VMD Documentation

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Abstract

In this documentation, the basic and intermediate documentation of VMD molecular dynamics visualization software from University of Illinois at Urbana-Champaign are provided. This documentation includes user guide for opening and loading molecular structure files, change drawing options of molecular structures like CPK, tube, ribbon and etc., change color styles of molecular structures for better visualization, select different user interested atoms in a big molecular structure, create a multitask framework for molecular structure visualization, how to save your modified structure and how to render high resolution structures for high resolution three-dimensional visualization, how to study the trajectories and movement of molecular dynamics simulation of user interested structure, how to write basic scripts in VMD to have a programmable visualization filter, how to deal with multiple molecular structures, compare different molecular structures to have a better understanding of molecular dynamics simulation, statistical data analysis in VMD and finally run VMD on Clemson University Palmetto cluster as a high performance supercomputing.

Introduction

VMD which is an abbrevation for Visual Molecular Dynamics, is one of the most powerful molecular structure visualization packages which is distributed under University of Illinois at Urbana-Champagin affilation. This software can be used in several computational science areas like materials science, chemistry and biochemistry. VMD has a lot of unique features like, it can deal with large polymeric and biomolecular structures and it has high resolution rendering features that makes it suitable for high resolution visualization and also it can be used with high performance supercomputing facilities like Palmetto cluster in Clemson University to improve visualization performance of extra large molecular dyanmics simulation results by using parallel visualization techniques. According to VMD original documentation, the main features of VMD include:

- Three-dimensional molecular structure visualization by using user defined molecular drawing styles and coloring of molecular dynamics simulation results.
- VMD can support a wide range of molecular dynamics output file formats and there is no limit for size of molecular structures or trajectories.
- User defined atomic selection from a big molecular structure to analyze and visualize specific regions of whole data structure.
- VMD can be used to visualize volumetric data like position, displacement and velocity of atoms in molecular structures.
- Rendering high resolution data structures to have a better understanding of molecular structure and trajectories.
- VMD has a lot of statistical data analysis features to help users extract useful scientific information.
- VMD has a powerful tool to make movies and animations from molecular dynamics results.
- VMD can be used as a pre-processing software to prepare input files for molecular dynamics packages like NAMD, LAMMPS and GROMACS.
- VMD accepts Python and Tcl prgoramming scripts languages to create user defined programmable visualization filter.
- VMD accepts C/C++ programming source codes to create user defined programmable visualization filter.

In the next sections, we will try to provide a basic and intermediate coverage of these features to help interested students.

Downloading and installation of VMD

VMD software is distributed under University of Illinois at Urbana-Champaign affilation as an open source software which can be obtained easily in the official website of VMD software. In that official website, users may find a complete instructions for downloading and installation for three major operating systems: Windows, Linux and Mac OS X.

Downloading tutorials files

The files which is needed in this documentation can be easily obtained in the official website of VMD tutorials.

Single molecule visualization

As we mentioned before, in this section, we will learn how to open a molecular structure file, change the drawing options and coloring styles and how to render a high resolution data structure to obtain a publication quality image. Before starting this section, user should download the tutorials files as we mentioned in the last section. Also for the start, we used ubiquitin protein molecular structure which can be find the tutorials files folder as 1ubq.pdb. In order to open this file in VMD software, you should follow these steps:

1. Start VMD software. In the VMD main menu, choose File $\longrightarrow$ New Molecule... (Fig. 1). Then another windows as Fig. 2 will appear in your screen.

2. You should use Browse... option and find the 1ubq.pdb file and then don't forget to press the Load button in order to load the ubiquitin data structure.

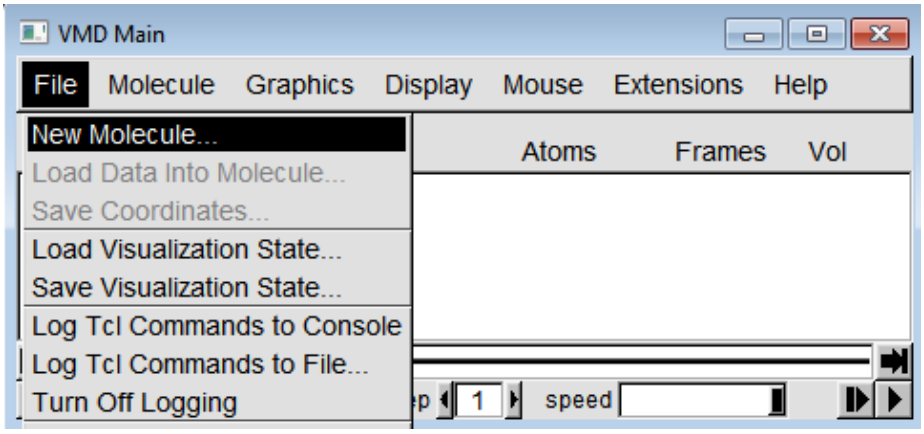

Figure 1: The main menu and New Molecule... option in the main VMD window.

Now you should see the ubiquitin molecular structure in your VMD OpenGL rendering window as it is shown in Fig. 3.

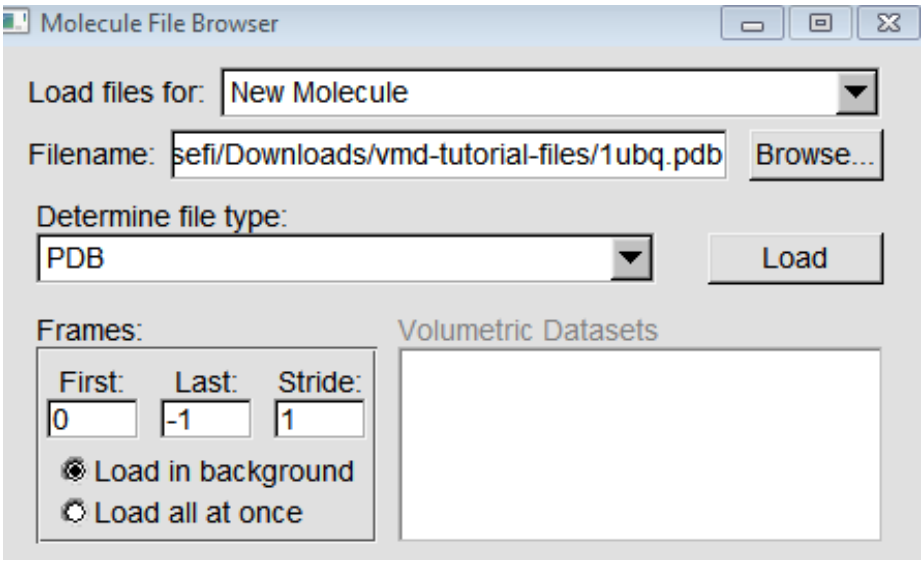

Figure 2: The browse and load button to open 1ubq.pdb file and load it to the VMD OpenGL window.

One of the interesting features of VMD is that if you type the first four letter of your interested protein structure, VMD can find it from pdb database and download it to your machine and you can load to see the visualization of that molecular structure. Now in order to change the drawing and color style of visualized ubiquitin protein structure, you should follow these steps:

1. In the VMD main menu, choose Graphics $\longrightarrow$ Representations. Then another windows will appear in your screen to change the drawing style.

2. Now you could change the drawing style in the Drawing Method tab. For example you could change it to CPK, Tube and Ribbon as is shown in Fig. 4.

Also in this Representation menu you can change the coloring style. You can use several representation for coloring style like atom types, mass, volumetric parameters like displacement, velocity and radial distance and also it can differentiate between alpha and beta molecular structures which is important for some biopolymers configurations. For example we changed the coloring style to radial distance in Tube drawing method and you can see the visualization of this molecular structure in Fig. 5.

Also in the Representation main menu you could change the selection of atoms. This feature help user to select different regions of interest in a big molecular structure to have more artistic three-dimensional visualization. Also this feature accepts the boolean operations like AND/OR to combine different selection methods and create a user defined visualization framework. For example if we choose the helix structures in selection method, you can see only helix molecular structures in Fig. 6.

As we mentioned before, we could create multiple representations. For example you hit the Create Rep. button, you could create multiple representations.

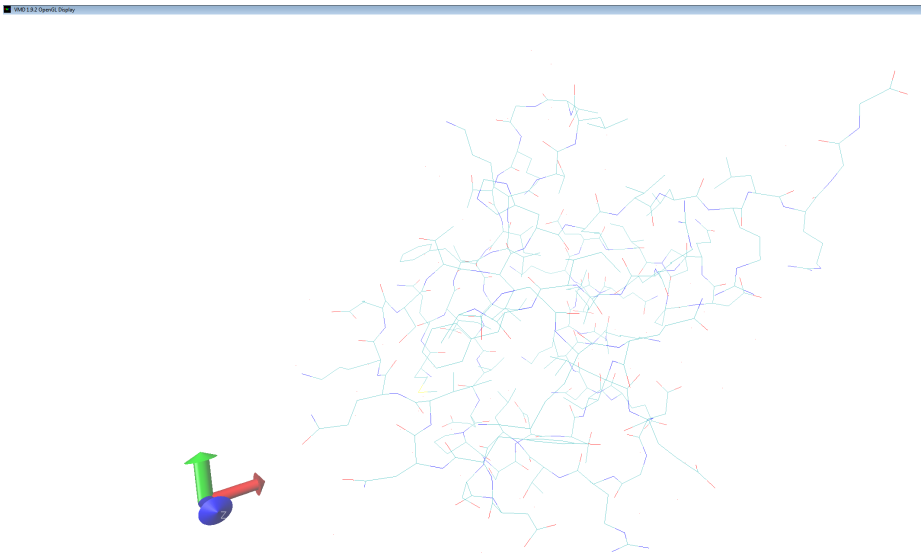

Figure 3: Loaded ubiquitin molecular structure in VMD OpenGL window.

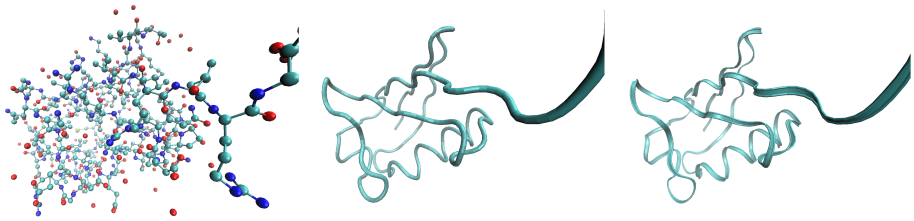

Figure 4: Three drawing method of ubiquitin molecular structure as CPK, Tube and Ribbon respectively.

For example we combined helix and all molecular structure and define different coloring styles to bold the helix structures in ubiquitin protein as is shown in Fig. 7.

Proteins and generally biopolymers have a complex molecular structure and scientists need to study the chemical effect of different structure explicity. In order to deal with complex biopolymers structures, VMD developed an extension as Sequence Viewer to pick different chemical bonds, chains and etc. more easily. You could see and pick different molecular sequeneces by using VMD main menu as Extension $\longrightarrow$ Analysis $\longrightarrow$ Sequence Viewer. For example we picked chain X and reside 68 of ubiquitin protein and it is shown as a yellow coloring style in Fig. 8.

Now in order to keep these settings and load it in the future, you could save the visualization state by using File $\longrightarrow$ Save Visualization State in the format of .vmd file extension.

As we said before, VMD has some unique high resolution rendering feature to create robust three-dimensional molecular visualization. You could change the resolution of different selection in Representation main menu and also by creating a molecular surface as a new representation and change the Material

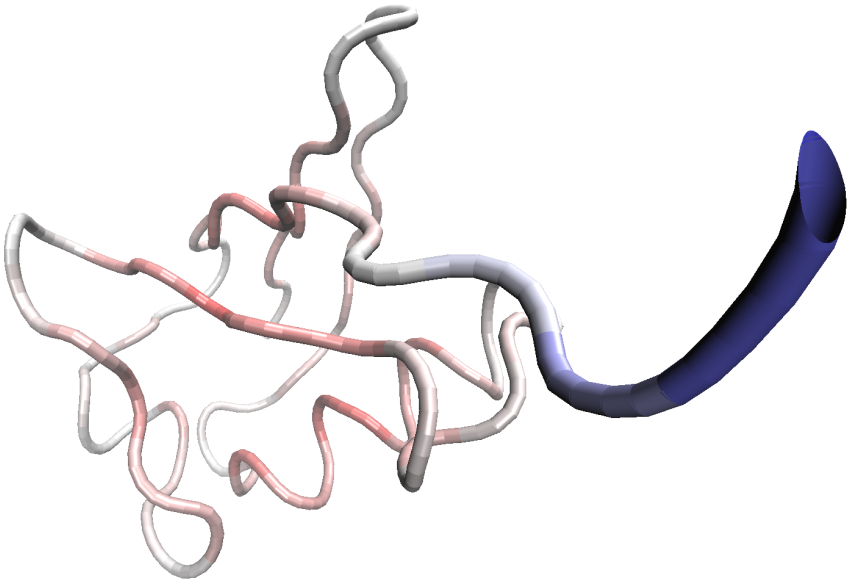

Figure 5: Radial coloring style is applied on Tube drawing method and is shown in VMD OpenGL window.

to transparent, we could create this unique three-dimensional molecular visualization as is shown if Fig. 9. Actually we used File $\longrightarrow$ Render option to create this high resolution image.

At this stage, you learned the basic operations of VMD and now we could move on to the intermediate level of molecular visualization. The first advanced visualization technique that we will study here is the movement and trajectories of molecular structures. Actually, we want to visualize the results of molecular dynamics simulation which is consist of molecular vibrations and displacement. In order to load movements and trajectories, you should load ubiquitin.psf and pulling.dcd files from tutorials folder and then you can see the ubiquitin protein which is surronded by water molecules that represents this protein in water solvent. Actually, this is the result of molecular dynamics simulation ubiquitin protein folding at water solvent. If you change the selections and select the protein and water molecules and pick some chain sequences you could see this three-dimensional molecular visualization as Fig. 10.

Now in the VMD main menu, you change the speed of animation and other options like zoom and etc. to promote movements of atomic trajectories of protein and water molecules. Also in Representation main menu if you go to the trajectory tab and in the Draw multiple frame you could choose multiple frames for visualization. For example if you choose 0:10:99 frames which means it will selects the frames from 0 to 99 by 10 steps and change the coloring method to Trajectory $\longrightarrow$ Timestep, you could find this colorful three-dimensional molecular visualization as is shown in Fig. 11.

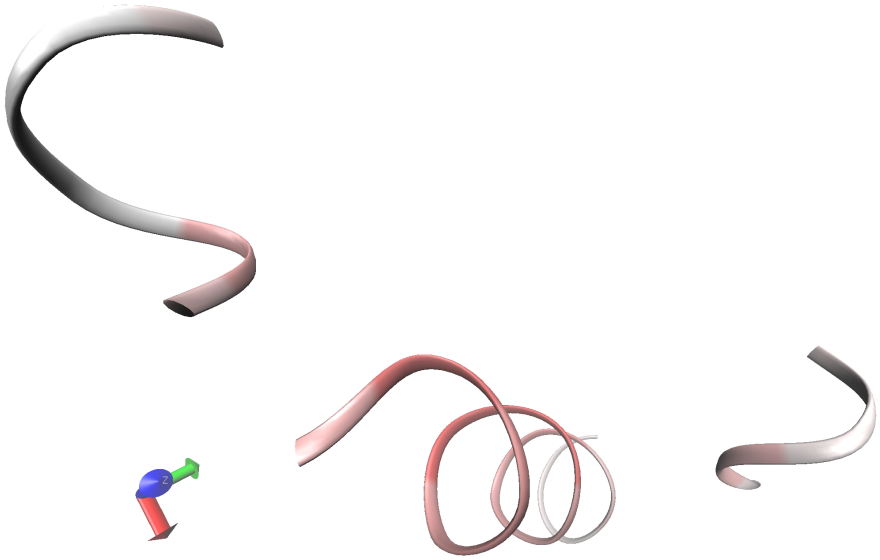

Figure 6: Helix is selected and is shown in VMD OpenGL window.

VMD scripting

For some advanced visualization techniques, we should use programmable filters. Actually, everything that we did up to this stage by using graphical user interface (GUI) of VMD software can be done by writing scripts. Moreover, you could add some new features to VMD by writing scripts. In order to write scripts for VMD by using Tcl programming language, you could go to the Extension $\longrightarrow$ Tk Console to open VMD Tk Console. After opening of VMD Tk Console you should see this as Fig. 12.

There are two basic commands in Tcl/Tk programming language as set and put. For example if say $set \quad x \quad 0.5$, It will change the value of x to 0.5. Also if we say $put \quad "x = \$x"$, it will print the value of x that we set before. You could see some examples as is shown in Fig. 13.

Also in order to perform some mathematical operations, we could use *expr* command in Tcl console. For example, if we say that $set \quad x \quad [expr \quad 8 - 3 * \$x]$, it will calculate $8 - 3 * x$ expression and set the value x as a result of that expression (Fig. 14).

Sometimes we need to do some iterative operations. Tcl provide a for loop like other programming languages that can do some repetitive operations. The syntax of for loop in Tcl programming language is as follows: $for \quad \{initialization\} \quad \{test\} \quad \{increment\} \quad \{commands\}$. Now if we want to calculate the expression of $8 - 3 * x$ for $x \in [0, 20]$ and save the results as a output.dat file on disk, we could write this expression (Fig. 15):

Now you should learned the basic concept of scripting by using Tcl language. So we could move on the specific VMD scripting to manipulate molecular structure and create visualization. For example if we want to load a .pdb file we could do this by using mol command as follows: $mol \quad new \quad 1ubq.pdb$. Note: if you see error that it says the 1ubq.pdb file doesn't exist, you should spec-

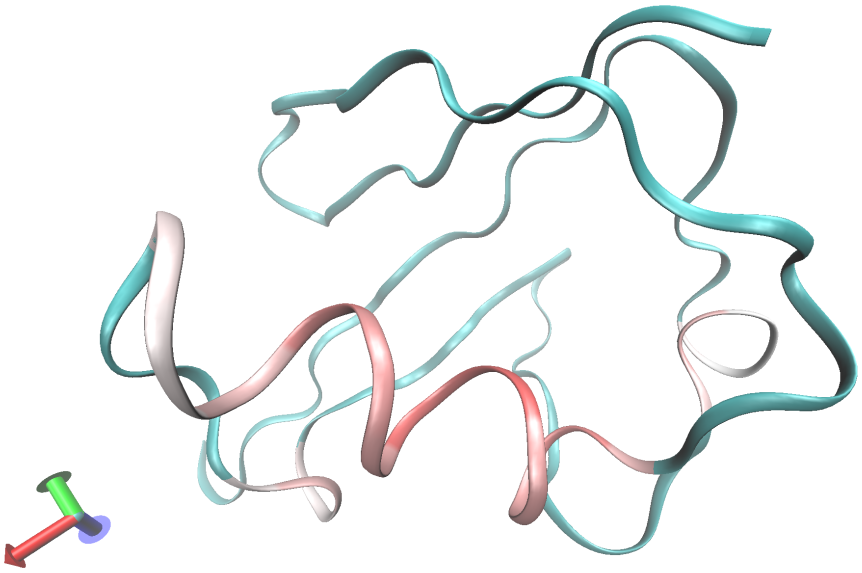

Figure 7: Create multiple representation of helix/all structure and assign different coloring styles to them and it is shown in VMD OpenGL window.

ify the complete address of tutorials folder. For example: $mol\ \ new\ \ C:/User/yousefi/Downloads/vmd-tutorial-files/1ubq.pdb$. Also if we want to do some operations only on specific regions of a big molecular structure, we could use atomselect command. The syntax of atomselect commands is: $atomselect\ \ molid\ \ selection$ which molid is molecule ID and selection is the name of the user defined selection. The example of using atomselect is: $set\ \ crystal\ \ [atomselect\ \ top\ \ "all"]$. This expression create a new selection which its name is crystal and select the last loaded molecular structure as top and also it will select all atoms instead of other selections like protein, waters or etc. Also you could gain some useful information by using Tcl scripts from your molecular structure which is loaded to VMD by using num command. For example if you type $\$crystal\ \ num$, it will shows you the number of atoms in the loaded molecular structure at that user defined selection (crystal). Also you could do some translational and rotational transformations to your molecular structure by using move command. For example you could move crystal molecular selection as $\$crystal\ \ moveby\ \ \{10\ \ 0\ \ 0\}$. This command will moves the crystal selection according to the $\{10\ \ 0\ \ 0\}$ translational vector. Also if you want to rotate your molecular selection you could use this command as $\$crystal\ \ move\ \ [transaxis\ \ x\ \ 40\ \ deg]$ which it will rotates the crystal selection along the x axis by 40 degree. One of the most powerful visualization tools which is available in VMD scripting is B-factor field. Actually you could move any computationally gained data to the parameter which is called B-factor field and visualize it as a colorful image. For example if you want to show the temperature gradient of molecular structure during movements, you could save temperature field to B-factor field of VMD and visualize it as colorful countor

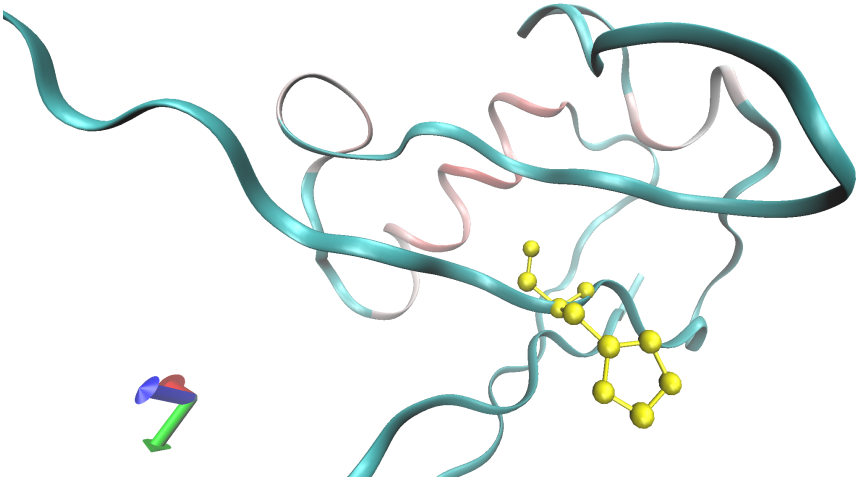

Figure 8: Pick chain X and reside 68 of ubiquitin molecular structure from sequence viewer option in VMD main menu.

in your molecular structure. In order to zero initialization of B-field factor you could use this command as $\$crystal \;\; set \;\; beta \;\; 0$. Also for example if you want to split hydrophobic and hydrophilic part of a biopolymer, you could do this by using $set \;\; sel[atomselect \;\; top \;\; "hydrophobic"]$ and this will creates a selection which contains the hydrophobic part of the molecular structure. And then you could change the beta parameter of this hydrophobic selection to 1 as $\$sel \;\; set \;\; beta \;\; 0$. Now you should see the hydrophobic and hydrophilic parts as is shown in Fig. 16. Also you could change the radius of atomic spheres for better visualization by using this command: $\$crystal \;\; set \;\; radius \;\; 1$ and $\$sel \;\; set \;\; radius \;\; 1.5$.

Now if you want to extract the name residues in the hydrophobic part of the ubiquitin protein, you could get the residue names by using this command: $\$sel \;\; get \;\; resname$. But it will show the all repititive residues. If you want to just pick the residues with alpha carbons you could do this by using: $set \;\; sel \;\; [atomselect \;\; top \;\; "hydrophobic \;\; and \;\; alpha"]$ and then $\$sel \;\; get \;\; resname$ and it will eliminates the repititive components. Now also you could get other useful information like residue ids and spatial coordinates by using these commands:
$\$sel \;\; get \;\; resid$, $\$sel \;\; get \;\; \{resname \;\; resid\}$ and $\$sel \;\; get \;\; \{x \;\; y \;\; z\}$. Also you could measure some geometric features of the user specified selection like center of mass and minimum and maximum of atomic spatial coordinates by using these commands: $measure \;\; center \;\; \$sel$ and $measure \;\; minmax \;\; \$sel$. When you finished your calculations, you could remove the selection by using: $\$sel \;\; delete$. Another option to write all these scripts is the writing the all commands in a file like beta.tcl and load it to the VMD Tcl Console by using $source \;\; beta.tcl$. Tcl programming language also can provide some drawing and geometrical features to construct molecular structures in a programmable way. For example if you want to draw a point you could use:

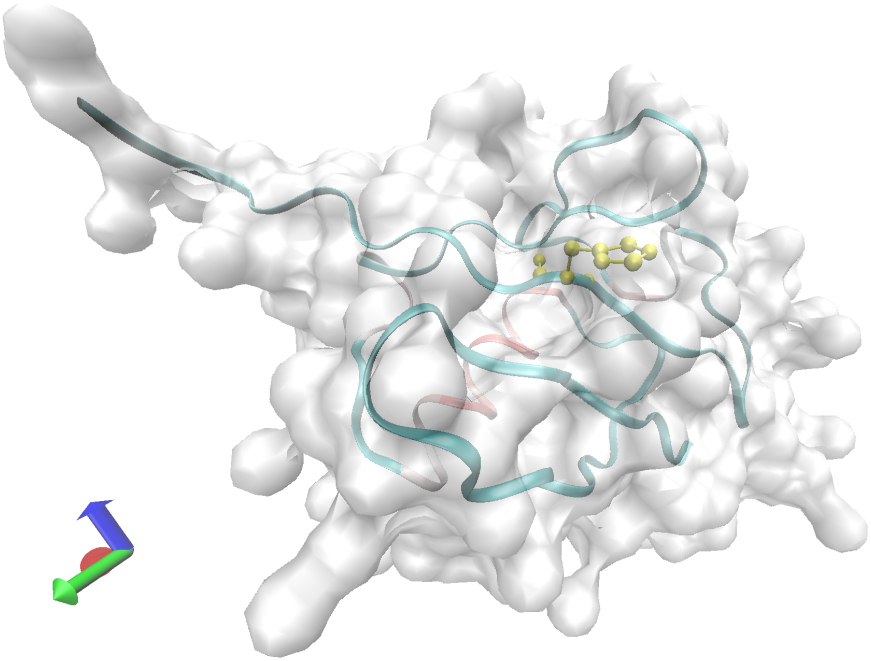

Figure 9: High resolution molecular visualization of ubiquitin protein.

graphics top point {0 0 10}
Also if you want to draw a line you could use:
graphics top line {−10 0 0} {0 0 0} *width* 5 *style solid*
Or if you want to change the style of the line to the dashed one you could use:
graphics top line {−10 0 0} {0 0 0} *width* 5 *style dashed*
You could draw some basic three-dimensional geometrical objects like cylinder, sphere and triangle by using these commands:
graphics top cylinder {15 0 0} {15 0 10} *radius* 10 *resolution* 60 *filled no*
graphics top cylinder {15 0 0} {15 0 10} *radius* 10 *resolution* 60 *filled yes*
graphics top cone {40 0 0} {40 0 10} *radius* 10 *resolution* 60
graphics top sphere {65 0 5} *radius* 10 *resolution* 60
graphics top triangle {80 0 0} {85 0 10} {90 0 0}
graphics top text {40 0 20} "*CCIT Visualization Group*"

You could get your commands' information by using: *graphics top list* and then get the specific information by using *graphics top info ID* which ID represents the ID of your command that could be shown by using list command. Also you could delete the specific object by using *graphics top delete ID*.

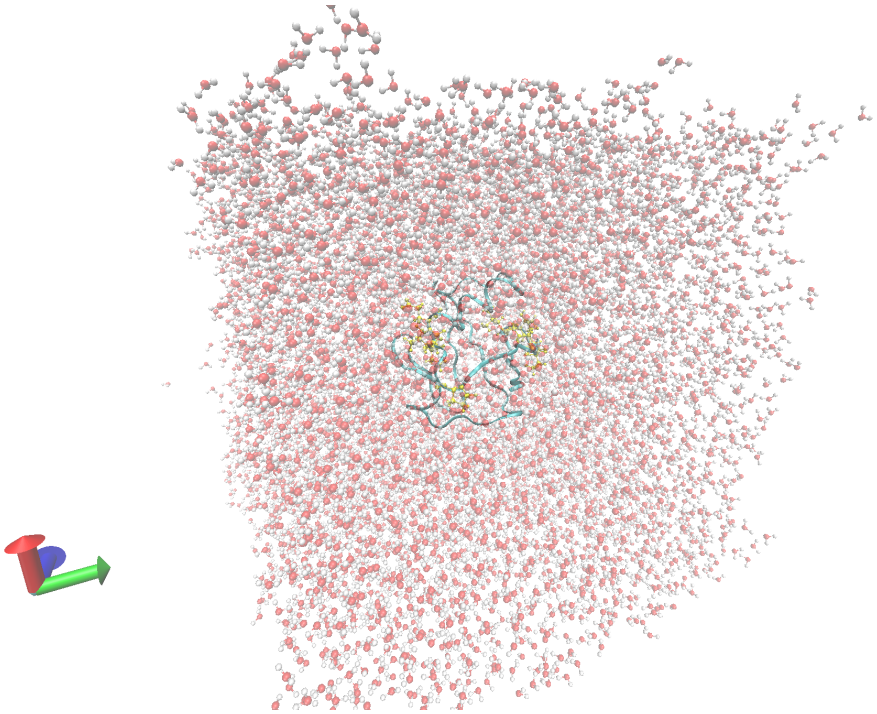

Figure 10: Ubiquitin protein in water solvent molecular visualization.

Multiple molecule visualization

Now we learned how to deal with single molecule and how to write some basic programmable filters by using Tcl programming language. In the advanced molecular visualization area, it is useful to learn how to deal with multiple molecular structure and how to visualize them in a meaningful way. Fortunately, VMD provide a powerful tool to deal with multiple complex molecular structures. In order to load multiple pdb files, you could do this from File $\longrightarrow$ New Molecule... main menu and load 1fqy.pdb and 1rc2.pdb files. After loading these two molecular structures, you should see both of them in your OpenGL windows as is shown in Fig. 17.

Now in order to make a meaningful comparison between these molecular structure we could use $measure \quad fit$ command. First we should create two selections from these two molecular structures and then calculate the translational vectors that can match these two molecular structures and then move one of them according to the calculated translational vectors. So you could find the commands in the seuqential order as:

$set \quad sel0 \quad [atomselect \quad 0 \quad all]$
$set \quad sel0 \quad [atomselect \quad 1 \quad all]$
$set \quad M \quad [measure \quad fit \qquad \$sel0 \qquad \$sel1]$
$\$sel0 \quad move \qquad \$M$

Also you could find the final structures as is shown in Fig. 18.

In order to compare multiple molecular structures according to their chemical

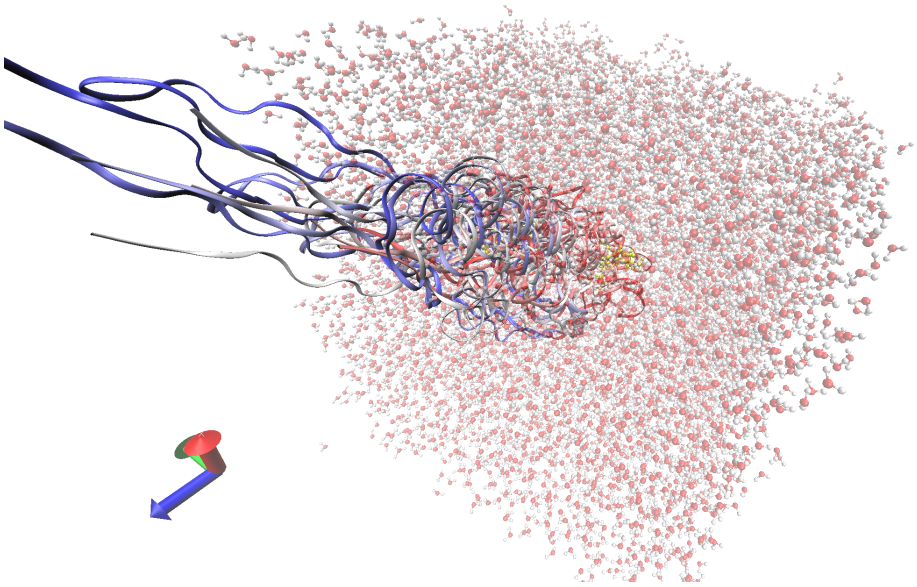

Figure 11: Trajectories of Ubiquitin protein in water solvent molecular visualization.

sequences and their alignments, we could use this provided method. You should load all 1fqy, 1rc2, 1lda and 1j4n molecular structures to the VMD. And then you should use Extensions $\longrightarrow$ Analysis $\longrightarrow$ MultiSeq menu and then you should remove the 1lda_X and 1j4n_X and then from Tools menu of MultiSeq you should choose Stamp Structural Alignment and you will see the aligned structure as is shown Fig. 19.

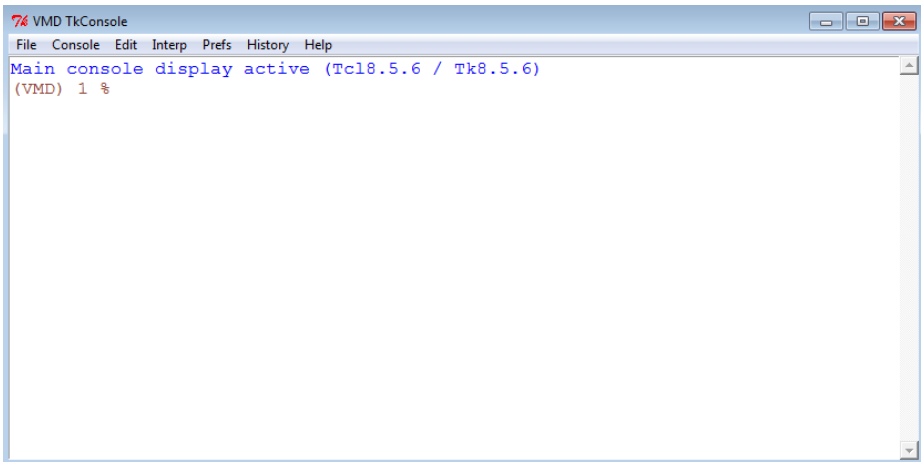

Figure 12: VMD Tk Console.

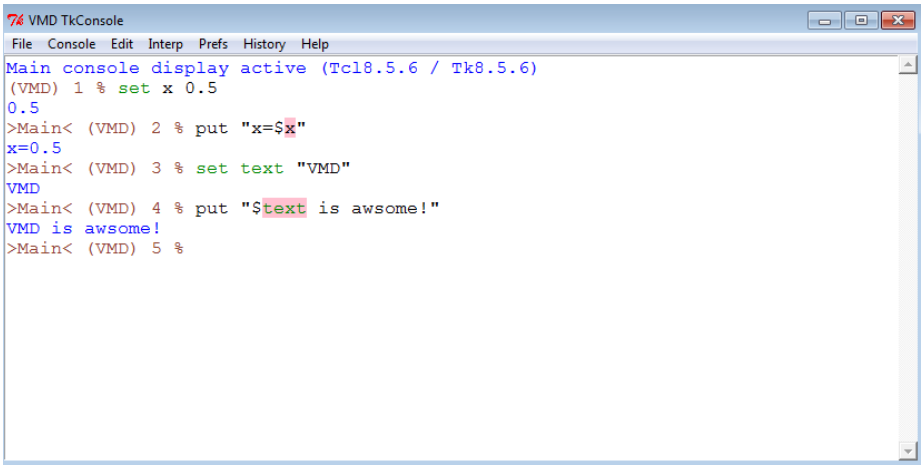

Figure 13: VMD Tk Console, set and put examples.

VMD statistical data analsysis

Statistical data analysis can help scientists to extract some useful information about molecular structures during their movements. One of the best statistical parameters which can be used as a tool to compare fold and unfold transformation of polymers is Root Mean Square Deviation (RMSD). In order to extract the RMSD parameter as a function of simulation time, you should load ubiquitin.psf and equilibration.dcd files. Then you could choose Extensions $\longrightarrow$ Analysis $\longrightarrow$ RMSD Trajectory Tool to extract the RMSD versus simulation time graph of ubiquitin protein during its molecular dynamics simulation. Now you should see these RMSD plots for ubiquitin as are shown in Fig. 20 and Fig. 21 (Note these two figures are taken from original VMD documentation which is distributed under University of Illinois Urbana-Champaign affilation and it is a reference to their work).

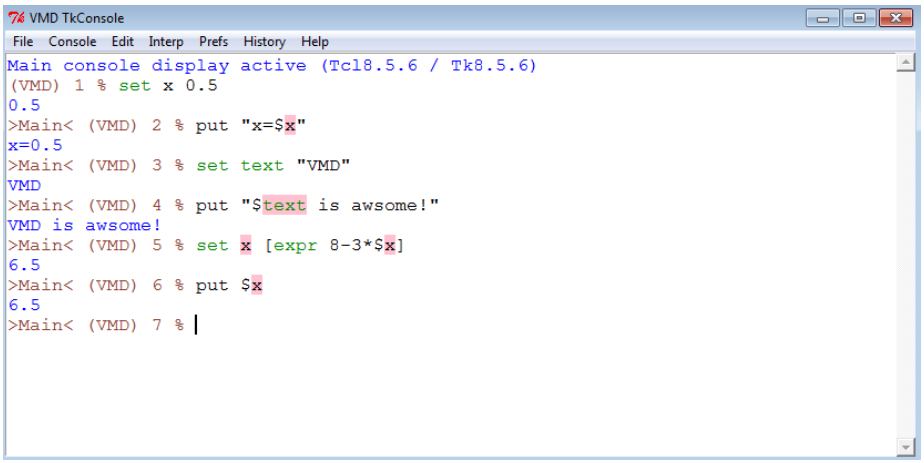

Figure 14: VMD Tk Console, expr example.

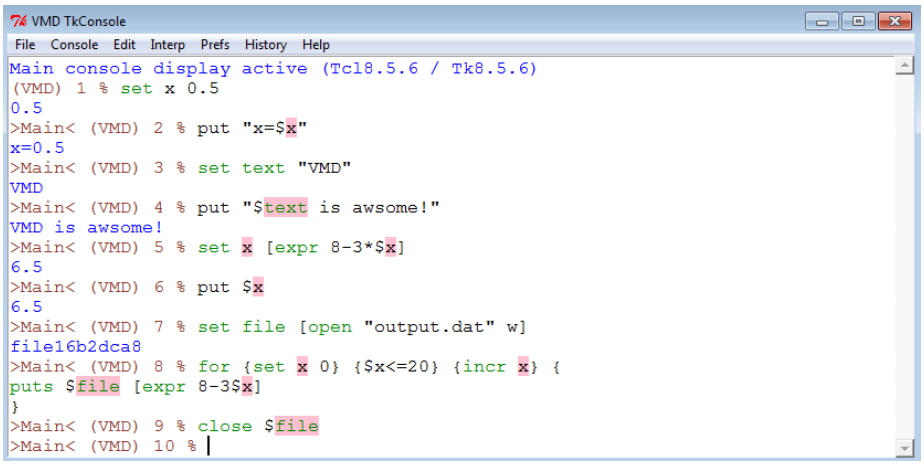

Figure 15: VMD Tk Console, for loop example.

Running VMD on Clemson University Palmetto cluster

First step in order to use VMD on Palmetto cluster is installing the VMD software on Palmetto because currently it is not available as a pre-compiled module. In order to install VMD on Palmetto cluster, you could download a pre-compiled of current version and then install it by following these simple steps:

1. Download current pre-compiled VMD software for Linux operating system by using these options: VMD LINUX_64 OpenGL, CUDA, OptiX, OSPRay. You could download it directly to your Palmetto user work path by using wget command.

2. You should unzip the downloaded file by using this command: tar -xvzf

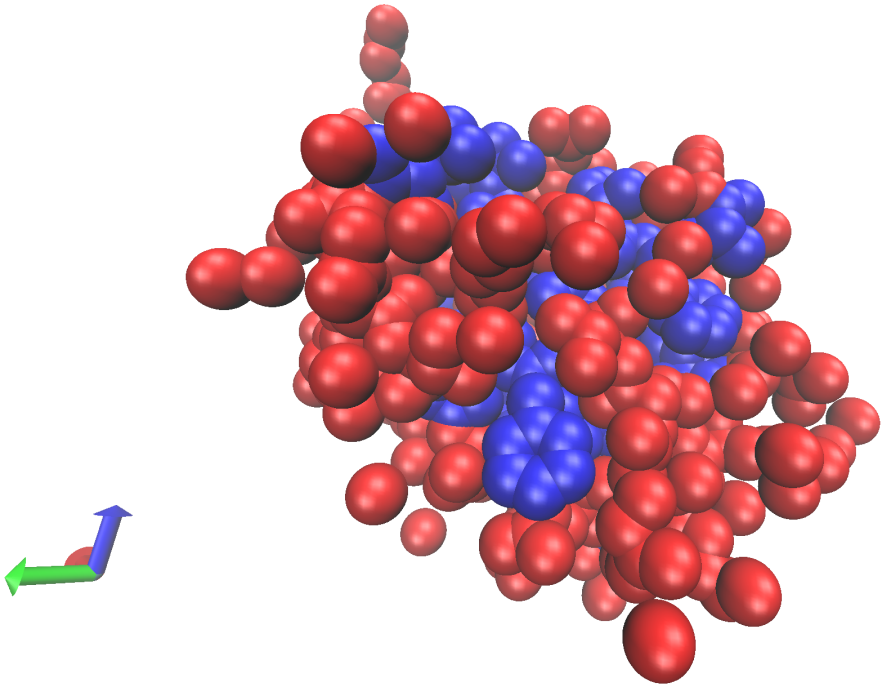

Figure 16: Hydrophobic and hydrophilic part of ubiquitin protein.

vmd-1.9.3.bin.LINUXAMD64-CUDA8-OptiX4-OSPRay111p1.opengl.tar.gz

3. Then by using mkdir command create two directories in your home path like this to store binary and library files of VMD: mkdir ∼/bin-vmd-1.9.3 && mkdir ∼/lib-vmd-1.9.3

4. You should go the vmd-1.9.3 main directory and change the binary and library install path manually by using this command: cd ∼/vmd-1.9.3 && vi ./configure

5. You should change the install_bin_dir to $install_bin_dir="/home/yousefi/bin-vmd-1.9.3" and change the install_library_dir to $install_library_dir="/home/yousefi/lib-vmd-1.9.3/$install_name".

6. Then you should run configure file by using this command: ./configure

7. Finally you should go the src directory and then use make install command like this: cd ∼/vmd-1.9.3/src && make install

8. Your binary and library files will be on bin-vmd-1.9.3 and lib-vmd-1.9.3 directories respectively.

Now you could run VMD on Palmetto cluster and you may find the binary executable file in bin-vmd-1.9.3 directory nad you could run it by using ./vmd

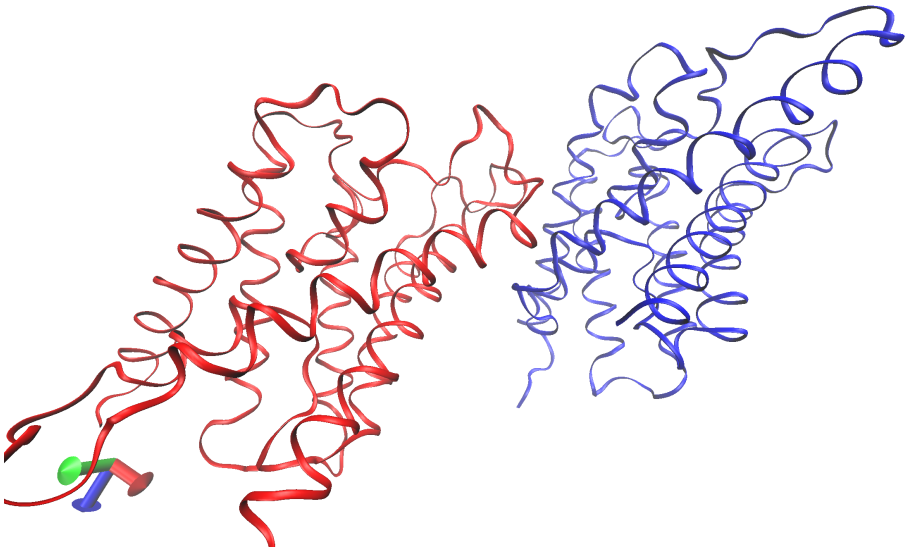

Figure 17: Two visualized proteins.

command. But prior to run VMD you should change your DISPLAY identification parameter by using this command: export DISPLAY=:0. If you do all these steps successfully, you should see the terminal information like Fig. 22.

So now you could use VMD on Palmetto cluster much faster and use it for big molecular structure visualization.

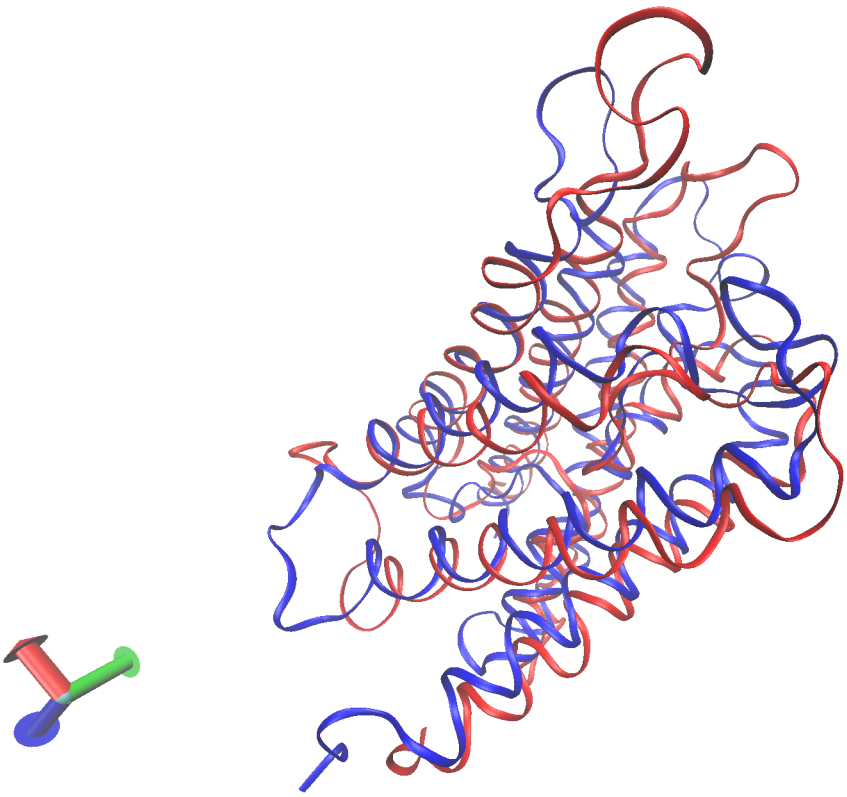

Figure 18: Final translated structures.

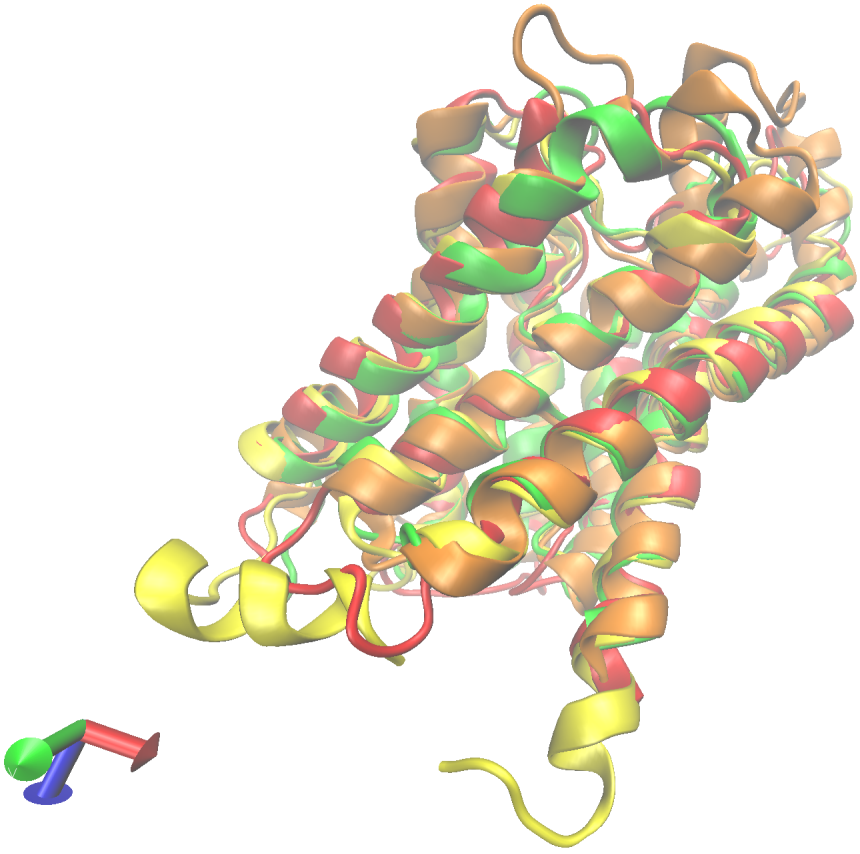

Figure 19: Aligned structures.

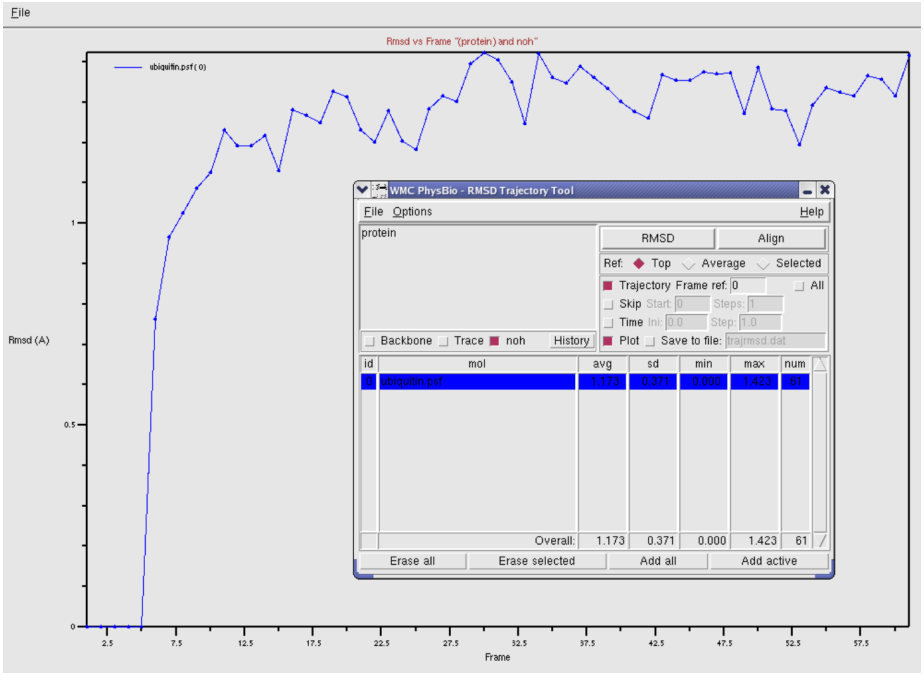

Figure 20: RMSD plot of ubiquitin protein.

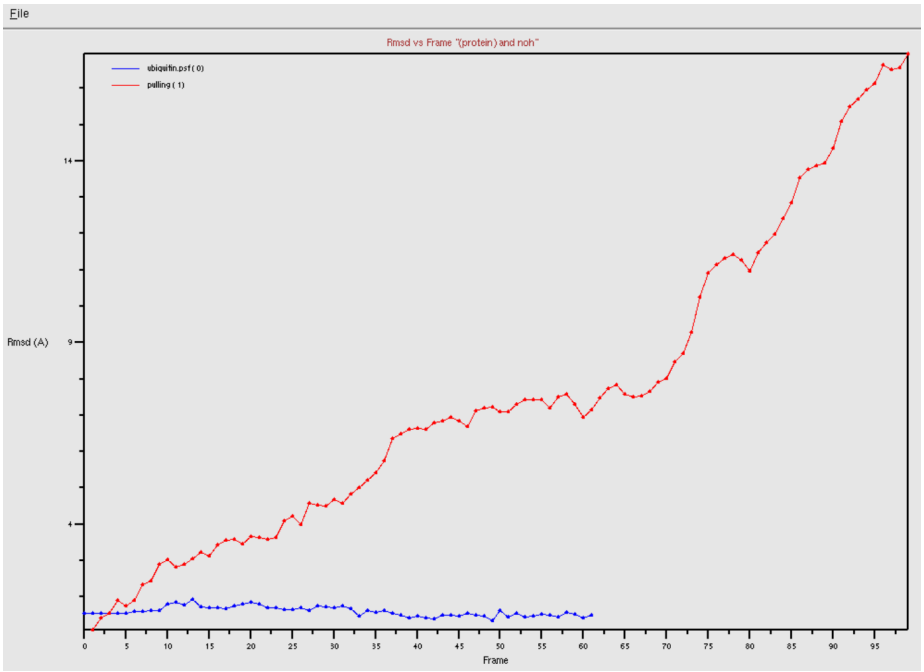

Figure 21: RMSD plots of ubiquitin protein in two conditions of with and without external force.

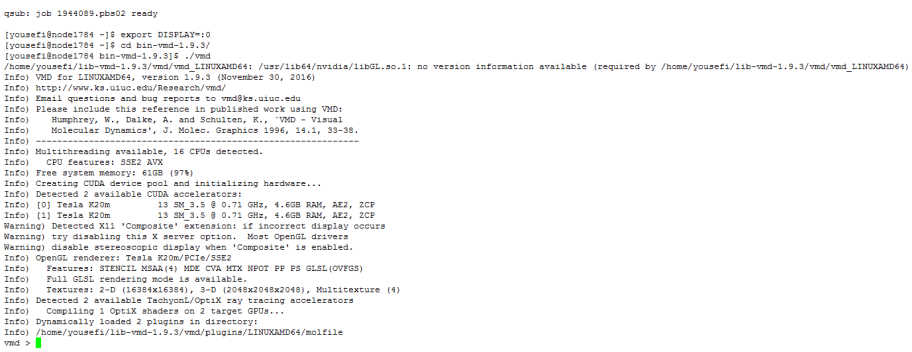

Figure 22: Terminal output after running VMD on Palmetto cluster.