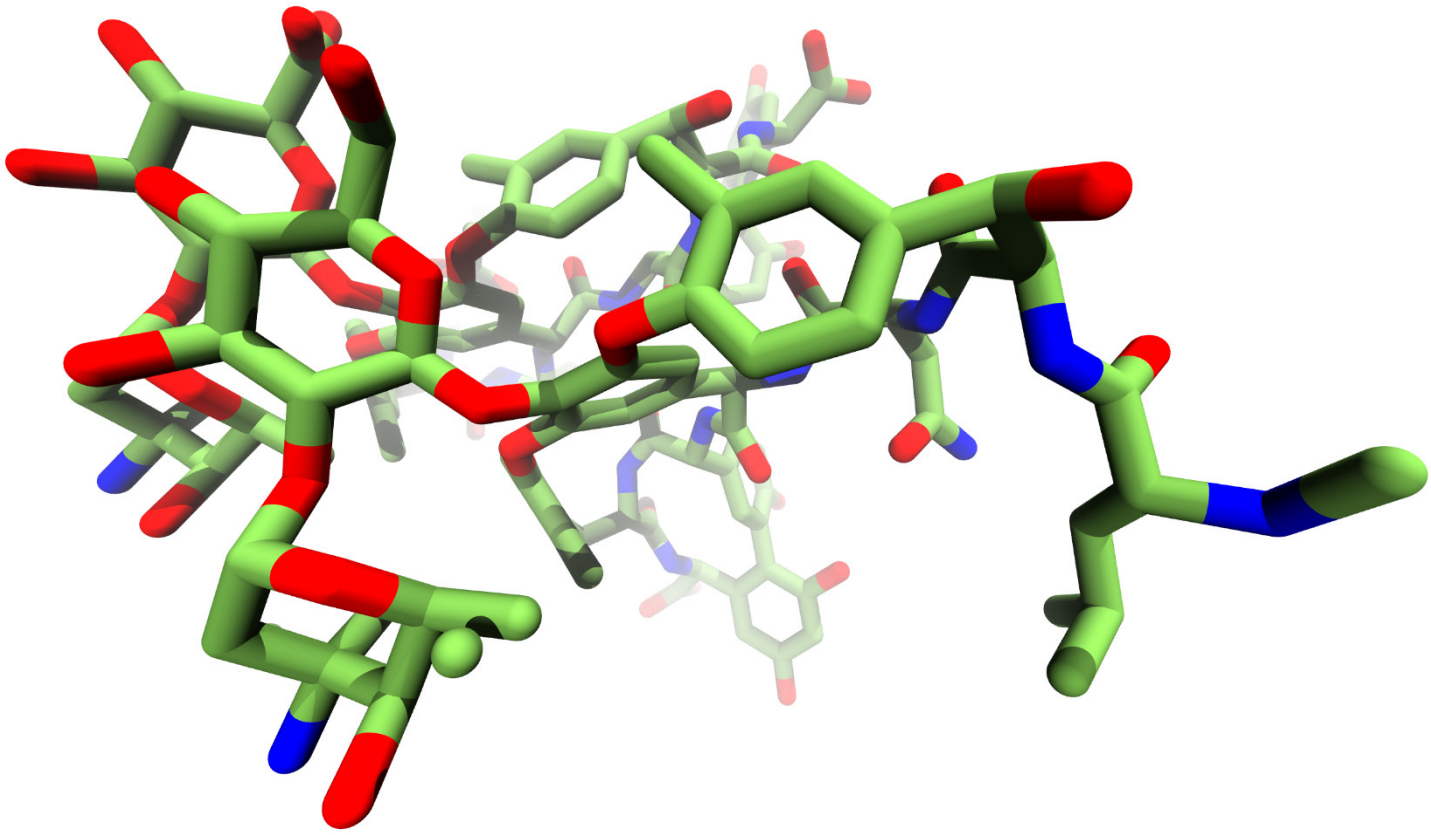
2019



Creating Publication Grade Renderings in VMD

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Contents

Required Software

VMD	Molecular visualization software
WinSCP	Graphical interface to interact with supercomputer
PuTTy	Supercomputer terminal

VMD Setup

Downloading VMD

VMD is a well packaged software and easy to install but some technical knowledge is required which this section will guide you through.

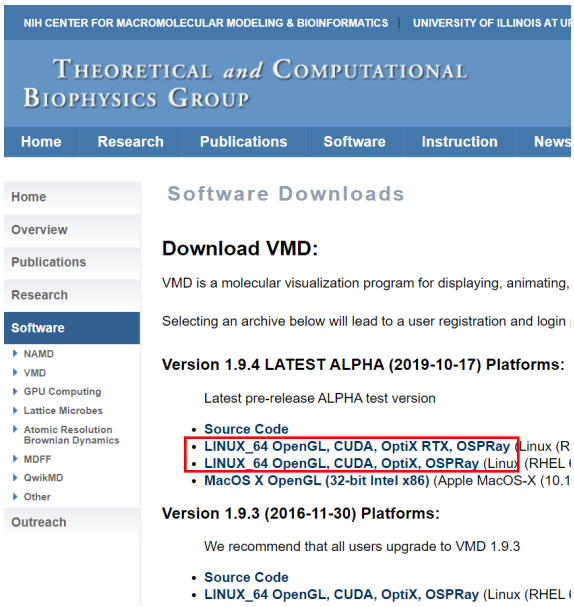

***Figure 1**. Current version of VMD*

1. Visit the VMD website download page. You have access to the current alpha versions undergoing testing as well as the current stable version.
2. Download one of the pre-release alpha test versions. As of the writing of this tutorial the current alpha is LINUX_64 OpenGL, CUDA, OptiX RTX, OSPRay.
3. In order to download VMD, there will be a brief registration window. Take a moment to fill this out accurately as it helps support the TCBG group the maintains VMD.
4. A compressed tar.gz will begin downloading
5. Log into a supercomputer terminal using PuTTy to begin the installation.
6. If you have not already, create a new folder called software in your home directory with the following command:

   ```
   -bash-4.2$ cd ~
   -bash-4.2$ mkdir software
   ```
7. Open WinSCP.
8. Drag the newly downloaded tar.gz to your software directory in WinSCP.

Installing VMD Locally

9. Once the tar.gz file is in your software directory, log into a supercomputer terminal using PuTTy to begin the installation.
10. Move the software folder:

    ```
    -bash-4.2$ cd /fslhome/software/
    ```
11. Extract the VMD files:

    ```
    -bash-4.2$ tar -zxvf vmd-1.9.4a38.bin.LINUXAMD64-CUDA10-OptiX600-RTX-OSPRay170.opengl.tar.gz
    ```
12. A new directory will be created called vmd-1.9.4a38 depending on your downloaded version
13. Move to the new directory:

    ```
    -bash-4.2$ cd /fslhome/software/vmd-1.9.4a38
    ```
14. Prior to installation some changes need to be made to the configure file located at ~/software/vmd-1.9.4.a38/configure
15. Open the new vmd-1.9.4a38 directory in WinSCP and navigate to the configure file.
16. You will need to tell VMD where you want it to install VMD. You will be editing lines 15-19, which look like this:

```
# Directory where VMD startup script is installed, should be in users'
paths.
$install_bin_dir="/fslhome/software/bin";

# Directory where VMD files and executables are installed
$install_library_dir="/usr/local/lib/$install_name";
```

17. The variable $install_bin_dir and $install_library_dir tell VMD where to install itself.
18. Make a new directory in your software directory for the VMD installation:
    -bash-4.2$ `cd /fslhome/software/vmd/`
    -bash-4.2$ `mkdir vmd`
19. Change these variables to your software directory path. It is easiest to change them with WinSCP. Lines 15-19 will now look something like this:

```
# Directory where VMD startup script is installed, should be in users'
paths.
$install_bin_dir="/fslhome/software/vmd/";

# Directory where VMD files and executables are installed
$install_library_dir="/fslhome/software/lib/vmd";
```

20. Save the file and run the configure file from the terminal with the following command making sure you are in the proper directory:
    -bash-4.2$ `cd /fslhome/software/vmd-1.9.4a38/`
    -bash-4.2$ `./configure`
21. A new *make file* has just been made in the src folder. We will now change to the src directory and install VMD:
    -bash-4.2$ `cd /fslhome/software/vmd-1.9.4a38/src/`
    -bash-4.2$ `make install`

Congrats! VMD has now been installed at /fslhome/software/vmd/ and you can now begin rendering!

Generating Renderings

Initializing VMD

This section will be system specific. Since I use VMD on Brigham Young University's Fulton Supercomputer Mary Luo, the commands will be optimized for Mary Luo's architecture.

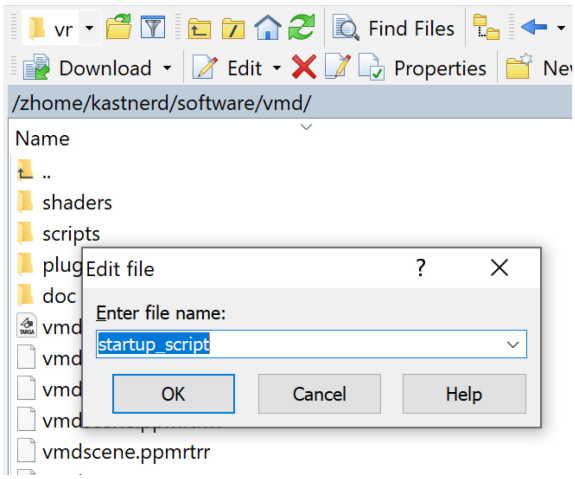

***Figure 2**. Create a startup_script.*

1. Create a script that will automatically run the commands needed for VMD startup. I recommend doing this through WinSCP.
2. Right click in vmd folder in WinSCP and choose new > file.
3. Name it *startup_script*.
4. Open the new file and copy paste the following code into the file:

```
JID=$(sbatch --time 4:00:00 -n 6 -N 1 --
gres=gpu:1 --mem=8G --wrap='sleep 4h' --parsable)
while [ $(squeue -j $JID -h -o %t) != R ]; do sleep 10; done
ssh -X $(squeue -j $JID -h -o %B)
```

5. Save the file.
6. This script will activate the CUDA GPU cores which are inactive by default.
7. Move to your VMD software:
   `-bash-4.2$ cd /fslhome/software/vmd/`
8. Execute the *startup_script*:
   `-bash-4.2$ source startup_script`
9. Since VMD needs to be visualized in order to do a rendering, PuTTy will not be sufficient. Luckily there is a web interface for the BYU supercomputer at the website https://viz.fsl.byu.edu:3443/
10. Navigate to this site preferably using Google Chrome and sign in with your credentials.
11. To initiate a session, choose:
    1) Launch Session
    2) XFCE
    3) Launch
    4) Terminal (black box)

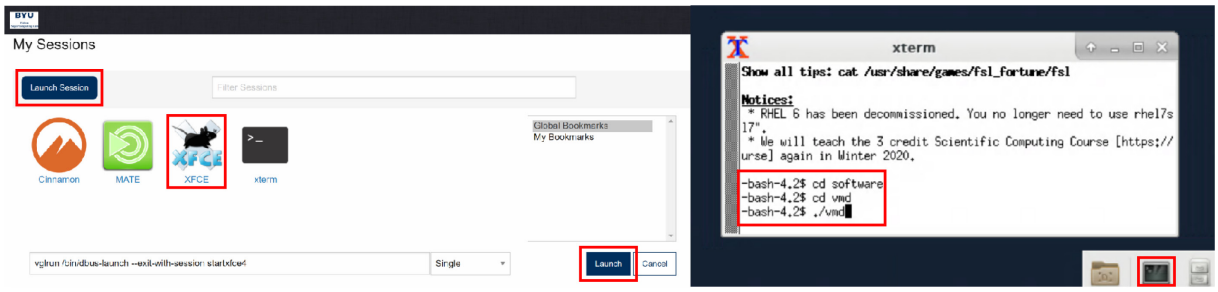

***Figure 3.** Initiating the online visualization terminal.*

12. Next move to your VMD folder and execute the software:

```
-bash-4.2$ cd ~/software/vmd
-bash-4.2$ ./vmd
```

Congrats! You just opened your first instance of VMD.

Setting the Stage

Now that VMD is open we will need to load or molecule of interest and begin setting up the visual environment to get the best rendering quality.

1. Obtain a PDB of interest or another structural file (MOL2, XTC, etc.). In this tutorial, we will work with Dr. Castle's favorite molecule Vancomycin (PDB: 1SHO).
2. Download the Vancomycin PDB from the Protein Database website: 1SHO

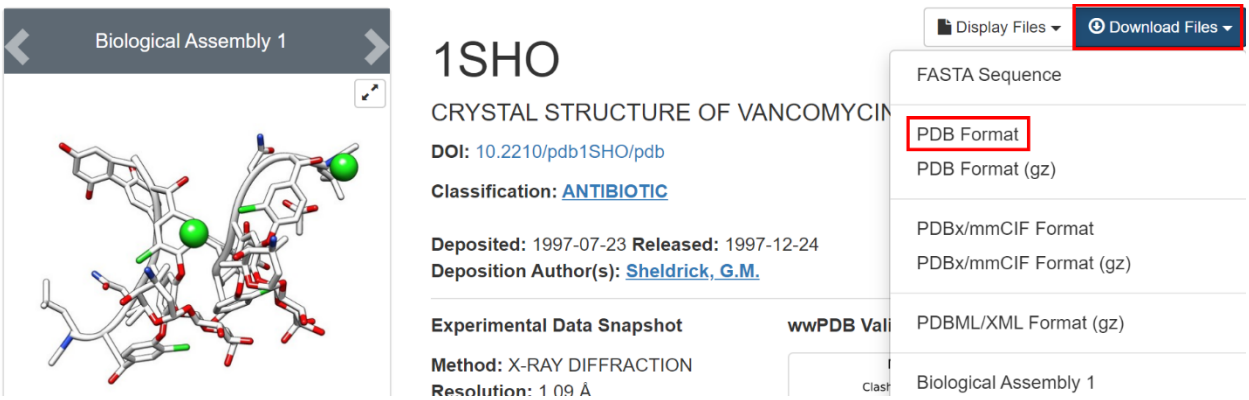

Figure 4. *Downloading from the PDB website*

3. Drag and drop it to your directory on the supercomputer via WinSCP. I recommend creating a new directory for this specific project:

```
-bash-4.2$ cd ~
-bash-4.2$ mkdir vancomycin
```

4. Open a 1SHO in VMD:
    1) File
    2) New Molecule…
    3) Browse…
    4) Navigate to ~/vancomycin/1aa5.pdb
    5) Select it and press OK

6) Load

5. You should now see a simple representation of vancomycin loaded in the OpenGL display and the "VMD Main" windows should display the molecule name (1aa5.pdb), the number of atoms (461) and the number of frames (1).
6. Next we will make some simple
7. Turn off the axes in the corner with:
    1) Display
    2) Axes
    3) Off
8. Turn the background white
    1) Graphics
    2) Colors…
    3) Categories > Display
    4) Names > Background
    5) Colors > white
9. Increase display rendering:
    1) Display
    2) Rendermode
    3) GLSL

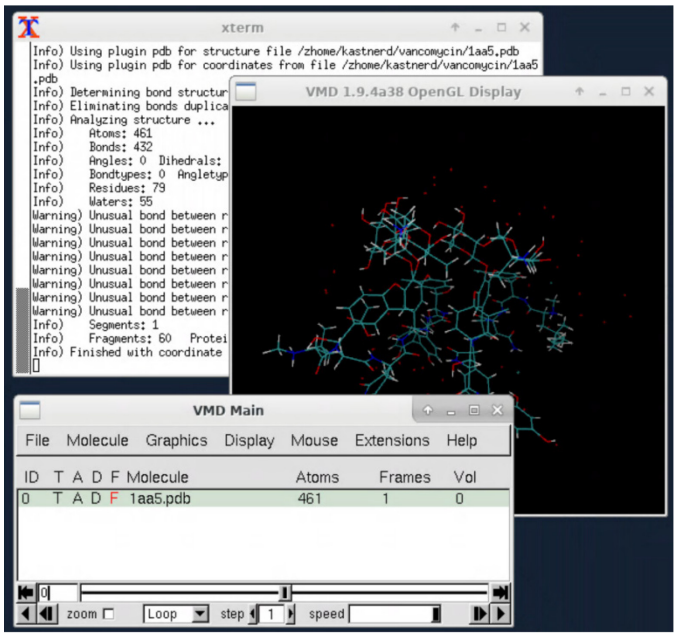

Figure 5. First view of VMD.

10. Position molecule use the rotate, translate, and scale tools:
    1) Mouse
    2) Rotate Mode, Translate Mode, or Scale Mode
11. Choose how VMD renders depth. You can use either perspective or orthographic:
    Note: Orthographic is simplifier and is preferred for publications but perspective is dynamic and interesting and should be used for posters, tweets, and other eye-gripping illustrations
    1) Display
    2) Perspective
12. Change depth fog:
    1) Display
    2) Display Settings…
    3) Cue Mode > Linear
    4) Cue Start > 1.25
    5) Cue End > 2.95

    Note: Changing *Cue Start* will change fog in the foreground and changing *Cue End* will change fog in background.
13. Change the rendering style:
    1) Coloring Method > Name
    2) Drawing Method > Licorice
    3) Material >AO Chalky
    4) Sphere Resolution > 100
    5) Bond Radius > 0.3
    6) Bond Resolution >100

Note: There are a ton of different materials to play with. I prefer AO chalky and opaque because they are the most common in publications.

14. Turn on ray traced shadows:
    1) Display
    2) Display Settings…
    3) Ray Tracing Options > Shadows > On
    4) Ray Tracing Options > AO Ambient > 0.20
    5) Ray Tracing Options > Amb. Occl. > On
    6) Ray Tracing Options > AO Direct > 1.00

    Note: Making the sum of AO Ambient and AO Direct greater than 1.0 gives the illusion that your image is brighter.
15. Change atom colors:
    1) Graphics
    2) Color…
    3) Categories > Name
    4) Names > C
    5) Colors > green

    Note: The default cyan color is fine but sometimes you may want to change the color, so I am demonstrating that process here. You can also play with the sliding color bars to get an off shade of green.
16. Before we begin rendering, it is good practice to save your visualization state:
    1) File
    2) Save Visualization State…
    3) Save as ~/vancomycin/vancomycin.vmd

Congrats! You have just set up a molecular environment and it is ready to be rendered.

Rendering

There are a lot of ways to render and most of them will look subpar. In this section we will do everything possible to get the most interesting and highest resolution image we can.

1. Open the rendering dialogue box:
    1) File
    2) Render…
2. A new dialogue called File Render Controls will open
3. Change the Render:
    1) Render the current scene using:
    2) Tachyon (internal, in-memory rendering)
4. Change the save location:
    1) Filename
    2) Browse
    3) ~/vancomycin/vancomycin.tga
5. Before we begin rendering will we need to change the resolution of display:
    1) Extension
    2) Tk Console
    3) Display resize 2000 2000

    Note: This will change the resolution to 2000 px by 2000 px. This will make the display giant and you will need to move it out of the way to continue working with the rendering prompt. In some versions you can also use the command "-res 2000 2000."
6. Return to the File Render Control Dialogue and choose render.

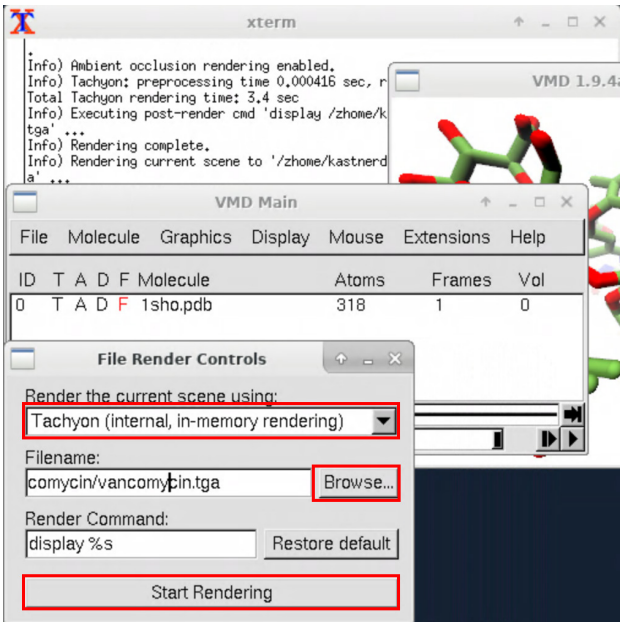

Figure 6. Rendering dialogue.

Congrats! You just rendered a TGA file of vancomycin.

Post Processing

Now that we have the output, we need to edit the file so that it is ready to be inserted in your paper!

1. Open WinSCP
2. Move the TGA file to your desktop
3. TGA files can be opened in Photoshop and converted to either PNG, JPEG, etc.
4. Crop it to the appropriate size.

Key Citations

1. Humphrey, W., Dalke, A. and Schulten, K., "VMD - Visual Molecular Dynamics", J. Molec. Graphics, 1996, vol. 14, pp. 33-38.
2. James C. Phillips, Rosemary Braun, Wei Wang, James Gumbart, Emad Tajkhorshid, Elizabeth Villa, Christophe Chipot, Robert D. Skeel, Laxmikant Kale, and Klaus Schulten. Scalable molecular dynamics with NAMD. Journal of Computational Chemistry, 26:1781-1802, 2005.