# Advanced Visualization in VMD

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### Outline

- Saving your VMD state
- Advanced materials + ray tracing
- Working with multiple viewpoints
- Live demo for movie making







## Saving your VMD state

- Creating a VMD scene might take a lot of work and time:
  - Graphical Representations
  - Viewpoint (camera location)
  - Other Customizations (colors, materials)
- Re-use VMD states
- VMD tutorial section 1.5

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resid 100				
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Drawing Metho CPK	d •	Default		

**Graphical Representations** 



### Advanced materials

- Pre-defined materials have different graphics properties
- Advanced materials might require appropriate render mode and display settings
- VMD tutorial section 1.6

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AOShiny	- 85	Delete	
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0.00		Ambient	
0.65		Diffuse	
0.50		Specular	
0.53		Shininess	
0.70		Mirror	
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0.00		OutlineWidth	
🗆 Angle-Modu	lated Trar	sparency	



https://www.ks.uiuc.edu/Research/vmd/current/ug/node88.html

#### Combining advanced materials + ray tracing options Example of RTChrome material

Render with	Snapshop	Tachyon	Tachyon

No

Ray Tracing Options					
Shadows	On 💌				
Amb. Occl.	Amb. Occl. On				
AO Ambient	((	(	0.80	•	*
AO Direct	"	1	0.30	•	*

Yes (shadows, AO)

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**Ray Tracing options** 

No

## Working with viewpoints: ViewChangeRender

- Viewpoints contain graphical reps and camera position / viewing angle
- ViewChangeRender allows to save and retrieve viewpoints to swap between focus points.
- Add viewpoints to create a movie with geometrical interpolation
- Combine with VMD Movie Maker plugin



### Stereoscopic rendering tutorial (VR)



#### VMD VR Movie Rendering for YouTube, Google Cardboard, GearVR, and Oculus Rift

Overview Publications

Home

Research

Software

BioCoRE

VMD Molecular

Graphics Viewe

**Dynamics Simulato** 

NAMD Molecular

Collaboratory

 MD Service Suite
 Structural Biology Software Database

Computational Facility One of the advanced features provided by VMD versions 1.9.3 and later is the ability to render omnidirectional stereoscopic 3-D images and movies, useful to create so-called "VR" movies on YouTube and for VR HMD movie players on devices such as GearVR, Oculus Rift, and others. The process of developing VR (omnidirectional stereoscopic) movies using VMD follows a series of steps:

- Set VMD renderer and rendering settings for VR/360 movies
- Render the movie
- · Encode the raw frames into a YouTube-compatible MP4
- Tag the MP4 movie with special YouTube-compatible metadata to indicate that it is
- a VR movie
- Upload the movie to YouTube, and mark it as 3-D/stereoscopic



VMD Example VR movies produced with panoramic and omnidirectional stereoscopic ray tracing techniques, described in DOI: 10.1016/j.parco.2015.10.015

#### VMD Renderers and Settings

At present, the special omnidirectional stereoscopic projection (OSP) and associated image formats are most easily used via the TachyonL-OptiX (aka "TachyonLOptiXInternal" in text commands) GPU-accelerated ray tracer in VMD. It can be used both for batch mode movies and for live interactive previewing. By default, the TachyonL-OptiX ray tracing engine uses the same camera projection mode that is selected in the main VMD graphical interface. Since the VMD OpenGL renderer is not yet capable of rendering the special OSPs and lighting modes needed for VR movies, the graphical interface in VMD doesn't yet provide a projection mode for OSP rendering, and it must be enabled by setting some environment variables, as described below. Variables can be set and unset either in the unix shell or within VMD itself, but they will not take effect until the next time the TachyonL-OptiX renderer runs to completion.

#### VMD Mailing List

VMD

Outreach

Download

- bash: export VARIABLE=1
  bash: export VARIABLE=
- VMD
- Tutorials
- tcsh: unsetenv VARIABLE
   vmd/tcl: set env(VARIABLE) <sup>2</sup>

tcsh: seteny VARIABLE=1

vmd/tcl: unset env(VARIABLE)

- VMD Manuals
- Environment variable and associated rendering results

Setting/unsetting an environment variable

- VMDOPTIXAOMAXDIST: change AO shadows from "infinit" to a maximum occlusion distance formulation. Units are specified in camera coordinates. This is
  needed within virus capsids or other dark areas that would otherwise be completely dark, and which would otherwise look "2-D" if only the VR headlight was used.
  A good starting value would be in the range 0.5 to 10, increasing to collect more shadow, or decreasing to collect less shadow.
- VMDOPTIXHEADLIGHT: set to enable a VR-camera-centered "headlight". This light works just like the standard VMD directional lights, but it is always positioned at the camera location.
- VMDOPTIXEQUIRECTANGULAR: set to enable the omnidirection projection
- VMDOPTIXSTEREO: set to enable stereoscopic rendering

Other more specialized environment variables and associated rendering results

 VMDOPTIXNODESTROYCONTEXT: set to speed up batch-mode movie rendering -- when set all subsequent environment variable changes will be ignored until unset again

#### **Rendering the Movie**

For early testing purposes, the movie can be rendered at low or moderate resolutions, e.g. 512x512, 1024x1024, or 2048x2048, which will both speed up rendering and also speed up YouTube uploading and associated post-processing. Final completed movies should be rendered at either 3840x2160 or 4096x4096 resolution, to ensure good quality playback on the latest generation smartphones that have 2560x1404 displays.

#### https://www.ks.uiuc.edu/Research/vmd/minitutorials/vrmovies/