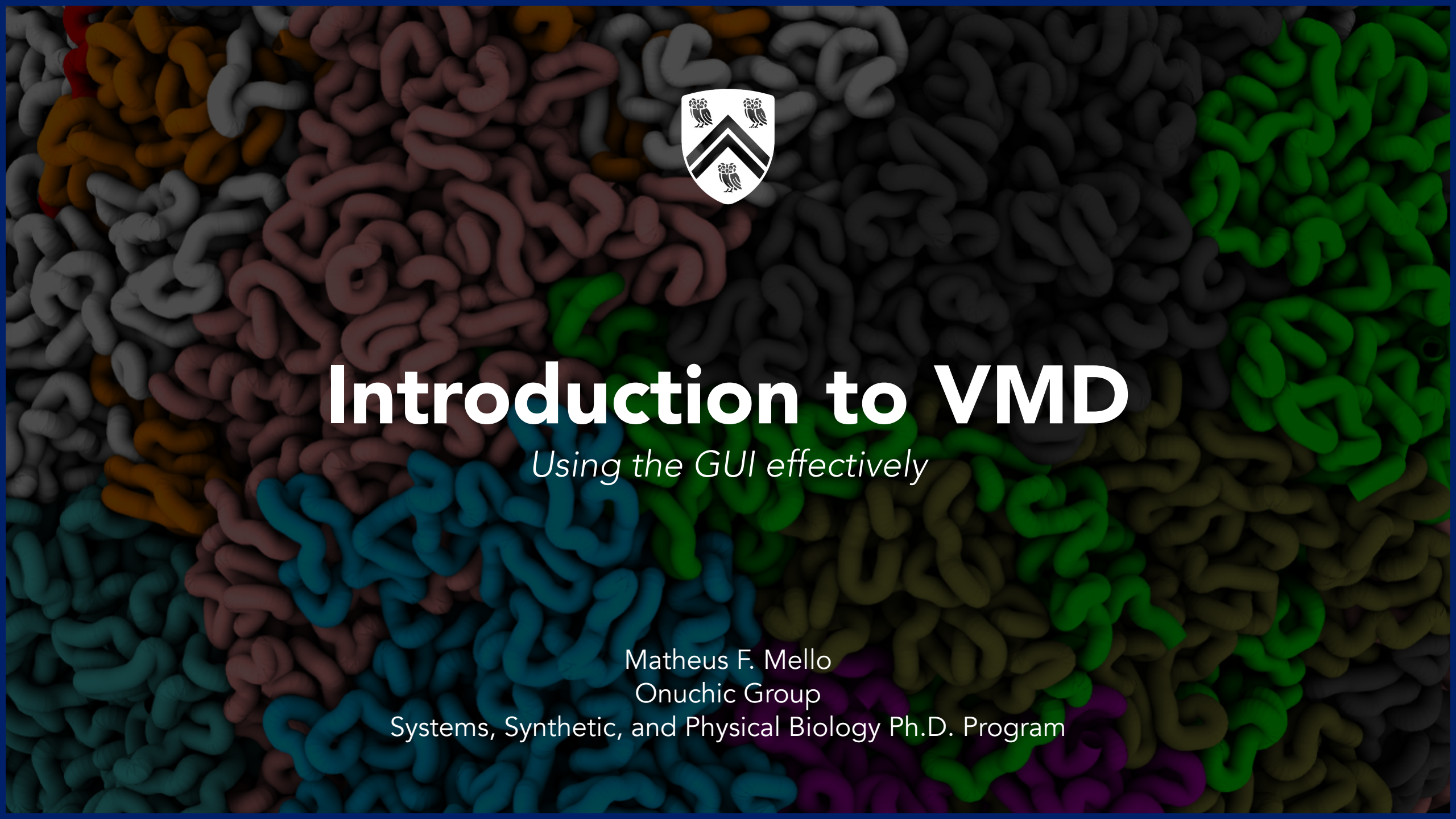


Introduction to VMD

Using the GUI effectively

Matheus F. Mello
Onuchic Group
Systems, Synthetic, and Physical Biology Ph.D. Program

Agenda

Installing VMD

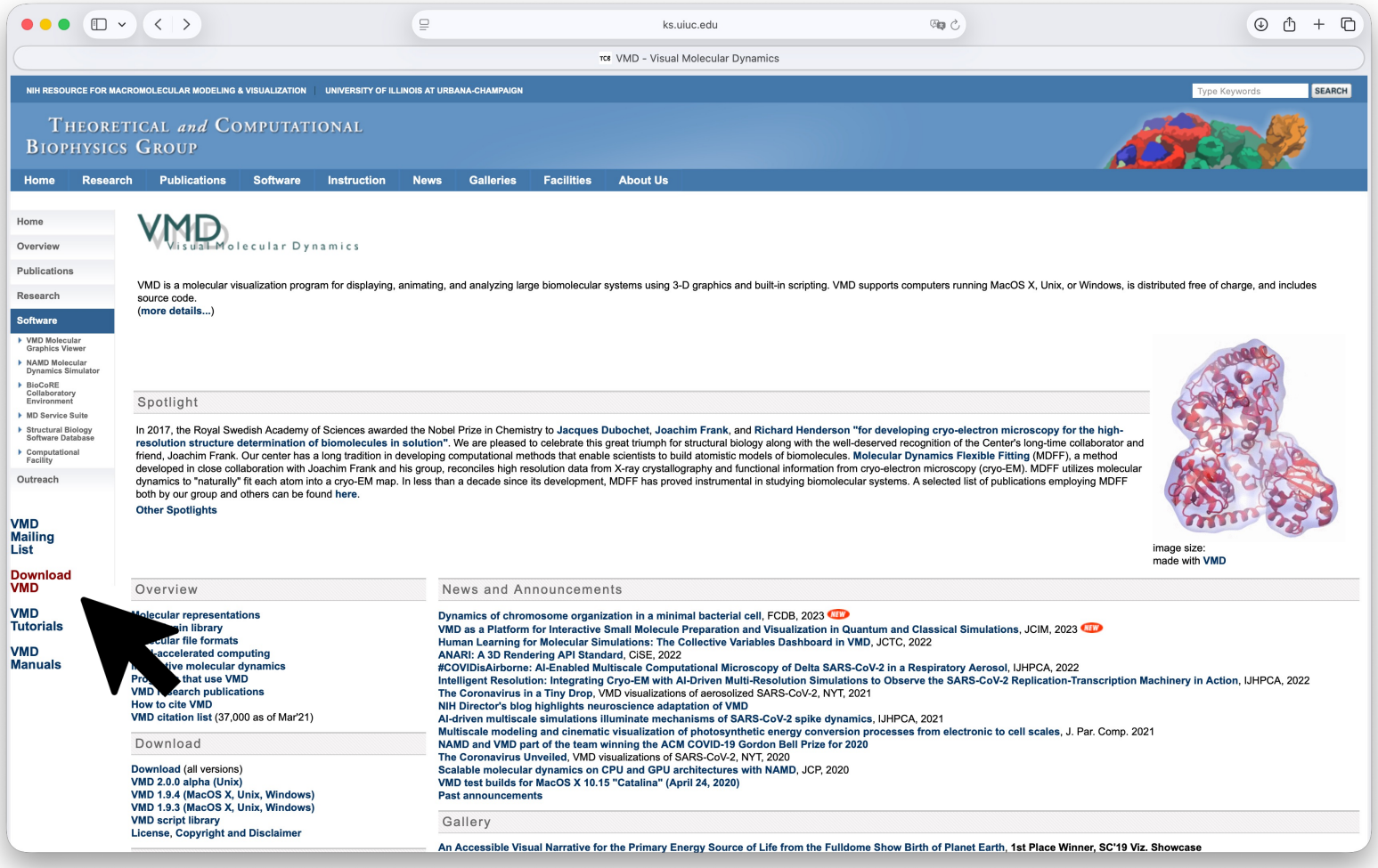
Basic UI elements

Rendering images

Rendering videos

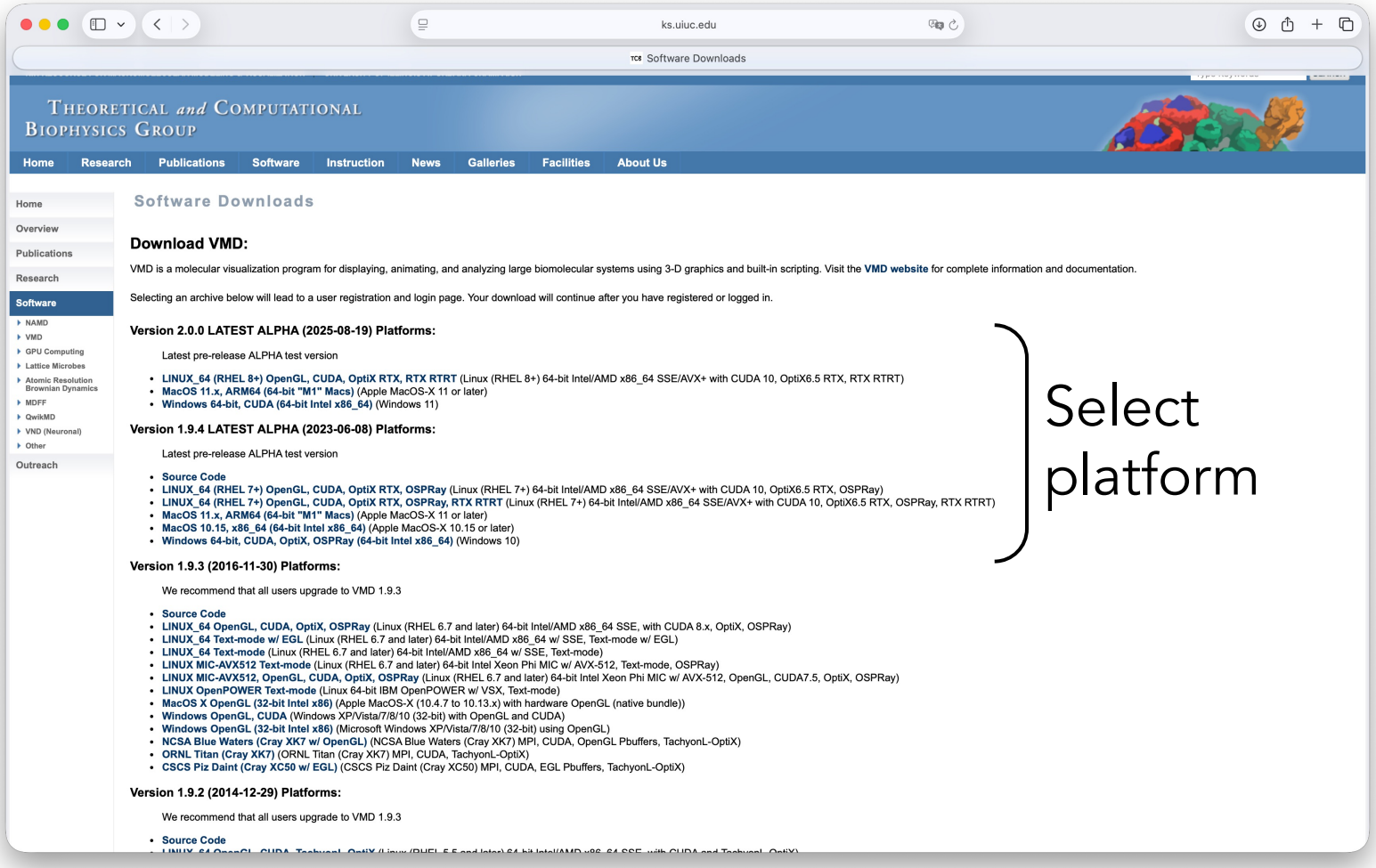
Visual Molecular Dynamics, VMD

VMD Website

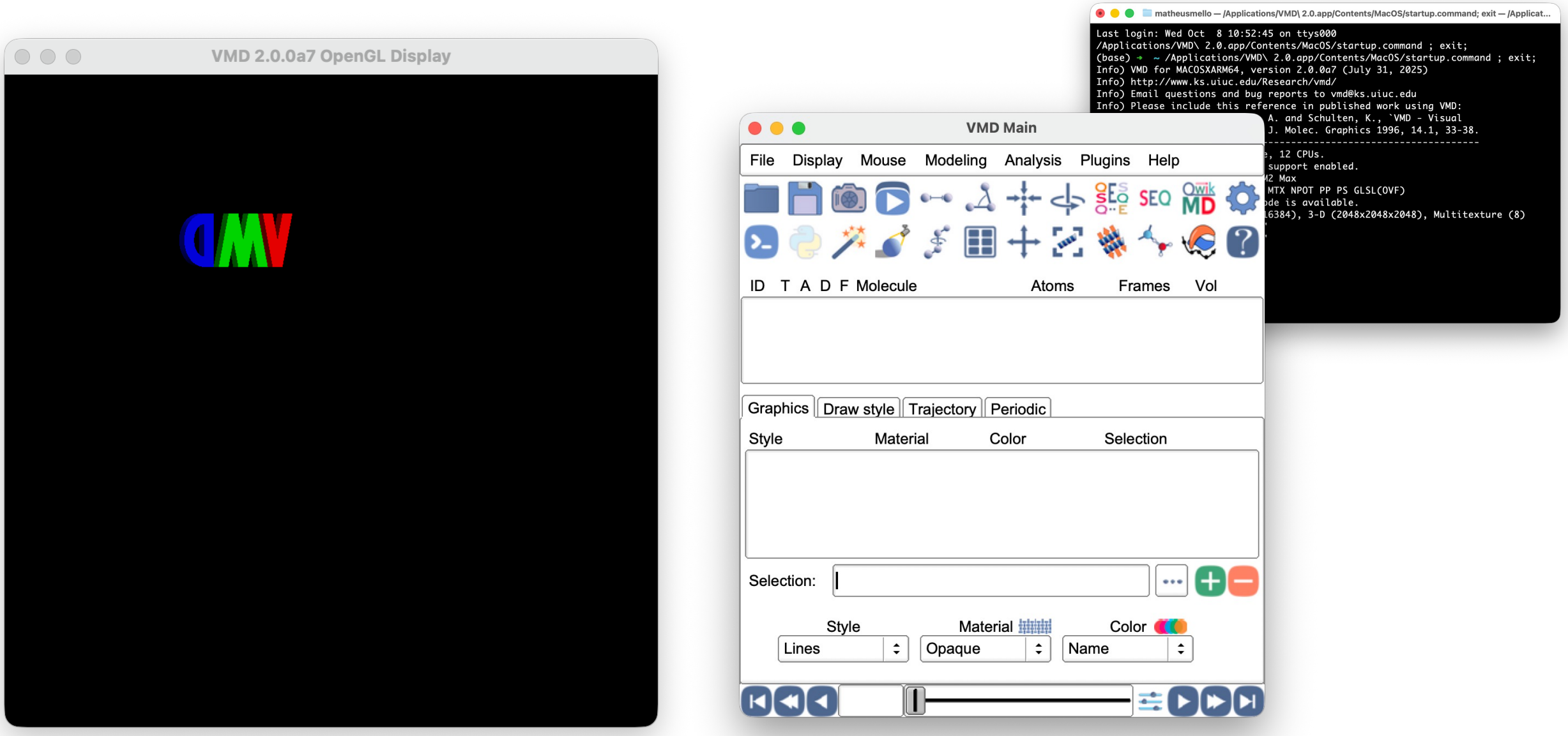


Visual Molecular Dynamics, VMD

VMD Website

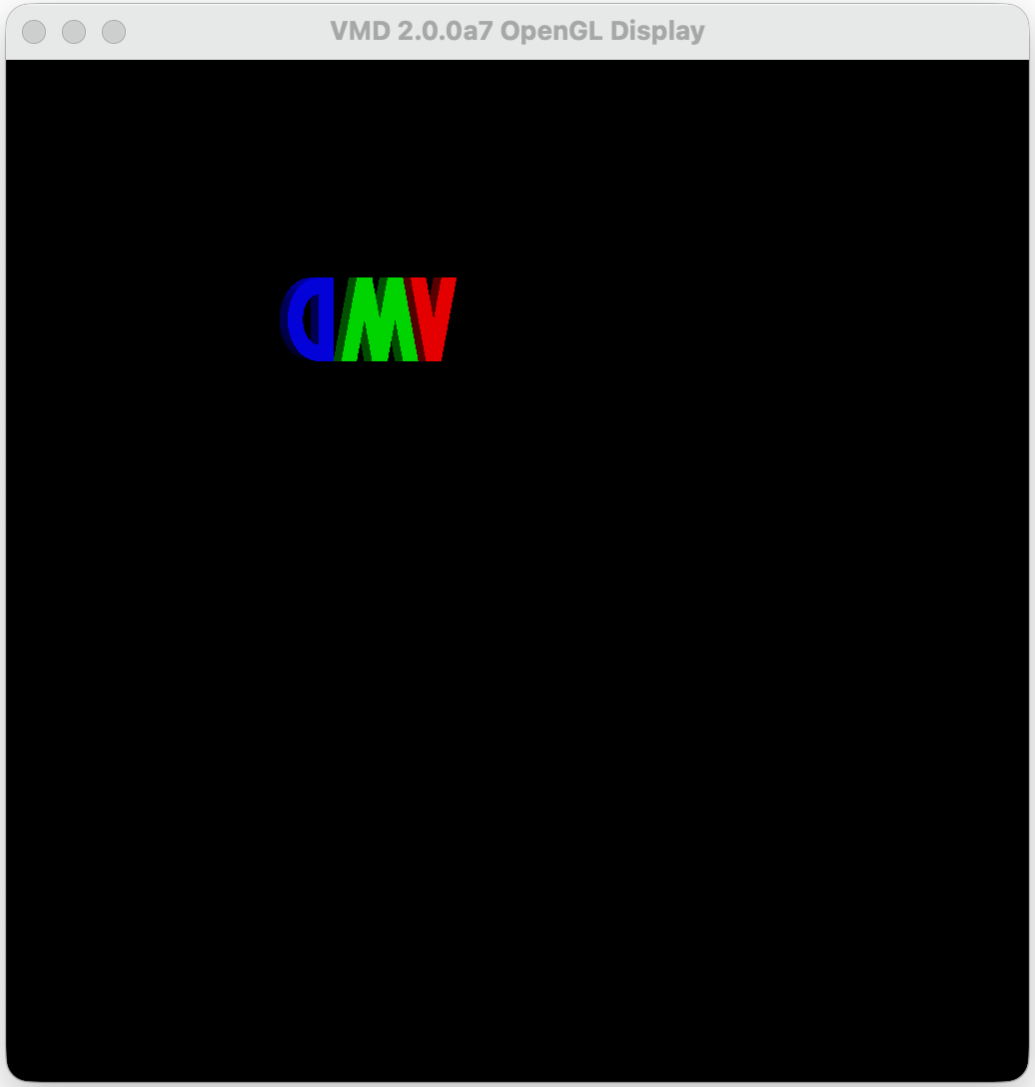


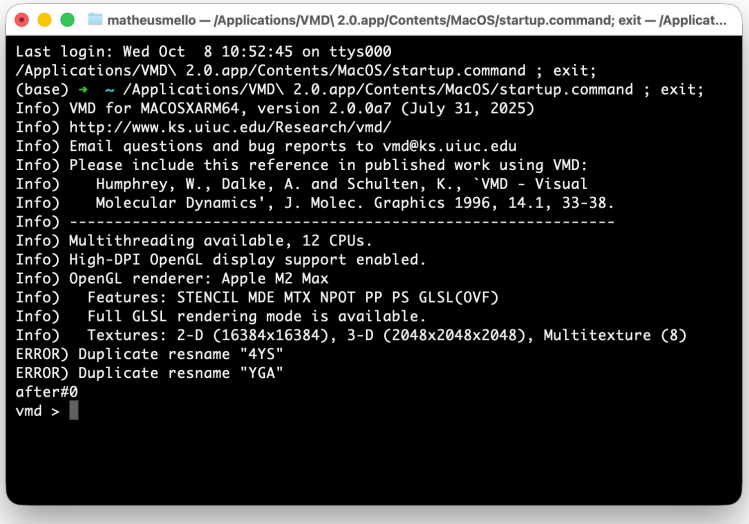
Opening VMD

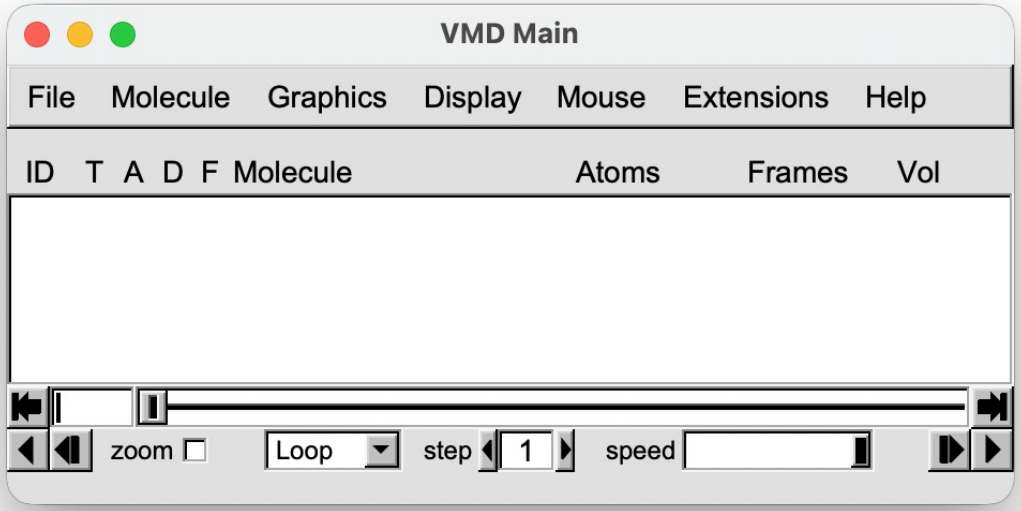


version 2.0.0

Opening VMD

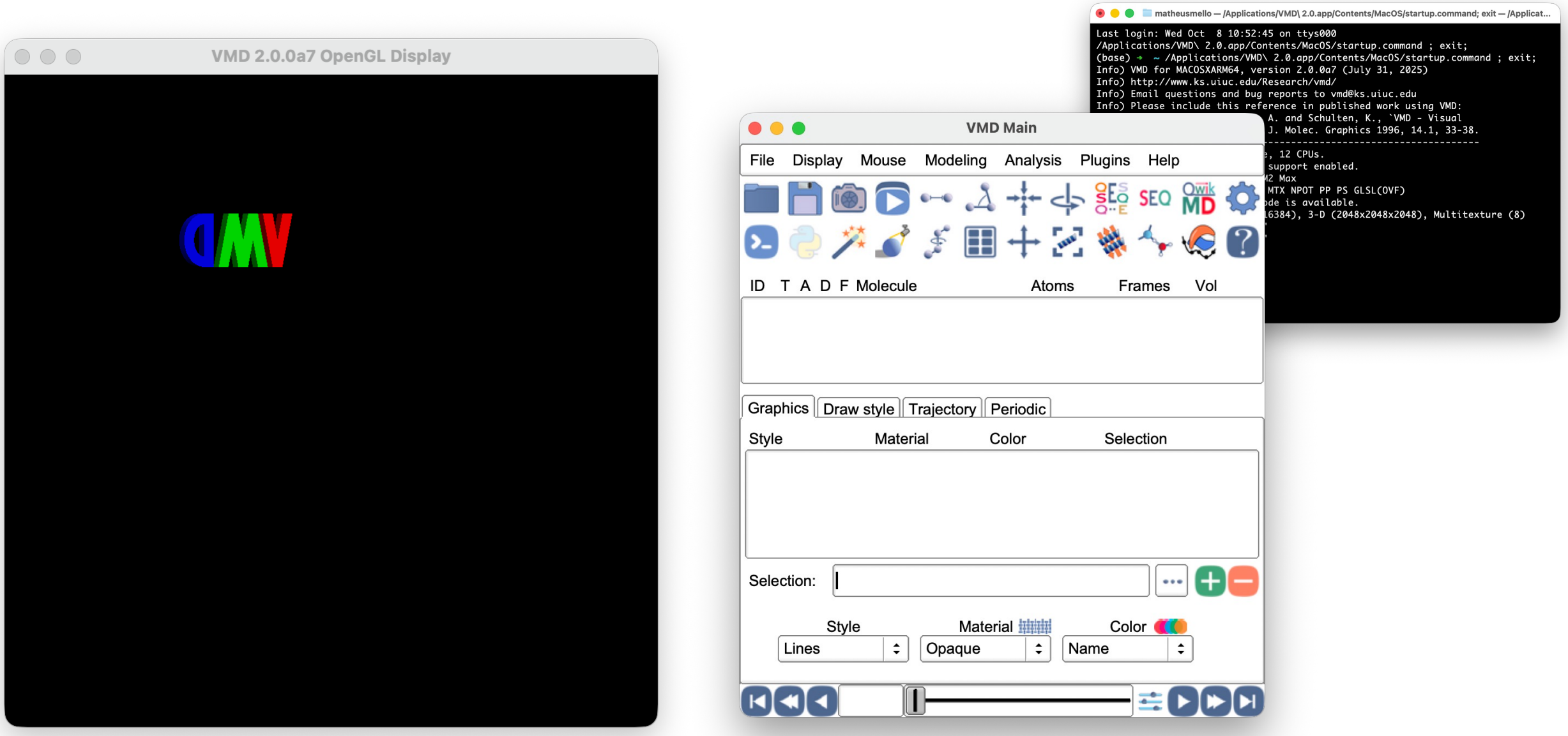






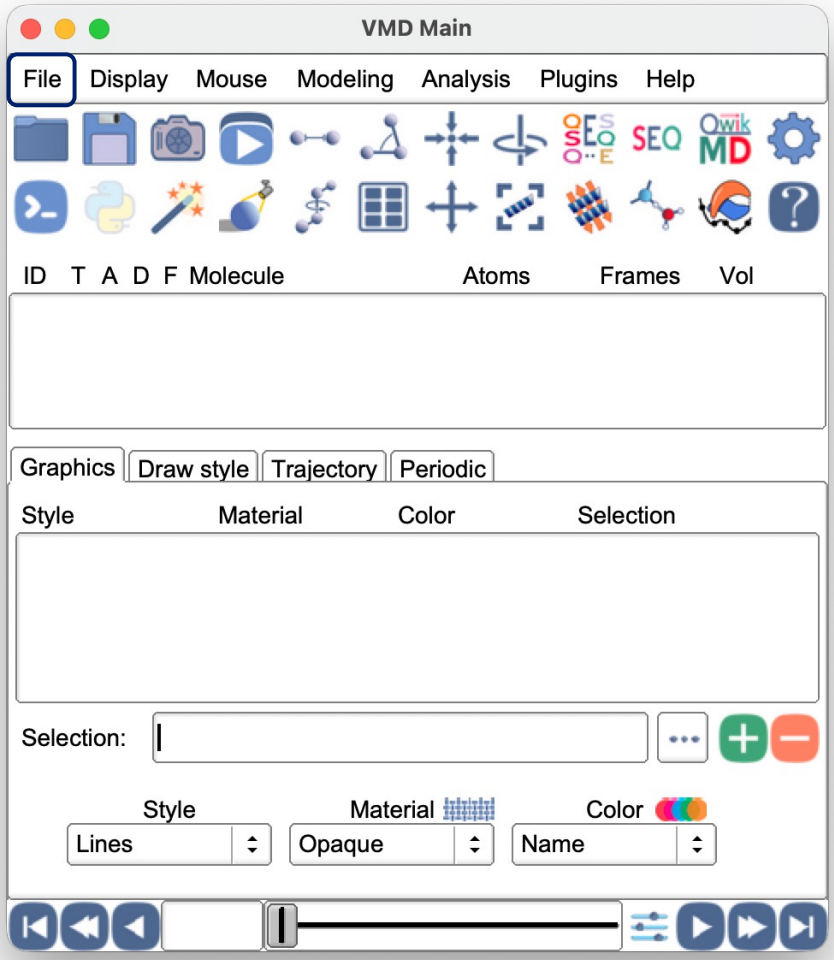
version 1.9.4

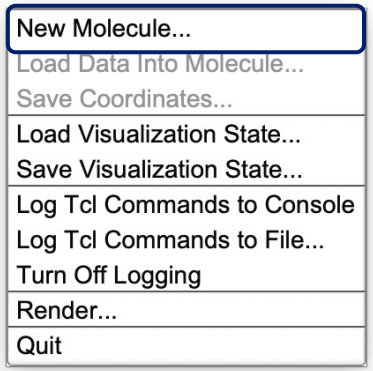
Opening VMD

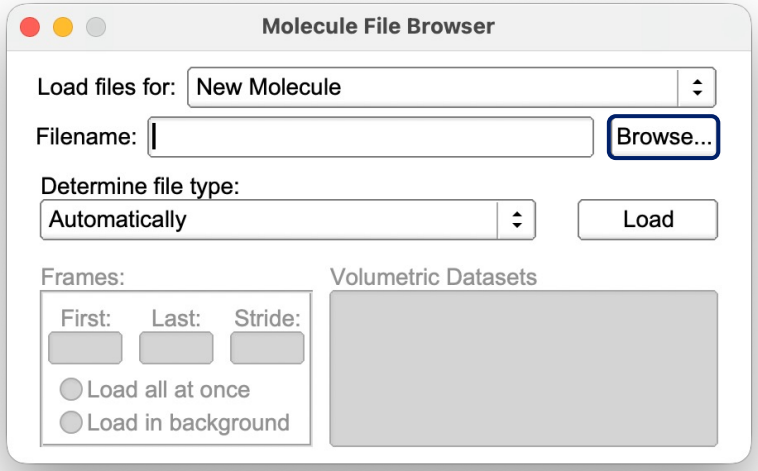


version 2.0.0

Loading a molecule





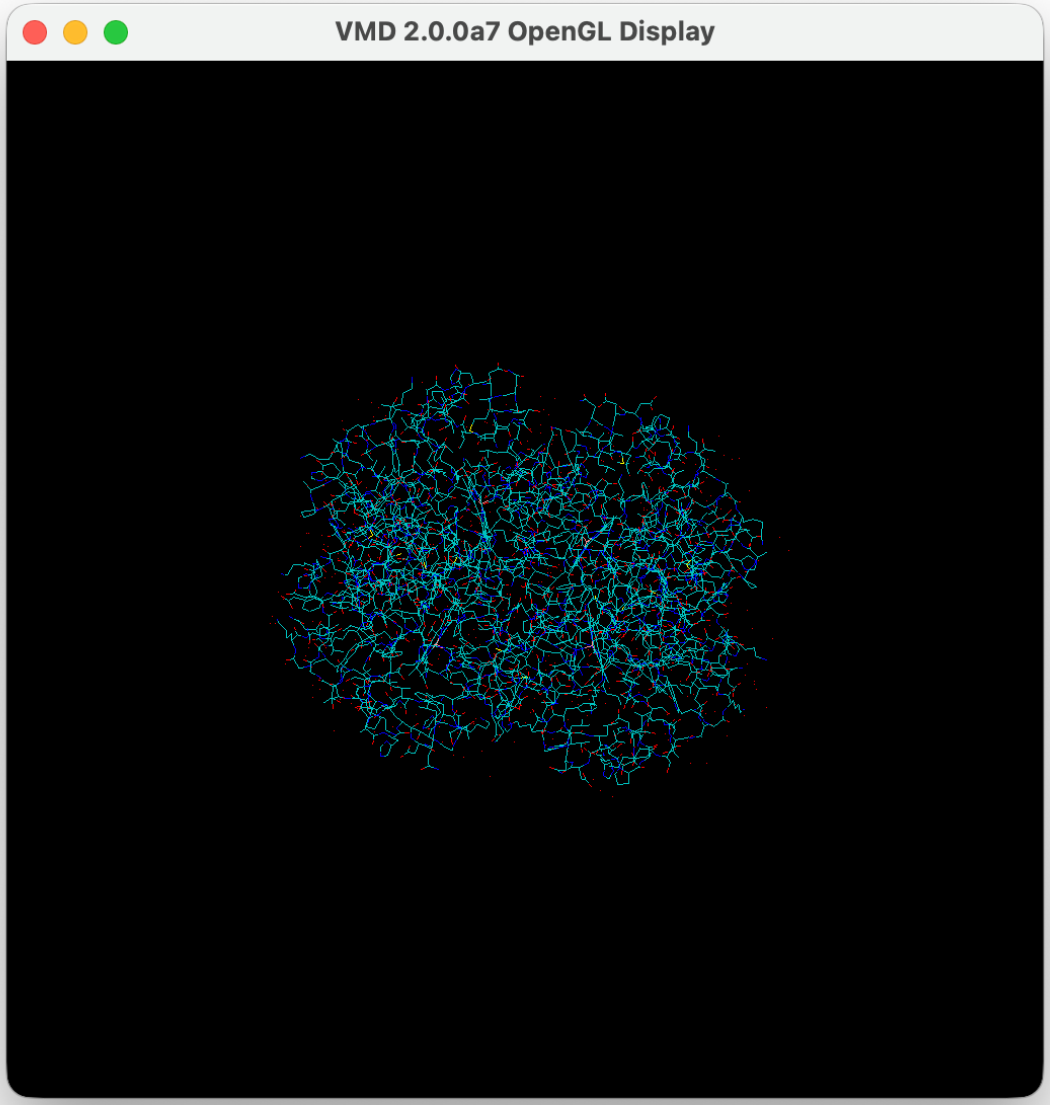


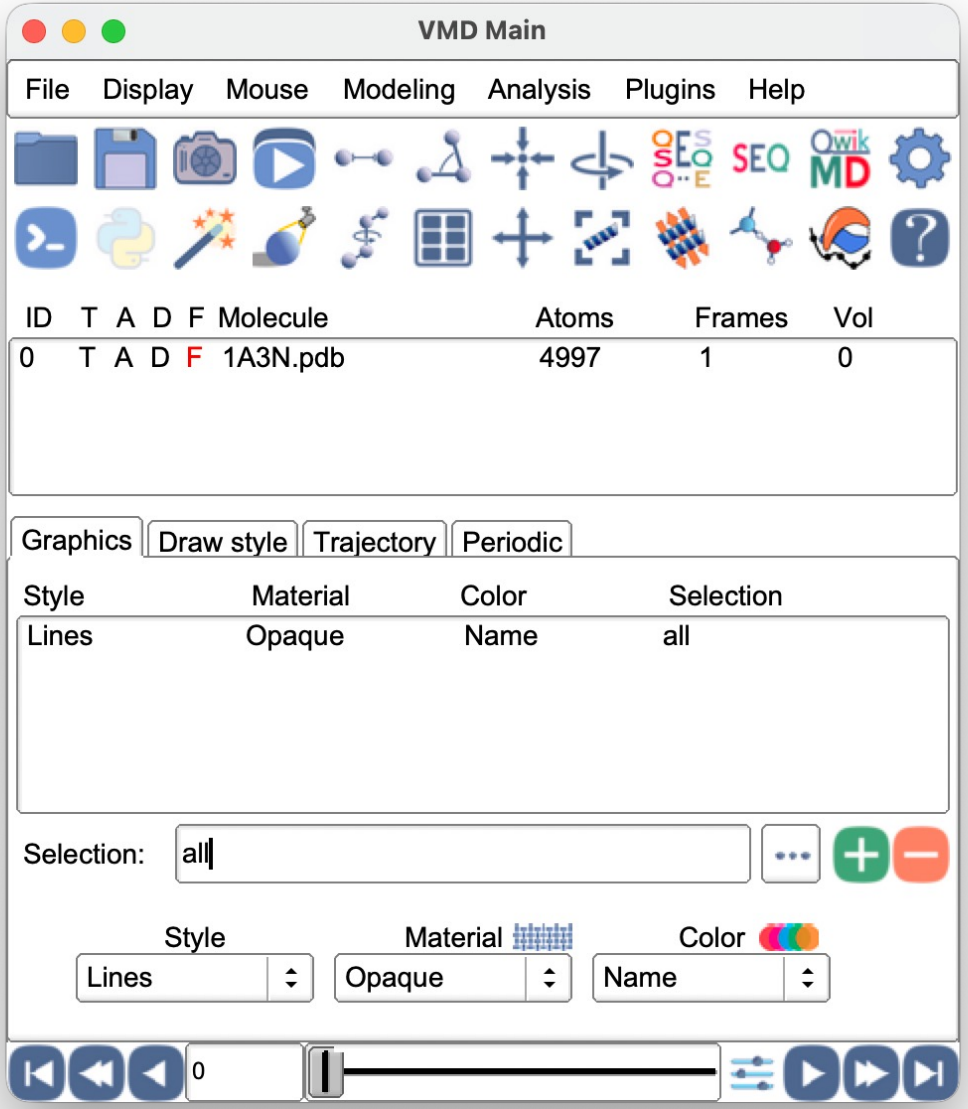
Download PDB

Also at: https://github.com/Whitford/ctbp-techtalks

version 2.0.0

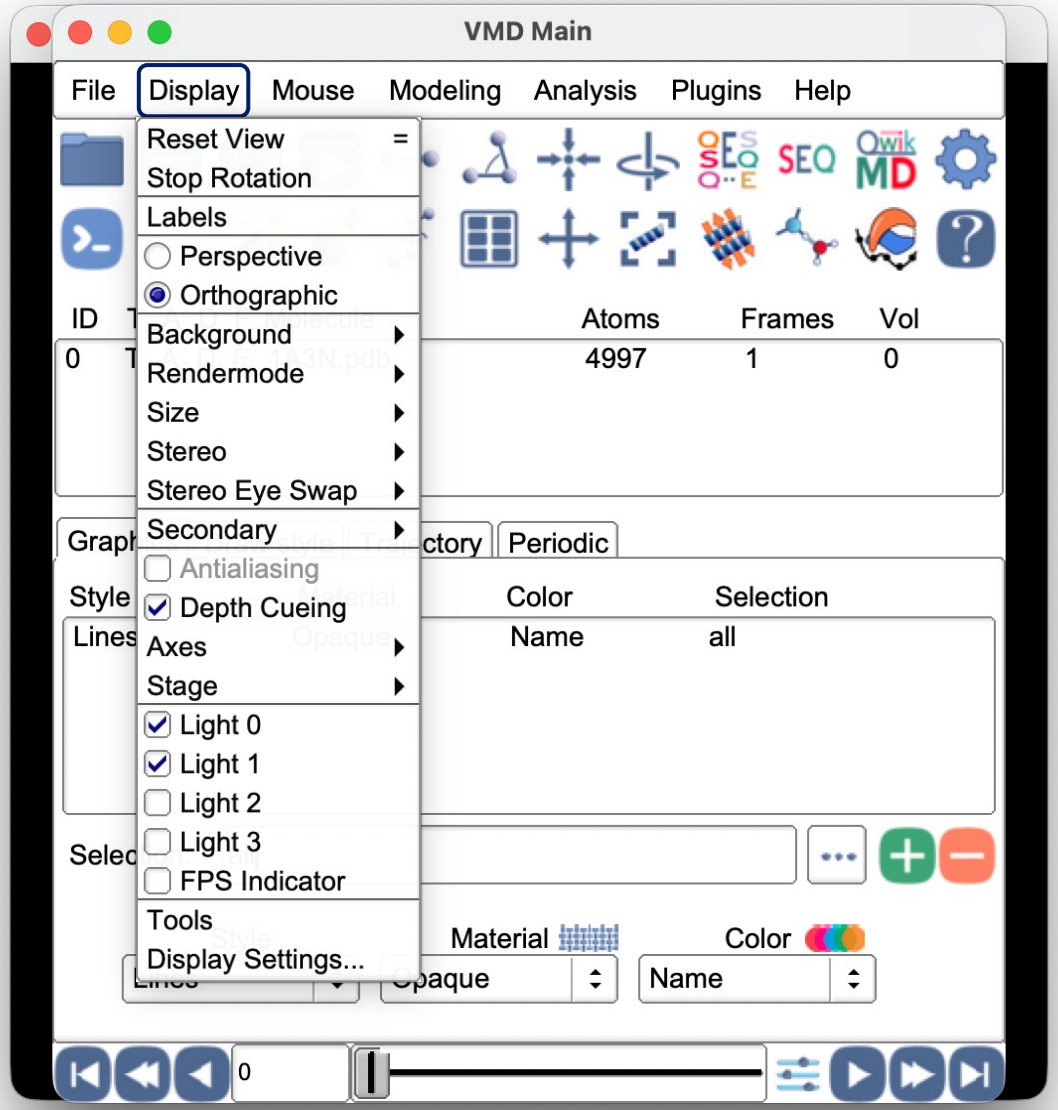
Loading a molecule





version 2.0.0

Changing Display options



We can change under `Display`:

`Perspective > Orthographic`

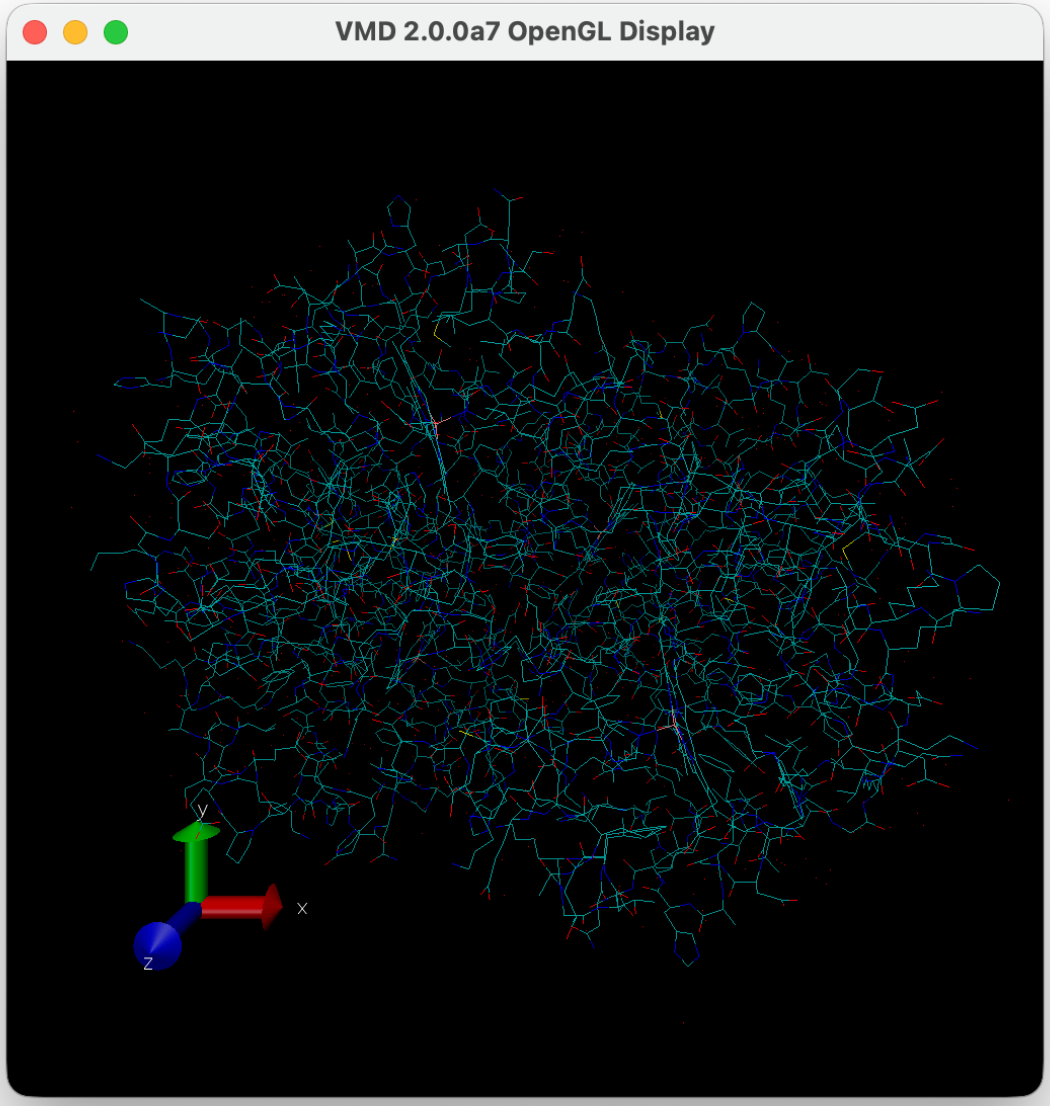
`Axes > Off`

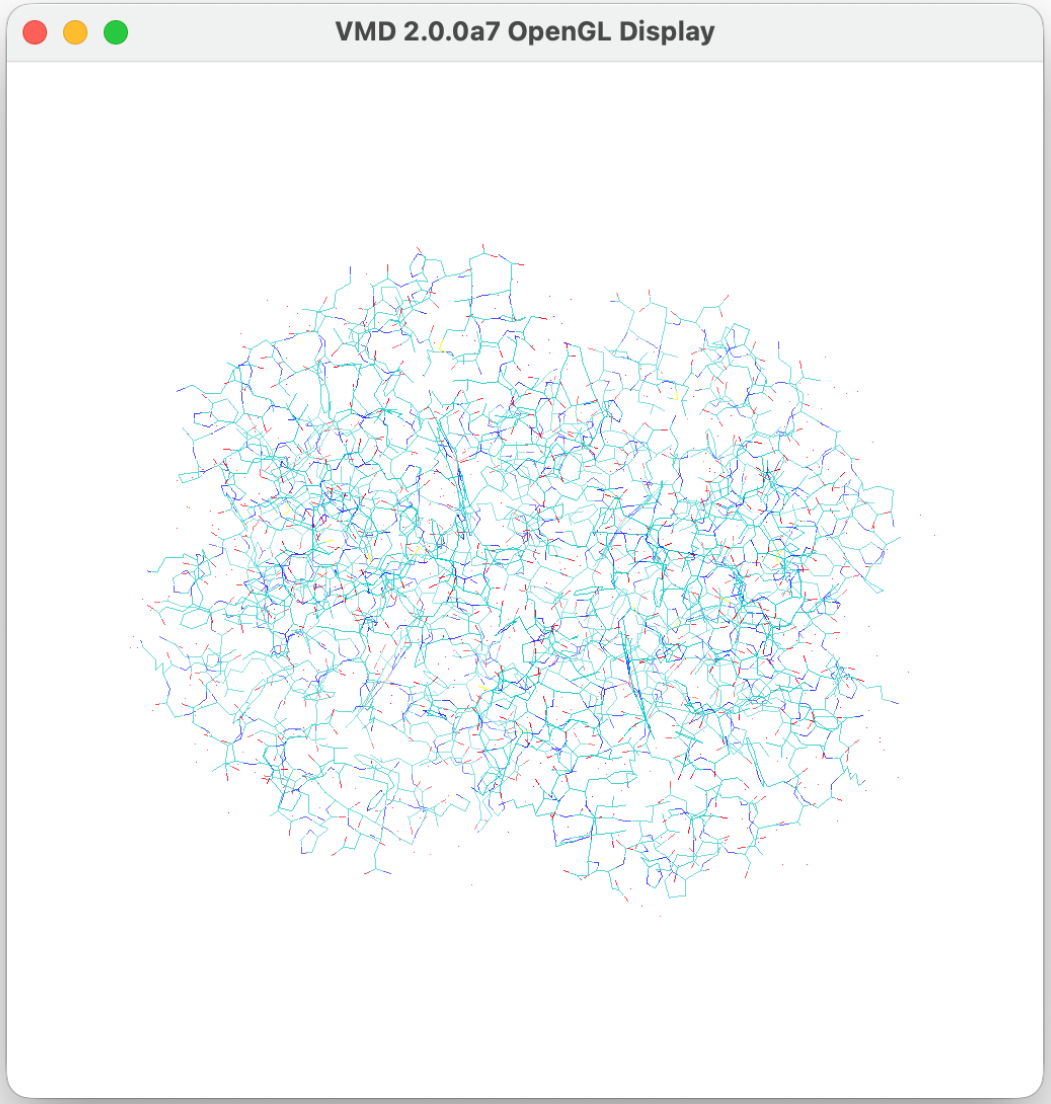
`Background > White`

In version 1.9.4

`Graphics > Colors > Display > Background`

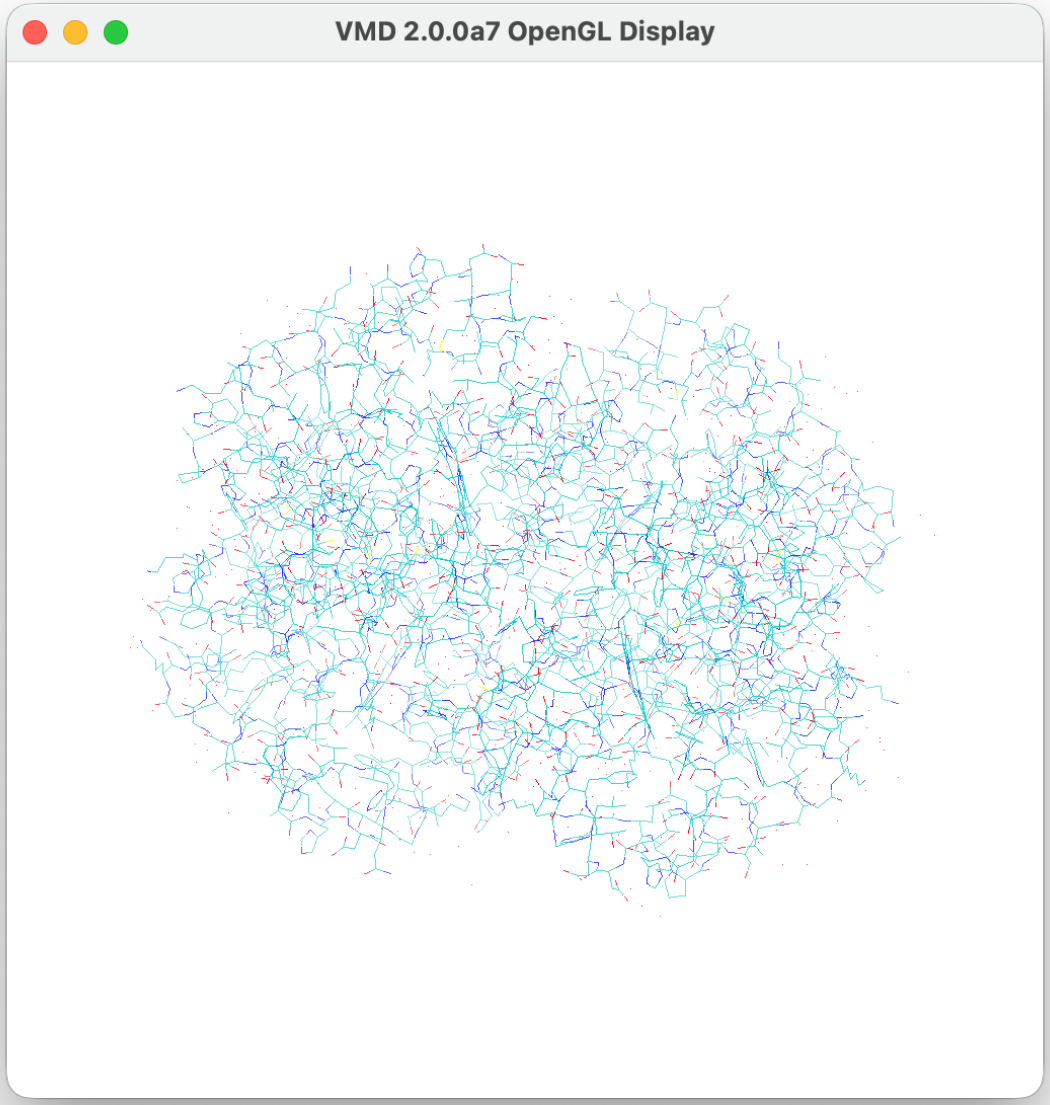
Changing Display options

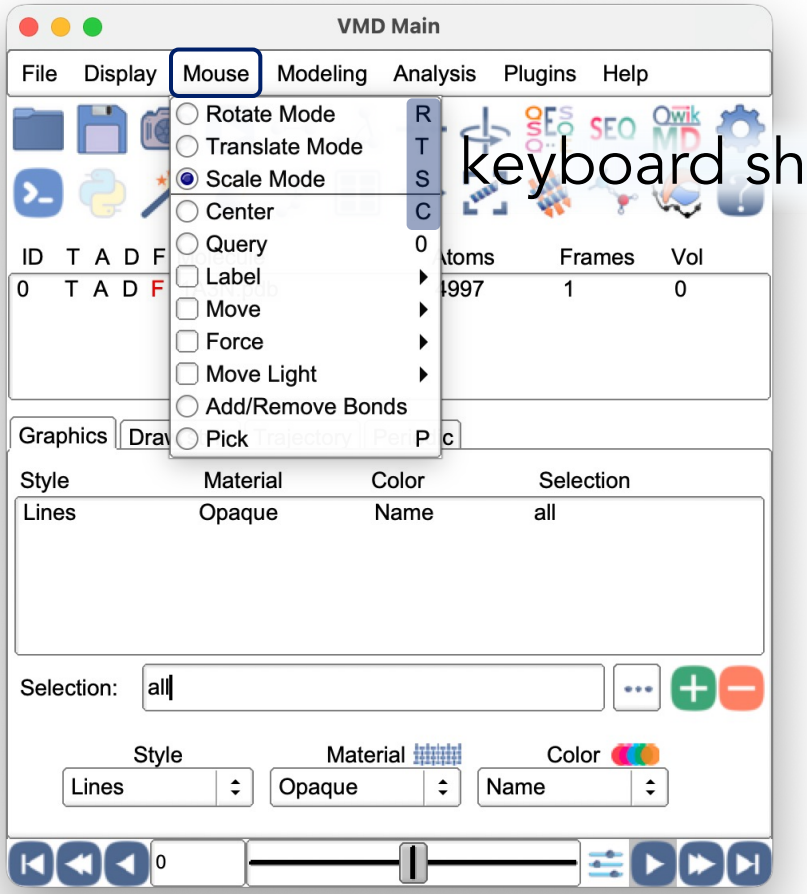




version 2.0.0

Exploring mouse actions

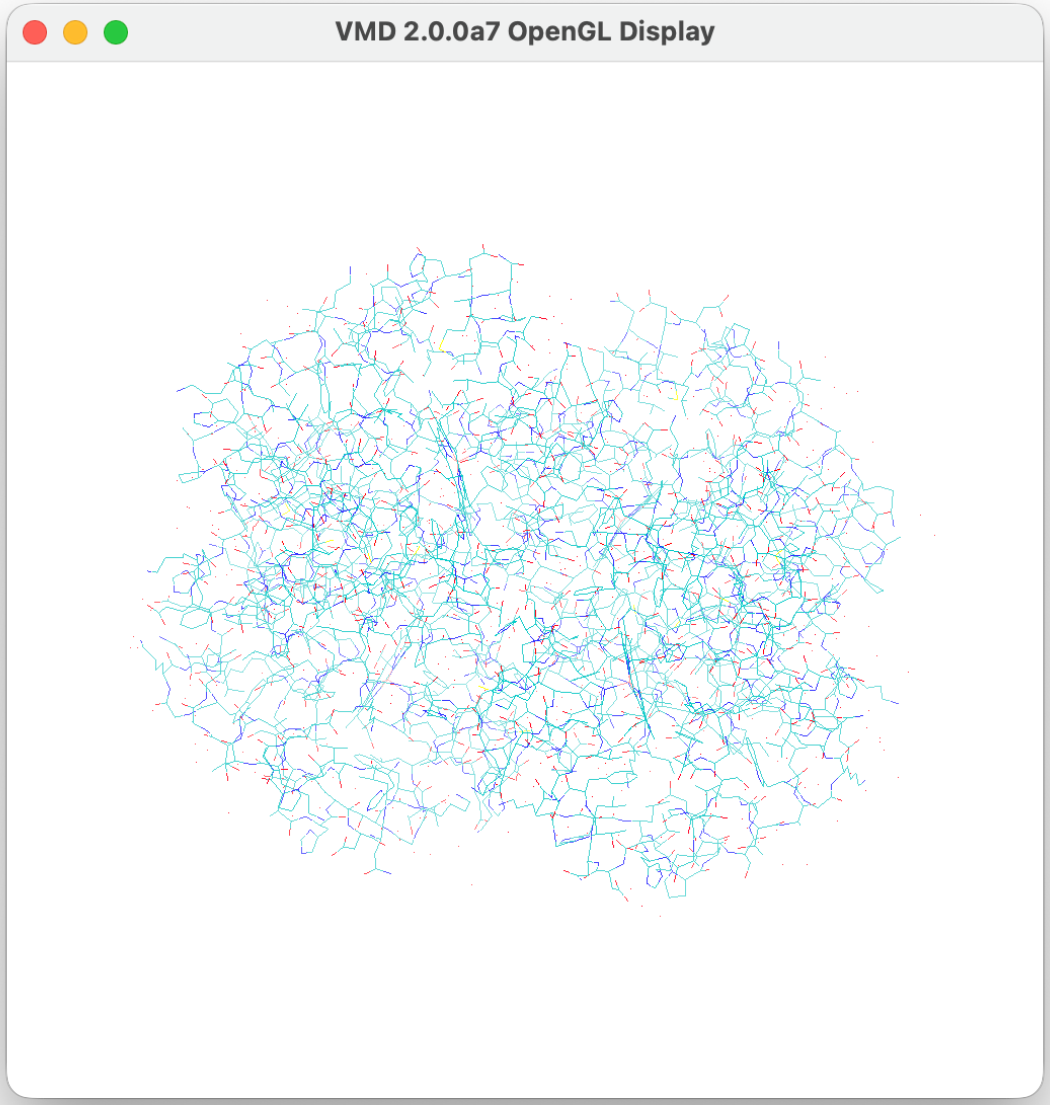


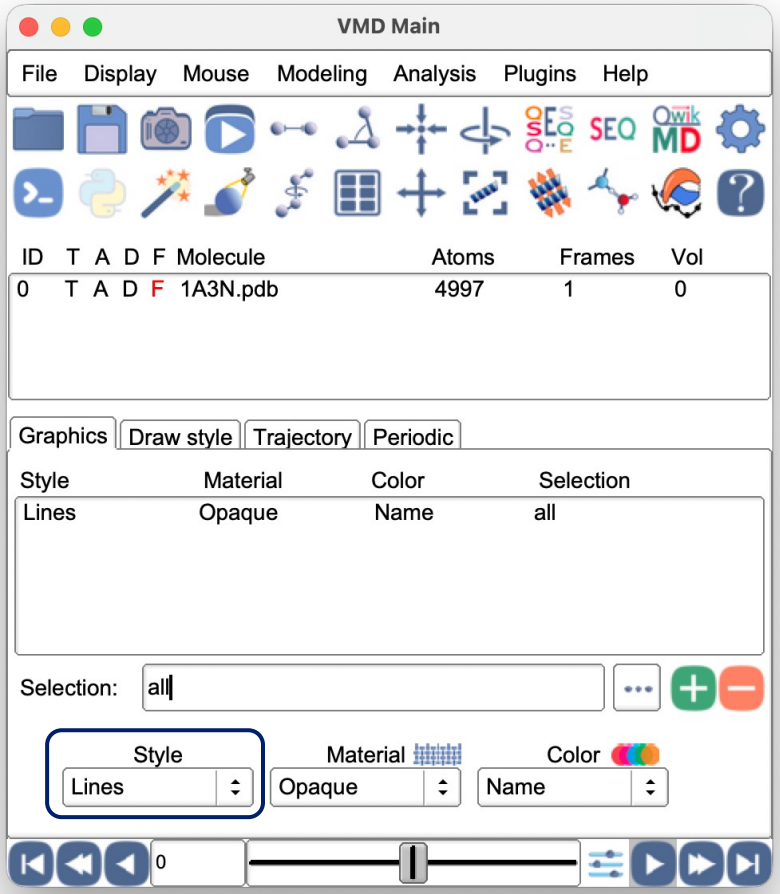


keyboard shortcuts

version 2.0.0

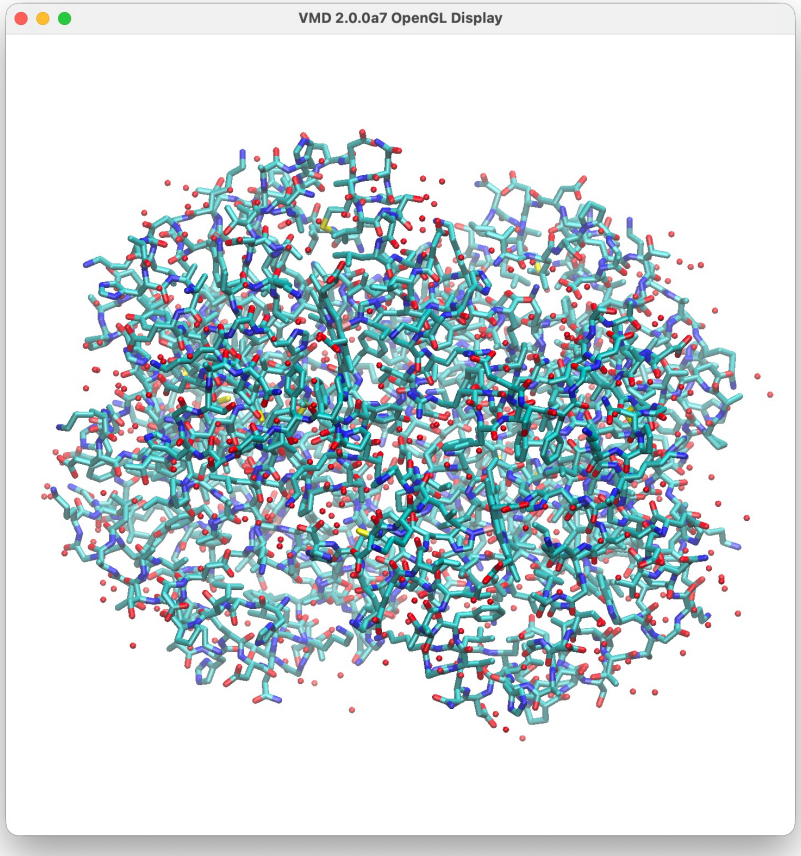
Changing the representation style



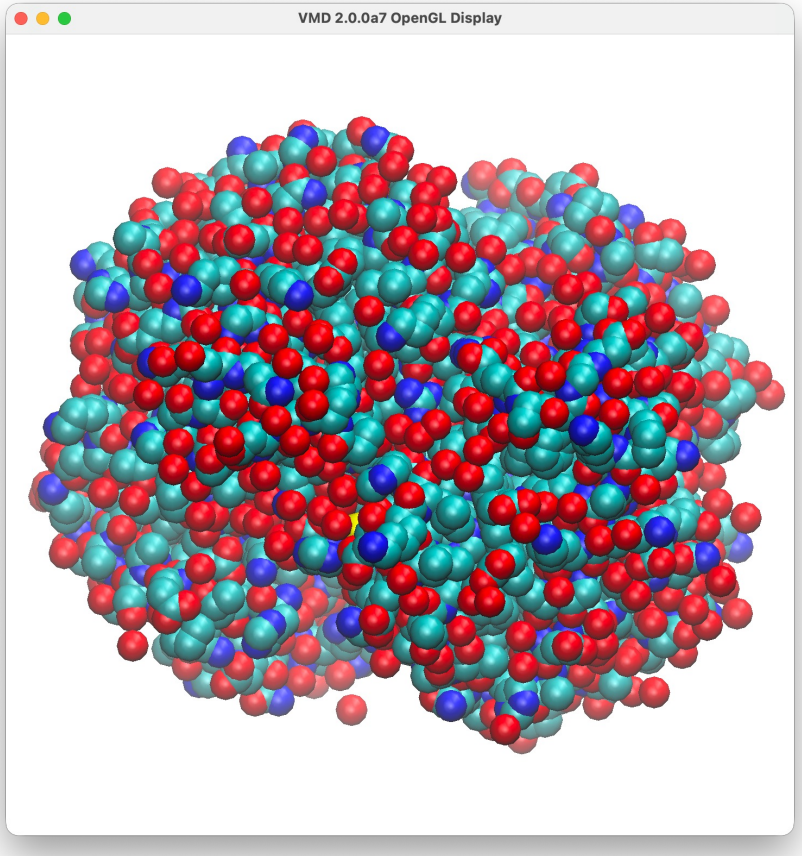


Changing the representation style

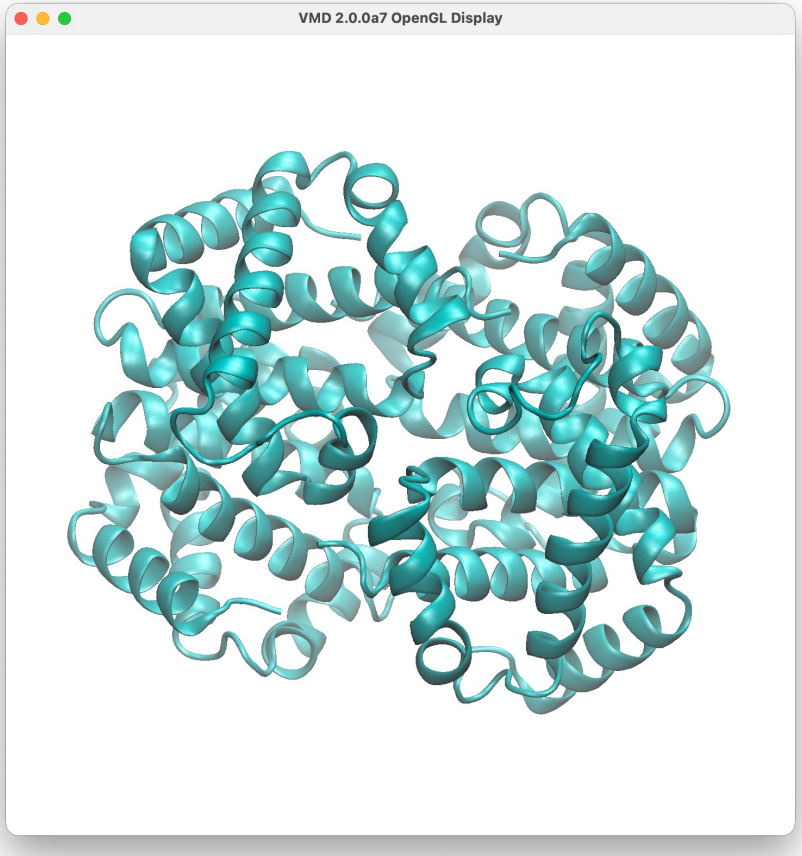
Licorice

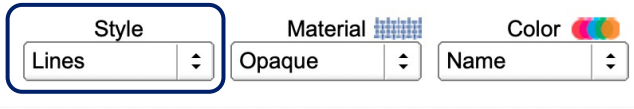


VDW



NewCartoon

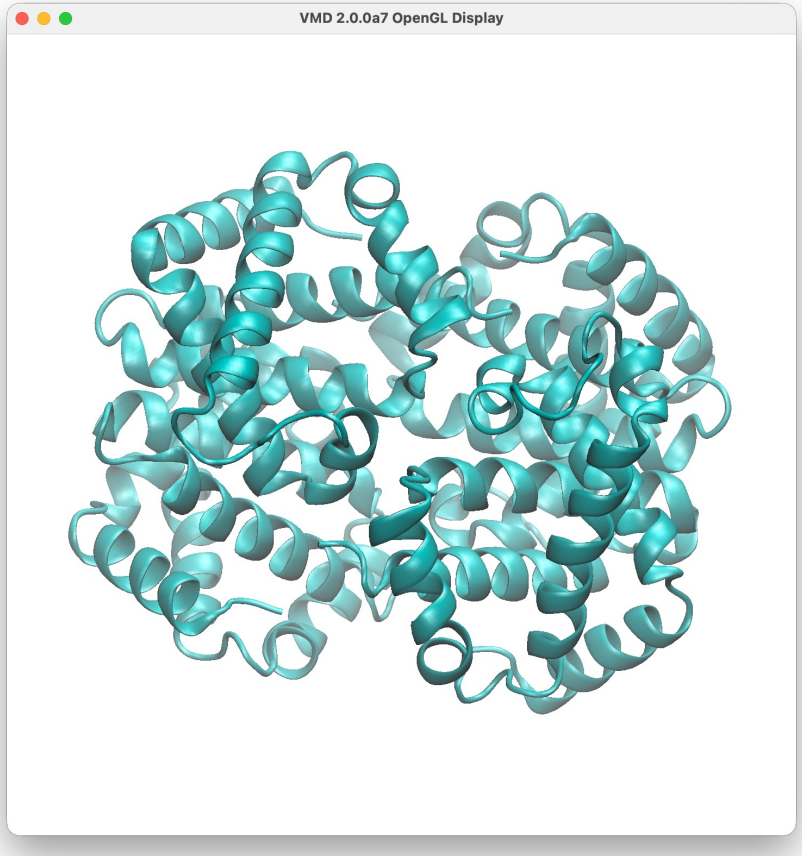




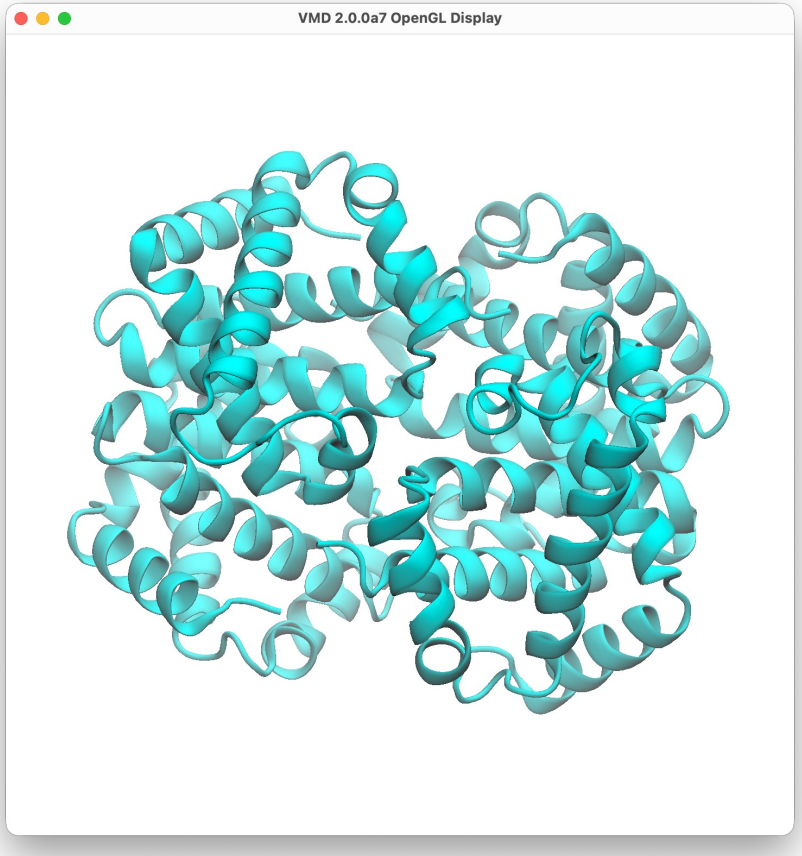
version 2.0.0

Changing the representation material

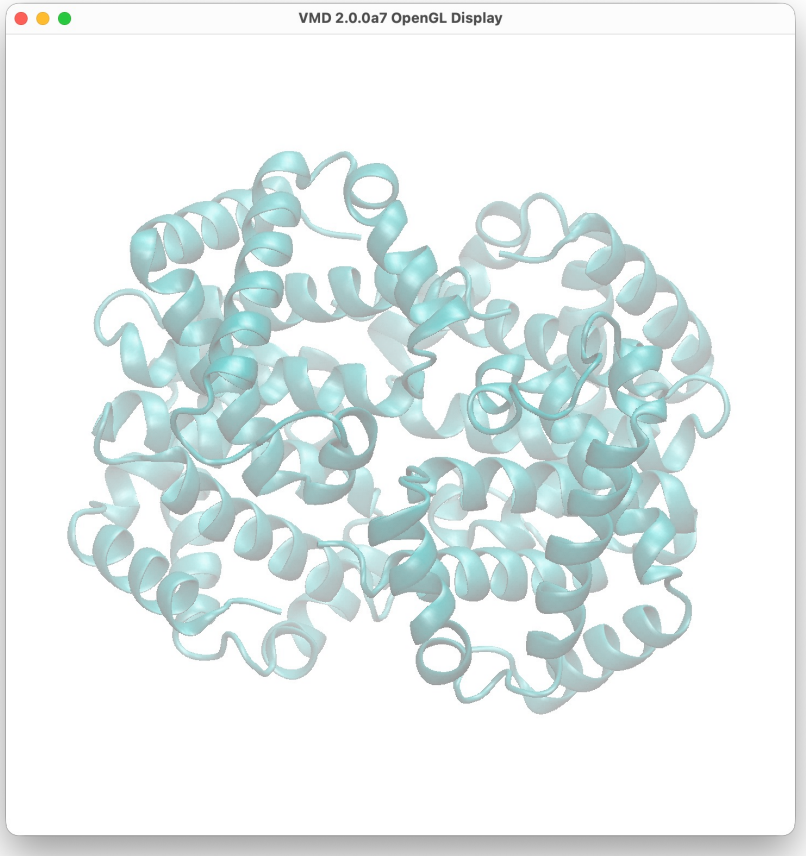
Opaque



AOChalky



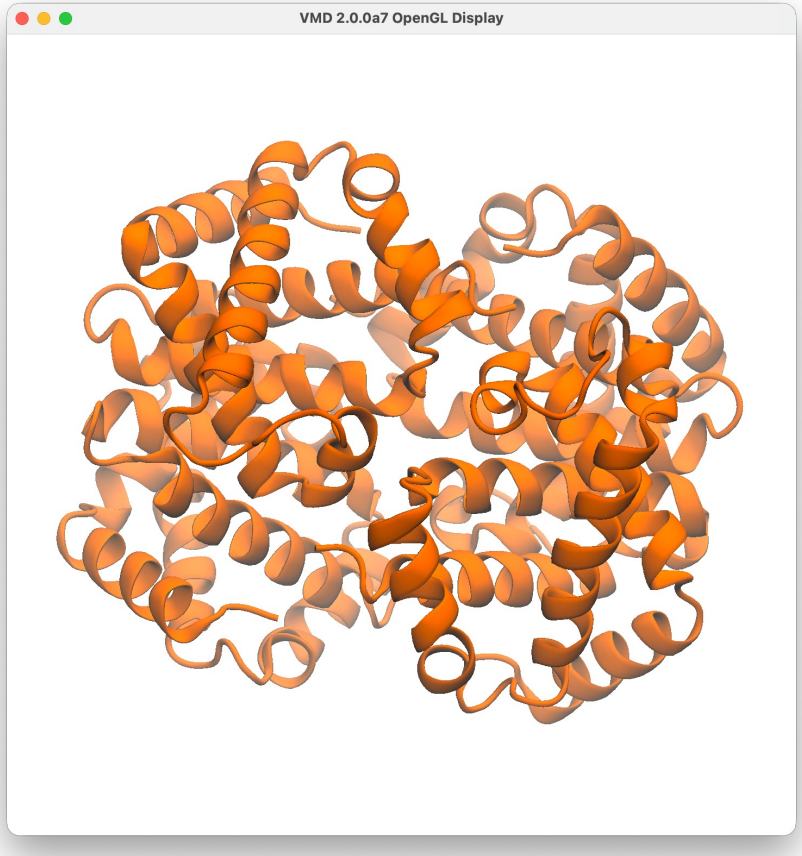
Transparent



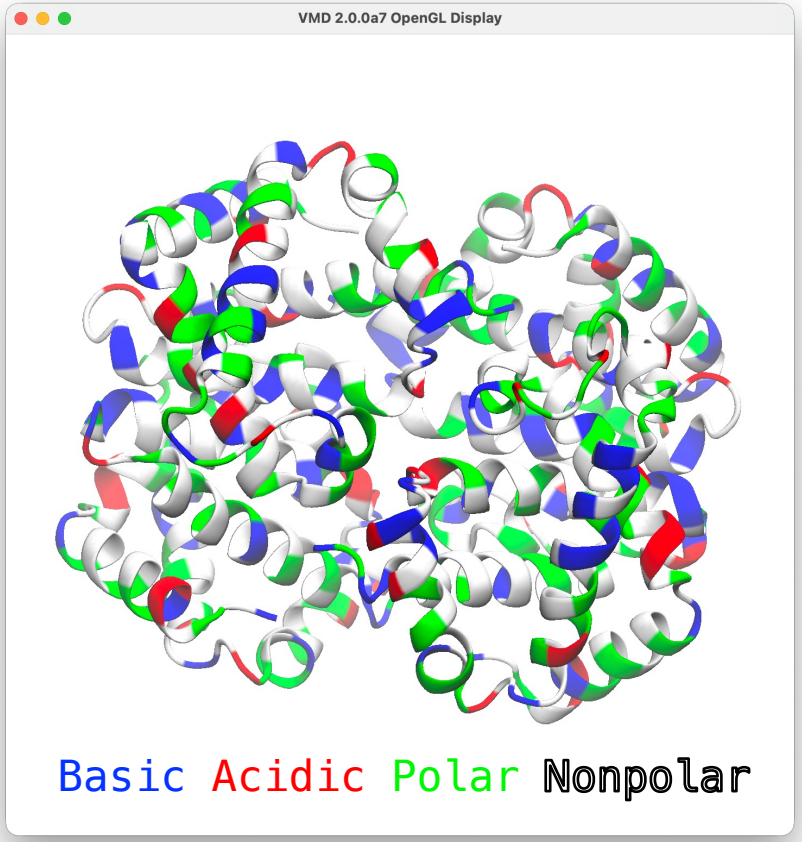
version 2.0.0

Changing the representation colors

ColorID (31)



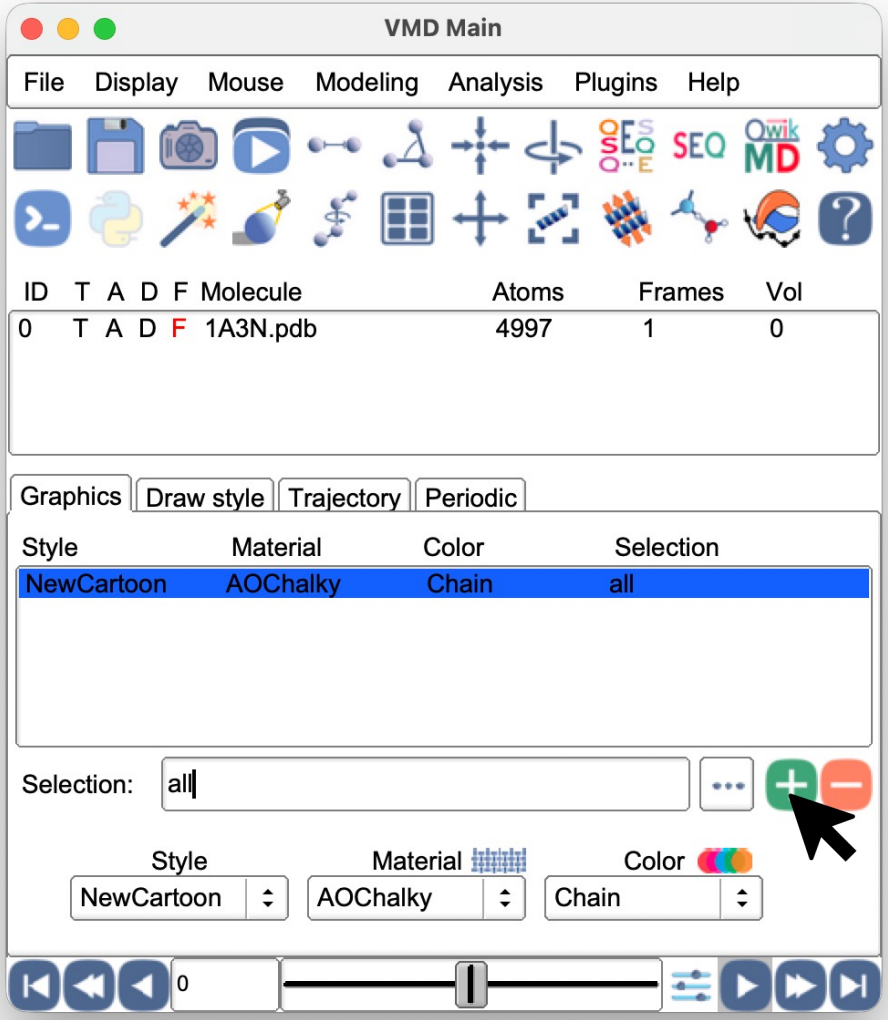
ResType

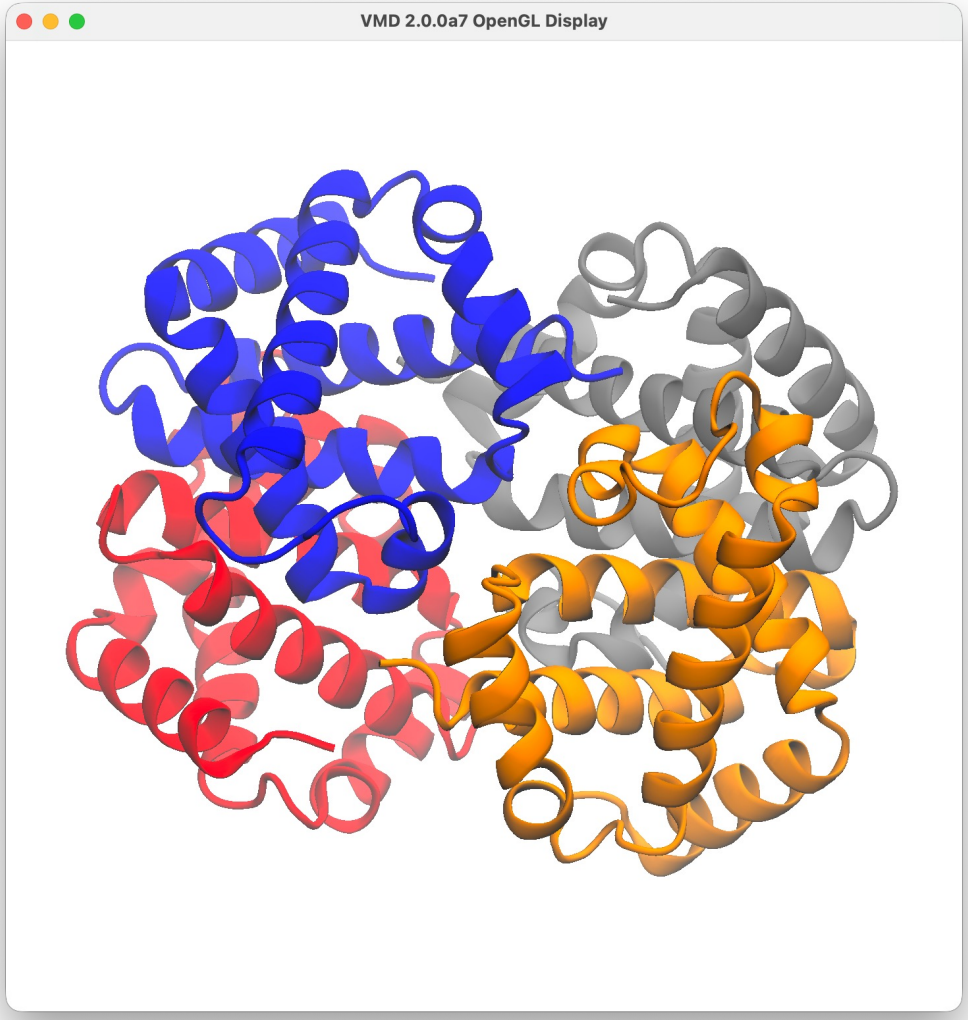


Chain

version 2.0.0

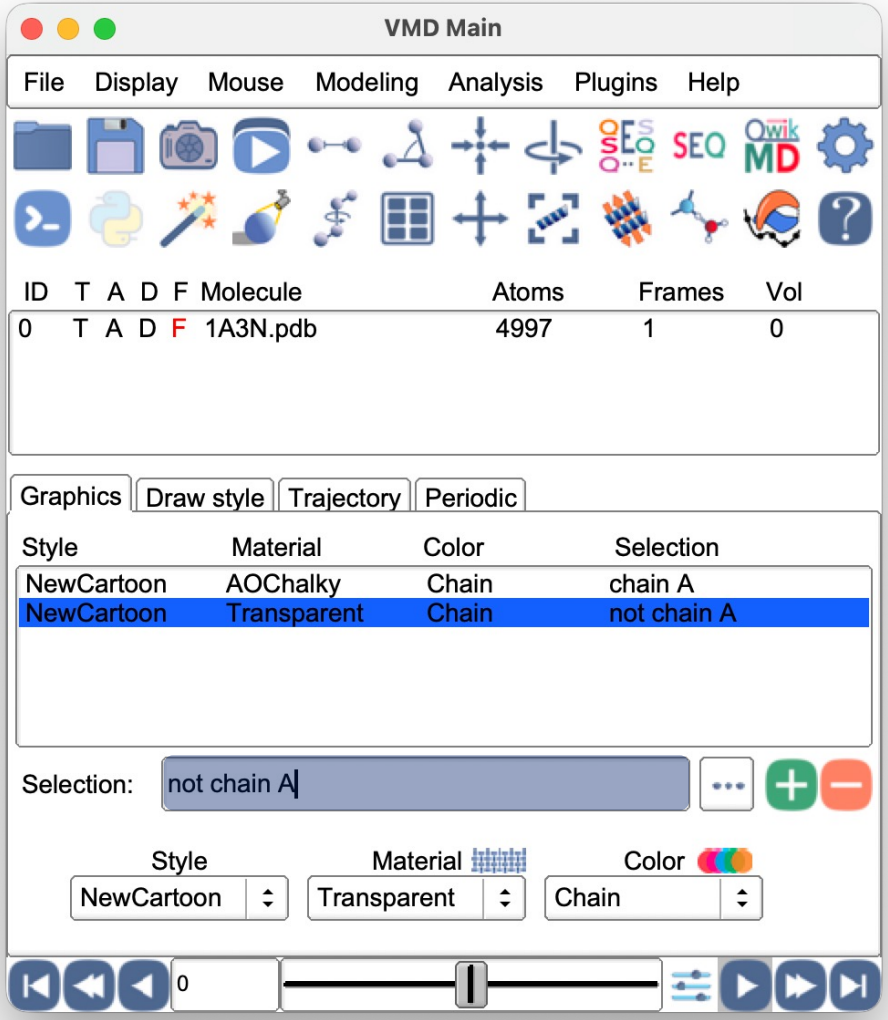
Adding different representations and selections

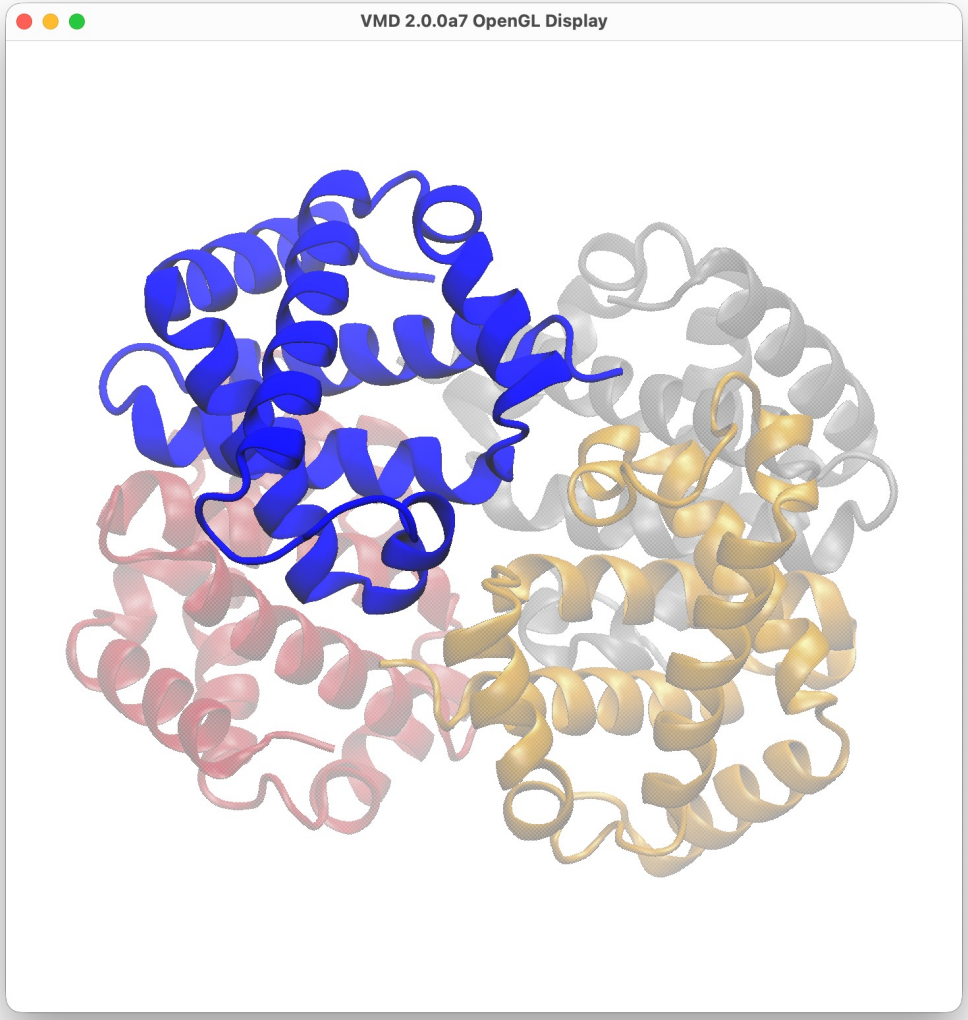




version 2.0.0

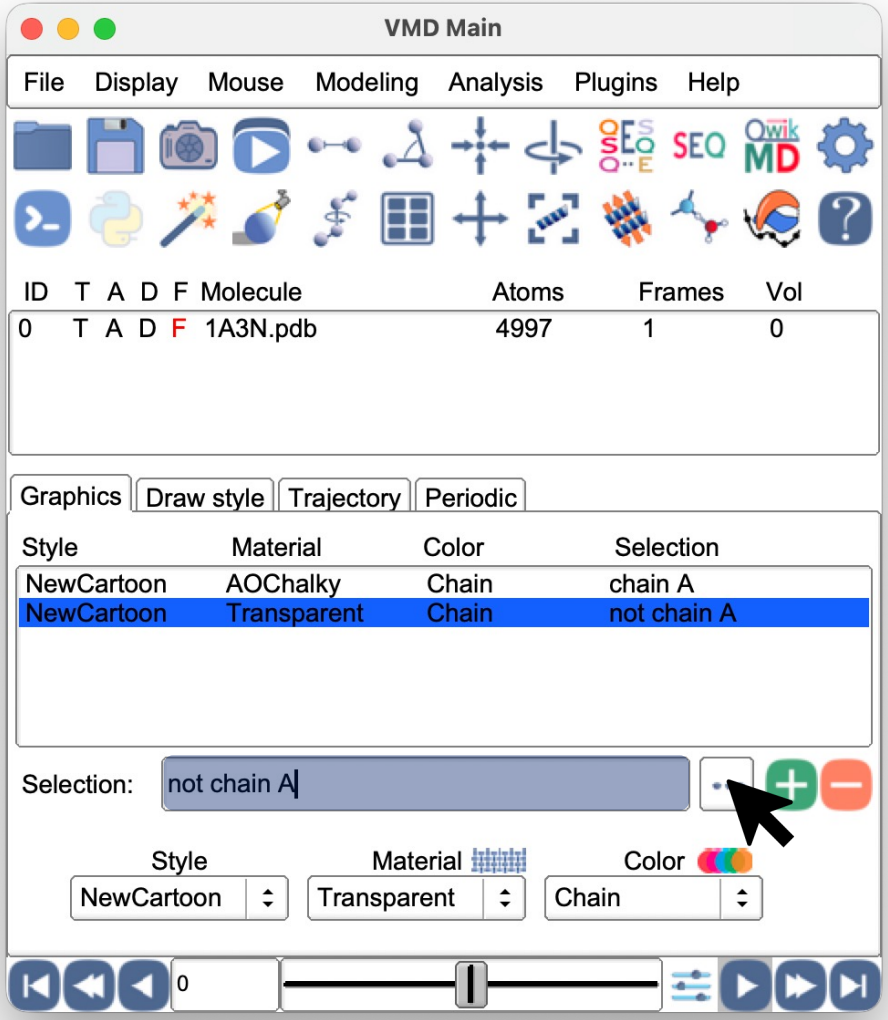
Adding different representations and selections

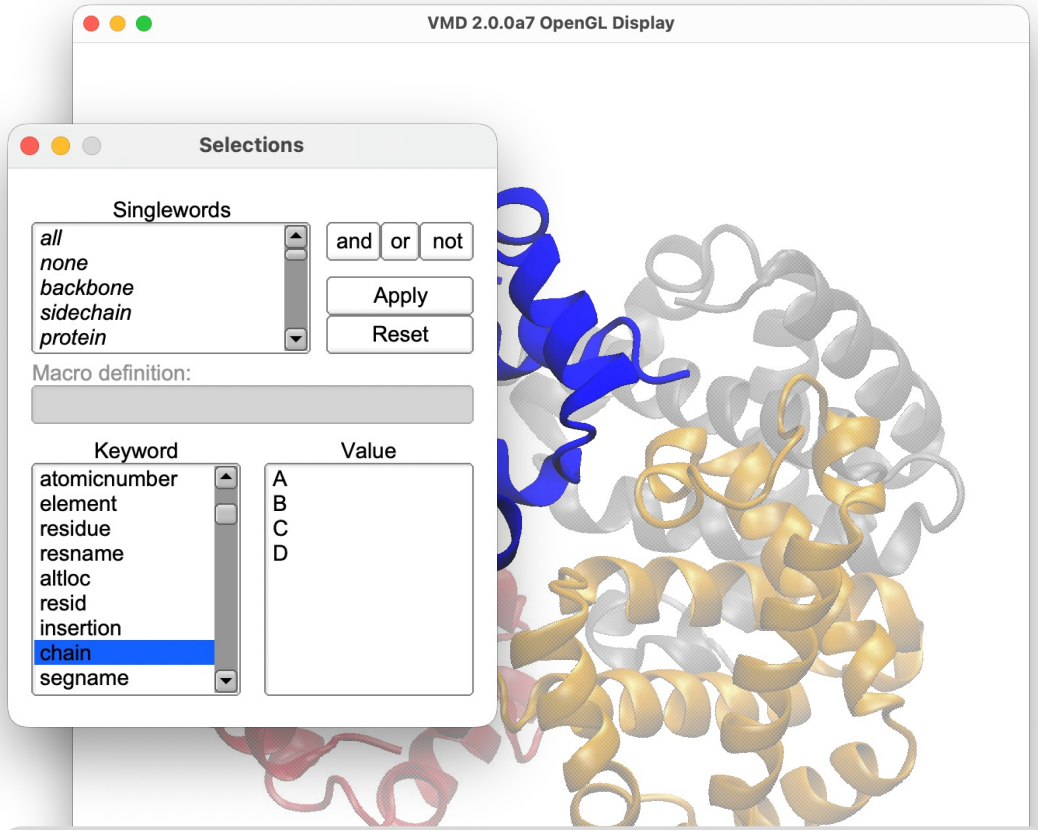




version 2.0.0

Adding different representations and selections

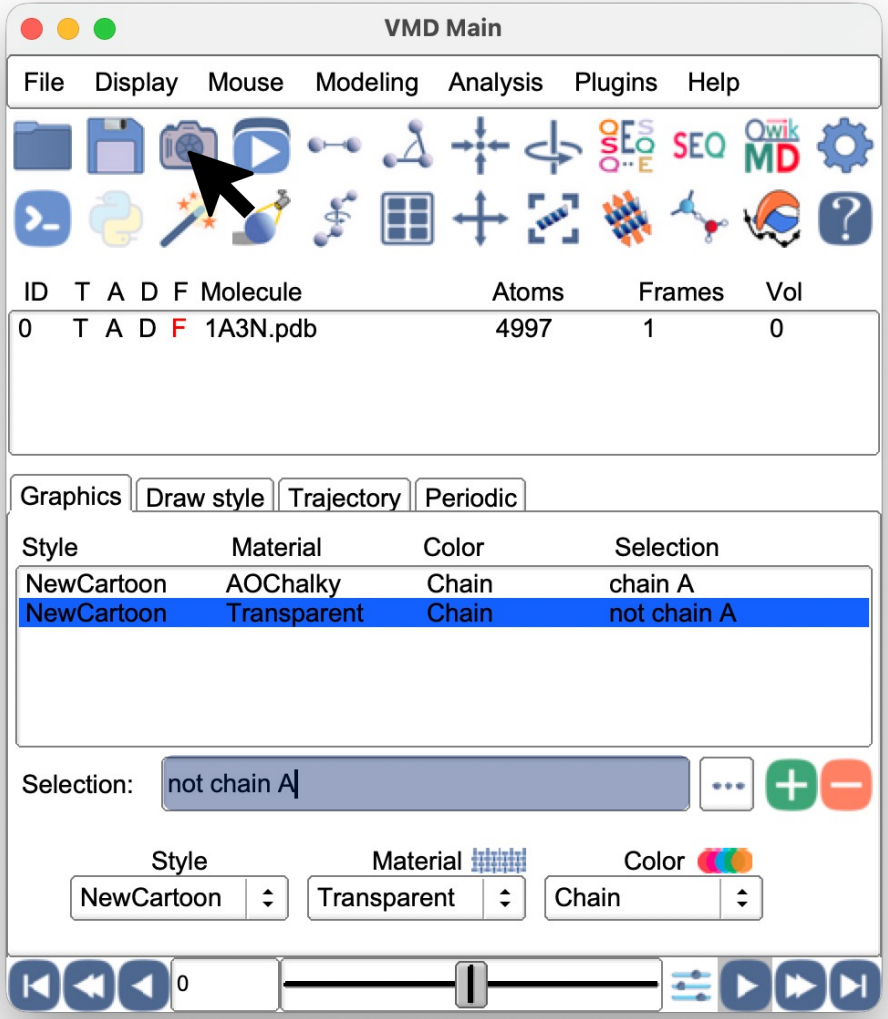




`Selections` window helps identify possible selections

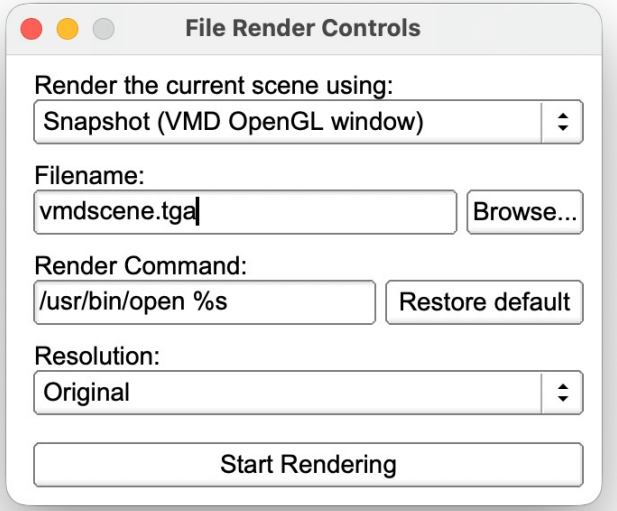
version 2.0.0

Rendering images



Alternatively: `File > Render`

(version 1.9.4)

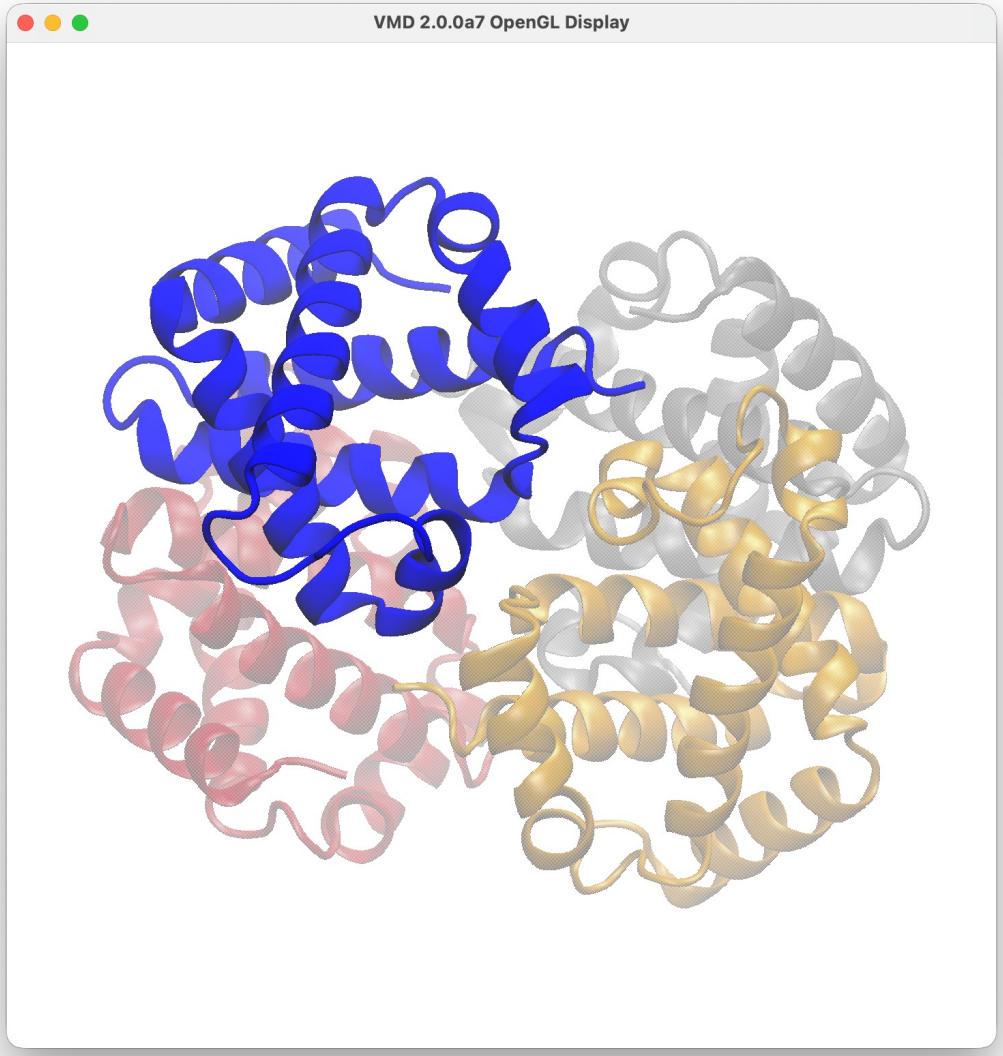


rendering engine

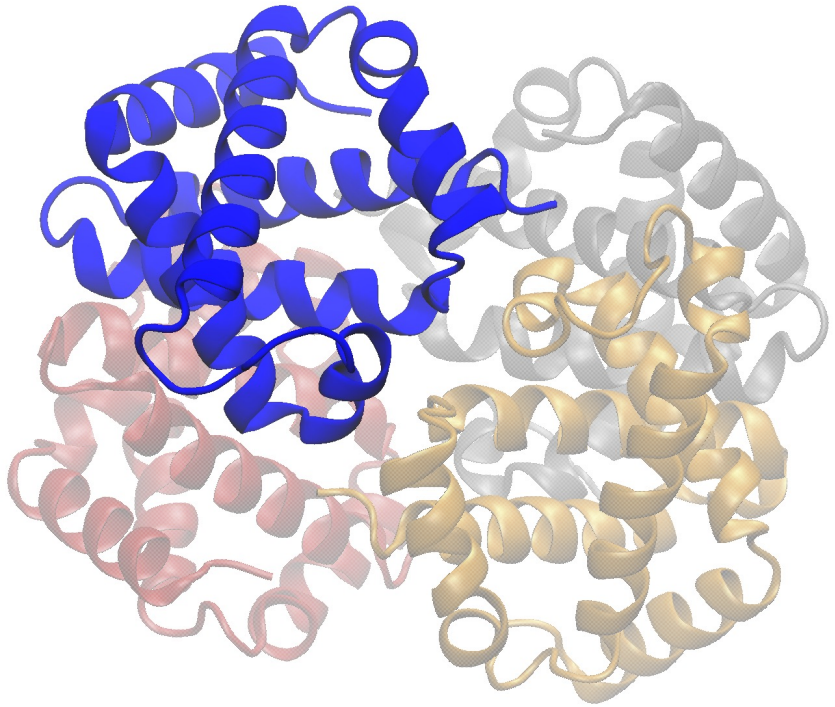
folder/file name

version 2.0.0

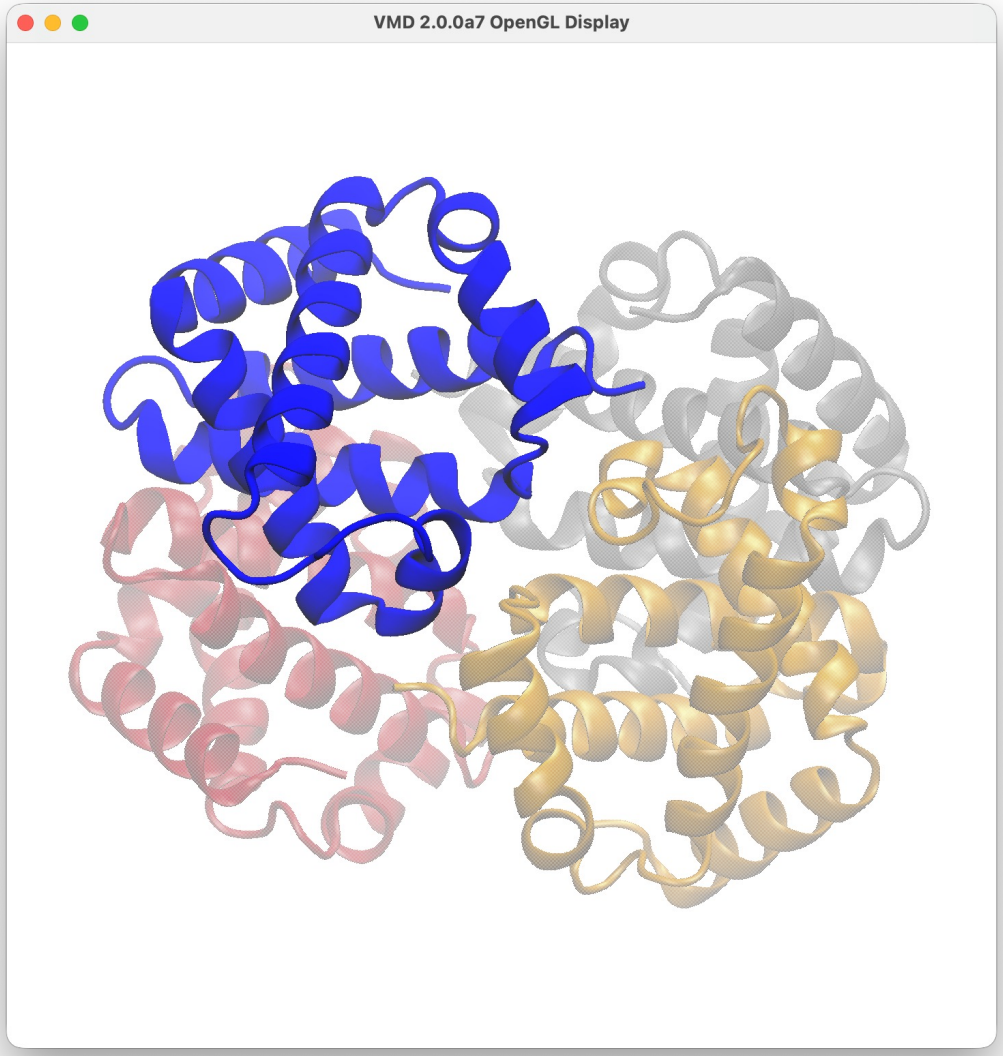
Rendering images



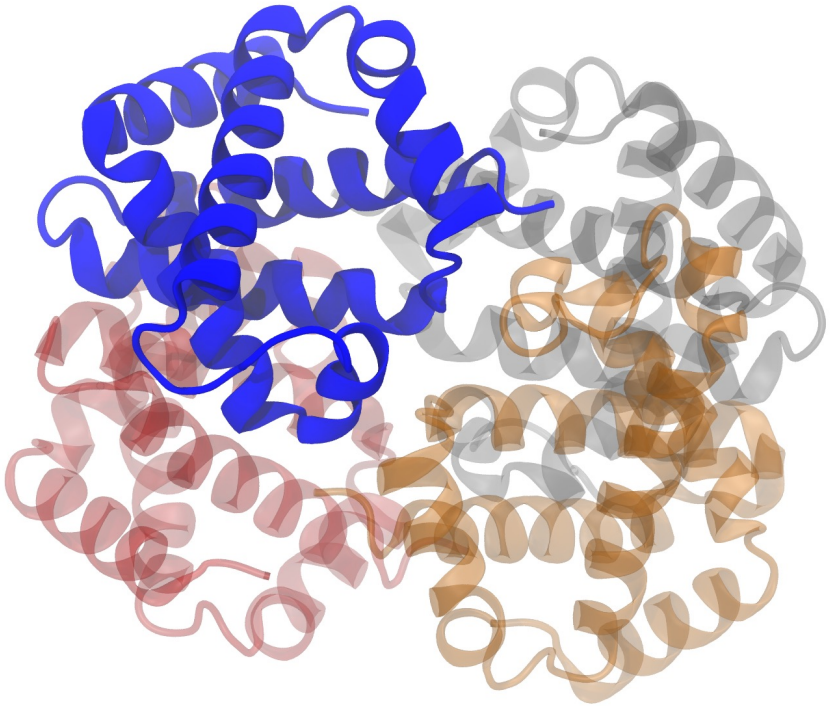
Snapshot



Rendering images

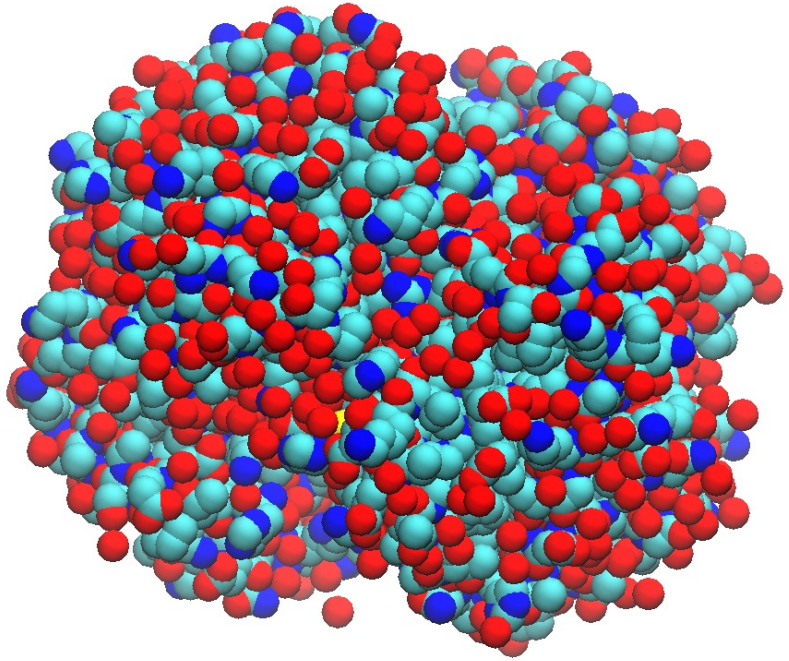


Tachyon Internal

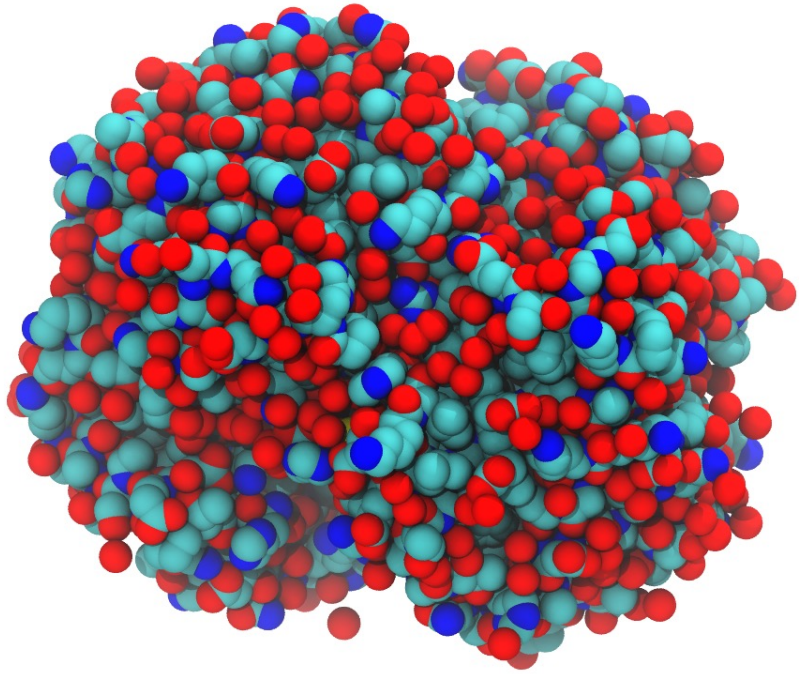


Rendering images

`Snapshot`

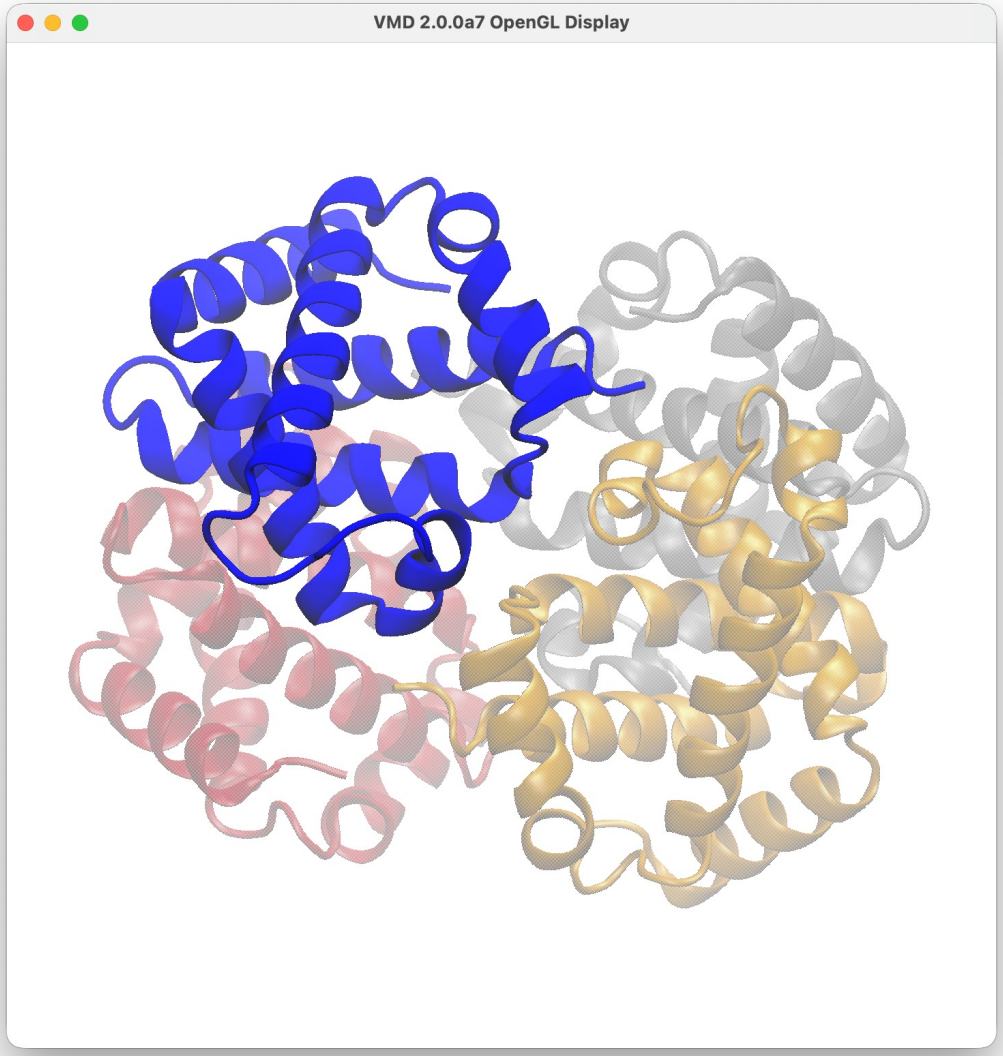


`Tachyon Internal`

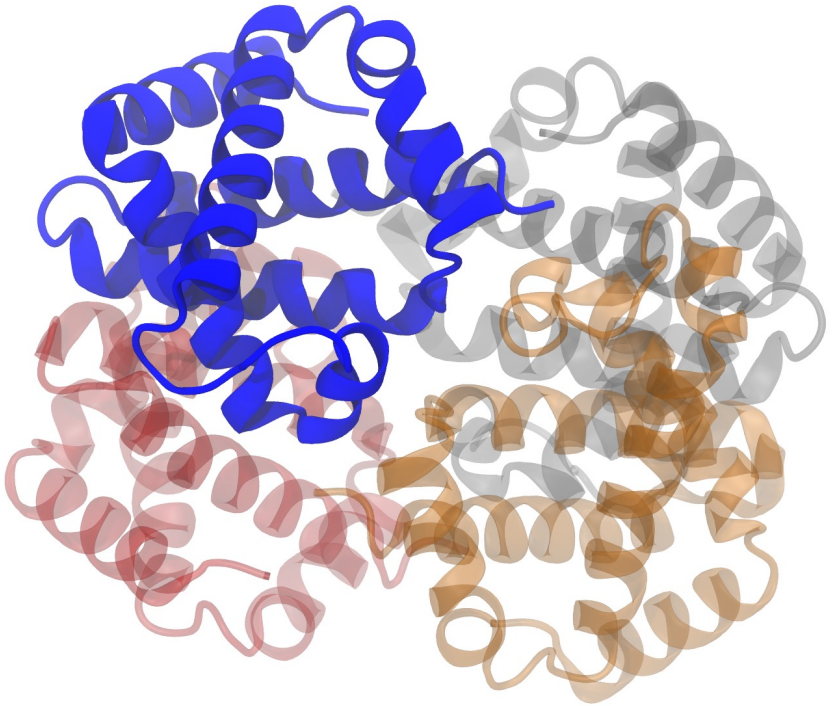


Shadows and the depth cueing become more apparent in `Tachyon`

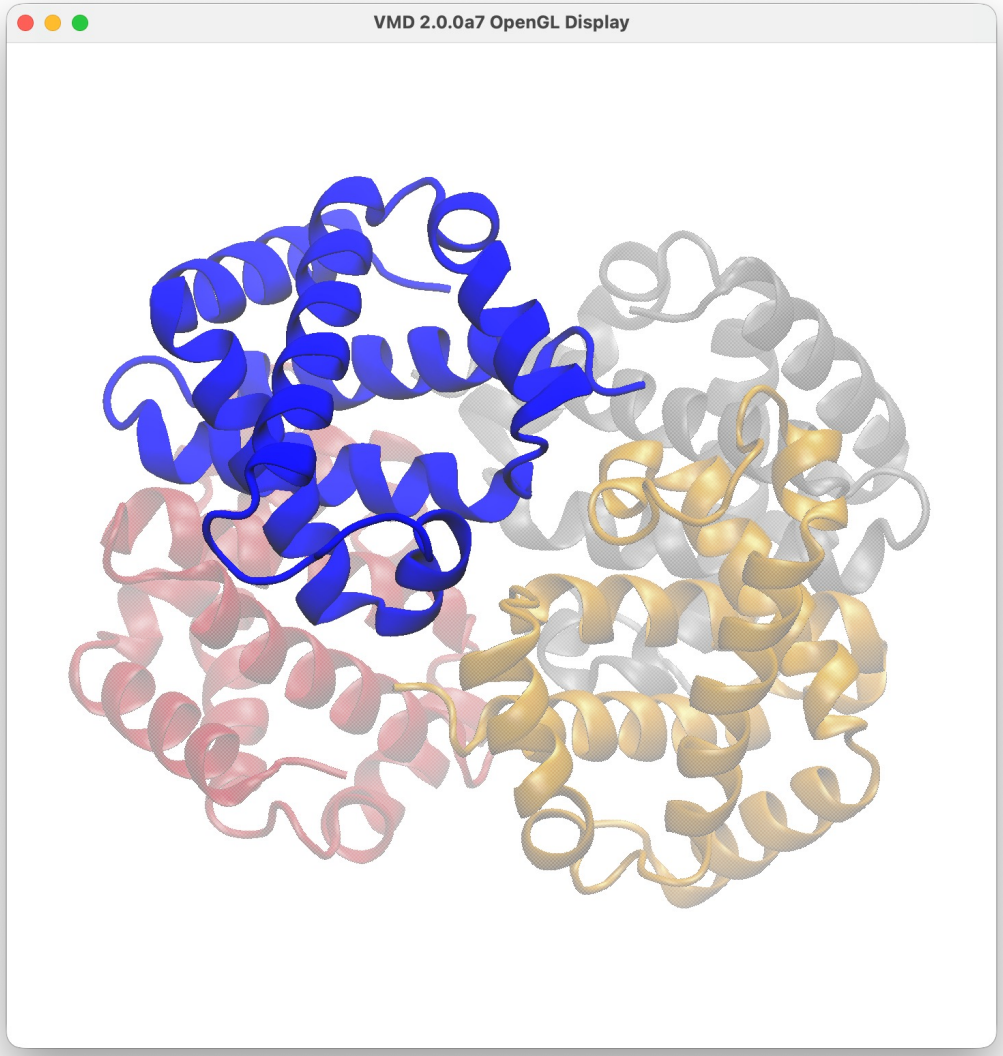
Rendering images



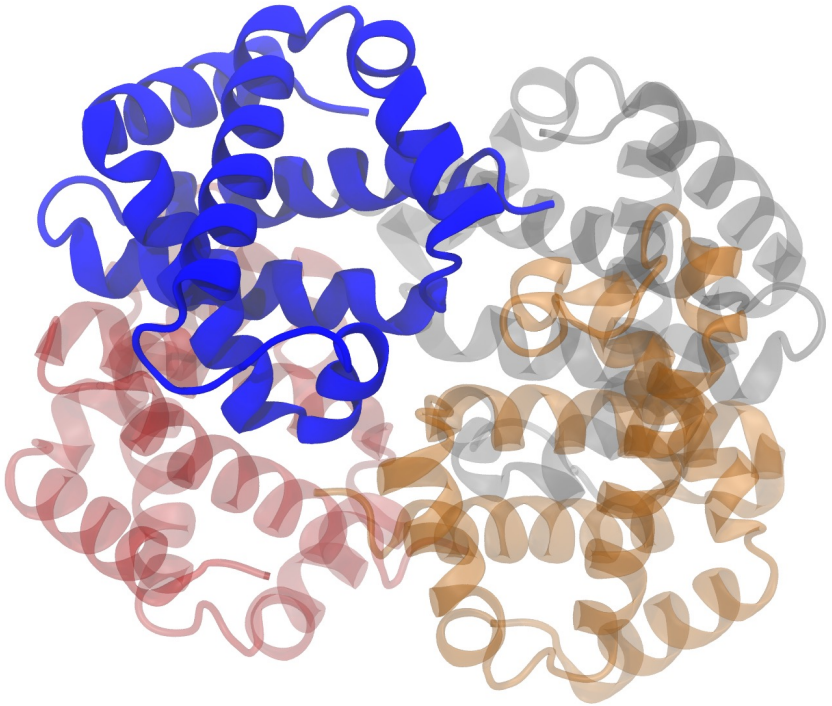
Tachyon Internal



Rendering images



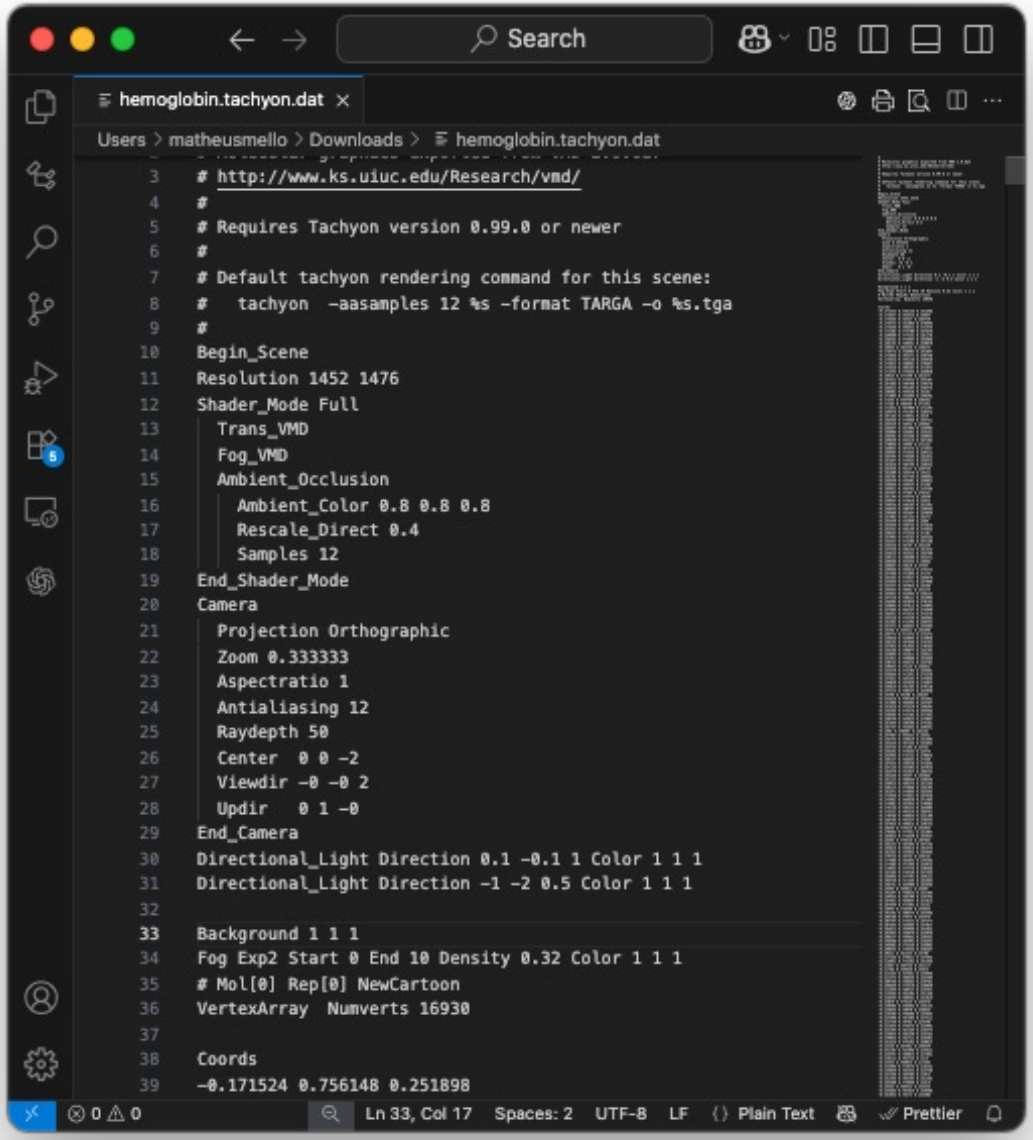
Tachyon



Note that a `.dat` file was generated

version 2.0.0

Rendering images

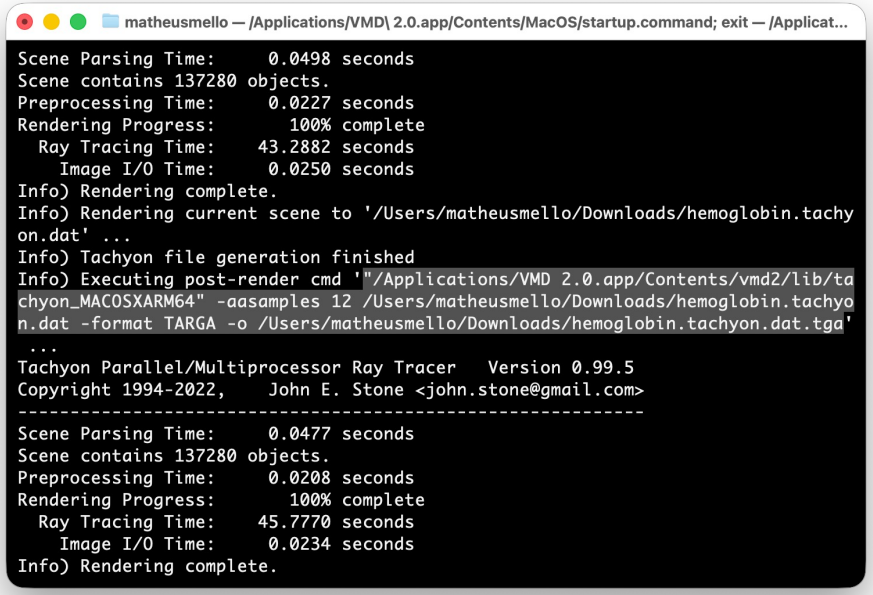


`.dat` file: configures the scene

Some things we can change:

- `Resolution > 500 500`
- `Fog | Density 0.32 > 0.30`

VMD terminal

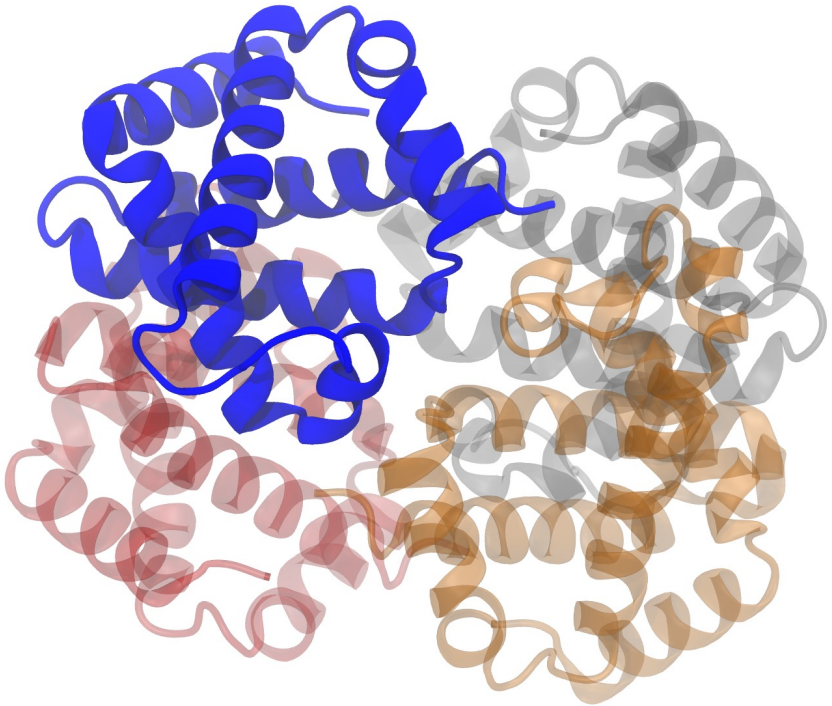


Copy rendering command

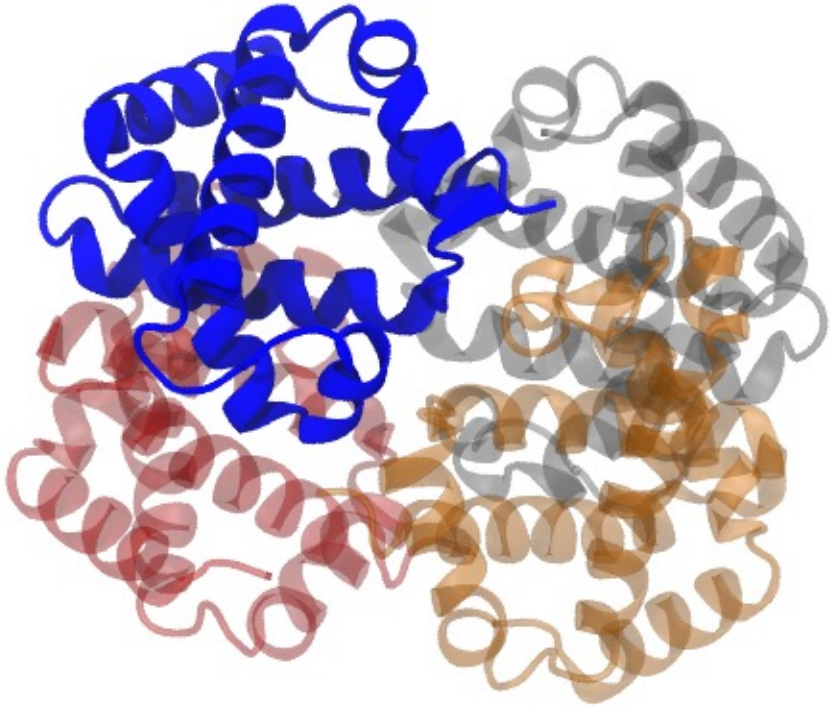
version 2.0.0

Rendering images

Tachyon



edited .dat file



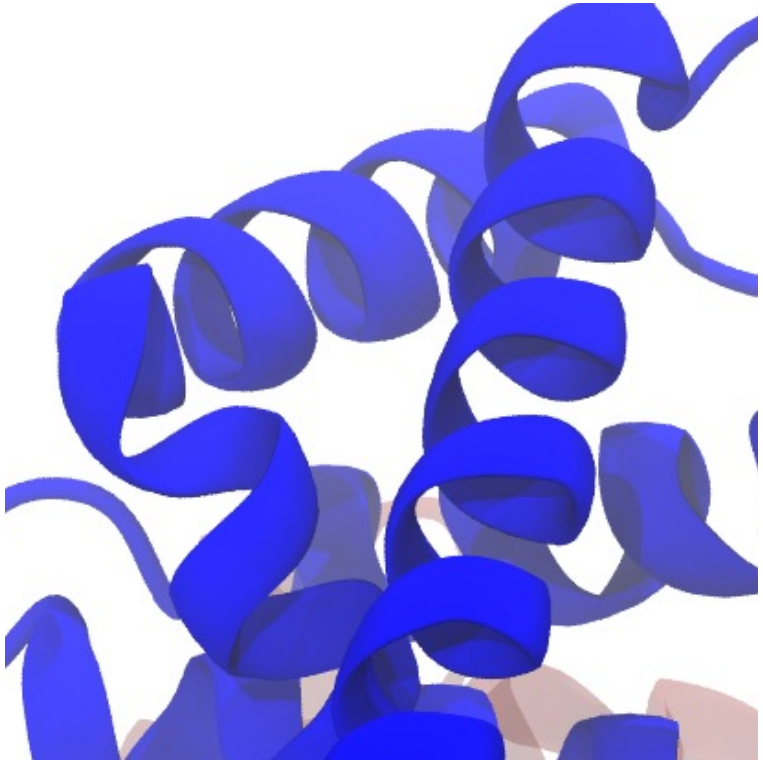
On a new terminal

```
"/Applications/VMD 2.0.app/Contents/vmd2/lib/tachyon_MACOSXARM64" -aasamples 12
hemoglobin.tachyon.edited.dat -format TARGA -o hemoglobin.tachyon.edited.dat.tga
```

version 2.0.0

Rendering images

Tachyon



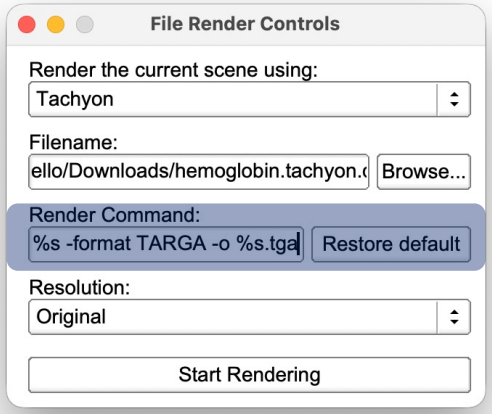
edited .dat file

On a new terminal

```
"/Applications/VMD 2.0.app/Contents/vmd2/lib/tachyon_MACOSXARM64" -aasamples 12
hemoglobin.tachyon.edited.dat -format TARGA -o hemoglobin.tachyon.edited.dat.tga
```

Rendering images

We can also change the rendering command:



Default command:

```
"/Applications/VMD 2.0.app/Contents/vmd2/lib/tachyon_MACOSXARM64"
-aasamples 12 %s -format TARGA -o %s.tga
```

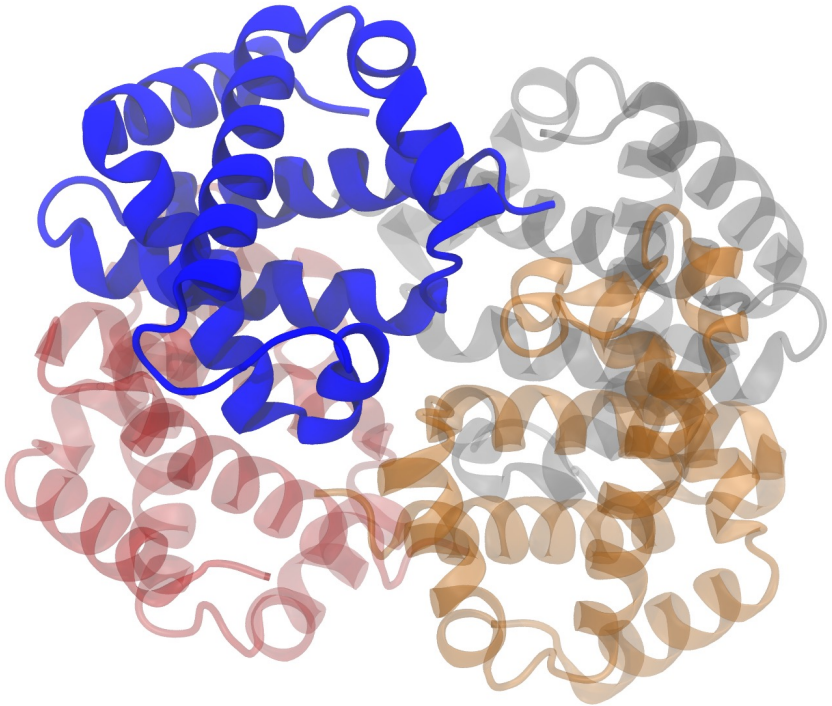
We can add:

```
"/Applications/VMD 2.0.app/Contents/vmd2/lib/tachyon_MACOSXARM64" -
aasamples 12 %s -fullshade -auto_skylight 1.4 -format TARGA -o %s.tga
```

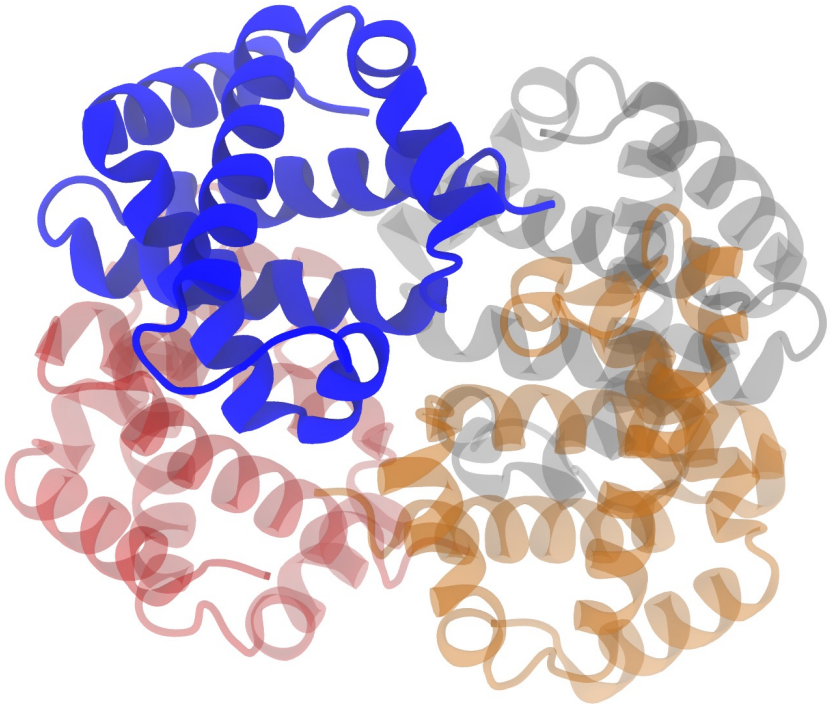
It will take considerably longer to render

Rendering images

Tachyon



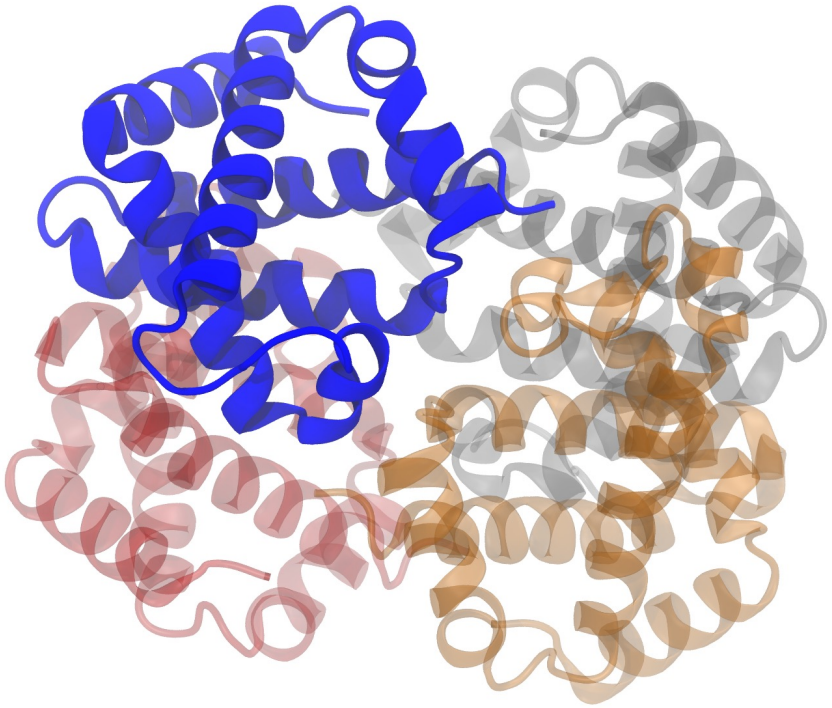
“Fancy” Tachyon



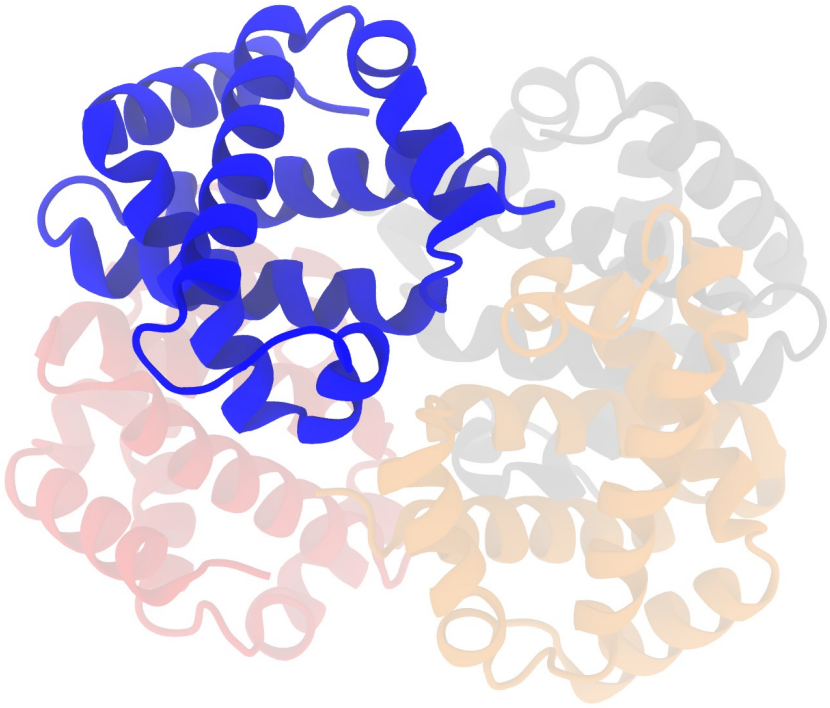
version 2.0.0

Rendering images

Tachyon

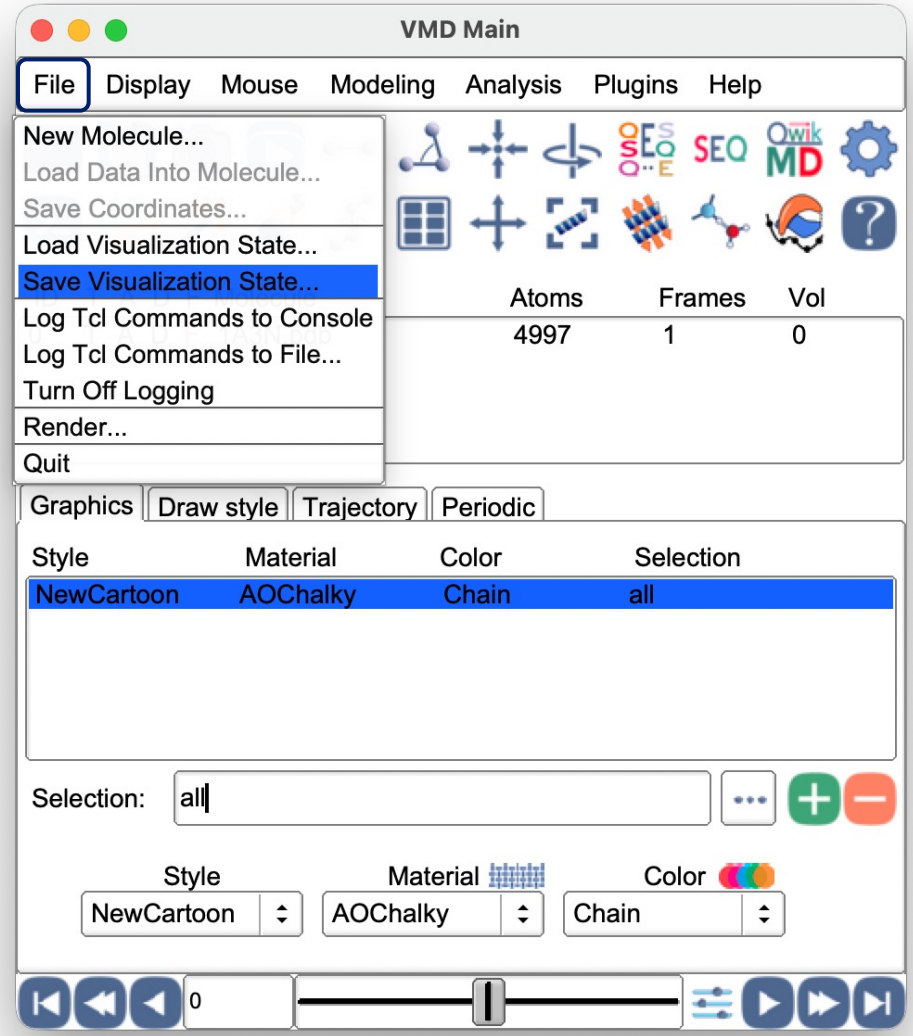


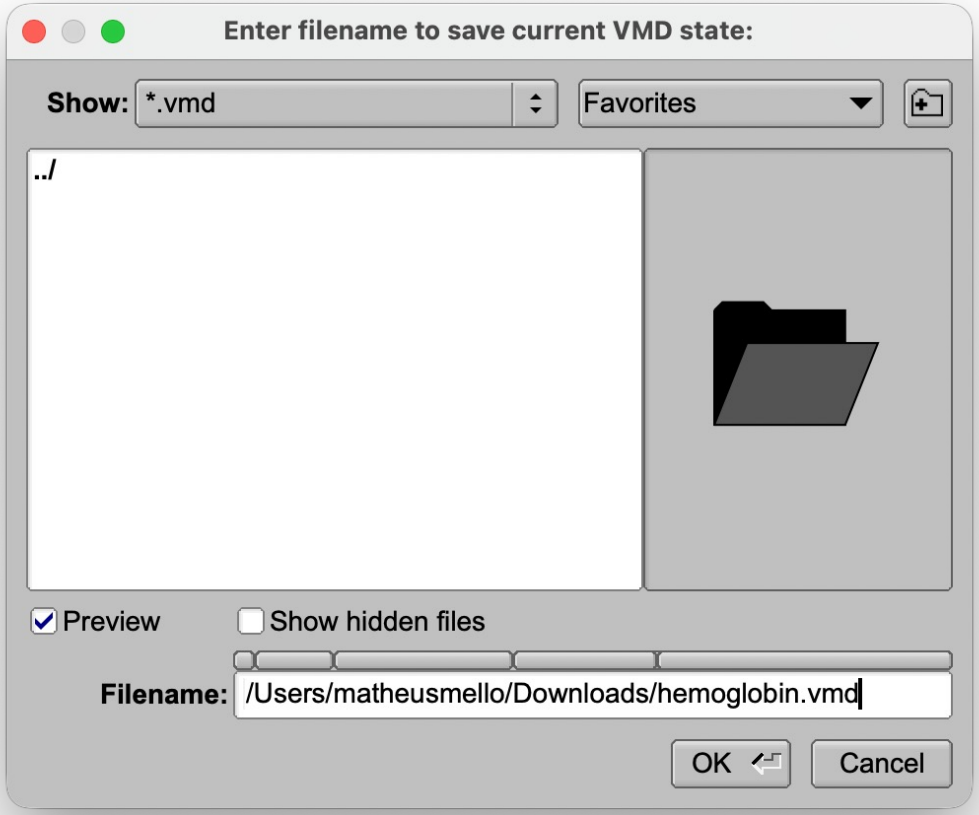
"Fancy" Tachyon



For transparent objects, we can add `-trans_max_surfaces 1`

Saving current scene

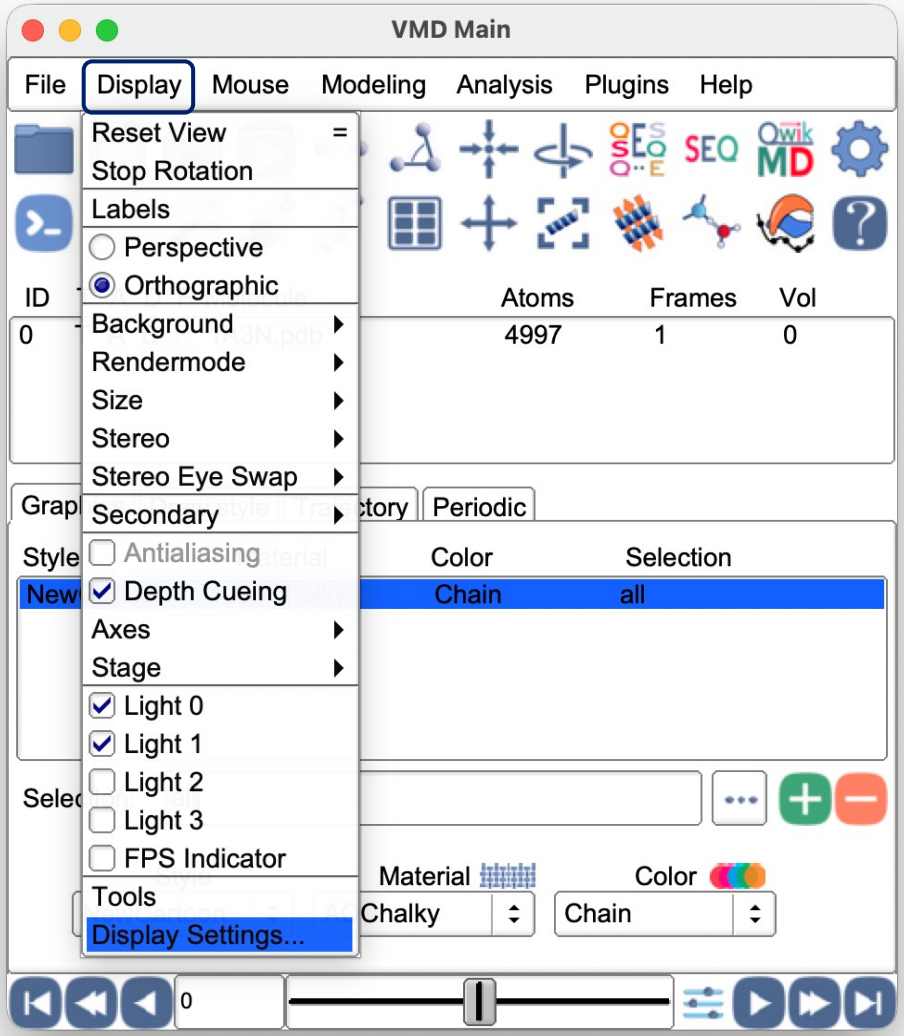


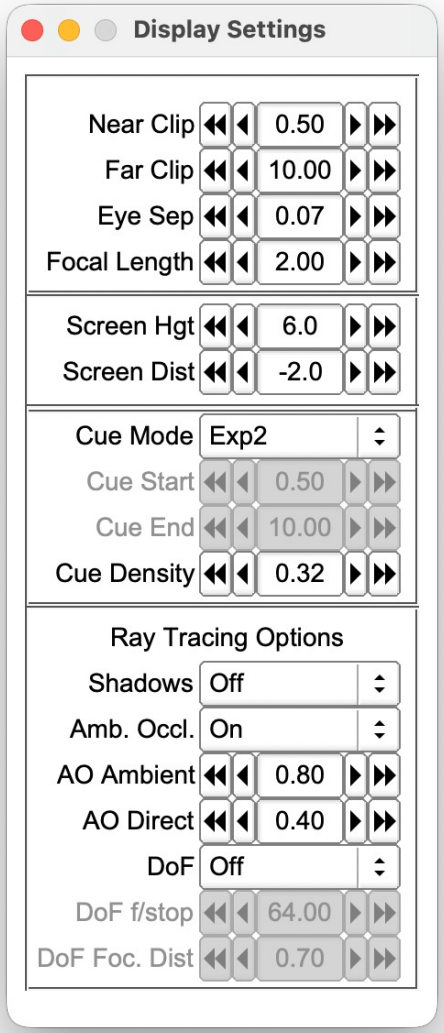


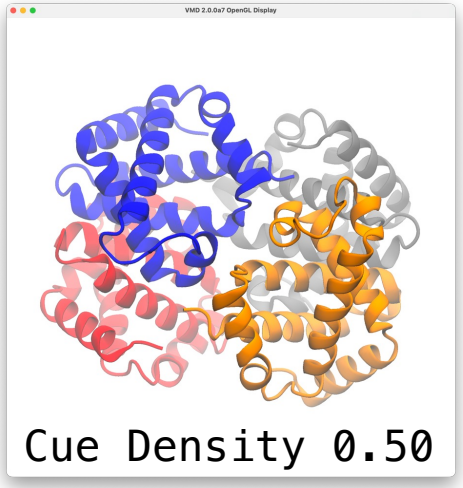
Useful to save the scene of a presentation or publication figure

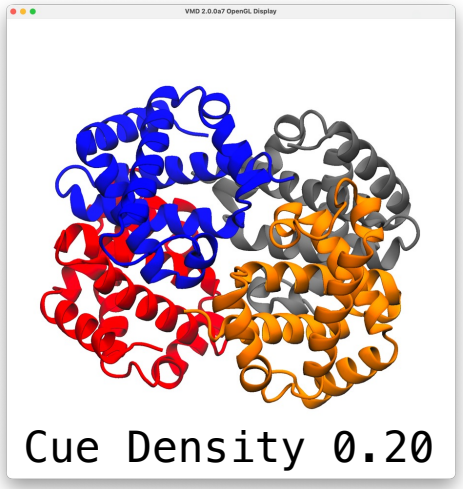
version 2.0.0

Advanced options



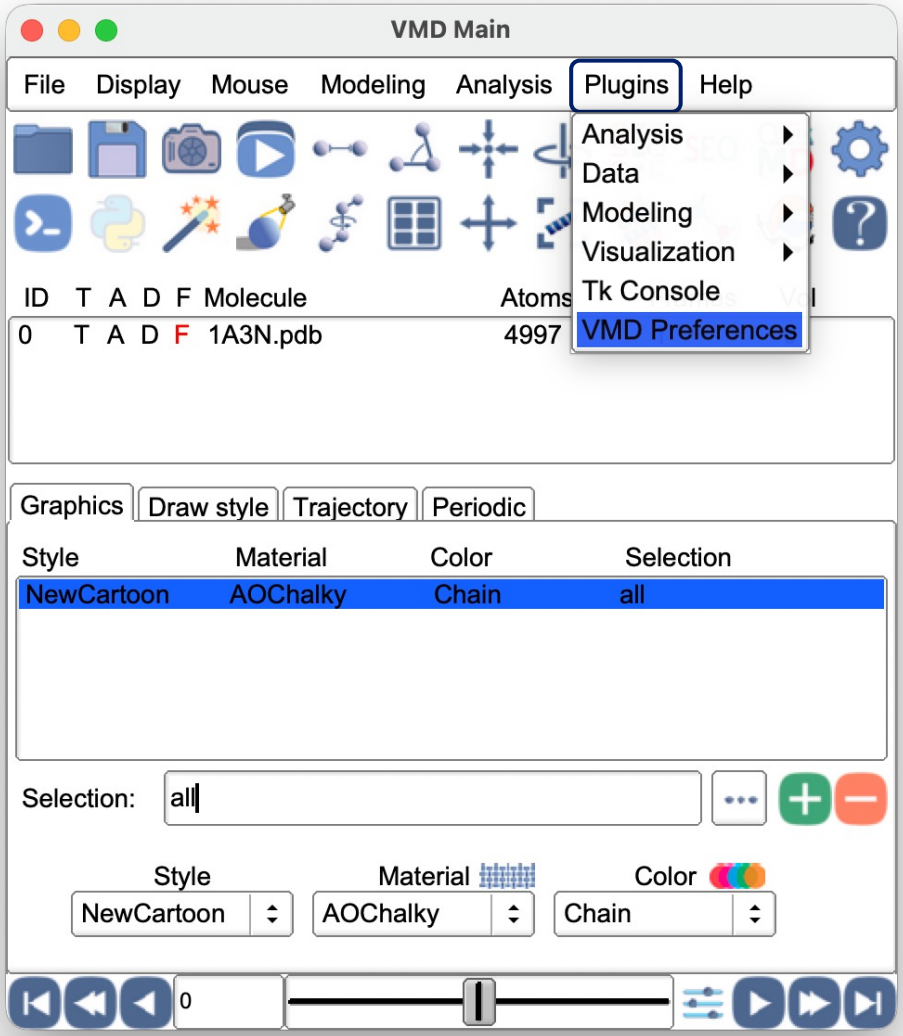




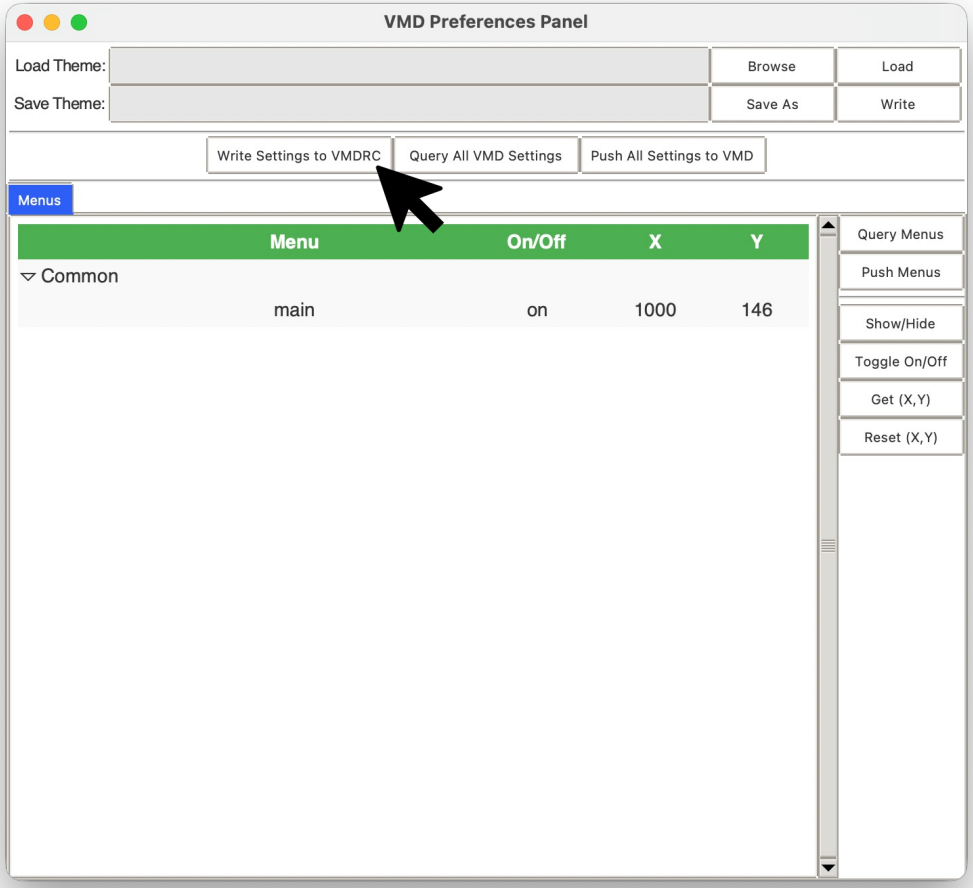


version 2.0.0

Advanced options



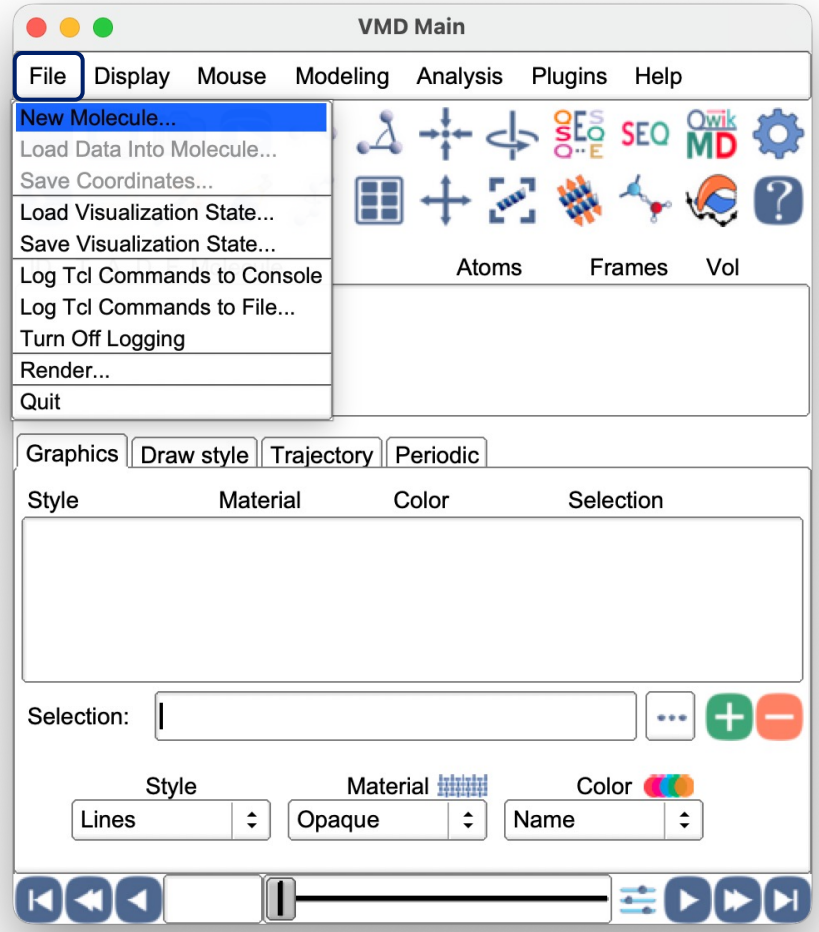
Save current settings, to apply every time VMD opens:

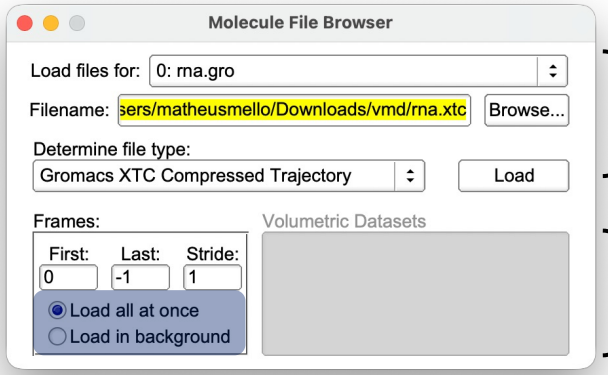


version 2.0.0

Managing trajectories

Load RNA model (`rna.gro`) and trajectory (`rna.xtc`)





The trajectory file is loaded on top of the topology file

`Load all at once` loads faster, especially for larger systems

Note that the molecule leaves the field of view

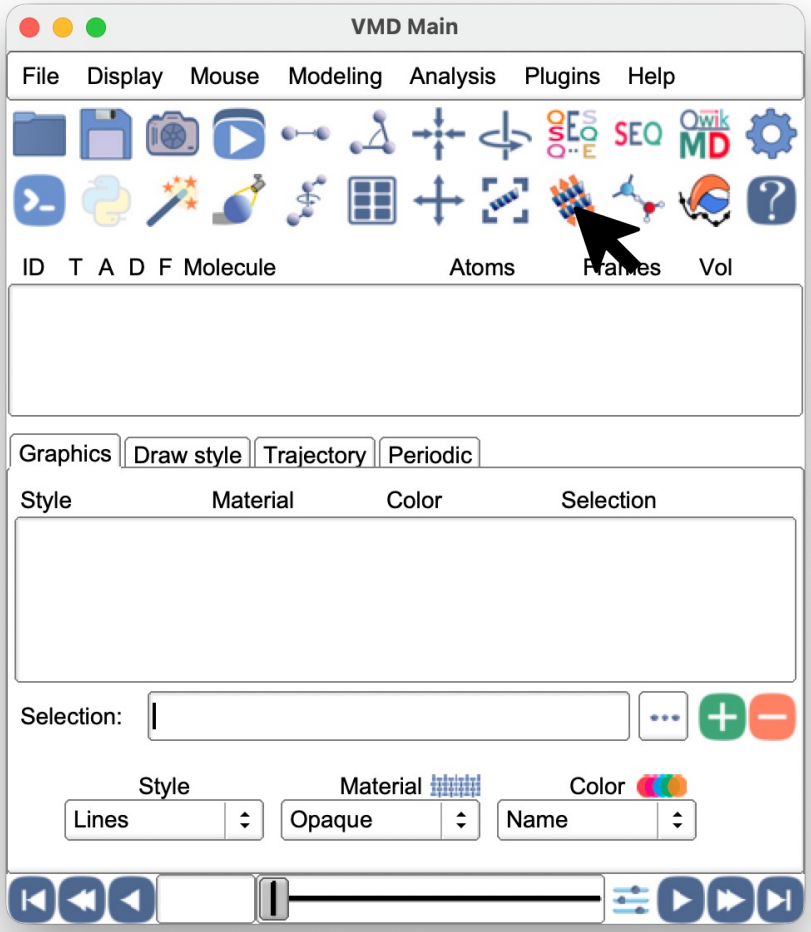
Solutions:

- press '=' to reset view
- align trajectory to first frame

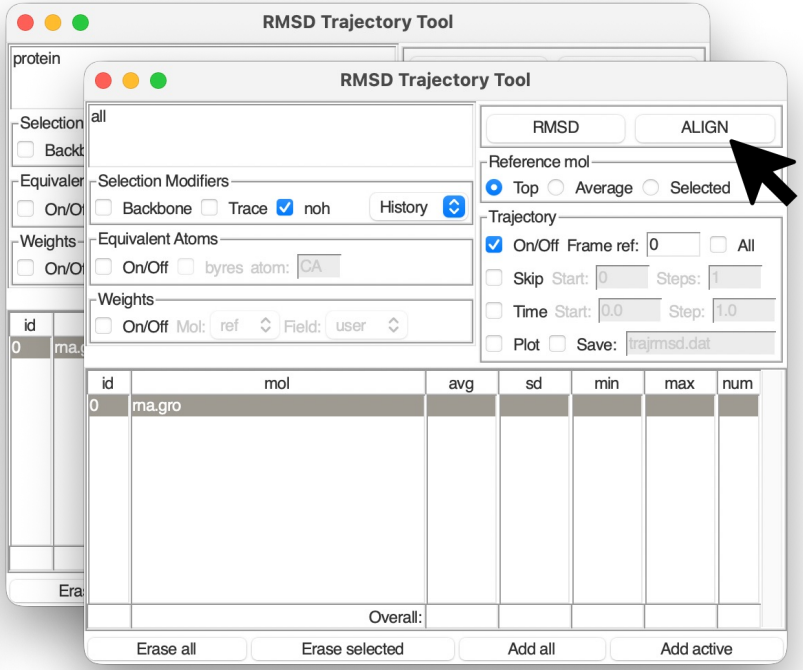
version 2.0.0

Aligning trajectories

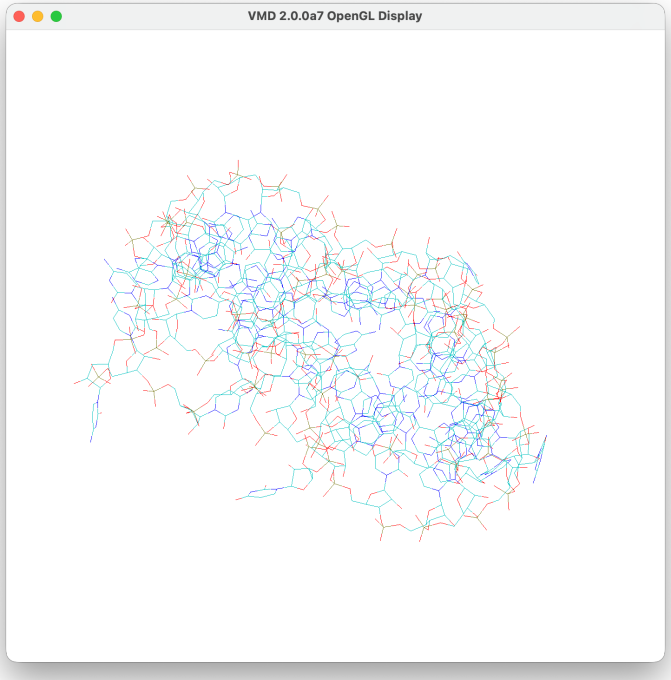
Open RMSD Trajectory tool



Change selection and align



Reset view (=)

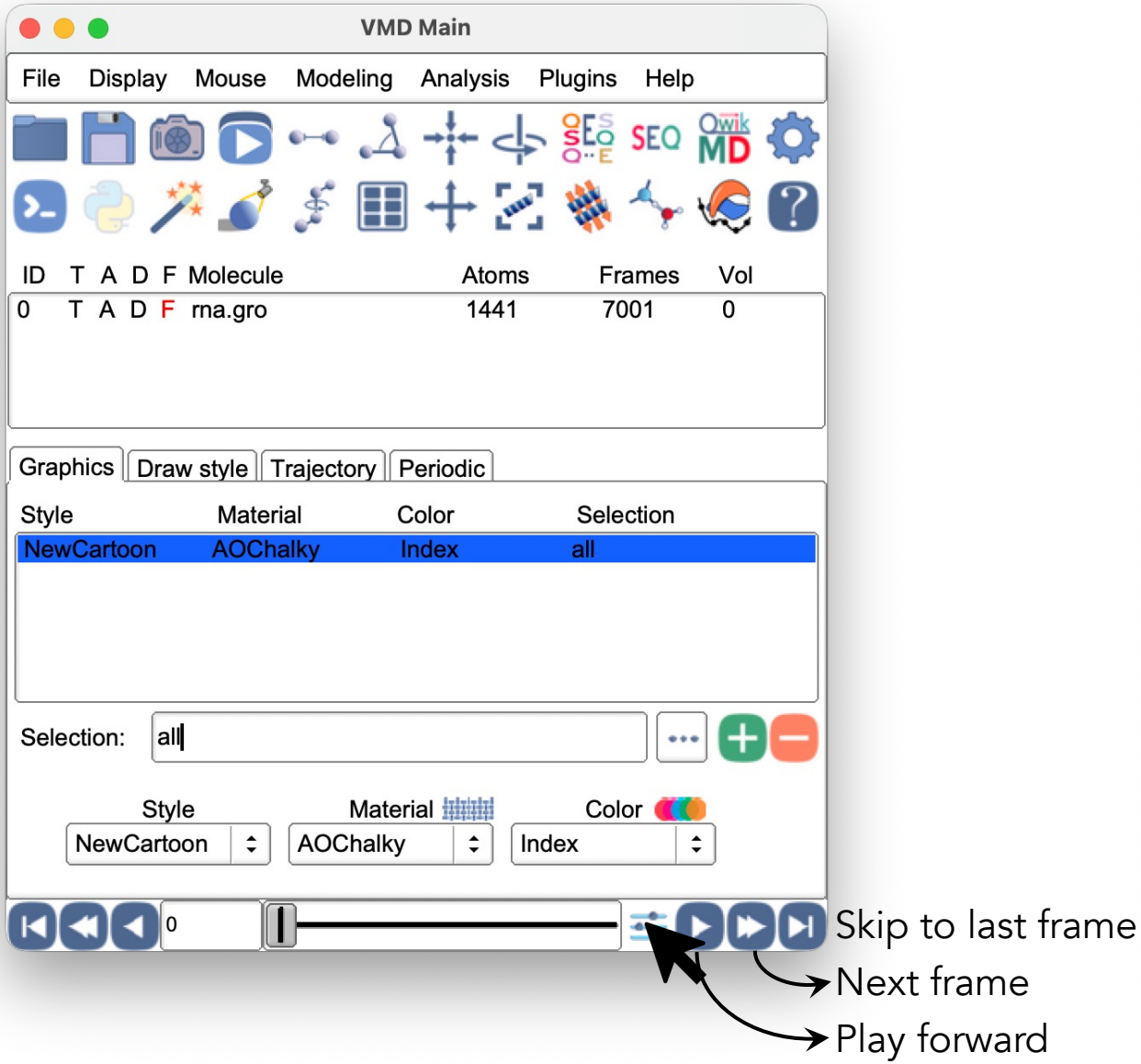


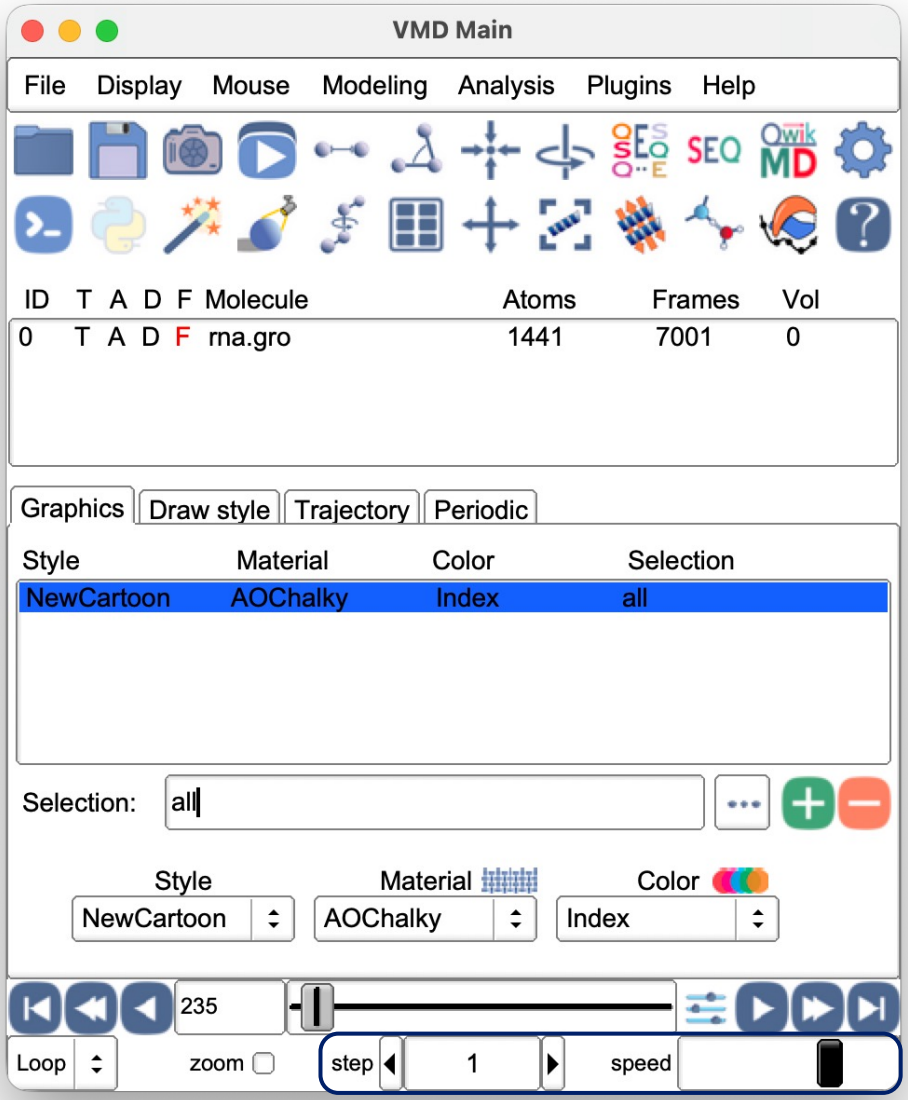
Try a custom selection and explore a representation that you like!

Alternatively : `Extensions > Analysis > RMSD Trajectory Tool`

version 2.0.0

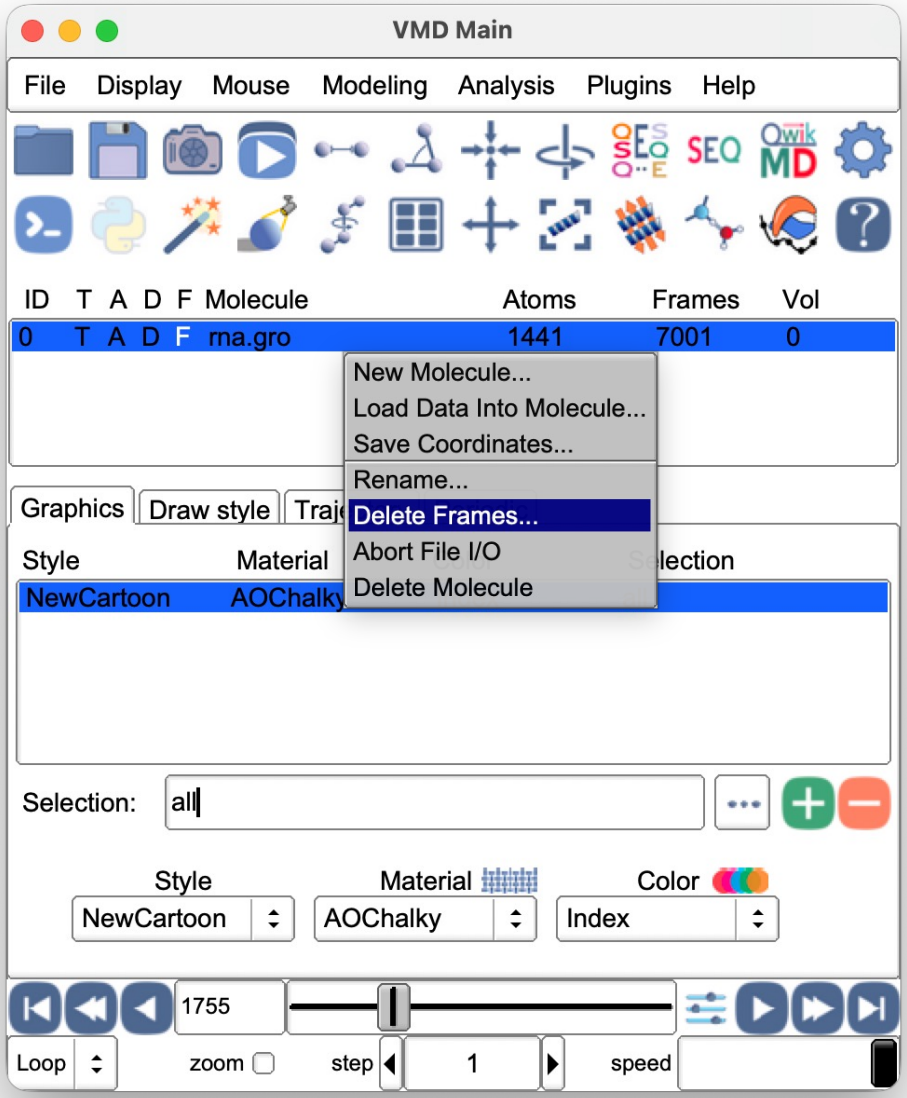
Managing trajectories



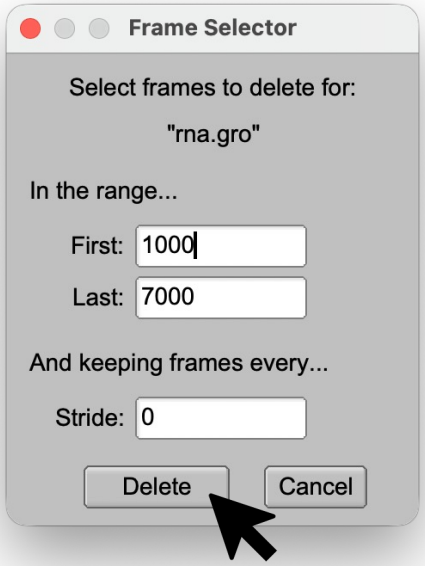


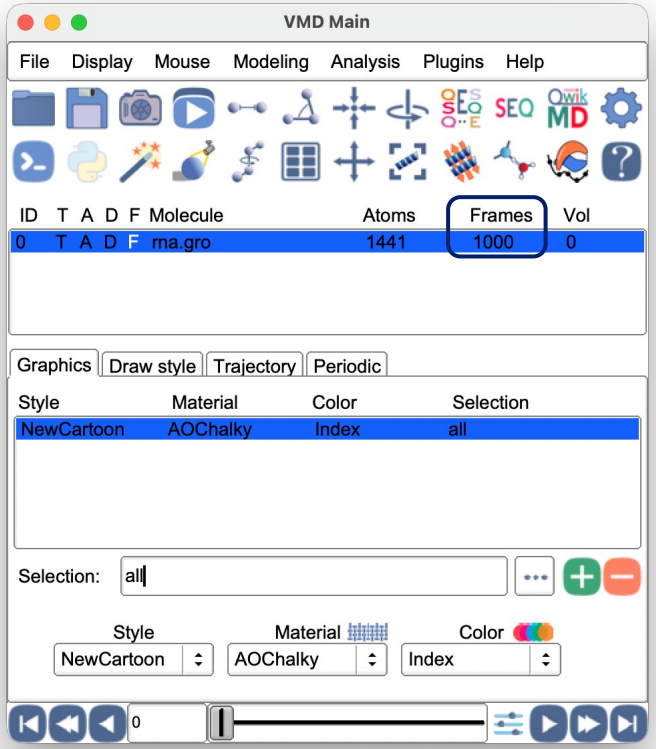
version 2.0.0

Managing trajectories



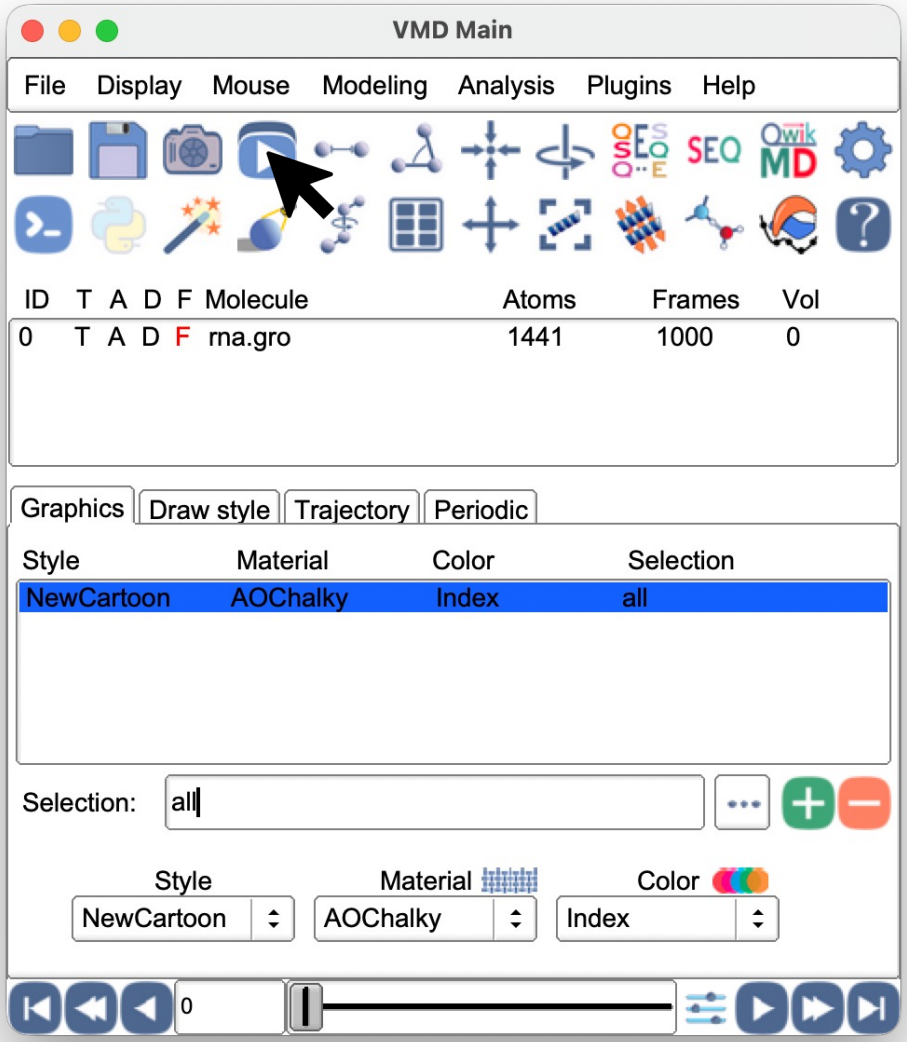
The trajectory is quite long!
Let's keep only the first 1,000 frames.





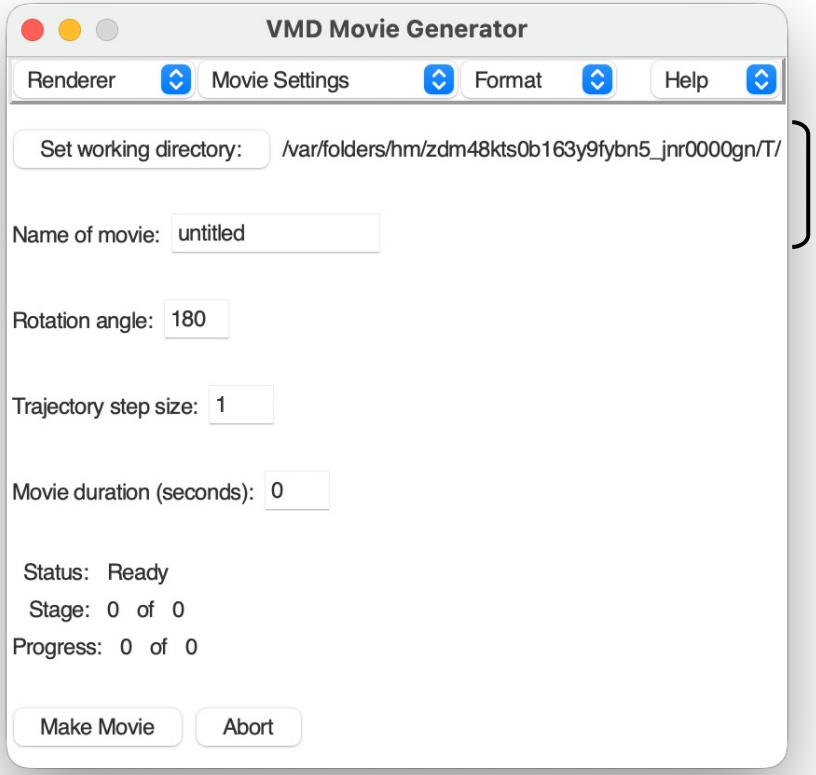
version 2.0.0

Rendering videos



Alternatively: `Extensions > Visualization > Movie Maker`

(version 1.9.4)



Set the proper directory

Name your movie

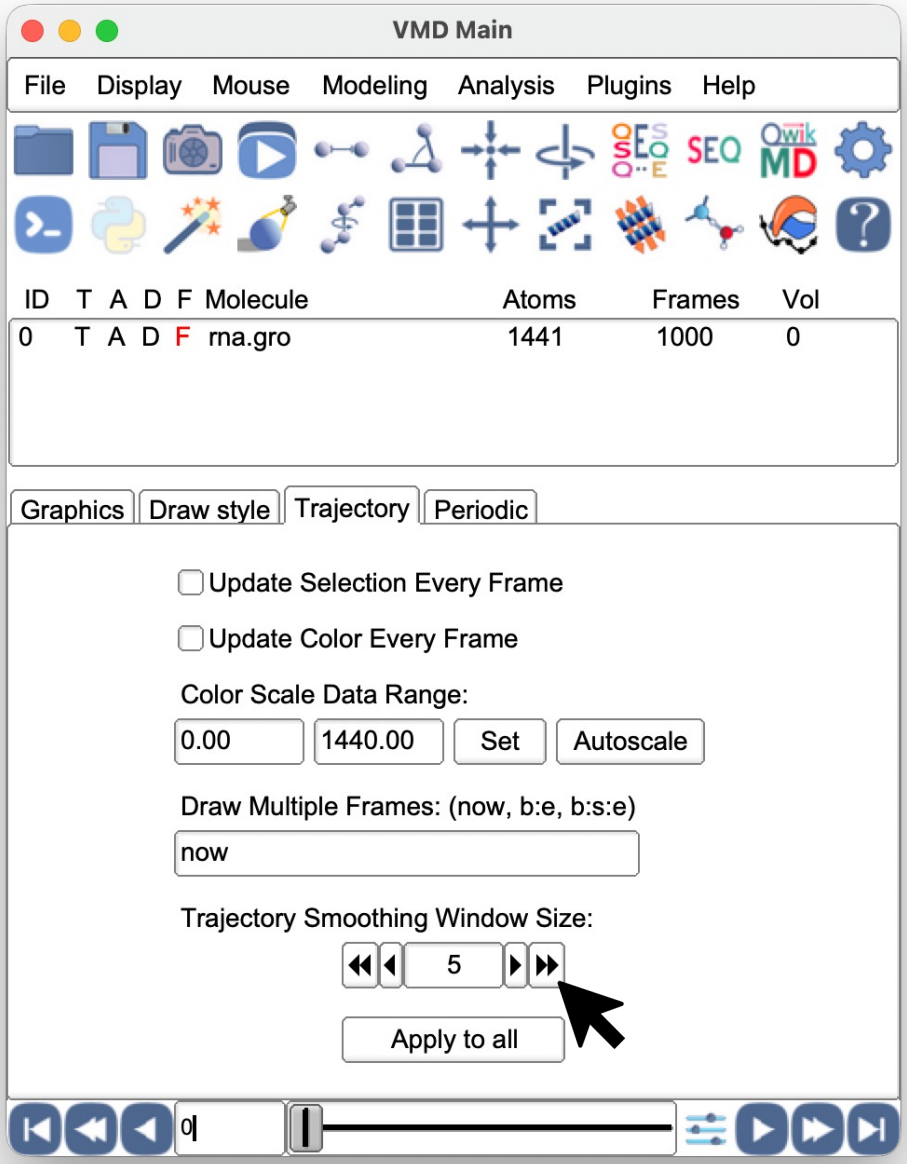
version 2.0.0

Rendering videos

Our results so far…

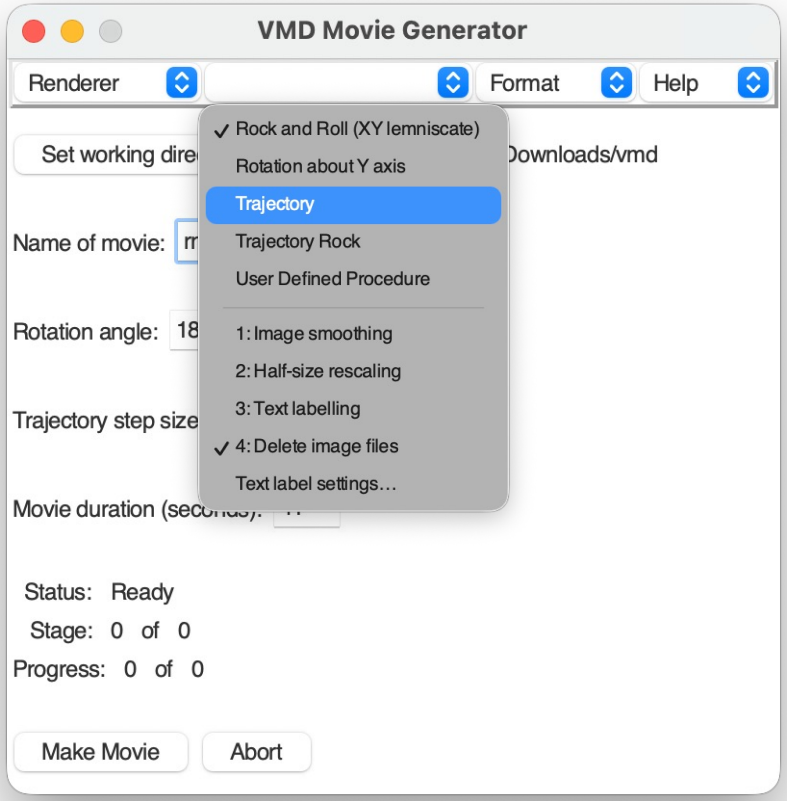
version 2.0.0

Rendering videos



Change `Movie Settings` to `Trajectory`

You can also change the renderer to `Tachyon`, but the rendering time will increase significantly



version 2.0.0

Rendering videos

`Smoothing = 5`

`Smoothing = 0`

Questions?