PWSCF: first steps

What can I learn in this lecture ?

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How to run PWscf (pw.x) in self-consistent mode for Silicon

How to get the band structure of Silicon along the main symmetry directions

How to draw charge density map of Silicon in a given plane

How to calculate the density of state of Silicon

What are the basic convergence parameters to have under control

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symmetry directions

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How to deal with metals (Aluminum, Copper)

How to deal with spin polarized systems (Nickel)

How to perform structural relaxations (CO [1d] , Aluminum (001) [2d])

How to perform an DFT+U calculation (FeO)

Download example file TutorialQE.tgz and unpack it.

This will create a sub-directory named TutorialQE containing several files.

Move to the TutorialQE directory and check its content

```
 prompt> cd TutorialQE

 prompt> ls
Aluminum  Copper  FeO  Nickel  RELAX  Silicon

+ some additional files that will be discussed later
```

Self-consistent calculation for Silicon in the diamond structure

Move to the Silicon directory

```
prompt> cd Silicon
```

Inspect input file si.scf.in (a copy of it can be found in the reference directory) and notice that it is an scf calculation (default value)

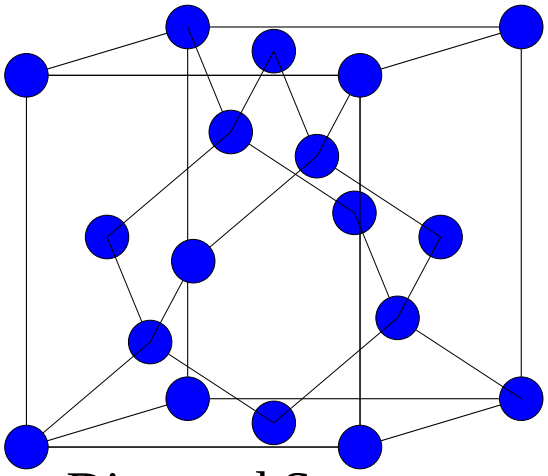
```
calculation = 'scf'  ! this line is actually not there !
```

The outdir and pseudo_dir directory are defined in such a way that

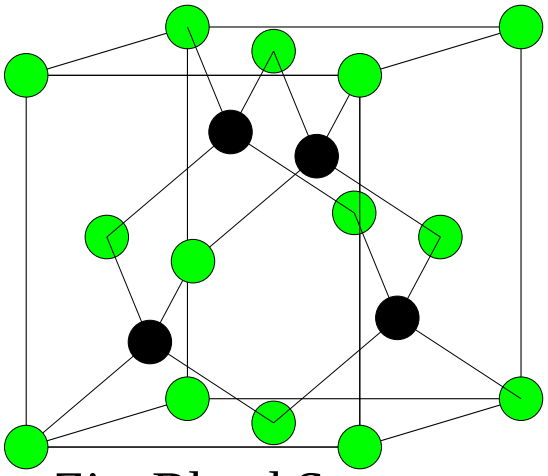
```
outdir = 'temporary directory for large files'
          example: /scratch/"my_name"/espresso
pseudo_dir = 'directory where pp-files are kept'
          example: "espresso_dir"/pseudo
```

Check that these directories exist, have read/write permission and that pseudo_dir contains the pseudopotential file Si.pz-vbc.UPF for Silicon

How the crystal structure is defined ?



Diamond Structure



ZincBlend Structure

check in the input file

```
How the Bravais lattice is selected ?
How many and which parameters are needed to completely
  define Bravais lattice geometry ?
How many atoms in the unit cell ?
How many different atomic species ?
Which ones ?
Where the atoms are located in the unit cell ?
```

You can check the syntax and allowed values for the input variables at the web page
www.quantum-espresso.org/wp-content/uploads/Doc/INPUT_PW.html

Brillouin zone sampling

BZ sampling is performed using 2 Chadi-Cohen special points for the fcc lattice.

check in the input file how k-points are provided manually

```
 k-points are given (default) in cartesian coordinates
  in unit of 2pi/celldm(1)
k-point weights need not add-up to 1,
  they are later normalized
```

This is equivalent to a 2 2 2 shifted grid of points in the BZ.

You can modify the input to use this format if you wish.

For an introduction to special points techniques see for instance

A. Baldereschi, *Phys. Rev. B* **7**, 5212 (1973).
D.J. Chadi e M.L. Cohen, *Phys. Rev. B* **8**, 5747 (1973).
H.J. Monkhorst e J.D. Pack, *Phys. Rev. B* **13**, 5188 (1976).

run pw.x code

```
prompt> espresso_dir/bin/pw.x < si.scf.in > si.scf.out
```

look at outdir and its content

```
prompt> ls /scratch/my_name/espresso
silicon.pot  silicon.rho  silicon.save  silicon.wfc
```

examine the output file and look how convergence proceeds

```
prompt> grep -e 'total energy' -e estimated si.scf.out
     total energy              =     -15.79103344 Ry
     estimated scf accuracy    <       0.06376674 Ry
     total energy              =     -15.79409289 Ry
     estimated scf accuracy    <       0.00230109 Ry
     total energy              =     -15.79447822 Ry
     estimated scf accuracy    <       0.00006291 Ry
     total energy              =     -15.79449510 Ry
     estimated scf accuracy    <       0.00000448 Ry
!    total energy              =     -15.79449593 Ry
     estimated scf accuracy    <       0.00000005 Ry
```

You can encapsulate all these operations by using a shell script that can be reused and modified as needed

Inspect run_si_scf script and understand its logics and the use of the auxiliary file environment_variables in order to customize the definition of pseudo_dir and outdir directories and define the path to espresso_dir.
Do not bother about the (empty) $PARA_PREFIX variable for now.

Execute the script

```
prompt> ./run_si_scf
```

and verify that the result is the same as before, except for a different choice for outdir.

We can further automatize the procedure and submit the work to be executed to the batch queue by creating a job file and submitting to the queue.
This also allows to use more processor elements (properly defining PARA_PREFIX), chosing the execution queue etc.

Examine and understand the submit script and use it to submit the run_si_scf script to the queue system

```
prompt> ../submit run_si_scf
```

You can monitor the execution by typing

```
prompt> qstat
```

In order to remove myjob and its log files you can execute

```
prompt> ../clean_log
```

Bands at high-symmetry points in silicon:

Compare file si.nscf.in with si.scf.in and check how it is set for a non-self-consistent calculation in the three high symmetry points:
Γ = (0,0,0), X=(1,0,0)$\frac{2\pi}{a}$ and L=(1/2,1/2,1/2)$\frac{2\pi}{a}$

```
 calculation='nscf' in CONTROL namelist
nbnd=8 (4 valence + 4 conduction) in SYSTEM namelist
the three k-points are given in the K_POINTS card
 K_POINTS
 3
 0.0 0.0 0.0   1
 1.0 0.0 0.0   2  WEIGHTS ARE MEANINGLESS IN NSCF CALCS
 0.5 0.5 0.5   3
```

DO NOT MODIFY outdir or prefix,
DO NOT REMOVE files from the scratch area

Bands at high-symmetry points in silicon:

run pw.x code

```
prompt> espresso_dir/bin/pw.x < si.nscf.in > si.nscf.out
```

OR

```
prompt> .../submit run_si_nscf
```

look at the output

```
 how many iteration have been performed ?
which potential is used in the diagonalization ?
which wfcs are used as initial guess ?
is the charge density and/or the total energy computed ?
```

Band structure calculation for silicon:

Compare file si.bands.in and si.nscf.in and verify that the only difference is that a k-point list is provided that describes a path in the BZ along the Λ, Δ and Σ directions.

run pw.x code

```
prompt> espresso_dir/bin/pw.x < si.bands.in > si.bands.out
```

Now collect band results for plotting:
inspect the file bands.in in order check to the needed input then run bands.x

```
prompt> espresso_dir/bin/bands.x < bands.in > bands.out
```

Verify the content of the file bands.out and bands.dat. Take note of the value of the valence band maximum at Γ and then run plotband.x interactively providing the appropriate input.

```
prompt> espresso_dir/bin/plotband.x
```

OR you can do all this together by executing

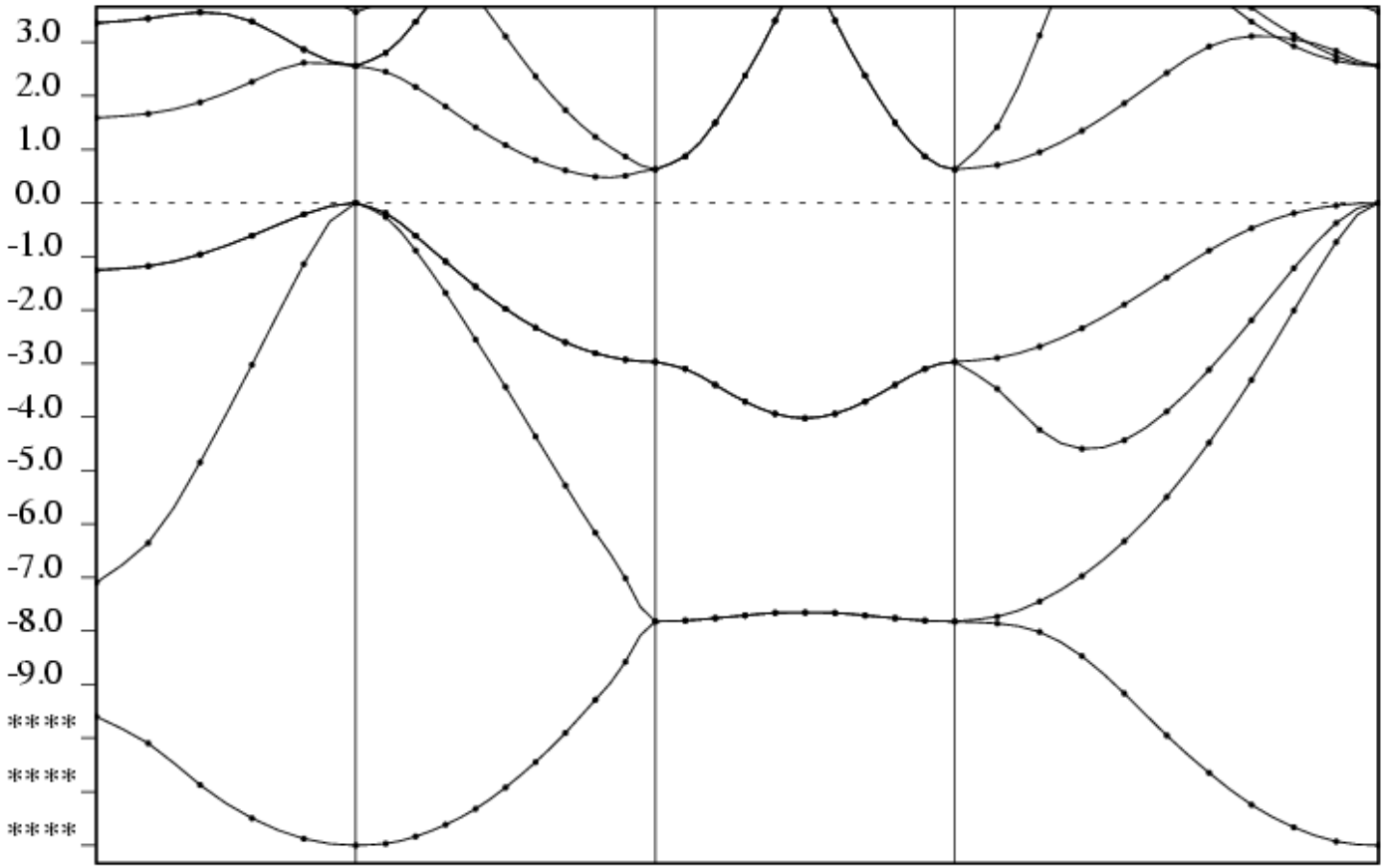
```
prompt> .../submit run_si_bands
```

Band structure calculation for silicon:

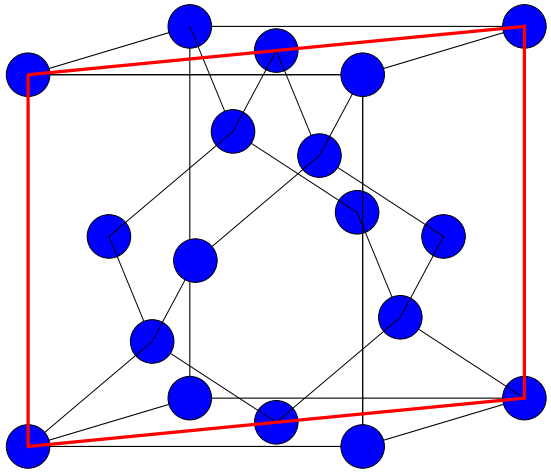
```
 prompt> espresso_dir/bin/plotband.x
input file > bands.dat
Reading    8 bands at   36 k-points
Range: -5.6680 16.4950eV  Emin, Emax > -6.0 10.0
high-symmetry point:  0.5000 0.5000 0.5000
high-symmetry point:  0.0000 0.0000 0.0000
high-symmetry point:  0.0000 0.0000 1.0000
high-symmetry point:  0.0000 1.0000 1.0000
high-symmetry point:  0.0000 0.0000 0.0000
output file (xmgr) > si.bands.xmgr
bands in xmgr format written to file si.bands.xmgr
output file (ps) > si.bands.ps
Efermi > 6.337
deltaE, reference E (for tics) 1.0, 6.337
bands in PostScript format written to file si.bands.ps
```

Band structure calculation for silicon:

```
prompt> ghostview si.bands.ps
```



Charge density plot for silicon in the (1-10) plane:



Inspect file si.pp_rho.in to understang how the desired plane is defined and then run the postprocessing code (pp.x) to extract the charge density (plotnum=0)

```
prompt> espresso_dir/bin/pp.x < si.pp_rho.in
```

You can check the syntax and allowed values for the input variables at the web page www.quantum-espresso.org/wp-content/uploads/Doc/INPUT_PP.html

```
prompt> espresso_dir/bin/pp.x < si.pp_rho.in
     Program POST-PROC v.2.1cvs starts ...
     Today is 25Sep2005 at 21:41:44

     Reading file silicon.save ...       only dimensions
     read complete

     Reading file silicon.save ...       all except wavefuctions
     read complete

     nbndx  =      8  nbnd   =      8  natomwfc =      8  npwx   =      200
     nelec  =   8.00  nkb    =      8  ngl    =     43

     Calling punch_plot, plot_num =   0
     Writing data to file  sicharge
     Reading header from file  sicharge
     Reading data from file  sicharge

     Writing data to be plotted to file si.rho.dat
     Min, Max, imaginary charge:     0.003289    0.088720    0.000000
     Plot Type: 2D contour              Output format: plotrho.x
```

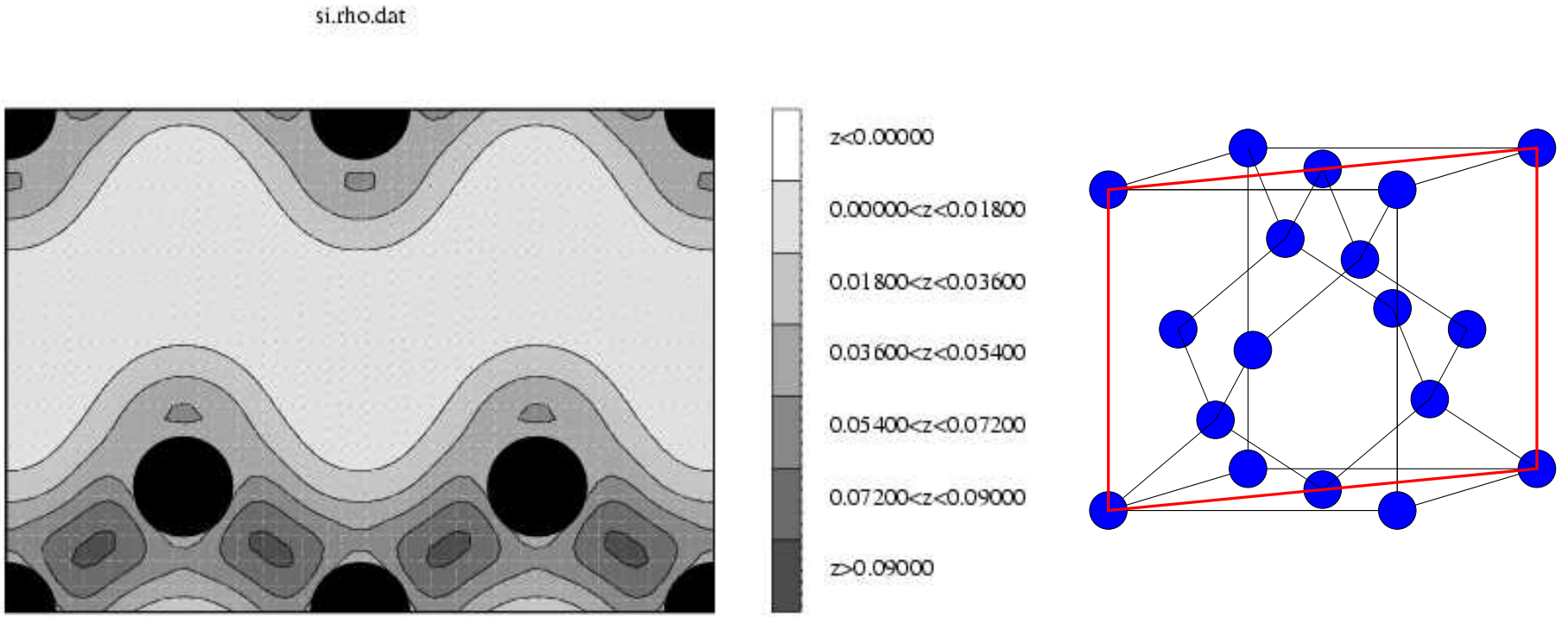
Charge density plot for silicon in the (1-10) plane:

run interactively plotrho.x to produce the plot

```
prompt> espresso_dir/bin/plotrho.x
input file > si.rho.dat
r0    :    0.0000   0.0000   0.0000
tau1  :    1.0000   1.0000   0.0000
tau2  :    0.0000   0.0000   1.0000
read   2 atomic positions
output file > si.rho.ps
Read  56 * 40  grid
Logarithmic scale (y/n)? > n
Bounds:      0.002839     0.093110
min, max, # of levels > 0 0.09 6
```

Charge density plot for silicon in the (1-10) plane:

```
prompt> ghostview si.rho.ps
```



Density of States for Silicon:

Compare file si.dos.in with si.bands.in and check how it is set for a non-self-consistent calculation on a regular grid of points in the BZ.

```
 calculation='nscf' in CONTROL namelist
nbnd=8 (4 valence + 4 conduction) in SYSTEM namelist
occupations='tetrahedra' in SYSTEM namelist
k-point grid is defined in the K_POINTS card
 K_POINTS automatic
 8 8 8 0 0 0
```

DO NOT MODIFY outdir or prefix,
DO NOT REMOVE files from the scratch area

Density of States for Silicon:

run pw.x code to produce the plot

```
prompt> espresso_dir/bin/pw.x < si.dos.in > si.dos.out
```

Now collect results in a DOS file:

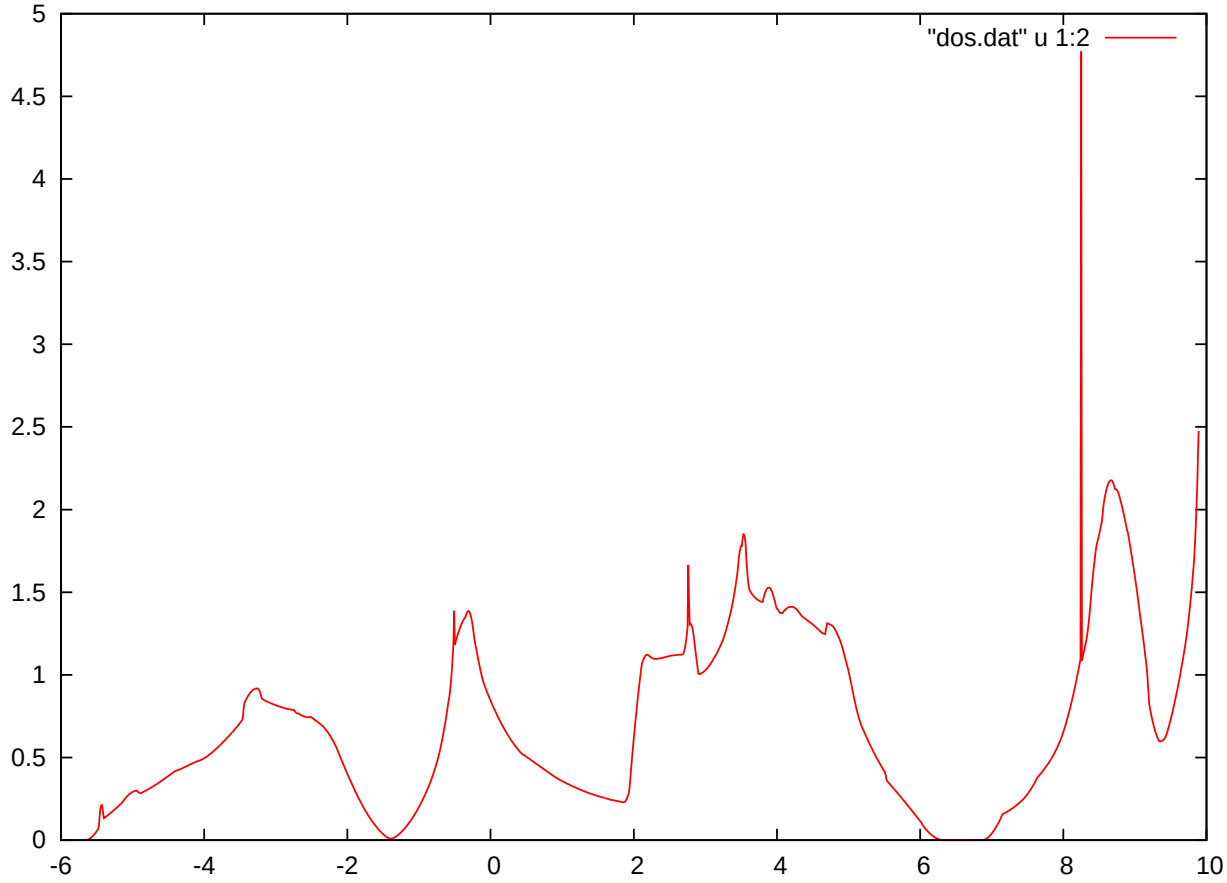
Inspect file dos.in in order to check the needed input parameters and run dos.x code

```
prompt> espresso_dir/bin/dos.x < dos.in > dos.out
```

Verify the content of file dos.out and dos.dat and visualize the DOS by (for instance) gnuplot

```
prompt> gnuplot
gnuplot> plot "dos.dat" u 1:2 w l
```

```
prompt> gnuplot
gnuplot> plot "dos.dat" u 1:2 w l
```



can be improved with denser grids

Convergence Parameters in a PW code:

- Convergence w.r.t. kinetic energy cutoff

- Convergence w.r.t. k-points

Convergence w.r.t. kinetic energy cutoff:

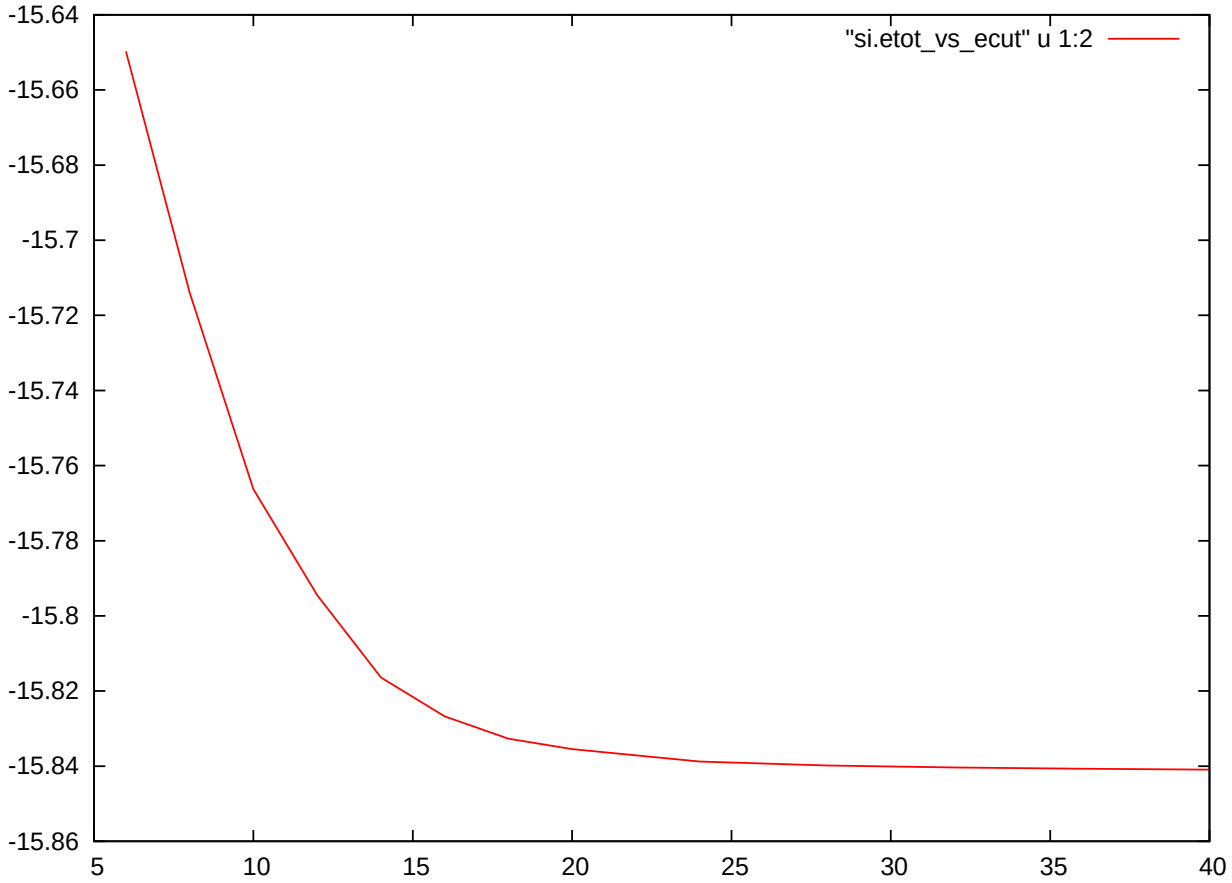
Changing the value of ecutwfc in the SYSTEM namelist in si.scf.in input file to 16, 20, 24 ... Ry and collecting the corresponding total energies one can reproduce the data in si_etot_vs_ecut file;

```
 prompt> cat si.etot_vs_ecut
6.0000 -15.64970592
8.0000 -15.71391639
10.0000 -15.76626748
12.0000 -15.79449593
14.0000 -15.81640517
16.0000 -15.82676464
18.0000 -15.83267689
20.0000 -15.83546695
24.0000 -15.83876531
28.0000 -15.83981308
32.0000 -15.84034461
36.0000 -15.84069586
```

Convergence w.r.t. kinetic energy cutoff:

Plot the data in si_etot_vs_ecut and notice the monotonic convergence.

```
prompt> gnuplot
gnuplot> plot "si.etot_vs_ecut" u 1:2 w l
```



Convergence w.r.t to cutoff is a property of the pseudopotential

Convergence w.r.t. k-points:

Changing k-point grid in the K_POINTS input block in si.scf.in using automatic grids with nk=2,4,6

```
 K_POINTS automatic
  2 2 2 1 1 1
```

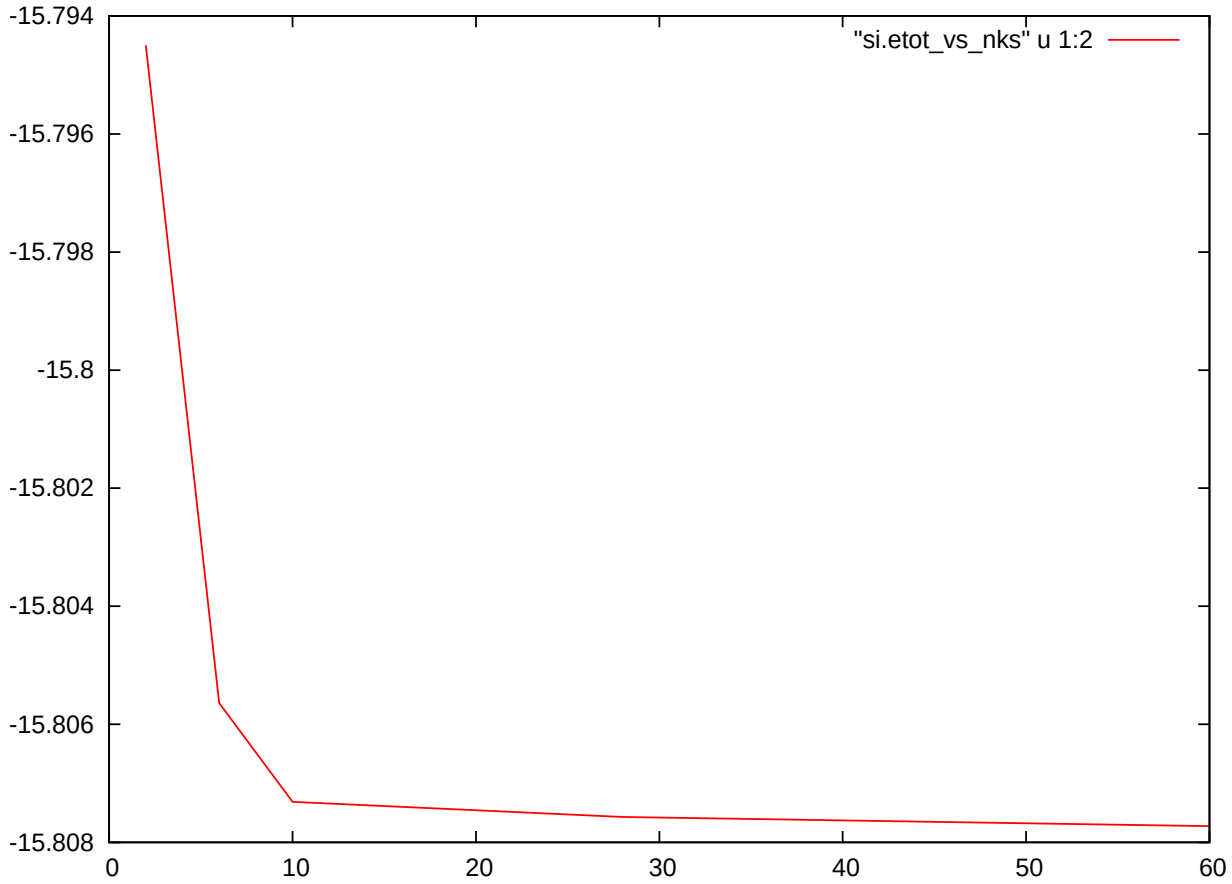
and collecting the corresponding total energies one can reproduce the data in si.etot_vs_nks file;

```
 prompt> cat si.etot_vs_nks
2 -15.79449593
6 -15.80564003
10 -15.80731236
28 -15.80757128
60 -15.80772572
```

Convergence w.r.t. k-points:

Plot the data in si.etot_vs_nks.

```
prompt> gnuplot
gnuplot> plot "si.etot_vs_nks" u 1:2 w l
```



Convergence is not necessarily monotonic ;

There is no variational principle w.r.t. k-points number.

A metallic example: Aluminum

Move to the Aluminum directory

```
prompt> cd ../Aluminum
```

Edit input file al.scf.in and check that it is an scf calculation for a metallic system.

Notice the use of variables occupations, smearing, degauss;

You can check the syntax and allowed values for the input variables at the web page www.quantum-espresso.org/wp-content/uploads/Doc/INPUT_PW.html

Run pw.x code

```
prompt> espresso_dir/bin/pw.x < al.scf.in > al.scf.out
```

Notice in the output file that nbnd is automatically set to a value larger than nelec/2 and that Efermi is computed.

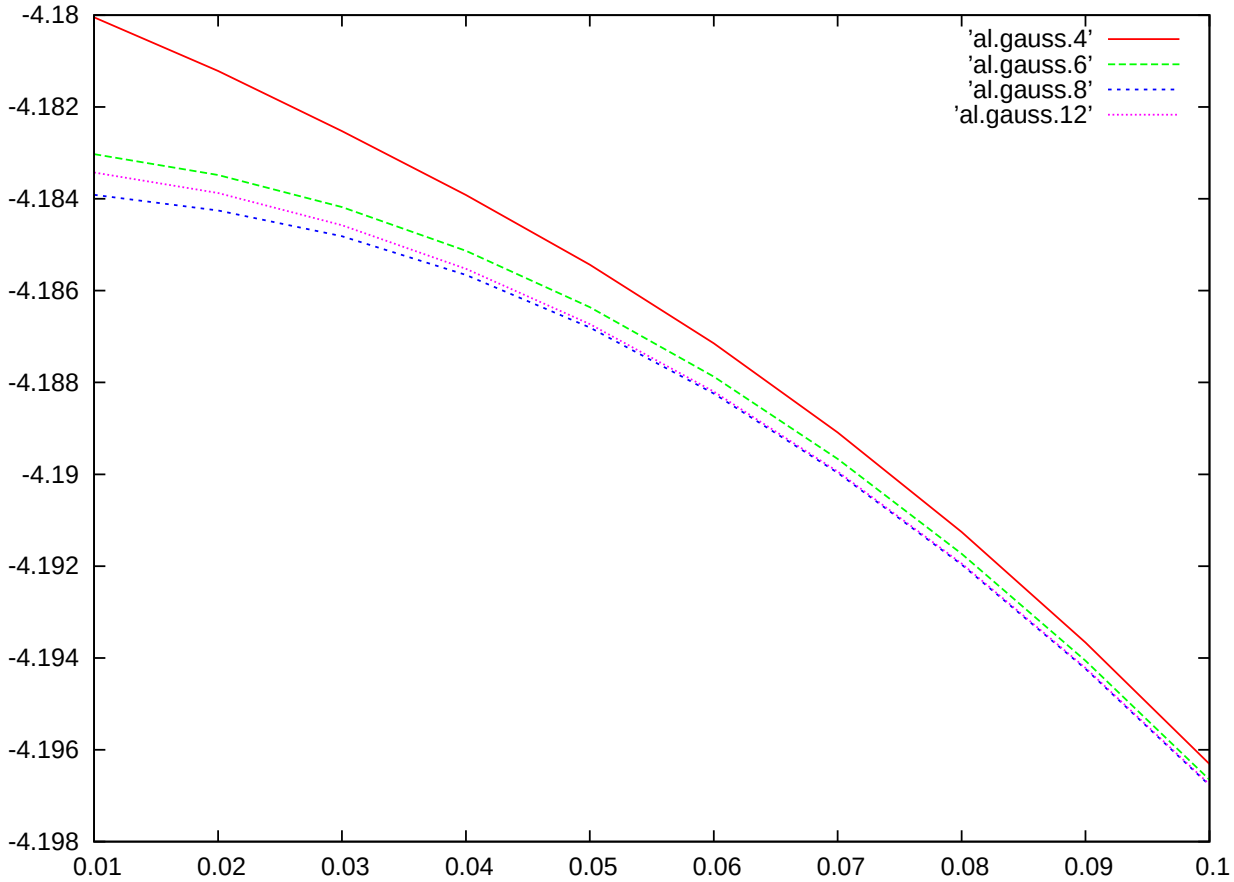
Convergence with respect to degauss/smearing ...

K-point convergence in the metallic case is more delicate than in the insulating case.

By editing al.scf.in and varying variables smearing
[gaussian (gauss), marzari-vanderbilt (m-v), methfessel-paxton (m-p)]
and degauss [0.06, 0.07, 0.08, 0.09, 0.10, ...]
one can reproduce the results collected in al.gauss.6, al.m-v.6, al.m-p.6, ... files.

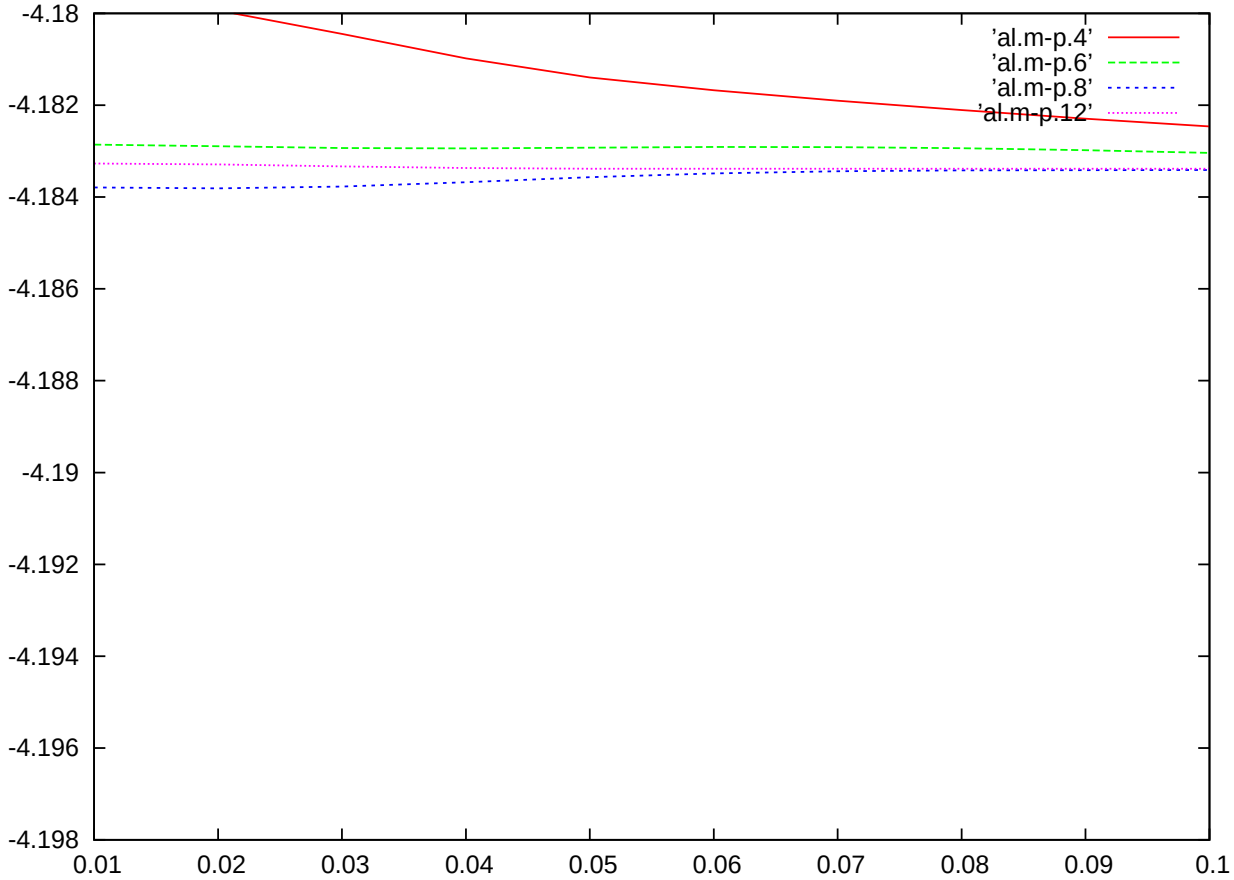
Convergence with respect to degauss/smearing ...

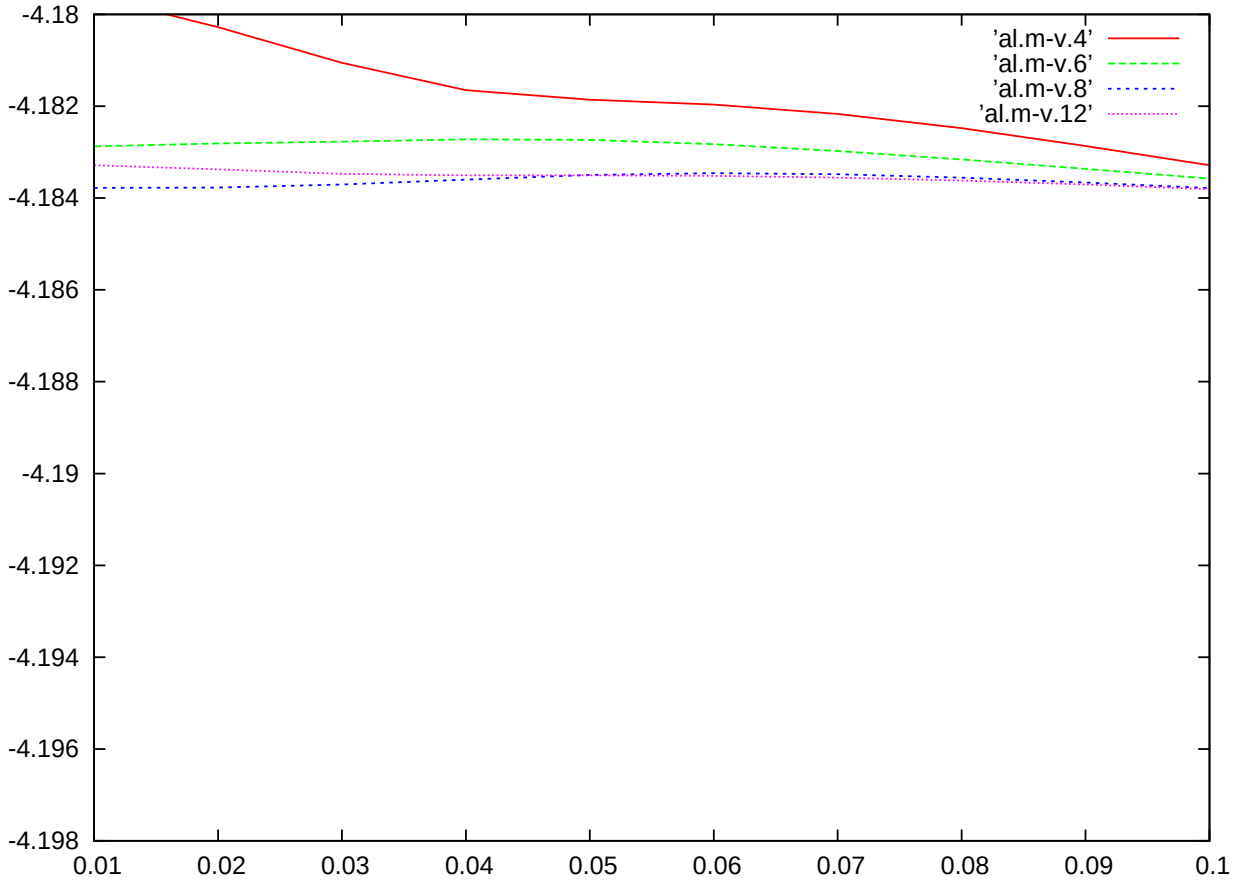
Plot the content of al.gauss.4, al.gauss.6, al.gauss.8, al.gauss.12, and similarly for m-v and m-p



Notice that for metals convergence is SLOW

It can be improved by using m-v or m-p.


-4.18
-4.182
-4.184
-4.186
-4.188
-4.19
-4.192
-4.194
-4.196
-4.198
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
0.1
'al.m-p.4'
'al.m-p.6'
'al.m-p.8'
'al.m-p.12'


-4.18
-4.182
-4.184
-4.186
-4.188
-4.19
-4.192
-4.194
-4.196
-4.198
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
0.1
'al.m-v.4'
'al.m-v.6'
'al.m-v.8'
'al.m-v.12'

A 3d metal: Copper

Move to the Copper directory

```
prompt> cd ../Copper
```

Inspect input file cu.scf.in and check that it is an scf calculation for a metallic system.

Notice that this is a metallic calculation.

Copper pseudopotential is an US-PP: ecutrho $> 4\times$ecutwfc

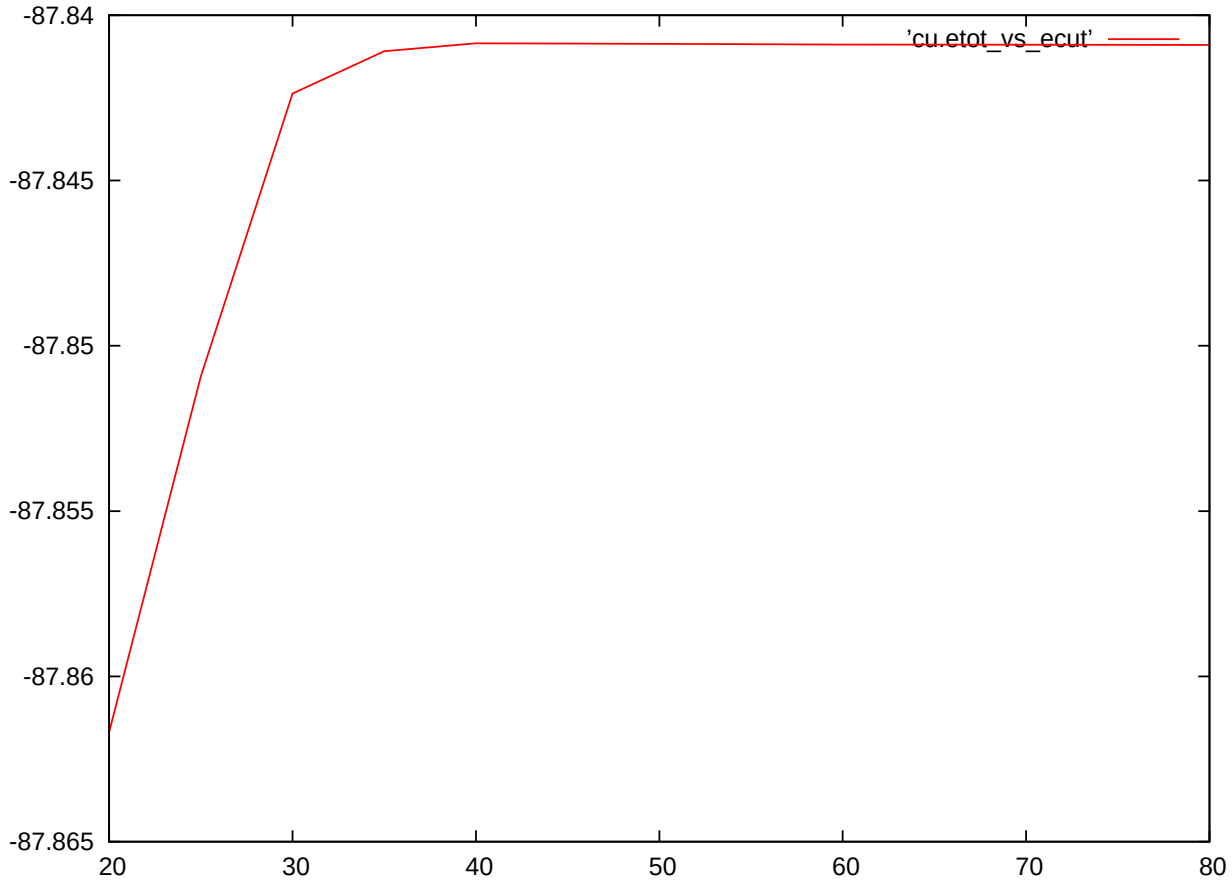
Run pw.x

```
prompt> espresso_dir/bin/pw.x < cu.scf.in > cu.scf.out
```

Notice the different number of calls and timing of the cft3 and cft3s routines.
Why it is convenient to introduce a different cutoff for wfcs and rho ?

Chose ecutwfc and ecutrho for Copper

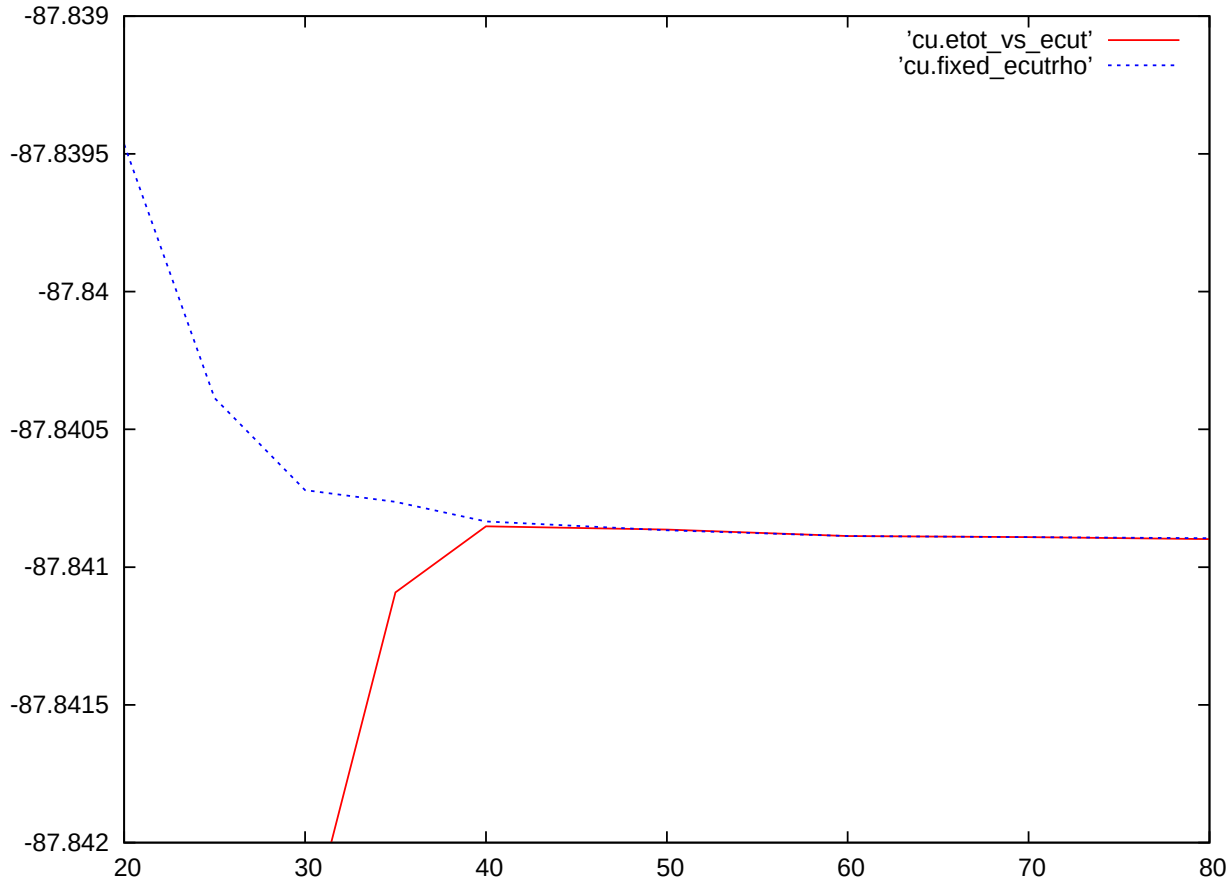
Look for convergence with the default value of ecutrho $= 4 \times$ ecutwfc



Notice that the behavior may look non varational due to the inaccurate evaluation of integrals involving the augmentation charge.

Chose ecutwfc and ecutrho for Copper

Once ecutrho is fixed in such a way that the integration is performed properly repeat the scan w.r.t. ecutwfc to find out if it can be safely reduced.



A magnetic example: Nickel

Move to the Nickel directory

```
prompt> cd ../Nickel
```

Inspect input file ni.scf.in and check that it is an scf calculation for a metallic system.

Notice the use of variables nspin and starting_magnetization.

Notice that this is a metallic calculation.

Nickel pseudopotential is an US-PP: ecutrho $> 4\times$ecutwfc

Run pw.x

```
prompt> espresso_dir/bin/pw.x < ni.scf.in > ni.scf.out
```

Notice that the number of k-points is doubled w.r.t non-magnetic case

Notice different number of calls and timing of cft3 and cft3s routines.
Why it is convenient to introduce a different cutoff for wfcs and rho ?

Stuctural Relaxation

Move to the RELAX directory and check its content

```
 prompt> cd ../RELAX
prompt> ls
Al001        CO
```

Relaxation of CO molecule in a box

Move to the CO sub-directory

Inspect the input file co.rx.in and notice that calculation="relax" and that an additional namelist &ions is persent.

How is an isolated molecule defined in this input ?

check in the input file

```
 What is the Bravais lattice ?
What is the lattice parameter ?

How many atoms in the unit cell ?
How many different atomic species ?
Which ones ?

What type of Brillouin zone sampling is performed ?
why ?
```

run pw.x code

```
prompt> espresso_dir/bin/pw.x < co.rx.in > co.rx.out
```

examine output file and look how relaxation proceeds

```
prompt> grep -e ! -e BFGS co.rx.out
!    total energy              =     -43.09625765 Ry
     BFGS Geometry Optimization
!    total energy              =     -43.09665632 Ry
!    total energy              =     -43.10970996 Ry
!    total energy              =     -43.10976481 Ry
!    total energy              =     -43.10976799 Ry
     End of BFGS Geometry Optimization
```

the relaxation kept fixed one of the two atoms

```
can you identify where in the input this was set ?
```

remove this constraint and repeat the calculation

```
 does the relaxation reach the same result ?

why ?

is it equivalent ?
```

A surface slab example: Aluminum (001)

move to Al001 sub-directory

Inspect the al001.rx.in input file and visualize the input by xcrysden

```
prompt> xcrysden --pwi al001.rx.in
```

and verify that this represents a (001) Al surface in the repeated slab geometry

```
How many layers ?
How many atoms per layer ?
How wide is the vacuum space ?
```

Run pw.x

```
prompt> espresso_dir/bin/pw.x < al001.rx.in > al001.rx.out
```

How many iterations are necessary ?

What is the final interlayer relaxation for the surface layers ?

compare al001.rx.in input with al001.damp.in

What are the differences ?
Why the atomic mass of Al is set to 1.0 ?
What would be necessary to change if the real mass would be used ?

Run pw.x

```
prompt> espresso_dir/bin/pw.x<al001.damp.in>al001.damp.out
```

How many iterations are necessary ?
Is the final result equivalent to the previous case ?

To complete the exercise one should monitor the convergence with respect to

```
number of slab layers
thickness of the vacuum region
```

A Tansition Metal Oxide : FeO

plain LDA/GGA give a metallic GS while experimentally FeO is an insulator.

DFT+U may be needed to open a gap in the bands associated to the localized 3d orbitals

```
Hubbard_U(ityp)
```

An appropriate starting point for the occupation of the localized orbitals may be needed

```
starting_ns_eignvalue(m,ispin,I)
```

U can be computed from firs principles [M.Cococcioni and SdG, PRB 71, 035105 (2005)]

```
Hubbard_alpha(ityp)
```

THE END