EPW School 2026 Cheat Sheet

Installed executables, Frontera/VISTA environment setup, GPU build/run commands, I/O troubleshooting, and file downloads

1. Installed executables and environments

Use these shared locations during the school. For most calculations, add the appropriate code directory to PATH or call executables from the corresponding bin directory.

Item	Path	Use
EPW v6.1s	/work2/05193/sabyadk/shared/EPW_6.1s/q-e	Main EPW v6.1s installation.
Quantum ESPRESSO 7.6 develop branch for Frontera GPU	/work2/05193/sabyadk/shared/QE_7.6devGPU/q-e	GPU-enabled QE develop installation on Frontera.
Quantum ESPRESSO 7.6 develop branch with EPW 6.1	/work2/05193/sabyadk/shared/QE_7.6dev/q-e	QE develop installation including EPW 6.1.
Wannier90 v3.1.0	/work2/05193/sabyadk/shared/W90/wannier90-3.1.0	Wannier90 installation for tutorials requiring Wannierization.
NVHPC compiler on Frontera	/scratch3/05193/sabyadk/nvidia/hpc_sdk_24.7	Needed only if building GPU-enabled QE on Frontera.
Virtual environment for EPWpy + EPW v6.1s	/work2/05193/sabyadk/shared/Virtual_env/venv/bin	Only for the last EPWpy tutorial on VISTA.

2. Running EPW v6.1s

EPW v6.1s was compiled with HDF5, so load the HDF5 module before running.

```
module load hdf5/1.10.4
export PATH=/work2/05193/sabyadk/shared/EPW_6.1s/q-e/bin:$PATH
```

Example launch pattern:

```
mpirun -np 1 pw.x -in scf.in > scf.out
```

3. Running QE v7.6devGPU on Frontera

Start an RTX development session before running GPU-enabled QE:

```
idev -N 1 -n 4 -p rtx-dev
```

Then load the GPU build environment:

```
module purge
deactivate
source /work2/05193/sabyadk/shared/QE_7.6devGPU/clean.sh
export PATH=/work2/05193/sabyadk/shared/QE_7.6devGPU/q-e/bin:$PATH
```

Expected mpirun: The clean.sh script prints the MPI launcher it will use:
/scratch3/05193/sabyadk/nvidia/hpc_sdk_24.7/Linux_x86_64/24.7/comm_libs/12.5/hpcx/hpcx-2.19/ompi/bin/mpirun

Launch calculations in the same manner as the non-GPU case, but disable CPU binding:

```
mpirun -np 1 --bind-to none pw.x -in scf.in > scf.out
```

4. Building GPU-enabled QE on Frontera, if needed

For the QE GPU tutorial, the recommended approach is to source the provided environment file instead of manually reconstructing the NVHPC environment.

```
source /work2/05193/sabyadk/shared/QE_7.6devGPU/clean.sh
```

Configure QE with CUDA support as follows:

```
./configure --enable-parallel --enable-openmp \
  --with-cuda=/scratch3/05193/sabyadk/nvidia/hpc_sdk_24.7/Linux_x86_64/24.7/cuda/12.5 \
  --with-cuda-cc=75 \
  --with-cuda-runtime=12.5 \
  --with-cuda-mpi=no
```

5. EPWpy environment on VISTA

For the last tutorial on VISTA, use the EPWpy + EPW v6.1s virtual environment:

```
source /work2/05193/sabyadk/shared/Virtual_env/venv/bin/activate
```

6. I/O troubleshooting

6.1 Frontera

If the wall time is more than about 2-3 times the CPU time without OpenMP, the run may be slowed by I/O. Set Lustre striping in the working directory before launching the calculation:

```
lfs setstripe -c 8 $PWD
```

6.2 VISTA

For similar MPI-IO slowdowns on VISTA, use the following OpenMPI/ROMIO settings. For the last ROMIO_FSTYPE_FORCE line, use either $SCRATCH or the specific folder where MPI-IO occurs.

```
export OMPI_MCA_fs=ufs
export OMPI_MCA_fs_ufs_lock_algorithm=1
export OMPI_MCA_io=^ompio
export ROMIO_FSTYPE_FORCE="ufs:$SCRATCH"
# OR, for a specific working folder:
export ROMIO_FSTYPE_FORCE="ufs:/path_to_working_folder_where_MPIIO_occurs/"
```

7. Downloading tutorial files from Google Drive

Tutorial files can be downloaded directly with wget by using the Google Drive file ID.

```
FILEID="1b8Mhsoc58sxeRZiuVIOh5qwvtG5so0FP"
FILENAME="Mon.4.Giannozzi.tar"

wget --no-check-certificate \
  "https://drive.google.com/uc?export=download&id=${FILEID}" \
  -O "${FILENAME}"
```

For a link such as:

```
https://drive.google.com/file/d/1b8Mhsoc58sxeRZiuVIOh5qwvtG5so0FP/view?usp=drive_link
```

the file ID is:

```
1b8Mhsoc58sxeRZiuVIOh5qwvtG5so0FP
```