scf and band structure calculations for Cu (metal)

- No input files available, but should be generated for practice.
- Next two slides explain where changes need to be done for scf calculations.
- Follow the similar procedure to find dos and band structure for Cu.

Input help:
http://www.quantum-espresso.org/Doc/INPUT_PW.html

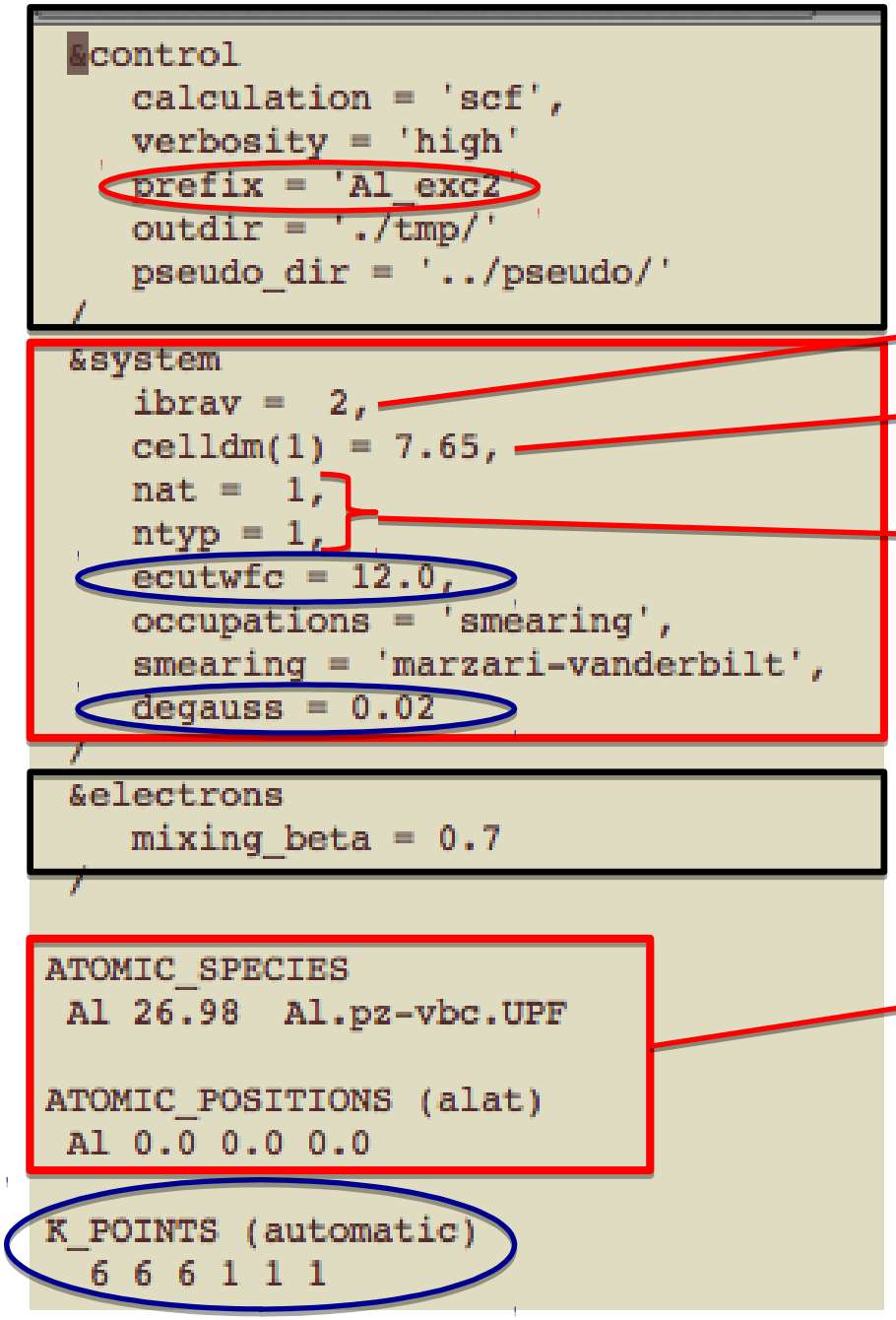
```
 &control
    calculation = 'scf',
    verbosity = 'high'
    prefix = 'Al_exc2'
    outdir = './tmp/'
    pseudo_dir = '../pseudo/'
 /
 &system
    ibrav =  2,
    celldm(1) = 7.65,
    nat =  1,
    ntyp = 1,
    ecutwfc = 12.0,
    occupations = 'smearing',
    smearing = 'marzari-vanderbilt',
    degauss = 0.02
 /
 &electrons
    mixing_beta = 0.7
 /

ATOMIC_SPECIES
 Al 26.98  Al.pz-vbc.UPF

ATOMIC_POSITIONS (alat)
 Al 0.0 0.0 0.0

K_POINTS (automatic)
  6 6 6 1 1 1
```

- Not system dependent!
- “prefix” should be changed preferably to avoid overwriting of wavefunctions and charge density.



1. What is the crystal structure for Cu?
2. Cu experimental lattice constant as a starting point?
3. Number of atoms in the unit cell?
4. How many different types of elements?

Need to specify which element, which pseudopotential, and atomic positions correct?

Convergence tests required for the new pseudopotential!!