Steps followed:

1. Activate intel compiler: . /opt/intel/oneapi/setvars.sh
2. Configuration: ./configure MPIF90=mpiifort CC=mpiicc F90=ifort -enable-parallel --with-libxc --with-libxc-prefix='/opt/etsf'

Output:

*The following libraries have been found: BLAS\_LIBS= -lmkl\_intel\_lp64 -lmkl\_sequential -lmkl\_core LAPACK\_LIBS= FFT\_LIBS= LIBXC\_LIBS= -L/opt/etsf/lib -lxcf03 -lxc Please check if this is what you expect.*

1. Make.inc

**DFLAGS** = -D\_\_DFTI -D\_\_LIBXC -D\_\_MPI

**IFLAGS** = -I$(TOPDIR)/include -I$(TOPDIR)/FoX/finclude - I/opt/intel/oneapi/mkl/latest/include -I/opt/etsf/include

**LD\_LIBS** = -L/opt/etsf/lib -lxcf90 –lxc *(As you suggested)*

**BLAS\_LIB** = -L${MKLROOT}/lib/intel64 -lmkl\_scalapack\_ilp64 -lmkl\_blacs\_intelmpi\_ilp64- lpthread -lm –ldl

**LAPACK\_LIB** = same as above (Took from intel advisor website)

**FFT\_LIB** = same as above

**MPI\_LIBS**= -L/opt/intel/oneapi/mpi/2021.2.0/lib/ -lmpi

**LIBXC\_LIBS** = -L/opt/etsf/lib -lxcf90 -lxc

1. Make –j 2 pw

Output:

/home/flame/Downloads/test\_qe/new/q-e-qe-6.7.0/upflib/radial\_grids.f90:364: undefined reference to `dptsv\_' libupf.a(upf\_invmat.o): In function `upf\_invmat\_mp\_invmat\_': /home/flame/Downloads/test\_qe/new/q-e-qe-6.7.0/upflib/upf\_invmat.f90:41: undefined reference to `dgetrf\_' /home/flame/Downloads/test\_qe/new/q-e-qe-6.7.0/upflib/upf\_invmat.f90:43: undefined reference to `dgetri\_' /opt/intel/oneapi/mkl/latest/lib/intel64/libmkl\_scalapack\_ilp64.so: undefined reference to `slaq5\_' /opt/intel/oneapi/mkl/latest/lib/intel64/libmkl\_scalapack\_ilp64.so: undefined reference to `dlarrv\_' /opt/intel/oneapi/mkl/latest/lib/intel64/libmkl\_scalapack\_ilp64.so: undefined reference to `sisnan\_' /opt/intel/oneapi/mkl/latest/lib/intel64/libmkl\_scalapack\_ilp64.so: undefined reference to `dgemv' /opt/intel/oneapi/mkl/latest/lib/intel64/libmkl\_scalapack\_ilp64.so: undefined reference to `dlaebz\_' (series of these lines appeared)

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Makefile:60: recipe for target 'virtual\_v2.x' failed make[1]: \*\*\* [virtual\_v2.x] Error 1 make[1]: Leaving directory '/home/flame/Downloads/test\_qe/new/q-e-qe-6.7.0/upflib' Makefile:194: recipe for target 'libupf' failed make: \*\*\* [libupf] Error 1 make: \*\*\* Waiting for unfinished jobs....

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a - ParO/paro\_k.o a - ParO/pcg\_k.o a - ParO/paro\_gamma\_new.o a - ParO/paro\_k\_new.o a - DENSE/rotate\_HSpsi\_gamma.o a - DENSE/rotate\_HSpsi\_k.o a - DENSE/rotate\_wfc\_gamma.o a - DENSE/rotate\_wfc\_k.o ranlib libks\_solvers.a make[1]: Leaving directory '/home/flame/Downloads/test\_qe/new/q-e-qe-6.7.0/KS\_Solvers'

1. **Input file**

**PP file taken from qE website SCAN Pseudo-potential**

&control calculation = 'scf' prefix='O', etot\_conv\_thr = 1e-5 forc\_conv\_thr = 1e-4 pseudo\_dir = '/home/flame/Downloads/test\_qe/new/q-e-qe-6.7.0/SSSP\_precision\_pseudos' outdir= '/home/flame/Downloads/test\_qe/new/q-e-qe-6.7.0/fresh/oxygen/' restart\_mode='from\_scratch', wf\_collect=.true. / &system input\_dft = 'scan' degauss = 1.4699723600d-02 ecutwfc = 7.5000000000d+01 ibrav= 0, nat= 1, ntyp= 1 / &electrons conv\_thr = 1e-7 / ATOMIC\_SPECIES O 16 O.SCAN.UPF ATOMIC\_POSITIONS bohr O 1.00000000000000 0.00000000000000 0.00000000000000 K\_POINTS gamma CELL\_PARAMETERS {bohr} 30.0000000000000 0.00000000000000 0.00000000000000 0.00000000000000 30.0000000000000 0.00000000000000 0.00000000000000 0.00000000000000 30.0000000000000

1. **pw.x < o\_scf.in > o\_scf\_new2.out**

**Output:**

Current dimensions of program PWSCF are: Max number of different atomic species (ntypx) = 10 Max number of k-points (npk) = 40000 Max angular momentum in pseudopotentials (lmaxx) = 3 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%% Error in routine set\_dft\_from\_name (1): SCAN: unrecognized dft %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%