Reference manuals

VMD

Petr Kulhanek

kulhanek@chemi.muni.cz

National Center for Biomolecular Research, Faculty of Science
Masaryk University, Kotlářská 2, CZ-61137 Brno

VMD

http: //www.ks.uiuc.edu/Research/vmd/

Program for visualization of molecules. Available after free registration for MS Windows and Linux.

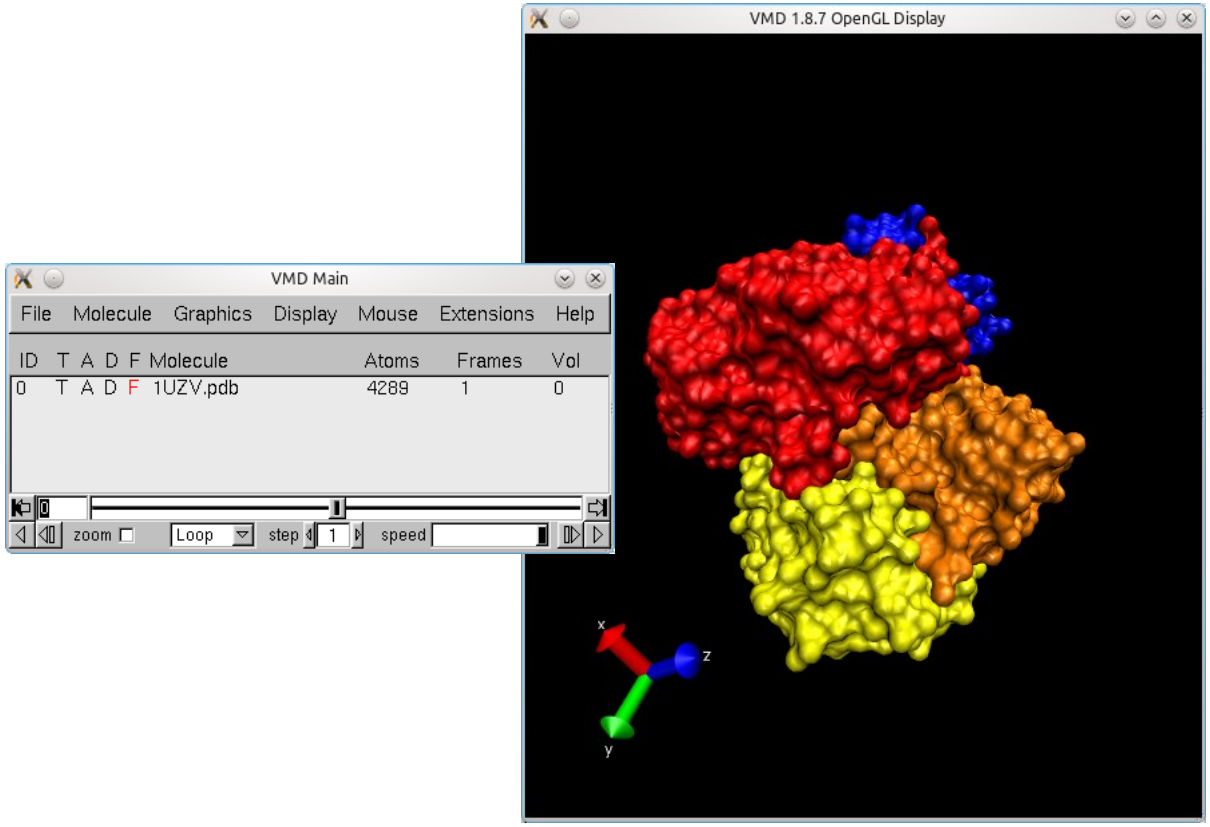
VMD program

http://www.ks.uiuc.edu/Research/vmd/

The program is used to visualize (bio)molecules and to analyze the results of molecular dynamics simulations. The program is freely available (requires registration) and is also available for the MS Windows operating system.

Starting the program:

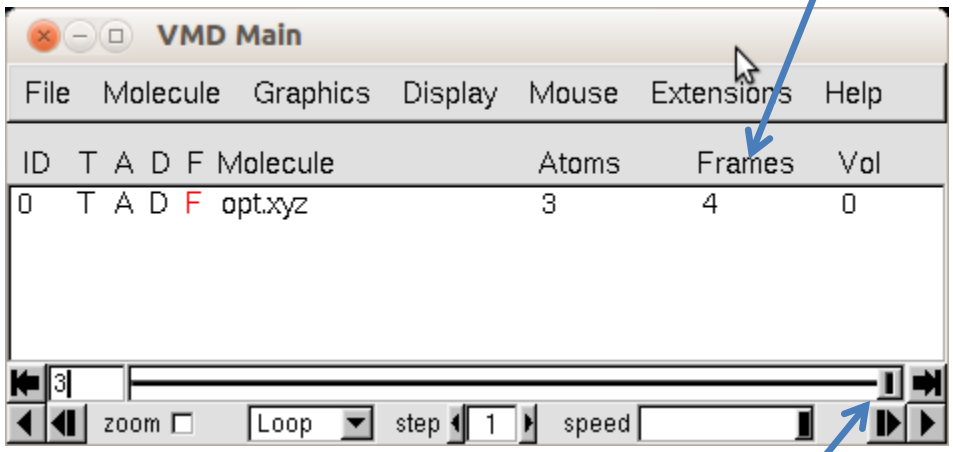
```
$ module add vmd
$ vmd
```



Geometry optimization visualization

Load **xyz** trajectory (optimization process) extracted by the script **extract-gopt-xyz** from the module **qmutil** into the vmd program.

number of optimization steps

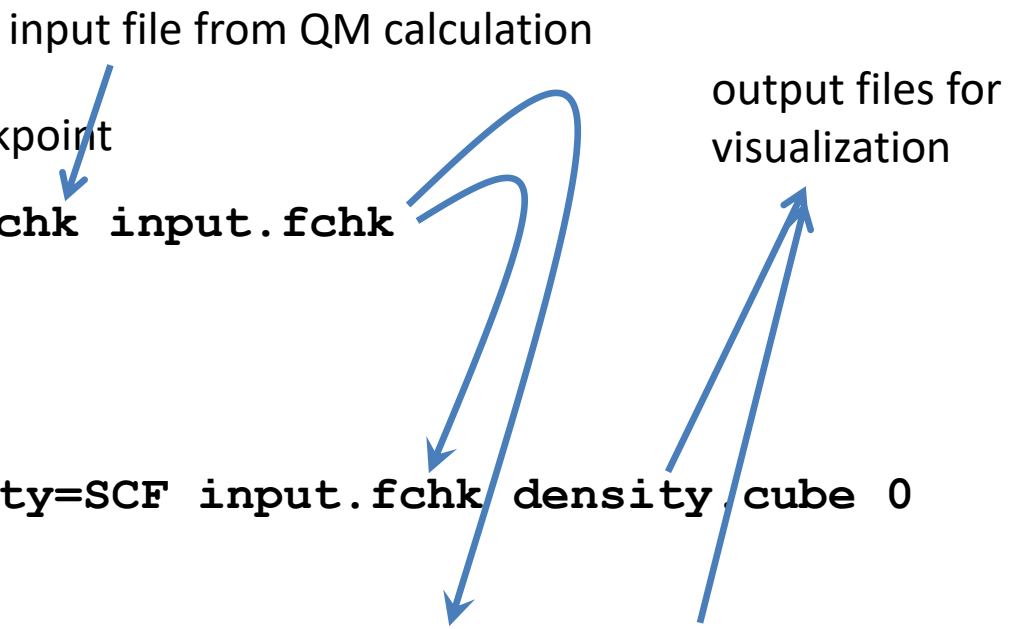


moving between individual geometries

Volumetric data

Preparing volumetric data

Volumetric data (**cube** files) can be created by the program **cubegen** from formatted checkpoint, which is a file containing a wave function (coefficients).



Procedure:

1) preparation of formatted checkpoint

```
$ formchk     input.chk input.fchk
```

2) calculation of volumetric data
   1) electron density

```
$ cubegen 0 Density=SCF input.fchk density.cube 0
```

   1) electrostatic potential

```
$ cubegen 0 Potential=SCF input.fchk potential.cube 0
```

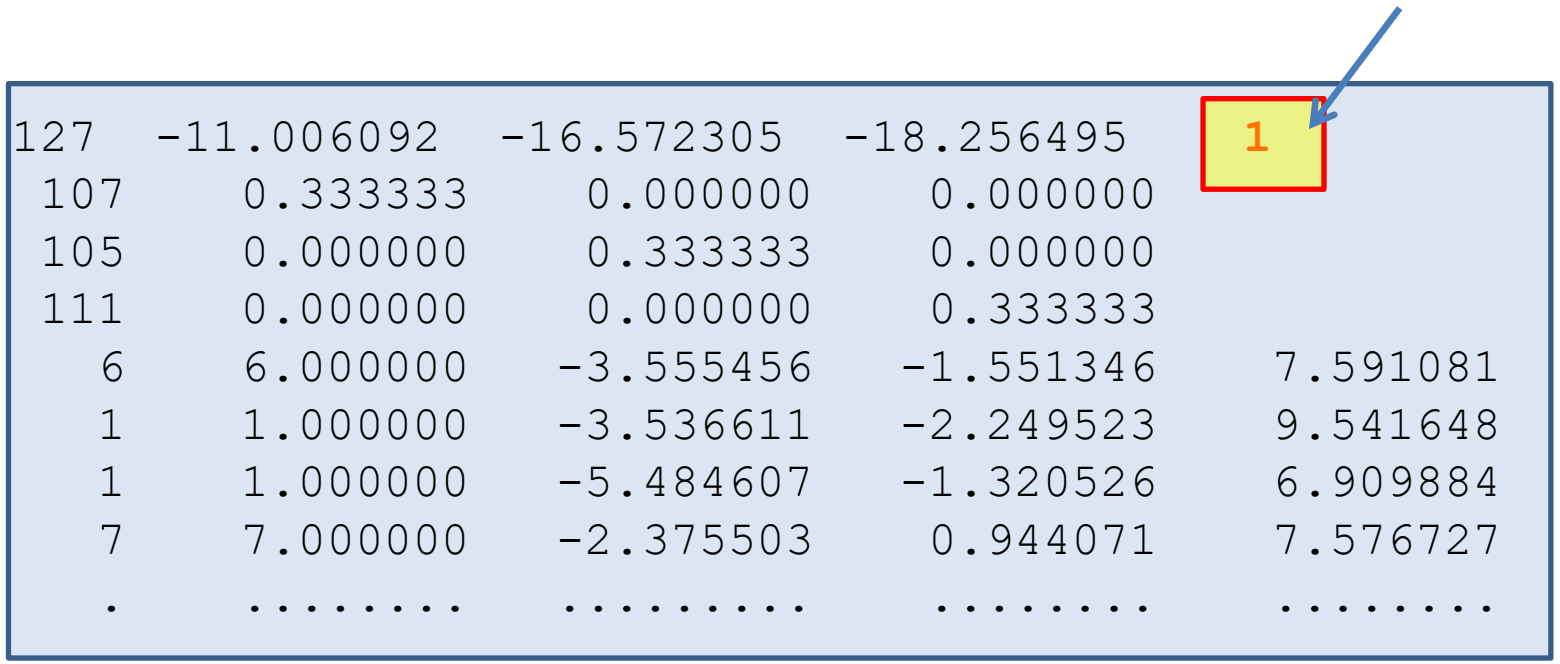
formchk and **cubegen** are from the module **gaussian**.

Documentation:
http://gaussian.com/g_tech/g_ur/u_formchk.htm
http://gaussian.com/g_tech/g_ur/u_cubegen.htm

Adjustment of cube files

VMD cannot load cube files created in some old versions of the gaussian program. The files must first be edited manually. Open the file in a text editor and edit it according to the instructions below.

this number must be deleted, the rest of the file remains unchanged



```
127  -11.006092  -16.572305  -18.256495    1
 107    0.333333    0.000000    0.000000
 105    0.000000    0.333333    0.000000
 111    0.000000    0.000000    0.333333
   6    6.000000   -3.555456   -1.551346    7.591081
   1    1.000000   -3.536611   -2.249523    9.541648
   1    1.000000   -5.484607   -1.320526    6.909884
   7    7.000000   -2.375503    0.944071    7.576727
   .    ........    ........    ........    ........
```

Visualization of volumetric data

Volumetric data (cube files created by the program cubegen) can be loaded directly into the vmd program. In the default visualization, the molecule is displayed in a line model without volumetric data.

Volumetric data can be displayed as (Representations):

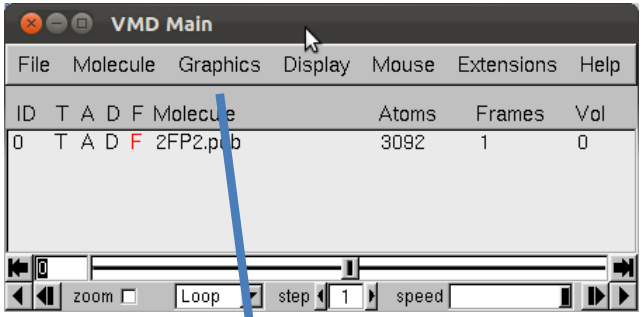
- isosurface
- volumeslice

Map[ping of electrostatic potential to isosurface with electron densities:

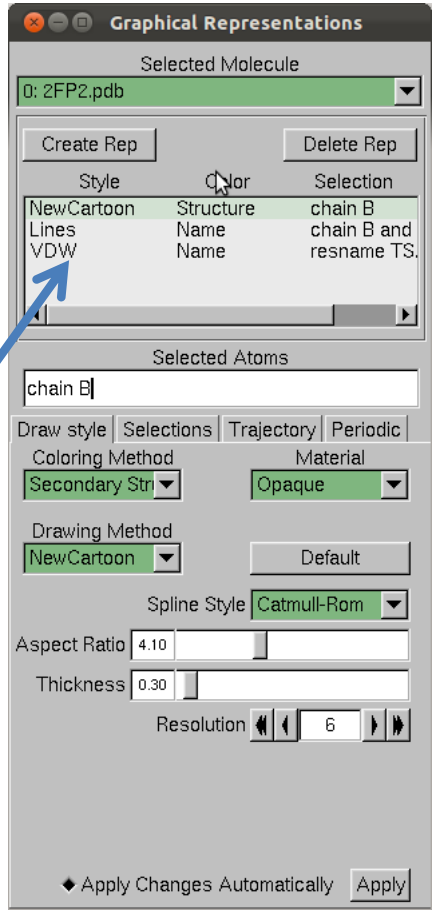
1) load the density and electrostatic potential into one molecule
2) display isosurface of the electron density
3) for isosurface, choose coloring (Coloring Method) according to volumetric data (Volume) - select the electrostatic potential, the range of colors is set in the tab Trajectory (Color Scale Data Range)

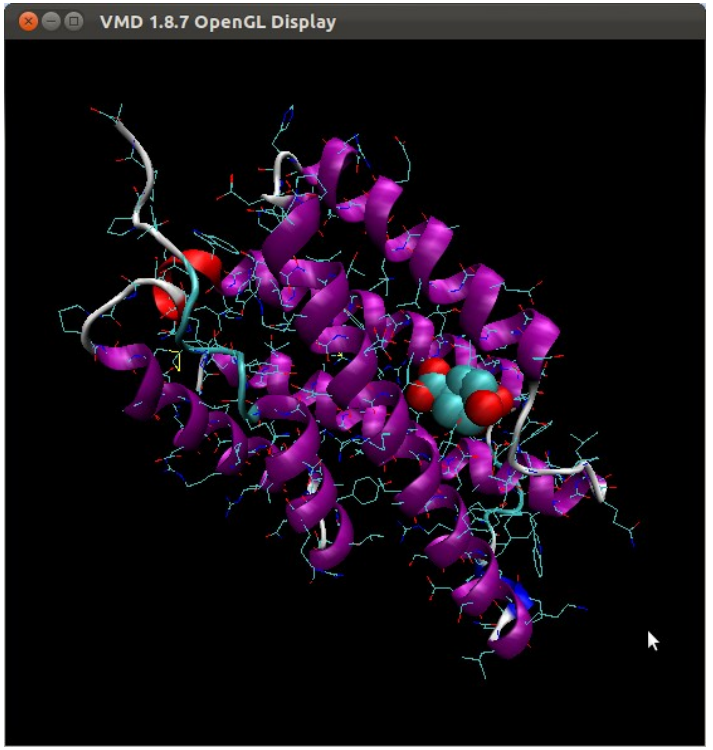
Graphic representations

VMD program – change of models



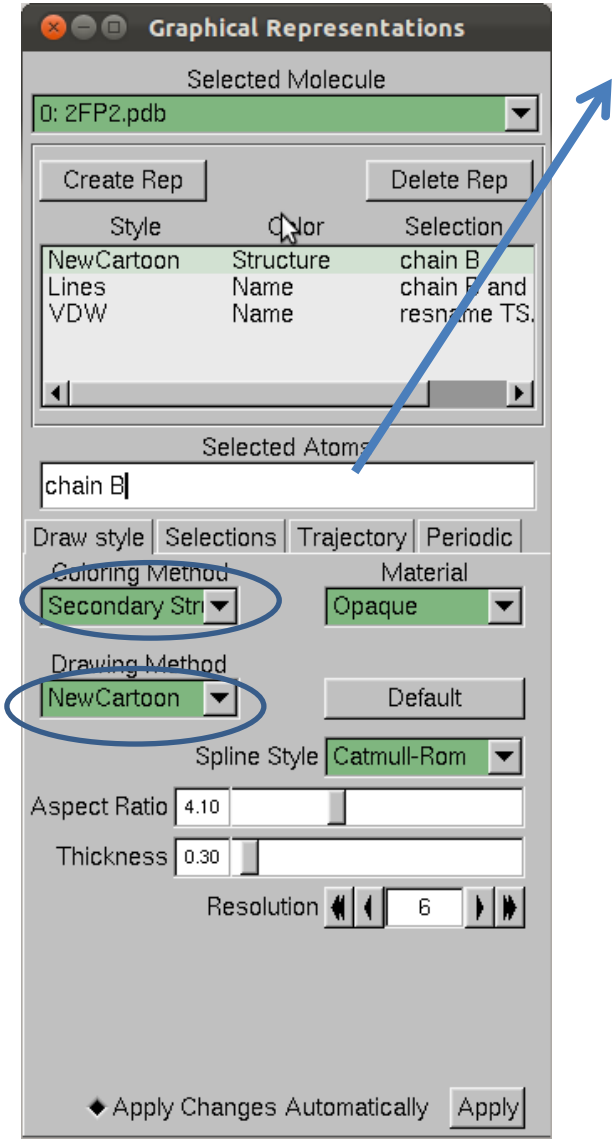
Representation





double-clicking on a line deactivates the graphical representation

VMD program – change of models



Selection (mask) of a part of a molecule:

protein	- select all amino acids
water	- select all water molecules
chain X	- select chain X
resname X	- select a residue named X
resid X	- select a residue with number X
within 5 of Y	- select all atoms that are 5 Å away from the atoms in Y mask
not hydrogens	- do not display hydrogen atoms

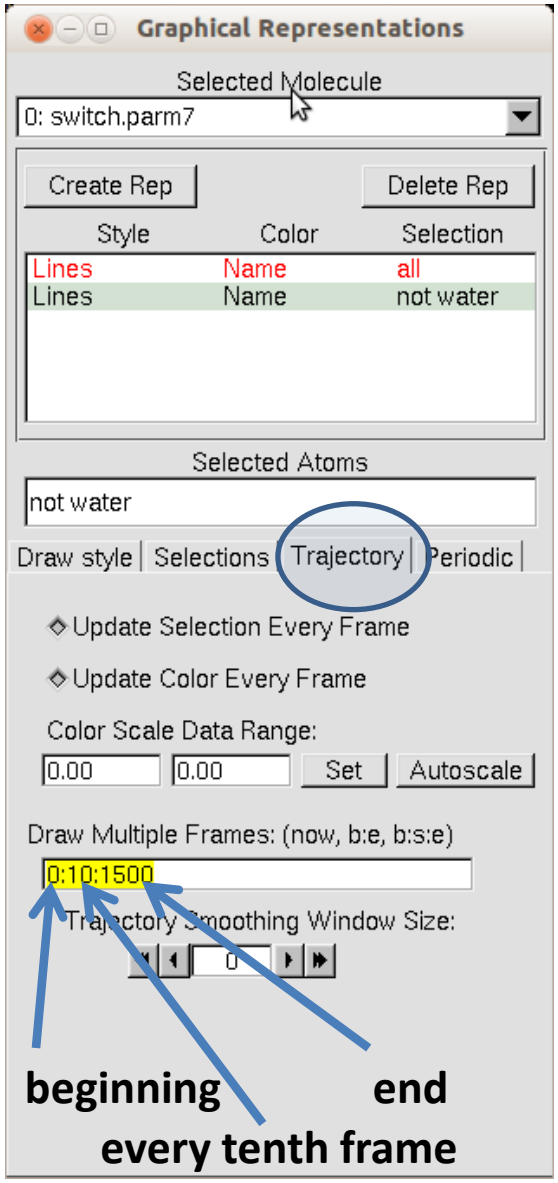
Examples:

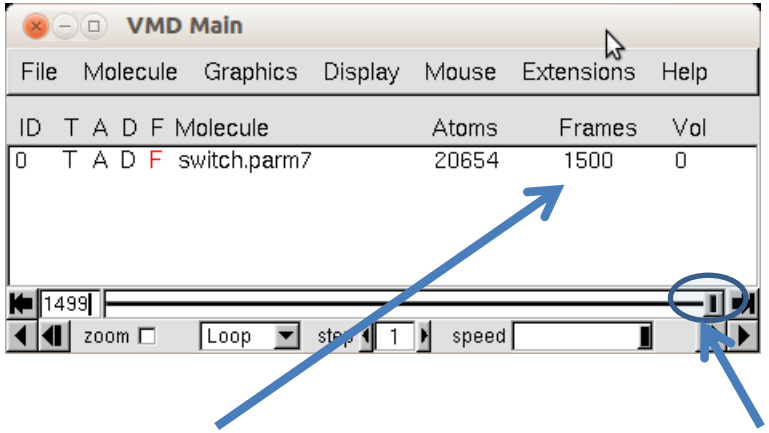
chain A
chain A B C
resname ASP GLU
resid 1
resid 1 to 100
within 6 of resid 100

residue can be an amino acid, ligand, or part of a ligand

Trajectories

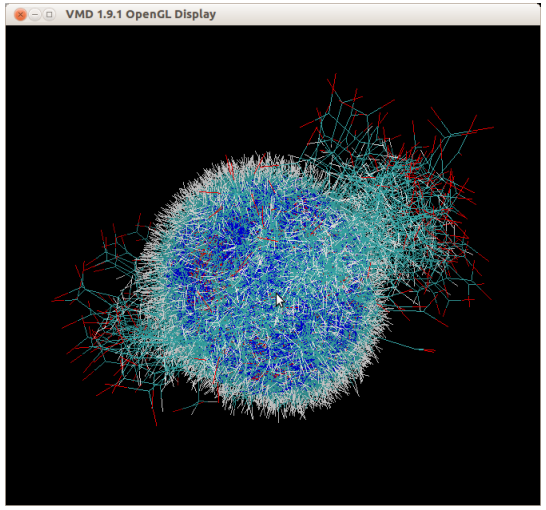
Analysis of trajectories

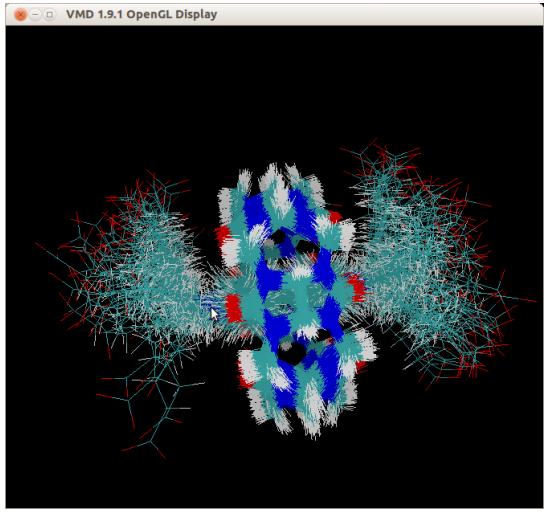




number of frames in trajectory

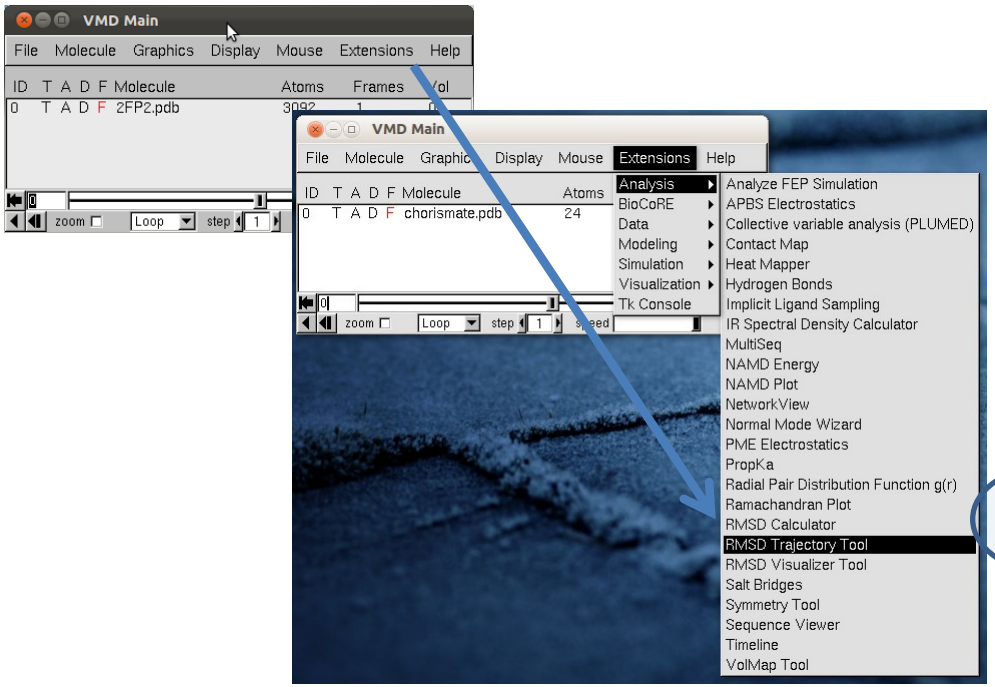
scroll between trajectory frames





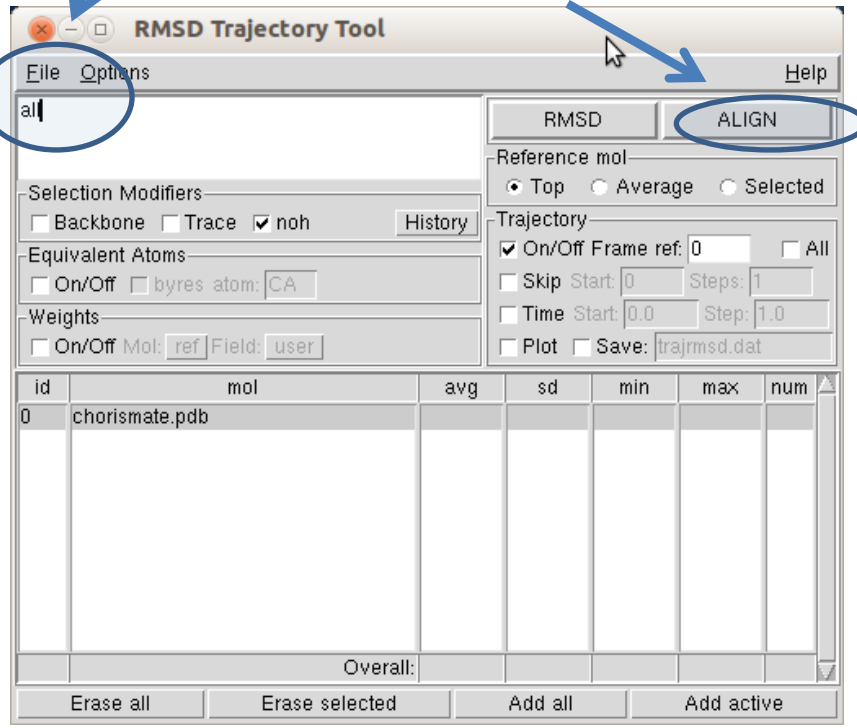
before and after removing the translational-rotational movements

Removing TR movements



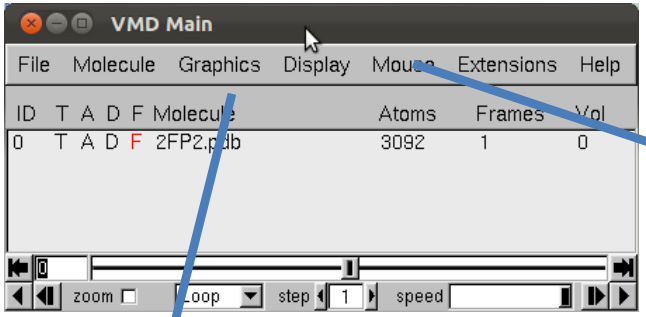
Change to "all“ (all atoms), or to the part of the molecule we want to perform the superimposition to

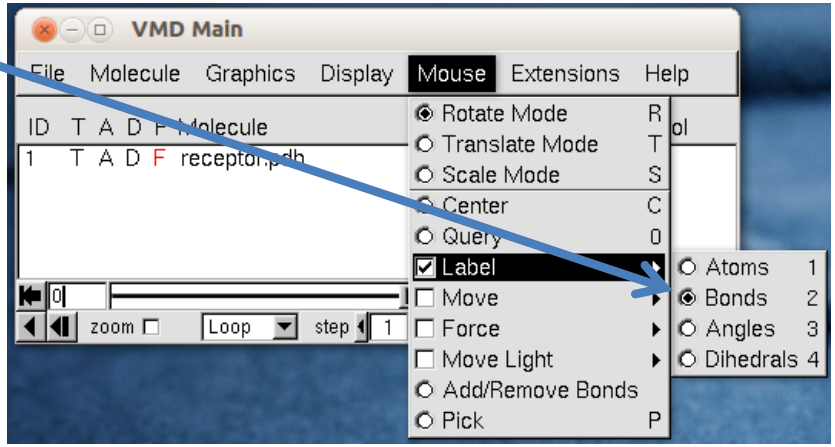
Removes the translational-rotational motion of selected atoms

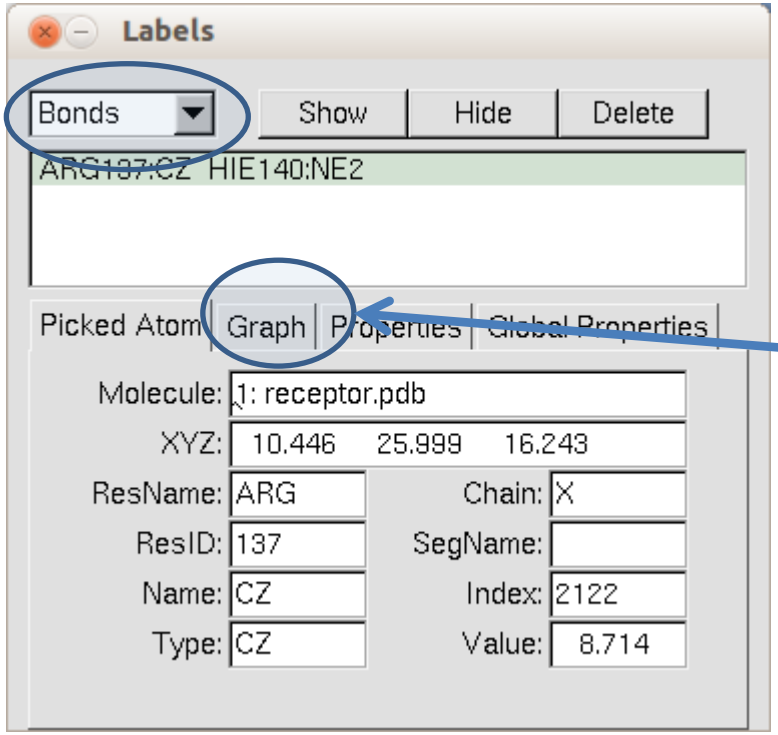


When evaluating the course **trajectories** it is advisable to remove **translational-rotational (TR) motions** of the whole system. This will make visual analysis of movements easier.

Measurement

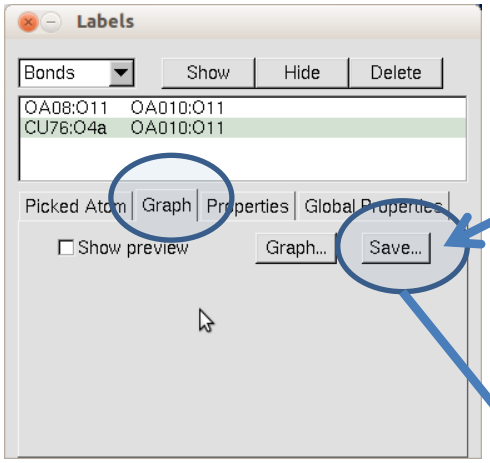






if we have a loaded trajectory, time course of the measured distance is displayed

Histogram analysis



Save to disk as a text file. File (e.g., distance.txt) contains two columns: the frame number and the measured value.

For other setting of histogram program, see:

```
$ histogram -h
```

```
$ module add cats
$ histogram -c 2 distance.txt distance.hist
```

analyze the second column, i.e., the measured value