Tutorial

Quantum ESPRESSO has a package called `ev.x` that can be used to calculate the bulk modulus of a material. `ev.x` basically offers calculation of 4 equation of states, namely: These equation of states give the equilibrium volume (lattice constant in case of cubic) as well as the bulk modulus and it's first derivative.

The procedure is pretty simple. You first need to calculate the energy of the system at different volumes of unit cell. So you would basically need to run several SCF calculations at different values of lattice parameters (thereby different volumes) and note down the corresponding energies in a `text` file. For cubic systems you can have the lattice parameter in the first column and the Energy in the second column, while for non-cubic systems, you'd note down the volumes in the first column.

A typical file would look like this:

Let's say this text file is called: `volvsE.txt`

Now, we can use this to get the Murnaghan [1] equation of state which is very popular among the scientific community.
Murnaghan EOS is given by:

$$E(V) = E(V_0) + \frac{B_0 V}{B_0'}\left[\frac{(V_0/V)^{B_0'}}{B_0' - 1} + 1\right] - \frac{B_0 V_0}{B_0' - 1}$$

Now you just need to run `ev.x` from the command-line (terminal) and supply inputs to the following prompts:

```
manas@ubuntu:~$ /home/manas/qe-6.1/bin/ev.x
Lattice parameter or Volume are in (au, Ang) > Angstrom
Assuming Angstrom
Enter type of bravais lattice (fcc, bcc, sc, noncubic) > sc
Enter type of equation of state :
1=birch1, 2=birch2, 3=keane, 4=murnaghan > 4
Input file > volvsE.txt
Output file > eos
```

Once, the calculation is done you should have file (`eos.txt`) that looks like this:

```
# equation of state: murnaghan.          chisq =   0.6924D-06
# a0 =  8.7452 a.u., k0 = 1242 kbar, dk0 =  4.28 d2k0 =  0.000 emin = -634.20782
# a0 =  4.62774 Ang, k0 = 124.3 GPa,  V0 =   668.81 (a.u.)^3,  V0 =   99.11 A^3

#########################################################################
# Lat.Par       E_calc        E_fit       E_diff    Pressure      Enthalpy
# Ang             Ry            Ry           Ry       GPa           Ry
#########################################################################
  4.16740    -633.83860    -633.83794    -0.00066      82.43     -631.10164
  4.26740    -634.00049    -634.00169     0.00120      53.17     -632.10480
  4.36740    -634.10886    -634.10932     0.00046      32.03     -632.88498
  4.46741    -634.17399    -634.17341    -0.00058      16.62     -633.49405
  4.56740    -634.20433    -634.20331    -0.00102       5.33     -633.97144
  4.66740    -634.20659    -634.20601    -0.00058      -3.01     -634.34714
  4.76740    -634.18643    -634.18675     0.00033      -9.21     -634.64438
  4.86740    -634.14847    -634.14952     0.00105     -13.85     -634.88113
  4.96740    -634.09643    -634.09731     0.00088     -17.34     -635.07134
  5.06740    -634.03350    -634.03242    -0.00108     -19.98     -635.22607
```

Example output file generated from ev.x

This contains information of the equilibrium volume, bulk modulus and it's derivative and the minimum energy.

You can use the above generated data to create a neat plot of the equation of state (as you'd see in many publications), using gnuplot. The following shell script, plots the calculated data-points from file `volvsE.txt` as well as the fitted equation of state curve. [NOTE: This shell script is for cubic systems only. You'd need to modify the code to implement it for non-cubic systems]

Create a file called script.sh and add the following code to it:

```
#!/bin/bash
a="$1"
k="$2"
dk="$3"
emin="$4"
V=$(echo "$a*$a*$a"|bc)
echo "
set terminal png size 1000,500
set output 'EOSplot.png'
set xlabel 'Volume (Ang^3)'
set ylabel 'Energy (Ry)'
set title 'Equation of state'
#set key box linestyle 1
f(x)= "$emin"+(x*10**(-30)*"$k"*10**9/"$dk"*(("$V"/x)**"$dk"/("$dk"-1)+1)-
"$k"*10**9*"$V"*10**(-30)/("$dk"-1))/(1.6*10**(-19)*13.6)
plot f(x) w l title 'Murnaghan EOS fit', 'volvsE.txt' u 1:2 w points pointtype 7
pointsize 2 title 'Calculated data-points'
set terminal postscript enhanced color solid 22
set output 'EOSplot.eps'
set xlabel 'Volume (Ang^3)'
set ylabel 'Energy (Ry)'
set title 'Equaiton of state'
set autoscale
```

```
plot f(x) w l title 'Murnaghan EOS fit', 'volvsE.txt' u 1:2 w points pointtype 7
pointsize 2 title 'Calculated data-points'
set term x11" >EOSplotScript.p
```

Now save the file and open the terminal and run the command:
`chmod u+x script.sh`

Now simply run the script by providing the four arguments, in the following order: lattice parameter, bulk modulus, derivative of BM, and minimum energy.

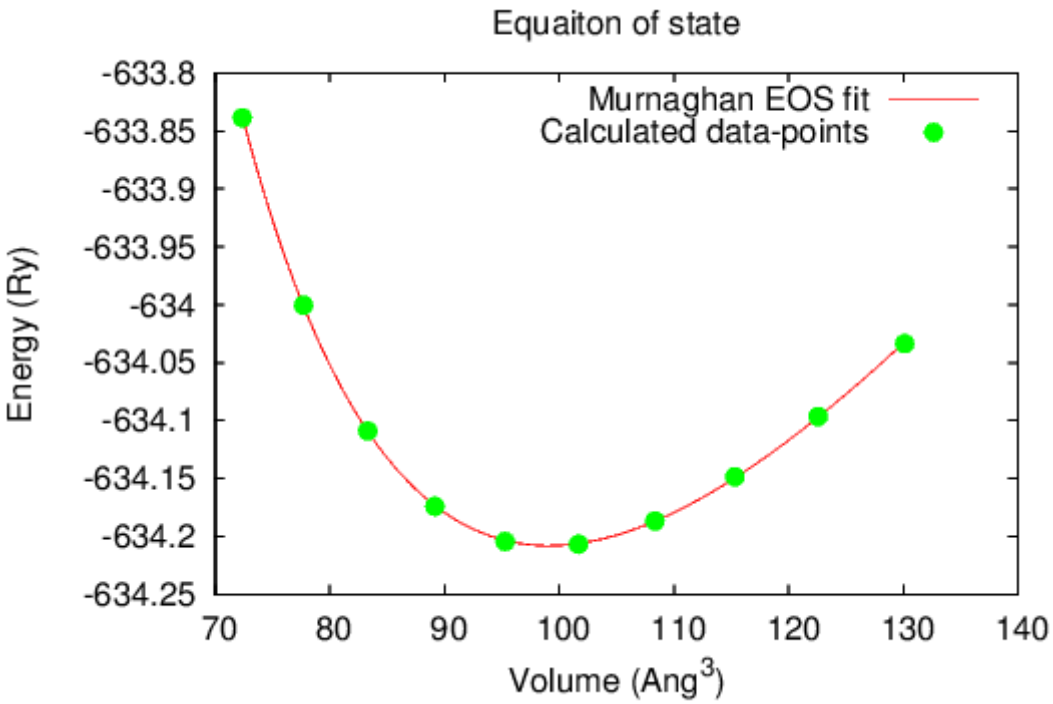
Example: `./script.sh 5.5 81 3.9 -588.656`

The above command will create a gnuplot script file called: `EOSplotScript.p`

This can then be run using gnuplot using the following command:
`gnuplot ./EOSplotScript.p`

When you run this command, it will generate a PNG image as well as an EPS file.

The output looks like this:



Example of the PNG and EPS file generated by the above script

References

[1] F.D. Murnaghan, Proceedings of the National Academy of Sciences **30**, 244 (1944).

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I'm a physicist specializing in theoretical, computational and experimental condensed matter physics. I like to

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