HOW TO USE *GAMESS*

1 Login

Use the `ssh` icon on the Desktop. Go to `File`→`Connect`. Type for the `Host Name`:

`theochem1.la.asu.edu`

and

`your␣first␣name␣and␣last␣name␣initial`

for the `User Name`. E.g., for Mike Brown, type

`mikeb`

Password:

`Please try to memorize the password and do not write it down anywhere`

After you login into the system for the first time, please change the password from that given to you to your own by typing

`passwd`

You need to press Enter after each command you type!

2 Input file

You need to create an input file which specifies which molecule is being calculated and which packages are used. An example input file can be found in your directory as `example.inp`. First copy it to another file:

```
cp example.inp newfile.inp
```

Then edit the new file with an editor. Without graphical interface, the following editors can be used: `vi`, `vim`, `xemacs`. A short list of `vi` and `xemacs` command is attached. Use `man vi` or `man xemacs` for a general reference. In order to check your input file, use EXETYP=CHECK in the $CONTRL group.

In order to get help on a particular GAMESS input do

`gmshelp topic`, e.g. `gmshelp scf`

Type `q` to exit.

The full documentation on GAMESS input is available in the file:

`/usr/scr/chm546/INPUT.DOC`

Do `vi ../INPUT.DOC` to see the input documentation. There are also postscript and pdf files: `/usr/src/chm546/INPUT.DOC.pdf` and `/usr/src/chm546/INPUT.ps`. You may copy these files or any of your outputs to your computer by using the SSH Secure File Transfer protocol (link icon on the Desktop, drag-and-drop is available).

3 Running GAMESS

In order to run GAMESS type:

```
gms input > output.log&
```

Here, `input` is the name of the input file (with `.inp` extension) and output is the name of an output file of your choice. The results will be also written to the `input.dat` file. If you want to rerun the program with the same input file, you need first to remove the `input.dat` file:

```
rm input.dat
```

The file `input.dat` may be used upon a corresponding modification to runs on the next level of the theory. You can do, e.g.

```
cp input.dat input1.inp
```

and then run

```
gms input1 > output1.log&
```

Please use `gms` instead of the GAMASS code rungms since the alias `gms` lowers the priority of your job relative to jobs of regular users.

4 Graphical output

You can obtain graphical outputs by specifying corresponding options in the $CONTRL group. Specifying MOLPLT=.TRUE. generates the output file for the program molplt at the end of the corresponding .dat file. Extraction of this file with the extension .mol allows to you to visualize the molecule by running

```
molplt file
```

E.g., if you have created the file water.mol, you will need to issue

```
molplt water
```

Giving `xw` or `ps` options will allow you to view the molecule in the X-terminal (if you have it) or create a Postscript wile (`water.ps`). If you want to have a PDF file, you will need to convert a PS file into a PDF file by

```
ps2pdf water.ps
```

You can send your PS file to the printer by issuing the command

```
lpr -P 129.219.49.237 water.ps
```

In order to draw contour plots of molecular orbitals, there is a program called `pltorb`. GAMESS will make an almost complete input file for PLTORB if you give the input $CONTRL PLTORB=.TRUE. $END, even for EXETYP=CHECK runs.

5 Exiting

Please do not forget to exit. Go to `File`→`Exit`.