Visual Molecular Dynamics (VMD) tutorial

1 Introduction

VMD (Visual Molecular Dynamics) is a powerful tool to visualize, model and analyse various molecular systems. It is developed and freely distributed by the Theoretical and Computational Biophysics Group at the University of Illinois at Urbana-Champaign. You can download the tool for free from here `http://www.ks.uiuc.edu/Research/vmd/`, but the tool is already installed for you on the workstation. This tutorial gives a short overview on how to load and visualize structures and trajectories from MD simulations. For detailed tutorial, including how to do analysis using VMD refer to `http://www.ks.uiuc.edu/Training/Tutorials/vmd/tutorial-html`.

1.1 Start VMD from the command line

Simply type into your shell window

  `vmd`

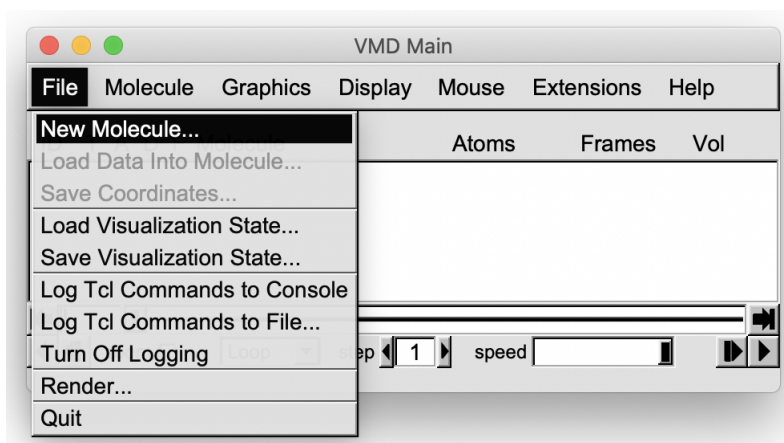To open a structure file (`pdb` or `gro` format), use e.g.

   `vmd protein.gro`

To load frames from a compressed trajectory (`xtc`) to a structure, use e.g.

   `vmd protein.gro protein_fitted.xtc`
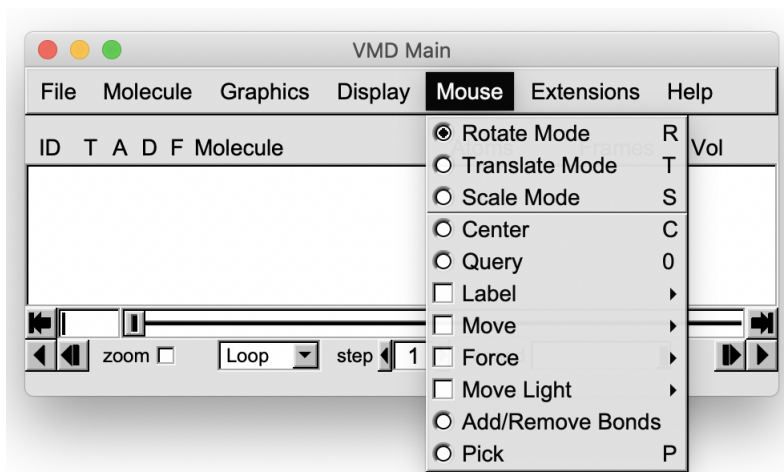
1.2 Loading structure file

Run VMD. This will cause three windows to appear on the screen. If you started a plain VMD session, PDB or GRO files can be loaded from the **VMD Main** window by going to the **File** menu and clicking on **New Molecule**. You can then browse for the PDB file. Once you load the file, the three-dimensional molecular structure will appear in the **OpenGL window**.

1.3 Interaction Modes

The user can interact with the molecule in a variety of ways . The user can rotate, translate and scale (zoom) the molecule. Each of these interactions modes can be accessed via the **Mouse** menu in the **VMD Main** window or using a shortcut key listed below. After the interaction mode has been selected, click
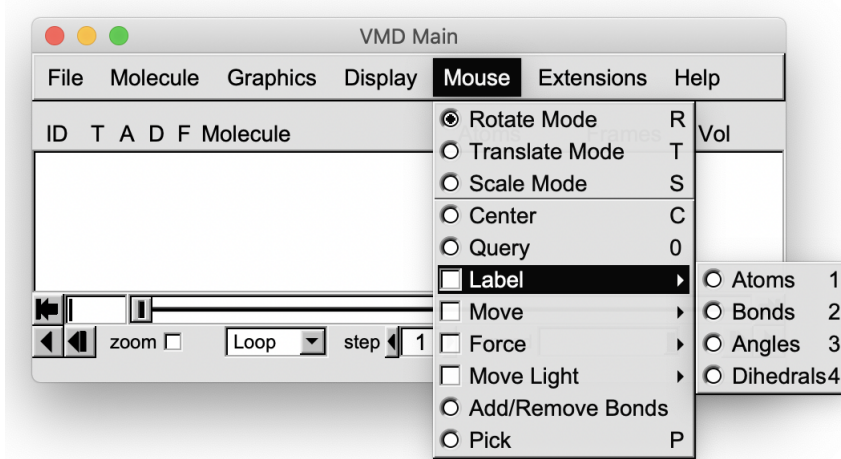
on the **OpenGL** window with the left mouse button and drag the mouse. By default, VMD starts in **Rotate Mode**.


```
Mode        Shortcut Key        Description
Rotate          r           Rotates the molecule
Translate       t           Translates the molecule
Scale           s           Scales the molecule (zoom)
Center          c           Centers on an atom
```

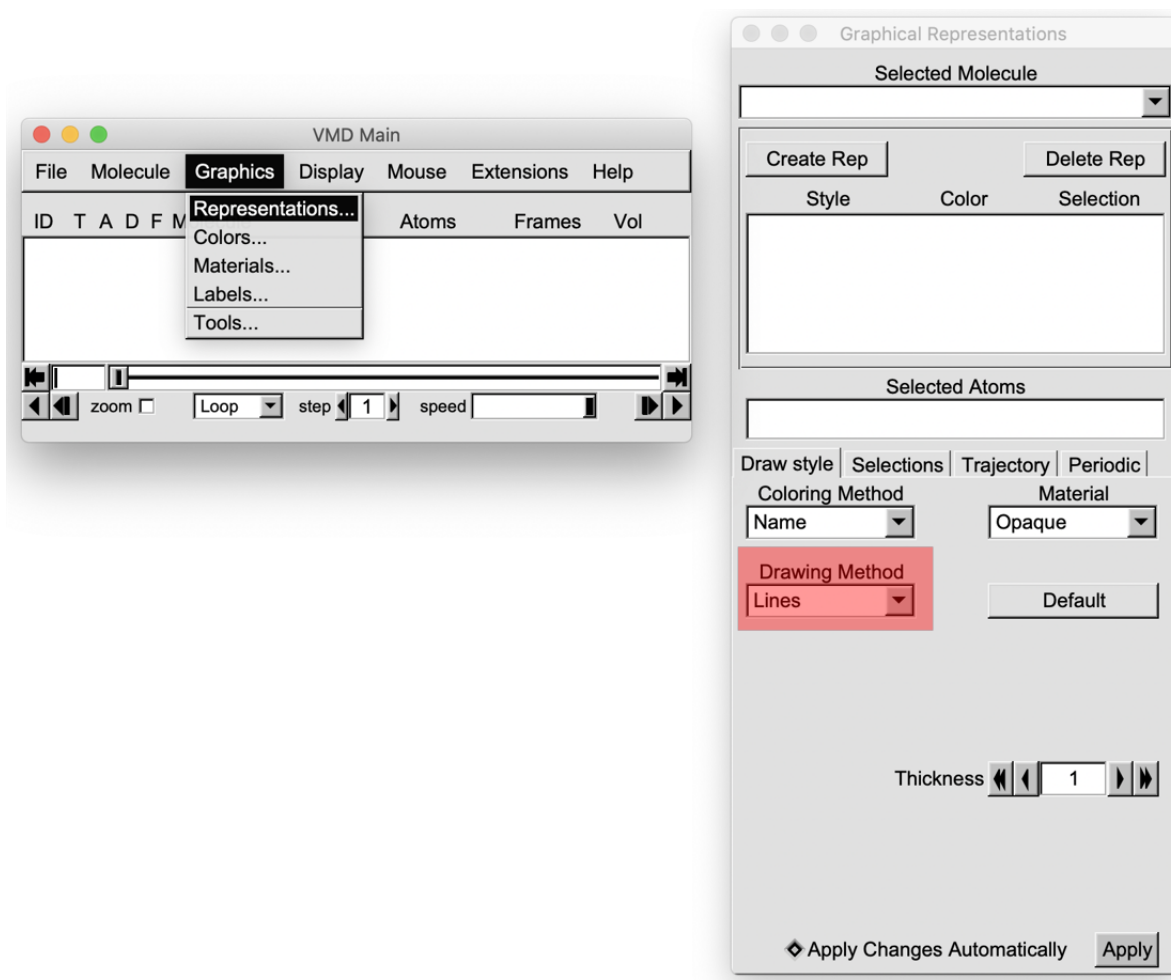## 1.4 Measuring Structural Features

You can place labels that specify the distance between two atoms, the angle formed by three atoms and the dihedral angle formed by four atoms. To do so, select the particular feature you would like to label from the Mouse menu in the VMD Main window or using a shortcut key listed below. Then click on the atoms you would like to measure.


```
Feature         Shortcut Key        Description
Bond length         2           Distance between two atoms
Angle               3           Angle between three atoms
```

```
Dihedral Angle      4          Dihedral angle between four atoms
```

1.5 Changing the Drawing Method

Atoms and molecules can be visualized with various drawing methods. To change the drawing method, go to **Graphics → Representations** and then click on the **Drawing Method** menu.

```
Drawing Method          Description
Lines                   Default method
HBonds                  Draws hydrogen bonds
VDW                     Space filling visualization
CPK                     Ball and stick visualization
Licorice                Stick visualization
Ribbons/New Ribbons     Draws backbone of DNA/protein as a ribbon
Cartoon/New Cartoon     Draws secondary structure of proteins
Surf                    Draws a surface around the molecule
Beads                   Draws residues as beads
```

1.6 Changing the Coloring Method

You can change the way atoms and molecules are colored. This can be done by going to **Graphics →
Representations** and then clicking on the **Coloring Method** menu. By default, VMD starts with the
Name method that colors atoms as listed below.

```
Default Coloring Method (Name)
Hydrogen     White
Carbon       Cyan
Oxygen       Red
Nitrogen     Blue
Phosphorus   Brown
Sulfur       Yellow
```

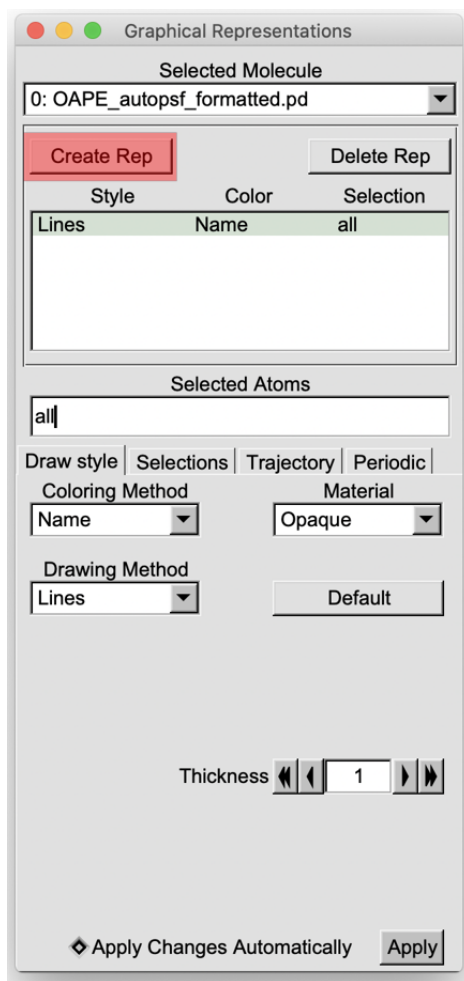## 1.7 Changing the Selected Atoms

You can choose to visualize a subset of the atoms in the PDB file by changing the text in the **Selected
Atoms** box in the **Graphical Representations** window (Graphics → Representations). To determine
what selections are available, click on the **Selections** tab of the **Graphical Representations** window.

```
Some Common Atom Selections
Atom Selection          Description
all                 Show all atoms
protein             Show only protein atoms
backbone            Displays backbone atoms
noh                 Do not display hydrogen atoms
resname X           Displays atoms of residue X
name X              Display atoms named X
resid X             Display residue number X
```
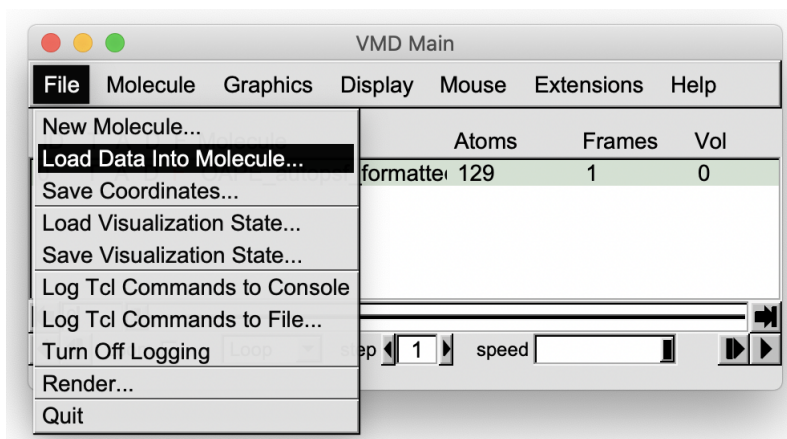
1.8 Superimposing Representations

You can superimpose multiple representations to emphasize certain features of a molecule. To generate
a new representation, click on **Create Rep** in the **Graphical Representations** window. You can then
apply new drawing methods, coloring methods and/or atom selections to this new representation.
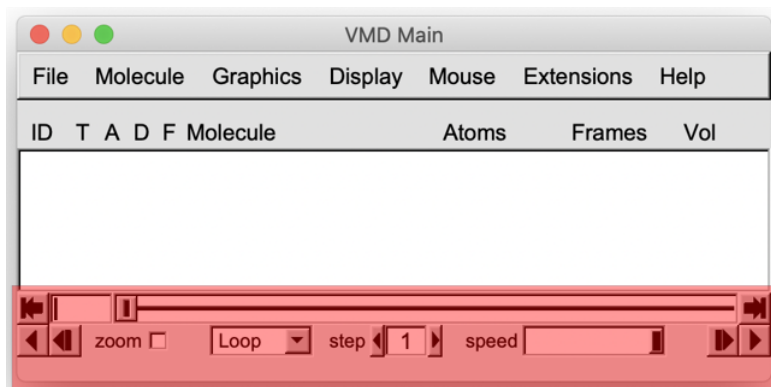
1.9 Loading and Playing a Trajectory

VMD can play an animation of a molecule if provided with a trajectory file. Like PDB files, trajectory files come in many different formats. To load a trajectory right click on the molecule name in the **VMD Mai** window and select **Load Data Into Molecule**. Then browse and select the desired trajectory.
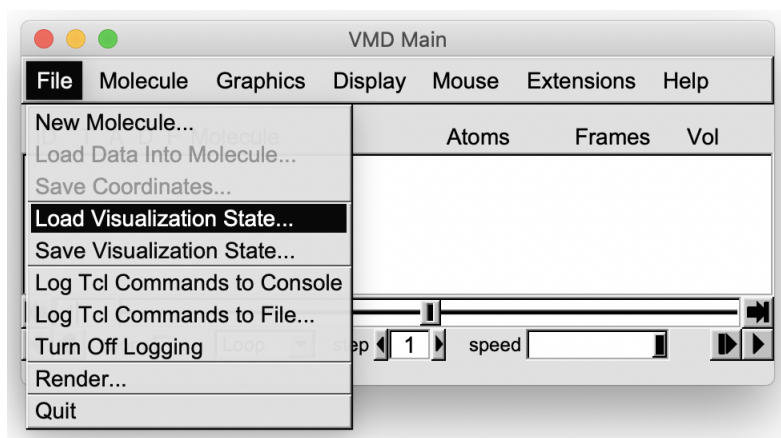
The trajectory can be played using the arrow buttons at the bottom of the **VMD Main** window. The speed can be adjusted with the slider in the bottom right hand corner.

1.10 Saving/Loading a State File

After applying your own visualization style to the PDB file, you can save your work in a VMD state file. You can then load the state file at a later time and it will load the PDB file along with the changes that you made. State files have a .vmd file extension. To save a state file, go to **File → Save State** in the **VMD Main** window. To load a state file, go to **File → Load Visualization State**.
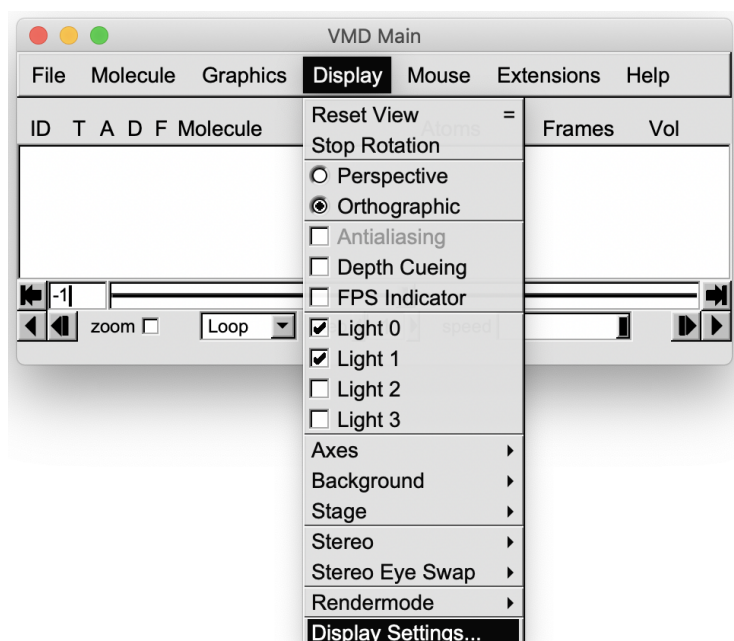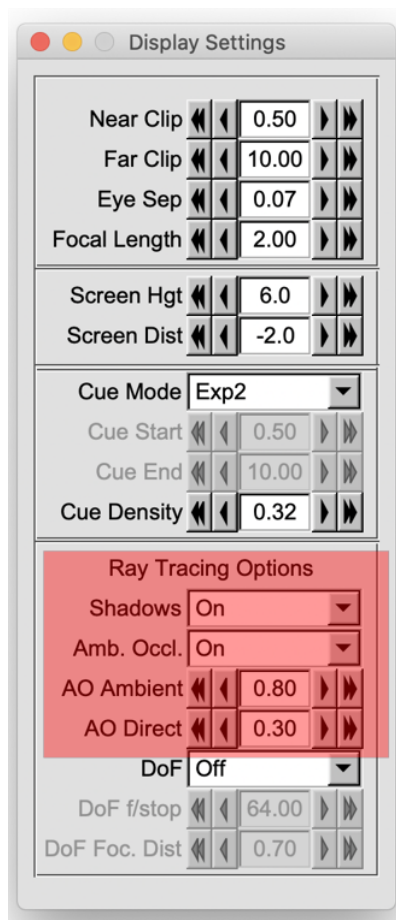
1.11 Saving an Image

To save a screenshot of the contents of the **OpenGL** window in the **File** menu of the **VMD Main** window go to: **File → Render → Start Rendering** Using the default renderer takes a screen shot of the VMD OpenGL window and saves it as an image.

1.12 Saving an Image with Lighting and Shadow Effects

You can also save images that include lighting and shadow effects. First, specify the strength of the lighting by going to **Display → Display Settings**

Turn **Shadows** and **Ambient Occlusion** on. Adjust **AO Ambient** and **AO Direct** to your desired value (values of 0.80, 0.30 usually works pretty well).

Go to **File** → Render and choose **TachyonInternal** as the renderer and click "Start Rendering". It may take a few minutes to render the scene.