Quantum Espresso 101

introduction and basic applications

Dr. H. C. Nguyen (Bob)

ICIQ
Institut Català d'Investigació Química

15 December 2017

Outline

1 Introduction

Outline

1. Introduction
2. Input of QE

Outline

1. Introduction
2. Input of QE
3. Job submission

Outline

1. Introduction
2. Input of QE
3. Job submission
4. Output of QE

Outline

1. Introduction
   - Capabilities
   - Code Compilation
   - Parallelization
2. Input of QE
3. Job submission
4. Output of QE

Introduction

DFT code with many capabilities

- Ground-state calculations.
- Structural Optimization.
- Transition states and minimum energy paths.
- Ab-initio molecular dynamics.
- Response properties (DFPT).
- Spectroscopic properties.
- Quantum Transport.
- Quantum Monte Carlo.

Capabilities

Ground-state calculations

- Self-consistent total energies, forces, stresses;
- Kohn-Sham orbitals; (Plane waves)
- Norm-conserving, ultrasoft and PAW pseudo-potentials available;
- Several exchange-correlation functionals: from LDA to GGA 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;
- Scalar relativistic and fully relativistic calculations.

Capabilities

Structural Optimization

- GDIIS with quasi-Newton BFGS preconditioning;
- Damped dynamics.

Transition states and minimum energy paths

- Nudged Elastic Band method (NEB);
- Meta-Dynamics, using the PLUMED plug-in.

Ab-initio molecular dynamics

- Born-Oppenheimer Molecular Dynamics (PWscf package);
- Car-Parrinello Molecular Dynamics (CP package).

Capabilities

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, using the D3Q package;
- Infrared and (non-resonant) Raman cross-sections;
- EPR and NMR chemical shifts, using the QE-GIPAW package.
- Phonons for 2D heterostructures

Capabilities

Spectroscopic properties

- X-ray Absorption Spectra (XSpectra package);
- Time-Dependent Density Functional Perturbation Theory (TurboTDDFT package);
- Electronic excitations with Many-Body Perturbation Theory (GW), using the YAMBO or GWL package;

Capabilities

Quantum Transport

- Ballistic Transport (PWCOND package);
- Coherent Transport from Maximally Localized Wannier Functions, using the WanT code;
- Maximally-localized Wannier functions and transport properties, using the WANNIER90 code.
- Kubo-Greenwood electrical conductivity using the KGEC code.

Capabilities

Quantum Monte Carlo

- Direct interface with CASINO, (not included by default);
- Post-processing with QMCPACK (not included by default).

Main differences with VASP:

- QE is open source = license free
- QE is a bunch of codes of non-homogeneous quality
- Inconsistencies between versions

Code Compilation

In theory, very easy...

Working architectures

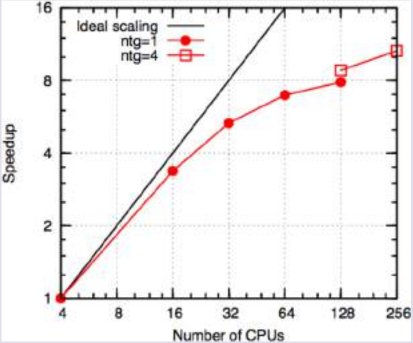
- HPC: IBM SP and BlueGene, Cray XT, Altix, Nec SX,...
- Personal workstations: HP, IBM, SUN, Intel, AMD, ...
- OS: Linux, Windows, Mac OS-X
- Exotic: Playstation 3, Debian in a Nokia N900, ...

In practice, be thankful to your computer technician (Martin) who has to deal the with complex library dependencies (MPI/OpenMPI) and multiple recompilations needed for each add-on and numerous executables. Please install the basic serial version on your local machine for post-processing.

Parallelization

Scalability for small systems

Typical speedup vs number of processors:
128 Water molecules (1024 electrons) in a cubic box 13.35 Å side, Γ point. PWscf code on a SP6 machine, MPI only.
ntg=1 parallelization on plane waves only
ntg=4 also on electron states



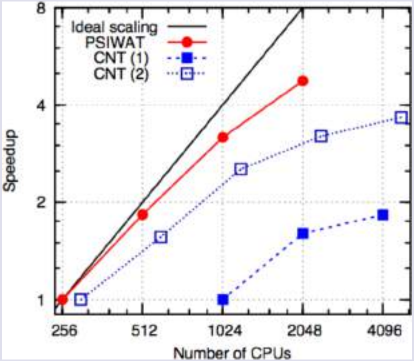
Parallelization

Scalability for medium systems

PSIWAT: Thiol-covered gold surface and water, 4 k-points, 10.59x20.53x32.66 Å^3 cell, 587 atoms, 2552 electrons. PWscf code on CRAY XT4, parallelized on plane waves, electron states, k-points. MPI only.

CNT(1): nanotube functionalized with porphyrins, Γ point, 1532 atoms, 5232 electrons. PWscf code on CRAY XT4, parallelized on plane waves and electron states, MPI only.

CNT(2): same system as for CNT(1). CP code on a CRAY XT3, MPI only.



Outline

1 Introduction

2 Input of QE
- Syntax
- Single point calculation
- Geometry optimisation
- LDOS
- Bader Charge
- Workfunction
- Solvation

3 Job submission

4 Output of QE

Syntax of QE

QE is a collection of programs that work together.

Single point calculation, Geometry/Cell Optimisation, BO-MD : pw.x
DOS : pw.x → dos.x
STM images, integrated LDOS : pw.x → pp.x
Workfunction : pw.x → pp.x → average.x
LDOS, Löwdin Charge, polarization : pw.x → projwfc.x
Bader Charge: pw.x → pp.x → bader
Vibration, phonons : pw.x → ph.x
IR and Raman cross sections: pw.x → dynmat.x
CP-MD : cp.x → cppp.x
TD-DFT : turbo_lanczos.x, turbo_spectrum.x, turbo_davidson.x
NEB: neb.x

Documentation available in (http://www.quantum-espresso.org/users-manual/input-data-description/) or guessing from the source code if not available...

Structure of the input data of pw.x

```
&CONTROL
...
/
&SYSTEM
...
/
&ELECTRONS
...
/
[ &IONS ... / ] → only for relax
[ &CELL ... / ] → for vc-relax
ATOMIC_SPECIES
ATOMIC_POSITIONS
K_POINTS
```

Single point calculation

pw.x < INPUT > OUTPUT

Example with H_2O: USPP_D2H2O-scf.in

```
&CONTROL
calculation = 'scf' ,  → scf= self-consistent single point calculation
restart_mode = 'from_scratch' ,→ New calculation
wf_collect = .true.  , → required flag for future restart
prefix = 'USPP_D2H2O' , → restart name folder
verbosity = 'high' ,→ write all information in output file
etot_conv_thr = 1.0D-9 ,→ in Ry
forc_conv_thr = 1.0D-5 ,→ in Ry/bohr
tstress = .true.  ,→ calculate stress
tprnfor = .true.  , → calculate forces
!dipfield = .true.  ,→ it is commented (only for slab calculation)
```

```
&SYSTEM
ibrav = 1, → cubic simple
A = 15 , → in ANGSTROM
nat = 3 , → number of atoms
ntyp = 2,  → number of types of atoms
ecutwfc = 40.0 ,  → kinetic energy cutoff for wavefunctions (Ry)
ecutrho = 320.0 ,  → kinetic energy cutoff for charge density (Ry)
input_dft = 'PBE' ,  → use PBE Exchange-correlation functional
occupations = 'smearing' ,  → gaussian smearing for metals
degauss = 0.02 , → gaussian spreading (Ry)
smearing = 'gaussian' , → ordinary Gaussian spreading
nspin = 2 , → spin-polarized calculation (collinear)
starting_magnetization(1) = 0.0,
starting_magnetization(2) = 0.0,
vdw_corr = Grimme-D2, !  DFT-D2 dispersion correction
nosym = .true.  !For isolated atom
assume_isolated = 'makov-payne'→ ONLY FOR CUBIC SYSTEMS
```

`&ELECTRONS`
`electron_maxstep = 800,` → max step for scf calculation
`conv_thr_init = 1e-4 ,` → threshold used for the first scf cycle
`conv_thr = 1e-9 ,` → threshold for the first scf cycle
`startingpot = 'atomic' ,` → starting potential = atomic charge
`startingwfc = 'random' ,` → Slower start of scf wfc but safer
`adaptive_thr = .true. ,` → adaptive conv_thr
`mixing_beta = 0.514,` → if convergence bad reduce that number
`diagonalization = 'david' ,` → much faster than cg but less stable
`/`

`ATOMIC_SPECIES`

`O 15.99990 O.pbe-van_ak.UPF` → says which pseudopotential to use

`H 1.00790 H.pbe-van_ak.UPF`

`ATOMIC_POSITIONS angstrom` → positions in angstrom

`O 4.960864866 4.932204696 10.000041372` → TYPE X Y Z (1 1 1)

`H 5.926442340 5.064579477 9.999978448`

`H 4.592692795 5.834600215 9.99998018`

`K_POINTS Gamma`

You can choose to freeze an atom with 0 0 0 after TYPE, X, Y, Z

Geometry optimisation

```
&CONTROL
calculation = ’relax’ ,
...
&SYSTEM
...
&ELECTRONS
...
&IONS
ion_dynamics = ’bfgs’ ,
trust_radius_min = 1.D-5 ,
ATOMIC_SPECIES
...
ATOMIC_POSITIONS
...
K_POINTS Gamma
```

LDOS

DOS and LDOS can be computed after an scf/relax calculation as long as a restart folder has been correctly created

```
projwfc.x < $INPUT > $OUTPUT
```

```
&PROJWFC
prefix = 'USPP.001_G_D2H2O' , → folder name of the restart
!outdir = '/home/hnguyen/espresso_tmp',  → output dir
DeltaE = 0.01 , → in eV
Emin = -15.0 , → in eV
Emax = 15.0 ,  → in eV
ngauss = 0,  → Simple Gaussian
degauss = 0.001469972, !  =0.02 eV → in Ry
pawproj = .false.  , → true only for PAW
/
```

Bader Charge part 1

You MUST use PAW pseudopotential to compute Bader charges in QE.
After a scf calculation you need to run
pp.x < INPUT > OUTPUT

```
&INPUTPP
prefix = 'prefix' ,
filplot = 'prefix' ,
plot_num = 17,
/
&PLOT nfile = 1 ,
weight(1) = 1.0,
fileout = 'prefix.charge.cube' ,
iflag = 3 ,
output_format = 6 ,
/
```

This create a .cube file that can be read by the program bader (not included in QE).

Bader Charge part 2

After step1, execute

```
bader -v file.charge.cube
```

This will creates 3 files ACF.dat, AVF.dat, BCF.dat.

ACF.dat contains the coordinates of each atom, the charge associated with it according to Bader partitioning, percentage of the whole according to Bader partitioning and the minimum distance to the surface.

BCF.dat contains Bader maxima

AVF.dat contains Bader volumes

For practical reasons, it is highly recommended to rename these files before scripting large data set.

```
mv ACF.dat prefix.ACF.dat
mv AVF.dat prefix.AVF.dat
mv BCF.dat prefix.BCF.dat
```

The Bader charges will be written in prefix.ACF.dat

Workfunction step 1

After a scf/relax calculation, restart with pp.x:

pp.x < INPUT > OUTPUT

```
&inputPP
prefix = 'Fe.USPP.001_2x2_145_full_D2' ,
outdir='/home/hnguyen/espresso_tmp',
plot_num=11
filplot = 'Fe.USPP.001_2x2_145_full_D2.pot'
/
&plot
iflag=3,
output_format=3,
nx = 1,
ny = 1,
nz = 1,
/
```

Workfunction step 2

After step 1 , run average.x

average.x < INPUT > OUTPUT

```
1
Fe.USPP.001_2x2_145_full_D2.pot
1.D0
1440
3
3.835000000
```

NB: There is no manual for the program average.x

Solvation

Solvation is added with the Environ-0.2 add-on. An additional file called exactly "environ.in" must be put in the same folder as your calculation.

```
&ENVIRON
!
verbose = 0
environ_thr = 1.d-1
environ_type = 'water'  → set solvent to water
tolrhopol = 1.d-11
mixrhopol = 0.6
!mixtype = 'pcg' !    → preconditioner is buggy don't use it
/
```

Outline

1 Introduction

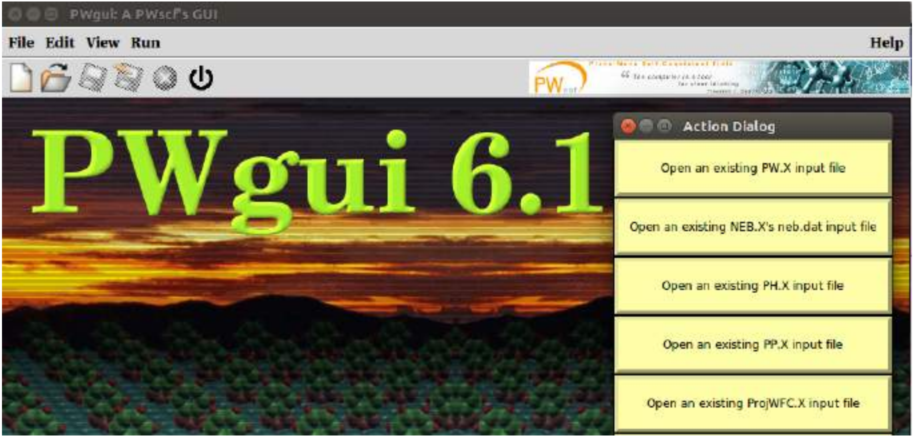
2 Input of QE

3 Job submission
- Local
- tekla
- CSUC
- cesvima
- MN4

4 Output of QE

How to submit job?

Before sending a job, make sure that your input is correct with *pwgui* a GUI for writing QE input and check the syntax. If *pwgui* cannot open your input, you screwed up.


PWgui: A PWscf's GUI
File
Edit
View
Run
Help
PWscf
PWgui 6.1
Action Dialog
Open an existing PW.X input file
Open an existing NEB.X's neb.dat input file
Open an existing PH.X input file
Open an existing PP.X input file
Open an existing ProjWFC.X input file

Local machine

Environment setup

After a clean install of qe-6.1, setup the qe environment by adding all the **executables** and **scripts** to your PATH in your *.bashrc*

```
### Quantum Espresso path
# QE 6.1
export PATH="$PATH:/home/hnguyen/Downloads/qe-6.1/PW/tools"
export PATH="$PATH:/home/hnguyen/Downloads/qe-6.1/bin"
```

Setup working directories

You must setup a directory of where your Pseudopotentials are and where is the directory for temporary files

```
export ESPRESSO_PSEUDO=/home/hnguyen/espresso_pseudo
export ESPRESSO_TMPDIR=/home/hnguyen/espresso_tmp
###Needed memory for VASP and QE
ulimit -s unlimited
```

Local machine

Put all your input files in the same folder and run them

```
pw.x <prefix.in > prefix.out1
projwfc.x < prefix_LDOS.in > prefix_LDOS.out grep

'polarization' prefix_LDOS.out >
prefix_LDOS.out.polarization
grep 'charge' prefix_LDOS.out > prefix_LDOS.out.charge
```

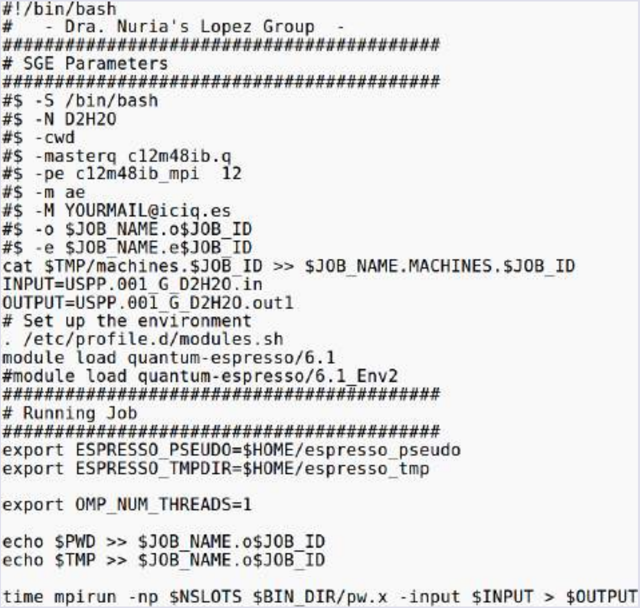
tekla

Only 12m48ib.q and c24m128ib.q have qe-6.1 installed.
You need to create two folders in your $HOME directory:
`$HOME/espresso_pseudo` where you put all your pseudo potentials (O.pbe-van_ak.UPF and H.pbe-van_ak.UPF)
`$HOME/espresso_tmp` is where all the outputs will be. Put all the .in and .lsf12 files there. Edit `#$ -M YOURMAIL@iciq.es` with your email to receive notification when job is finished.
Submit *USPP.001_G_D2H2O.lsf12*

```
qsub USPP.001_G_D2H2O.lsf12
```

When it is done, it will create a human readable output USPP.001_G_D2H2O.out1 and a folder USPP.001_G_D2H2O for restart and postprecessing.

USPP.001_G_D2H2O.lsf12



```
#!/bin/bash
#   - Dra. Nuria's Lopez Group  -
##########################################
# SGE Parameters
##########################################
#$ -S /bin/bash
#$ -N D2H2O
#$ -cwd
#$ -masterq c12m48ib.q
#$ -pe c12m48ib_mpi  12
#$ -m ae
#$ -M YOURMAIL@iciq.es
#$ -o $JOB_NAME.o$JOB_ID
#$ -e $JOB_NAME.e$JOB_ID
cat $TMP/machines.$JOB_ID >> $JOB_NAME.MACHINES.$JOB_ID
INPUT=USPP.001_G_D2H2O.in
OUTPUT=USPP.001_G_D2H2O.out1
# Set up the environment
. /etc/profile.d/modules.sh
module load quantum-espresso/6.1
#module load quantum-espresso/6.1_Env2
##########################################
# Running Job
##########################################
export ESPRESSO_PSEUDO=$HOME/espresso_pseudo
export ESPRESSO_TMPDIR=$HOME/espresso_tmp

export OMP_NUM_THREADS=1

echo $PWD >> $JOB_NAME.o$JOB_ID
echo $TMP >> $JOB_NAME.o$JOB_ID

time mpirun -np $NSLOTS $BIN_DIR/pw.x -input $INPUT > $OUTPUT
```

tekla

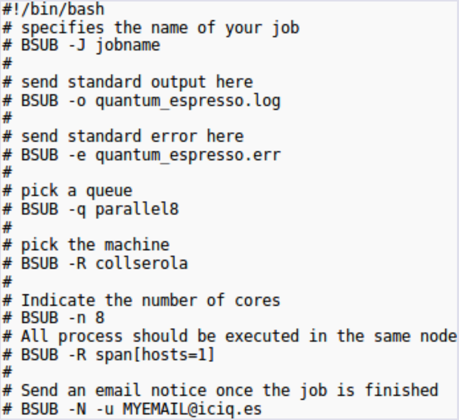
You can, after the geometry optimisation, submit a PDOS calculation

```
qsub USPP.001_G_D2H2O_LDOS.lsf12
```

When finished, it will create a directory in PDOS/USPP.001_G_D2H2O_LDOS containing all the projected DOS and the total DOS (USPP.001_G_D2H2O.pdos_tot) in text format. You can used your favourite program to plot the DOS. Löwdin charges will be in USPP.001_G_D2H2O_LDOS.out.charge and polarization will be in USPP.001_G_D2H2O_LDOS.out.polarization

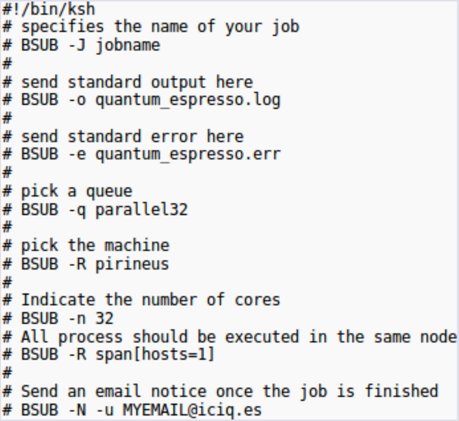
CSUC

collserola



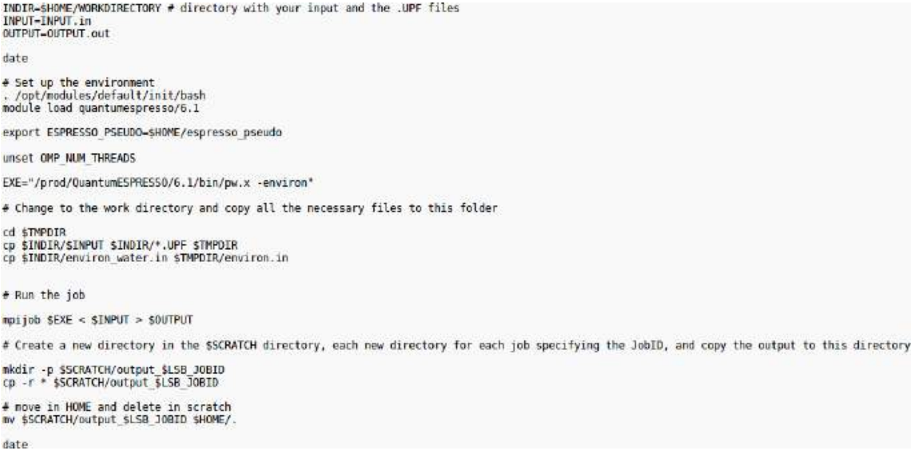
```
#!/bin/bash
# specifies the name of your job
# BSUB -J jobname
#
# send standard output here
# BSUB -o quantum_espresso.log
#
# send standard error here
# BSUB -e quantum_espresso.err
#
# pick a queue
# BSUB -q parallel8
#
# pick the machine
# BSUB -R collserola
#
# Indicate the number of cores
# BSUB -n 8
# All process should be executed in the same node
# BSUB -R span[hosts=1]
#
# Send an email notice once the job is finished
# BSUB -N -u MYEMAIL@iciq.es
```

pirineus



```
#!/bin/ksh
# specifies the name of your job
# BSUB -J jobname
#
# send standard output here
# BSUB -o quantum_espresso.log
#
# send standard error here
# BSUB -e quantum_espresso.err
#
# pick a queue
# BSUB -q parallel32
#
# pick the machine
# BSUB -R pirineus
#
# Indicate the number of cores
# BSUB -n 32
# All process should be executed in the same node
# BSUB -R span[hosts=1]
#
# Send an email notice once the job is finished
# BSUB -N -u MYEMAIL@iciq.es
```

CSUC



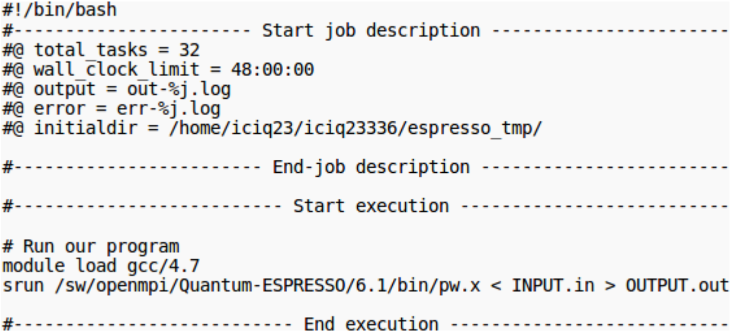
```
INDIR=$HOME/WORKDIRECTORY # directory with your input and the .UPF files
INPUT=INPUT.in
OUTPUT=OUTPUT.out

date

# Set up the environment
. /opt/modules/default/init/bash
module load quantumespresso/6.1

export ESPRESSO_PSEUDO=$HOME/espresso_pseudo

unset OMP_NUM_THREADS

EXE="/prod/QuantumESPRESSO/6.1/bin/pw.x -environ"

# Change to the work directory and copy all the necessary files to this folder

cd $TMPDIR
cp $INDIR/$INPUT $INDIR/*.UPF $TMPDIR
cp $INDIR/environ_water.in $TMPDIR/environ.in


# Run the job

mpijob $EXE < $INPUT > $OUTPUT

# Create a new directory in the $SCRATCH directory, each new directory for each job specifying the JobID, and copy the output to this directory

mkdir -p $SCRATCH/output_$LSB_JOBID
cp -r * $SCRATCH/output_$LSB_JOBID

# move in HOME and delete in scratch
mv $SCRATCH/output_$LSB_JOBID $HOME/.

date
```

job are send with the command:

```
bsub< jobname.lsf
```

cesvima

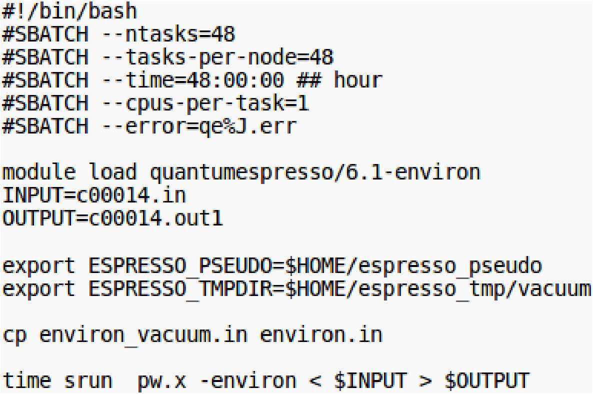
Warning: cesvima does not have environ installed!



```
#!/bin/bash
#----------------------- Start job description -----------------------
#@ total_tasks = 32
#@ wall_clock_limit = 48:00:00
#@ output = out-%j.log
#@ error = err-%j.log
#@ initialdir = /home/iciq23/iciq23336/espresso_tmp/

#------------------------ End-job description ------------------------

#-------------------------- Start execution --------------------------

# Run our program
module load gcc/4.7
srun /sw/openmpi/Quantum-ESPRESSO/6.1/bin/pw.x < INPUT.in > OUTPUT.out

#--------------------------- End execution ---------------------------
```

Jobs are sent CESVIMA queue with
`jobsubmit jobname.sh`

MN4



```
#!/bin/bash
#SBATCH --ntasks=48
#SBATCH --tasks-per-node=48
#SBATCH --time=48:00:00 ## hour
#SBATCH --cpus-per-task=1
#SBATCH --error=qe%J.err

module load quantumespresso/6.1-environ
INPUT=c00014.in
OUTPUT=c00014.out1

export ESPRESSO_PSEUDO=$HOME/espresso_pseudo
export ESPRESSO_TMPDIR=$HOME/espresso_tmp/vacuum

cp environ_vacuum.in environ.in

time srun  pw.x -environ < $INPUT > $OUTPUT
```

To submit an environ job to MareNostrum4

```
sbatch script.lsf
```

Outline

1 Introduction

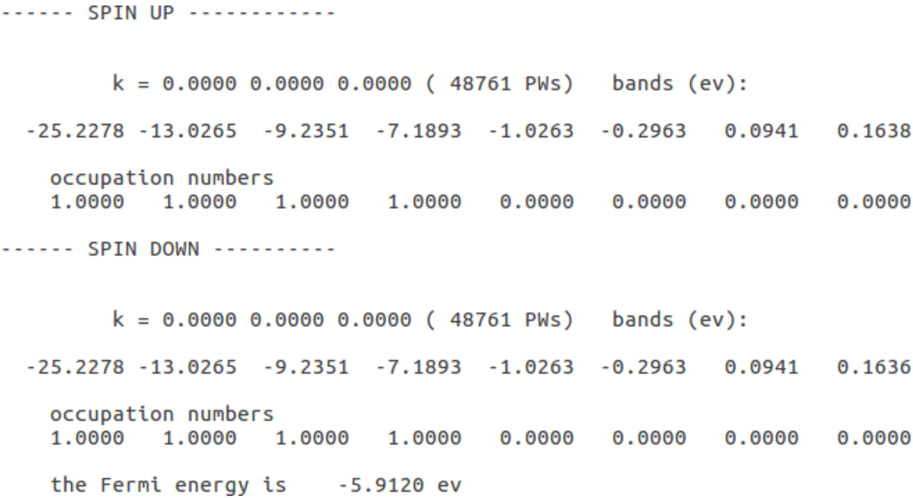
2 Input of QE

3 Job submission

4 Output of QE
- Output format
- xcrysden

Output format

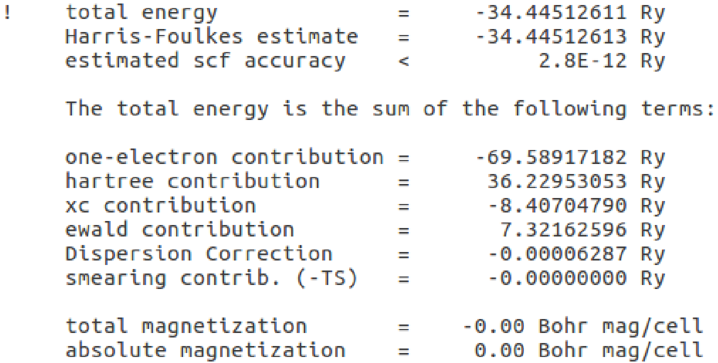
End of *scf* calculation:



```
------ SPIN UP ------------


         k = 0.0000 0.0000 0.0000 ( 48761 PWs)   bands (ev):

  -25.2278 -13.0265  -9.2351  -7.1893  -1.0263  -0.2963   0.0941   0.1638

    occupation numbers
    1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

------ SPIN DOWN ----------


         k = 0.0000 0.0000 0.0000 ( 48761 PWs)   bands (ev):

  -25.2278 -13.0265  -9.2351  -7.1893  -1.0263  -0.2963   0.0941   0.1636

    occupation numbers
    1.0000   1.0000   1.0000   1.0000   0.0000   0.0000   0.0000   0.0000

    the Fermi energy is    -5.9120 ev
```

Output format

End of *scf* calculation:



```
!    total energy              =     -34.44512611 Ry
     Harris-Foulkes estimate   =     -34.44512613 Ry
     estimated scf accuracy    <          2.8E-12 Ry

     The total energy is the sum of the following terms:

     one-electron contribution =     -69.58917182 Ry
     hartree contribution      =      36.22953053 Ry
     xc contribution           =      -8.40704790 Ry
     ewald contribution        =       7.32162596 Ry
     Dispersion Correction     =      -0.00006287 Ry
     smearing contrib. (-TS)   =      -0.00000000 Ry

     total magnetization       =    -0.00 Bohr mag/cell
     absolute magnetization    =     0.00 Bohr mag/cell
```

Output format

End of *relax* calculation:

```
    Final energy = -34.4451261118 Ry
Begin final coordinates
ATOMIC_POSITIONS (angstrom) → same format as input
O 4.960991383 4.932452337 10.000042692
H 5.926598065 5.064299775 9.999977700
H 4.592410553 5.834632277 9.999979608
End final coordinates
```

xcrysden

Geometrical structures can be visualized with *xcrysden* (already installed on your desktop by default). *xcrysden* can open .xsf and .asxf file than can be produced for input:

```
pwi2xsf.sh USPP.001_G_D2H2O.in > USPP.001_G_D2H2O.in.xsf
```

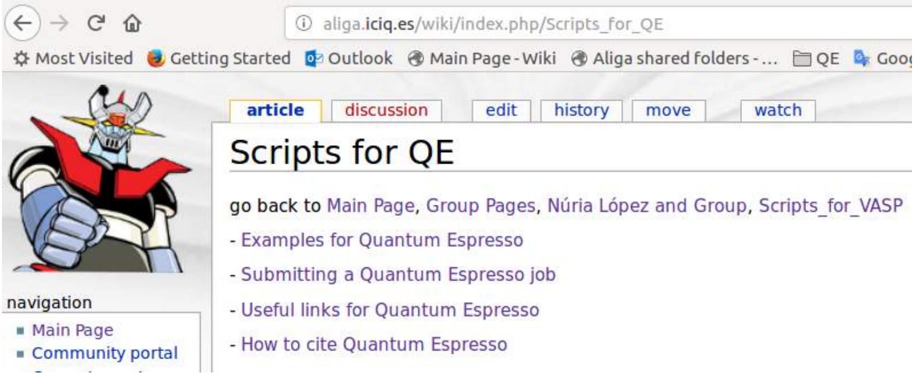
and output:

```
pwo2xsf.sh -lc
USPP.001_G_D2H2O.out1>USPP.001_G_D2H2O.out1.xsf
pwo2xsf.sh -a
USPP.001_G_D2H2O.out1>USPP.001_G_D2H2O.out1.axsf
```

The last one (axsf) creates a movie of all intermediate steps.

Group wiki

Examples are available on the wiki:
http://aliga.iciq.es/wiki/index.php/Scripts_for_QE



Scripts for QE

go back to Main Page, Group Pages, Núria López and Group, Scripts_for_VASP

- Examples for Quantum Espresso

- Submitting a Quantum Espresso job

- Useful links for Quantum Espresso

- How to cite Quantum Espresso