Practical 4 – Molecular Dynamics

Learning Objectives

- Perform *ab initio* molecular dynamics calculations on simple systems.
- Investigate factors affecting energy conservation, etc.
- Use various tools to visualize and analyze the results.

N_2 Dimer

As a simple example, we will explore the system discussed in the lecture – the N_2 dimer.

1. Download the input files

```
wget http://www-users.york.ac.uk/~mijp1/teaching/grad_FPMM/files/4.tar.gz
```

2. Unzip and untar the files, then move into the new directory

```
gunzip 4.tar.gz
tar -xvf 4.tar
cd N2
```

3. Run this and then read the **`N2.castep`** file – see how the MD information is reported. Plot a graph of temperature vs. time – does it look correct?

Hint: try

```
grep Temp N2.castep | awk '{print c++,$3}' > N2.T
```

to get a 2-column file of temperature vs MD step. You can then plot this using `xmgrace` or `gnuplot` etc. Is there an initial transient?

4. What is the effect of electronic convergence (**`cut_off_energy`**, **`elec_energy_tol`** , etc) on the energy conservation? What is the effect of changing the time step or the thermostat used? Plot a graph of "Hamilt Energy" vs MD step to see.

5. Make a movie of your dynamics. Load the `N2.md` file in **`jmol`** and use Tools/Animate to see it in action.

6. Calculate the average bond length, as a function of temperature – is the system harmonic or anharmonic?

Hint: try something like this:

```
grep ' N          1' N2.castep | awk '{print $4,$5,$6}' >
N2.r1
grep ' N          2' N2.castep | awk '{print $4,$5,$6}' >
N2.r2
paste N2.r1 N2.r2 | awk '{print c++,10.0*sqrt(($4-$1)^2+($5-
$2)^2+($6-$3)^2)}' > N2.r12
```

NB the number of spaces matters! There should be 10 spaces between N and 1 in the first command. Ask a demonstrator if you do not understand these Linux commands!

H_2 Molecule

Copy the N2.cell and N2.param files to a new directory, and edit them to create a suitable set of input files for the H_2 molecule. Use CASTEP to run MD on this new system for a similar amount of time.

- *Do you have any problems?*
- *How can you solve them?*

Extension activities

If you wish to explore further, you can use MD to study any system (aperiodic, supercell, bulk, etc.) that you are interested in. There are many properties that can be calculated sampled within an MD run. For example, if you have population analysis turned on, set **`md_sample_iter=10`** to re-calculate it every 10 steps during the MD run.

You can also analyse the resulting MD trajectory using tools such as **`mdtep`** (that is included by the `module load phys/CASTEP` command).

Using MDTEP

MDTEP is designed as an example of a basic CASTEP .md file analyser. You are welcome to extend it! To use it you should **`wget`** **`http://www-users.york.ac.uk/~mijp1/teaching/grad_FPMM/files/mdtep_sample.input`** and customize it as you wish and put it in the directory with your MD run. You can then use it to analyse your MD run using:

```
mdtep mdtep_sample.input
```