Information for the 2021 Virtual School on Electron-Phonon Physics and the EPW code

Hands-on session

Hands-on based on QE v6.7 and EPW v5.4Beta

1. Preparation

There are two ways to follow the hands-on during the school:

(1) **Running on the Frontera cluster [recommended]**

▶ Connect with X11 support on Frontera:

Note: Some tutorials use the plotting software such as gnuplot and you are advised to connect with X11 support on Frontera. If you encounter a connection problem, etc., you can connect without X11 support. For further information on Frontera, please see the page at https://frontera-portal.tacc.utexas.edu/user-guide/admin/ .

```
$ ssh -Y USER_NAME@frontera.tacc.utexas.edu (or ssh -X ...)
```

Then you will need to enter your password and the second authentication with the TACC Token app that you can download on your phone from the Android/Apple shop. Please see the following page for further information (download link for TACC token app, etc.) about multifactor authentication at TACC: https://portal.tacc.utexas.edu/tutorials/multifactor-authentication

▶ Export the code PATH variable:

```
$ export PATHQE=/work2/06868/giustino/EPW-SCHOOL/q-e
```

Note: You will need to redo this export every time you login.

▶ Running jobs on the Frontera compute nodes:

Below is a sample jobscript you can use for job submission (copy and paste might not work).

```
#!/bin/bash
#SBATCH -J myjob
#SBATCH -o myjob.o%j
#SBATCH -e myjob.e%j
#SBATCH -N 1               # This line should not be changed.
#SBATCH -n 8               # Number of MPI tasks can be controlled here.
#SBATCH -t 01:30:00        # Run time (hh:mm:ss)
#SBATCH -A EPW-SCHOOL      # This line should not be changed.
#SBATCH -p small           # This line should not be changed.
#SBATCH --reservation=EPW-SCHOOL-06-13-2021 # Each day of the class the date (06-13) should be updated.

module purge
module load TACC

# Launch MPI code...
# Use ibrun instead of mpirun or mpiexec
ibrun /work2/06868/giustino/EPW-SCHOOL/q-e/bin/pw.x -input scf.in > scf.out
```

Several variants are also allowed, but you should follow the four instructions below:

1. Use the system default collection of modules. If you made any changes to modules, you have to restore them to the default modules: `make purge; module load TACC`

2. Run jobs by submitting batch jobs with sbatch; do not use an interactive session.
3. Use one node: the maximum number of MPI tasks per node is 56.
4. Add the following three SBATCH directives to your jobscript (copy and paste might not work):

```
#SBATCH -A EPW-SCHOOL
#SBATCH -p small
#SBATCH --reservation=EPW-SCHOOL-06-13-2021 # Each day of the class the date (06-13) should be updated.
```

You can then submit your job using:

```
$ sbatch SCRIPT_NAME.sh
```

You can see the status of your running job by doing:

```
$ squeue -u USER_NAME
```

▶ Copying and extracting the tutorial tarballs:

The tutorial tarballs sit in /work2/06868/giustino/EPW-SCHOOL/. Please copy the tutorial tarball into your scratch directory using:

```
$ cp /work2/06868/giustino/EPW-SCHOOL/XXX.X.XXXXX.tar $SCRATCH
```

(2) **Running on your own desktop or local cluster**

Note: We are not supporting this option. If you have trouble compiling the code on your own machine, please use the method 1 above.

▶ Download the code for the school:

```
$ wget https://docs.epw-code.org/_downloads/q-e-EPWv5.4Beta.tar.gz
```

Then untar it and go inside the folder. Then issue:

```
$ ./configure (additional options would be required.)
```

and then

```
$ make epw pp
$ cd test-suite/not_epw_comp ; make
$ cd EPW/ZG_displacement/src ; make
$ cd EPW/ZG_displacement/src/local ; ./compile_ifort.sh (or ./compile_gfortran.sh)
```

Note: If you want to run the parallel version of Wannier90, you need to install it in `YOUR_PATH/q-e/wannier90-3.1.0-par`

Then export the path where you installed it:

```
$ export PATHQE=YOUR_PATH/q-e
```

2. Other things to know about the EPW calculations will be covered during Hands-On Intro: Running EPW [9:20-10AM (PDT) on Tuesday 15 June].