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) 
Whenever you have opened a new terminal window, give the command

```
conda activate qespresso
```

(if not, you will have no access to the executable pw.x)

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
```

note 1: the warning that might appear about site occupancies is harmless.
note 2: if you would have closed your terminal and/or the virtual machine and you want to come back and continue, then you first must decend into the folder where this cif file is (`cd workQE/basic`) before giving the cif2cell command. It looks for the cif file only in the folder from where you give the cif2cell command.

7. Open the file you have just generated:

```
nano basic.in
```

note: you are of course free to use any other text editor instead of 'nano', if you are familiar with one in the linux environment.

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:

- In a web browser on your laptop, i.e. not inside the virtual machine, go to http://www.quantum-espresso.org/pseudopotentials and click on the link with 'ready to use PP tables are available here). You can start a browser in the virtual machine too if you prefer, but there is no harm in using the browser on your laptop as you usually do. *Note: we will use this procedure only to get this specific Si example started. At the end of the document you'll find another procedure which you have to go through once in order to have pseudopotential files for all elements available within your virtual machine.*

- click on the element you need
- copy the url of the first item in the table (in this case: http://pseudopotentials.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 (`workQE/basic`, if you followed the naming example of this document), and type there
  `wget http://pseudopotentials.quantum-espresso.org/upf_files/Si.pbe-n-kjpaw_psl.1.0.0.UPF`
- highlight the name of the UPF file that has been put in your folder (here: Si.pbe-n-kjpaw_psl.1.0.0.UPF), right-click on it and copy the name
- in basic.in, remove the word `Si_pseudo`, right-click and paste the name you just copied ther, 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 (these instructions are for the `nano` text editor – if you use another text editor, the way of saving and closing will be different).

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
```

Addendum:

Procedure to install a set of pseudopotential files for all elements, which you will be able to use for all your calculations.

- Go to https://www.quantum-espresso.org/pseudopotentials/
- Click on the link to the Standard Solid State PPs (https://www.materialscloud.org/discover/sssp/table/efficiency)
- Click on the blue download button 'Pseudos' to download the library. It will download a tar.gz file with a long name, here abbreviated as SSSP.tar.gz.
- Bring this file via the shared folder to Quantum Mobile, and copy it from there to the top folder where you have your subfolders with calculations. Unzip and unfold the file there by the commands:
    - gunzip SSSP.tar.gz
    - tar -xvf SSSP.tar
- Now you'll have a folder with one pseudopotential file per element. Take note of the name of the files for the elements you need (UPF files).
- In your calculation folder, where you have your Quantum Espresso input file, set the pseudo_dir variable to the location of this pseudopotential folder, for instance:
- pseudo_dir='/home/max/work/my-pseudo-library',

- Now you can list under the ATOMIC_SPECIES block the name of the UPF files you have taken note of. The folder name does not to be repeated, as it is already contained in the pseudo_dir variable.

For any calculation you will make from now on, it is sufficient to look up what is the file name for the pseudopotential for that element in your library folder, and to specify that file name in the ATOMIC_SPECIES block.