Building the libraries and packages required for 3D spectral code

First of all, update gfortran and set the most updated version as the default gcc compiler.

1- Install Intel MKL 10.0 (tarball can be found in ~/packages) which is then to be installed using install.sh in the home directory. Go to your installation directory (/opt/intel/mkl/10.0.1.14/interfaces/lapack95) and change the following line in the makefile and run it:

```
FC= gfortran
make
```

Copy the module files to "working_directory/include".

2- Install Python 2.7.18 (or similar) which is needed for PETSC.

3- Install an implementation of MPI (need mpif90 and ifort). I had a better experience with MPICH (follow the readme file for installation).

4- To build NETCDF-fortran you need to install NETCDF-C, and for NETCDF-C you need HDF5 and Zlib:

- Follow the instructions below: https://www.unidata.ucar.edu/software/netcdf/documentation/NUG/getting_and_building_netcdf.html

- Use version HDF5-1.8.9 or higher (1.8.22 in my case) and install with parallel I/O support.

- When you compile NETCDF-C after HDF5 and Zlib you might get an error about curl.h which means you have to install the following package:

```
$ sudo apt-get install libcurl4-openssl-dev
```

- After building NETCDF -C you can now build NETCDF-fortran. Follow the instructions here (try "Building with static libraries"): https://www.unidata.ucar.edu/software/netcdf/docs/building_netcdf_fortran.html

```
$ NCDIR=/usr/local

$ CPPFLAGS="-I${NCDIR}/include -I${H5DIR}/include -I${ODIR}/include"
LDFLAGS="-L${NCDIR}/lib -L${H5DIR}/lib -L${ODIR}/lib -L/home/mpich_installation_directory/lib"
LD_LIBRARY_PATH=${NCDIR}/lib:${H5DIR}/lib:${ODIR}/lib
LIBS="-lnetcdf -lmpi -lhdf5_hl -lhdf5 -lz -lcurl" ./configure --disable-shared --prefix=${NCDIR}
```

- Download and compile Lapack95. You need the module files such as "f95_lapack" to load in "ModBasicMath.f90". Follow the readme file and change the following lines in the makefile:

```
FC= gfortran -ffree-form
FC1= gfortran -ffixed-form
OPTS0=

$ make single_double_complex_dcomplex
```

Copy the module files to “working_directory/include”.

- Download Blas (eg. 3.8.0) and Lapack (eg. 3.9.1) and compile them.
- Install Valgrind.
- Install PETSC by introducing the directories of Blas and Lapack:

```
 $ ./config/configure.py -with-cc=mpicc --with-fc=mpif90 --with-blas-lib=/blas-directory/BLAS-3.8.0/blas_LINUX.a
--with-lapack-lib=/lapack-directory/liblapack.a --with-valgrind-dir=/valgrind-directory --with-shared=0

$ make all check
```

- Install FFTW (best to use module files).
- Finally, run the following command first before compile the code:

```
 $ export
LD_PRELOAD=/opt/intel/oneapi/mkl/2021.2.0/lib/intel64/libmkl_def.so.1:/opt/intel/oneapi/mkl/2021.2.0/lib/intel64/libmkl_av
x2.so.1:/opt/intel/oneapi/mkl/2021.2.0/lib/intel64/libmkl_core.so:/opt/intel/oneapi/mkl/2021.2.0/lib/intel64/libmkl_intel_threa
d.so
```

It tells the compiler to search for the required shared libraries in the directories listed above.