CASculator Manual

1. **Installing the CASculator**
2. **Using the CASculator**

1. Installing the CASculator

a. Install python on your local machine:
   i. visit https://www.python.org/download/ and download the installer for python 2.7.8. Get the 64-bit version if possible as I'm not 100% sure the 32-bit version works for some reason. Follow the instructions to install
   ii. Append python to your path on Windows. To doso on Windows 7:
      1. Go to Computer\System properties\ Advanced system settings\. Click on Environment Variables and under User variables click edit to append the following to the variable PATH (it may need to be added under Sytem Variables rather than User Variables):
         a. \ C:\Python27;C:\Python27\Lib\site-packages\;C:\Python27\Scripts\;

b. Load python 2.7 on your remote machine by adding the following to your .cshrc file:
   i. module load python/2.7.5
      1. 2.7.3 (on Mason)

c. Install the python graphics module wxpython:
   i. http://www.wxpython.org/download.php#msw and download the appropriate binary and follow the installation instructions. Make sure that you download a compatible version (32-bit/64-bit for Python 2.7).

d. Install a python SFTP module called paramiko:
   i. First you need to download and install pycrypto: http://www.voidspace.org.uk/python/modules.shtml#pycrypto. Click the appropriate installer and follow the instructions
   ii. Also download something called ecdsa: https://pypi.python.org/pypi/ecdsa
      1. Click the green download button and extract the download folder using 7zip or some other utility until you can see a folder called dist.
         a. Open the command prompt on windows and cd into the dist\ecdsa-0.11 directory. You may need to extract again after you see the dist folder to get to the ecdsa folder.
         b. Issue the command: python setup.py build
         c. Issue the command: python setup.py install
   iii. Download the paramiko source: https://pypi.python.org/pypi/paramiko/1.14.0
      1. Extract to get to the dist folder and extract again to reveal the paramiko-1.14.0 folder.
      2. cd into the paramiko folder and again type python setup.py build followed by python setup.py install into the command prompt.

e. The following are python modules that should be installed by default (sqlite3 and pexpect).
f. Add the script unix2dos.sh to your bin folder and make it executable with chmod +x unix2dos.sh
g. You will need to authenticate your computer with winSCP against the server. For each server that you plan to add, you will probably need to authenticate your local machine with WinSCP. To do so, use the command prompt to open the winscp console. Navigate to the CASculator directory and type:
    i. winscp.exe /console
    ii. Type the following in the winscp console window:
        1. open sftp://username:"password"@servername
        2. Type yes or y when prompted
h. Copy the file casculator.py (the py file not the compiled python file) to your bin folder. The command line version and GUI have been combined into one module so you don't have to worry about which one is which. Make sure to alias the program with:
    i. alias cask 'python /N/u/username/BigRed2/bin/casculator.py'

2. Using the CASculator

a. Using the command line:
    i. The command line interface has been changed so that keywords are now used for arguments rather than putting them in a particular order. The following are the available commands:

Command	Result
-active	Gets the active space
-atom	Gets orbitals for a selected atom above the threshold value (Uses ORCA numbering for atom#)
-dorbs	Gets orbitals with d-orbital character above threshold value
-orbital	Selects an orbital type
-range	Selects orbitals within a given numerical range
-res	Changes the plotting resolution from 40 to 80
-plot	Plots the selected orbitals
-thresh	Changes the orbital composition percentage for selected orbitals (10% is the default)

So if the calculation id was DC_test, you would navigate to that directory and then issue the appropriate command. I think you only need to specify the minimum number of letters that make the command unique so 'd' would also be accepted for 'dorbs' and 'ac' for 'active', but not just 'a' because 'a' could stand for 'atom' or 'active'.

If you wanted to plot the active space for DC_test you would call the following:

```
cask DC_test –active –plot
```

If you wanted to plot all orbitals that have > 5% d-orbital character:

```
cask DC_test –dorbs –t 5 –plot
```

If you wanted just the dxy orbital on a particular atom. In this case the cobalt atom which is atom 0 in the ORCA output file. Presently, the atom and orbital commands must be specified together. You cannot ask for all orbitals on a single atom or all orbitals of just one type.

```
cask DC_test –atom Co0 –orbital dxy –plot
```

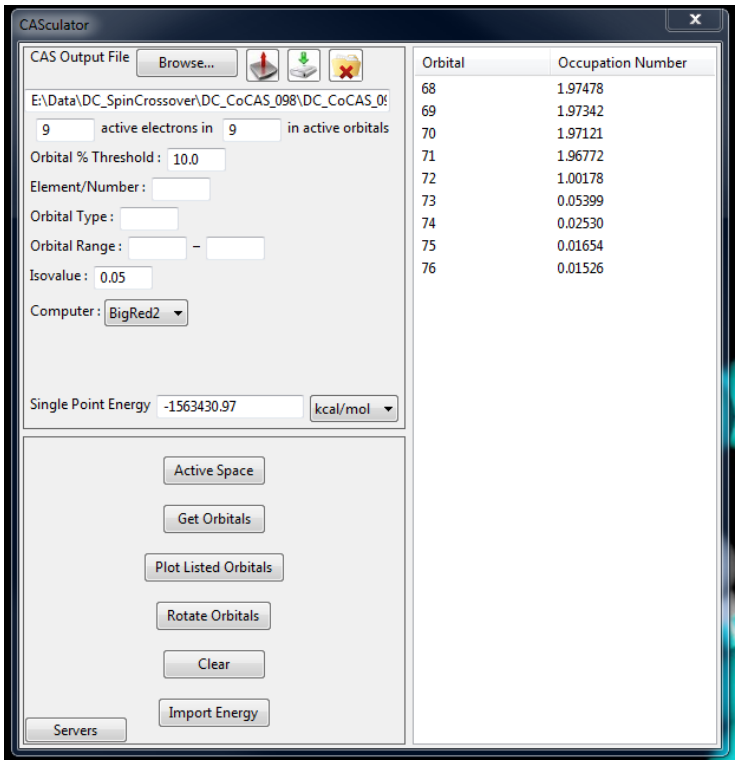
The –range command will print all of the occupation numbers of orbitals within a given range. It will not show the % composition (this will soon be included). However, you should still be able to plot a range of orbitals with the following, where 75 is the first orbital you want to plot and 85 is the last:

```
cask DC_test –range 75 85 -plot
```

The –plot keyword can also be used with a list of numbers if the orbitals you want to plot are not consecutively numbered. The following plots orbitals 68, 78, and 252.

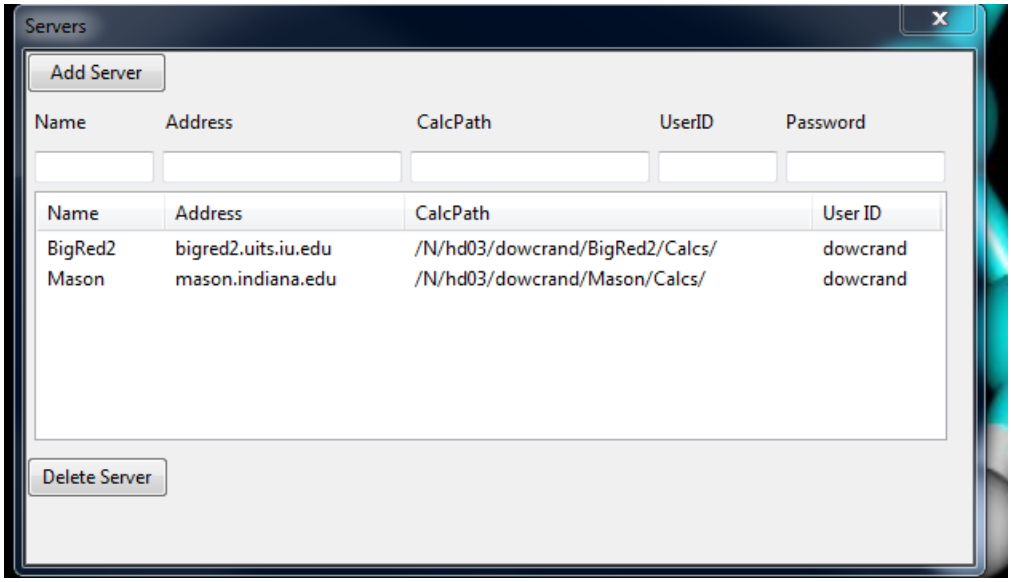
```
cask DC_test –plot 68 78 252
```

b. Using the GUI
    i. Copy the CASculator folder to your desktop and double click on the cas_gui.py file. Alternatively navigate to the folder using the Windows command prompt and open the program with:
        1. Python cas_gui.py



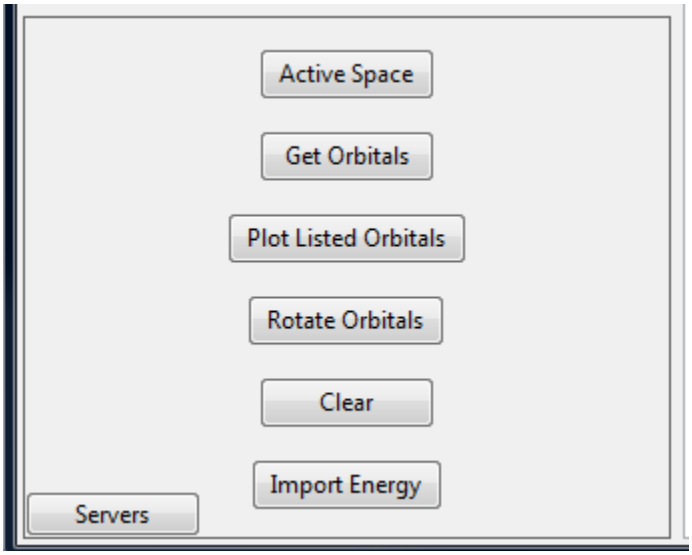
ii. All of the command line features are replicated in the GUI. Please note that I haven't been able to add all of the error checking functions that I want to so, if you are doing something wrong, the CASculator probably won't warn you.
iii. First open an output file using the Browse button in the upper left hand corner. The path to this output file will be displayed in the textboxes below along with the number of active electrons and active orbitals.
iv. The threshold field functions just like the –t keyword on the command line
v. The element#/orbital type and orbital range also function like their command line counterparts.
vi. You may change the isovalue when viewing orbitals using the isovalue textbox
vii. To populate the list of computers click on the servers button in the lower lefthand corner of the CASculator.
    1. Fill in the textboxes with the appropriate information and click add server to add the information to the server database. The password is encrypted prior to storage.
    2. Servers may be deleted using the 'Delete Server' button.
viii. The three buttons to the right of the 'Browse' button enable you to transfer folders and files between your local machine and added servers.
    1. The first button with the red arrow is the **'Upload'** button and transfers the folder of the currently selected output file to the selected server.
    2. The middle button with the green arrow is the **'Download'** button and collects the folder of the currently selected output file from the selected server.
    3. The third button with the red 'X' is the **'Delete'** button and will delete the presently selected output file and folder from the selected server.

NOTE: Be careful when transferring files. I am fairly certain that the CASculator will not corrupt .gbw files, but you may want to make copies of them elsewhere (at least at first) to ensure nothing goes wrong if you do not want to repeat the calculation.

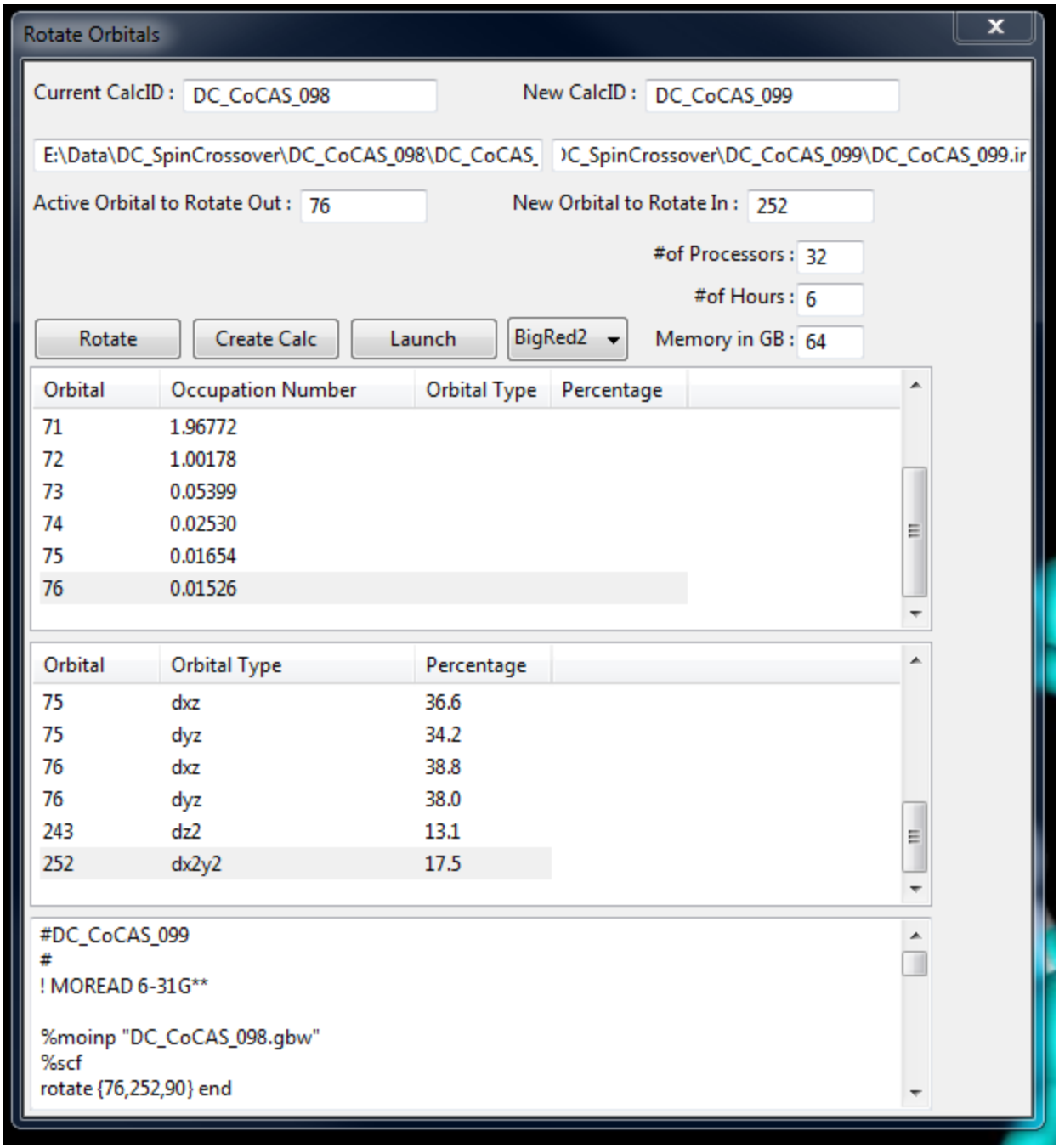


ix. The following buttons are extremely useful:

1. The active space button populates the active space with occupation numbers in the list on the right hand side of the CASculator.
2. The 'Get Orbitals' button will get all selected orbitals above the threshold value. If the Element/Number and Orbital Type fields are not empty the selected atom and orbital type will be used to populate the list. Similarly, if the orbital range field is full, the desired range of orbitals and their occupation numbers will fill the list. By default the Get Orbitals button will select the metal d-orbitals if none of the other boxes are filled.



3. The 'Plot Listed Orbitals' button will plot any orbitals that are currently listed by the CASculator. The CASculator will transfer the gbw file to the server and then download the generated cube files. **Again, as the CASculator will be transferring the gbw file to the server and back, you may want to make a copy to ensure it is not accidentally corrupted.**
4. **The 'Clear' button clears the list**
5. The 'Import Energy' button gets the Single Point Energy and populates the text field at the bottom of the upper left-hand panel. Units can be selected from kcal/mol, eV, hartrees and kJ/mol.
6. The 'Rotate Orbitals' button allows you to generate new input files quickly from previous calculations and rotate in/out desired orbitals.
    a. Make sure that you have selected the ouput file that you want to serve as the basis for your new calculation.
    b. Click the 'Rotate Orbitals' button and you should see the following:



c. Enter a CalcID for the new calculation.

d. You may either type the numbers of the orbitals to rotate in and out or select them by double-clicking from the lists below. The top list is the active space orbitals and the bottom is the list of the metal d-orbitals with >10% character (I will work to make this listing more flexible).

e. If you click on ‘Rotate’ the bottom text field will be populated with the text for the new input file. This can be edited as necessary. The appropriate rotate command should be added.
f. Clicking ‘Create Calc’ will generate the new input file and copy over the gbw file and xyz file from the template calculation.
g. Clicking ‘Launch’ will call create calc and then submit via msub or jsub to the selected computer.