Visualization Tips

Paul Whitford

CTBP

9/22/21

The point…

- This is a collection of easy-to-implement tips that I have picked up over the years… i.e. this is not comprehensive.
- Hopefully they can help as you design figures for manuscripts, or movies.
- These tips can help get you pointed in the right direction, so that you can make figures that more clearly communicate your scientific thoughts.

- Disclaimer: Some of these slides were accompanied by interactive demonstrations, so some descriptions may seem vague.

Topics

- Making movies
  - Perspectives and time sequences
  - Rendering frames
  - Editing frames
  - Post-processing (making the movie)

- Making figures
  - Generating high-res images
  - Basics of editing vector graphics
  - A trick for bitmaps

VMD – the only real option

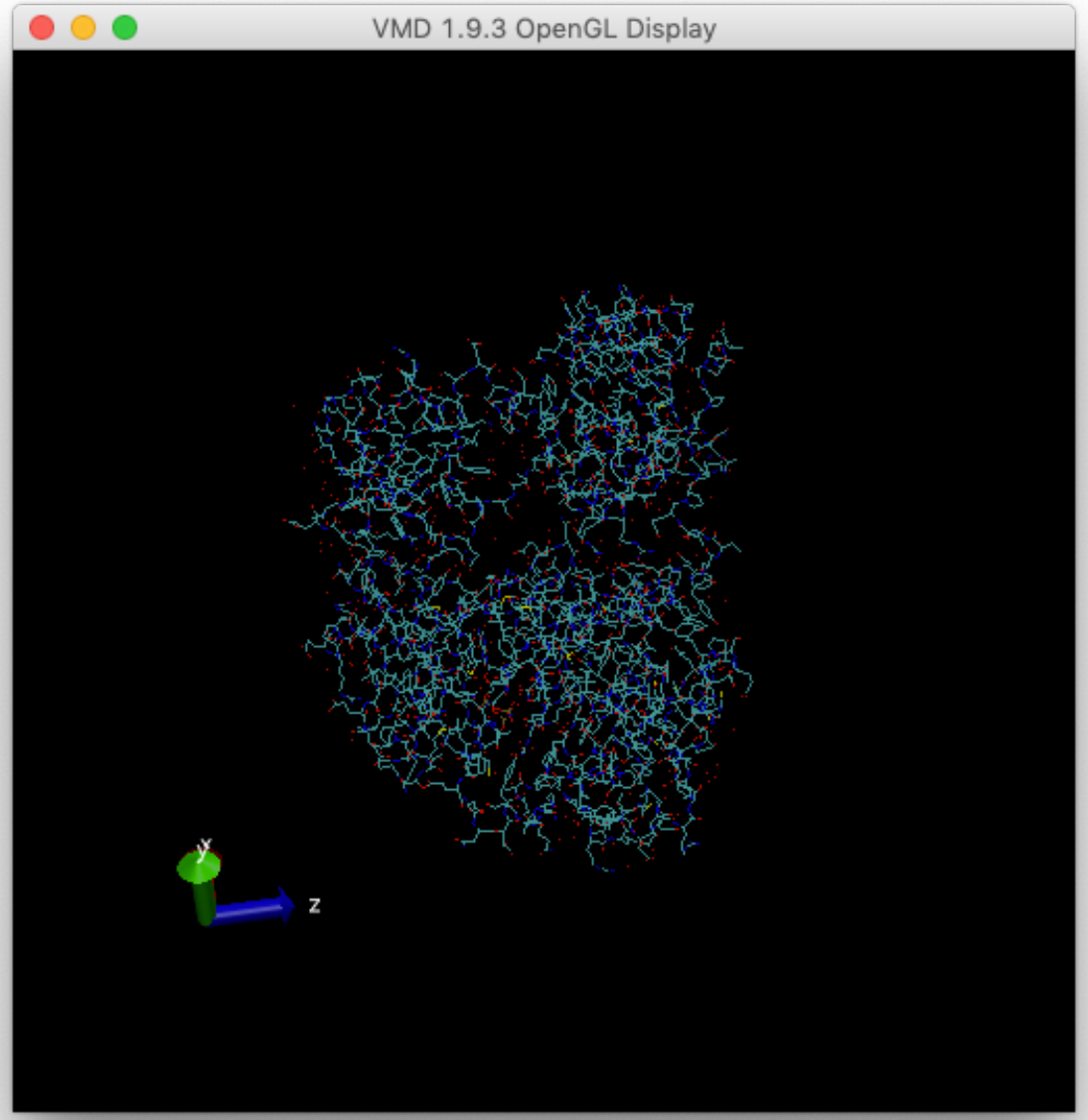
- Steps to generating a good image
  - Select a perspective
  - Select a representation
  - Export the scene
  - Render a high-quality version

- We will use Tachyon, though other renderers are available.

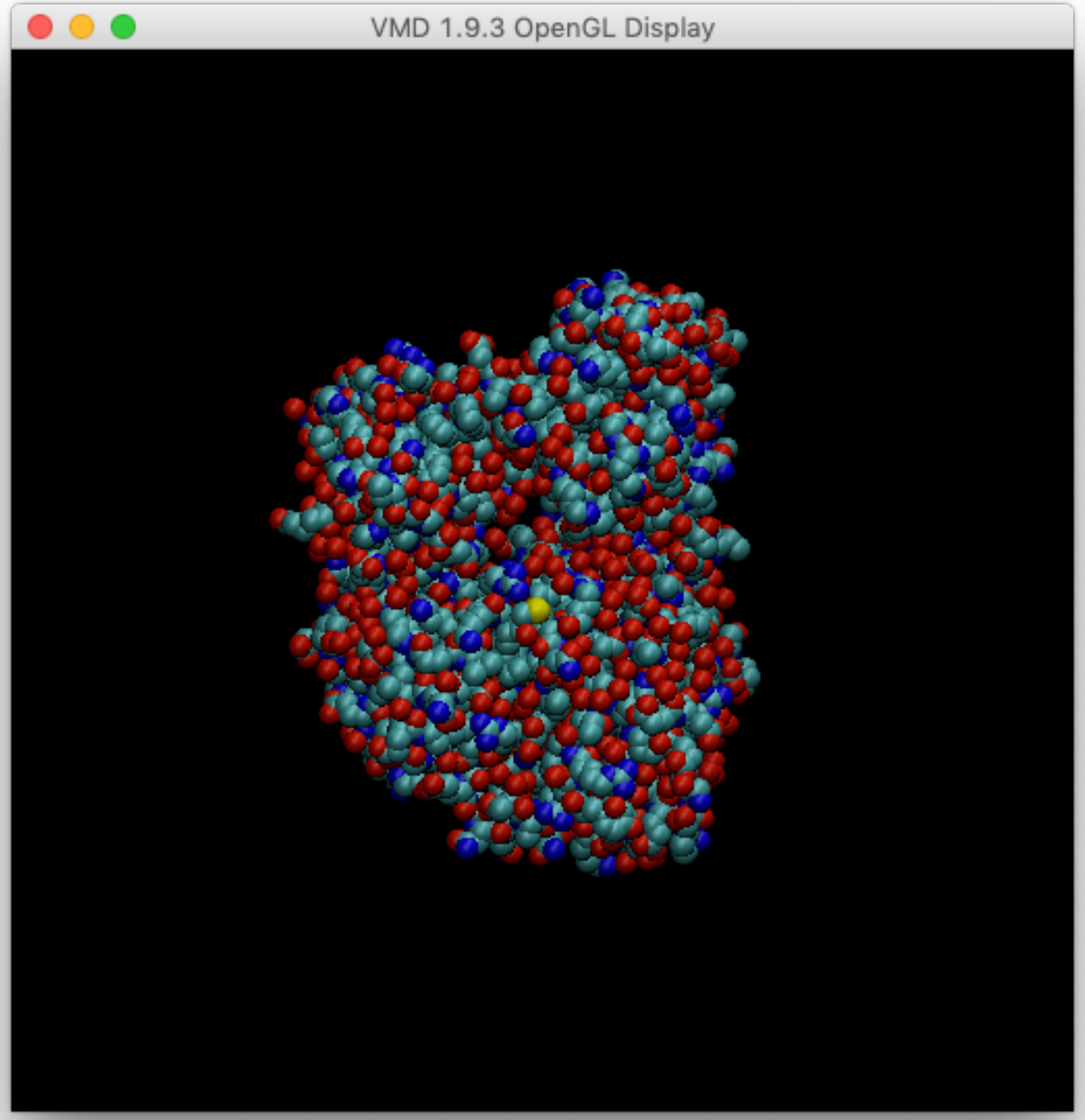
Load a PDB

For this, load the PDB file 2SRC.pdb

> vmd 2src.pdb



- Hide axes
- Recommend white background
- Select vdw representation



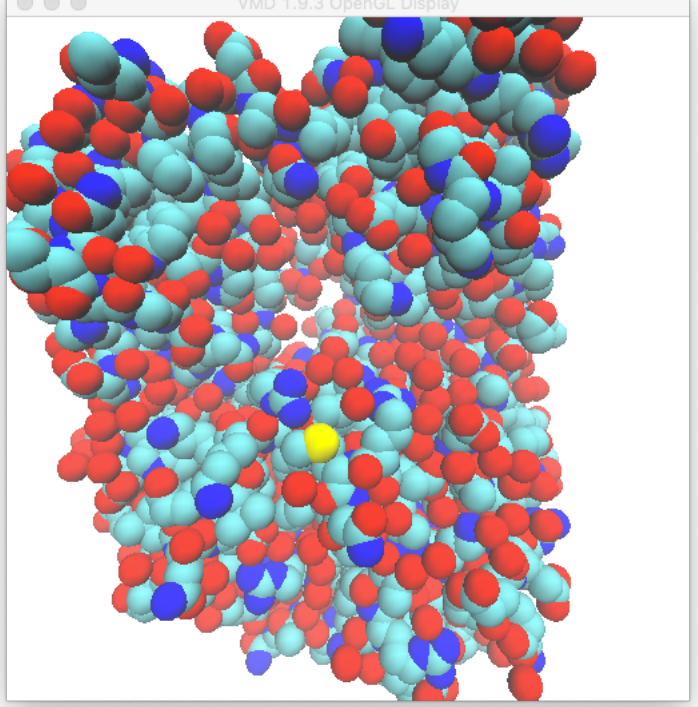
recommendation

- Always use Orthographic

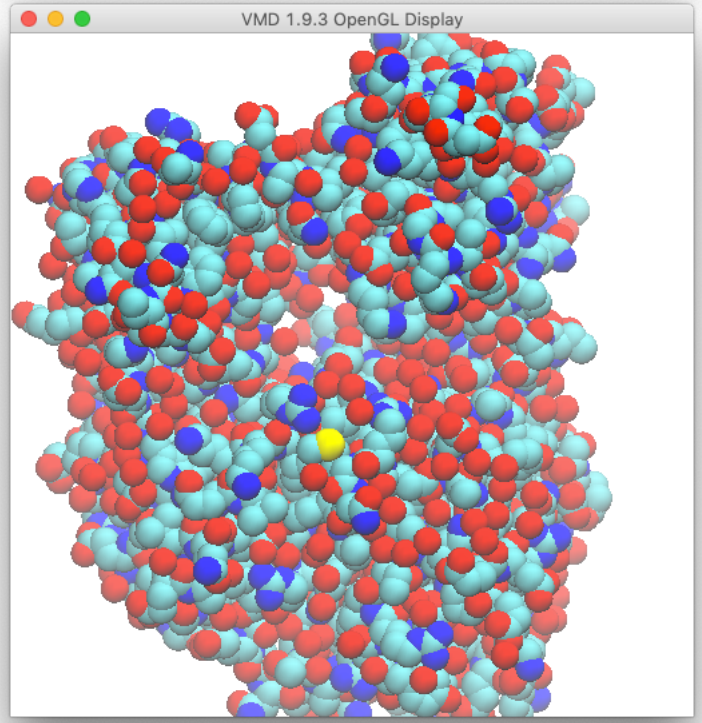
In VMD Main window:

> Display -> Orthographic

Default - Perspective



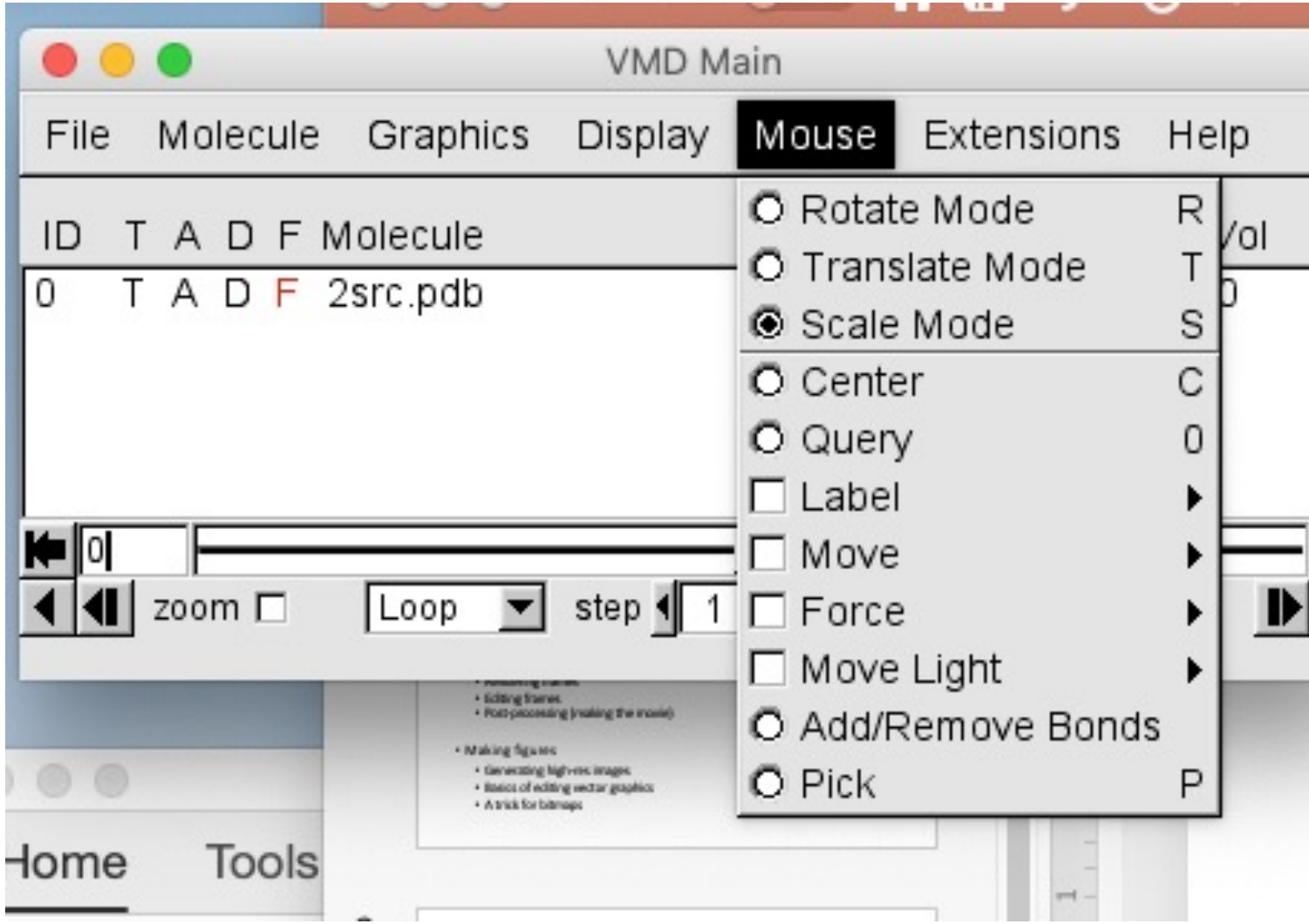
Orthographic –
Avoids distortion



Basic tip

- Get used to navigating the different mouse modes
  - Rotate
  - Translate
  - Scale
  - **Center (often overlooked)**

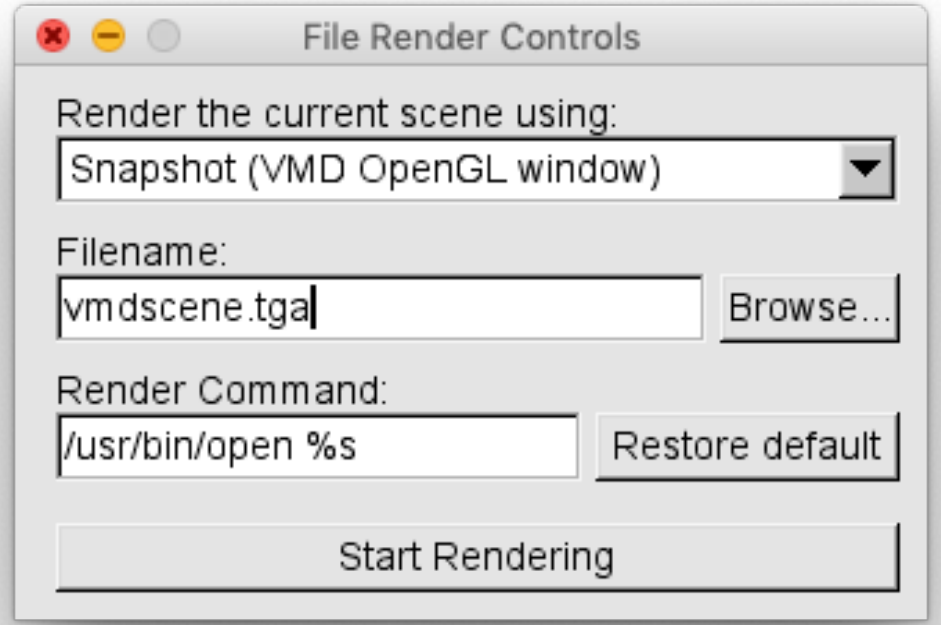
Keyboard shortcuts are on the right of each menu (e.g. T changes to translate mode)



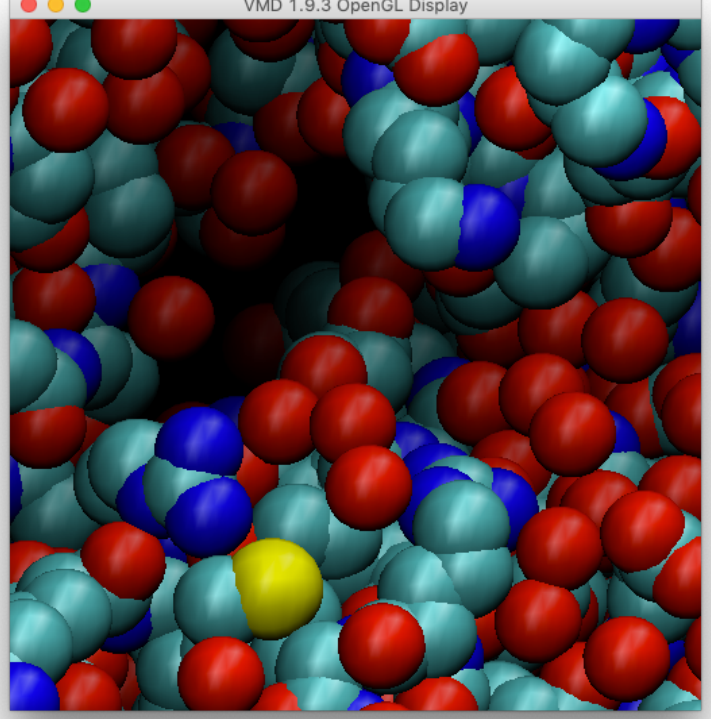
Zoom in and render

To render: File -> render

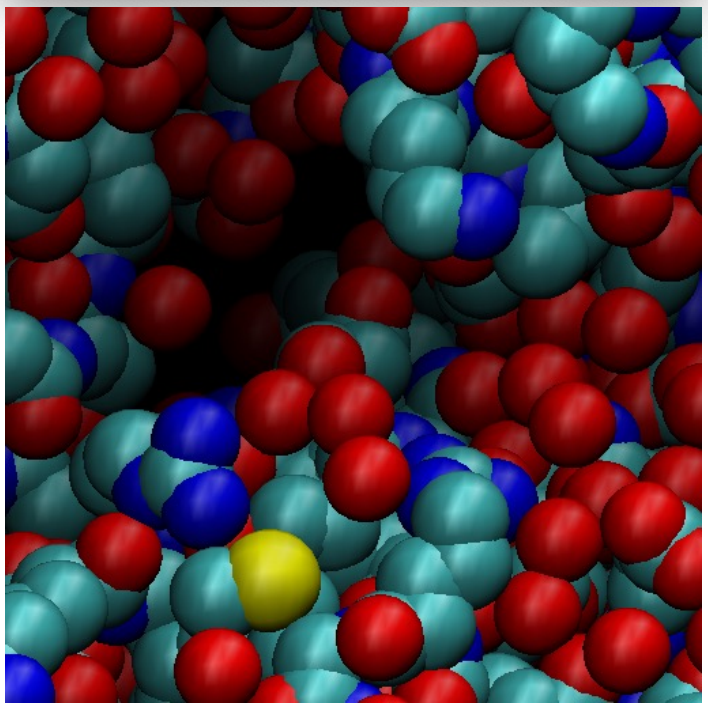
Use default Snapshot rendering



display

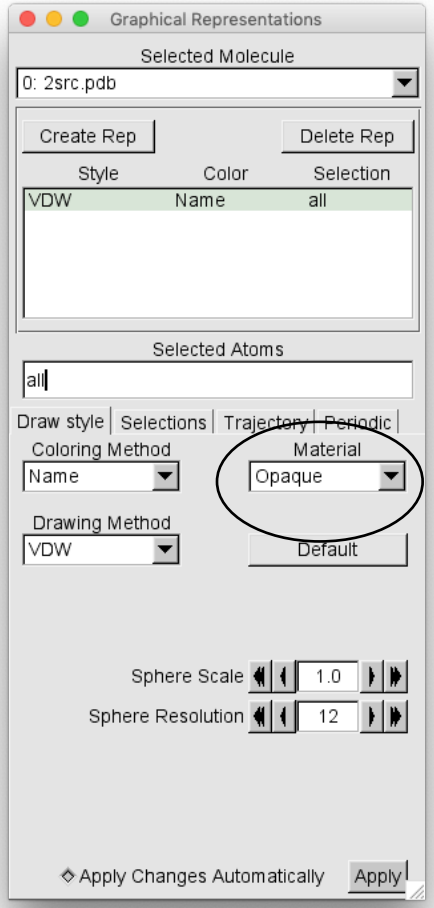


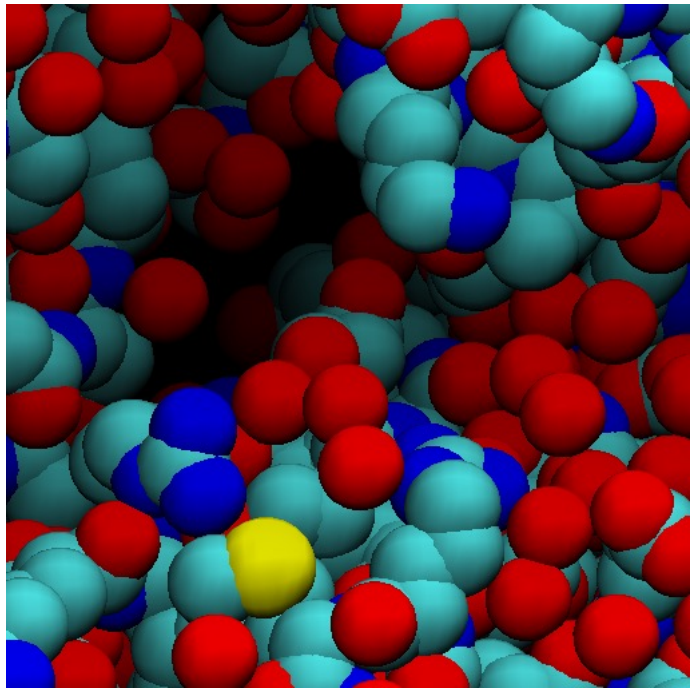
Snapshot –
What you see is what you get



Let’s try to make things look a bit better

- We will use Ambient Occlusion (AO)
- Change the material of your selection
  - Select AOChalky
- Now, re-render with snapshot





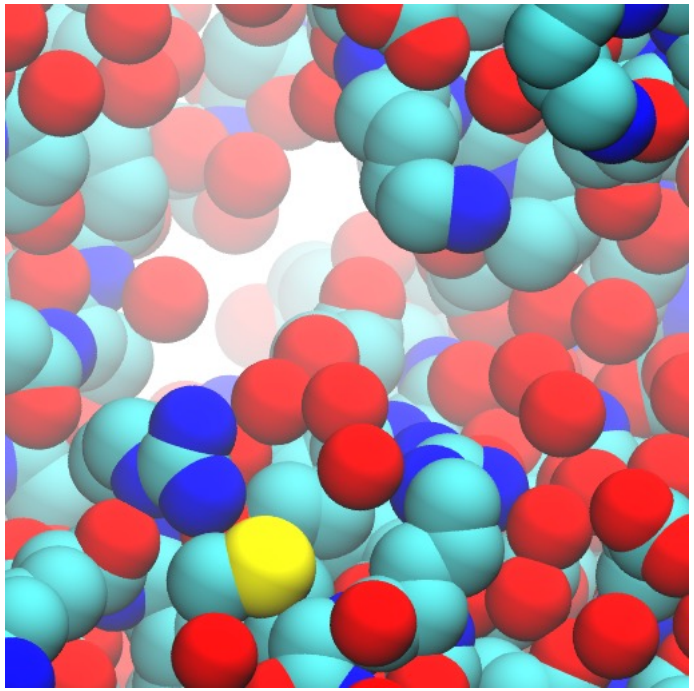
No real improvement….

Render again, turning on AO

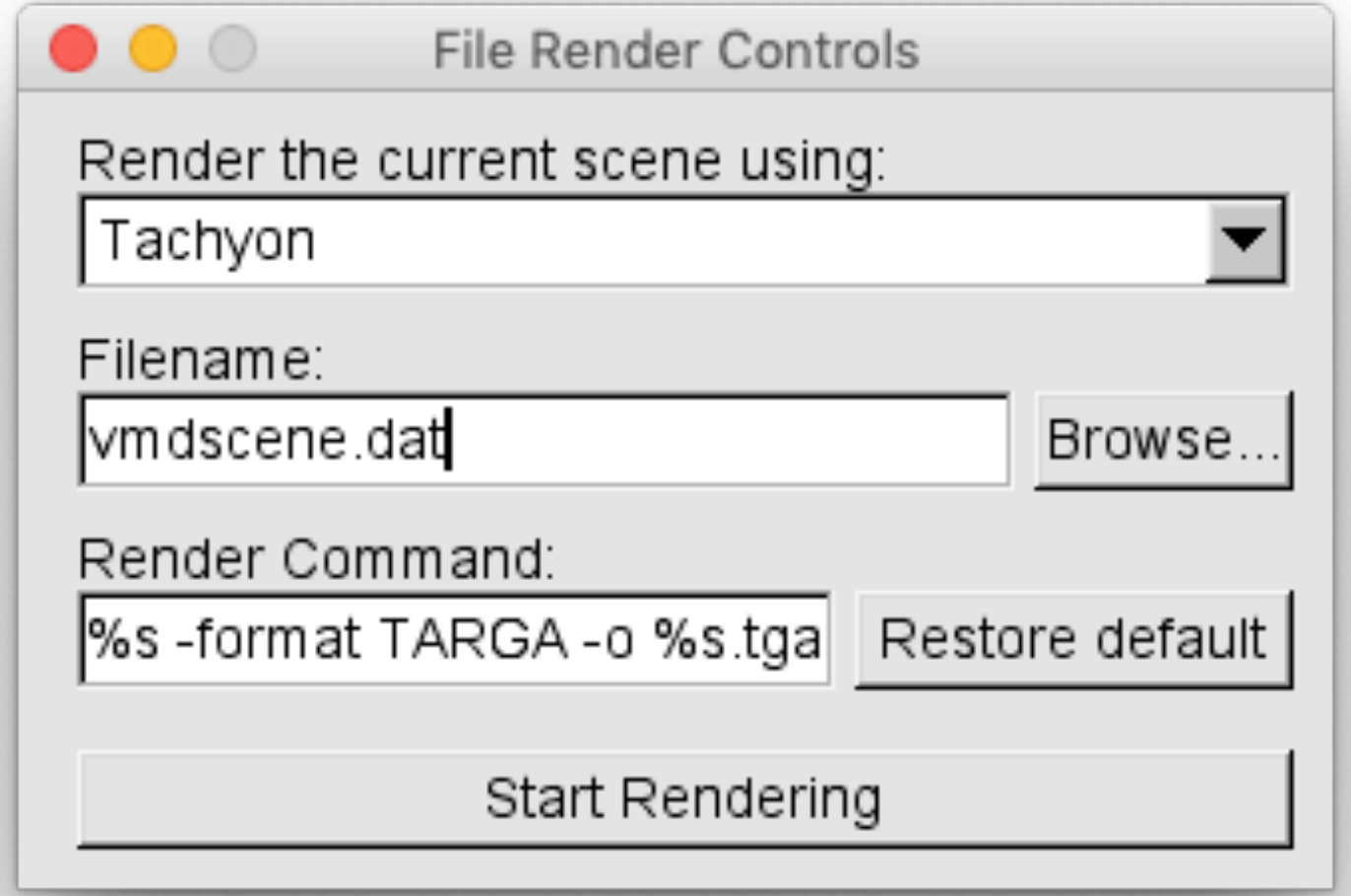
We will use Tachyon

This will generate two files:

vmdscene.dat
vmdscene.dat.tga



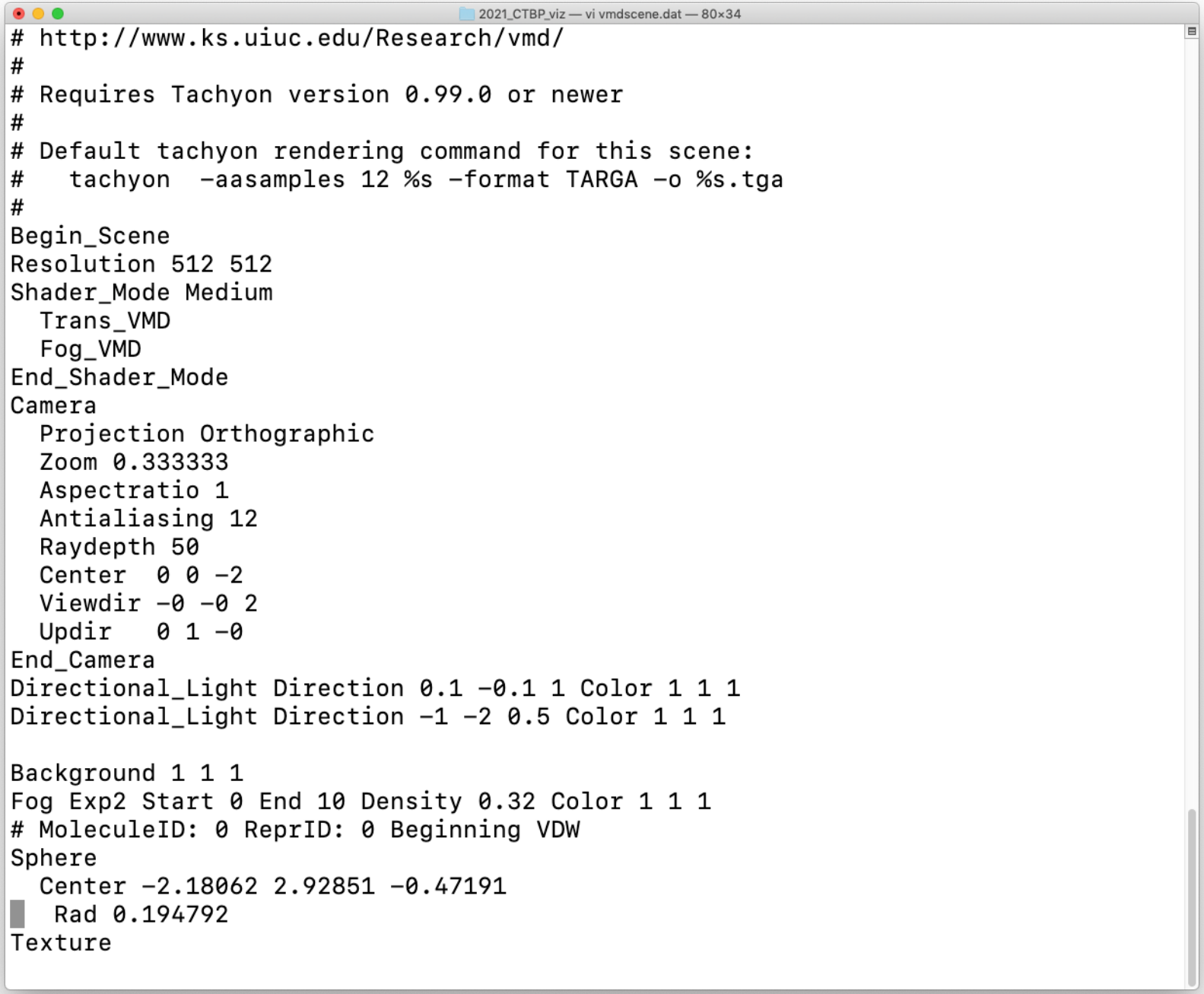
vmdscene.dat.tga looks even worse….



Open the .dat file

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

- At this point, we no longer necessarily need VMD.



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

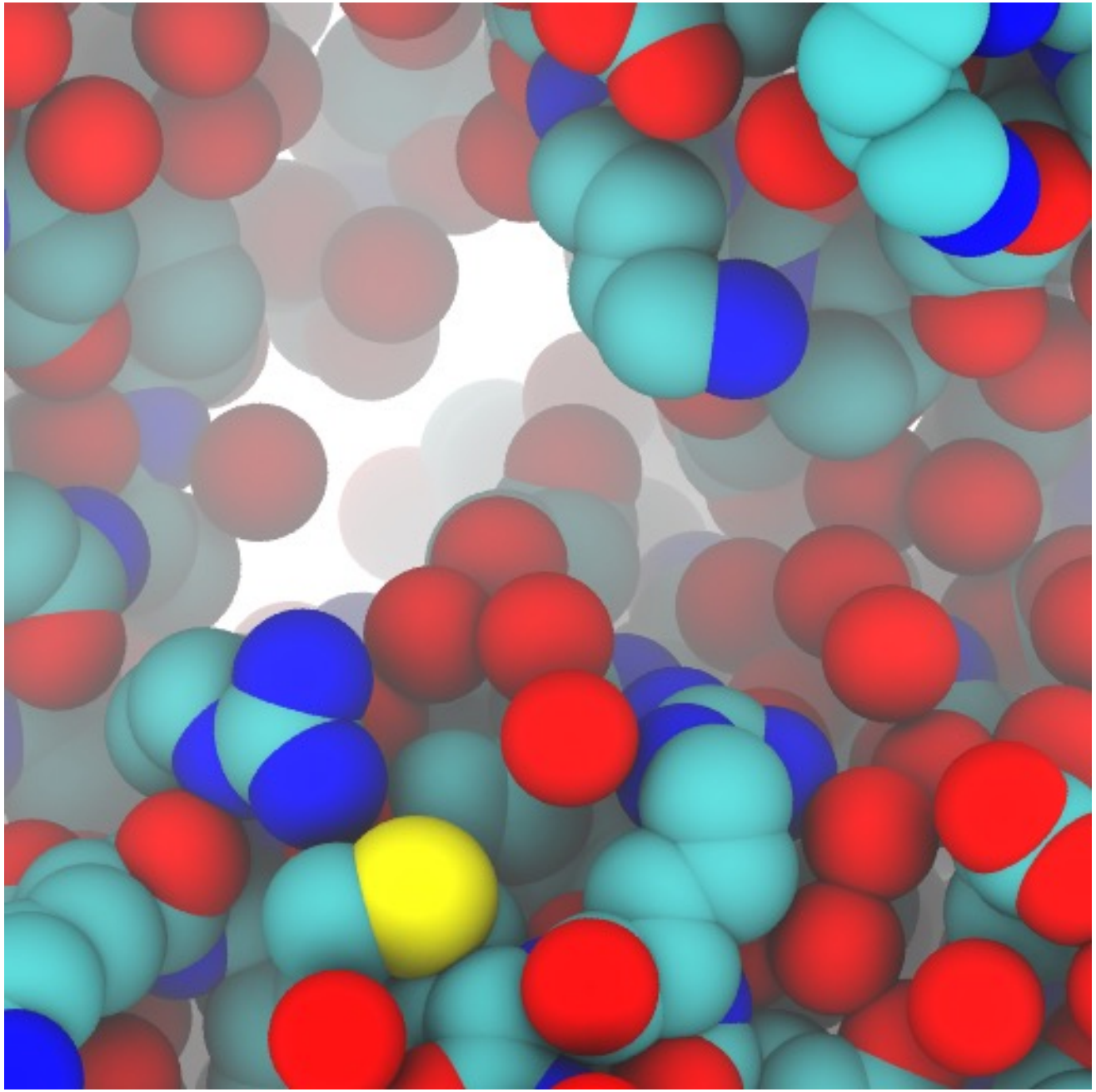
$tachyon just refers to your locally-available version

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

If too slow, add “–res 200 200” to your Tachyon call, to make a smaller test version of your image.

Looks better, but oversaturated. Perhaps too much light

Let’s try again with light at 1.2



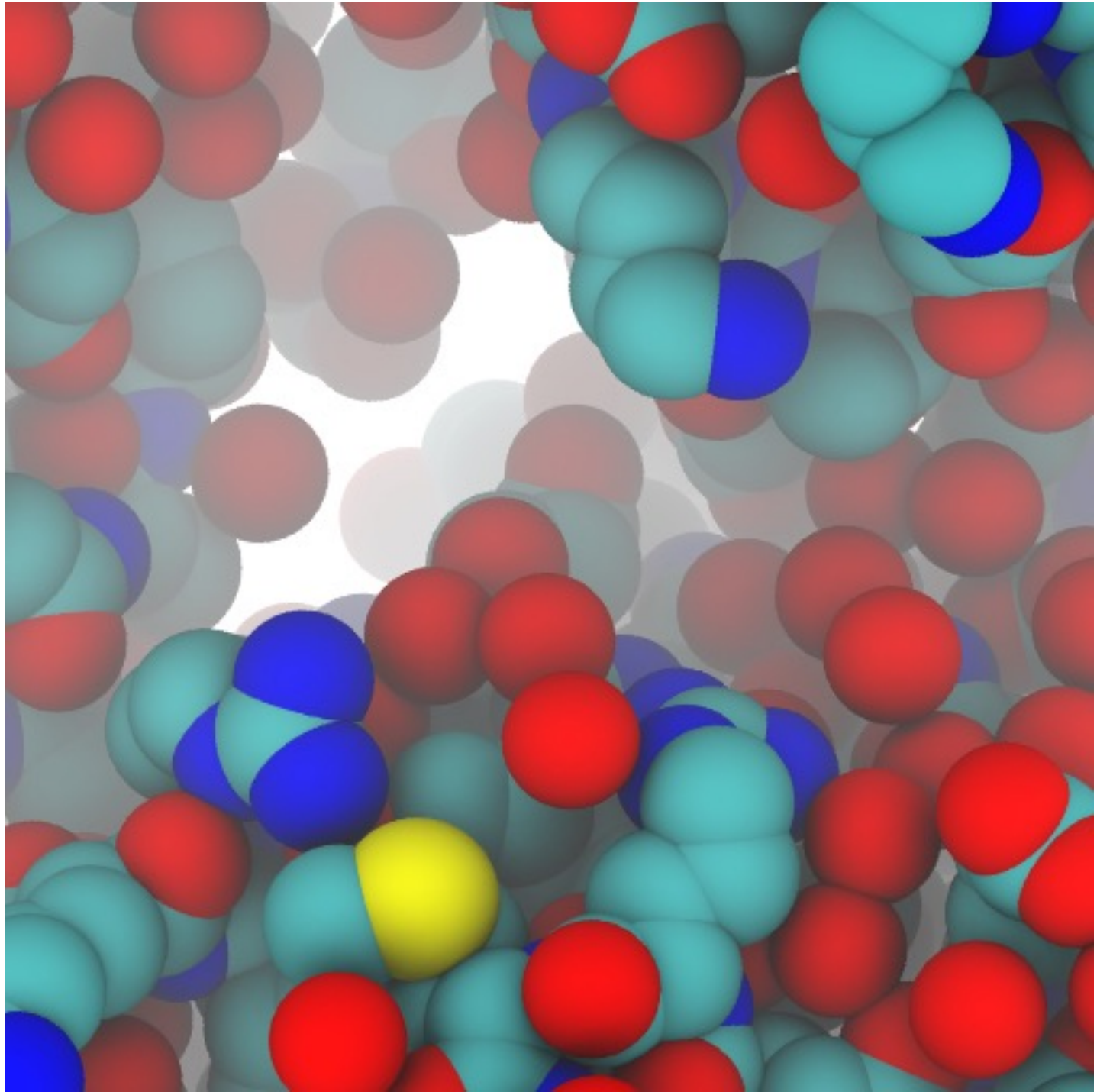
Better, but we can hardly see the atoms in back.

Too much depth queueing

Two options to correct:

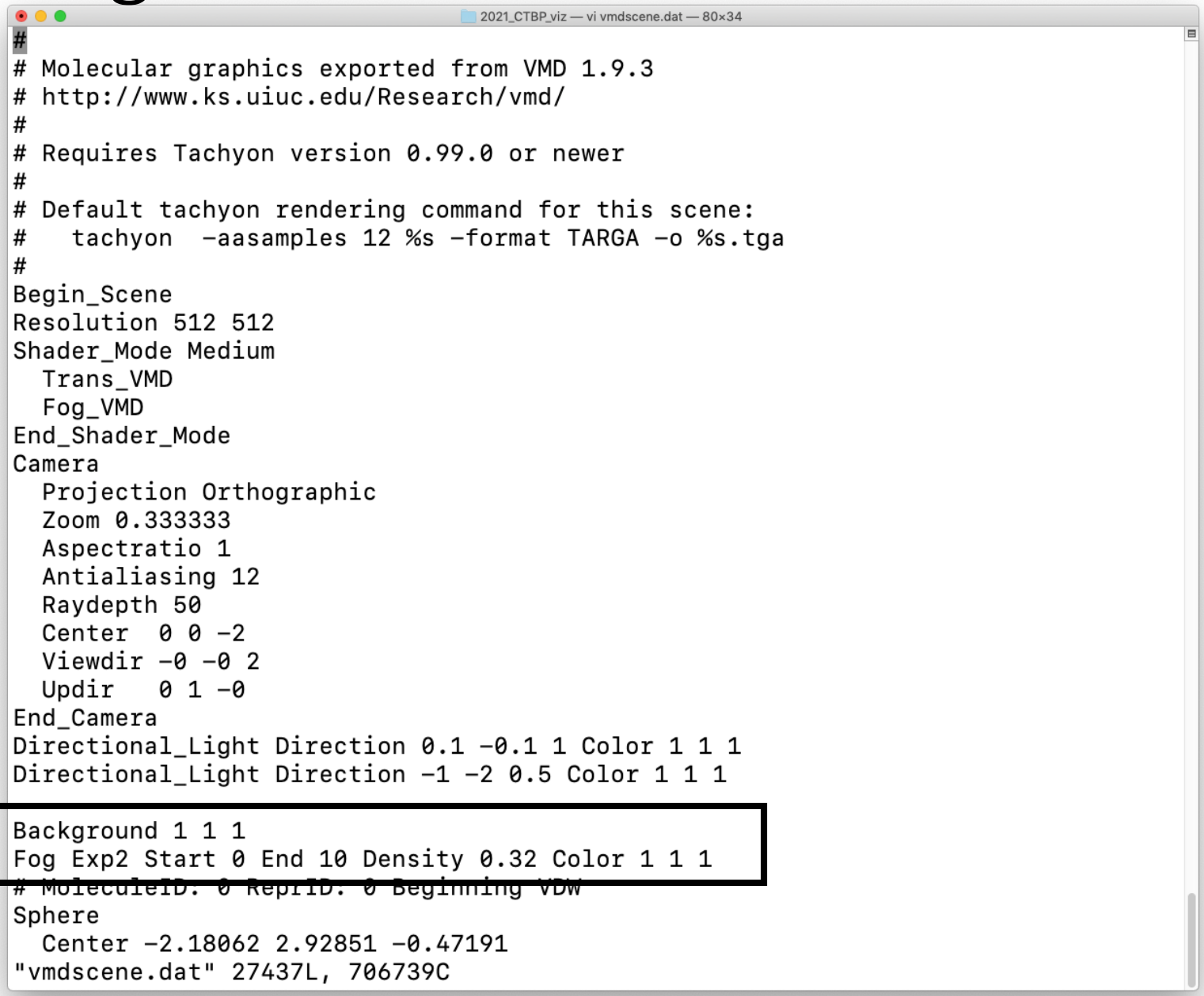
Change Cue Density under:
Display -> Display Settings
This would require us to regenerate the scene

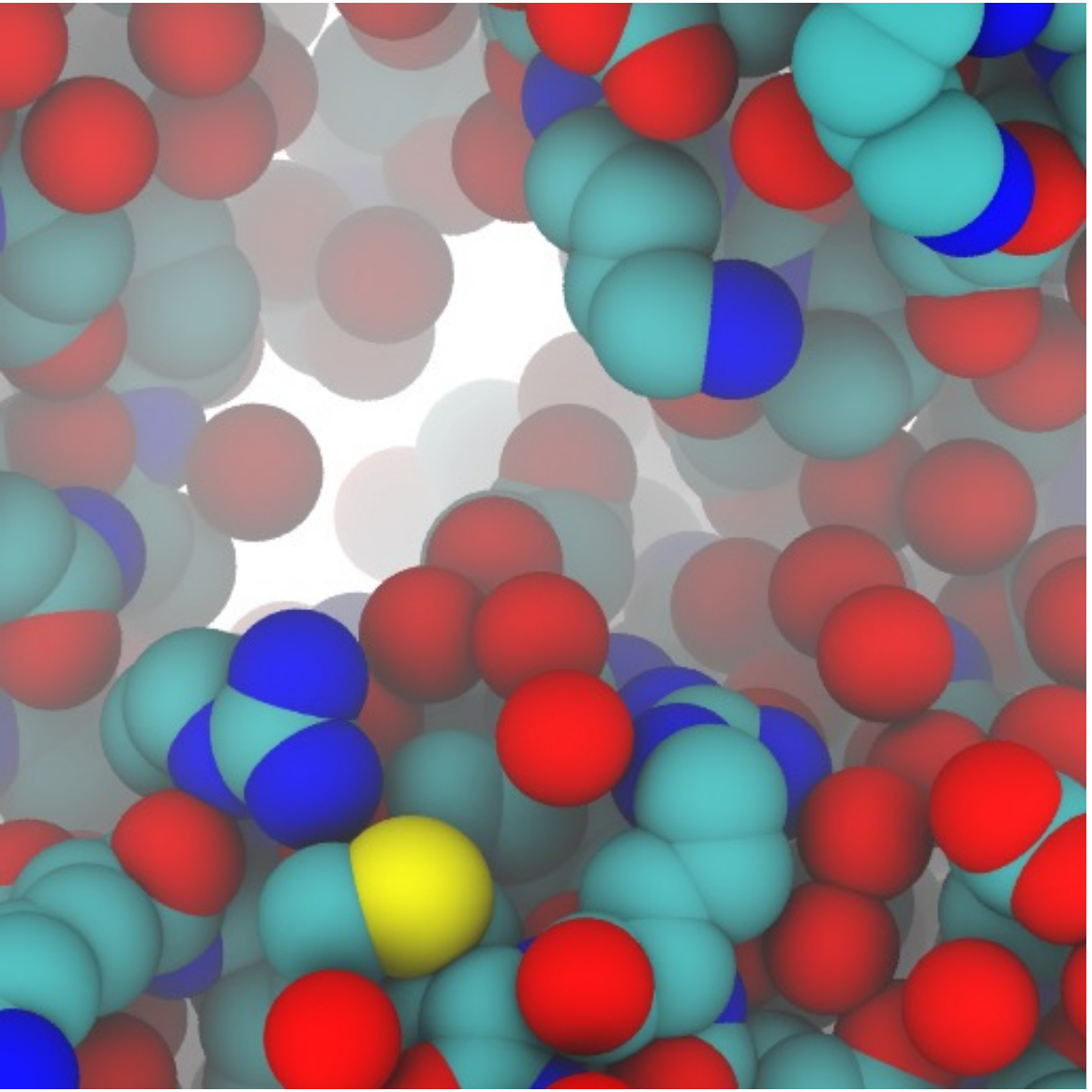
Change the scene file directly (recommended)



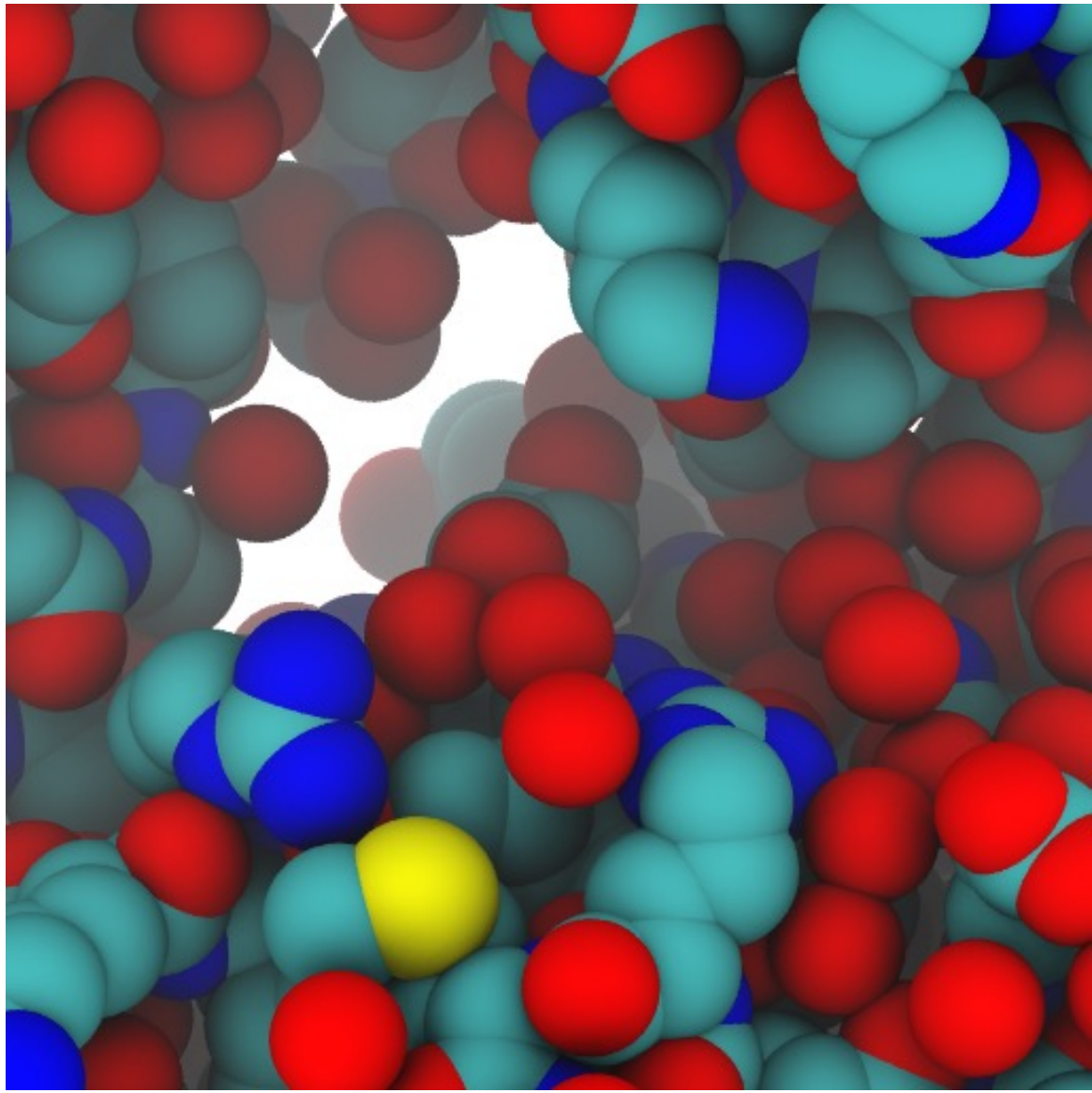
Change the scene using vi

- We will change the Density value (0.32) to 0.2
- Rerender with Tachyon





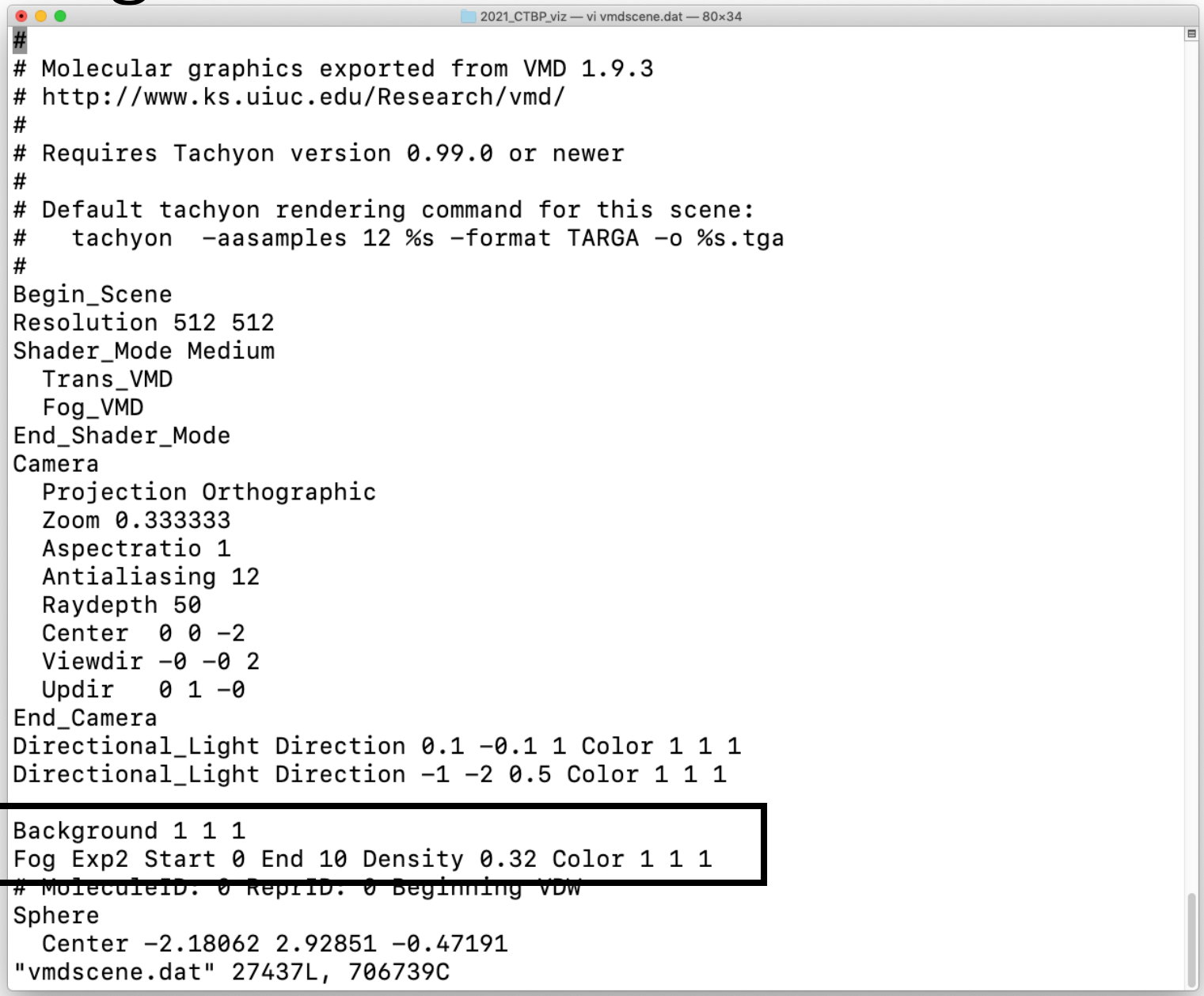
Density 0.32



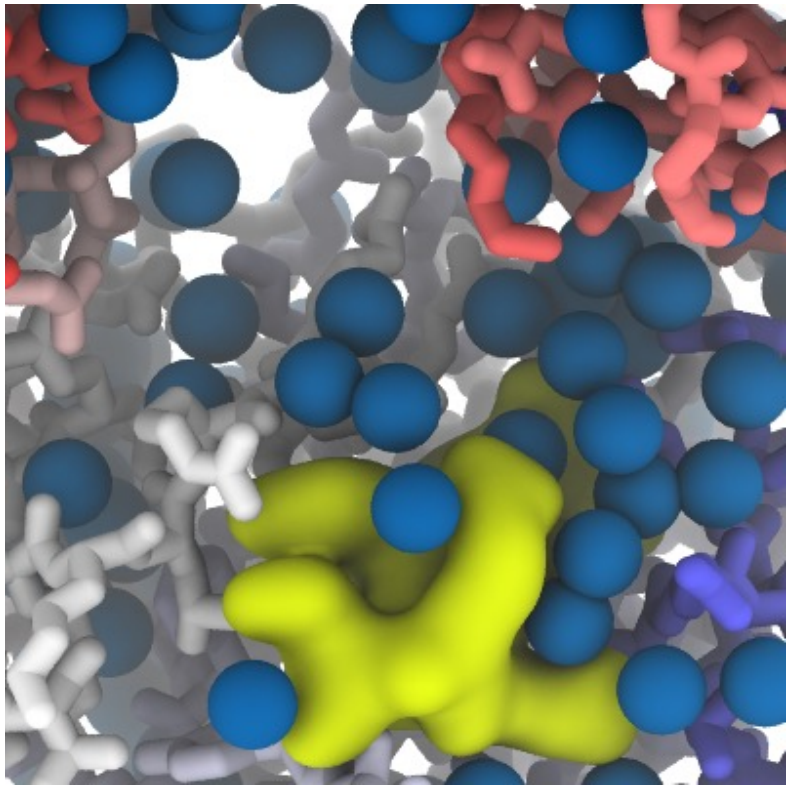
Density 0.2

Change the scene using vi

- Anything can be changed
  - Materials of individual objects
  - Colors
  - Background
  - Lighting
  - Antialiasing (12 is default, and usually ok)
- Highly recommend playing around with the scene directly
  - Can enable script-based modifications to movie frames…



General tips



- Only show atoms that are in view
  - Even particles that are not in view will cast shadows
- Most striking representations
  - Vdw
  - Licorice (expensive to render, see right)
    - Desirable to use thicker bond radius than the default
    - May want higher sphere resolution than 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.
- Remember, Tachyon is parallel! Use an interactive cluster node with many cores. A good image of a relatively large system (or high-res version for a poster) can easily take 5-20 minutes on a multi-core node.

Making an actual figure for a manuscript

- I always use Inkscape (free) or Adobe Illustrator ($$$$)
- Vector graphics support
  - So, export all elements you want to include in .svg format. For a simple figure, we will use gnuplot
  - In gnuplot, issue the following commands

    set terminal svg
    set output "example.svg"
    plot sin(x),cos(2x)

    Will generate example.svg (svg for Scalable Vector Graphic, which is very portable)

Image processing example

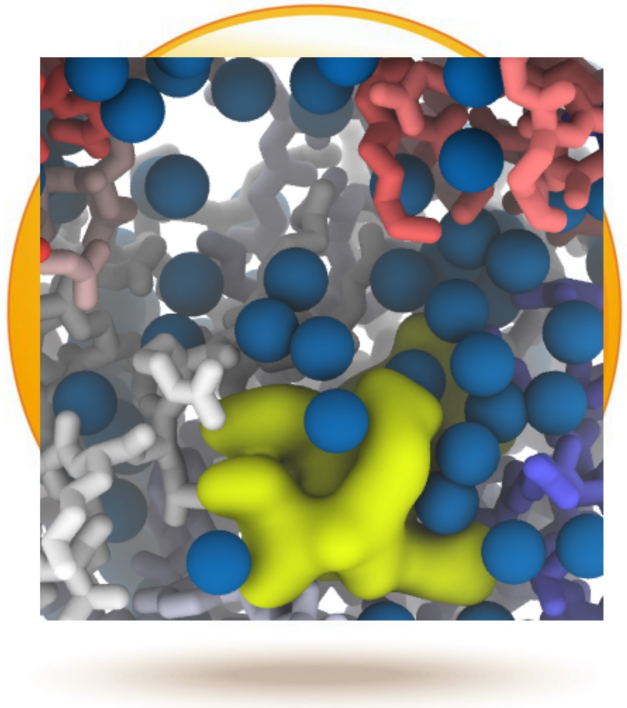
- Select the image, right click and select “ungroup”
- Now you can manipulate different elements
  - may have to repeatedly ungroup things
- In Inkscape:
  - Make lines thicker than you think is sane. Remember, the image is small in a paper
  - Delete all characters and replace them using the Text tool in Inkscape
    - Makes them easier to modify later
  - Make text larger than is comfortable. See reason above.
  - Make different types of labels the same size (axis labels same size, but different from legends)

Basic tips

- Adding text on top of graphics can be ugly
  - Consider a semi-transparent box underneath the text, but on top of the molecule.
- Clipping images can be helpful, especially for saving wasted space.
- Lock image aspect ratios

A nice side trick (use Gimp for this)

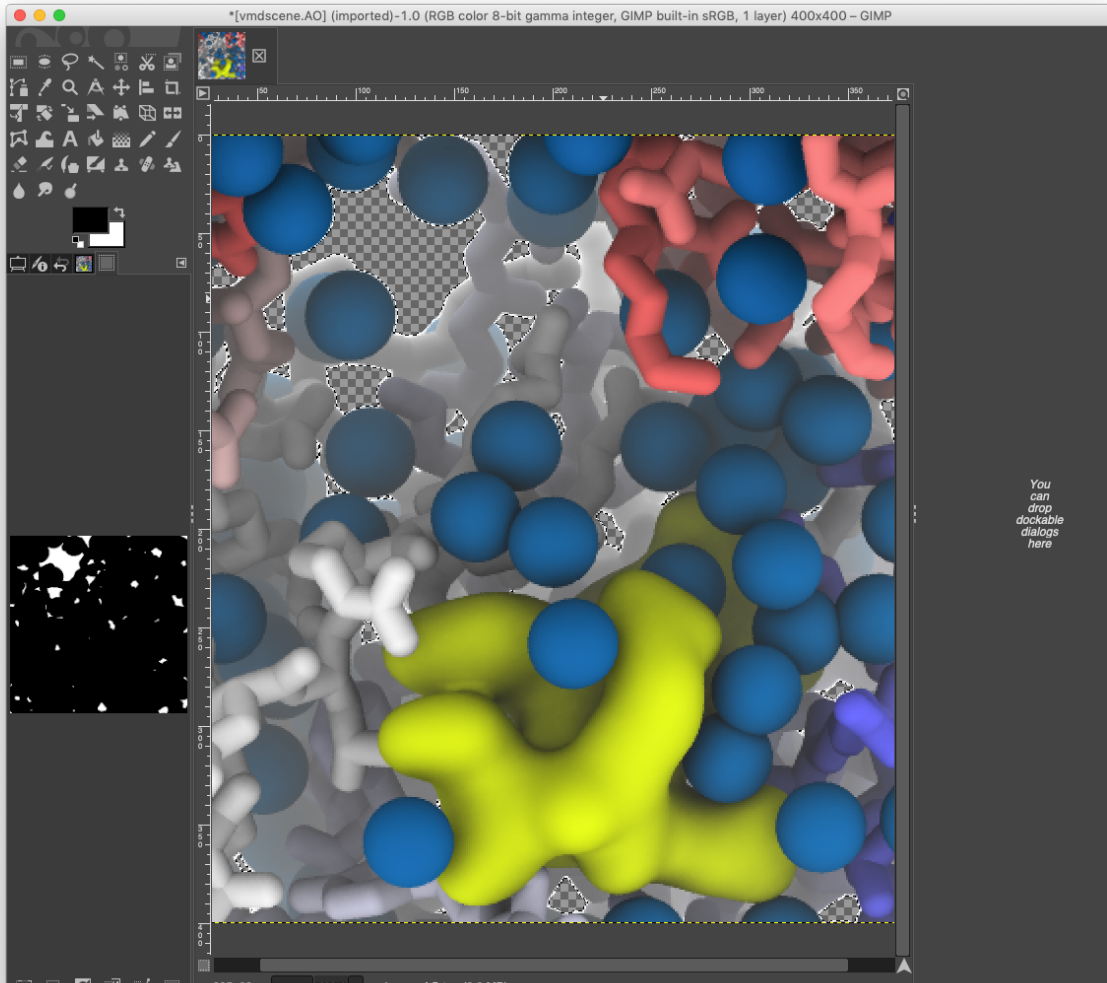
- Let’s have someone look at us from behind our molecule
- If we just place the molecule image on top, we can’t see the image beneath

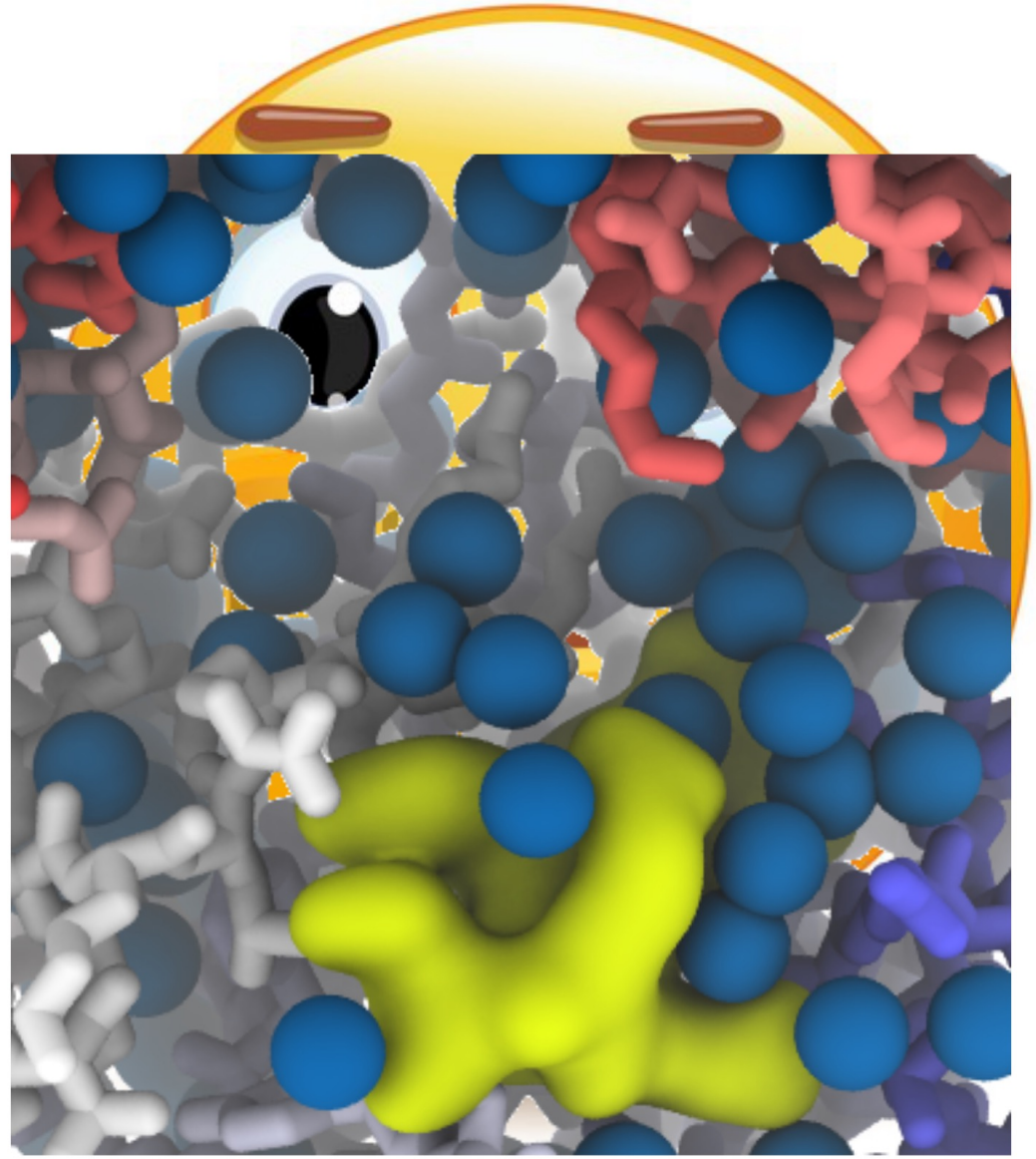


Use the alpha channel (Gimp)

- Turn on alpha channel (controls transparency)
- In Gimp
  - Layer -> Transparency -> Add Alpha Channel
  - Select all white and remove it
    - Select -> By Color
    - Then click the color you want to select
    - Delete with the “delete” key
    - After deleting, should look like image on right
  - Export as a PNG file (other formats can work)

- Now you can use the PNG in Inkscape to make a layered image





Topics

- Making movies
  - Perspectives and time sequences
  - ~~Rendering frames~~
  - Editing frames
  - Post-processing (making the movie)

- ~~Making figures~~
  - ~~Generating high-res images~~
  - ~~Basics of editing vector graphics~~
  - ~~A trick for bitmaps~~

Movie Making: Changing perspective

From the Tk Console in VMD, ”source” the file viewpoint.tcl

This will allow us to save perspectives and move between them

Rotate your system to a view that you like and type “save_vp 1” in Tk

Translate/rotate/zoom to a different view and type “save_vp 2” in Tk

Move between them with “move_vp 1 2”

If you want to save the scene of each frame during the transition, use:

> move_vp_render 1 2 0 . Move

Moves between 1 and 2. Indexes the frames starting with 0. Writes them to the current directory. Gives each name the prefix “Move”. Will write 50 scenes (number can be changed)

Next you will need to run Tachyon on each frame (use a cluster)

Movie Making: incrementing frames

- In Tk, source the file “movie_stuff.tcl”
- To watch the frames of interest:
  - > increment_np 1 20 1
  - “_np” for no picture
- When ready to save the frames
  - > increment 1 20 1
  - This will write out a scene for each frame

- Note: trajectory smoothing can be defined in the Representation window. Settings will apply during rendering.

Movie Making Tip

- Make proc of the full visualization process before rendering. You can then watch it before writing a lot of stuff…
- i.e. used move_vp and increment_np
- See examples in movie_stuff.tcl (commented out procs)

Let’s pull it all together - Adobe Premiere