How to create new VMDMagazine Packages

1. Introduction

VMDMagazine was developed with the goal of visualizing scientific information without requiring any prior knowledge of the user in the area of molecular visualization or even molecular modeling. This means that the users (teachers and students) do not have to worry about the handling of molecular visualization software or in the preparation of such types of visualizations that normally involve complex selection steps and the upload of multiple files and scripts.

In this tutorial, a brief overview is given to create new VMDMagazine packages.

2. How to create new Files

In the following sections it will be described how new packages for VMDMagazine can be prepared. Each package is basically a new directory that contain all the files required to show the chemical structure in VMD together with the subtitle, and animation.

2.1. Step 1: Package directory

This directory can have any name, but the inclusion of characters such as #,$, or similar ones should be avoided.

This directory should then be included in the main directory that is read by the VMDMagazine. The main directory can be changed in the options menu of VMDMagazine (File source directory).

In the new directory (for example *example*), the following files must exist:
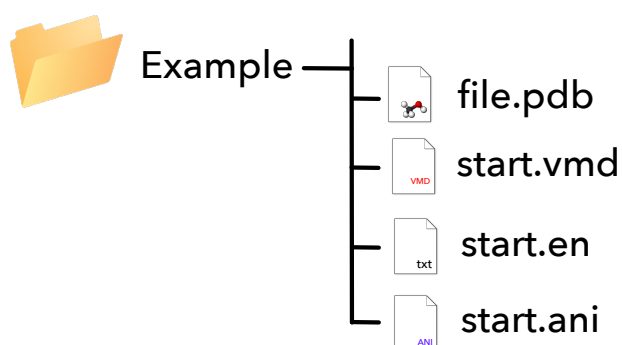
Each of these files will be briefly described in the next sections.

2.2. Step 2: Coordinates files `(file.pdb)`

This file must contain the coordinates of molecules that are displayed in the VMD

main windows. It can have any format that can be recognized by the VMD software, such as PDB, XYZ, MOL2, etc.

To visualize macromolecules, such as proteins, the format PDB is the one that is most commonly used. These files can be obtained from several sources such as the protein databank ([www.rcsb.org)](www.rcsb.org). Other and smaller molecules can also be built using specific software as it is the case of the open source software Avogadro (https://avogadro.cc)..

Once file containing the coordinates of a molecular system has been created, for example file.pdb, it should be moved to the directory that was created in step 1.

2.3. **Step 3:** creation of the start.vmd file

In this step, the file start.vmd will be created. This file is a specific format of VMD that will provide the visualization of the molecule that was saved in step 2, such color of the atoms, representation, etc.

To create this file one has first to load the molecule into the VMD software. Afterwards, the representations and colors of the molecule can be changed using the VMD menu Graphics>Representations (Figure 1). Additional information on how this can be done can be found in many VMD tutorials available in the web.
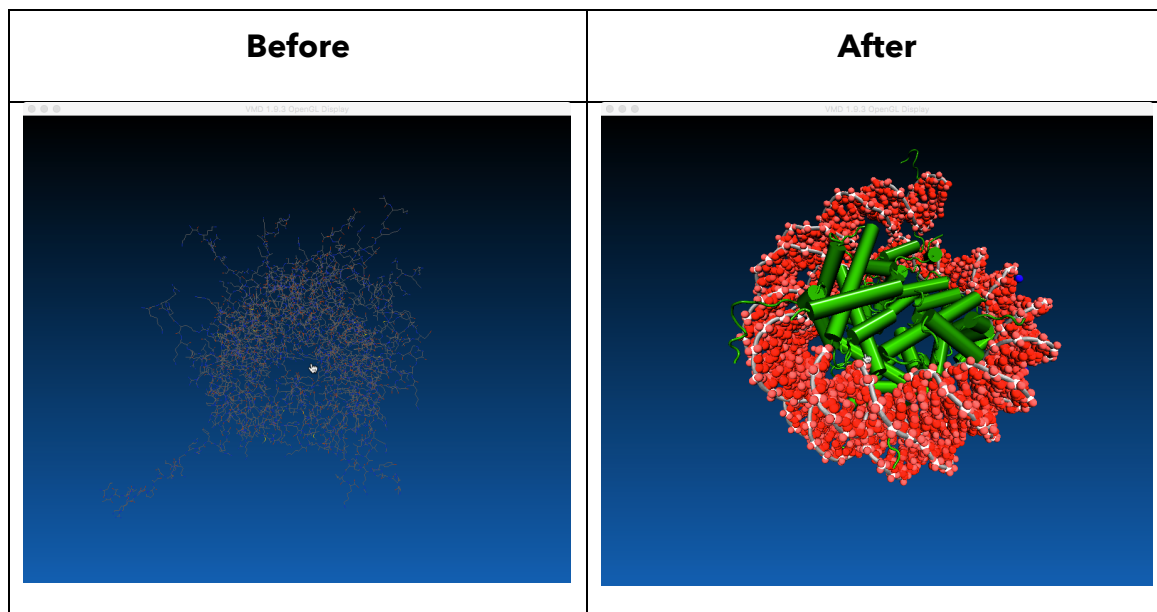
Before	After

Figure 1: Changing the representation and colors of the atoms in a molecule (pdb code: 1AOI)

Once all the modifications on the structure of the molecule have been done, the visualization state file has to be saved (start.vmd) . This is done in the VMD menu File>Save Visualizartion State. The file must be saved with the name start.vmd in the directory that was created in step 1.
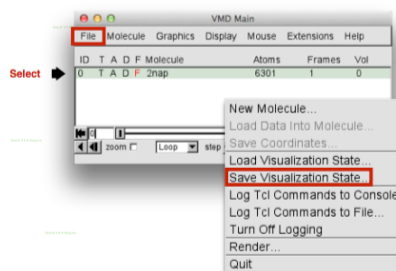

Figure 2: Save the VMD visualization state.

In order to prevent the problems of the path of the file containing the coordinates (file.pdb) and is linked in the start.vmd file, we have to open it with a text editor and remove the path from the line that starts with the command *mol new* as shown in Figure 3.

```
display projection    Perspective
display nearclip set 0.500000
display farclip  set 10.000000
display depthcue   on
display cuestart    0.500000
display cueend      10.000000
display cuedensity 0.320000
display cuemode     Exp2
mol new /Users/pscprgueira/Desktop/untitled.pdb type pdb first 0 last -1 step 1 filebonds 1 autobonds 1 waitfor all
mol delrep 0 top
mol representation Lines
mol color Name
mol selection {all}
mol material Opaque
mol addrep top
mol selupdate 0 top 0
mol colupdate 0 top 0
mol scaleminmax top 0 0.000000 0.000000
mol smoothrep top 0 0
mol drawframes top 0 {now}
mol clipplane center 0 0 top {0.0 0.0 0.0}
```

new line | mol new untitled.pdb type pdb first 0 last -1 step 1 filebonds 1 autobonds 1 waitfor all

Figure 3: Change the path of the start.vmd file

2.4. Step 4: creation of the start.en file

The file start.en holds the subtitles that are displayed in the vmdMagazine plug-in.

The format of this file is a standard txt, but it is possible to setup different font types,

font sizes and different colours. The font type and size can be changed using the

keyword: -font {*A B C*}, where *A* is the font type, *B* the font size and *C* the font style

(normal, bold or italic). The colour of the text can also be changed using the

keyword: -fill *D*, where *D* stands for the name of the colour. For example, the text

after the keywords: -font {Helvetica 14 bold} – colour Green, will display the text in

bold, font Helvetica, size 14 and in green.

The default language of the subtitles is English, but other languages can be created

and chosen by the user. The language pack depends solely on the extension of the

file that contains the description of the scene (for instance, start.en stands for

5

English, start.pt for Portuguese, etc). If the language pack does not exist for the selected language, the English version is set as default.

An example of start.en file is provide in figure 4.

```
-font {Helvetica 14 bold}

-fill Green

Diamond

-font {Helvetica 14 bold}

-fill White

Diamond is the hardest known natural material on the Mohs scale of mineral hardness, where hardness is
defined as resistance to scratching and is graded between 1 (softest) and 10 (hardest). Diamond has a
hardness of 10 (hardest) on this scale.

In these structures each carbon atom is covalently bonded to four other carbon atoms.This arrangement of
carbon atoms gives rise to a tetrahedral structure. These small tetrahedrons combine to form a rigid three
dimensional network.

(…)

-fill White

-font {Helvetica 12}

source of the file
```

Figure 4: Example of the start.en file that provides the subtitles to VMDMagazine.

2.6   **Step 5:** creation of the start.ani file

This file is optional and should only be used if the one want to include some sort of animation to the chemical structure that is displayed in the VMDMagazine.

There are several ways to create the animations. All of them must be based on the capabilities of the VMD software. The ones that are described below were created specifically to be used with VMDMagazine.

A. Roll

USAGE: VBox::Roll *times steps yangle xangle*

> *times* - number of times to animate the sequence
> *steps* - number of frames per complete sequence
> *angle* - Y-axis arc angle to sweep over
> *xangle* - X-axis arc angle to sweep over (yangle / 2.0 or so is a good option)

EXAMPLE: VBox::Roll 500 4000 45 45

B. Rotate Axis

USAGE: VBox::TranslateAxis *times vec deg*

> *times* - number of times to animate the sequence
> vec - vector where the translation should take place
> *deg* - degree of the translation

EXAMPLE: VBox::TranslateAxis 5000 {1 0 0} 2

C. Rotate Axis

USAGE: VBox::TranslateAxis *times vec deg*

> *times* - number of times to animate the sequence
> vec - vector where the translation should take place
> *deg* - degree of the translation

EXAMPLE: VBox::TranslateAxis 5000 {1 0 0} 2

D. Movie

USAGE: VBox::Movie *file time*

     file   - file saved with the view change render plugin of VMD (Extensions-Visualization>ViewChangeRender)
     time – time of the animation

     Note: The file must be saved in the directory that was created in step 1

EXAMPLE: VBox::Movie movie.txt 20