computing and visualizing charge density differences

This document describes how to compute the *charge density difference* (*) by Quantum Espresso, and how to visualize it in 3 (or is it 4?) dimensions.

(*) by *charge density difference*, we mean here "charge density minus superposition of atomic densities" (quote from the QE input reference document). The opposite quantity (superposition of free atom densities minus the charge density of the crystal) is used equally often. You always have to check which of both definitions is used before interpreting a picture in a book or paper.

In this document, we will use rocksalt (NaCl) as the example.

First make a regular DFT calculation for rocksalt, starting from this cif file, with this pseudopotential for Na and this pseudopotential for Cl, with ecutwfc=60, ecutrho=360 and a 15x15x15 k-mesh. Pay particular attention to `prefix` and `outdir`: the names/choices you take for these, will need to be used later on in other files as well.

This is how your input file for a regular pw.x calculation should look like (make it yourself, starting from the cif file):

```
&CONTROL
  calculation='scf',
  outdir='.',
  prefix='NaCl',
  pseudo_dir='.',
  verbosity='low',
  tprnfor=.true.,
  tstress=.true.,
/

&SYSTEM
  ibrav=2,
  celldm(1)=10.6591135892d0,
  nat=2,
  ntyp=2,
  ecutwfc=60,
  ecutrho=360,
  input_dft='pbe',
  occupations='smearing',
  smearing='mv',
  degauss=0.005d0,
/

&ELECTRONS
  conv_thr=1d-08,
  mixing_beta=0.7d0,
/

ATOMIC_SPECIES
  Cl 35.453000d0 Cl.pbe-n-kjpaw_psl.0.1.UPF
  Na 22.989800d0 Na.pbe-spn-kjpaw_psl.0.2.UPF


ATOMIC_POSITIONS {crystal}
  Na   0.0000000000d0   0.0000000000d0   0.0000000000d0
  Cl   0.5000000000d0   0.5000000000d0   0.5000000000d0

K_POINTS {automatic}
  15 15 15 0 0 0
```

After having run this calculation, prepare an input file for PP (the Post-Processing tool of QE). The file can have any name, let's call it here `ppinput.in`. This is how it should look like (explanations are given underneath):

```
&INPUTPP
  prefix='NaCl',
  outdir='.',
  filplot='ppoutputfile.txt',
  plot_num=9,
/

&PLOT
  nfile=1,
  iflag=3,
  output_format=6,
  fileout='myplot.cube',
  e1(1)=1.0,e1(2)=0.0,e1(3)=0.0,
  e2(1)=0.0,e2(2)=1.0,e2(3)=0.0,
  e3(1)=0.0,e3(2)=0.0,e3(3)=1.0,
  x0(1)=1.0,x0(2)=0.0,x0(3)=0.0,
  nx=101,ny=101,nz=101,
/
```

These are the meanings of the lines in this file:

&INPUTPP block : this instructs pp.x to calculate the requested quantity (yet not to plot it)

prefix : this should be exactly the same as 'prefix' in the preceding pw.x calculation.

outdir : this should be exactly the same as 'outdir' in the preceding pw.x calculation.

filplot : name of a file that will contain the requested object, albeit in a format that cannot yet be visualized. Possible error information will be in this file as well.

plot_num = 9 : for this value, pp.x will calculate the 'charge difference density', defined as "charge density minus superposition of atomic densities". See the QE input reference manual for other values of plot_num, to calculate other quantities (charge density, potential, spin density, STM-image,…)

&PLOT block : this instructs pp.x to write (part of) the quantity calculate in the previous step into a format that can be read by plotting tools.

nfile = 1 : for a charge difference density there will be only one file to plot

iflag = 3 : this instructs to create a three-dimensional plot

output_format = 6 : this instructs to write the three-dimensional plot into the "cube" format (a file format that can be generated and/or visualized by many programs, stemming from the Gaussian code).

fileout = 'myplot.cube' : the file in cube format that contains your final image. You can use any file name here. The *.cube extension is logical, yet not strictly necessary.

Then comes a set of 4 coordinates. The first three define three vectors that together span the volume that will be plot. These three vectors must be orthogonal to each other. The 4th set of coordinates defines the origin from which these vectors start.

The last line contains the number of grid points for which plottable data will be generated, along each of the three vectors specified above.

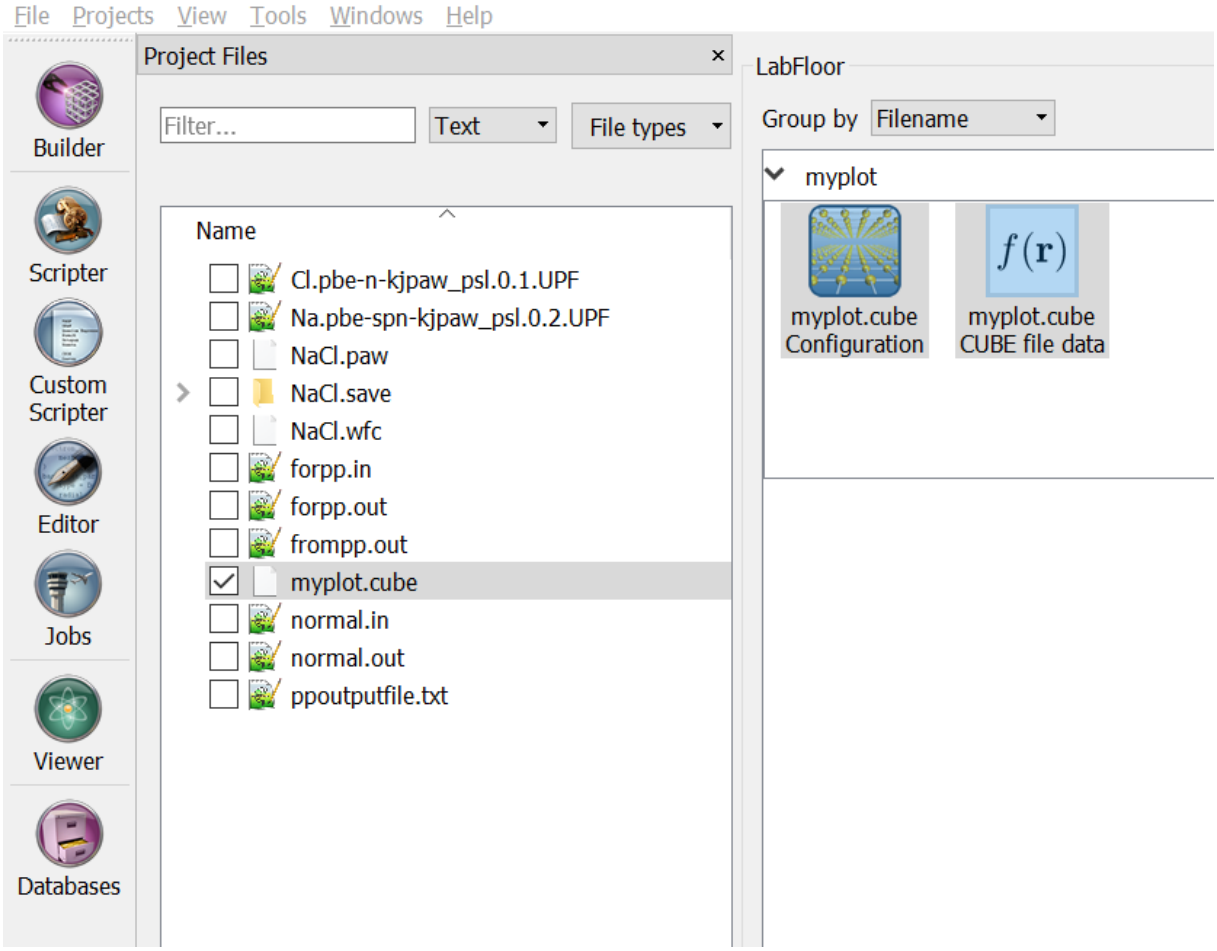
Once you prepared this file (named ppinput.in), run pp.x:

pp.x -input ppinput.in > ppoutput.out

(as usual, in Windows the command is pp, not pp.x).

Displaying the charge difference density in VNL :

Open a VNL project for the folder in which you ran the calculations above. In the left column, check/select the file ‘myplot.cube’. Then go to the Labfloor at the right, and click ‘myplot’. You will see a ‘Configuration’ and ‘CUBE file data’ appearing on the Labfloor:



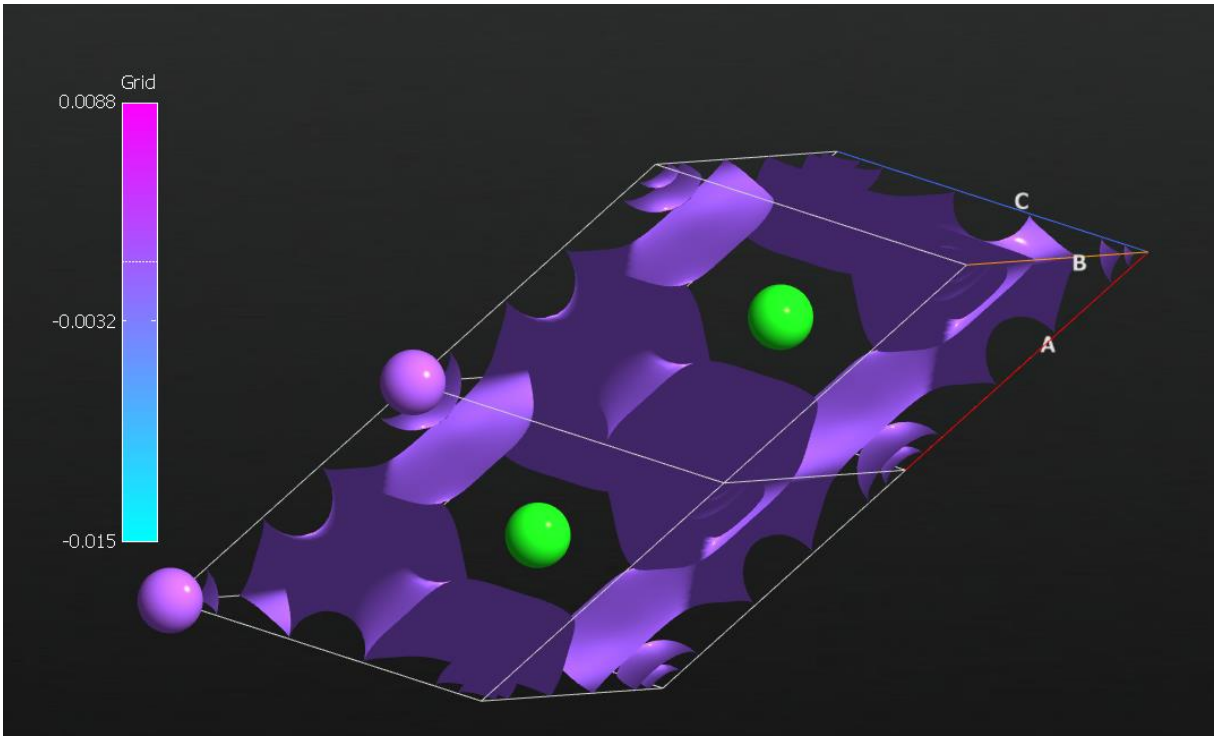
Select both of these objects, and drag them onto the ‘Viewer’ icon on the left.

You will get a ‘Drop selection?’ window. Select both ‘Grid configuration’ and ‘Grid values’, then OK. Select ‘Isosurface’ in the next window (for 2D plots, you can select ‘Cut plane’).

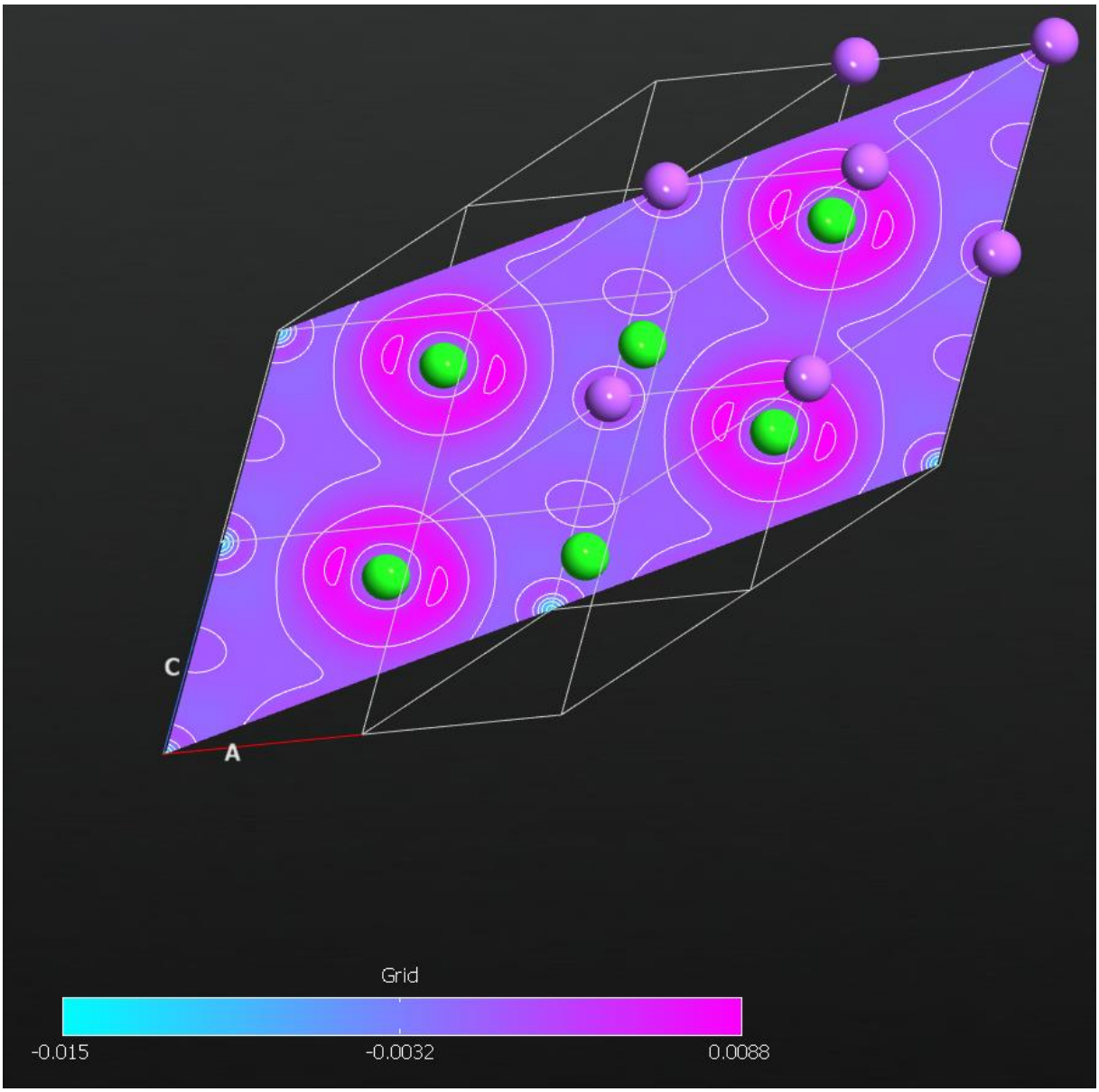
A unit cell picture will appear. From the list of items at the right hand side, select ‘Properties’ (you might need to scroll down):

- Use the ‘isovalue’ slider to select the isovalue you want to plot.
- Use ‘color map’ to use the color scheme you like.
- In the ‘repetition’ block, you can select a larger number of unit cells, to see better the extended 3D view (increase the values in the three ‘upper’ boxes to 2, or 3, or…).
- If you go to the display window, you can hold the right mouse button and drag the crystal around, to view the isosurface from all directions.

If you have selected ‘cut plane’ rather than ‘isosurface’, you get a plane with a color scheme in that plane to indicate the different values. By ‘position’ and ‘rotation’ you can drag that plane through the unit cell. Check/select ‘isolines’ to see isolines on the surface. The repetition block allows to draw multiple unit cells. In the display window itself, you can rotate the crystal by holding the right-handside mouse button.



Example of an isosurface picture for NaCl.



Example of the difference density in one plane for NaCl.