



Guide to Running Quantum ESPRESSO

What is Quantum ESPRESSO

Quantum ESPRESSO is an integrated suite of open-source computer codes for electronic-structure calculations and materials modelling at the nanoscale. It is based on density-functional theory, plane waves, and pseudopotentials.

Quantum ESPRESSO has evolved into a distribution of independent and inter-operable codes in the spirit of an open-source project. The Quantum ESPRESSO distribution consists of a “historical” core set of components, and a set of plug-ins that perform more advanced tasks, plus a number of third-party packages designed to be inter-operable with the core components. Researchers active in the field of electronic-structure calculations are encouraged to participate in the project by contributing their own codes or by implementing their own ideas into existing codes.



Quantum ESPRESSO Functionality

Ground-state calculations (Self-consistent total energies, forces, stresses, Kohn-Sham orbitals, separable norm-conserving and ultrasoft (Vanderbilt) pseudo-potentials, PAW (Projector Augmented Waves, structural optimization, several exchange-correlation functionals: from LDA to generalized-gradient corrections (PW91, PBE, B88-P86, BLYP) to meta-GGA, exact exchange (HF) and hybrid functionals (PBE0, B3LYP, HSE), VdW corrections (DFT-D) or nonlocal VdW functionals (vdw-DF), Hubbard U (DFT+U), Berry’s phase polarization, spin-orbit coupling and noncollinear magnetism),

Structural optimizations (GDIIS with quasi-Newton BFGS preconditioning, damped dynamics),

Transition states and minimum energy paths (Nudged Elastic Band method (PWneb), Meta-Dynamics using the PLUMED plug-in),

Ab-initio molecular dynamics (Car-Parrinello molecular dynamics (CP), Born-Oppenheimer molecular dynamics (PWscf)),

Response properties (DFPT) (Phonon frequencies and eigenvectors at any wavevector, full phonon dispersions; inter-atomic force constants in real space, translational and rotational acoustic sum rules, effective charges and dielectric tensors, electron-phonon interactions, third-order anharmonic phonon lifetimes, infrared and (non-resonant) Raman cross-sections, EPR and NMR chemical shifts using the GIPAW method),

Spectroscopic properties (K- and L₁-edge X-ray Absorption Spectra (XSpectra), Time-Dependent Density Functional Perturbation Theory (TD-DFT), electronic excitations with

Many-Body Perturbation Theory using YAMBO package, electronic excitations with Many-Body Perturbation Theory using GWL package)..

Step 1 - Log in

The examples used in this guide are configured to run on the Cardiff Skylake *Hawk* cluster. Connect to *hawklogin.cf.ac.uk* with your Supercomputing user credentials using your preferred method (e.g. PuTTY from a Windows machine or ssh from any Linux terminal, thus

```
ssh -l your_username hawklogin.cf.ac.uk
```

The steps below involve typing commands (**in bold font**) in the terminal window.

Step 2 - Load a Quantum ESPRESSO module

In common with most of the application guides in this series, we assume at the outset that the module of choice would be selected from those originally available on HPC Wales. Thus, a necessary first step would be to gain access to that module set by issuing the commands

```
module purge  
module load hpcw
```

Note that the “module purge” command is required to prevent any unintentional collision with pre-existing modules. Subsequently issuing the module command

```
module avail hpcw
```

will provide visibility of and access to the entire set of HPCW modules.

A number of Quantum ESPRESSO binary packages are available. Note that in common with most other software packages on the system, these are built with the Intel compiler.

List pre-installed Quantum ESPRESSO versions:

```
module avail quantumespresso
```

Load the default version (5.2.1):

```
module load quantumespresso
```

Confirm the loaded modules. All dependencies are handled automatically via the module file:

```
module list
```

Step 3 - Create a directory

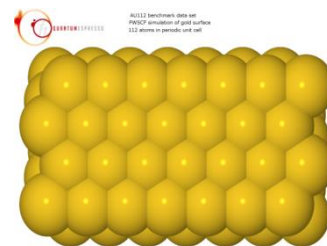
From your home directory, create a directory to hold the Quantum ESPRESSO data:

```
cd ~  
mkdir espresso-5.2
```

Step 4 - Obtain a test case

A validation and benchmark test cases are provided with the installation at:

```
/app/chemistry/quantumespresso/5.2.1/example
```



The directory `/app/chemistry/quantumespresso/5.2.1/inputFiles` contains the required input files.

Copy the benchmark job script to your user space:

```
cd ~/espresso-5.2
cp -rip
/app/chemistry/quantumespresso/5.2.1/example/benchmark/run_esp
resso.AUSURF112.SLURM.q .
```

Note that the SLURM job script points to the location of the required input files. The benchmark case is Au₁₁₂, a 112-atom gold surface (see figure), with 2,158,381 G vectors, two k-points, and FFT dimensions (180, 90, 288).

Step 5 - Submit a parallel job

Now you are ready to run this test case with the supplied job script

```
run_espresso.AUSURF112.SLURM.q
```

From your working directory, submit the job using:

```
sbatch run_espresso.AUSURF112.SLURM.q
```

Check the job queue using: `squeue`

When execution commences, a file called `AUSURF112_NCPUS=160.id-<Job_ID>.out` is created in the espresso-5.2 directory that holds the job output - many temporary files are generated and routed to the user's scratch directory, `run_espresso-AUSURF112_120-procs_id-<Job_ID>`, created by the job (where `<Job_ID>` is the ID assigned by the SLURM queuing system).

The job should take around 8.5 minutes using 160 cores if the case runs successfully.

The file `AUSURF112_NCPUS=160.id-<Job_ID>.out` should contain all the output and point to successful completion of the job.

Compare your job output with the output file

```
/app/chemistry/quantumespresso/5.2.1/example/benchmark/AUSURF1
12_NCPUS=160.id-14825.out
```

Step 6 – More Test Cases

More test cases are distributed with Quantum ESPRESSO. They can be found at

```
/app/chemistry/quantumespresso/5.2.1/example/inputFiles
```

The GRIR443 benchmark arises from a PRACE benchmarking suite. This is a simulation of a carbon–iridium complex (C₂₀₀Ir₂₄₃), with 2,233,063 G-vectors, eight k-points, and FFT dimensions (180, 180, 192). To run the benchmark, repeat the steps shown in the case above i.e.

Copy the benchmark job script to your user space:

```
cd ~/espresso-5.2
cp -rip
/app/chemistry/quantumespresso/5.2.1/example/benchmark/run_esp
```

```
resso.GRIR443.SLURM.q .
```

From your working directory, submit the job using:

```
sbatch run_espresso.GRIR443.SLURM.q
```

The job should take around 22 minutes using 160 cores if the case runs successfully. The file `GRIR443_NCPUS=160.out.id-<Job_ID>.out` should contain all the output and point to successful completion of the job.

To create a new case, refer to the Quantum ESPRESSO documentation available at

```
/app/chemistry/quantum-espresso/5.0.2/sb/intel-13.0/intel-4.1/Doc
```

and <http://www.quantum-espresso.org/resources/users-manual/>

PDF versions of sections of the manual are also available at:

<http://www.quantum-espresso.org/resources/users-manual/specific-documentation.>

References

Official Quantum ESPRESSO website: <http://www.quantum-espresso.org/>

A list of major projects related to Quantum ESPRESSO development, albeit incomplete, with information on their status and future directions can be found at <http://www.quantum-espresso.org/resources/road-map/>

Quantum ESPRESSO User Documentation, <http://www.quantum-espresso.org/resources/users-manual/specific-documentation.>