# Getting started with Quantum Espresso for APAC HPC-AI Competition

## 1. Overview

Quantum Espresso (QE) is a suite of first-principles codes designed for electronic-structure calculations and materials modelling. It is a powerful tool to study materials properties at nanoscale and fast screen the potential candidates for certain application.

In this competition, we will use QE to complete the HPC task I, which is running a SCF calculation to obtain the total energy of $CeO_2$. The goal is to achieve the best parallel performance on a supercomputing cluster for this specific computational job.

## 2. Access QE

### 2.1. Compilation from source code

The source code of QE can be downloaded from https://gitlab.com/QEF/q-e.

- Ensure MPI library can be found
- Use `make pw` to specify the plane wave code

### 2.2. Load modulefile on Gadi

Multiple versions of QE have already been pre-installed on Gadi supercomputer under the path: /apps/qe. There are also some handy commands to help you inspect the available software using Environment Modules. Simply type in:

```
module avail qe
```

which would print out the following content on the terminal:

```
------------------------------------------- /apps/Modules/modulefiles -------------------------------------
--

qe/6.4.1  qe/6.6  qe/6.7.0  qe/6.8  qe/6.8-gpu  qe/7.0
```

This tells you all the available versions of QE currently accessible on Gadi.

If we want to have a closer look at the information of the newest qe/7.0, we can use the *display* or *show* command:

```
module display qe/7.0
-------------------------------------------------------------------
/apps/Modules/modulefiles/qe/7.0:

module          load openmpi/4.1.2
prepend-path    PATH /apps/qe/7.0/bin
```

```
setenv          ESPRESSO_PSEUDO /apps/qe/7.0/pseudo
setenv          TMPDIR /scratch/dy3/jf1411/tmp
setenv          TMP_DIR /scratch/dy3/jf1411/tmp
conflict        qe
setenv          QE_BASE /apps/qe/7.0
setenv          QE_ROOT /apps/qe/7.0
setenv          QE_VERSION 7.0
module-whatis   {qe, version 7.0}
-------------------------------------------------------------------
```

To load QE into your current work environment, you can use the *module load* command

```
module load qe/7.0

Loading qe/7.0

  Loading requirement: openmpi/4.1.2
```

Then the loaded modulefiles can be inspected by:

```
module list

Currently Loaded Modulefiles:

 1) openmpi/4.1.2(default)   2) qe/7.0
```

# 3. Job submission for the competition task

## 3.1. Input files

- CeO2.in – includes all the parameters to set up a SCF calculation using QE
- Pseudopotentials – under the folder name /pseudo. The choice of pseudopotentials for Ce and O atoms is from Standard solid-state pseudopotentials (SSSP).

## 3.2. Submission script

Submission script is used to configurate the resources used for the PBS jobs and the command for the execution of Quantum Espresso. Parameters related to the CPU parallelism should also be set in this file. A sample of submission script for testing QE on Gadi is provided here:

```
#!/bin/bash

#PBS -l walltime=00:10:00

#PBS -l ncpus=48

#PBS -l mem=190gb

#PBS -l software=qe

#PBS -l wd

module load openmpi/4.1.2
```

```
module load qe/7.0
export OMP_NUM_THREADS=1
mpirun pw.x -npool 1 -ndiag 1 -inp CeO2.in > CeO2.out
```

# 4. Tunables/Non-Tunables

The computational resources consumed by Quantum Espresso are closely related to the model setup and the selected optimisation algorithm. To fairly assess the submitted answers from participants, we provide some more detailed explanation of the parameter setup in the CeO2 energy calculation.

## 4.1. Parameters can be modified:

Jobs should be tested on a single node then scale up to the maximum of 32 nodes (e.g. for the normal nodes on Gadi supercomputer, it would be 32 × 48 = 1536 cores). The key parameters to test out are in the submission script:

- Number of processes (-np)
- Number of pools (-npool)
- Diagonalization (-ndiag)
- Number of openMP threads (OMP_NUM_THREADS)

Parameters should be optimised to reach the optimal performance, i.e. the shortest CPU time for calculating the energy.

## 4.2. In contrast, parameters that are directly associated with the model accuracy are NOT allowed to be modified:

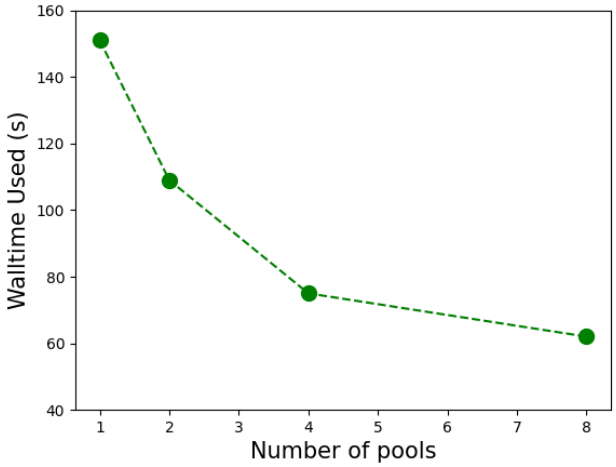
- The input file (CeO2.in), which includes the number of iterations, convergence threshold, cutoff energies, … etc.
- Pseudopotentials.

## 4.3. For teams that decide to compile their own versions of QE (optional), things that can be considered changing are:

- Version of compilers

## 5. Assessment

Teams should experiment the parallelization parameters and identify the optimal combination for this specific task. The trend of the CPU time change should also be discussed using figures or tables. A sample figure (which is NOT plotted from the $CeO_2$ data in our competition task) is provided here.




## 6. Reference

- Input File Description of pw.x: https://www.quantum-espresso.org/Doc/INPUT_PW.html
- Gadi user guide for QE: https://opus.nci.org.au/display/Help/Quantum+ESPRESSO