfftw3
  X   LIBX options:            -DLIBXC -I/home/username/libxc-6.2.2/include
      LIBXC-LIBS:              -L/home/username/libxc-6.2.2/lib -lxcf03 -lxc
...
Selection: S
...
     Press RETURN to continue
...
 Shared Memory Architecture? (y/N):y
  Do you know/need a command to bind your jobs to specific nodes?
  (like taskset -c). Enter N / your_specific_command: N
...
  Do you have MPI, ScaLAPACK, ELPA, or MPI-parallel FFTW installed and intend
   to run finegrained parallel?
...
   (y/N) y
...
    Your compiler: mpiifort
...
 Do you want to use a present ScaLAPACK installation? (Y,n): Y
...
 Do you want to use the MKL version of ScaLAPACK? (Y,n):Y
  Do you use Intel MPI? (Y,n):Y
...
 Is this correct? (Y,n): Y
...
 Do you want to use ELPA? (y,N):
N

     Press RETURN to continue
...
   Please specify your parallel compiler options or accept the recommendations (Enter - default)!:

   Please specify your parallel OMP_SWITCH (type "del" to blank it)
   or accept the recommendations (Enter - default)!:
```

Please specify your MPIRUN command or accept the recommendations (Enter - default)!:

Press RETURN to continue
...
Current settings:

Parallel compiler : mpiifort
SCALAPACK_LIBS : -lmkl_scalapack_lp64 -lmkl_blacs_intelmpi_lp64
FFTW_PLIBS : -lfftw3_mpi
ELPA_OPT :
ELPA_LIBS :
FPOPT(par.comp.options): -O -FR -mp1 -w -prec_div -pc80 -pad -ip -DINTEL_VML -traceback -assume buffered_io -I$(MKLROOT)/include
OMP_SWITCH : -qopenmp
MPIRUN command : mpirun -np _NP_ -machinefile _HOSTS_ _EXEC_

parallel execution:

RP_LIBS : $(R_LIBS)
...
Selection: S
...
Press RETURN to continue
...
Selection: Q
...
Selection: A
...
Compile time errors (if any) were:
<= It should be blank here if successful.
Check file compile.msg in the corresponding SRC_* directory for the compilation log and more info on any compilation problem.

Press RETURN to continue
...
Please enter the full path of the perl program: /usr/bin/perl
...
Press RETURN to continue
...
Please enter the full path to your temporary directory: /tmp
...
Press RETURN to continue
…

9. If it is the first time installing WIEN2k on the computer, enter in the terminal:

```
username@computername:~/WIEN2k$ ./userconfig_lapw
...
 Specify your prefered editor (default is emacs):
    editor shall be: gedit


   Set editor to  gedit (Y/n) Y

    Specify your prefered DATA directory, where your cases should be
    stored (for  /home/username/WIEN2k, just enter RETURN key):
    DATA directory: /home/username/wiendata

    Set DATA directory to  /home/username/wiendata (Y/n) Y
...
   Specify your prefered scratch directory, where big case.vector files
    can be stored (Recommended is a local directory (maybe /scratch), not a
    NFS directory. For your working directory, just enter RETURN key):
    scratch directory:

   Set scratch directory to  working directory (Y/n) Y

    Specify your program to read pdf files (default is okular)
    (on some Linux systems use xpdf, evince, pdfstudio, ...):evince
...
    Set PDFREADER to  evince (Y/n) Y

WIEN2k can use OpenMP parallelization on multicore computers.
For details please read the "Parallelization section" of the Usersguide.
Your present computer has 6 cores, but more than 4 (8) cores is useless.
How many cores do you want to use by default (4):1

    Set OMP_NUM_THREADS to  1 (Y/n) Y


!!!  The following lines will be added to your .bashrc file if you continue !!!
    A copy of your current .bashrc will be saved under  .bashrc.savelapw !

# added by WIEN2k: BEGIN
# ------------------------------------------------------
alias lsi="ls -aslp *.in*"
alias lso="ls -aslp *.output*"
alias lsd="ls -aslp *.def"
alias lsc="ls -aslp *.clm*"
alias lss="ls -aslp *.scf* */*scf"
```

```
alias lse="ls -aslp *.error"
alias LS="ls -alsp |grep /"
alias pslapw="ps -ef |grep "lapw""
alias cdw="cd /home/username/wiendata"
if [ "$OMP_NUM_THREADS" = "" ]; then export OMP_NUM_THREADS=1; fi
#export LD_LIBRARY_PATH=.....
export EDITOR="gedit"
export SCRATCH=./
if [ "$WIENROOT" = "" ]; then export WIENROOT=/home/username/WIEN2k; fi
export W2WEB_CASE_BASEDIR=/home/username/wiendata
export STRUCTEDIT_PATH=$WIENROOT/SRC_structeditor/bin
export PDFREADER=evince
export PATH=$WIENROOT:$STRUCTEDIT_PATH:$WIENROOT/SRC_IRelast/script-
elastic:$PATH:.
export OCTAVE_EXEC_PATH=${PATH}::
export OCTAVE_PATH=${STRUCTEDIT_PATH}::

ulimit -s unlimited
alias octave="octave -p $OCTAVE_PATH"
# ----------------------------------------------------
    Do you want to continue (Y/n)? Y
...
    Edit .rhosts file now? (y/N) N
...
username@computername:~/WIEN2k$ source ~/.bashrc
...
```

10. To setup or start w2web, enter in the terminal:

```
username@computername:~/WIEN2k$ w2web
#############################################################################
# w2web starter                                          #
# Copyright (C) 2001 luitz.at                                 #
#############################################################################
w2web installer on host computername

#############################################################################
# w2web installer                                         #
# Copyright (C) 2001 luitz.at                                 #
#############################################################################

Checking for Installation in /home/username/.w2web/computername

Creating /home/username/.w2web
Creating /home/username/.w2web/computername
conf directory does not exist - creating it.
```

logs directory does not exist - creating it.
sessions directory does not exist - creating it.
tmp directory does not exist - creating it.

Installing w2web files ...
Please answer these questions for proper installaltion.
Just press enter for the default value of (in brackets).

Please enter the username: [admin] username
Please enter the password: [password] password
username:password
Remember these. You will need them when you log in.

Select the port to run on: [7890]
Running on port 7890

Please enter this system's hostname: [computername] localhost
Using localhost

Is this your master node?: [y] y
Installing... Attempting to start now...

Trying to start /home/username/WIEN2k/SRC_w2web/bin/w2web
w2web server started, now point your web browser to
http://localhost:7890

done.

11. The WIEN2k 23.2 installation is now complete. To test if WIEN2k installed okay or not, run the TiC example. Additional details of the TiC example are given in the WIEN2k 23.1 usersguide (section “3 Quick Start” starting on page 13) [1].

[1] http://susi.theochem.tuwien.ac.at/reg_user/textbooks/usersguide.pdf