

## VMD - *continued*: Making Movies

(This section can be used immediately after Desktop Molecular Graphics)

VMD (<http://www.ks.uiuc.edu/Research/vmd/>) is a free program developed at the Theoretical and Computational Biophysics Group at the University of Illinois at Urbana-Champaign for the visualization and animation of biological (macro) molecules. See also <http://www.scripps.edu/rc/training/unixslides/vmd.pdf>

### LABORATORY EXERCISES

#### 1 -VMD-Exercise H: Starting VMD and opening a molecule



#### OPTIONAL

This exercise summarizes the methods seen in the Desktop Molecular Graphics section.

- **Double click on the VMD icon** or select it within the task-bar.
- On the “**VMD Main**” window menu select “**File > New Molecule...**” this will open the “Molecule file browser.”
  - Click the “**Browse**” button to select a PDB file in your folder within yet another window. – For example use “hrv2-3C-1CQQ.pdb” - Click “**Open**”
  - Click “**Load**”
- The selected PDB file is now loaded within VMD
- VMD Main: **Graphics > Representations**
- Click on the “**Create Rep**” button
  - a. Create Rep (button)
  - b. Within the “Selected Atoms” **Edit one representation to “protein”**
  - c. **Edit the other to “not protein”**
- **Resize** the VMD OpenGL display to the size you want your movie. Don’t make it too large and don’t make it too small either.
- Using the mouse **highlight the “Rep” selection of the “not protein”**
  - **Coloring Method: Name**
  - **Drawing Method: Licorice**
- Using the mouse **highlight the “Rep” selection of the “protein”**
  - **Coloring Method: Pos**
  - **Drawing Method: Surf**
- **Orient** your image, this will be the start position for the movie.
- **Change the background** to white if you wish:
  - VMD Main: Colors > Display > background > white
- VMD Main: **Display > Orthographic**
- VMD Main: **Display > Depth Cue**



## 2 VMD-Exercise I: Making movies with VMD

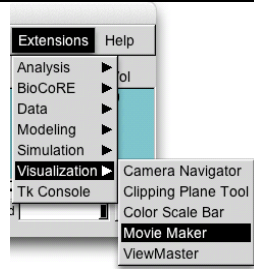
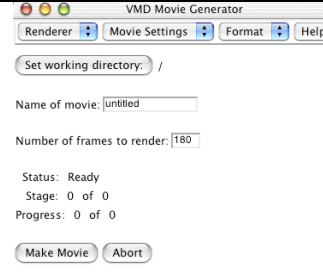
**INFO - Prerequisites:** making movies with VMD requires that other software packages be installed. The DMC classroom is already set-up for using the VMD movie-making scripts. The Unix/MacOSX solution is free while the windows version requires the installation of the VideoMach shareware package. Some installing information is given at the end of this tutorial.

As of this writing the relevant information is located on the VMD web site at <http://www.ks.uiuc.edu/Research/vmd/plugins/vmdmovie/>

However: even if the required software for making movies is not installed on your computer, VMD will nevertheless make all the individual frames that can later be assembled into a movie, for example with Apple's QuickTime™ Pro (Macintosh and Windows) or a shareware such as Animagic (Windows) or freeware GIMP (Unix, Mac OS X) to make animated GIF.

**TASK**

- within the “VMD Main” window select the **“Extensions > Visualizations > Movie Maker”** menu. This will open the “VMD Movie Generator” interactive window.

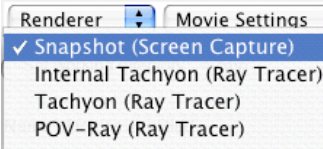
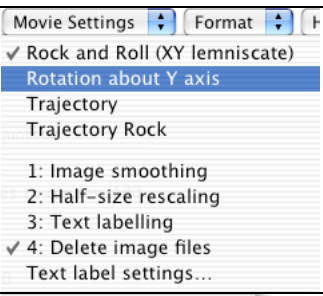
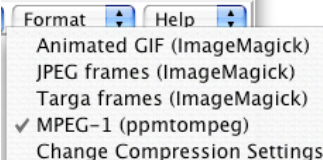



- Verify** the settings in the 3 pull-down menus within “VMD Movie Generator”
  - Render:** Should set on **“Snapshot”**

*Note:* if this option creates strange images (most possible under Windows) change to “Internal Tachyon” which is slower but would work.
  - Movie Settings:** To make a rotation of the molecule **change the “Rock and Roll” setting to “Rotation about Y axis.”**

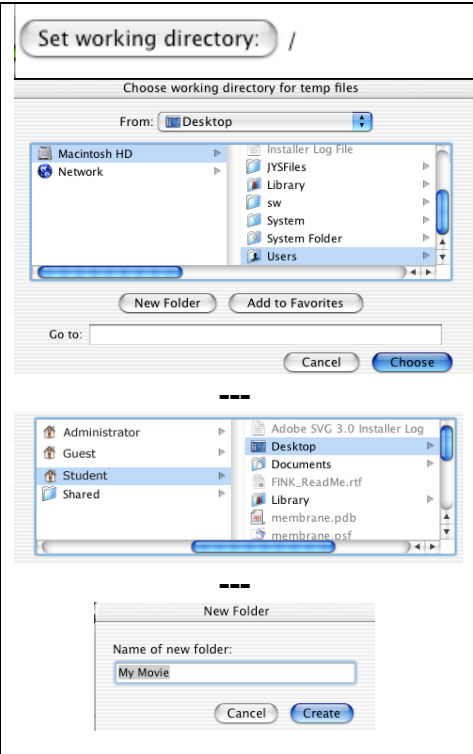
*Note:* if you want to *keep the frames*, then **uncheck the “4: Delete image files”** as illustrated.
  - Keep** the preselected “MPEG-1” selection
 

*Note:* if you want to place your movie on a web site select “Animated GIF” but note the animated GIF files are larger than MPEG-1 files.

- **Set working directory:** the default working directory is “/” (also called “root”) which would be the main hard drive on Mac OS X often named “Macintosh HD” this is where movies and frames are saved.
  - If you want to change the working directory somewhere on the “Desktop” click on the button “Set working directory”
  - Click “Users”
  - Click “BNMC”
  - Click “Desktop”
  - Click “New Folder”
  - Name your folder “My Movie”
  - Click “Create”
  - Your working folder is now set on the desktop

**Note:** On Windows systems the desktop is available within the C:\Windows directory



- **Name your movie “movie-1”** or choose a name you like.
- **Set the number of frames to 36** if you are making a “Rock and Roll” movie, otherwise set this number to **360** if you selected earlier “Rotation about Y axis” (the default is 180).

Name of movie:

Number of frames to render:

- **Make your movie: Press the “Make movie”** button.

*You can watch the progress of the movie making on the “VMD Display” as well as on the “VMD Movie Generator” window by looking at the “Status,” “Stage,” and “Progress” information provided.*

**Note:** The 360 Y-rotation takes a few minutes since there are more frames. If you made a mistake you can click “Abort” and reset your parameters. The temporary files will be discarded automatically.

Number of frames to render:

Status: Rendering

Stage: 2 of 8

Progress: 25 of 360



### 3 -VMD-Exercise J: Finding and viewing your movies

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a. Finding your movies:

The movies are created within the “working directory” which you have set earlier. If you have not set the working directory your movie will be in the default working directory of “/” which is the main hard drive on a Mac OS X computer. If you still don’t know or cannot find your movie use the menu “File > Find...” (Macintosh) or “Start > Find Programs and Files...” (Windows) and search for the movie name you have given, e.g. “My Movie.”

b. Playing your movies:

The movies will have either a .gif or .mpg attached to the name you had given. However depending on the settings of the computer you are using these filename extensions may not be visible. These filename extensions are a way for your computer to know the format of these animations and will warn you if you try to delete them.

Playing MPEG-1 files: your default multimedia player should automatically play the MPEG-1 files. Your default player is likely to be “QuickTime™” on an Apple computer and “Windows Media Player” on a Windows system.

Playing animated GIF files: animated GIF files may play within your default media player just like the MPEG-1 files, but you may have to use the “File > Open...” menu sequence to open it. Animated GIF files play well within web browsers (Netscape, Internet Explorer, Safari, Mozilla etc.).

c. Using your movies:

MPEG-1 files can be used for presentation or inserted within a PowerPoint presentation to illustrate your molecule. MPEG-1 images can also be made a part of a web page, however the viewer will need the appropriate plug-in (to see the movie within the browser) or appropriate media player (the movie will be downloaded and played).

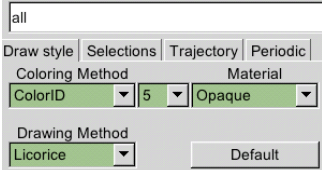
Animated GIF files can be used as an image on the web. Inserted as a regular GIF image file it will still be an animation. The advantage is that this does not require any plug-in for the viewers to see your animation as it is the case for QuickTime, MPEG or FLASH animations.



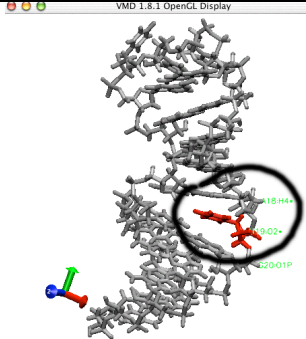
## 4 -VMD-Exercise K: Movies from NMR multiple PDB files

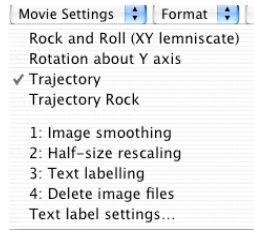
Usually NMR structures are published as both a series of 10 to 20 possible models, as well as an “average” model. The average structure contains a single set of PDB coordinates, while the other file contains a series of PDB structures within the same file. Each structure starts with the PDB record “**MODEL #**” (where # is a number) and ends with “**ENDMDL**” record line. Some software can sometimes only see the first model in a multiple file, others can be used to animate them. Here we will animate a file containing 20 models with VMD.

### ✓ TASK

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| <ol style="list-style-type: none"> <li>1) open VMD and load PDB file <b>1NYZ.pdb</b> <ol style="list-style-type: none"> <li>a. VMD Main: <b>File &gt; New Molecule</b></li> <li>b. <b>Browse...</b> (find 1NYZ.pdb in window)</li> <li>c. <b>Open</b></li> <li>d. <b>Load</b></li> </ol> </li> </ol> | <p><u>Note</u>: as the molecule opens you can notice it “wiggle” as the 20 models are loaded.</p>   |
| <ol style="list-style-type: none"> <li>2) VMD Main: <b>Display &gt; Orthographic</b></li> </ol>  |   |
| <ol style="list-style-type: none"> <li>3) VMD Main: <b>Graphics &gt; Representations</b> <ol style="list-style-type: none"> <li>a. Coloring Method: <b>ColorID 5</b></li> <li>b. Drawing Method: <b>Licorice</b></li> </ol> </li> </ol>  |    |
| <ol style="list-style-type: none"> <li>c. <b>Create Rep</b> button</li> <li>d. <b>Edit</b> new rep to “<b>resid 19</b>”</li> <li>e. Coloring Method: <b>ColorID 3</b></li> <li>f. Drawing Method: <b>Licorice</b></li> </ol>   | <p>This command selects residue <b>19</b> (a U) to be represented differently than the rest of the molecule, here ColorID 3 is orange. You can select an other color scheme, e.g. <b>6</b> (gray) for the RNA and <b>1</b> (red) for U19. You can also make the background white if you wish.</p> |

**Note: “resid” keyword is different than “residue” keyword. First residue is internally renamed residue 0 (zero) by VMD. Therefore to select residue 19 we would have to select “residue 18” ... or simply “resid 19”**

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| <p>4) Scale the image within the window and orient it so that residue 19 is on your right, showing its stacking position, in a side-way view.</p> |  |
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| <p>5) VMD Main: <b>Extensions &gt; vmdmovie</b></p> <p>6) Set parameters within VMD Movie Generator top menus:</p> <ol style="list-style-type: none"> <li>Render: Snapshot (screen capture)</li> <li>Movie Settings:             <ol style="list-style-type: none"> <li><b>Trajectory</b></li> <li><b>Uncheck 4:</b> Delete image files</li> </ol> </li> <li>Format: MPEG-1</li> </ol> <p>7) Set parameters within the rest of the window:</p> <ol style="list-style-type: none"> <li>Set working directory: <b>create a folder</b> on the desktop and name it e.g. <b>NMR</b></li> <li>Name of movie: <b>u19</b> (.mpg will be appended automatically)</li> <li>Number of frames to render: 20 (default, because there are 20 models)</li> </ol> |  |
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8) **Click Make Movie** button

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| <p>9) The movie will be saved within the working directory (NMR), you can double click on it, it should automatically open within QuickTime Player in the BNMC classroom.</p> <p>10) You can engage the menu “Movie &gt; Loop” to have it loop continuously.</p> | <p><u>Note:</u> the movie speed is about 30 frames per second.</p> |
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11) If you inspect the NMR directory, you will see two series of image frames: the original \*.rgb or tga frames and those converted to \*.ppm by ImageMagick in the background.

Note: PDB entry 1NYZ has now been replaced by 1SY4



✓ **INFO - Supplemental Information:** Installing software pre-requisites for movie making with VMD 1.8.x on Mac OS X. You will need to have administrator privilege (password) to accomplish this.

- 1) X11 is automatically present on newer OS X versions (starting with 10.5)
- 2) Download "Fink" from <http://fink.sourceforge.net/download/> :  
Download Fink Binary Installer for current version for later OS.  
Help is available at <http://homepage.mac.com/sao1/fink/#top8>

*Although there is a graphical interface ("Fink Commander"), for sake of simplicity the following will describes the line command method of installation of binaries:*

- 3) Launch a "Terminal" (located in Macintosh HD : Applications : Utilities : Terminal)
- 4) Within the terminal type the following commands a the % or \$ prompt:
  - a. % fink selfupdate-cvs
  - b. % fink install system-xfree86
  - c. % fink list
  - d. % sudo apt-get install imagemagick-nox
  - e. % sudo apt-get install netpbm
  - f. % rehash

*This should install all the necessary binary files for making movies from VMD. Note that you will be asked a password for administrative privilege, and that more binaries dependences may be installed at the same time.*

*Note for Windows users from the VMD script home page  
<http://www.ks.uiuc.edu/Research/vmd/plugins/vmdmovie/>*

*On Windows, the program VideoMach is currently required for all movie generation tasks. It is a shareware program and is available for trial download from the VideoMach web site. Registration costs \$19 for non-commercial use, and \$49 for commercial use."*

*Note: the Videomatch web site is at  
<http://www.gromada.com/videomach.html>*

**- End of VMD Movie -**

