VMD Visualization Tips

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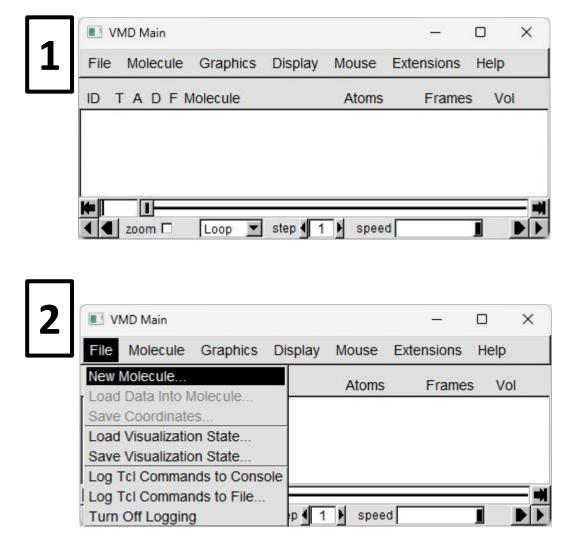
CTBP

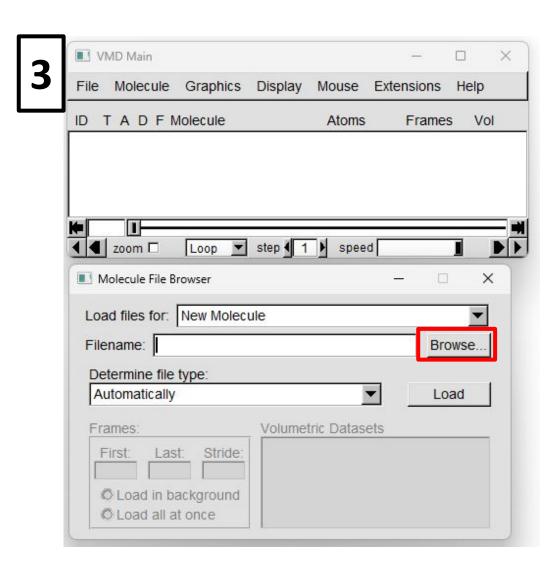
09/04/23

Topics

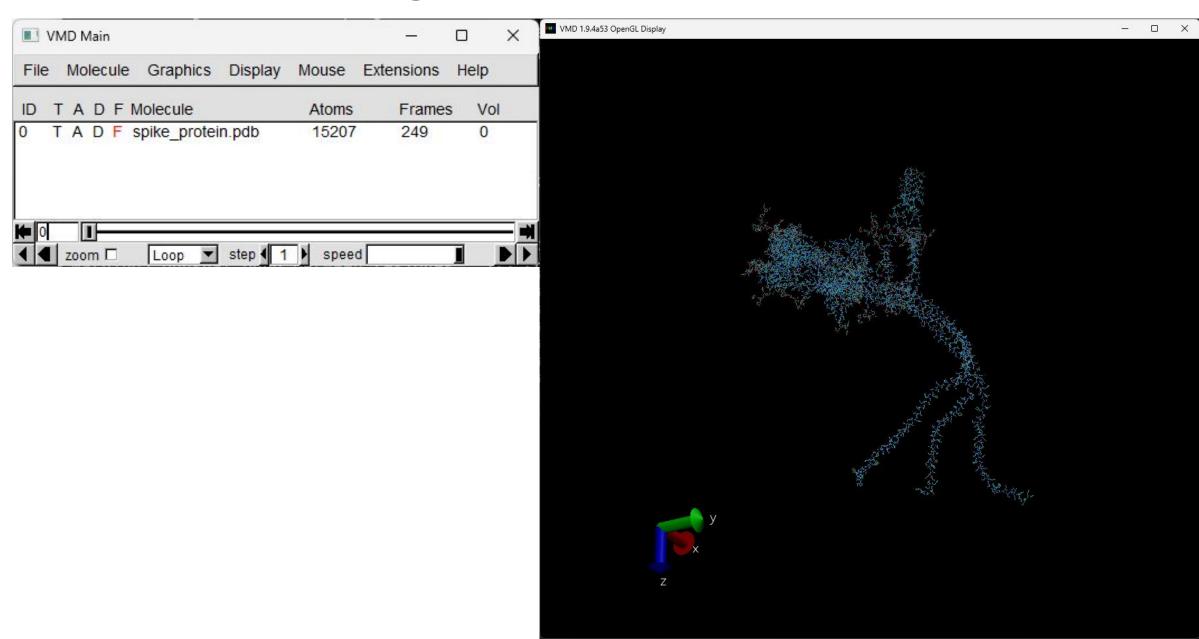
- Rendering images
 - Perspectives
 - Colors, representations, viewpoints
 - Rendering frames
 - Editing frames
- Making a movie
- Other visuzalation tips

VMD – Loading a molecule



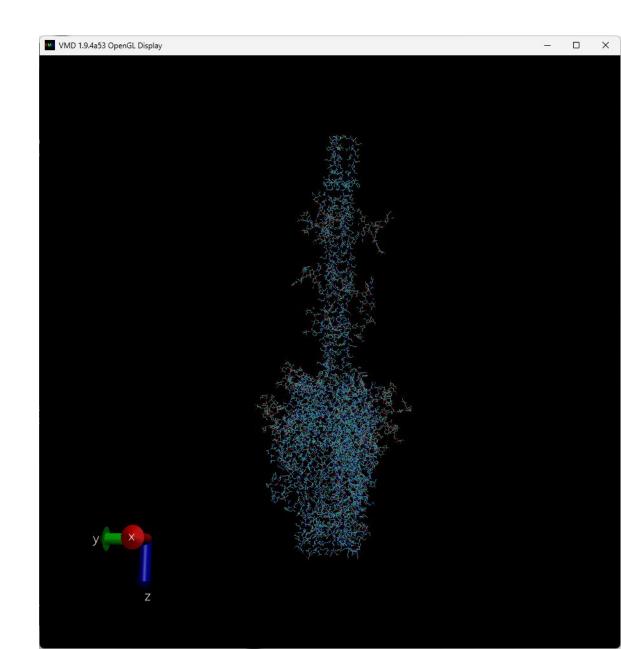


VMD – Loading a molecule



VMD – perspective

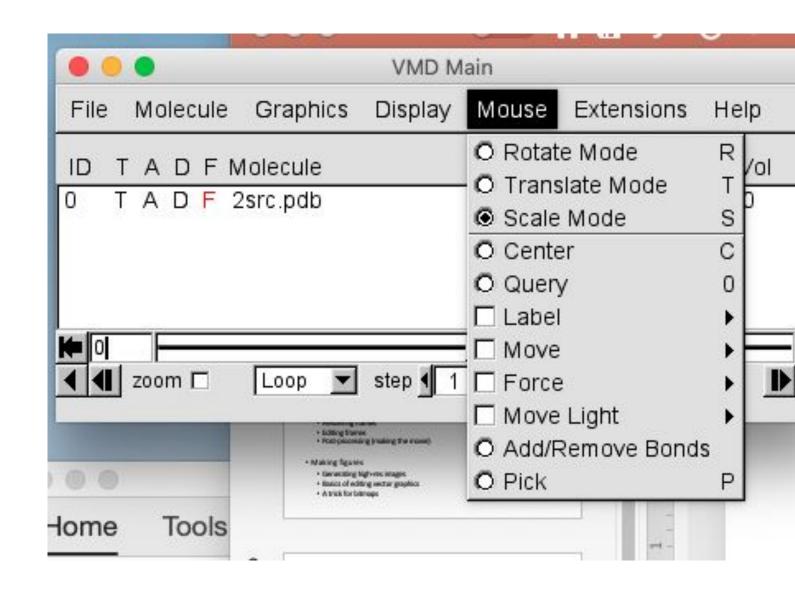
- Selecting a perspective
 Orthographic > Perspective
- Hide axes



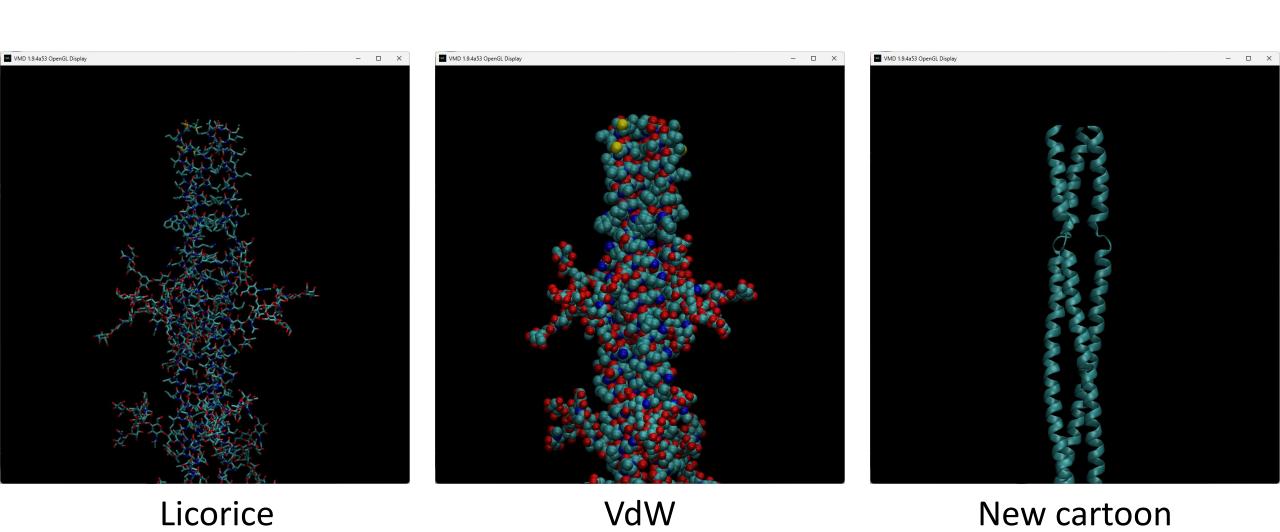
VMD – Move around

- Get used to navigating the different mouse modes
 - Rotate
 - Translate
 - Scale
 - Center

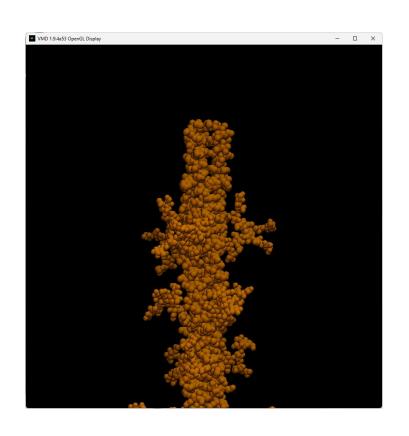
Keyboard shortcuts are on the right of each menu (e.g. T changes to translate mode)

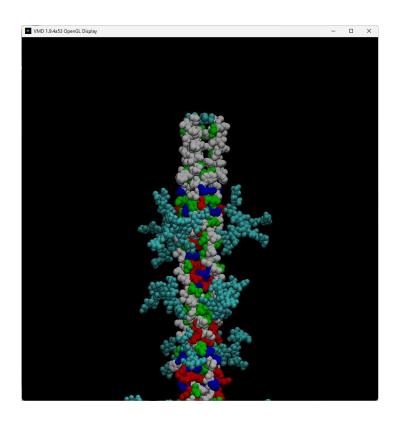


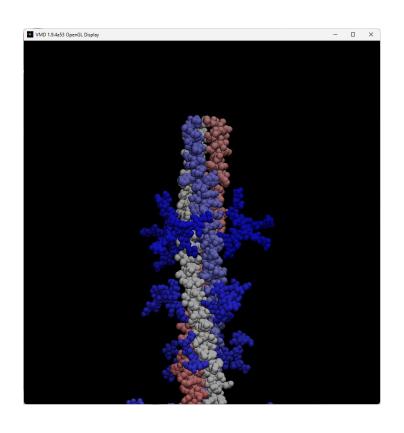
VMD – Representations



VMD – Colors

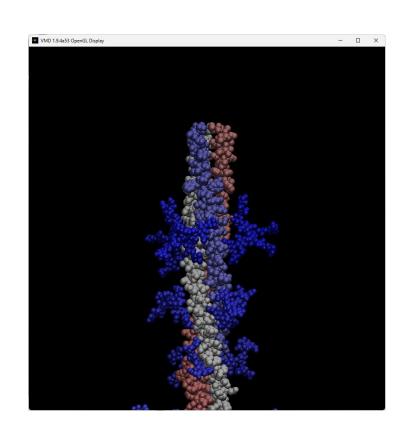


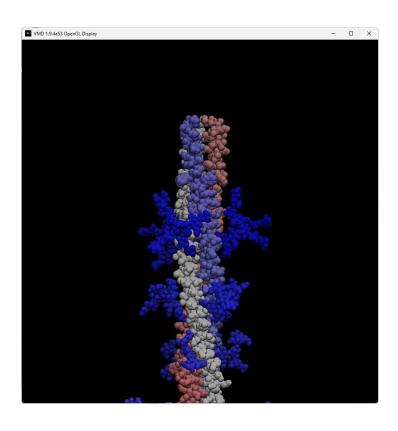


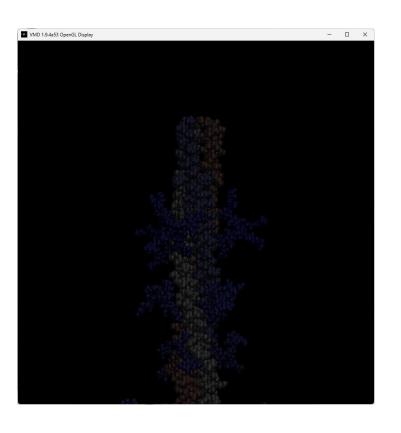


ColorID ResType Index

VMD – Material







Opaque

AOChalky

Transparent

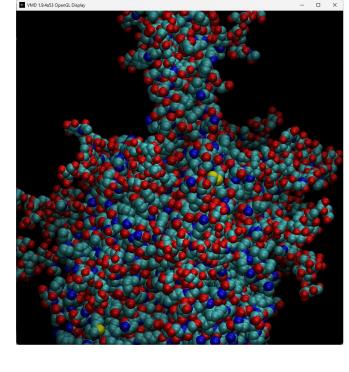
VMD 1.9.4a53 OpenGL Display ■ Graphical Representations — Selected Molecule 0: spike protein.pdb Create Rep Delete Rep Selection Style Color NewCartoon Chain Licorice ColorID 3 not protein Selected Atoms all Draw style | Selections | Trajectory | Periodic | Coloring Method Chain EdgyShiny **Drawing Method** NewCartoon Default Spline Style Catmull-Rom ▼ Aspect Ratio 4.10 Thickness 0.30 Resolution (10)) Apply Changes Automatically

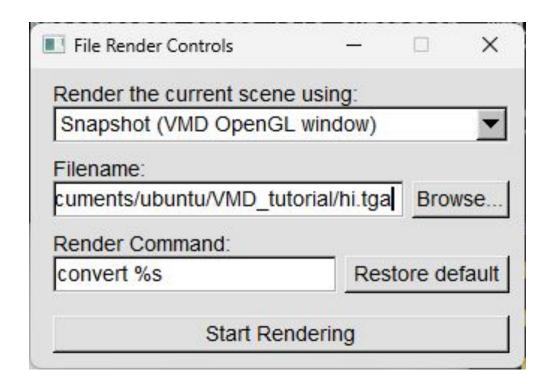
Representations again (but cooler)

Zoom in and render

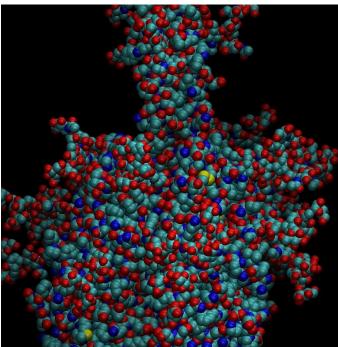
To render: File -> render

display

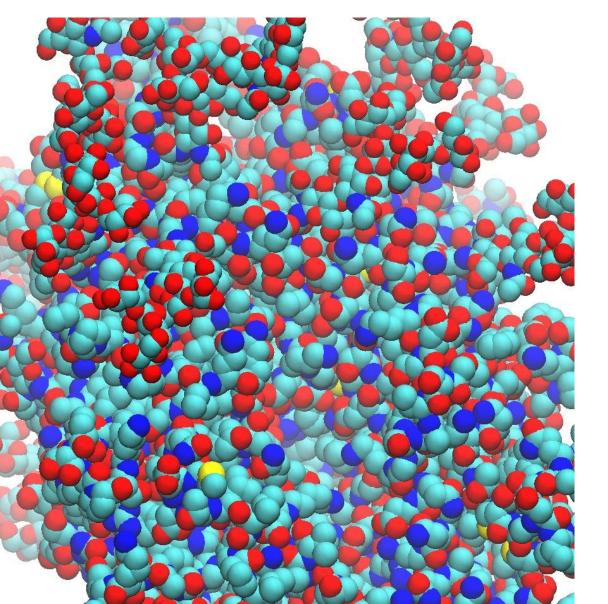




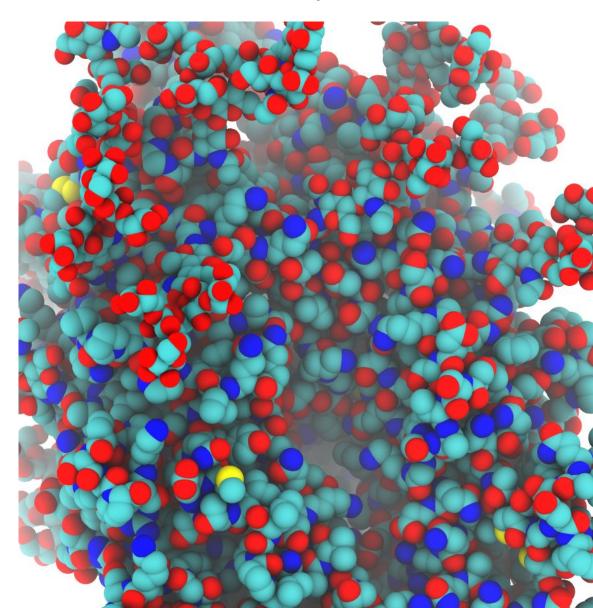
Snapshot – What you see is what you get



Built in rendering

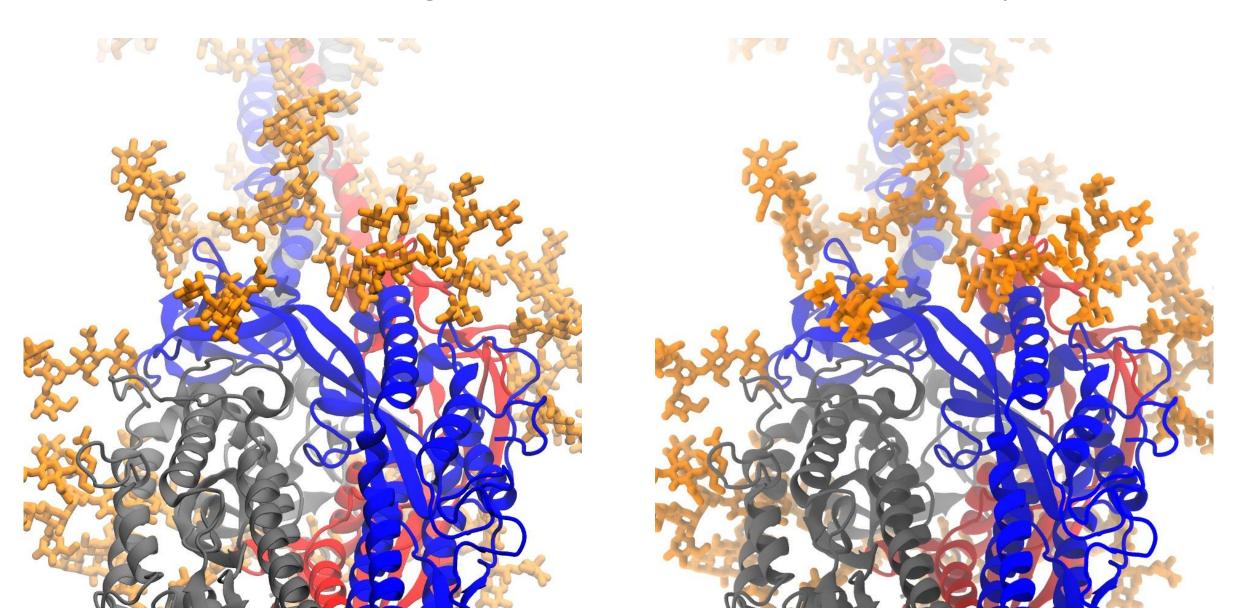


Tachyon

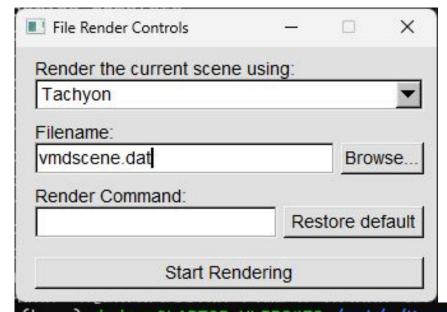


Built in rendering

Tachyon



Render with tachyon



tachyon -fullshade -auto_skylight 1.4 file.dat -o output.tga

```
(base) dodero@LAPTOP-VLIR34F9:/mnt/c/Users/doder/Documents/ubuntu/VMD_tutorial$ tachyon -fullshade
-auto_skylight 1.4 file.dat -o output.tga
Tachyon Parallel/Multiprocessor Ray Tracer
                                             Version 0.99
Copyright 1994-2013, John E. Stone <john.stone@gmail.com>
Scene Parsing Time:
                        0.9152 seconds
Scene contains 389373 objects.
Preprocessing Time:
                        0.2244 seconds
Rendering Progress:
                          100% complete
  Ray Tracing Time:
                      111.5722 seconds
    Image I/O Time:
                        0.0366 seconds
```

Let's use the .dat file to render

Directly call Tachyon

Use the command:

tachyon -fullshade -auto_skylight 1.4 vmdscene.dat -o vmdscene.AO.tga

You may notice rendering is very slow. This is a good sign.

If too slow, add "-res 200 200" to your tachyon call, so make a smaller version.

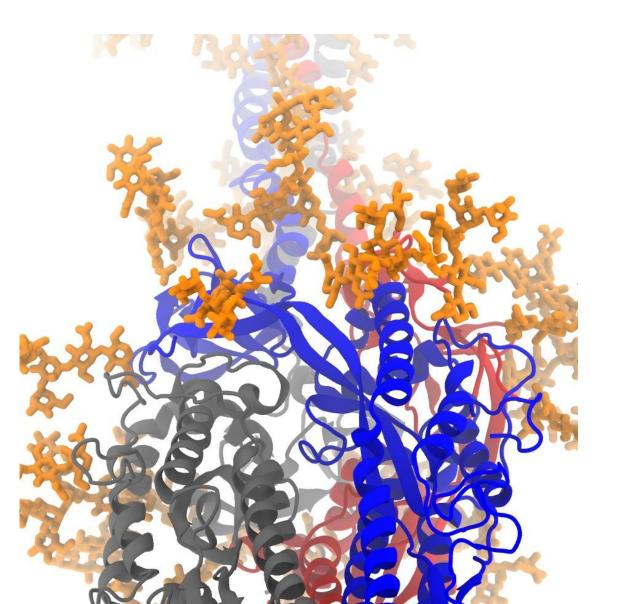
Open the .dat file

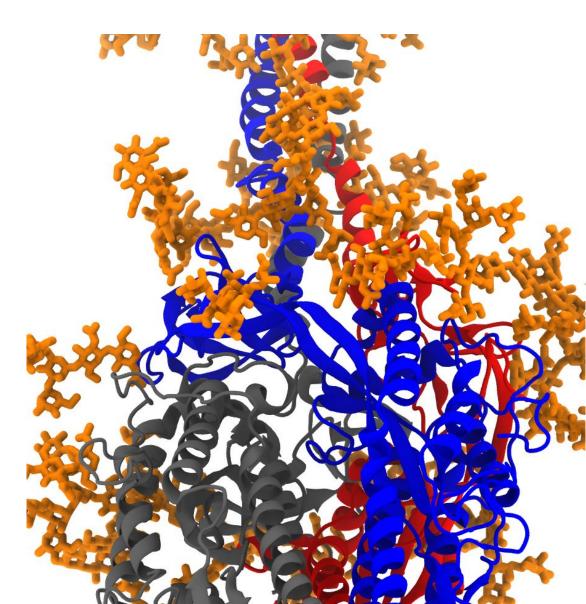
- Defines the scene
 - Perspective
 - Objects
 - Colors
 - Shading
 - Fading (fog)
 - Material
 - Everything...

 At this point, we no longer necessarily need VMD.

```
# http://www.ks.uiuc.edu/Research/vmd/
# Requires Tachyon version 0.99.0 or newer
# Default tachyon rendering command for this scene:
    tachyon -aasamples 12 %s -format TARGA -o %s.tga
Begin_Scene
Resolution 512 512
Shader_Mode Medium
  Trans_VMD
  Fog_VMD
End_Shader_Mode
Camera
  Projection Orthographic
  Zoom 0.333333
  Aspectratio 1
  Antialiasing 12
 Raydepth 50
  Center 0 0 -2
  Viewdir -0 -0 2
 Updir 0 1 -0
End Camera
Directional_Light Direction 0.1 -0.1 1 Color 1 1 1
Directional_Light Direction -1 -2 0.5 Color 1 1 1
Background 1 1 1
Fog Exp2 Start 0 End 10 Density 0.32 Color 1 1 1
# MoleculeID: 0 ReprID: 0 Beginning VDW
Sphere
  Center -2.18062 2.92851 -0.47191
Rad 0.194792
Texture
```

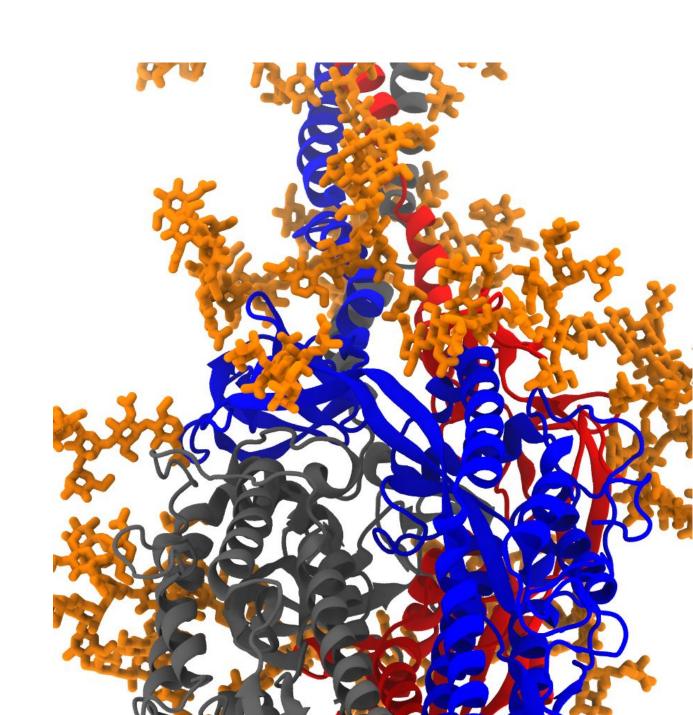
Foggy Less fog





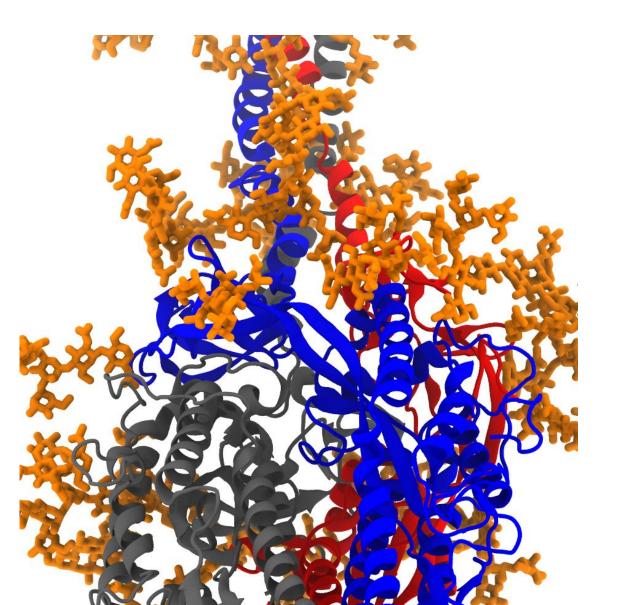
Light intensity and oversaturation

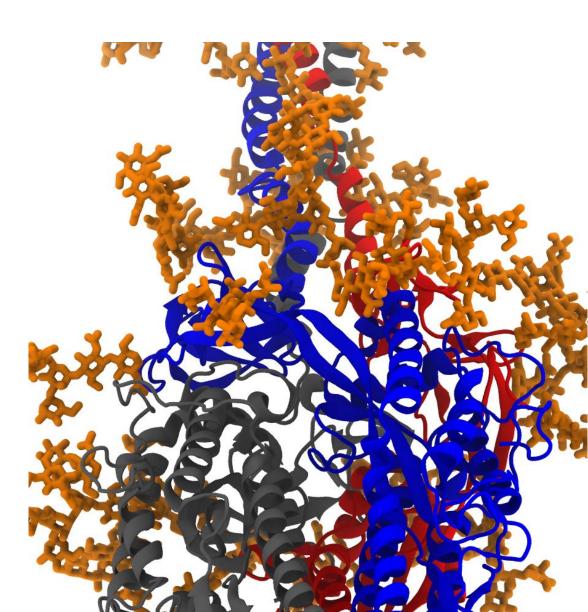
tachyon -fullshade -auto_skylight 1.2 vmdscene.dat -o vmdscene.AO.tga



Saturated

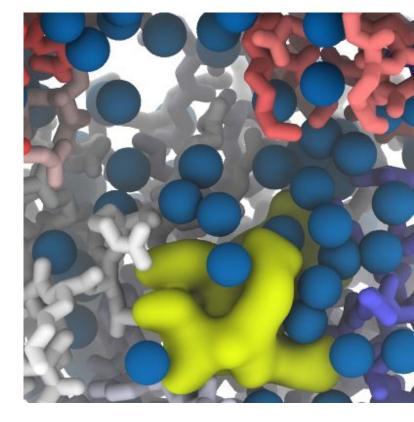
Less saturated





General tips

- Only show atoms that are in the frame
- Even particles that are not in view will cast shadows
- Best representations
 - Vdw
 - Licorice (expensive to render, see right)
 - Use thicker bond radius than the default
 - May want higher sphere resolution the default
 - Tubes
 - Quicksurf
- AO often results in darker images than in the display. Plan accordingly
- Remember you can reassign colors in terms of RGB values in the scene file
- For a publication, expect to render, re-render and repeat.... You only get one chance to catch the reader's eye.
- Tachyon is parallel! Use an interactive cluster node with many cores. A good image can take 5-20 minutes on a multi-core node.



Tk console

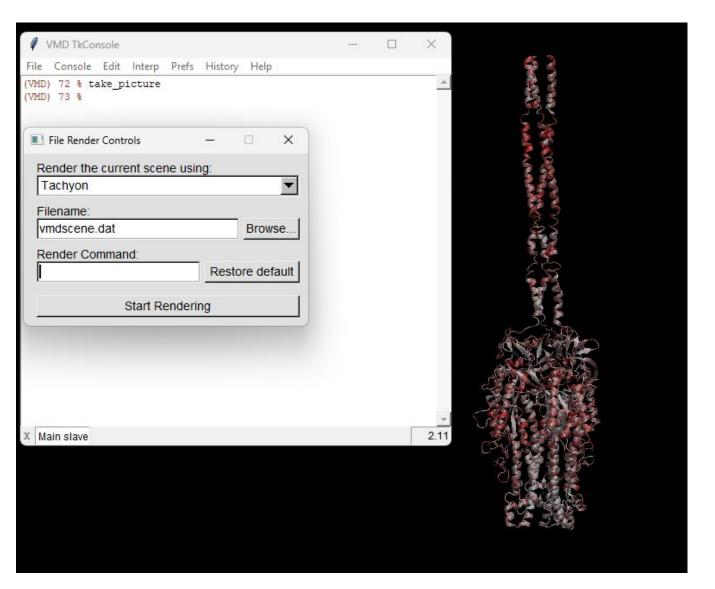
Let's play with scripting

Open the tk console and source visualization.tcl (bag of goodies)

take_picture
colorByFile
colorByResid
tricolor_scale
bicolor_scale
align_pi
rotate_axis
increment_np
increment

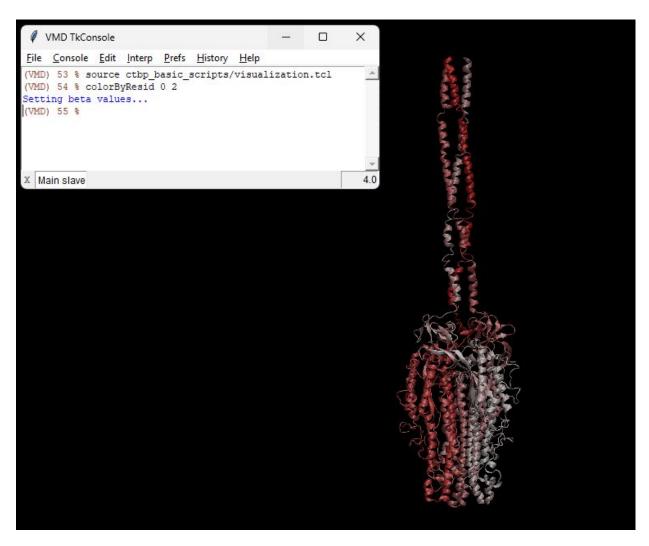
save_vp move_vp move_vp_render retrieve_vp write_vps

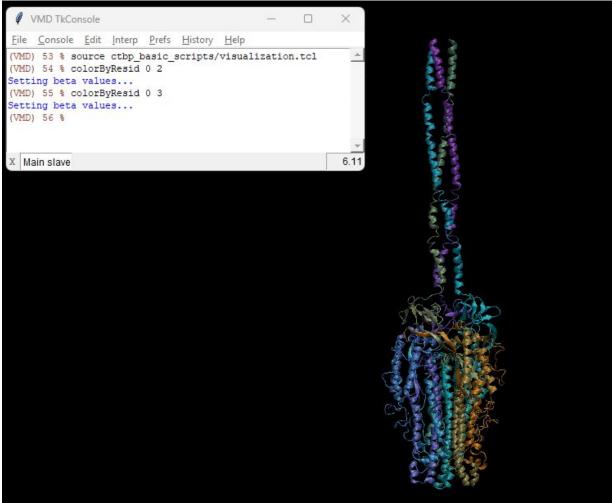
Tk console - take_picture



Renders display into .dat file

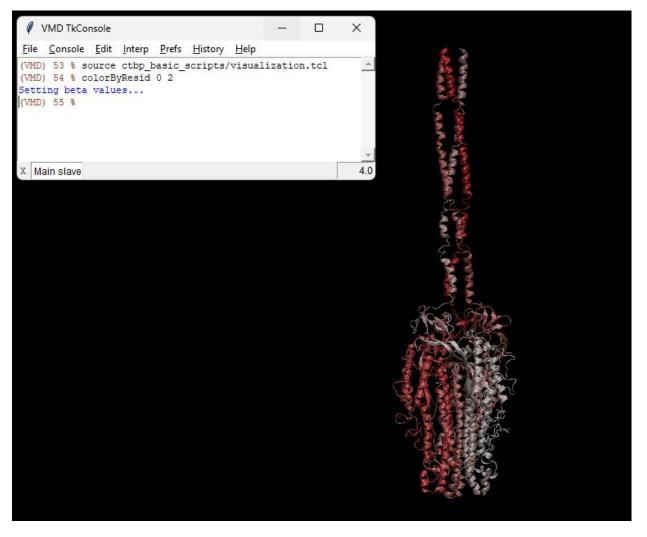
Tk console - colorByResid



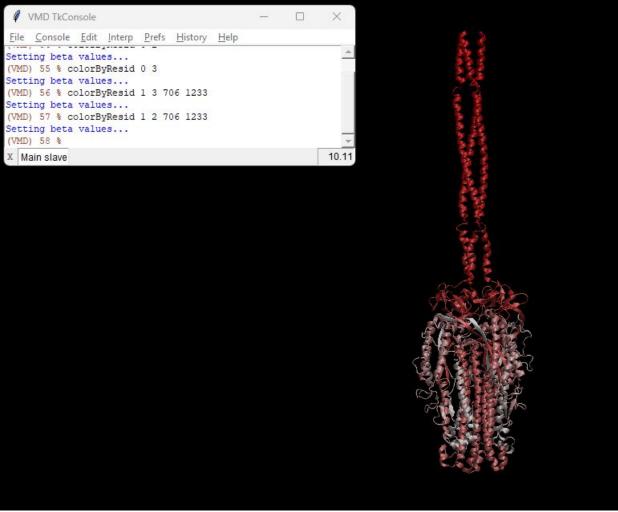


Tk console - colorByResid

GRO

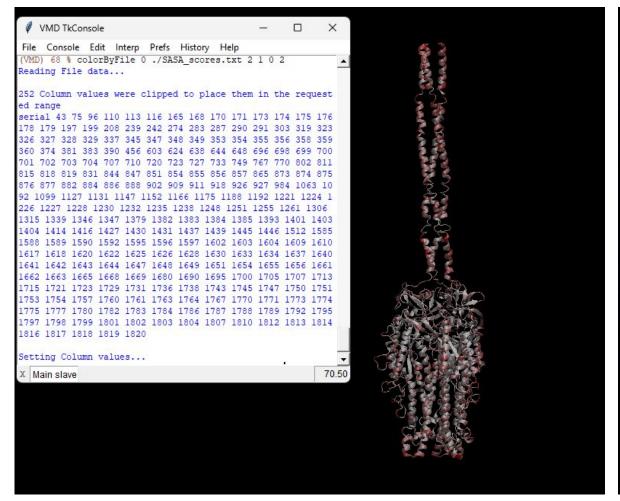


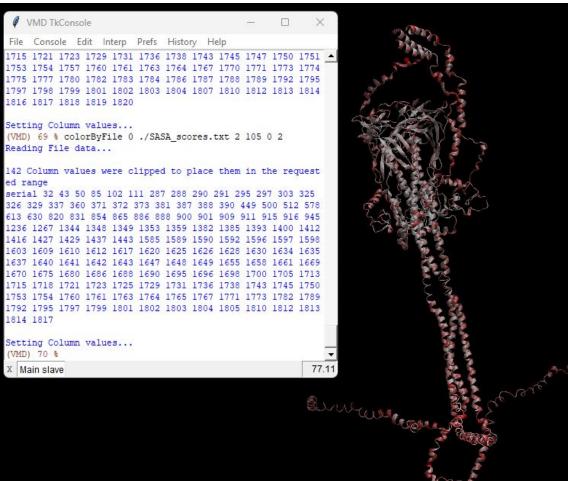
PDB



Tk console - colorByFile

SASA: Solvent Area Surface Area

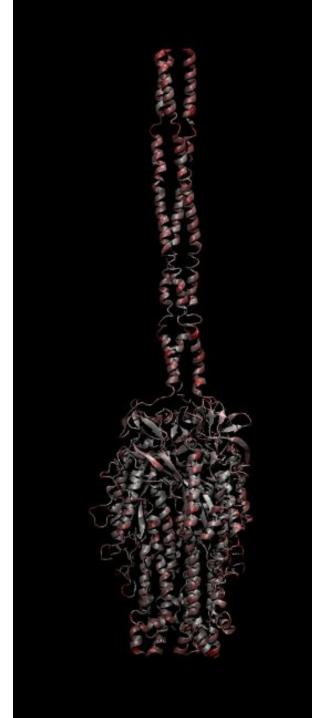




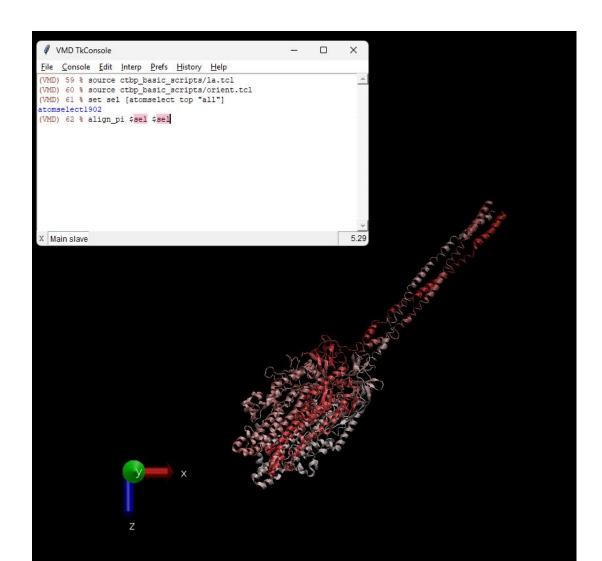
Tk console - colorByFile

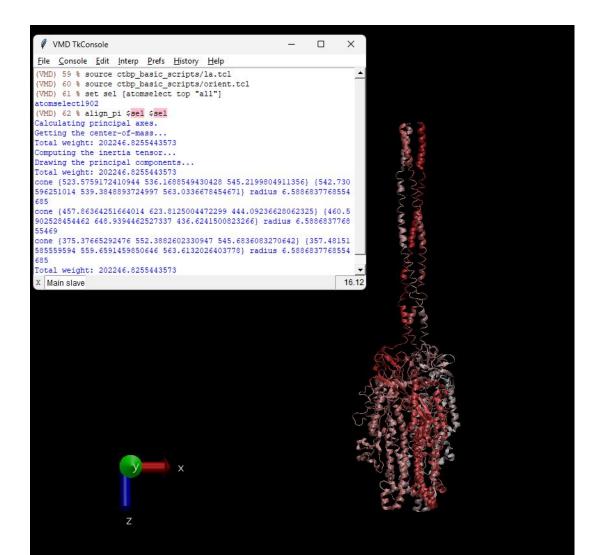
SASA: Solvent Area Surface Area

```
File Console Edit Interp Prefs History Help
(VMD) 71 % for {set i 1} {$i < 249} {incr i 10} {
colorByFile 0 ./SASA scores.txt 2 $i 0 2
take picture
Reading File data...
252 Column values were clipped to place them in the requested range
  Main slave
```

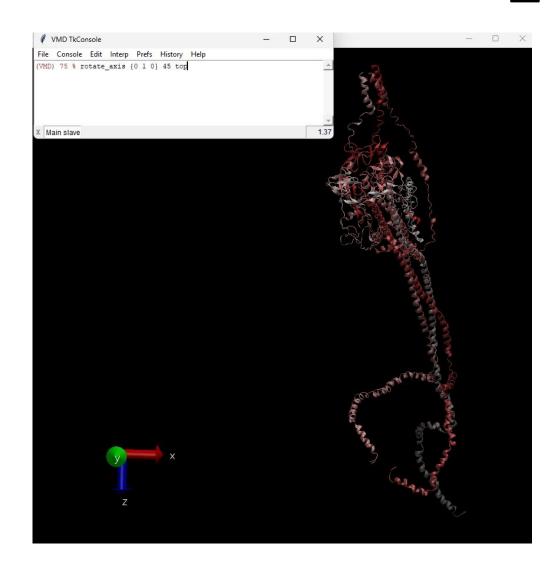


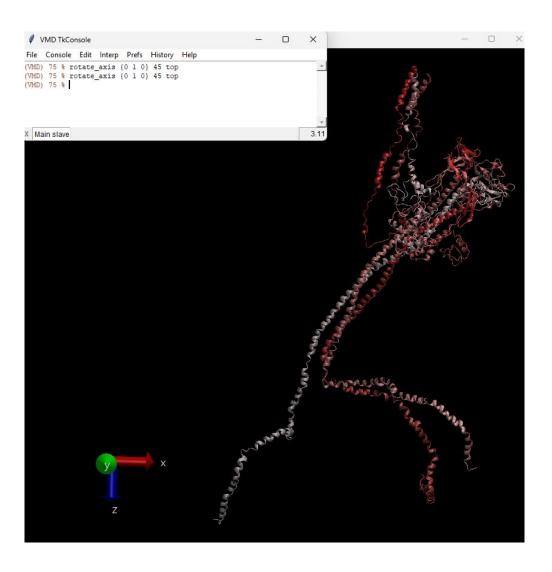
Tk console - align_pi





Tk console - rotate_axis

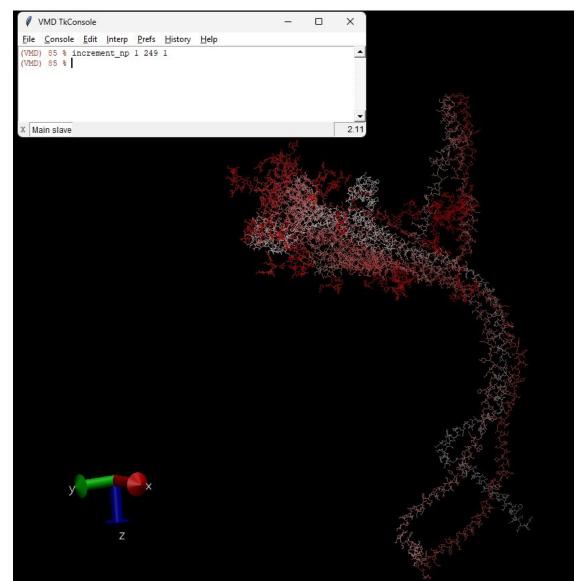




Tk console - rotate_axis

```
for {set i 1} {$i < 249} {incr i 10} {
  rotate_axis {0 1 0} 10 top
  display update
}</pre>
```

Tk console - increment(_np)



increment_np 1 249 1

To render increment 1 249 1

Tk console - Viewpoints

save_vp vpID

retrieve_vp vpID

move_vp vpID_1 vpID_2

move_vp_render vpID_1 vpID_2 first_frameID dirName
filePrefixName morph_frames=50

write_vps

Tk console - Merging everything together

```
source ctbp basic scripts/la.tcl
source ctbp basic scripts/orient.tcl
source ctbp_basic scripts/visualization.tcl
source vps.tcl
retrieve_vp 1
animate goto 0
#mol representation NewCartoon 0.3 10 4.1
colorByFile 0 ./SASA scores.txt 2 1 0 2
move vp render 1 2 0 . move 20
move vp 120
#RENDER WITH TACHYON LATER
for {set i 1} {$i < 360} {incr i 2} {
rotate axis {0 1 0} 2 top
display update
#take picture
#RENDER WITH TACHYON LATER
```

move_vp_render 2 1 0 . move 20

increment np 1 249 1

Tk console - Merging everything together

```
mol new ./spike_protein.gro
mol addfile ./sample_trajectory.xtc 0
```

source ctbp_basic_scripts/la.tcl source ctbp_basic_scripts/orient.tcl source ctbp_basic_scripts/visualization.tcl source vps.tcl

retrieve_vp 1

mol representation NewCartoon 0.3 10 4.1 mol material AOChalky color Display Background white colorByFile 0 ./SASA scores.txt 2 1 0 2

```
for animate goto 1
move_vp_render 1 2 0 . move 20

for {set i 1} {$i < 360} {incr i 10} {
  rotate_axis {0 1 0} 10 top
  take_picture
  }

move_vp_render 2 1 20 . move 20
  increment 1 249 5

exit</pre>
```

VMD without looking - Command line

vmd -e sample_script.tcl -dispdev text

vmd -e sample_script_2.tcl -dispdev text



VMD without looking - Command line

vmd -e sample_script.tcl -dispdev text

vmd -e sample_script_2.tcl -dispdev text

