ONETEP Workshop: running a simple geometry optimization

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Aim: To run a geometry optimization on an ethene molecule

We will run a geometry optimization on an ethene molecule. First create a working directory:

```
> cd
> mkdir ethene
> cd ethene
```

Copy the pseudopotential files **hydrogen.recpot** and **carbon.recpot** from the **quality_control/PSEUDOS** directory of the ONETEP distribution:

```
> cp ~/ONETEP-2.2.0/quality_control/PSEUDOS/hydrogen.recpot .
> cp ~/ONETEP-2.2.0/quality_control/PSEUDOS/carbon.recpot .
```

Create a new input file called ethene.dat and follow the example input files available at the workshop URL: http://www.tcm.phy.cam.ac.uk/onetep/workshop for which you'll need the user name **Kernel** and password **Ngwf2008!**

The main difference from yesterday is that you'll need to set the **task** keyword:

```
task = GeometryOptimisation
```

Initially, try running a calculation with an energy cutoff of about 450eV, NGWF radii of about $5.5a_0$ and a cubic simulation cell of side-length $40a_0$.

You may then want to try running further calculations by varying the following parameters:

- **cutoff_energy**
- NGWF radii in the **species** block
- **geom_max_iter**
- **ngwf_threshold_orig**
- size of the simulation cell in the **lattice_cart** block

The output consists principally of two files: **ethene.onetep** (the main output file) and **ethene.geom**

ethene.geom contains a block of information for each geometry optimization iteration, which looks like:

```
3
              -1.37014664E+001     -1.37014664E+001                      <-- E
               6.00000000E+001      0.00000000E+000      0.00000000E+000  <-- h
               0.00000000E+000      6.00000000E+001      0.00000000E+000  <-- h
               0.00000000E+000      0.00000000E+000      6.00000000E+001  <-- h
  C     1      2.12454516E+001      1.98806591E+001      2.00641343E+001  <-- R
  H     1      2.23095241E+001      2.13673969E+001      2.10799465E+001  <-- R
  H     1      2.23041930E+001      1.84694367E+001      1.90960354E+001  <-- R
  C     1      1.87541519E+001      2.01191244E+001      1.99345619E+001  <-- R
  H     1      1.76958907E+001      2.15304250E+001      2.09042225E+001  <-- R
  H     1      1.76907888E+001      1.86309579E+001      1.89210995E+001  <-- R
  C     1     -2.64214320E-002      3.57284349E-002      1.15858705E-002  <-- F
  H     1      1.24731218E-003     -7.07702548E-003     -1.51569912E-003  <-- F
  H     1      7.76179733E-003     -1.56081442E-002     -7.99423616E-003  <-- F
  C     1      2.66831747E-002     -3.58706441E-002     -1.28682024E-002  <-- F
  H     1     -7.80712364E-003      1.55413529E-002      8.21231486E-003  <-- F
  H     1     -1.46372865E-003      7.28602594E-003      2.57995233E-003  <-- F
```

The first line is the iteration number.
The second line is the total energy.
The next three lines are the lattice vectors.
The next *N* lines (where *N* is the number of atoms) give the atomic coordinates.
The following *N* lines give the atomic forces.
All values are in Hartree atomic units.

Create a new file **ethene_energy.dat** in a text editor and enter the values of the energy (from the **.geom** file) as a column of data (see the examples "files for plotting" on the workshop webpage) and plot using gnuplot:

```
> gnuplot
> plot with lines 'ethene_energy.dat'
```

Similarly, you can keep track of the maximum rms force on the ions at each iteration of the minimization by running **grep** on the **.onetep** output file:

```
> grep "|F|max" ethene.onetep
```

which should give you something like:

```
|   |F|max   |    1.916149E-001 |   2.0000000E-002  |    Ha/Bohr  | No    |  <--  BFGS
|   |F|max   |    1.358384E-001 |   2.0000000E-002  |    Ha/Bohr  | No    |  <--  BFGS
|   |F|max   |    9.173846E-002 |   2.0000000E-002  |    Ha/Bohr  | No    |  <--  BFGS
:
:
```

The second column is the calculated value of $|F|_{max}$, the third column is the threshold you are trying to achieve (determined by the **geom_force_tol** input parameter), the fourth column provides the units, and the fifth column informs you as to whether convergence of the force has been achieved.

Create a new file **ethene_force.dat** in a text editor and enter the values of the $|F|_{max}$ as a column of data (see the examples "files for plotting" on the workshop webpage) and plot it using gnuplot:

```
> gnuplot
> plot with lines 'ethene_force.dat'
```

You may want to investigate the way in which the rate of convergence of the total energy and the force varies with energy cutoff and with NGWF radius.

You can use the perl script **geom2xyz** (available from the workshop website) to generate an **xyz** file containing the atomic coordinates at each iteration of the geometry optimization:

```
> geom2xyz ethene.geom
```

produces a file **ethene.xyz** which you can visualize using, for example, the XCrysDen package.