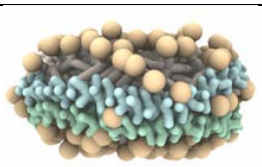
Illustrations using Visual Molecular Dynamics (VMD)

Michael Dolan 11/03/09



Exercise 1: Creating Representations and Rendering

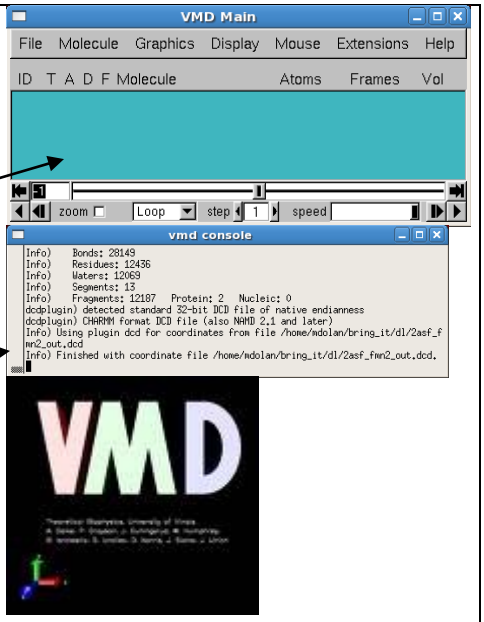
Opening VMD

1. Click on the VMD icon. This will open three windows:

VMD Main
Interfaces and extensions are available from the menu interface.

vmd console
Text commands are typed in the console window.
Also shows results of an executed GUI command.

VMD 1.8.6 OpenGL Display
Molecules are displayed and manipulated in this graphics window



Loading a molecule

2. In the Main window, click:

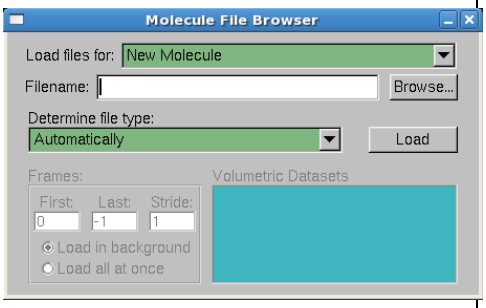
   File >> New Molecule

   The Molecule File Browser window opens.

3. Click Browse. The 'Choose a molecule file' window opens.

4. Navigate to /Desktop/vmd_illustration and double-click 1snc.pdb. In the Molecule File Browser window, click Load.

   A crystal structure of a *Staphylococcal* nuclease will appear in the Display window.



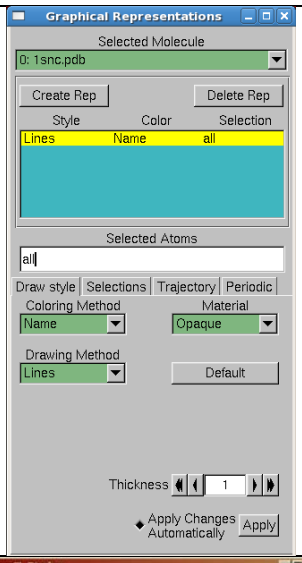
Creating a representation

Note: 1snc.pdb contains a ligand, waters and a calcium atom.

5. In the VMD Main window, click Graphics >> Representations. The Graphical Representations window opens.

6. In the Selected Atoms field, change 'all' to 'protein' and hit return. Only the protein atoms are displayed.

7. Change the Coloring Method to ColorID. Choose a color in the adjacent pulldown menu that appears.

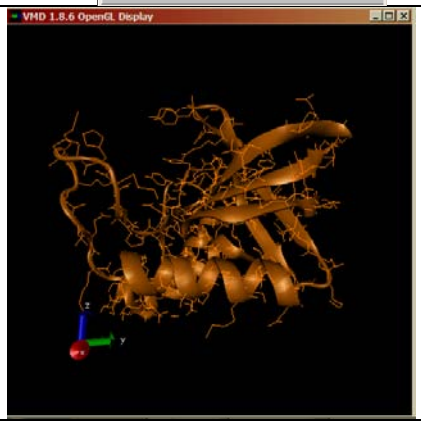


8. In the Graphical Representations window, click the 'Create Rep' button. A second representation line of text is added.

9. With the second line of text highlighted, change the Drawing method to New Cartoon. A ribbon is drawn through the protein.

10. Experiment by changing the 'Thickness' and 'Resolution' settings.

11. From the Material menu, select 'Glossy.'



Multiple representations

12. Our goal is to display the ligand, but we do not know its name. In the Graphical Representations dialog, click the Create Rep button. A third representation line of text is added.

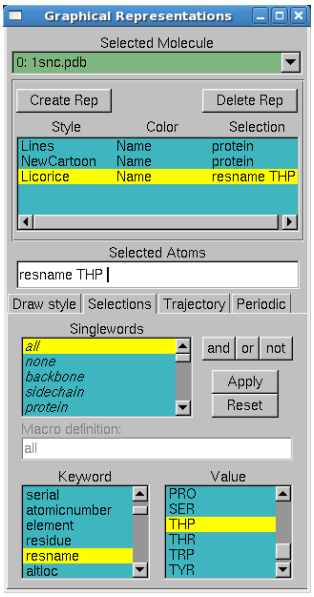
13. Change the Drawing Method to Licorice.

14. Delete 'protein' from the Selected Atoms field.

15. Click on the Selections tab. In the Keyword section, double-click on 'resname'. The 'resname' keyword appears in the Selected Atoms field. A list of residue names appear in the Value section. Double-click 'THP' in the Value section. The 'THP' string appears in the Selected Atoms field. Hit return.

    The ligand appears rendered as licorice.

16. Under the Draw Style tab, change the Coloring Method to 'Name.' This colors the ligand atoms based on type.



17. Click the Create Rep button. In the Selected Atoms text field, replace the 'resname THP' text with 'resname CA' and hit return. This displays the calcium atom.

18. Change the Drawing Method to VDW.

19. Click the Create Rep button.

20. In the Selected Atoms text field, replace the 'resname CA' text with 'resid 41' and hit return.

21. Change the Drawing Method to Licorice.

    Note: A convenient way to locate and highlight residues is by using the Sequence Viewer. Go to: Extensions >> Analysis >> Sequence Viewer

Changing default colors

22. Choose Display >> Background >> Gradient

    The background is changed to a gradient of color.

23. Choose Graphics >> Colors

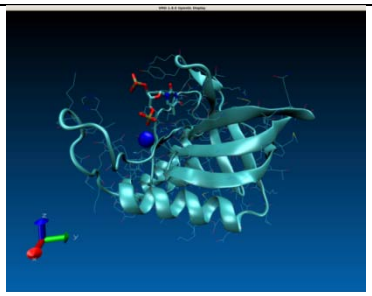
    The Color Controls window opens.

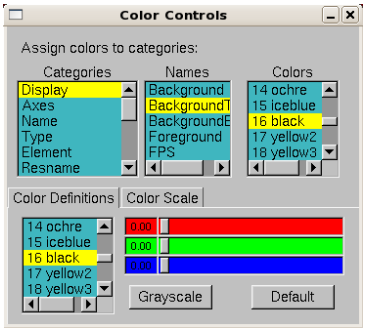
24. Click 'Display' in the Categories section.
    Click 'BackgroundTop' in the Names section.
    Choose a color in the Colors section.

    The background top color updates in the Display window.

25. Repeat above for 'BackgroundBot' in the Names section.

    Note: Do not delete this protein. We'll need it for the next exercise.





Exercise 2: Making images, saving, formats

Note: To undisplay the axes, go to: Display >> Axes >> Off

1. In the VMD Main window, select:

   File >> Render

   The File Render Controls window opens.

2. From the 'Render using' pulldown menu, select 'TachyonInternal'

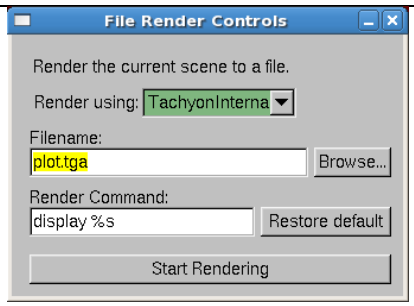
3. Click Start Rendering

   A Preview window (specific to Mac OS) is opened displaying the rendered image.

4. In the Preview window, choose File >> Save As

5. Enter a name for the plot, select the Desktop as the location to save, and change the format to PNG. Click Save.

   The file is saved to the Desktop with a .png extension.



Exercise 3: Creating surfaces and mapping properties

Notes: This exercise will show one to how to add a solvent accessible surface to a molecule and "map" electrostatic calculation results to the surface. Electrostatic properties have already been calculated using the APBS (Adaptive Poisson-Boltzmann Solver) program. VMD provides support for both the execution of APBS and the visualization of the resulting electrostatic potentials.

(This exercise adapted from http://cholla.wustl.edu/baker/classes/nbcr/tutorial1/#introduction-sect)

Loading the .pqr file

Note: The .pqr file is simply a .pdb formatted file with charge and atomic radii added to the occupancy and b-factor columns. This is one format that can be read by the APBS program. A webservice is available to create a .pqr file: http://pdb2pqr-1.wustl.edu/pdb2pqr/

1. Clear the VMD Main window by right clicking on the 1snc.pdb entry and choosing Delete Molecule.

2. Read the 1myk.pqr file into VMD:

   File >> New Molecule; Browse; Load

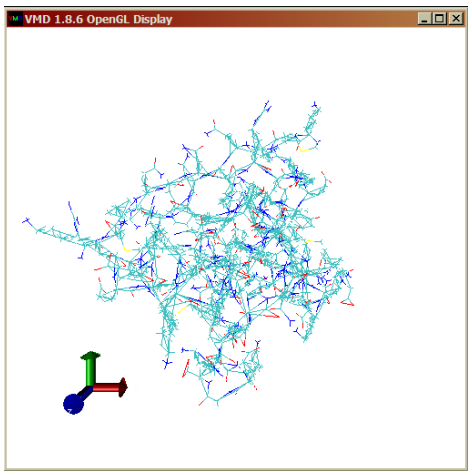
Loading the .dx file

Note: A .dx file is generated by APBS and contains volumetric data from which isocontours may be generated.

3. In the VMD Main window, select and right click the 1myk.pqr entry.

4. Select 'Load Data Into Molecule…'

5. Browse to the pot.dx file. Click Load.



Electrostatics visualization - isocontour

1. In the VMD Main window, choose:

   Graphics >> Representations

2. In the Graphics Representations window, click 'Create Rep' and change Drawing Method to 'Isosurface.'

3. Change Draw from 'Points' to 'Solid Surface' and Material to 'Transparent'

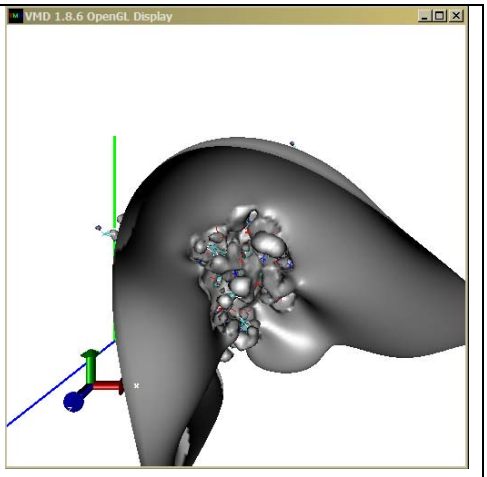
4. The current isovalue is '0.' Change this value to 1.

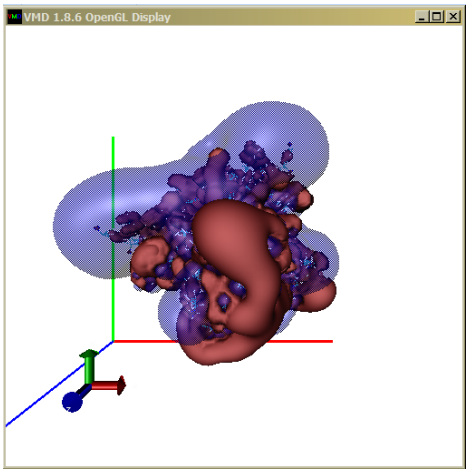
5. For the Coloring Method, choose 'ColorID' and set to 0. This will color the positive isocontour blue.

6. Click Create Rep. Change the isovalue value to -1 and the ColorID to 1. This will color the negative isocontour red. Change the Material to 'BrushedMetal.'

7. Follow Exercise 2 to create and view the transparent surface.

   Note: To render on the fly, go to the VMD Main window and choose: Display >> Rendermode >> GLSL





Electrostatics visualization – Mapping the potential at the surface

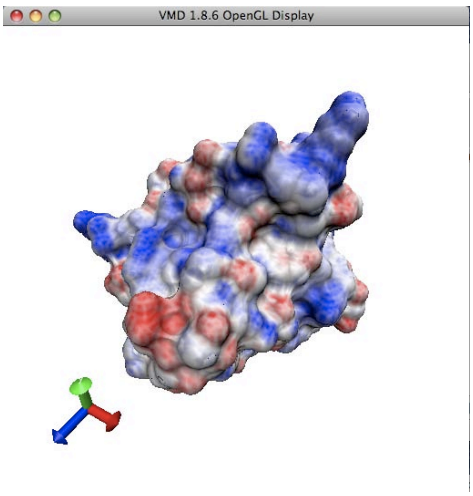
1. Delete the two isocontours using the Delete Rep button in the Graphical Representations window.

2. Click the Create Rep button.

3. Change the Drawing Method to 'Surf' and Coloring Method to 'Volume.'

   This will add a solvent accessible surface to the protein.

4. Go to the Trajectory tab and change 'Color Scale Data Range' to -10 to 10. Click Set.



Exercise 4: Using Tachyon ambient occlusion lighting

The Tachyon ray tracer (included with VMD) has the ability to render scenes with "ambient occlusion" lighting. This lighting technique mimics some of the effects that occur under conditions of omnidirectional diffuse illumination, e.g. outdoors on an overcast day.

1. From the VMD Main dialog, go to: File >> Load State

   Read in 1e79.vmd.

   Note: A .vmd file contains a saved "state" for a molecule. That is, it can store colors, renderings, labels etc. so that they don't have to be recreated again and again.

2. In the VMD Main window, go to: Display >> Display Settings
3. In the Display Settings dialog, find the External Renderer Options.
   Turn ON Shadows.
   Turn ON Amb. Occl.

   Note: In most cases, an ambient light coefficient ranging from 0.7 to 1.0 and a direct lighting coefficient of 0.1 to 0.4 are most appropriate and yield the best results.

4. In the VMD Main window, go to: File >> Render
5. In the File Render Controls dialog, change 'Render using' to TachyonInternal.
6. Click Start Rendering.

   An image appears in the Preview window rendered using ambient occlusion. Notice the depth of the object and the shadows.

   Note: Selecting a Material such as 'Diffuse' or 'AOShiny' in the Graphical Representation dialog, yields the best results for ambient occlusion.

Additional information

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

Obtaining APBS
http://apbs.wustl.edu/MediaWiki/index.php/APBS_electrostatics_in_VMD
http://apbs.sourceforge.net/

Ambient occlusion lighting information
http://www.ks.uiuc.edu/Research/vmd/minitutorials/tachyonao/

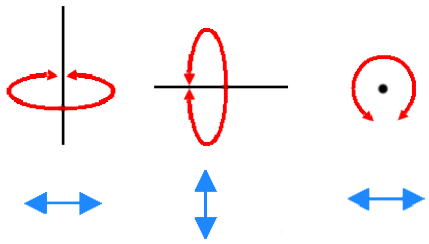
Molecule Manipulation

Press R on the keyboard.

Left mouse button = rotate the molecule

Center mouse button = rock the molecule.

Rotation mode

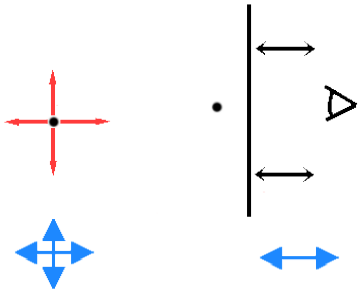


Press T on the keyboard.

Left mouse button = translate the molecule

Center mouse button = move clipping plane

Translation mode

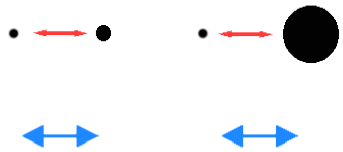


Press S on the keyboard.

Left mouse button = scale the molecule

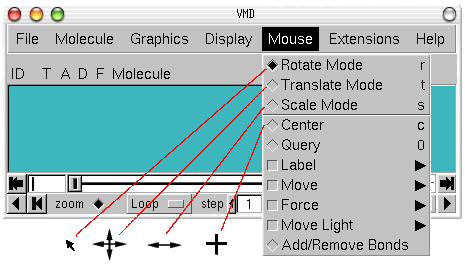
Center mouse button = greatly scale the molecule

Scale mode



Press C on the keyboard and click any atom.

Left mouse button = center the molecule around atom



Note: Modes can also be accessed using the Mouse menu in the VMD Main window.