CPLC Summer School 2009
VMD Mini Tutorial

VMD Developer:
John Stone

This tutorial is an abbreviated version of the TCBG VMD tutorial:
http://www.ks.uiuc.edu/Training/Tutorials/
Tutorial files were taken from the Titin Case Study by Mu Gao and Eric Lee:
http://www.ks.uiuc.edu/Training/CaseStudies/pdfs/titin.pdf
Tutorial prepared by Jen Hsin.
Contents

1 Basic Figure Rendering in VMD ........................................... 3
   1.1 Setting the display background ........................................ 3
   1.2 Creating representations ........................................... 3
   1.3 Rendering .............................................................. 6

2 Basic Movie Making in VMD ............................................. 7
   2.1 Single-frame movies ................................................. 7
   2.2 Trajectory movies .................................................... 8

Introduction

VMD (Visual Molecular Dynamics) is a molecular visualization and analysis program designed for biological systems such as proteins, nucleic acids, lipid bilayer assemblies, etc. It is developed by the Theoretical and Computational Biophysics Group at the University of Illinois at Urbana-Champaign. Among molecular graphics programs, VMD is unique in its ability to efficiently operate on multi-gigabyte molecular dynamics trajectories, its interoperability with a large number of molecular dynamics simulation packages, and its integration of structure and sequence information.

Figure 1: Example VMD renderings.

In this mini tutorial (the tutorial should take ~20 minutes), you will play with two major capabilities of VMD: publication-quality figure rendering, and movie making. You will need two files, which should have been prepared for you: I27-wat.psf and I27-pulling.dcd. Your TA should have given you a quick 10-minute VMD course on manipulation of molecules and loading of trajectory data.
1 Basic Figure Rendering in VMD

In this section you will learn how to render images with VMD. We will use the protein I27 as an example molecule. I27 is a part of the large muscle protein, titin, responsible for muscle extension and contraction.

1.1 Setting the display background

Before you render a figure, you want to make sure you set up the OpenGL Display background the way you want. Nearly all aspects of the OpenGL Display are user-adjustable, including background color.

1 In the VMD Main window, choose Graphics → Colors. The Color Controls window should show up. Look through the Categories list and select Display. In Names, select Background. Finally, choose white in Colors. Your OpenGL Display now should have a white background.

2 When making a figure, we often don’t want to include the axes. To turn off the axes, select Display → Axes → Off in the VMD Main window.

1.2 Creating representations

Depending on what molecular aspects one would like to display, molecular representations are created accordingly to render an informative figure. Here, as an example, we will create representations that showcase the shape of the waterbox and the secondary structure of the protein.

1 Both I27-wat.psf and I27-pulling.dcd should be loaded.

2 Make sure frame 0 is the one displayed. To do so, drag the slider at the bottom of the VMD Main window all the way to the left. Your VMD Main window should look like Figure 2.

3 Open the Graphical Representations window (Graphics → Representations...), and delete or hide any representation you might have created previously. Create the following two representations:

MSMS and Surf drawing styles. In Table 1, water box will be rendered in the MSMS representation, which requires an external software that is not installed on the Mac machines. If you are using a Mac machine, instead of the MSMS drawing style, use Surf instead. Both drawing styles portrays the volumetric shape of the water box, but the latter does not require an external software.
1 BASIC FIGURE RENDERING IN VMD

4 The transparent waterbox is looking very unclear at the moment. In the VMD Main window, choose Display → Rendermode → GLSL. This mode uses your 3D graphics card to render the scene with real-time ray-tracing of spheres and alpha-blended transparency. You should see that the rendering quality of the water box is a lot better now.

5 To view the protein better, the transparency of the water box can be increased. Go to Graphics → Materials..., and highlight Transparent. Slide the scroll bar next to Opacity to change the opacity to 0.15.

6 By default VMD draws molecules in the “Perspective” mode that provides strong size-based visual depth cues. For this reason the perspective mode does not preserve scale relationships or parallelism of lines, and molecules can appear distorted. In the VMD Main window, click on the Display menu, and switch from Perspective to Orthographic mode, and see if you can detect the difference (Figure 3).

7 Your OpenGL Display window should now look like Figure 4.
Playing with molecular representations. As seen in Table 1, a molecular representation has various parameters defining its coloring method, drawing style, and material. Each of these parameters has a long list of options, and each of these options can be further adjusted by the user (we saw, as an example, that the material "Transparent" can be adjusted). VMD users are encouraged to play around with these abundant options to find their favorite molecular representations.

Figure 3: Difference between Perspective and Orthographic modes (shown here is the same view of the same molecule; water is not shown for clarity).

Figure 4: An example VMD rendering of a protein immersed in a waterbox.
1.3 Rendering

Now we will try out some renderers equipped in VMD.

1 Choose File → Render... in the VMD Main window. The File Render Controls window will appear on your screen.

2 In the File Render Controls window, you can choose which renderer you want to use in the scroll-down menu, as well as the file name of your image. Select snapshot for now (which is the default option), type in a filename of your choice, and click Start Rendering button on the bottom of the window.

3 An image-processing application should open automatically with the resulting image file. Close this window when you are done viewing the image to continue using VMD.

4 Try to render again using different rendering method, particularly TachyonInternal and POv3 (see the note below before trying to render image with POV3). Compare the quality of the images created by different renderers.

POV3 renderer. Some features in VMD uses external applications, and such is the case for POV3 renderer. If you are using a Mac, POV3 will not work since the appropriate supporting software is not installed. If you are using a Linux machine, you can try POV3, but it will take a few minutes. Shorten the rendering time by making the OpenGL Display window much smaller.
2 Basic Movie Making in VMD

Here basic movie making with VMD is introduced. You will make two different types of movies: single-frame movies and trajectory movies.

Software requirements. If you cannot successfully make movies with VMD, it’s possible that you’re missing some softwares required for generating movies. All the required softwares are freely available, and to find what software you need, please see the VMD Movie Plugin page at http://www.ks.uiuc.edu/Research/vmd/plugins/vmdmovie/.

Users of the Mac machines will not be able to render movies for now, and they are encouraged to join the Linux users for this section. Two movies generated by following the steps below have also been provided as an example (single-frame.mpg and trajectory.mpg).

1. Hide or delete the representation for water drawn in MSMS (or Surf) style.

2.1 Single-frame movies

1. Movie making is quite simple in VMD using the Movie Maker plugin. In the VMD Main window, go to menu item Extensions → Visualization → Movie Maker. The VMD Movie Generator window will appear (Figure 5).

![Figure 5: The VMD Movie Generator window.](image)
2 Click on the Movie Settings menu in the VMD Movie Generator window, and select Rotation about Y axis. In this mode, the “camera” looking at the molecule will rotate by a given degree (180° by default), providing a 3D perception of the protein.

3 You may want to change the path of the output movie file by clicking on the Set working directory: button and entering a preferred path. After that, change Rotation angle: to 360°, and change Movie duration (seconds): to 5. Make sure no other window is overlapping the OpenGL Display window, and click Make Movie.

4 Once rendering is finished, open and view the movie with a compatible application (for example, mplayer on a Linux machine). The movie should be 5 seconds long, showing a full rotation of the protein.

5 Click on the Format menu in the VMD Movie Generator window. You can select which software to use for making movie, which will change the output file type of the movie. For example, the Animated GIF option makes .gif movies that are easy to display within a web browser.

2.2 Trajectory movies

1 Now we will make a movie of the trajectory, which is in our case a simulated unraveling of the protein. Play the trajectory by using the animation control panel on the bottom of the VMD Main window (Figure 2). Adjust the size of the OpenGL Display window so that the protein fits in the window at all frames of the trajectory.

2 In the VMD Movie Generator window, select Movie Settings → Trajectory, give this movie a different name, and click Make Movie. Note that the length of the movie is automatically set 24 frames per second. For a trajectory, duration of the movie can be decreased, but cannot be increased.

3 Play the movie you just made. You can see that the protein is being pulled apart with so much fluctuation that it is difficult to observe the motion of the protein. Motion of the molecule can be smoothed by setting a trajectory smoothing window.

4 In the Graphical Representations window, select the representation of the protein, and click on the Trajectory tab. At the bottom, the Trajectory Smoothing Window Size option was set to zero (Figure 6). Increase this setting to 10, and make a trajectory movie again with a different name.
Play again the new movie with trajectory smoothing. You should see that the rupture of the protein is more visible now with less fluctuations.

This is the end of the mini VMD tutorial. If you have some spare time, feel free to try out other options in the VMD menu tabs. When you are done, quit VMD.
Final Remarks

In this mini tutorial we are only able to take a quick glimpse of VMD’s figure and movie making capabilities. There are many other more detailed tutorials available, either on a specific VMD tool or on a scientific topic. You can find many useful documentations, including the comprehensive VMD User’s Guide, in the VMD homepage [http://www.ks.uiuc.edu/Research/vmd/](http://www.ks.uiuc.edu/Research/vmd/). If you have any question on using VMD, we encourage you to subscribe to the VMD mailing list [http://www.ks.uiuc.edu/Research/vmd/mailing_list/](http://www.ks.uiuc.edu/Research/vmd/mailing_list/)

Citing VMD

The development of VMD is funded by the National Institute of Health. Proper citation is a primary way in which we demonstrate the value of our software to the scientific community, and is essential to continued NIH funding for VMD. All published work which utilizes VMD should include the primary VMD citation at a minimum: