

# CHPC Student Cluster Competition 2022

## Quantum ESPRESSO

Quantum **ESPRESSO** (op**En**-**S**ource **P**ackage for **R**esearch in **E**lectronic **S**tructure, **S**imulation, and **O**ptimization) is an integrated suite of computer codes for electronic-structure calculations and materials modeling at the nanoscale. It is based on density-functional theory, plane waves, and pseudopotentials.

Refer to [https://www.quantum-espresso.org/Doc/user\\_guide](https://www.quantum-espresso.org/Doc/user_guide) for detailed usage and installation instructions. The flash drive you have been provided contains the current release of Quantum ESPRESSO for use in the competition. Additionally, to successfully build Quantum Espresso you will require:

- **FORTRAN** compiler and **MPI** wrapper,
- Implementations of **BLAS**, **LAPACK**, **SCALAPACK** and *optionally* **FFTW** libraries.

## Benchmark

The **AUSURF112** benchmark, as the name suggests, consists of 112 Gold (AU) atoms in a layered sheet configuration.

```
$ git clone https://github.com/QEF/benchmarks.git
$ cd benchmarks/AUSURF112
$ mpirun -np <NUM_PROCS> <MPI_FLAGS> pw.x -inp ausurf.in
```

You must **SUBMIT TWO RESULTS**, one for a **SINGLE NODE** and one for your entire **CLUSTER**. Ideally the performance scaling should be linear, (i.e. three nodes *‘should’* complete the problem three times as fast as a single node run). The key scoring metric is the final wall clock time, where your submission to the judges must include:

- `pw.x` binary,
- Single node and cluster `run_qe.sh` scripts,
- Single node and cluster `qe_log_**` files, and
- The simulation output files `ausurf.wfc1`.

## MPI Profiler

Run an **IPM** (or any other) MPI Profiler for the `ausurf.in` benchmark, across your entire cluster and submit the output report that details the usage of the most predominant MPI calls.