Use a computer command line

Introduction

If we wish to use computers to predict properties of molecules, study reaction mechanisms or solve crystal structures, we first need to learn how to talk to the computer! You will be running all the programs used in the computational chemistry labs in a terminal or a console (such as those used on Unix systems). This is actually the easiest and most powerful way to do things, and it works pretty much the same way on everything (Windows, Mac and Unix).

You have to be careful to type commands exactly as written in the laboratory manual. Commands are case sensitive and a simple mistake such as a missing space or dash will cause problems.

The focus of this section is solely on talking to the computer. It is necessary to go through this handout because if you don't understand these commands you will have an extremely difficult time doing the lab, as you will waste more time trying to understand how to talk to the computer than understanding the results.

2. Handy hints

- Use this section during the labs, refer to it when necessary.
- Ask us if you need help or don't understand an instruction
- Use TAB to autocomplete commands
- Use the up and down keys on the command line to go through your previous commands (it remembers!)
- You are allowed to use the internet to look up terms you don't understand or if you need more detailed help with something and we are unavailable.

3. Common commands

- Changing directories (folders): *cd path/to/new/directory*
- Go up/back a directory: *cd ..*
- Return to home directory: *cd ~*
- Print working directory (or "What folder am I in?"): *pwd*
- List everything in your directory: *ls*
- Read manual for help with commands: *man command name*

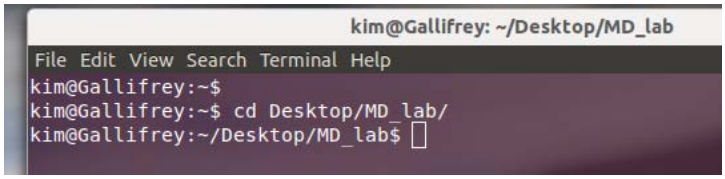

Figure 1: Using cd. The terminal first states the user name@computer name:current directory$ and then waits for you to enter commands. For example, here the user was kim, computer is called

Gallifrey and the current directory is ~ (the symbol for the home directory). On the next line we have changed to the MD lab folder on the desktop (note the capital!) and the third line shows we are then in that directory and awaiting the next command.

4. Viewing and editing files

You can choose to use the non-graphical command-line editor vim (or emacs or pico if you are familiar with them) as an alternative to the simple notepad editor. Microsoft Word or equivalent is not recommended as it inserts hidden symbols that might make your calculation crash. The advantage of using command-line editors is that you can work more quickly by using the keyboard and avoid the mouse. Although vim might be awkward to use at first it makes editing files much more efficient once used properly.

YOU MUST BE IN THE DIRECTORY WHICH CONTAINS THE FILE TO VIEW AND EDIT IT.

To open a file with vim type in the command line: *vi filename.inp*

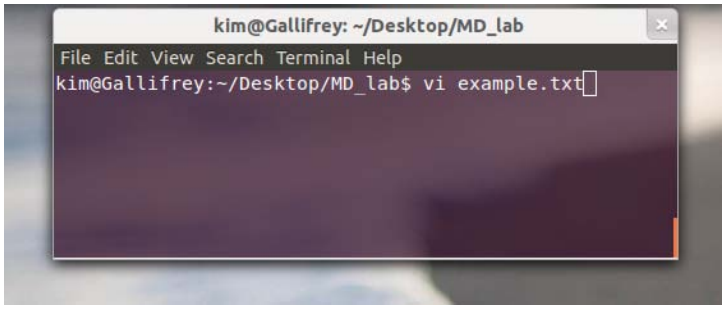

Figure 2: Opening file 'example.txt' with vim. To navigate through the file use the up/down arrow and pageup/pagedown keys To make changes press the Insert[1] or 'i' key. When you are finished press Esc.

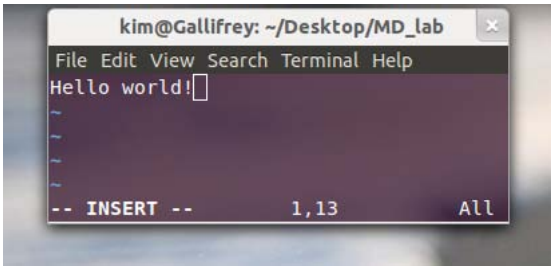

Figure 3: Inside vim in Insert mode, as is visible by the bottom left status. The user has typed the message "Hello world!".

To undo press Esc then 'u' to cycle back one change at a time or 'U' to undo all changes
To save changes press Esc and type :w to write (save) the file
To close the file press Esc and then type :wq if changes have been made or :q! to quit without saving changes (take care!)

[1] If you press Insert twice or 'r' you will enter replace mode instead of insert mode -this can be exited by pressing Esc

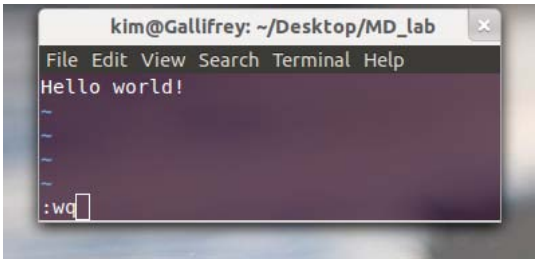

Figure 4: Leave Insert mode using ESC then type :wq to write (save) and quit vim. If you wish to save the file under a new name type :w new filename.

5. Exercise

Look at the screenshot below and fill in the worksheet. Use the 'Explanation' box to briefly explain what the corresponding command did in the given example. This should take no more than 10 mins.

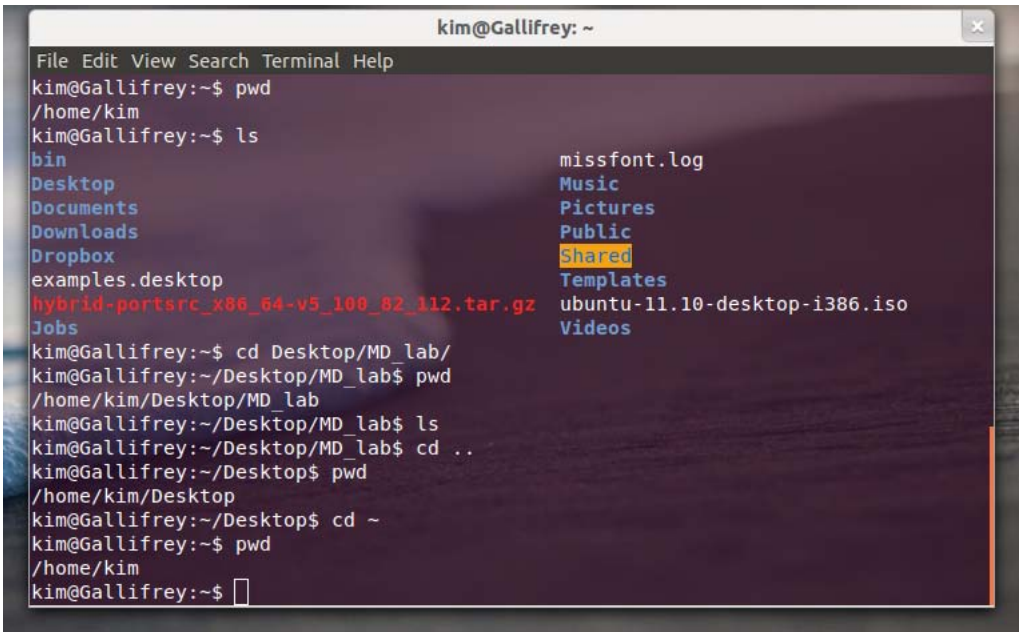

Figure 5: Fill in the accompanying spreadsheet with what is happening for each step in the screenshot.

CHEM3002 Terminal commands worksheet

Command	Current directory	Explanation
pwd	/home/kim (also denoted as ~)	We start off in the home directory. PWD is "print working directory" i.e. print to the screen what the current directory is.
ls		
cd Desktop/MD_lab		
pwd		
ls		
cd ..		
pwd		
cd ~		
pwd		