Molecular Modeling in Process Engineering

2023/2024

Project 0

Getting started

Let's familiarize with a commandline-based environment and practice elementary tasks such as browsing, creation, and manipulation of text files and folders. Let's then move on to learn about QM codes and associated utilities such as output-visualization software. Finally, let's try to run some actual QM calculations on the spot. You are expected to complete each task by the next practical, at which point results will be discussed.

Recommended approach:

1. Think about how to do what is requested in the following, one point at a time.
2. Try to do it.
3. If unsuccessful, ask for help and take note of the answer.

Tasks:

(0.1) Fire up the virtual machine.
(0.2) Log in as 'ospite' (password: lezione).
(0.3) Open Terminal.
(0.4) Digit 'tcsh' and press ENTER.

cd NAME	changes directory to NAME ('..' moves up one directory)
ls (NAME)	lists the content of the NAME directory ('.' for current directory)
cp OLD NEW	creates a copy of OLD named NEW
mv OLD NEW	rename/move OLD into NEW
grep 'STRING' NAME	searches text STRING into file(s) called NAME
mkdir NAME	creates a new directory called NAME
rm NAME	deletes NAME
cat NAME	prints on screen the content of NAME
more NAME	prints on screen the content of NAME, one page at a time
head NAME	prints on screen the first 10 lines of NAME
tail NAME	prints on screen the last 10 lines of NAME
df (PATH)	reports file system disk usage
du (PATH)	reports file disk usage
wc NAME	reports lines, words, and bytes counts for file NAME
Pwd	reports current directory full path
vi (NAME)	fires up VIM text file editor (and loads file NAME)
man COMMAND	shows a manual page COMMAND (any of the above red words)

VIM is a text editor, read the manual and check out keyboard commands at https://vim.rtorr.com/
The output of any command that prints text on screen (such as 'ls', 'du', or 'wc') can be filtered by using the 'grep' command and searching for certain strings, as in COMMAND | grep 'STRING'
Selecting text with your mouse copies it, even over multiple lines, and pressing the middle mouse button pastes it at the current cursor location

(1.1) Browse the 'qm' folder and snoop around subdirectories therein.
(1.2) Find out which file is the largest and where it is located.
(1.3) Create your own subdirectory inside 'qm'.
(1.4) Move into this subdirectory.
(1.5) Find the full path to this subdirectory
(1.6) Create a text file with a list of all files named 'tmp.chk' found inside 'qm' and subdirectories.
(1.7) Mess around with this file: rename it, create a copy or ten, and whatnot.

molden NAME	open NAME file for visualization, accepts *.chk and *.molden
Gaussian manual page: https://gaussian.com/man/ Molpro manual page: https://www.molpro.net/manual/	

(2.1) Read g09 input file 'qm/start.com' and try to understand its content.
(2.2) Read g09 output file 'qm/start.log' and try to understand its content.
(2.3) Figure out what the calculation is about.
(2.4) Now visualize the output file using the molden command.
(2.5) Check out molpro input file 'qm/ch4_caspt2/ch4_react/ch4.com'.
(2.6) Check out molpro output file 'ch4.out' in the same directory.
(2.7) Figure out what the calculation is about.
(2.8) Now open 'molpro.molden' in molden for a graphical ouput.

g09 NAME &	runs g09 in background using instructions from NAME input file
molpro NAME &	runs MOLPRO in background using instructions from NAME input file

(3.1) Optimize the geometry of a CH4 molecule on g09.
(3.2) Optimize the geometry of a C3H8 molecule on MOLPRO.