

## 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 L<sub>1</sub>-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 example used in this guide is configured to run on the Swansea Sandy Bridge cluster. Connect to `login.hpcwales.co.uk` with your HPC Wales user credentials using your preferred method (e.g. PuTTY from a Windows machine or ssh from any Linux terminal), then `ssh sw-sb-log-001` to connect to the Swansea system.

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

## Step 2 - Load a Quantum ESPRESSO module

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 (5.0.2):

```
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-5.0
```

## Step 4 - Obtain a test case

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

```
/app/chemistry/quantumespresso/5.0.2/example
```

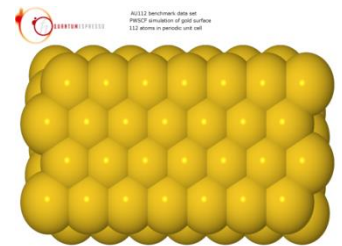
The directory `/app/chemistry/quantumespresso/5.0.2/inputFiles` contains the required input files.

Copy the benchmark job script to your user space:

```
cd ~/espresso-5.0
```

```
cp -rip
```

```
/app/chemistry/quantumespresso/5.0.2/example/benchmark/run_esspresso.AUSURF112.SLURM.q .
```



Note that the SLURM job script points to the location of the required input files. The benchmark case is Au<sub>112</sub>, 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=64.id-<Job\_ID>.out* is created in the espresso-5.0 directory that holds the job output - many temporary files are generated and routed to the user's scratch directory, *run\_espresso-AUSURF112\_64-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 30 minutes using 64 cores if the case runs successfully. The file *AUSURF112\_NCPUS=64.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/quantum.espresso/5.0.2/example/benchmark/AUSURF112_NCPUS=64.id-583.out
```

## Step 6 – More Test Cases

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

```
/app/chemistry/quantum.espresso/5.0.2/example/inputFiles
```

The GRIR443 benchmark arises from a PRACE benchmarking suite. This is a simulation of a carbon–iridium complex (C<sub>200</sub>Ir<sub>243</sub>), 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-5.0
```

```
cp -rip
```

```
/app/chemistry/quantum.espresso/5.0.2/example/benchmark/run_espresso.GRIR443.SLURM.q .
```

- From your working directory, submit the job using:

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

- The job should take around 73 minutes using 64 cores if the case runs successfully. The file *GRIR443\_NCPUS=64.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/users-manual/>

A PDF version of all sections of the manual is also available at:

[http://www.quantum-espresso.org/wp-content/uploads/Doc/user\\_guide.pdf](http://www.quantum-espresso.org/wp-content/uploads/Doc/user_guide.pdf).

## 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/road-map/>

Quantum ESPRESSO User Documentation, [http://www.quantum-espresso.org/wp-content/uploads/Doc/user\\_guide.pdf](http://www.quantum-espresso.org/wp-content/uploads/Doc/user_guide.pdf)