```
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.
/home/users/mollabashi/expands/openmpi/bin/mpirun
/home/users/mollabashi/expands/v21.1/lapw1
/opt/exp_soft/local/generic/gcc/6.2.0/bin:/opt/exp_soft/generi
c/intel/compilers_and_libraries/linux/bin/intel64:/home/users/mollab
ashi/expands/v21.1:/home/users/mollabashi/expands/v21.1/SRC_structed
itor/bin:/home/users/mollabashi/expands/v21.1/SRC_IRelast/script-
elastic:/home/users/mollabashi/expands/openmpi/bin:/home/users/molla
bashi/expands/fftw/bin:/usr/lib64/qt-
3.3/bin:/bin:/usr/local/bin:/usr/bin:/usr/local/sbin:/usr/sbin:/sbin
:.:/home/users/mollabashi/expands/v21.1:.:/home/users/mollabashi/exp
ands/openmpi/bin/
/home/users/mollabashi/expands/v21.1
/opt/exp_soft/local/generic/intel/mkl/lib/intel64:/opt/exp_soft/loca
l/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/compi
lers_and_libraries/linux/lib/intel64:/home/users/mollabashi/expands/
openmpi/lib:/home/users/mollabashi/expands/fftw/lib::/home/users/mol
labashi/expands/fftw/lib:/home/users/mollabashi/expands/openmpie/lib
        linux-vdso.so.1 =>  (0x00007ffc5a316000)
        libpthread.so.0 => /lib64/libpthread.so.0
(0x00002b302431f000)
        libm.so.6 => /lib64/libm.so.6 (0x00002b302453b000)
        libdl.so.2 => /lib64/libdl.so.2 (0x00002b302483d000)
        libiomp5.so =>
/opt/exp_soft/local/generic/intel/compilers_and_libraries/linux/lib/
intel64/libiomp5.so (0x00002b3024a41000)
        libmkl_scalapack_lp64.so =>
/opt/exp_soft/local/generic/intel/mkl/lib/intel64/libmkl_scalapack_l
p64.so (0x00002b3024e47000)
        libmkl_blacs_openmpi_lp64.so =>
/opt/exp_soft/local/generic/intel/mkl/lib/intel64/libmkl_blacs_openm
pi_lp64.so (0x00002b3025772000)
        libmkl_intel_lp64.so =>
/opt/exp_soft/local/generic/intel/mkl/lib/intel64/libmkl_intel_lp64.
so (0x00002b30259b5000)
        libmkl_intel_thread.so =>
/opt/exp_soft/local/generic/intel/mkl/lib/intel64/libmkl_intel_threa
d.so (0x00002b30266d5000)
```

```
        libmkl_core.so =>
/opt/exp_soft/local/generic/intel/mkl/lib/intel64/libmkl_core.so
(0x00002b3029fc0000)
        libmpi_usempif08.so.40 =>
/home/users/mollabashi/expands/openmpi/lib/libmpi_usempif08.so.40
(0x00002b302e601000)
        libmpi_usempi_ignore_tkr.so.40 =>
/home/users/mollabashi/expands/openmpi/lib/libmpi_usempi_ignore_tkr.
so.40 (0x00002b302e839000)
        libmpi_mpifh.so.40 =>
/home/users/mollabashi/expands/openmpi/lib/libmpi_mpifh.so.40
(0x00002b302ea45000)
        libmpi.so.40 =>
/home/users/mollabashi/expands/openmpi/lib/libmpi.so.40
(0x00002b302ecb0000)
        libc.so.6 => /lib64/libc.so.6 (0x00002b302eff4000)
        libgcc_s.so.1 =>
/opt/exp_soft/local/generic/gcc/6.2.0/lib64/libgcc_s.so.1
(0x00002b302f3c2000)
        /lib64/ld-linux-x86-64.so.2 (0x00002b30240fb000)
        libopen-rte.so.40 =>
/home/users/mollabashi/expands/openmpi/lib/libopen-rte.so.40
(0x00002b302f5d8000)
        libopen-pal.so.40 =>
/home/users/mollabashi/expands/openmpi/lib/libopen-pal.so.40
(0x00002b302f89e000)
        librt.so.1 => /lib64/librt.so.1 (0x00002b302fbdd000)
        libutil.so.1 => /lib64/libutil.so.1 (0x00002b302fde5000)
        libz.so.1 => /lib64/libz.so.1 (0x00002b302ffe8000)
        libifport.so.5 =>
/opt/exp_soft/local/generic/intel/compilers_and_libraries/linux/lib/
intel64/libifport.so.5 (0x00002b30301fe000)
        libifcoremt.so.5 =>
/opt/exp_soft/local/generic/intel/compilers_and_libraries/linux/lib/
intel64/libifcoremt.so.5 (0x00002b302413c000)
        libimf.so =>
/opt/exp_soft/local/generic/intel/compilers_and_libraries/linux/lib/
intel64/libimf.so (0x00002b303042c000)
        libintlc.so.5 =>
/opt/exp_soft/local/generic/intel/compilers_and_libraries/linux/lib/
intel64/libintlc.so.5 (0x00002b3030aaf000)
        libsvml.so =>
/opt/exp_soft/local/generic/intel/compilers_and_libraries/linux/lib/
intel64/libsvml.so (0x00002b3030da0000)
        libirng.so =>
/opt/exp_soft/local/generic/intel/compilers_and_libraries/linux/lib/
intel64/libirng.so (0x00002b3032870000)
        linux-vdso.so.1 =>  (0x00002b44fad3b000)
        libpthread.so.0 => /lib64/libpthread.so.0
(0x00002b44faf3d000)
        libm.so.6 => /lib64/libm.so.6 (0x00002b44fb159000)
        libdl.so.2 => /lib64/libdl.so.2 (0x00002b44fb45b000)
```

```
        libiomp5.so =>
/opt/exp_soft/local/generic/intel/compilers_and_libraries/linux/lib/
intel64/libiomp5.so (0x00002b44fb65f000)
        libfftw3_mpi.so.3 =>
/home/users/mollabashi/expands/fftw/lib/libfftw3_mpi.so.3
(0x00002b44fba65000)
        libfftw3.so.3 =>
/home/users/mollabashi/expands/fftw/lib/libfftw3.so.3
(0x00002b44fbc7d000)
        libfftw3_omp.so.3 =>
/home/users/mollabashi/expands/fftw/lib/libfftw3_omp.so.3
(0x00002b44fbf8a000)
        libmkl_intel_lp64.so =>
/opt/exp_soft/local/generic/intel/mkl/lib/intel64/libmkl_intel_lp64.
so (0x00002b44fc191000)
        libmkl_intel_thread.so =>
/opt/exp_soft/local/generic/intel/mkl/lib/intel64/libmkl_intel_threa
d.so (0x00002b44fceb1000)
        libmkl_core.so =>
/opt/exp_soft/local/generic/intel/mkl/lib/intel64/libmkl_core.so
(0x00002b450079c000)
        libmpi_usempif08.so.40 =>
/home/users/mollabashi/expands/openmpi/lib/libmpi_usempif08.so.40
(0x00002b4504ddd000)
        libmpi_usempi_ignore_tkr.so.40 =>
/home/users/mollabashi/expands/openmpi/lib/libmpi_usempi_ignore_tkr.
so.40 (0x00002b4505015000)
        libmpi_mpifh.so.40 =>
/home/users/mollabashi/expands/openmpi/lib/libmpi_mpifh.so.40
(0x00002b4505221000)
        libmpi.so.40 =>
/home/users/mollabashi/expands/openmpi/lib/libmpi.so.40
(0x00002b450548c000)
        libc.so.6 => /lib64/libc.so.6 (0x00002b45057d0000)
        libgcc_s.so.1 =>
/opt/exp_soft/local/generic/gcc/6.2.0/lib64/libgcc_s.so.1
(0x00002b4505b9e000)
        /lib64/ld-linux-x86-64.so.2 (0x00002b44fad19000)
        libimf.so =>
/opt/exp_soft/local/generic/intel/compilers_and_libraries/linux/lib/
intel64/libimf.so (0x00002b4505db4000)
        libsvml.so =>
/opt/exp_soft/local/generic/intel/compilers_and_libraries/linux/lib/
intel64/libsvml.so (0x00002b4506437000)
        libirng.so =>
/opt/exp_soft/local/generic/intel/compilers_and_libraries/linux/lib/
intel64/libirng.so (0x00002b4507f07000)
        libintlc.so.5 =>
/opt/exp_soft/local/generic/intel/compilers_and_libraries/linux/lib/
intel64/libintlc.so.5 (0x00002b4508272000)
```

```
        libopen-rte.so.40 =>
/home/users/mollabashi/expands/openmpi/lib/libopen-rte.so.40
(0x00002b45084ea000)
        libopen-pal.so.40 =>
/home/users/mollabashi/expands/openmpi/lib/libopen-pal.so.40
(0x00002b45087b0000)
        librt.so.1 => /lib64/librt.so.1 (0x00002b4508aef000)
        libutil.so.1 => /lib64/libutil.so.1 (0x00002b4508cf7000)
        libz.so.1 => /lib64/libz.so.1 (0x00002b4508efa000)
        libifport.so.5 =>
/opt/exp_soft/local/generic/intel/compilers_and_libraries/linux/lib/
intel64/libifport.so.5 (0x00002b4509110000)
        libifcoremt.so.5 =>
/opt/exp_soft/local/generic/intel/compilers_and_libraries/linux/lib/
intel64/libifcoremt.so.5 (0x00002b450933e000)
 LAPW0 END
2.314u 0.128s 0:01.57 154.7%   0+0k 198640+504io 10pf+0w
starting parallel lapw0 at Wed May 19 14:30:51 CEST 2021
-------- .machine0 : 2 processors
[1] 19029
----------------------------------------------------------------------
------
By default, for Open MPI 4.0 and later, infiniband ports on a device
are not used by default.  The intent is to use UCX for these
devices.
You can override this policy by setting the btl_openib_allow_ib MCA
parameter
to true.

  Local host:              e1098
  Local adapter:           mlx5_0
  Local port:              1


----------------------------------------------------------------------
------
----------------------------------------------------------------------
------
WARNING: There is at least non-excluded one OpenFabrics device
found,
but there are no active ports detected (or Open MPI was unable to
use
them).  This is most certainly not what you wanted.  Check your
cables, subnet manager configuration, etc.  The openib BTL will be
ignored for this job.

  Local host: e1098
----------------------------------------------------------------------
------
 LAPW0 END
[e1098:19029] 1 more process has sent help message help-mpi-btl-
openib.txt / ib port not selected
```

```
[e1098:19029] Set MCA parameter "orte_base_help_aggregate" to 0 to
see all help / error messages
[e1098:19029] 1 more process has sent help message help-mpi-btl-
openib.txt / no active ports found
[1]    Done                          mpirun -np 2 -machinefile
.machine0 /home/users/mollabashi/expands/v21.1/lapw0_mpi lapw0.def
>> .time00
2.848u 2.203s 0:05.30 95.0%    0+0k 12728+664io 82pf+0w
```