Quantum ESPRESSO

Purpose: Electronic structure, materials modelling
Latest version: 7.1
License: Free of use
GNU GPL_ext-link
Website: *https://www.quantum-espresso.org/_ext-link*

Quantum ESPRESSO is a suite for electronic structure calculations and simulation of nano-structured materials.

The core of Quantum ESPRESSO are density functional theory (DFT) electronic calculations using plane-wave basis sets and pseudo-potential.

SLURM Submit script example

For more information use the ***Job Script Generator***.

Sbatch options:

The options shown in the example are detailed below. For more information and a more comprehensive list of available options, see the ***sbatch command page***.

- **-J**: Name for the job's allocation.
- **-e**: Name of the stderr redirection filename.
- **-o**: Name of the stdout redirection filename.
- **-p**: Name of the partition (queue) where the job will be submitted.
- **-n**: Number of tasks.
- **-c**: Number of cores per task.

qe_example.slm

```
#!/bin/bash
#SBATCH -J qe_example
#SBATCH -e qe_example.err
#SBATCH -o qe_example.out
#SBATCH -p std
#SBATCH -n 1
#SBATCH -t 00-01:00

module purge
module load apps/quantumespresso/6.2.1

##
#  Modify the input and output files!
INPUT_FILE=qe_example.inp
OUTPUT_FILE=qe_example.log
export ESPRESSO_PSEUDO=${SCRATCH}/pseudo

##
#  You don't need to modify nothing more
cp -r ${SLURM_SUBMIT_DIR}/{pseudo,${INPUT_FILE}}
${SCRATCH}
cd ${SCRATCH}

srun pw.x -i qe ${INPUT_FILE} > ${OUTPUT_FILE}

cp ./${OUTPUT_FILE} ${SLURM_SUBMIT_DIR}
```

- **-t**: Set the job's time limit. If the job don't finish before the time runs out, it will be killed.

Software execution information:

The environment variable *ESPRESSO_PSEUDO* indicates where the pseudo-potentials files are located.

The executable used (***pw.x***) should change depending on the calculation kind (***more info_ext-link***).