VMD

Visual Molecular Dynamics

User Guide

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small things considered

Introduction

VMD (Visual Molecular Dynamics) is a software package for the 3D visualization, modeling and analysis of molecular systems. It is developed and freely distributed by the Theoretical and Computational Biophysics Group at the University of Illinois at Urbana-Champaign. VMD is a powerful instrument used in **real** scientific research. Additionally, it is also a highly effective teaching tool. This is an abbreviated guide that covers the download, installation and use of VMD. For a tutorial, see http://www.ks.uiuc.edu/Training/Tutorials/vmd/tutorial-html. Further questions can be sent to Bob Johnson: bobjohnson1981@gmail.com.

Download and Installation

1. Go to http://www.ks.uiuc.edu/Research/vmd

2. Click on "Download VMD" on the left side of the screen.

3. Choose the version you wish to download

    Windows users should select:
    Windows OpenGL (Microsoft Windows XP/Vista/7 (32-bit) using OpenGL)

    Mac users should select:
    MacOS X OpenGL (Intel x86) (Apple MacOS-X (10.4.7 or later) with hardware OpenGL (native bundle))

    Users of older Macs[1] may have to select:
    MacOS X OpenGL (PowerPC) (Apple MacOS-X (10.4.7 or later) with hardware OpenGL (native bundle))

4. Register a username and password

5. Download the file

6. Windows users: To install, run the file that was download and follow the installation instructions

7. To run VMD:

    Windows users: Click on VMD from the Start Menu
    (located in **Programs→University of Illinois→VMD** by default)

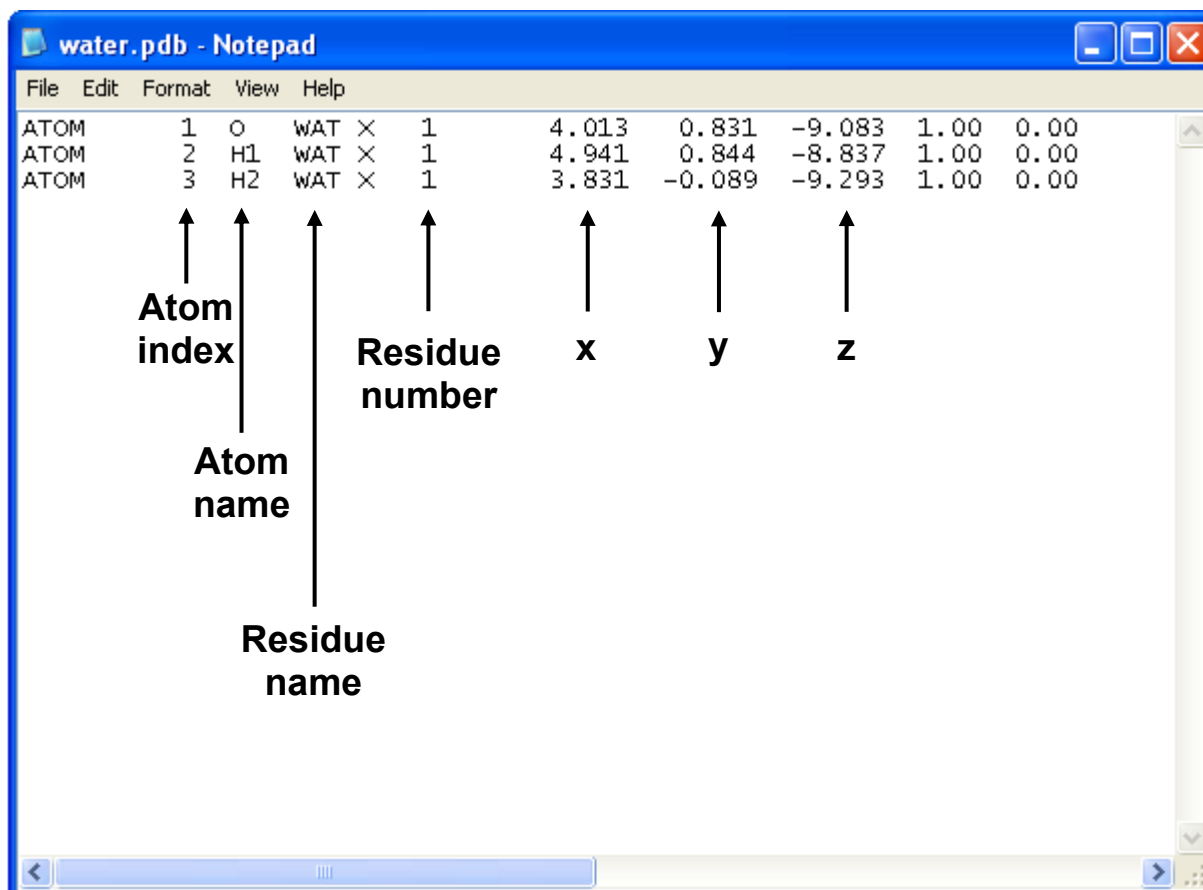   Mac users: Run the .dmg file

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[1] To determine what type of processor is in your Mac, go to the **Finder** and choose **About this Mac** from the **Apple Menu**

VMD Input – PDB Files

VMD accepts many types of input files. However, among the most common types are **PDB** (Protein Data Bank) files which have the .pdb file extension. You can find PDB files on the web for many molecules ranging from small organic molecules to large biomolecules like proteins and DNA. Normally, you can simply load these files into VMD without viewing or editing their content. However, to use VMD effectively, it is important to know some of the basics about these files.

PDB files contain a list of atoms along with their three-dimensional coordinates. Each atom has an **index** and a **name**. Collections of atoms are grouped into **residues**. Each residue has its own number.

Below is a sample PDB file of a single water molecule. There are three atoms: an oxygen named **O**, a hydrogen named **H1** and another hydrogen named **H2**. These three atoms are grouped into a residue named **WAT**.

```
water.pdb - Notepad
File   Edit   Format   View   Help
ATOM       1   O    WAT  X    1        4.013     0.831    -9.083    1.00    0.00
ATOM       2   H1   WAT  X    1        4.941     0.844    -8.837    1.00    0.00
ATOM       3   H2   WAT  X    1        3.831    -0.089    -9.293    1.00    0.00
```

Atom index

Atom name

Residue number

Residue name

x   **y**   **z**

A sample PDB file for hemoglobin, a more complicated molecule, is shown below. The molecule is divided up into many residues with each residue representing a single amino acid. Orange and blue boxes are drawn around the first two residues – a valine (VAL) and leucine (LEU) amino acid, respectively.

Many biological molecular structures are composed of several subunits that are held together by noncovalent (hydrogen bonds, van der Waals forces, etc.) interactions (e.g. double-stranded DNA). Within a PDB file, these subunits are collections of residues grouped into a **chain** designated by a single letter code in the fifth column.
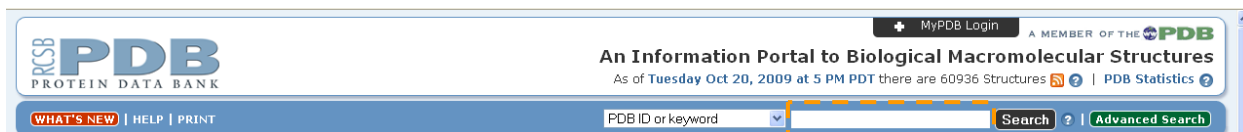
Finding PDB Files

PDB files for many molecules can be found on the web by simply typing "<molecule> pdb" into a search engine. Here, <molecule> is the name of whatever molecule you are interested in. This is usually the best place to start. You can also visit sites such as:

- **Bob Johnson's VMD Resource Page** (www.sas.upenn.edu/~robertjo/pdb)
- **Klotho** (http://www.biocheminfo.org/klotho)
- **Protein Data Bank** (http://www.pdb.org)
- **Nucleic Acids Data Bank** (http://ndbserver.rutgers.edu)

Using the Protein Data Bank

The Protein Data Bank contains PDB files for thousands of proteins whose structure has been resolved experimentally and is an indispensible resource in modern biological research.

Go to www.pdb.org. Type the name of the protein of interest in the search box and click **Search**.

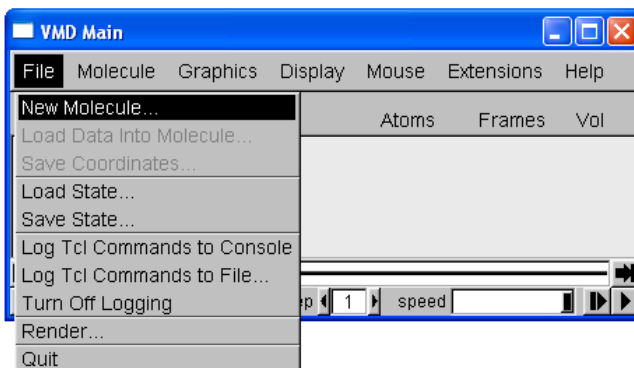As an example, here are the first few search results for "myoglobin".

Usually, there are multiple entries for the protein of interest. The entries may differ in the experimental methods or conditions used to resolve the protein's structure. You may have to browse through several entries before you find the right protein. However, for educational purposes, oftentimes the differences are negligible.

Clicking on the title of the entry will transfer you to a page that contains further information about the protein and links to download the PDB file. For example, below is the entry for "CRYSTAL STRUCTURE OF RECOMBINANT SPERM WHALE MYOGLOBIN UNDER 1ATM OF XENON". To download the PDB file, click **Download Files** in the upper right hand corner.

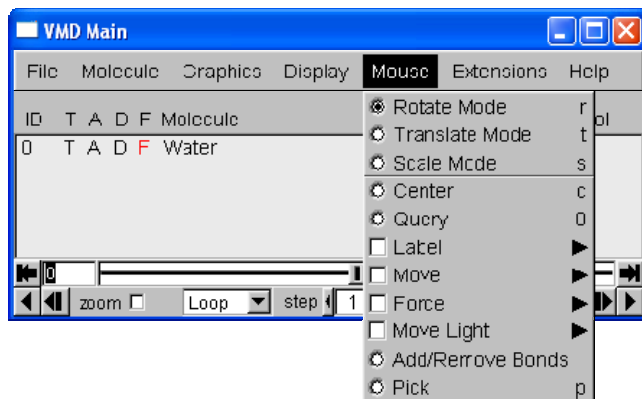Click on **PDB File (Text)** to download the PDB file.

Loading a PDB File

Run VMD. This will cause three windows to appear on the screen. PDB 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**.
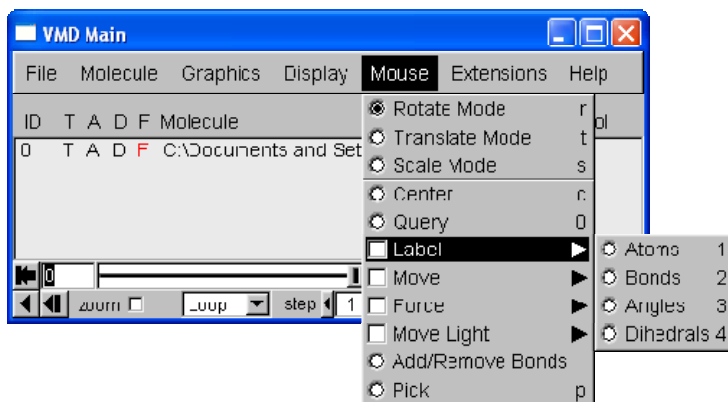

Interaction Modes

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**.

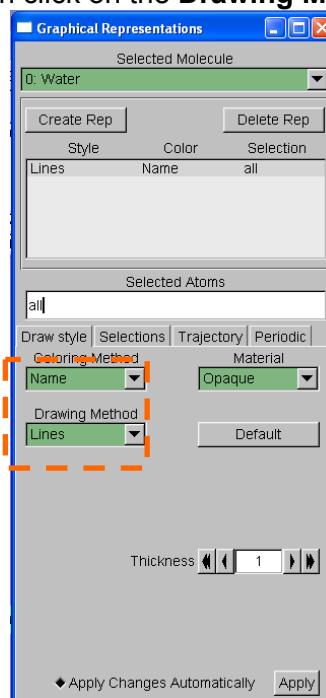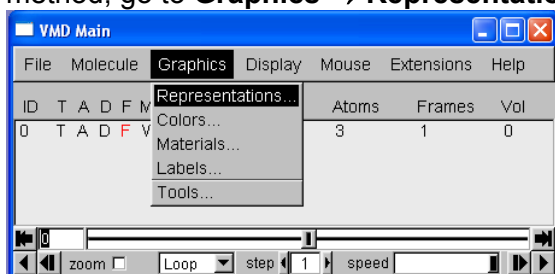| Mode	Shortcut Key	Description
Rotate	r	Rotates the molecule
Translate	t	Translates the molecule
Scale	s	Scales the molecule (zoom)
Center	c	Centers on an atom

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

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

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)

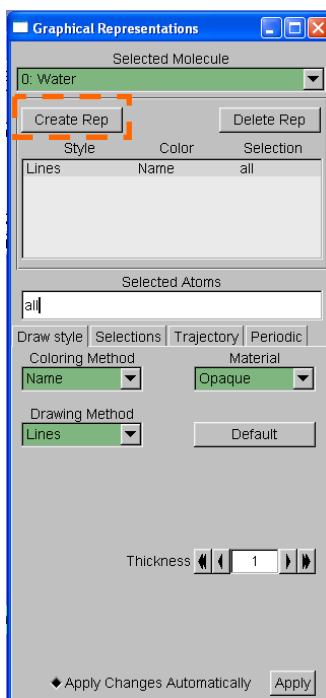| Hydrogen	White
Carbon	Cyan
Oxygen	Red
Nitrogen	Blue
Phosphorus	Brown
Sulfur	Yellow

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

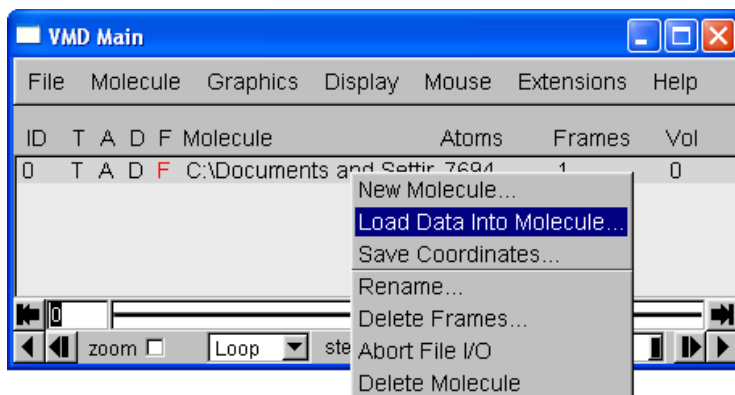| Atom Selection	Description
all	Show all atoms
protein	Show only protein atoms
backbone	Displays backbone atoms
noh	Do not display hydrogen atoms
resname X	Displays atoms of residue X
name X	Display atoms named X
resid X	Display residue number X

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.
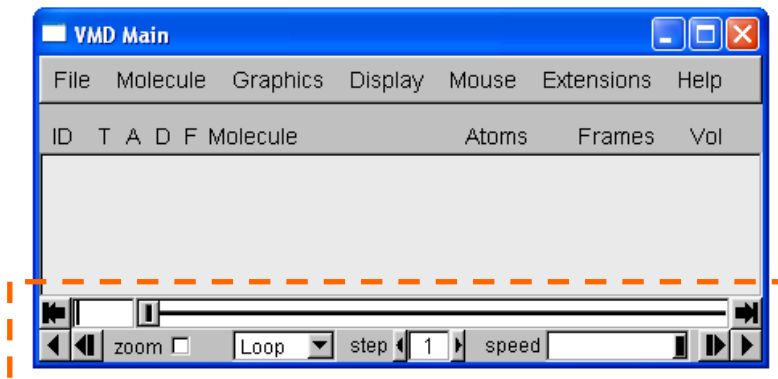

Loading and Playing a Trajectory

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 Main** window and select **Load Data Into Molecule**. Then browse and select the desired trajectory.
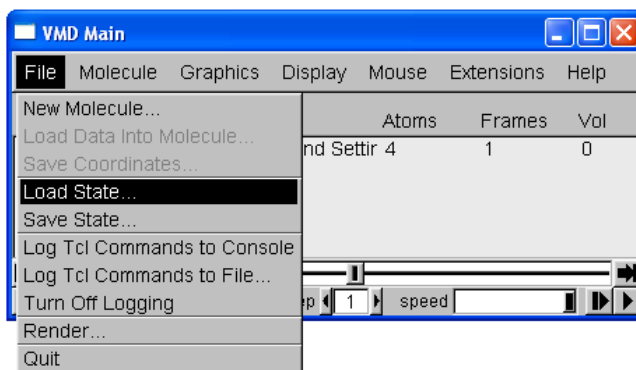
The trajectory can be played using the arrow buttons at the bottom of the **VMD Main** window. The speed can be adjusted with the slider in the bottom right hand corner.

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 State**.
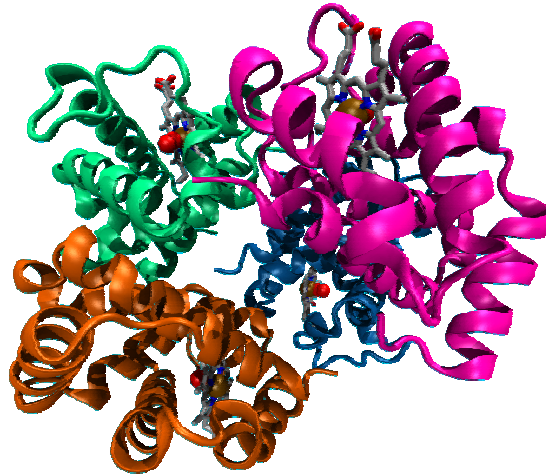

Saving an Image

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**
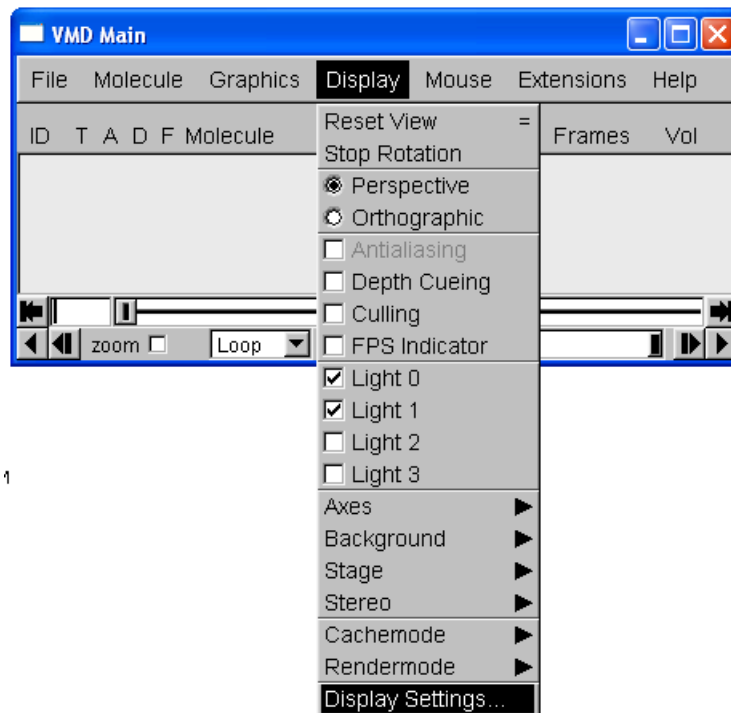
Using the default renderer takes a screen shot of the VMD OpenGL window and saves it as an image.

Saving an Image with Lighting and Shadow Effects

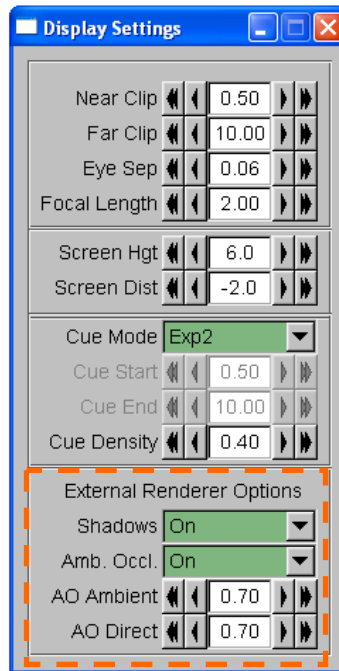You can also save images that include lighting and shadow effects (see figure below of hemoglobin).

First, specify the strength of the lighting by going to **Display → Display Settings**

Turn **Shadows** and **Ambient Occlusion** on. Adjust **AO Direct** and **AO Direct** to your desired value (values of 0.70 for both 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.