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PWSCF
First examples

(much more in espresso-3.1.1/examples directory!)

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A pw.x input file


```
 &CONTROL
                       title = 'Silicon bulk' ,
                 calculation = 'scf' ,
                restart_mode = 'from_scratch' ,
                      outdir = 'your directory for temporary files/' ,
                  pseudo_dir = 'your directory containing pseudopotentials/' ,
                      prefix = 'silicon' ,
 /
 &SYSTEM
                        ibrav = 2,
                   celldm(1) = 10.20,
                         nat = 2,
                        ntyp = 1,
                     ecutwfc = 18.0 ,
 /
 &ELECTRONS
                    conv_thr = 1.0d-8 ,
                mixing_mode = 'plain' ,
                mixing_beta = 0.7 ,
           diagonalization = 'david' ,
 /
ATOMIC_SPECIES
   Si   28.08600  Si.vbc.UPF
ATOMIC_POSITIONS
   Si       0.000000000    0.000000000    0.000000000    1  1  1
   Si       0.250000000    0.250000000    0.250000000    1  1  1
K_POINTS tpiba
10
   0.125000000    0.125000000    0.125000000       1.000000000
   ...
```

Described in detail in the file ESPRESSO/Doc/INPUT_PW

Graphical User Interface

1) Download stand-alone application (http://www-k3.ijs.si/kokalj/pwgui/download.html):

```
wget www-k3.ijs.si/kokalj/pwgui/download/pwgui-linux-x86.zip
```

2) Unzip / untar file:

```
unzip pwgui-linux-x86.zip
```

3) Execute:

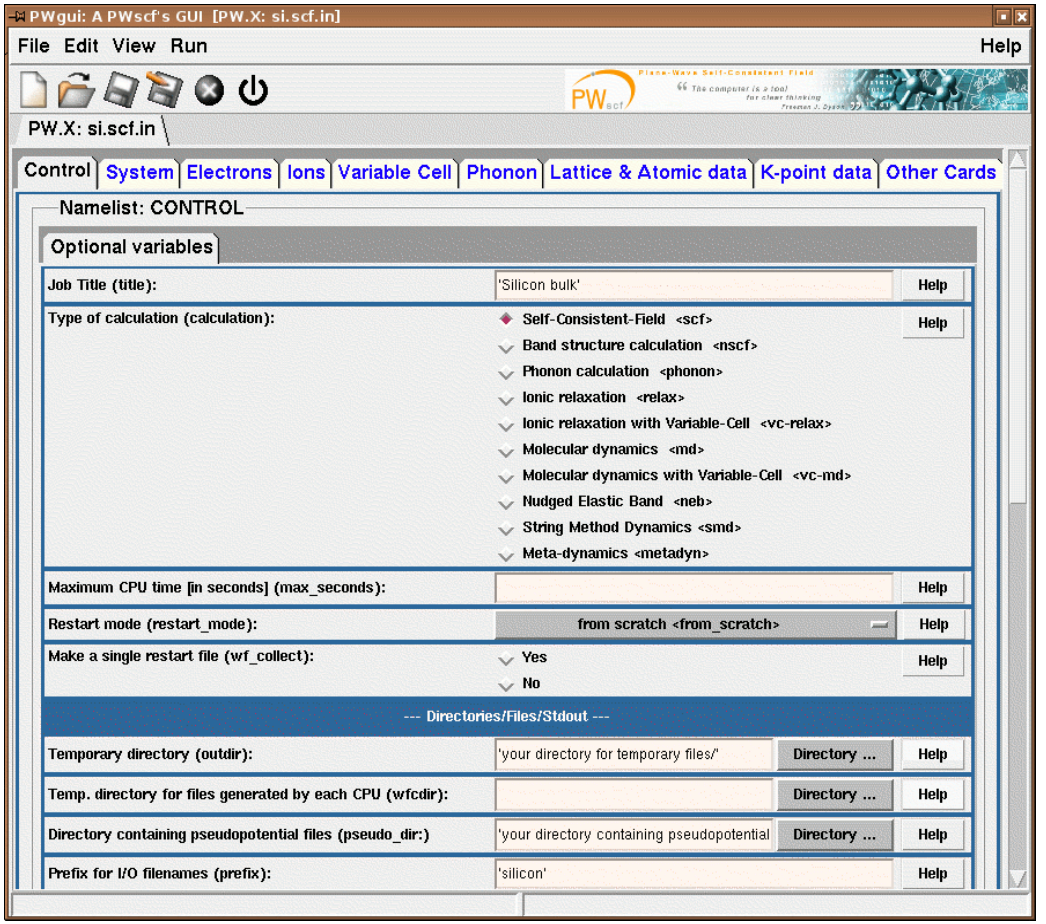
```
./pwgui
```

4) Open / create new input file

5) Save the input file

6) Run the calculation:

```
pw.x < input > output
```



GUI in practice:

DEMOCRITOS
DEmocritos MOdeling Center for Research In aTOmistic Simulation INFM

Open file si.scf.in (File – Open – Open Pw.x Input – si.scf.in)

Set your directories:

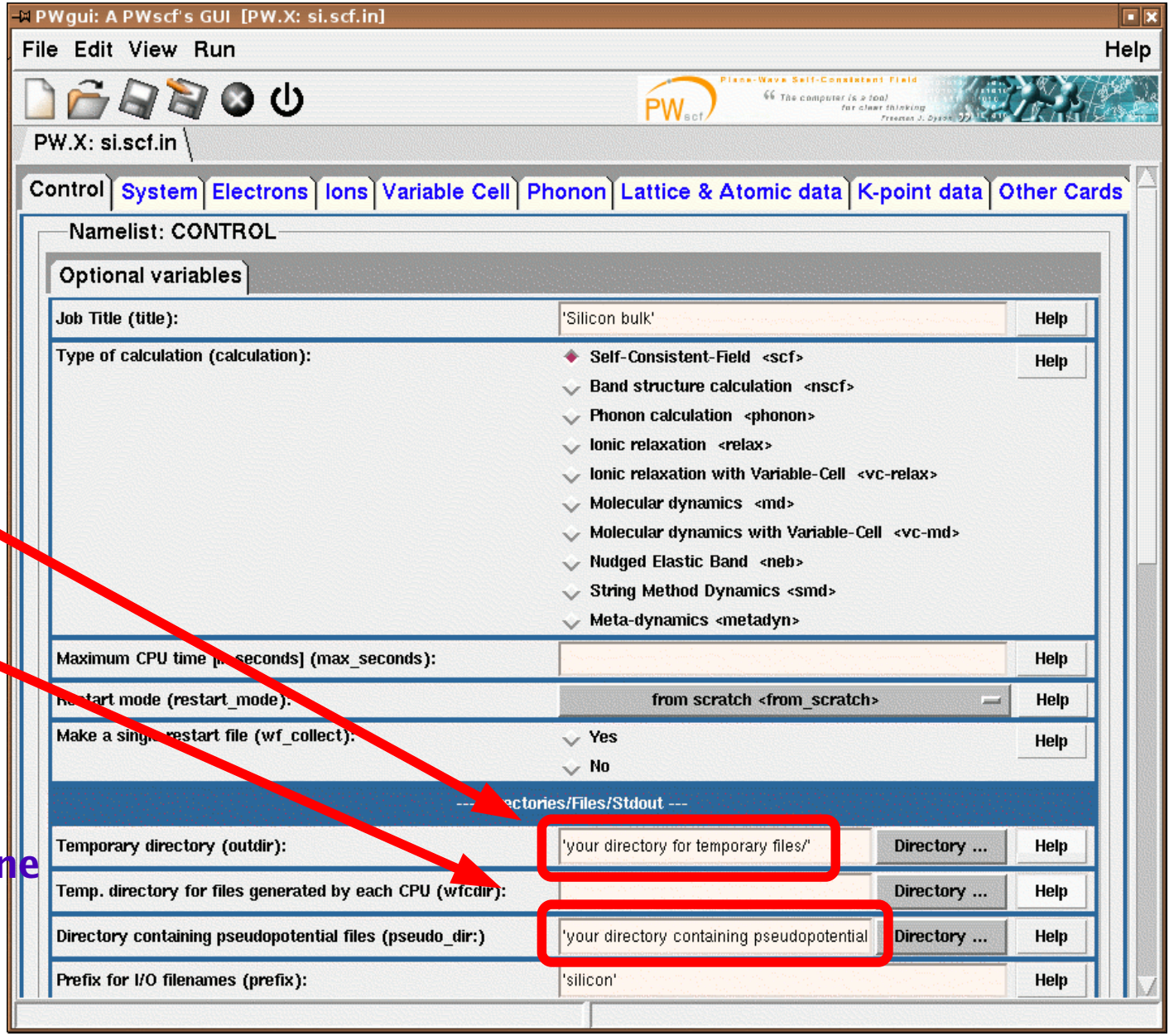
`outdir`
(containing temporary files)

`pseudo_dir`
(containing pseudopotentials)

Save (File – Save)

Copy to computing machine

Run calculation



And now the output file

Scroll the output file (type less si.scf.out**): informations on the system**

```
     Version // Title ...

     bravais-lattice index     =            2
     lattice parameter (a_0)   =      10.2000  a.u.
     unit-cell volume          =     265.3020 (a.u.)^3
     number of atoms/cell      =            2
     number of atomic types    =            1
     kinetic-energy cutoff     =      18.0000  Ry
     charge density cutoff     =      72.0000  Ry
     convergence threshold     =      1.0E-08
     beta                      =       0.7000
     number of iterations used =            8  plain     mixing
     Exchange-correlation      =  SLA  PZ   NOGX NOGC (1100)
     celldm(1)=  10.200000  celldm(2)=   0.000000  celldm(3)=   0.000000
     celldm(4)=   0.000000  celldm(5)=   0.000000  celldm(6)=   0.000000

     crystal axes: (cart. coord. in units of a_0)
               a(1) = ( -0.500000  0.000000  0.500000 )
               a(2) = (  0.000000  0.500000  0.500000 )
               a(3) = ( -0.500000  0.500000  0.000000 )

     reciprocal axes: (cart. coord. in units 2 pi/a_0)
               b(1) = ( -1.000000 -1.000000  1.000000 )
               b(2) = (  1.000000  1.000000  1.000000 )
               b(3) = ( -1.000000  1.000000 -1.000000 )

  [...]
```

And now the output file

Scroll the output file: informations on atoms and pseudopotentials

```
 [...]

     PSEUDO 1 is Si          zval =  4.0   lmax= 1   lloc= 0
     (in numerical form:   431 grid points, xmin =  0.00, dx = 0.0000)

     atomic species   valence    mass     pseudopotential
        Si             4.00    28.08600     Si( 1.00)

     48 Sym.Ops. (with inversion)


   Cartesian axes

     site n.     atom                  positions (a_0 units)
         1           Si  tau(  1) = (   0.0000000   0.0000000   0.0000000  )
         2           Si  tau(  2) = (   0.2500000   0.2500000   0.2500000  )

 [...]
```

And now the output file

Scroll the output file: informations on K points and FFT

```
 [...]

     number of k points=   10
                       cart. coord. in units 2pi/a_0
        k(    1) = (   0.1250000   0.1250000   0.1250000), wk =   0.0625000
        k(    2) = (   0.1250000   0.1250000   0.3750000), wk =   0.1875000
        k(    3) = (   0.1250000   0.1250000   0.6250000), wk =   0.1875000
        k(    4) = (   0.1250000   0.1250000   0.8750000), wk =   0.1875000
        k(    5) = (   0.1250000   0.3750000   0.3750000), wk =   0.1875000
        k(    6) = (   0.1250000   0.3750000   0.6250000), wk =   0.3750000
        k(    7) = (   0.1250000   0.3750000   0.8750000), wk =   0.3750000
        k(    8) = (   0.1250000   0.6250000   0.6250000), wk =   0.1875000
        k(    9) = (   0.3750000   0.3750000   0.3750000), wk =   0.0625000
        k(   10) = (   0.3750000   0.3750000   0.6250000), wk =   0.1875000

     G cutoff =  189.7462  (   2733 G-vectors)     FFT grid: ( 20, 20, 20)

     nbndx   =     16  nbnd    =      4  natomwfc =      8  npwx    =      350
     nelec   =   8.00  nkb     =      8  ngl     =      65

 [...]
```

And now the output file

Scroll the output file: the self-consistent field loop starts

```
 [...]

     Initial potential from superposition of free atoms

     starting charge    7.99901, renormalised to    8.00000
     Starting wfc are atomic

     total cpu time spent up to now is      0.36 secs

     Self-consistent Calculation

     iteration #  1     ecut=    18.00 ryd     beta=0.70
     Davidson diagonalization with overlap
     ethr =  1.00E-02,  avg # of iterations =  2.0

     Threshold (ethr) on eigenvalues was too large:
     Diagonalizing with lowered threshold

     Davidson diagonalization with overlap
     ethr =  7.75E-03,  avg # of iterations =  1.0

     total cpu time spent up to now is      0.92 secs

     total energy              =   -15.84097415 ryd
     estimated scf accuracy    <     0.06141563 ryd

 [...]
```

And now the output file

Scroll the output file: the self-consistent field loop converges

```
 [...]

     total energy              =   -15.84452724 ryd
     estimated scf accuracy    <     0.00000006 ryd

     iteration #  6     ecut=    18.00 ryd     beta=0.70
     Davidson diagonalization with overlap
     ethr =  7.18E-10,  avg # of iterations =  2.7

     total cpu time spent up to now is      1.88 secs

     End of self-consistent calculation

          k = 0.1250 0.1250 0.1250 (   335 PWs)   bands (ev):

    -5.6040   4.6468   5.9568   5.9568

 [...]
```

And now the output file

Scroll the output file: summary of energy, forces, and stress tensor

```
 [...]
!    total energy              =   -15.84452726 ryd
     estimated scf accuracy    <        8.8E-10 ryd

     band energy sum           =     0.66828316 ryd
     one-electron contribution =     4.79352695 ryd
     hartree contribution      =     1.07664132 ryd
     xc contribution           =    -4.81493686 ryd
     ewald contribution        =   -16.89975867 ryd

     convergence has been achieved

     Forces acting on atoms (Ry/au):

     atom    1 type  1   force =     0.00000000    0.00000000    0.00000000
     atom    2 type  1   force =     0.00000000    0.00000000    0.00000000

     Total force =     0.000000     Total SCF correction =     0.000000


     entering subroutine stress ...

          total   stress  (ryd/bohr**3)                   (kbar)     P=  -10.23
  -0.00006958   0.00000000   0.00000000        -10.23       0.00       0.00
   0.00000000  -0.00006958   0.00000000          0.00     -10.23       0.00
   0.00000000   0.00000000  -0.00006958          0.00       0.00     -10.23
 [...]
```

And now the output file

Scroll the output file: saving data file (restart, post processing, ...) and timing informations

```
 [...]

     Writing output data file silicon.save

     PWSCF        :     2.00s CPU time

     init_run     :     0.34s CPU
     electrons    :     1.52s CPU
     forces       :     0.01s CPU
     stress       :     0.07s CPU

     electrons    :     1.52s CPU
     c_bands      :     1.21s CPU (       7 calls,   0.173 s avg)
     sum_band     :     0.25s CPU (       7 calls,   0.036 s avg)
     v_of_rho     :     0.03s CPU (       7 calls,   0.004 s avg)
     mix_rho      :     0.00s CPU (       7 calls,   0.001 s avg)

     c_bands      :     1.21s CPU (       7 calls,   0.173 s avg)
     init_us_2    :     0.05s CPU (     170 calls,   0.000 s avg)
     cegterg      :     1.17s CPU (      70 calls,   0.017 s avg)

     sum_band     :     0.25s CPU (       7 calls,   0.036 s avg)

 [...]
```

Postprocessing: charge density

Let us plot the charge density of Si along the (110) plane.

1) Prepare input file **si.pp.in** with PWgui (see next slides):

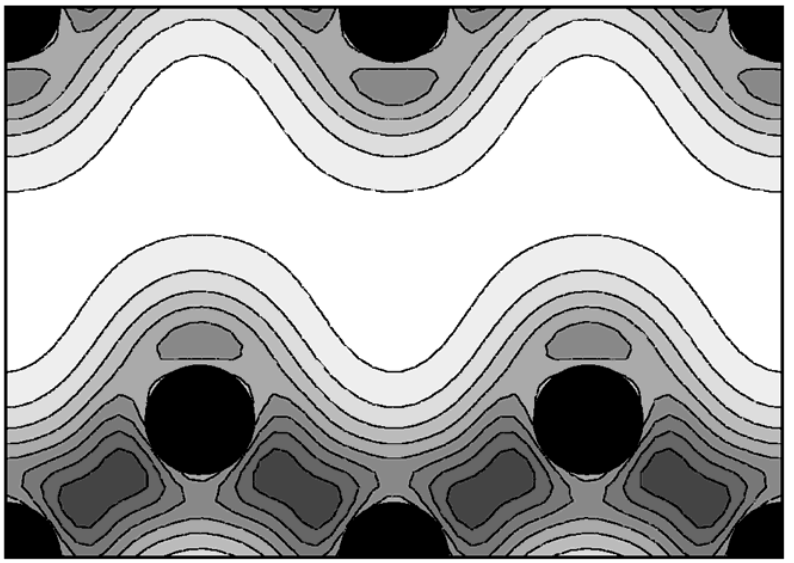
2) execute **pp.x**:

```
pp.x < si.pp.in > si.pp.out
```

(out of the many output formats available, let us choose the plotrho format)

3) execute **plotrho.x**:

```
plotrho.x
    Input file > silicon.charge110.dat
    r0    :    0.0000   0.0000   0.0000
    tau1  :    0.0000   0.0000   1.0000
    tau2  :    1.0000  -1.0000   0.0000
    read    2 atomic positions
    output file > silicon.charge110.ps
    Read   29 * 41   grid
    Logarithmic scale (y/n)? > n
    Bounds:       0.001411     0.087060
    min, max, # of levels > 0 0.09 10
```



4) Visualize postscript file

```
gv silicon.charge110.ps
```

For advanced and 3D graphics, use XCrySDen (www.xcrysden.org) or other formats

Postprocessing: charge density

Run PWgui and

0) Create a new PP.X input file

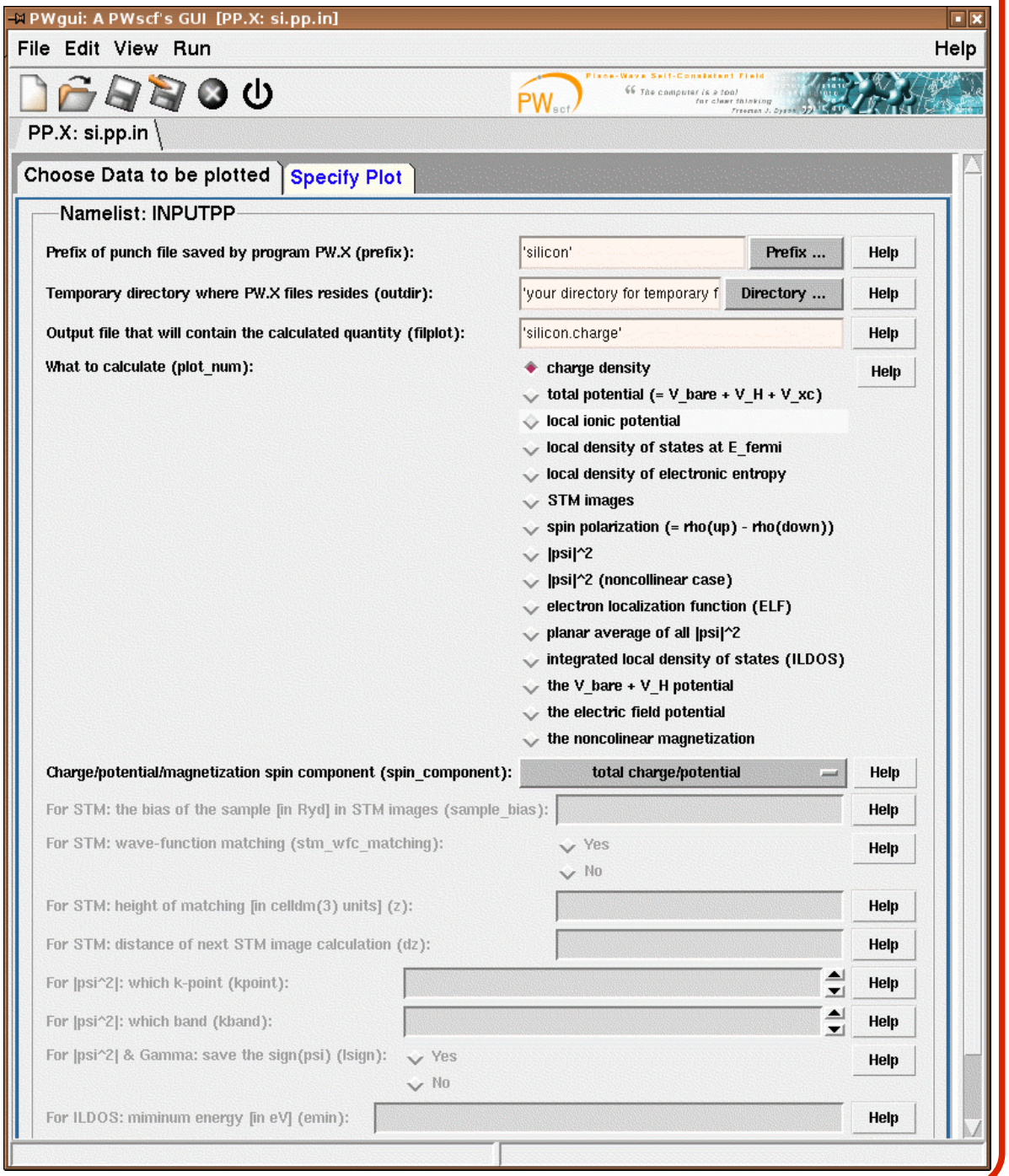
Be consistent with the SCF run:

1) `prefix` must be the same
2) `outdir` must be the same

3) Data will be saved in `filplot` in a raw format

4) Select quantity to plot (several choices)

5) Specify options

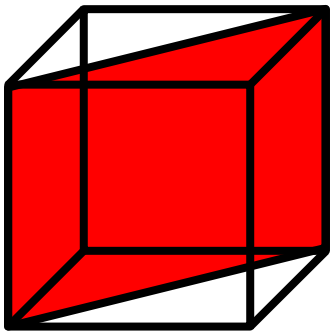


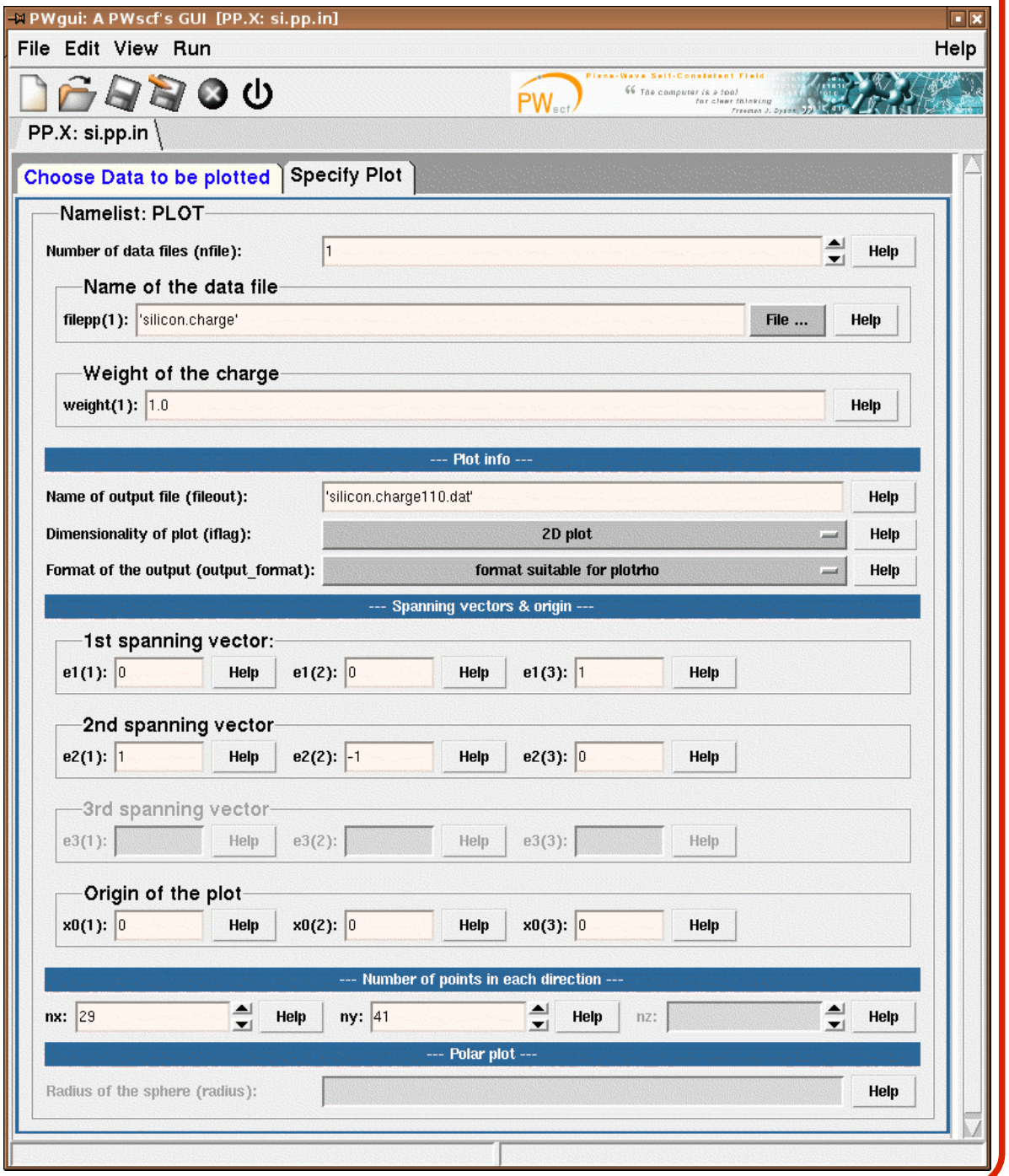
Postprocessing: charge density

6) Select the raw-data files to plot
(here, `filplot` as given before)

7) Select
the output file,
the kind of plot,
the output format (here `plotrho`)

8) Specify the region of the plot
(here, the 110 plane)

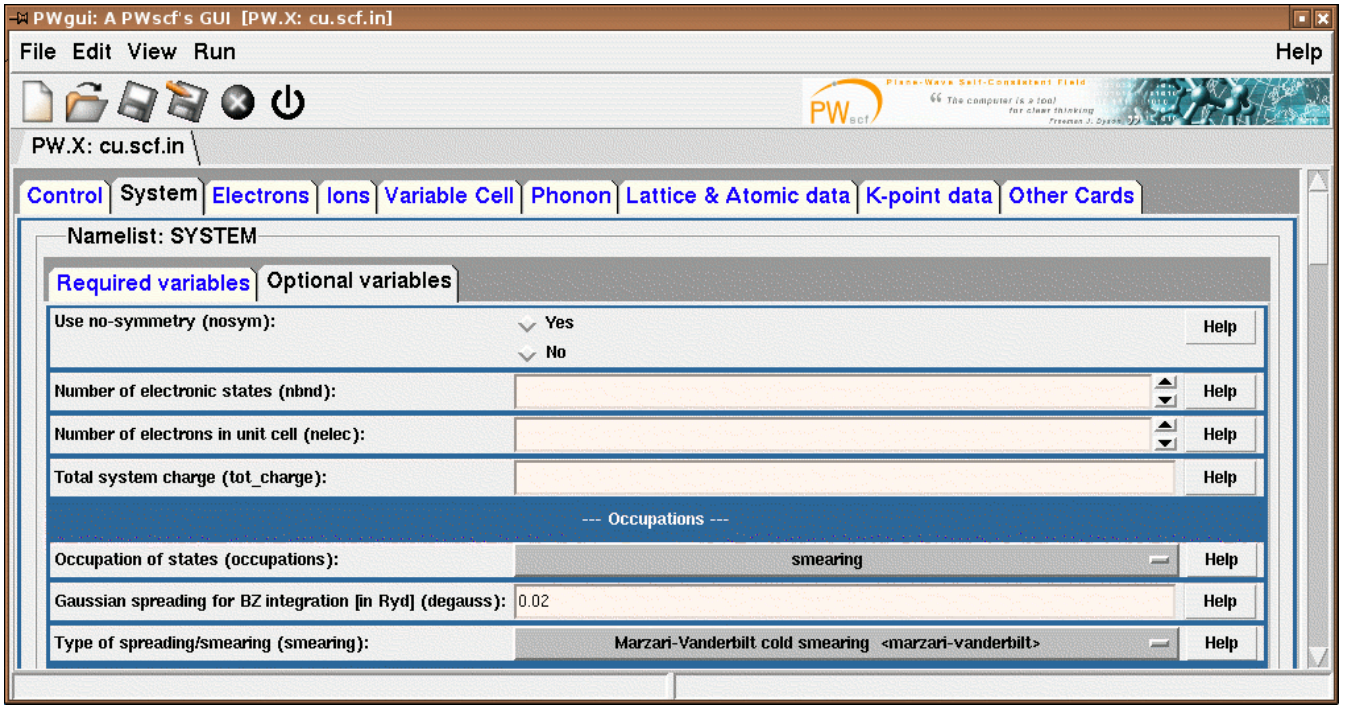




A metal: Cu bulk

Change number of atoms, coordinates, pseudopotentials, K-points, cutoffs, plus...

Set additional variables by using PWgui:



or directly editing the input file:

```
 &SYSTEM
                        [...]
                ecutrho = 300.0 ,
             occupations = 'smearing' ,
                 degauss = 0.02 ,
               smearing = 'marzari-vanderbilt' ,
 /
```

PWscf and XCrySDen

Atomic structure, forces, charge densities, dynamics, ... can be visualized by XCrySDen

Download from http://www.xcrysden.org, e.g. (choose the version for your machine):

```
wget http://www.xcrysden.org/download/xc-latest-linuxPC-static.tar.gz
```

Untar:

```
tar xzvf xc-latest-linuxPC-static.tar.gz
```

Install:

```
cd [xcrysden-directory]
./xcConfigure
```

Source your profile (or open a new terminal)

Visualize `pw.x` input/output files...

```
xcrysden --pwi si.scf.in
xcrysden --pwo si.scf.out
```

...files generated by `pp.x` (`output_format` 3, 5)...

```
xcrysden --xsf file.xsf
```

...animated files (NEB, ...)

```
xcrysden --axsf prefix.axsf
```