2024 School on Electron-Phonon Physics, Many-Body Perturbation Theory, and Computational Workflows

10-16 June 2024, Austin, TX

Hands-On Tutorial
QUANTUM ESPRESSO on GPUs

Hands-on based on today's development version of QE

In this session we will learn how to compile and run QUANTUM ESPRESSO for GPUs.
Logon to Frontera. Load the needed modules:

```
$ module load gcc mkl
$ module unload impi/19.0.9
```

It may be useful to prepare a script file like the following one:

```
#!/bin/bash
#SBATCH -J myjob            # Job name
#SBATCH -p rtx              # Queue (partition) name#
#SBATCH -o jobout.%j        # (optional) Name of stdout output file
#SBATCH -e joberr.%j        # (optional) Name of stderr error file
#SBATCH -N 1                # Total # of nodes
#SBATCH -n 4                # Total # of mpi tasks
#SBATCH -t 00:10:00         # Run time (hh:mm:ss)
#SBATCH -A DMR23030
#SBATCH --reservation= DMR23030_rtx_June_15

module load gcc mkl
module unload impi/19.0.9
NVHPC=/work2/05193/sabyadk/shared/NVHPC  # path to school material
export PATH=$NVHPC/Linux_x86_64/24.5/compilers/bin:$PATH
export MANPATH=$NVHPC/Linux_x86_64/24.5/compilers/man:$MANPATH
export PATH=$NVHPC/Linux_x86_64/24.5/comm_libs/mpi/bin:$PATH
```

Compilation

Start an interactive session on Frontera GPU partition:

```
$ idev -p rtx -N 1 -n 4 -t 00:15:00
```

(in this example, 1 node, 4 GPUs, 15 minutes). The compilation of QUANTUM ESPRESSO requires that the NVidia HPC standard development kit (SDK) is available, that the nvfortran compiler and related libraries are in the paths, etc. etc.. This is why you need to define the following variables:

```
NVHPC=/work2/05193/sabyadk/shared/NVHPC   # path to school material
export PATH=$NVHPC/Linux_x86_64/24.5/compilers/bin:$PATH
export MANPATH=$NVHPC/Linux_x86_64/24.5/compilers/man:$MANPATH
export PATH=$NVHPC/Linux_x86_64/24.5/comm_libs/mpi/bin:$PATH
```

To get a copy of QUANTUM ESPRESSO:

```
PATHSC=/work2/05193/sabyadk/stampede3/EPWSchool2024/tutorials/
tar -xf $PATHSC/qe-7.3.1.tar
```

There are two ways to compile the QUANTUM ESPRESSO distribution:

1. Using autoconf
2. Using CMake

▶ Compile using autoconf

```
$ cd qe-7.3.1
$ ./configure --with-cuda=$NVHPC_CUDA_HOME --with-cuda-cc=75 \
              --with-cuda-runtime=12.4  --without-scalapack  \
              --with-cuda-mpi
```

Note 1: with-cuda-cc depends upon the kind of GPU: use nvidia-smi –query-gpu=compute_cap –format=csv to find it (remove the dot: $7.5 => 75$)
Note 2: with-cuda-runtime depends upon the installed software
Note 3: -with-cuda-mpi ONLY if your hardware supports CUDA MPI
If there are no errors, compile:

```
$ make -j pw pp ph
```

(`-j` for parallel compilation; you may add whatever code you need, or specify `make all`). Links to executables are in `bin/`.
▶ Compile using CMake

```
$ cd qe-7.3.1
$ mkdir build
$ cd build
$ cmake -DCMAKE_C_COMPILER=nvc -DCMAKE_Fortran_COMPILER=nvfortran \
  -DQE_ENABLE_MPI_GPU_AWARE=ON -DQE_ENABLE_CUDA=ON -DQE_ENABLE_OPENACC=ON \
  -DQE_FFTW_VENDOR=FFTW3 -DNVFORTRAN_CUDA_VERSION=12.4 -DNVFORTRAN_CUDA_CC=75 ../
$ make [-jN]
```

Note the ../ at the end of the cmake command!
Finally you may run your first GPU run with QUANTUM ESPRESSO, e.g.:

```
export ESPRESSO_PSEUDO=./           # path to pseudopotential files
export ESPRESSO_TMPDIR=./tmpdir     # path to output data files
export OMP_NUM_THREADS=1
mpiexec -n 4 bin/pw.x < scf.in
```

(alternatively, `mpirun -np 4`) where scf.in is any valid (or even invalid) input for `pw.x`.

Running Quantum ESPRESSO

Download and unpack the input files of the tutorial of Monday:

```
$ cp $PATHSC/Mon.5.Giannozzi.tar .
$ tar -xvf Mon.5.Giannozzi.tar
```

▶ Run some or of all the tests that you run on CPU on Monday.
Note that each self-consistent or phonon calculation is quite small so do not expect a large speedup with respect to CPU execution. You may use 1 node (4 GPUs) and parallelize over k-points (`-nk 4`), then 2 or 4 nodes.
▶ Run a larger test
For a more significant test, you may try the input file `lpafa.in` contained in this file:

```
$ cp $PATHSC/Sat.2.Giannozzi.tar .
$ tar -xvf Sat.2.Giannozzi.tar
```

and compare it with CPU execution. It is a metal-organic framework containing 72 atoms
▶ Soft phonons in $BaTiO_3$ perovskite
The high-temperature structure of $BaTiO_3$ is cubic (Pm3m). The phonon modes are however *soft*: the structure is stabilized by anharmonicity. At lower temperature, the Ti atom moves away from the center of the O octahedron and becomes tetragonal (P4mm). The phonon modes are however still soft. A further transition brings $BaTiO_3$ to an orthorhombic (Amm2) structure. At even lower tenperature the Ti atoms moves in the $< 111 >$ direction and the structure becomes rhombohedral, with R3m (n.160) space group.
Can you compute the phonon modes for at least one of the two lower-temperature structures? For the R3m structure, it is convenient to start with a fake rhombohedral lattice equal to a simple cubic one and to displace the Ti, Ba and O atoms in the $< 111 >$ direction. Sample files can be found in `example_BaTiO3`.