VMD's Cheat Sheet

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VMD is one of the most versatile molecular viewer: it is free, it runs on Windows, Linux and Mac OS X, there is a huge community, plugins and scripts (the Tcl console allow you to write your own script). Last but not least, VMD is able to manage a lot (A LOT) of formats.

Open VMD from terminal:

vmd	run vmd
vmd file.xyz	open file with VMD. Mind that VMD tries to guess the file format from the file name. In this case VMD tries to open the file as xyz file.
vmd -tinker file.xyz	to open tinker files, specify the format with the option -tinker

Some shortcuts when focus on the view window:

1, 2, 3 or 4	select an atom, get the distance between two selected atoms, get the angle between three selected atoms or get the dihedral angles between four selected atoms, respectively.
7	allow to grab a fragment or molecule and displace it
=	reset view
s	zoom (also mouse wheel does this)
r	return in rotate mode
t	translate the entire system

The VMD main window

A number of controls are available directly from the main window. This windows can be divided in three main parts:

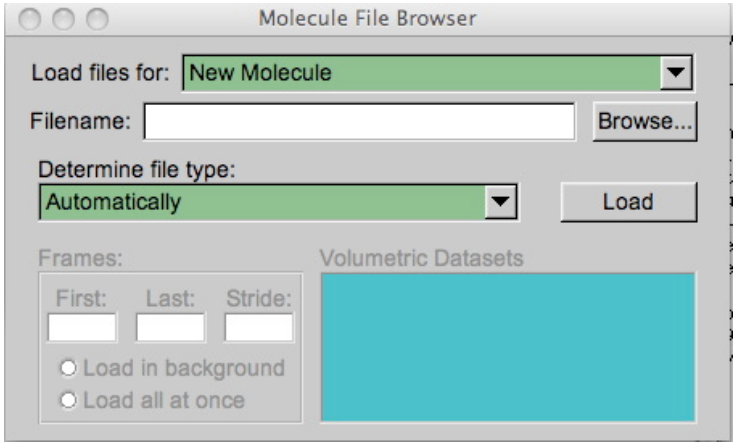
Menu Bar	Browse between different functions
Loaded molecules	display the molecules loaded in VMD
Trajectory controls	Control the trajectory

Useful info about Loaded Molecules part:

ID	id of the molecule. Useful to know when you make scripts
T	time line. Put the time for trajectory on a molecule
D	toggle on/off that molecule from the view windows
F	freeze the molecule: zoom, rotation, translation acts only on molecules that are not frozen
Molecule	name of the molecule
Atoms	number of atoms in the molecule
Frames	number of frames (a trajectory has more than one frame)

Trajectory controls

Load molecules in VMD (File -> New molecule):
To load a molecule in VMD you can also right-click on the main window



Load files for:

New Molecule	load a new molecule
Choose a loaded molecule	append new molecule to the selected one

Filename/**Browse**... select the file

Determine file type:

Automatically	let VMD try to guess the format or open the menu to choose manually the file format.

Frames:

load all at once	load a trajectory all in once, without showing all the frames
first/last/stride	load a part of trajectory

Load load the molecule

Graphical representations (Graphics -> Representations):

Another useful feature of VMD is the possibility to display only part of the molecules (e.g., specific fragments, atom types or atoms with specific atomic indices, ...) and to modify the style to display molecules or parts of it.

Use selected molecule menu to apply the changing to a specific molecule.

Create Rep/Delete Rep are use to create replica of the selected style or delete it

Selected atoms: choose the atom to be selected for the current representation:

E.g.:

all	all atoms
fragment x	only fragment x
not fragment x	all but fragment x
type C	all Carbon atoms C
index 20 21 22	only atoms 21, 22 and 23 in the structure. **Mind that numbering in VMD starts from zero, not one!**

More selection keywords can be combined using AND logical operator:

e.g.:

fragment 0 *and type* C

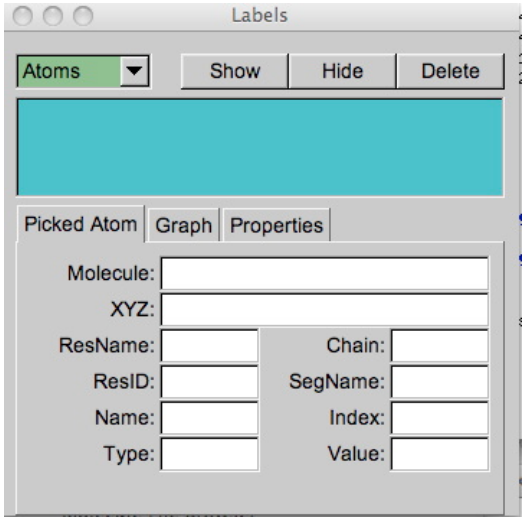
Some coloring methods:

Name	based on the name
Color	use only one color among those available

Drawing method: choose a style (VdW, lines,Bond, CPK, H-bonds, ...) Depending on the style, some controls are displayed in order to enhance the graphical representation, e.g. sphere/bond resolution, line thickness, ..

Labels (Graphics -> Labels):

Use labels windows to delete/hide labels on the view and/or retrieve information about selected atoms, distances, angles and dihedral angles.



This is quite self explaining...

Interesting is also the Graph submenu, which allows to draw a plot for the values assumed by the selected distance, angle or dihedral angle along the trajectory. The values can be saved in a text file. **Mind that the distances, angles and dihedrals are calculated considering the system NOT periodic**, so be careful to pbc artifacts: you may want to consider to use molgeom instead.