Quick tutorial

1. *Avogadro*

 Draw Tool to build molecules. Elements to be selected on the left, single click in the main window to put the atom.

 Navigate Tool is for rotating, zoom and moving your model.

 Selection Tool enables you to select atoms and/or fragments of your molecules.

 AutoOptimization Tool allows the geometry optimization with Molecular Mechanics, to refine your structure. A settings window appears on the left.

Avogadro official page
http://avogadro.openmolecules.net/wiki/Main_Page

2. *Linux/Unix commands*

ls
Lists the content of a directory.

cp *old_file new_file*
Copies the existing file *old_file* to the file *new_file*

mv *old_file new_file*
Renames the existing file *old_file* to the file *new_file*. CAUTION! If *new_file* already exists, it will be overwritten with NO chance to recover the lost data.

mkdir *dir_name*
Creates a new directory named *dir_name*

cd *dir_name*
Goes into the directory *dir_name*, where *dir_name* is the full path or a sub-directory of the current folder

cd
Goes back into your home directory

cd ..
Goes into the parent folder

rm *file_name*
Delete the file *file_name* if available. CAUTION! Once this command is executed, *file_name* is gone with NO chance to be recovered

man *command_name*
Opens the manual page for the command *command_name* (very useful in case of panic)

NOTE 1: to recall previous used commands, press the "Up" arrow at the command prompt until you reach the desired one.
NOTE 2: if you are not sure about the outcome of a command, just ask! (instead of trying it and making a catastrophe…)

3. File editing

Among the many available programs, you will use **vi** as a text editor.

vi *file_name*
Open *file_name* for editing. If *file_name* does not exist, an empty file will be shown

Commands in vi
vi works in different modes.

- Execute mode, the default: each key or combination can give commands of advanced editing (replacement, cut, copy, paste…);
- Input mode: the way you can write text, it is called by typing **i** while in execute mode.

The <Esc> key can switch from any mode back to the execute mode.

yy
Copies the line where the cursor is

p
Pastes previously copied lines after the line where the cursor is

dd
Delete the current line

:w
Saves the file with the name used to open the document (vi *file_name*)

:w *file_name*
Saves the file with the name *file_name*, which can be different from the initial name of the document

:q
Quit vi (if modifications are not saved, it will not work)

:q!
Quit vi discarding any modification

:x
Saves all modifications (like :w) and quits the editor (like :q)

4. Gaussian

Gaussian is a computational chemistry software to predict properties of molecules and reactions. Input file format guidelines are in the following.

Link 0 commands section
Lines starting with % symbol, to define how the program should run:

%mem
amount of RAM memory to be used during the calculation

%chk
checkpoint file name, a scratch file used by Gaussian

Route section
Starting with # symbol, to specify the kind of calculation, the method and the basis set:

#N, #P, #T
Amount of data in the output file, respectively normal, verbose and synthetic

method/basis_set other_options
Follows the output level, on the same line. Refer to the main tutorial (pp. 14 and following) or to the Gaussian manual for the available keywords.

Title section
Free and brief description of the calculation, preceded by a blank line, and followed by a blank line

Molecular charge and spin section
2 integers separated by a space, respectively the overall **charge** and **spin multiplicity**. NO BLANK LINES AFTER THIS SECTION.

Geometry specification sections
Molecular coordinates (Cartesian or Z-Matrix). To be followed by at least a blank line.

Avogadro will be used to generate input files starting from molecular structures:

- Once the molecular structure has been created, click on **Extension** menu, then choose **Gaussian**
- A dialog box for methods and properties selection will appear. Click **Generate** to create a Gaussian .com input file