Class 1: Getting Started

1. Use `rdesktop` to login to the Windows Terminal Server at `minsc.oerc.ox.ac.uk` (use your supercomputer login credentials). *Note:* please do not hammer the terminal server with large calculations.

2. Draw a toluene molecule in:

   ☐ GaussView

   ☐ Chem3D

   ☐ ArgusLab

   ☐ HyperChem

   ☐ Avogadro

   Observe the amount of effort required in each case.

3. Use GaussView version of toluene to save a .mol file. Read it with HyperChem and run geometry optimizations using (*Setup* menu, then *Compute* menu):

   ☐ Molecular dynamics (MM+)

   ☐ Semi-empirics (PM3)

   ☐ Hartree-Fock (STO-3G)

   ☐ DFT (B3LYP/STO-3G)

   Observe the time it takes to run each simulation. Save the PM3 geometry into a .mol file.

4. Read the .mol file with GaussView and set up a Gaussian03 job (*Calculate* menu) for toluene geometry optimization using DFT with B3LYP exchange-correlation functional and cc-pVDZ (reasonable accuracy) basis set. Save a Gaussian input file. Manually edit the resulting text file until it looks like this:

```
%Mem=500MB
%NProcShared=4
%Chk=toluene.chk
#p opt=tight b3lyp/cc-pVDZ

Toluene optimization.

0 1
 C                 -1.20826432   -1.19702571   -0.00001978
 C                 -0.00010596   -1.89475389   -0.00045387
 C                  1.20794073   -1.19772840    0.00016921
 C                  1.20818053    0.19769859    0.00002791
 C                  0.00027329    0.89519205   -0.00001716
 C                 -1.20805558    0.19780329    0.00035546
 H                 -2.16059560   -1.74676016   -0.00006116
 H                 -0.00060966   -2.99440897    0.00002760
 H                  2.16026400   -1.74761640    0.00046111
 H                  2.16080665    0.74706151    0.00046003
 H                 -2.16018155    0.74788069    0.00051772
 C                  0.00007157    2.43519202   -0.00018441
 H                 -0.86439991    2.79168866   -0.52027979
 H                 -0.01814478    2.79196553    1.00841900
 H                  0.88261929    2.79192142   -0.48880866
```

(coordinates will of course be different, also note that Gaussian requires a blank line at the end of each input file). Use SSH File Transfer client to upload the input file to your home directory on `hal.osc.ox.ac.uk`, then log out of the terminal server.

5. Launch a terminal window on your Linux box, use `ssh` to login to `hal.osc.ox.ac.uk` and load the Gaussian module (`module load gaussian03`). The scheduler is down at the moment, so we will be running on the head node. Rename your input file into `toluene.com` and launch Gaussian (`g03 toluene.com > toluene.log &`). Inspect the log file.

6. When the calculation finishes, log into the Windows server, download the log file and open it with GaussView with an option to load intermediate geometries ticked. Inspect the optimization trajectory.