a basic calculation with Quantum Espresso

Disclaimer: this document tells you 'how to', not 'why'. It is meant only to make you familiar with the practical procedure. Explanations about what every step really means, will follow gradually throughout the course.

1. Start your virtual machine for Quantum Espresso.

2. open a new terminal window (double-click the terminal icon in the left vertical bar)

3. if not yet done before: create a folder where you will perform all your Quantum Espresso calculations (call it workQE), and descend into that folder:

```
mkdir workQE
cd workQE
```

4. make a subfolder (called basic here, yet any name will do) where you will perform this particular calculation, and descend into it:

```
mkdir basic
cd basic
```

5. *(this step requires internet access)* download from a crystallographic database a file that contains a full specification of the crystal structure of silicon at room temperature. This file has the so-called cif-format, a common crystal structure definition format that is human-readable as well as machine-readable.

```
wget http://www.crystallography.net/cod/9008566.cif
```

6. Quantum Espresso reads crystal structure information in its own way. Translate the cif file to Quantum Espresso format, and store this into a file with the name 'basic.in' (same name header as the folder – this is not strictly required, yet it creates some natural order into your files):

```
cif2cell 9008566.cif -p quantum-espresso -o basic.in
```

(the warning that might appear about site occupancies is harmless)

7. Open the file you have just generated:

```
nano basic.in
```

8. after the 8 lines that start with '#', enter the following block of information:

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

```
   tstress=.true.,
/
```

The value for 'prefix' can be chosen freely – as you are going to do a basic calculation, it's reasonable to call it 'basic'. However, any name will do.

9. scroll down until you meet the &SYSTEM block. It will have a few lines (ibrav, A, nat, ntyp). In the latter three, you will recognize the lattice parameter of silicon in Ångstrom, the number of atoms in the unit cell, and the number of inequivalent atoms in the unit cell. Add the lines coloured in red, until the `&SYSTEM` block looks like this:

```
&SYSTEM
  ibrav = 0
  A =    5.43070
  nat = 2
  ntyp = 1
  ecutwfc=50,
  ecutrho=200,
  input_dft='pbe',
  occupations='smearing',
  smearing='mv',
  degauss=0.005d0,
/
```

10. After the `&SYSTEM` block, add the following `&ELECTRONS` block:

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

11. *(this step requires internet access)* Don't touch `CELL_PARAMETERS` and `ATOMIC_POSITIONS`. In the line `ATOMIC_SPECIES`, there is some work to do. For every element in the unit cell (in this case: only Si), do the following:

- go to http://www.quantum-espresso.org/pseudopotentials
- click on the element you need
- copy the url of the first item in the table (in this case: http://www.quantum-espresso.org/upf_files/Si.pbe-n-kjpaw_psl.1.0.0.UPF) (for later use: always check whether the chosen pseudopotential has the XC-functional you want – more on this in the next weeks)
- go to the folder in which your current calculation is being created, and type there
- `wget http://www.quantum-espresso.org/upf_files/Si.pbe-n-kjpaw_psl.1.0.0.UPF`
- copy the name of the UPF file that has been put in your folder (here: Si.pbe-n-kjpaw_psl.1.0.0.UPF)
- in basic.in, replace Si_pseudo by that name, such that the result is

```
ATOMIC_SPECIES
   Si   28.08500   Si.pbe-n-kjpaw_psl.1.0.0.UPF
```

12. After the atomic positions, add these lines (we will call this the k-mesh later on):

```
K_POINTS {automatic}
  7 7 7 0 0 0
```

13. close the file by 'ctrl-x' (=hold the ctrl key and type x), and then press 'y' to confirm that you want to save all changes to this file.

14. Now launch Quantum Espresso, and tell it to read its input from the basic.in file. Tell it it should write its output to basic.out :

```
pw.x -input basic.in > basic.out
```

This will take a few seconds (up to a minute) to finish.

15. verify whether your calculation finished correctly by opening the output file:

```
nano basic.out
```

The very bottom of the file should read:

```
=--------------------------------------------------------------
    JOB DONE.
=--------------------------------------------------------------
```

16. For now, we will extract only one of the many outputs in this file, namely the 'total energy' (we'll see later what it means). You find it near the end of the output file, in a line preceded by an exclamation mark:

```
!    total energy              =      -93.45255564 Ry
```

These steps will have to be performed many times during the course. It will become a routine. Perhaps you'll develop a strategy to make this faster and easier for yourself – feel free to do so.

As a summary, this is the entire basic.in file as it should look like after all modifications:

```
#**************************************************************************
#*                  Generated by cif2cell 1.2.10 2018-09-17 14:27
#*  T. Bjorkman, Comp. Phys. Commun. 182, 1183-1186 (2011). Please cite
generously. *
#*
#*              Data obtained from COD. Reference number : 9008566
#*                                      ()
#*          Wyckoff, R. W. G., Crystal Structures 1, 7-83 (1963)
#**************************************************************************

&CONTROL
  calculation='scf',
```

```
  outdir='.',
  prefix='basic',
  pseudo_dir='.',
  verbosity='low',
  tprnfor=.true.,
  tstress=.true.,
/

&SYSTEM
  ibrav = 0
  A =    5.43070
  nat = 2
  ntyp = 1
  ecutwfc=50,
  ecutrho=200,
  input_dft='pbe',
  occupations='smearing',
  smearing='mv',
  degauss=0.005d0,
/

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

CELL_PARAMETERS {alat}
  0.500000000000000   0.500000000000000   0.000000000000000
  0.500000000000000   0.000000000000000   0.500000000000000
  0.000000000000000   0.500000000000000   0.500000000000000

ATOMIC_SPECIES
  Si   28.08500  Si.pbe-n-kjpaw_psl.1.0.0.UPF

ATOMIC_POSITIONS {crystal}
Si   0.000000000000000   0.000000000000000   0.000000000000000
Si   0.250000000000000   0.250000000000000   0.250000000000000

K_POINTS {automatic}
  7 7 7 0 0 0
```