QUANTUM CHEMISTRY WITH *GAUSSIAN*: A *VERY* BRIEF INTRODUCTION

TARAS V. POGORELOV AND MIKE HALLOCK
SCHOOL OF CHEMICAL SCIENCES, UIUC

This tutorial is designed to help getting started with *Gaussian*. Single point energy calculation is performed on a single water molecule. Molecular orbitals are calcualted. Basic knowledge of Unix/Linux is assumed. Estimated time to complete this tutorial is 50 min.

1. Software

One will need: text editor, ssh client, and molecule builder.
Suggestions:
Molecule builder: Avogadro (http://sourceforge.net/projects/avogadro/files/)
Mac:
Text editors: TextEdit, Vim,
SSH client: built in Terminal , scp or Fugu for file transfers
PC:
Text editor: Notepad, vim
SSH client: putty, WinSCP for file transfer

2. Prepare Gaussian input file for a water molecule using Avogardo

Install Avogadro on your computer, if needed.
Open Avogadro and Select Element: Oxygen(8)
Click once anywhere is the main window and watch hydrogens being added making a water molecule.
Prepare *Gaussian* input file: Open Extensions, Gaussian.
Note: the coordinates are already listed in the *Gaussian* Input plugin.
Enter title: `water SP`
Select: `Calculation:` Single Point Energy, `Theory level:` RHF, `Basis:` 6-31G(d), `Charge:` 0, `Multiplicity:` 1.
Click: `Generate` button.
Save as: `water.com`

Date: February 10, 2010.

3. *Gaussian* single point calculation: interactively on triton (SCS' Linux cluster)

Copy *Gaussian* input file to triton using `scp` command.

```
> ssh triton
```

Make a directory `waterSP` in your home directory.

Copy *Gaussian* input file to triton using `scp` command.

Note: please see the Unix/Linux Primer if you need to refresh your knowledge of the OS.

Setup your environment:

```
> setenv g09root /share/apps/gaussian
> source $g09root/g09_login.csh
```

Start Gaussian job with prepared files:

```
> g09 < water.com
```

Note: `<` is the "pipe" flag to direct the input file to Gaussian

Output will be printed on the screen.

To direct output into a file add `> water.log` in the end.

Note: proceed to Appendix for an example of submitting a *Gaussian* calculation in queue. Please make sure to understand each line of the script.

4. *Gaussian* output: basic features

Open `water.log` in a text editor and locate the following: Input data, Standard orientation, Number of basis functions used, Single point energy, Symmetry, Mulliken charges.

Note: the energy is reported in A.U. please estimate how many significant digits are needed to guarantee sufficient accuracy. Define sufficient.

4.1. **Find data in the output without opening.** Close the output file and use `grep` to find the energy value, *without* opening the file. This can become important for larger systems, as the size of the output file will grow very fast.

5. Use *Gaussian* to calculate molecular orbitals

Copy `water.com` into `waterMO.com` and add in the end of the first line, after `SP` the following `Pop=Reg formcheck`. The former requests the data on molecular orbitals to be included into the output and the former asks to print what is called checkpoint file. It is used to restart calculations and to graph molecular orbitals.

Run the new calculation. Locate in the output file the following: the data mentioned above, molecular orbital coefficients, symmetries and energies of the MO's and HOMO/LUMO orbitals.

Note: the checkpoint `Test.FChk` was produced. This is an ASCII file which has MO information.

5.1. **Display molecular orbitals using Avogardo.** Copy `Test.FChk` to your computer where Avogardo is installed.

Start Avogardo. `File->Open Test.FChk`. To show surfaces go to `Extensions->Create Surfaces`.

To plot electrostatic potential select menu flags as shown on figure 1.

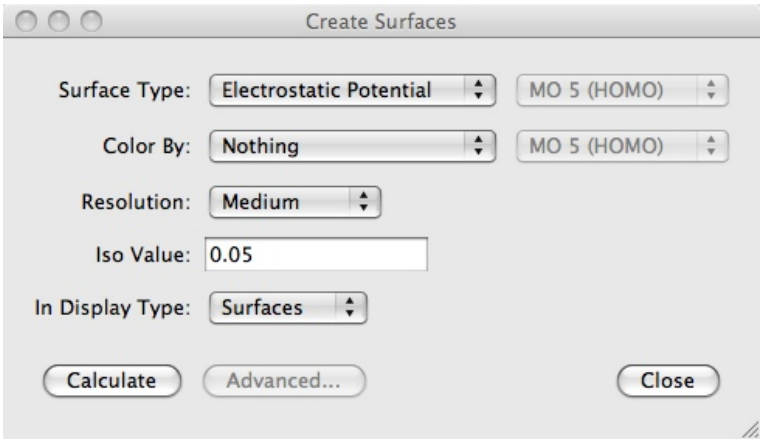

FIGURE 1. Avogadro Create Surface menu selection to plot electrostatic potential. Note: Isovalue is suggested by the program.

The result will look similar to figure 2

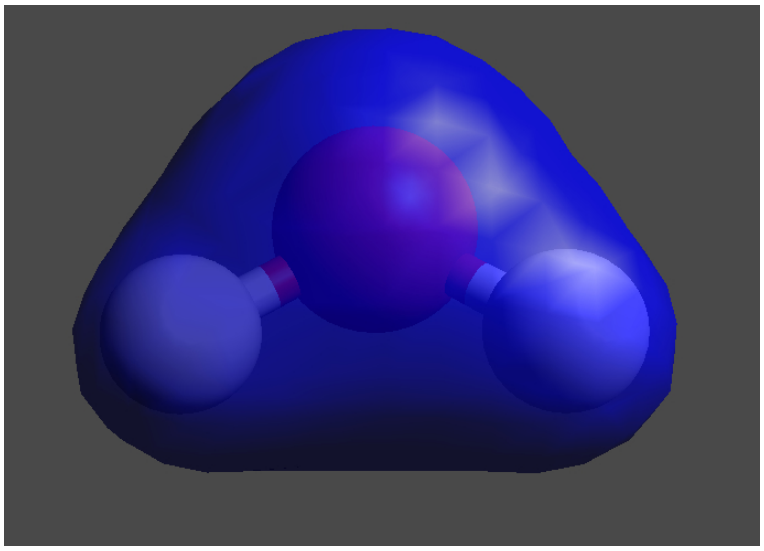

FIGURE 2. Electrostatic potential surface, isovalue: 0.05 e/au^3

Plot HOMO for water molecule. Select menu flags as shown on figure 3.

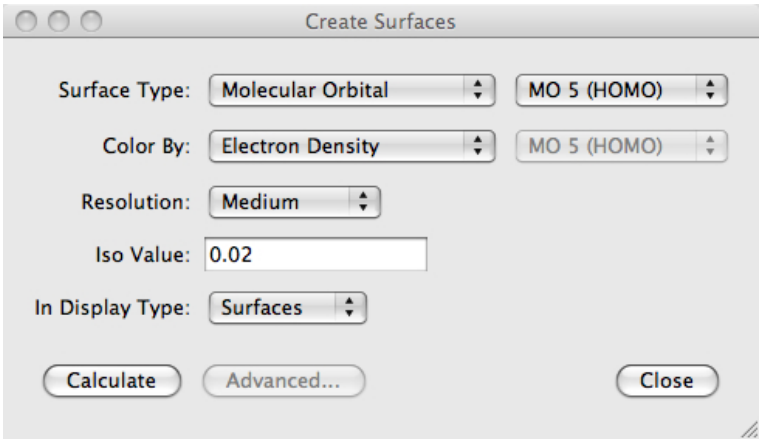

FIGURE 3. Menu selection for HOMO of water molecule

HOMO is shown on figure 4.

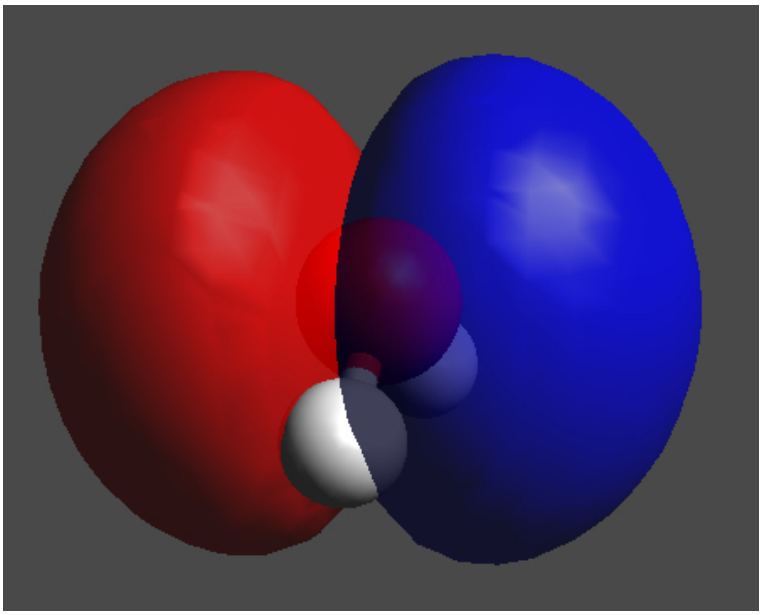

FIGURE 4. HOMO of a water molecule, isovalue 0.02 au

Use Avogardo to graph LUMO of a water molecule.

6. SUMMARY

This tutorial covered material to have one started using *Gaussian* for single point energy calculation, analyze the output, graph electrostatic potentials and molecular orbitals.

7. Contact

If you found errors/typos or have suggestions or comments on material in this tutorial please contact us at the SCS Computer Center. We are looking forward to hearing from you.

8. Appendix: Running *Gaussian* in queue on triton (Linux cluster)

Please make sure to understand each line of the shell script below. Edit it to match your file names.

Submit the queue script to the queue:

```
> qsub g09_qjob
```

Note: The following is probably not needed for the fast test job.

Check the status of your job:

```
> qstat
```

Delete the job if need:

```
> qdel
```

Study the shell script for queue submission open g09_gjob:

```
#!/bin/tcsh
#$ -cwd
#$ -pe default 1
#$ -q general
source /share/apps/gaussian/g09_login.csh
g09 input.com
```