

The script is:

```
#!/bin/tcsh

#SBATCH -N 1

#SBATCH -n 4

#SBATCH --mem 5000

#SBATCH -p standard

module load ifort

module load mkl

module load openmpi/4.1.0_gcc620

module load fftw/3.3.8_gcc620

setenv WIENROOT /home/users/mollabashi/codes/v21.1

which mpirun

which lapw1

echo $PATH

echo $WIENROOT
```

The result is:

```
gmp/5.1.3 load complete.

mpfr/3.1.2 load complete.

libmpc/1.0.1 load complete.

gcc/6.2.0 load complete.

ifort/19.1.3.304 load complete.

mkl/2020.0.4 load complete.

openmpi/4.1.0_gcc620 load complete.

fftw/3.3.8_gcc620 load complete.
```

/opt/exp_soft/local/generic/openmpi/4.1.0_gcc620/bin/mpirun

/home/users/mollabashi/codes/v21.1/lapw1

/opt/exp_soft/local/generic/fftw/3.3.8_gcc620/bin:/opt/exp_soft/local/generic/openmpi/4.1.0_gcc620/bin:/opt/exp_soft/local/generic/gcc/6.2.0/bin:/opt/exp_soft/local/generic/intel/compilers_and_libraries/linux/bin/intel64:/home/users/mollabashi/codes/v21.1:/home/users/mollabashi/codes/v21.1/SRC_structeditor/bin:/home/users/mollabashi/codes/v21.1/SRC_IReIast/script-elastic:/usr/lib64/qt-3.3/bin:/bin:/usr/local/bin:/usr/bin:/usr/local/sbin:/usr/sbin:/sbin:./home/users/mollabashi/codes/v21.1:.

/home/users/mollabashi/codes/v21.1

By adding the following lines:

echo \$LD_LIBRARY_PATH

ldd \$WIENROOT/lapw1_mpi

ldd \$WIENROOT/lapw0_mpi

The following lines are added to the result:

/opt/exp_soft/local/generic/openmpi/4.1.0_gcc620/lib:/opt/exp_soft/local/generic/intel/mkl/lib/intel64:/opt/exp_soft/local/generic/libmpc/1.0.1-2.el6/lib64:/opt/exp_soft/local/generic/mpfr/3.1.2-4.el6/lib64:/opt/exp_soft/local/generic/gmp/5.1.3-2.el6/lib64:/opt/exp_soft/local/generic/gcc/6.2.0/lib/gcc/x86_64-unknown-linux-gnu/6.2.0/32:/opt/exp_soft/local/generic/gcc/6.2.0/lib/gcc/x86_64-unknown-linux-gnu/6.2.0:/opt/exp_soft/local/generic/gcc/6.2.0/lib64:/opt/exp_soft/local/generic/gcc/6.2.0/lib:/opt/exp_soft/local/generic/intel/compilers_and_libraries/linux/lib/intel64

linux-vdso.so.1 => (0x00007fff41542000)

libpthread.so.0 => /lib64/libpthread.so.0 (0x00002ba9beba3000)

libm.so.6 => /lib64/libm.so.6 (0x00002ba9bedbf000)

libdl.so.2 => /lib64/libdl.so.2 (0x00002ba9bf0c1000)

libiomp5.so =>

/opt/exp_soft/local/generic/intel/compilers_and_libraries/linux/lib/intel64/libiomp5.so (0x00002ba9bf2c5000)

libmkl_scalapack_lp64.so =>
/opt/exp_soft/local/generic/intel/mkl/lib/intel64/libmkl_scalapack_lp64.so
(0x00002ba9bf6cb000)

libmkl_blacs_intelmpi_lp64.so =>
/opt/exp_soft/local/generic/intel/mkl/lib/intel64/libmkl_blacs_intelmpi_lp64.so
(0x00002ba9bfff6000)

libmkl_intel_lp64.so =>
/opt/exp_soft/local/generic/intel/mkl/lib/intel64/libmkl_intel_lp64.so (0x00002ba9c0238000)

libmkl_intel_thread.so =>
/opt/exp_soft/local/generic/intel/mkl/lib/intel64/libmkl_intel_thread.so
(0x00002ba9c0f58000)

libmkl_core.so => /opt/exp_soft/local/generic/intel/mkl/lib/intel64/libmkl_core.so
(0x00002ba9c4843000)

libmpi_usempif08.so.40 =>
/opt/exp_soft/local/generic/openmpi/4.1.0_gcc620/lib/libmpi_usempif08.so.40
(0x00002ba9c8e84000)

libmpi_usempi_ignore_tkr.so.40 =>
/opt/exp_soft/local/generic/openmpi/4.1.0_gcc620/lib/libmpi_usempi_ignore_tkr.so.40
(0x00002ba9c90ba000)

libmpi_mpi fh.so.40 =>
/opt/exp_soft/local/generic/openmpi/4.1.0_gcc620/lib/libmpi_mpi fh.so.40
(0x00002ba9c92c2000)

libmpi.so.40 => /opt/exp_soft/local/generic/openmpi/4.1.0_gcc620/lib/libmpi.so.40
(0x00002ba9c951e000)

libc.so.6 => /lib64/libc.so.6 (0x00002ba9c984f000)

libgcc_s.so.1 => /opt/exp_soft/local/generic/gcc/6.2.0/lib64/libgcc_s.so.1
(0x00002ba9c9c1d000)

/lib64/ld-linux-x86-64.so.2 (0x00002ba9be97f000)

libopen-rte.so.40 => /opt/exp_soft/local/generic/openmpi/4.1.0_gcc620/lib/libopen-
rte.so.40 (0x00002ba9c9e33000)

libopen-pal.so.40 => /opt/exp_soft/local/generic/openmpi/4.1.0_gcc620/lib/libopen-pal.so.40 (0x00002ba9ca0eb000)

librt.so.1 => /lib64/librt.so.1 (0x00002ba9ca3fd000)

libutil.so.1 => /lib64/libutil.so.1 (0x00002ba9ca605000)

libz.so.1 => /lib64/libz.so.1 (0x00002ba9ca808000)

libgfortran.so.3 => /opt/exp_soft/local/generic/gcc/6.2.0/lib/./lib64/libgfortran.so.3 (0x00002ba9caa1e000)

libquadmath.so.0 => /opt/exp_soft/local/generic/gcc/6.2.0/lib/./lib64/libquadmath.so.0 (0x00002ba9cad44000)

linux-vdso.so.1 => (0x00007ffded983000)

libpthread.so.0 => /lib64/libpthread.so.0 (0x00002b78ca922000)

libm.so.6 => /lib64/libm.so.6 (0x00002b78cab3e000)

libdl.so.2 => /lib64/libdl.so.2 (0x00002b78cae40000)

libiomp5.so =>
/opt/exp_soft/local/generic/intel/compilers_and_libraries/linux/lib/intel64/libiomp5.so (0x00002b78cb044000)

libmkl_intel_lp64.so =>
/opt/exp_soft/local/generic/intel/mkl/lib/intel64/libmkl_intel_lp64.so (0x00002b78cb44a000)

libmkl_intel_thread.so =>
/opt/exp_soft/local/generic/intel/mkl/lib/intel64/libmkl_intel_thread.so (0x00002b78cc16a000)

libmkl_core.so => /opt/exp_soft/local/generic/intel/mkl/lib/intel64/libmkl_core.so (0x00002b78cfa55000)

libmpi_usempif08.so.40 =>
/opt/exp_soft/local/generic/openmpi/4.1.0_gcc620/lib/libmpi_usempif08.so.40 (0x00002b78d4096000)

libmpi_usempi_ignore_tkr.so.40 =>
/opt/exp_soft/local/generic/openmpi/4.1.0_gcc620/lib/libmpi_usempi_ignore_tkr.so.40 (0x00002b78d42cc000)

libmpi_mpifh.so.40 =>
/opt/exp_soft/local/generic/openmpi/4.1.0_gcc620/lib/libmpi_mpifh.so.40
(0x00002b78d44d4000)

libmpi.so.40 => /opt/exp_soft/local/generic/openmpi/4.1.0_gcc620/lib/libmpi.so.40
(0x00002b78d4730000)

libc.so.6 => /lib64/libc.so.6 (0x00002b78d4a61000)

libgcc_s.so.1 => /opt/exp_soft/local/generic/gcc/6.2.0/lib64/libgcc_s.so.1
(0x00002b78d4e2f000)

/lib64/ld-linux-x86-64.so.2 (0x00002b78ca6fe000)

libopen-rte.so.40 => /opt/exp_soft/local/generic/openmpi/4.1.0_gcc620/lib/libopen-
rte.so.40 (0x00002b78d5045000)

libopen-pal.so.40 => /opt/exp_soft/local/generic/openmpi/4.1.0_gcc620/lib/libopen-
pal.so.40 (0x00002b78d52fd000)

librt.so.1 => /lib64/librt.so.1 (0x00002b78d560f000)

libutil.so.1 => /lib64/libutil.so.1 (0x00002b78d5817000)

libz.so.1 => /lib64/libz.so.1 (0x00002b78d5a1a000)

libgfortran.so.3 => /opt/exp_soft/local/generic/gcc/6.2.0/lib/./lib64/libgfortran.so.3
(0x00002b78d5c30000)

libquadmath.so.0 => /opt/exp_soft/local/generic/gcc/6.2.0/lib/./lib64/libquadmath.so.0
(0x00002b78d5f56000)