Class 3: Semi-empirics, Hartree-Fock and MP2

1. Use `rdesktop` to login to the Windows Terminal Server at `minsc.oerc.ox.ac.uk` (use your supercomputer login credentials).

2. Use `ssh` from either the Linux host or from the terminal server to login to `hal.oerc.ox.ac.uk` and load the Gaussian module (`module load gaussian03`).

3. Draw an ethylbenzene molecule in GaussView and use HyperChem to perform a preliminary structure optimization using the PM3 method.

4. Load the result back into GaussView and set up three Gaussian job for geometry optimization:

   - using HF/STO-3G method (minimal accuracy)
   - using HF/cc-pVDZ method (reasonable accuracy)
   - using HF/cc-pVQZ method (high accuracy)

Save the .gjf files to disk and edit them manually (in WordPad) until they look like this:

```
%Mem=4GB
%NProcShared=8
#p opt=tight uhf/cc-pvdz geom=connectivity

Ethylbenzene geometry.

0 1
 C                  0.79026691    0.36205306   -1.19971416
 H                  0.76510351    1.41894701   -1.36476563
 H                  1.79517766    0.05685955   -0.99499162
 H                  0.43474616   -0.14387156   -2.07295254
.....................................................
```

5. Copy the files to the supercomputer, change their extensions to .com and dos2unix them.

6. Create the run script (use vi, call the script geom.run) containing the following lines:

```
#!/bin/bash
#PBS -l select=1:mpiprocs=8
#PBS -l walltime=24:00:00
#PBS -V

cd $PBS_O_WORKDIR
GAUSS_SCRDIR=$TMPDIR
export GAUSS_SCRDIR

g03 ******.com
g03 ******.com
g03 ******.com
```

   (the last three lines should contain the names of your Gaussian input files). Make the script executable (`chmod +x geom.run`) and submit it to the supercomputer queue (`qsub geom.run`).

7. Inspect the logs for timing and the number of basis functions used in each case.

8. Repeat the calculations with `ump2` specified instead of `uhf` in the input file.

9. Run an RHF geometry optimization on a system containing two xenon atoms at the distance of 6 Angstroms from one another. Observe the attraction caused by BSSE.