VMD - Vissualization Tutorial

Loading into VMD

- For this tutorial I will be providing two frames with the same lipids, but different ratios
- We will start opening POPC_CHOL5.gro in VMD
    - `vmd POPC_CHOL5.gro`
    - If you are on windows you may have to load it from the GUI in vmd

We need to take a bit of a left turn from making images here and talk about your OS. Your OS will limit your imaging quality

- Linux - I am the best! VMD at 64 bit, high quality rendering, and full access to all libraries!
- Mac :
    - Pre M1 - I'm a solid choice! VMD at 64 bit, most access to libraries, and many rendering tools!
    - Post M1 - I am potentially the struggle bus
- Windows - I am here! VMD at 32 bit, most access to libraries, and high quality rendering!

Lets make your rendering consistent with the above knowledge

- Go to File > Log TLC Commands To Console
- Got to Extensions > TK Console
- Display > Rendermode:
    - Linux/Windows - GLSL
    - Mac - Acrobat3D (GLSL does not work well for transparent/translucent Materials for mac)
- Display > Orthographic
- Graphics > Colors
    - Gatergories > Display > Background > 8 white
- You should notice that a command appears in the TkConsole! We can use these commands and tell VMD to open with these as the default
- Go to `vi ~/.vmdrc` in your terminal (Windows users I'm sorry I have NO idea), and add

```
display projection Orthographic
display depthcue off
axes location Off
color Display Background white
display rendermode GLS
```

Graphical Representations

Vmd is open! We have lipids and water. We want to make this look pretty! So:

- VMD Main > Graphics > Representation

This is the Graphical Representations GUI. There are four tabs

- Draw style
- Selections
- Trajectory
- Periodic

We will only focus on Draw style today. In the Draw style talbe there are three drop down menus:

- Color Method - How we color our systems or selections
- Drawing Method - How we represent our system or selections
- Material - This is how we make our models "Pop"

Let's make a selection

Lets add Cholesterol

- Selected Atoms space enter `noh resname CHL1`. This will show only the cholesterol.
- In Drawing Method try:
    - Lines
    - VDW
    - CPK
    - Licorice
- Which looks best to you?

Now lets add in POPC.

- Click `Create Rep` and in the new Selected Atoms space `noh resname POPC`
- This is NOT easy to see the cholesterol and POPC!

Lets adjust our colors. Some rules to consider

- Colors too similar will make it hard to see things!
- Try contrasting colors
- Default colors are almost always bleh

Start with default for both selections : Coloring Method > Resname. So we can see the two molecules now, but booooooooy is it UGLY

Doing this for one selection at a time:

- Coloring Method > ColorID > play with the list!
    - My personal binary go to- cholesterol warm
    - Saturated cool
        - This is just me though! Find your style (*rather a style that other people can understand!*)

OK! We've got the start of a nice image!

- Back to your Graphical Representations
    - Your material is set to opaque. This material is fine for prototyping. Go through a few of the materials with the cholesterol selection.
    - Choose one you like and lets render an image!

Rendering

- File > Render > <Name.tga> > Start Rendering
- File > Render > Render the current scene using > TachyonL-GPU-accel > <Name.ppm> > Start Rendering
    - which is better?

Lets make it BETTER!

- Display > Display Settings
    - Shadows > On
    - Amb. Occl. > On
        - These settings will work your computer
    - Material > AOEdgy
    - Render!

Lets add water back in

- Graphical Representations make a new selection
    - water
    - Coloring Method > ColorID > 8
    - Drawing Method > Quick Surf
    - Material > :
        - GlassBubble
        - Ghost 1-3
        - Transparent
    - Which do you like more?
    - Render!

What if you need copy these settings to another simulation?

- We have two options. 1) Do it manually. 2) Clone it!
    - Start by loading POPC_CHOL50.gro
    - VMD Main > Extensions > Visualization > Clone Representation
        - From Molecule > 0
        - Clone

Lets look at two last things Custom Materials, and Custom Colors

This last section has a lot of options. I do not have an easy way to document them. So I will demonstrate how to go about it, and add a custom material at the bottom.

```
material add copy Goodsell
material rename Material25 Unlight
material change Diffuse Unlight 0.52
material change Outline Unlight 0.00
material change outlinewidth Unlight 0.16
material change Shininess Unlight 0.00
material change Specular Unlight 0.00```
```