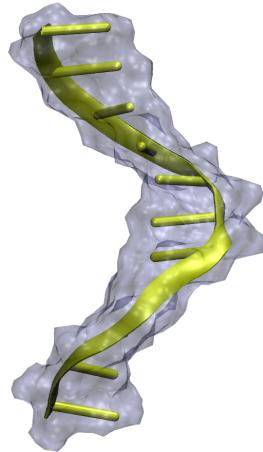


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Computational Biophysics Workshop

VMD Images and Movies Tutorial



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A current version of this tutorial is available at

<http://www.ks.uiuc.edu/Training/Tutorials/>

Join the `tutorial-1@ks.uiuc.edu` mailing list for additional help.

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Introduction

This tutorial is designed to give users of VMD an introduction to advanced techniques for making custom images and movies. The tutorial assumes that you already have a working knowledge of VMD. For the accompanying VMD tutorials go to:

<http://www.ks.uiuc.edu/Training/Tutorials/>

This tutorial has been designed for VMD versions 1.9.x, and should take about 3 hours to complete in its entirety.

The tutorial is subdivided into two separate units. In the first unit, we will look at the many options in VMD for the setup and production of images. The second unit is dedicated to trajectory use and the production of movies.

If you have any questions or comments on this tutorial, please email the TCB Tutorial mailing list at tutorial-l@ks.uiuc.edu. The mailing list is archived at http://www.ks.uiuc.edu/Training/Tutorials/mailing_list/tutorial-l/.

Required programs

The following programs are required for this tutorial:

- **VMD:** Available at <http://www.ks.uiuc.edu/Research/vmd/> (for all platforms)
- **MSMS:** Available at <http://www.scripps.edu/pub/olson-web/people/sanner/html/msms.home.html>
- **POV-Ray:** Available at <http://www.povray.org/download/> (for all platforms)
- **VMDMovie:** This plugin ships with VMD. However, please see <http://www.ks.uiuc.edu/Research/vmd/plugins/vmdmovie/> for platform-specific information regarding creation of MPEG movie files.

Getting Started

You can find the files for this tutorial in the `imgmvtut-files` directory. Below you can see in Fig. 1 the files and directories of `imgmvtut-files`.

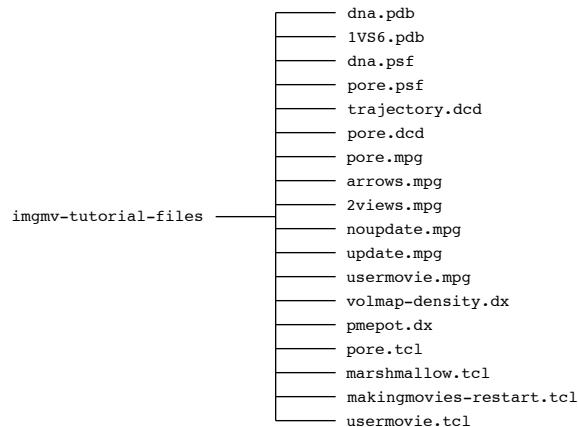


Figure 1: Directory structure of `imgmvtut-files`

To start VMD type `vmd` in a Unix terminal window, double-click on the VMD application icon in the `Applications` folder in Mac OS X, or click on the `Start → Programs → VMD` menu item in Windows.

Acknowledgments

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1 Working with Still Frames

In this section, we will look at some of the variety of ways VMD can work with still frames.

1.1 Graphical Representation Resolution

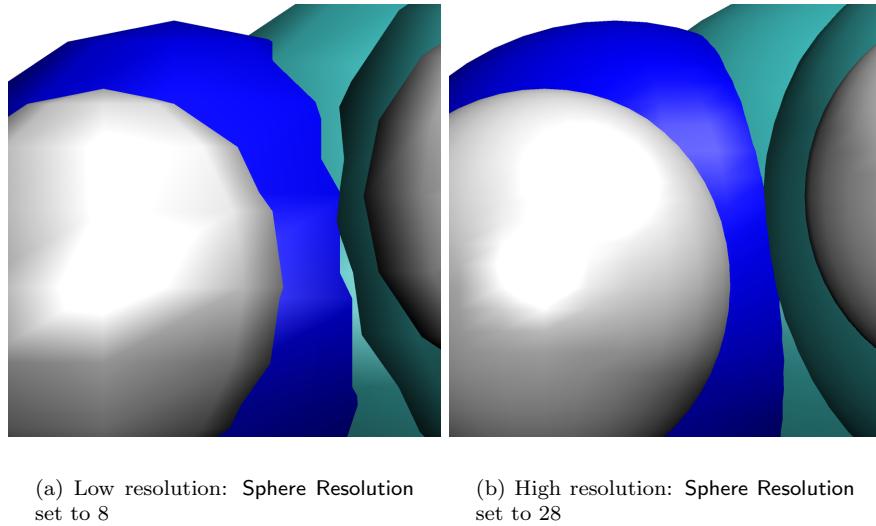
Objects are drawn with an adjustable resolution, allowing users to balance finesse of detail with drawing speed. The resolution setting directly controls the smoothness of the surface molecular representation, and the quality of lighting, texturing, and surface shading for interactive display. The resolution setting also affects the quality of external renderers, but with important differences which will be discussed later.

- 1 Load the files `dna.pdb` and `dna.psf`.
- 2 Show just the DNA, and use the VDW drawing method.
- 3 Zoom in on one or two of the atoms, either by using the scroll wheel on your mouse, or by using **Mouse → Scale Mode** (shortcut **s**) and clicking and dragging.
- 4 Notice that with the default resolution setting, the “spherical” atoms aren’t looking very spherical. In the Graphical Representations window, click on the representation you set up before for the DNA, and click on the **Draw Style** tab. Try adjusting the **Sphere Resolution** setting to something higher, and see what a difference it can make. (See Fig. 2.)

Many of the drawing methods have a resolution setting. Try a few different ones. When producing images, you can usually raise the resolution until it stops making a visible difference.

1.2 Colors and Materials

Nearly all aspects of the display are user-adjustable, including background and display mode colors, and material properties of the objects drawn. Material properties control the way that VMD calculates surface lighting and opacity of displayed objects. Material properties can be used to create dull matte surfaces, eye catching shiny or glass-like surfaces, and transparent ghost-like objects, each suiting different needs. Dull, matte, or diffuse materials are frequently used for background objects or low importance areas of structure, when one wishes to provide context but not draw too much attention, and are also well suited to production of high quality grayscale images. Shiny or glassy materials are useful to attract attention, and emphasize surface curvature with specular highlights. Shiny materials may be too “busy” for grayscale images, and tend to be best



(a) Low resolution: Sphere Resolution set to 8

(b) High resolution: Sphere Resolution set to 28

Figure 2: The effect of the resolution setting.

suited to use in color images. Opacity can be used to deemphasize areas of structure or to provide context, and can be particularly useful when superimposing several objects.

- 1 In the VMD Main window, choose **Graphics → Colors...**. Look through the **Categories** list. All display colors, e.g. the color of phosphorus atoms when coloring by name, are set here.
- 2 Now we will change the background color. In **Catagories**, select **Display**. In **Names**, now click **Background**. Finally, choose **white** in **Colors**.
- 3 When making a figure for a publication, we often don't want the axes showing. Select **Display → Axes → Off** to disable them.
- 4 You may have noticed the **Material** menu in the Graphical Representations window. Choose the DNA representation you made above, and experiment with the **Material** menu.



GLSL. Now is a good time to try out the GLSL Render Mode, if your computer supports it. In the VMD Main window, choose **Display → Rendermode → GLSL**. This mode uses your 3D graphics card to render the scene with real-time raytracing of spheres and alpha-blended transparency; see Fig. 3 for an example.

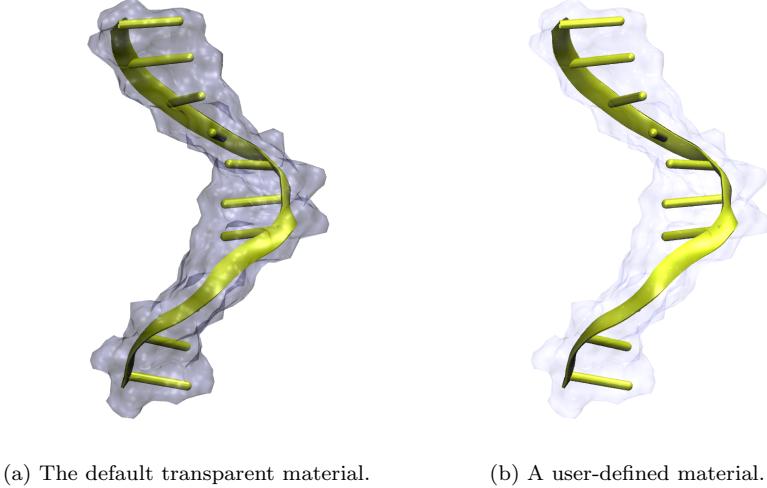


Figure 3: Examples of different material settings.

- 5** Now we'll make a new material. In the VMD Main window, choose **Graphics → Materials....** In the window that appears, you'll see a list of the materials you just tried out, and their adjustable settings. Click the **Create New** button, and give it the following settings:

Setting	Value
Ambient	0.62
Diffuse	1.00
Specular	0.87
Shininess	0.85
Opacity	0.11

See if you can reproduce Fig. 3(b) (Hint: use two representations of DNA.)

1.3 Depth Perception

Since the systems we are dealing with are three dimensional, VMD has multiple ways of representing the third dimension. In this section we will explore the use of VMD features which enhance or diminish depth perception.

- 1** The first thing to consider is the projection mode. In the VMD Main window, click the **Display** menu. Here we can choose either **Perspective** or **Orthographic**. In perspective mode, things nearer the camera appear

larger. Although perspective projection provides strong size-based visual depth cues, the displayed image will not preserve scale relationships or parallelism of lines, and objects very close to the camera may appear distorted. Orthographic projection preserves scale and parallelism relationships between objects in the displayed image, but greatly reduces depth perception. See Fig. 4 to see the difference this can make.

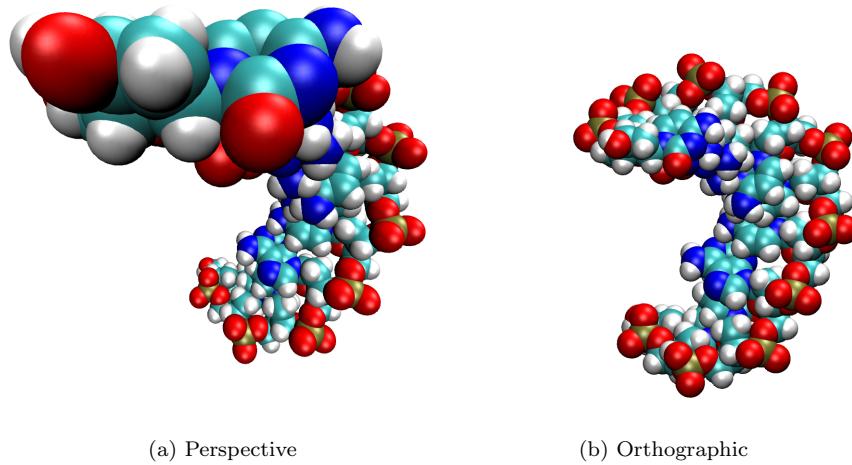


Figure 4: Comparison of perspective and orthographic projection modes. These were taken from above and to the side of the DNA.



Orthographic versus Perspective Mode. Orthographic mode tends to be more useful for analysis, because alignment is easy to see, while perspective mode is often used for producing figures and stereo images.

- 2 Another way VMD can represent depth is through so-called “depth cueing”. Depth cueing is used to enhance three-dimensional perception of molecular structures, particularly with orthographic projections. Choose **Display → Depth Cueing** in the VMD Main window. With depth cueing enabled, objects further from the camera are blended into the background. Depth cue settings are found in **Display → Display Settings**.... Here you can choose the functional dependence of the shading on distance, as well as some parameters for this function.



Linear Depth Cueing. If you choose **Cue Mode → Linear** in the **Display Settings** window, you can achieve dramatic shading across the subject of your figure by choosing the **Cue Start** and **Cue End** parameters. See Fig. 5 for an example of this.

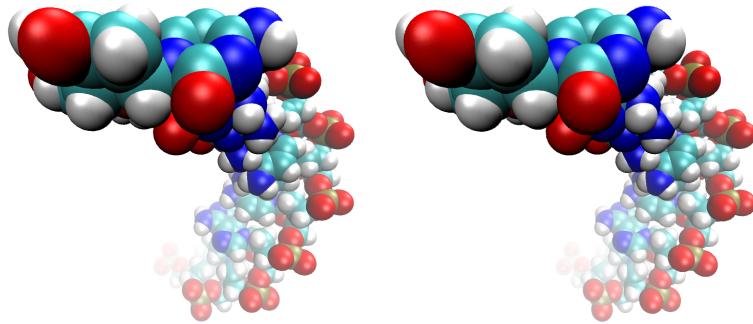


Figure 5: Stereo image of DNA, also showing linear depth cueing, with Cue Start = 1.5, Cue End = 2.75.

3 Finally, VMD can also produce stereo images. In the VMD Main window, look at the Display → Stereo menu, showing many different choices. Choose SideBySide, and return to Perspective mode as well. You should get something like that shown in Fig. 5

1.4 Rendering

By now we've seen some techniques for producing attractive figures in VMD interactively. In this section, we'll explore the use of the snapshot feature and external rendering programs to produce high quality image files. The interactive graphics display in VMD is performed by OpenGL and uses fast-but-elementary geometry, lighting, and transparency algorithms. In many cases, the interactive renderings created by VMD are adequate for use in presentations, movies, and small figures. The "snapshot" renderer saves the on-screen image and is handy for these cases. When one desires higher quality antialiasing, transparency, lighting, perfectly curved spheres, solid clipped volumes, or extremely high resolution images, renderers such as Tachyon and POV-Ray are better choices. Several of the supported renderers use ray tracing for high quality rendering of curved surfaces. Most of the supported renderers perform lighting calculations at every pixel, and so there's less need to set the graphical representation resolution parameters to high values. Renderers such as Tachyon and POV-Ray actually perform better and create nice images with very conservative representation resolution settings. Other rendering modes such as STL and VRML can be used to export the VMD molecular scene to a variety of rendering and animation tools, or for printing of 3-D solid models.

1 Rendering is a simple matter. Once you have the scene set the way you like it, simply choose File → Render... in the VMD Main window. In

the File Render Controls window that appears, you choose the renderer to use, choose the file name, and click Start Rendering.



Command Line. The Tk Console can be useful for setting up your scene in a precise way. Using `display resize <x> <y>`, you can set the size of the display window, and therefore also the size of the rendered image. Using the `rotate` and `scale` commands, you can change the camera angle and zoom. There is also a `render` command — the menu command above is simply a GUI front end.

- 2 Now let's actually render something. Try rendering the scene you have set up currently, using the renderers snapshot, TachyonInternal, and POV3.



Renderers. The snapshot renderer saves exactly what is already showing in your display window — in fact, if another window overlaps the display window, it will show up in the rendering as well! The other renderers reprocess everything, so it may not look exactly as it does in VMD. In particular, they don't "clip", or hide, objects very near the camera. If you select `Display → Display Settings...` in the VMD Main window, you can set `Near Clip` to 0.01 to get a better idea of what will appear in your rendering.

- 3 OK, now for something more challenging. Try to reproduce Fig. 6 as best you can. Think about which parts of the system to show, the drawing and coloring method, the projection mode, and the materials.

1.5 Volumetric Data

VMD has the ability to compute and display volumetric data. Volumetric data is data that is a function of position, e.g. density, potential, solvent accessibility, stored as a 3-D grid of values. VMD can display volumetric data in a few different ways. For this section, **please turn GLSL rendering off**, if it is on.



Creating Volumetric Data. VMD has a number of analysis plugins that compute volumetric data, notably the `VolMap` and `PMEpot` plugins.

- 1 Load the file `volmap-density.dx` by selecting our molecule in the VMD Main window, clicking `File → Load Data Into Molecule...`, then browsing to the file.



volmap-density.dx. This volumetric data set was generated by the `VolMap` plugin from a 1 ns simulation of the system we've been looking at, and shows the mass density of DNA averaged over the trajectory.

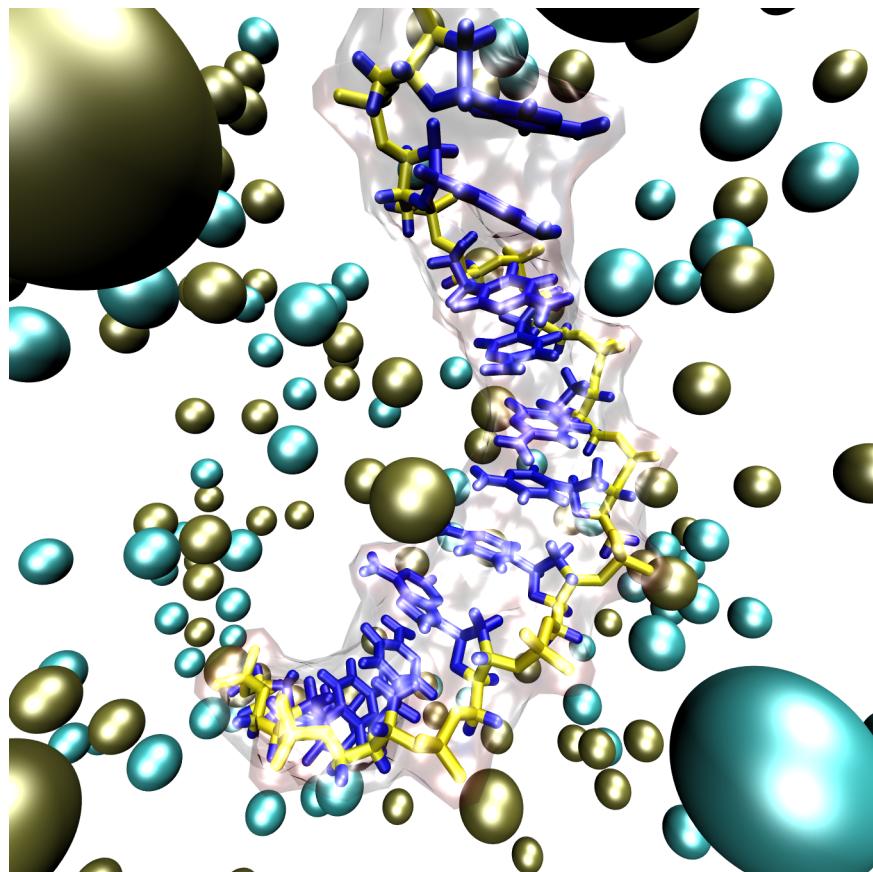


Figure 6: Example of POV3 rendering.

- 2 Our molecule now has one volumetric data set associated with it, as indicated by the “1” in the Vol column of the VMD Main window. Now we need a representation to display it. Create a new representation, and select VolumeSlice as the Drawing Method.
- 3 With the new representation still selected, set Slice Axis to Y, Render Quality to Medium, and Coloring Method to Volume.
- 4 Turn off all other representations, then type the following into the Tk Console window:

```
display resetview  
rotate x by -90
```

Play with the Slice Offset slider, which adjusts the y-coordinate of the slice. Different colors represent different numerical values of the volumetric data,

in this case mass density. When coloring by Volume, the color scale can be set in the Trajectory tab of the Graphical Representations window.

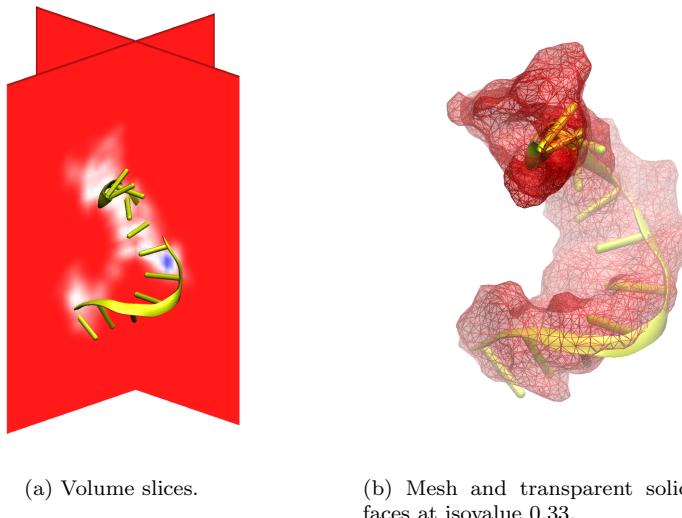


Figure 7: Different ways of showing volumetric data of DNA mass density.

- 5 Now make a similar slice representation for the x- and z-directions as well, and rotate you view with the mouse so that all three planes are visible. Fig. 7(a) shows an example with slice planes normal to the x- and y-axes.
- 6 Now for a more three-dimensional way of representing the data. Hide the current representations, then create a new one using the Isosurface drawing method. In the Draw menu, select Solid Surface. Now, you can see a surface of constant volumetric value, chosen using the Isovalue slider. As you choose higher values, you see the surface shrinks down around a core where the most average mass was located. Fig. 7(b) shows such an isosurface, represented by both a wire mesh and a transparent surface.
- 7 Another common way to represent volumetric data is by coloring other representations based on it. Load the file `pmeapot.dx` by selecting your current molecule, and choosing `File → Load Data Into Molecule...` in the VMD Main window.



pmeapot.dx. This file was generated from the same trajectory as the other volumetric dataset you've been using, this time from the last frame alone. As its name implies, it was made using the PMEpot plugin, which calculates electrostatic potential.

- 8 Now hide your current representations, and create a new one showing only DNA, with MSMS drawing style and Volume coloring style. The DNA surface is now colored based on the volumetric data value at each surface point. The color scale range is automatically set, but can be changed in the Trajectory tab of the Graphical Representations window.
- 9 We'll use the Color Scale Bar VMD plugin to show the color scale of the volumetric data. Choose Extensions → Visualization → Color Scale Bar in the VMD Main window.
- 10 Enable the Autoscale option, set the label color to black, and click Draw Color Scale Bar. This plugin will create a new molecule named Color Scale Bar that is “fixed”, meaning when you rotate or scale the scene, the color bar doesn't change.
- 11 You can move the color bar by unfixing its molecule and fixing the DNA molecule, then using the Translate mouse mode (shortcut T). Recall that a molecule is fixed or unfixed by double-clicking the “F” directly to the left of its name in the VMD Main window. An example is shown in Fig. 8.

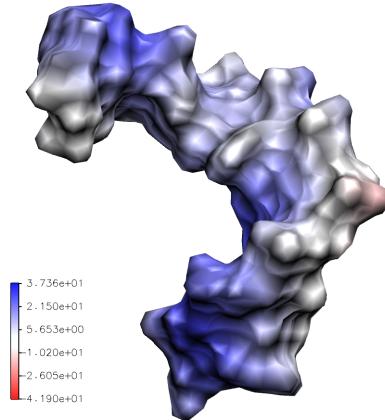


Figure 8: Example of coloring by volumetric data and use of the Color Scale Bar plugin.

1.6 Clipping Planes

In this section, we will learn one of the most useful techniques for producing clear figures: the clipping plane. Clipping planes allow us to look at cross-sections of the objects displayed, and can be applied very flexibly. We will learn how to use them by going through the steps of making Fig. 9.

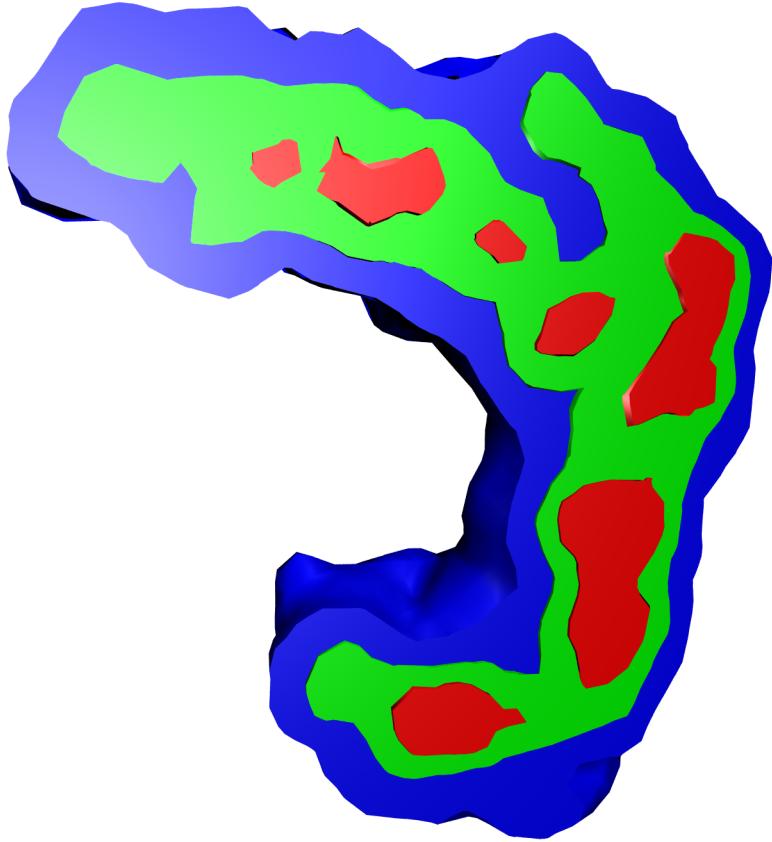


Figure 9: A three-dimensional contour plot, made through the use of clipping planes.

- 1** Start a fresh VMD session, and reload the files `dna.psf`, `dna.pdb`, and `volmap-density.dx`.
- 2** Create the representations in the following table. For each, select **Draw → Solid Surface** and **Show → Isosurface** in the **Draw style** tab. Once they're set up, you should see only a blue shell.

Drawing Method	Isovalue	Coloring Method
Isosurface	1.0	ColorID 1 (red)
Isosurface	0.6	ColorID 7 (green)
Isosurface	0.2	ColorID 0 (blue)

- 3** Now enter the following commands in the Tk Console:

```
mol clipplane status 0 0 0 2
mol clipplane status 0 1 0 2
mol clipplane status 0 2 0 2
```

Let's decipher this a bit. Every `mol clipplane` command is of the form
`mol clipplane <command> <clipid> <repid> <molid> <value>`.

Here, we have used the `status` command, which we use to enable the clipping planes. Thus, the first line refers to the first clipping plane of the first representation of the first molecule. The final 2 is the new status of each clip plane. Table 1 summarizes this command's usage.

<command>	Possible <value>s
<code>status</code>	0 (off), 1 (on), 2 (on, solid surface; material inherited from representation)
<code>normal</code>	"<x> <y> <z>", a vector pointing normal to the surface
<code>center</code>	"<x> <y> <z>", a vector pointing to the center of the surface
<code>color</code>	"<r> <g> ", an RGB triple specifying the color of the surface, if it is solid

Table 1: Summary of `mol clipplane` usage.



Multiple Clipping Planes. All of these numbers you give the `mol clipplane` commands show how flexible the command is — one may define up to six different clipping planes per representation!

- 4 Let's check the current settings of the clipping planes. Type the commands:

```
mol clipplane center 0 0 0
mol clipplane normal 0 0 0
```

and likewise for the other two clipplanes. By providing no new value, the command now print the current value instead of setting a new one. You should find that all clipplanes are centered at the origin, and with normal vector in the z-direction.

- 5 Now we'll use a trick to set the center and normal vectors interactively, using the Clipping Plane Tool VMD Plugin. Select `Extensions → Visualization → Clipping Plane Tool` in the VMD Main window. This tool will modify clipping planes of the molecules selected in the `Apply To` menu. The `Edit Clip Plane` buttons select which `clipid` will be edited. However, all representation clipping planes will be edited together, i.e. all the clipping planes we've created will get the same normal and center — exactly what we want.

- 6** You should now see cross-sections of the isosurfaces you created. Rotate down with the mouse. The clipping plane stays parallel to the screen, letting us choose the normal vector (the flip button inverts this vector). Try to set the normal vector so that we get a nice cross-section of the isosurfaces.
- 7** Now, adjust the position of the plane in the normal direction by using the Distance slider. Try to cut right through the center of the isosurfaces.
- 8** When you think you have a nice cross-section, click the Keep Aligned with Screen button to turn this feature off. Now, you can rotate the scene *without* changing the normal vector, letting you see your work from a different angle.
- 9** Before we close the Clip Tool window, click the Render plane as solid option near the bottom. This way, the status of our clipping planes will remain 2, as we set in the first step.
- 10** Now check the center and normal vectors of your clipping planes again, just as you did before. You should find that they have new values. For reference, here are the values used to produce Fig. 9:

Vector	Value
Normal	0.03 0.93 -0.36
Center	0.13 -1.17 13.78

- 11** Now we'll change the color of the planes to match the rest of the surface, using the following commands:

```
mol clipplane color 0 0 0 "1 0 0"
mol clipplane color 0 1 0 "0 1 0"
mol clipplane color 0 2 0 "0 0 1"
```

corresponding to red, green, and blue respectively.

Finally, before rendering, we need to shift two of the planes slightly, so that all three aren't in exactly the same place. Otherwise, we would only see one of the colors.

- 12** First decide a good shift direction — just reshew the axes, and see which direction is roughly normal to your planes. For the case of Fig. 9 above, this is the y-direction.
- 13** Now we'll move the plane for the largest contour 0.1 Å in the direction you chose, and the plane for the smallest contour by 0.1 Å in the opposite direction, using the axes to get the correct sign. You can do this by setting

the center to the value you found above, offset by the appropriate amount. For example,

```
mol clipplane center 0 0 0 "0.13 -1.27 13.78"  
mol clipplane center 0 2 0 "0.13 -1.07 13.78"
```

Now you're ready. Just hide the axes once more, and render using the POV renderer (the other renderers will not show the solid clipping plane surfaces.)

1.7 Visualizing Large Systems

Before moving on to trajectory topics, we will very briefly look at a script written by Jordi Cohen that uses volumetric data as a technique for visualizing large systems very clearly.

1 Start a new VMD session, and load the ribosome structure, PDB code 1VS6. Now is a great time to try out VMD's ability to download PDBs directly. If you have an active internet connection, simply type 1VS6 as the **Filename** in the Molecule File Browser window (menu item **File → New Molecule...**).

2 In the Tk Console, type the following commands:

```
source marshmallow.tcl  
marshmellify
```

3 This may take a minute or two to complete. When it does, you'll see that many new representations have been created, one for each chain of the ribosome. Examine the script to see how it works — it is surprisingly short for how much it does.

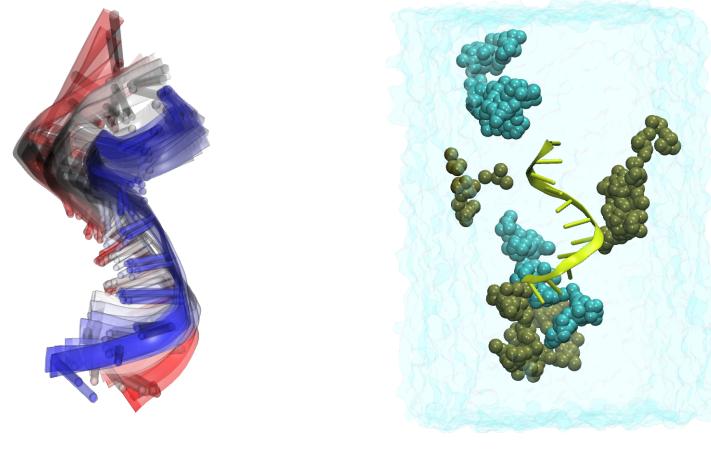
2 Working With Trajectories

In the second unit, you will learn how to work with trajectories.

2.1 Basics

In this section, we will learn how to smooth trajectories, show multiple frames at once, and make atom selections “follow” the trajectory.

- 1 Open VMD, and load the files `dna.psf` and `trajectory.dcd`. Before clicking **Load** in the Molecular File Browser window, look at the **Frames** section. Here you have precise control over how the file is loaded. Leave them at the default setting, so that all frames of the trajectory are loaded.
- 2 Set up a representation showing only the DNA, in the **NewCartoon** drawing style.
- 3 Play the animation, as you learned how to do in the VMD Tutorial. You may want to lower the speed!
- 4 The movement is not very smooth, due to thermal fluctuations. VMD can smooth the animation by averaging some number of frames. In the Graphical Representations window, select your DNA representation, and click the **Trajectory** tab. At the bottom, you see **Trajectory Smoothing Window Size** set to zero. As your animation is playing, increase this setting. Notice that the motion gets smoother and smoother as you go up.
- 5 Now we'll see how to display many frames at once. Create a new DNA representation, and hide the old one. (Hint: Select the old representation before hitting the **Create Rep** button, so that the new one already has the right selection and drawing style. Note that smoothing will be set to zero.)
- 6 Click the **Trajectory** tab again. Above the smoothing control, notice the **Draw Multiple Frames** control. It is set to **now** by default, which is simply the current frame. Enter **0:10:199**, which selects every tenth frame from the range 0 to 199.
- 7 Go back to the **Draw style** tab, and change the coloring mode to **Timestep**. This will draw the beginning of the trajectory in red, the middle in white, and the end in blue. Also set **Material** to **Transparent**.
- 8 We can also use smoothing, making the large-scale motion of the DNA more apparent. Set the smoothing window to 10. You should have something like Fig. 10(a).



(a) Image of every tenth frame showing at once, smoothed with a ten-frame window.

(b) Image of all frames showing at once, for two Na^+ ions and two Cl^- ions. Water is shown as a transparent MSMS surface.

Figure 10: Two examples of showing multiple frames at once.

9 Finally, we'll see how to make VMD "update" the selection each frame. Hide the representation showing all frames, and reshown your first representation, showing only DNA. Then make a new representation, with the selection text

```
ions and within 5 of segname ADNA
```

This will show all ions within 5 Å of the DNA.

10 Now play the trajectory. (A movie of the trajectory is provided as `noupdate.mpg`, and illustrated in Fig. 11.) Notice anything wrong? Although the ions may be near the DNA for a little while, they soon wander off, and are still shown despite no longer meeting the selection criteria. The **Update Selection Every Frame** option in the **Trajectory** tab of the Graphical Representations window remedies this, doing exactly what its name says. See Fig. 12



CatDCD. On Linux/Unix systems, VMD comes with the CatDCD program, which allows users to combine multiple trajectory files into one, with a variety of options.

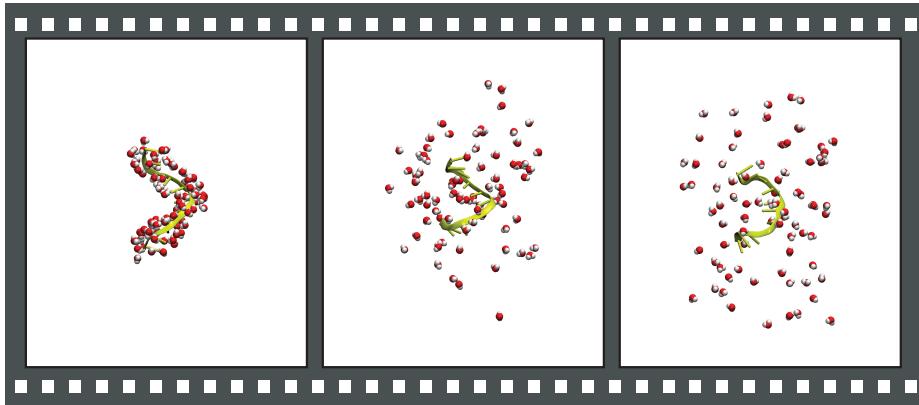


Figure 11: Movie `noupdate.mpg`.

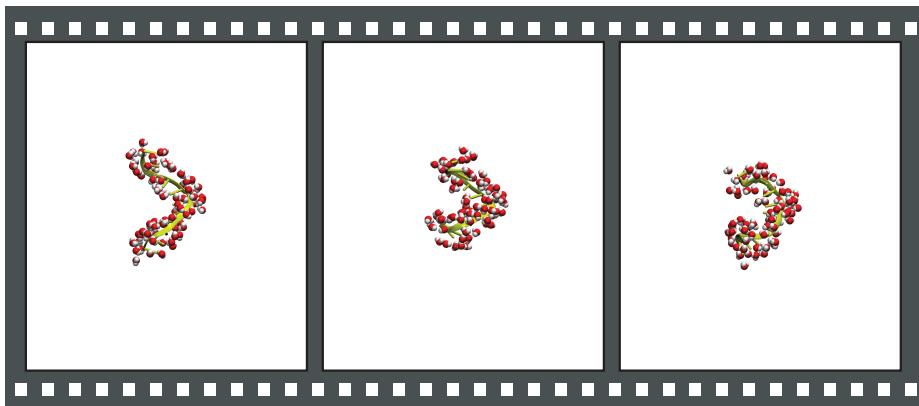


Figure 12: Movie `update.mpg`.

You now know the basics of working with trajectories. We will next look at some more advanced things we can do with them.

2.2 Advanced Trajectory Topic

In this section, we will explore an advanced technique for visualization. We will look at a trajectory from a simulation in which a “virtual pore” was collapsed around a short strand of DNA, and see how to use VMD to superimpose the position of the virtual pore at each timestep. Along the way we will learn about VMD’s custom graphics capabilities.

- 1** Start a fresh VMD session, and load the files `pore.psf` and `pore.dcd`, and set up a representation showing just the DNA.
- 2** For this section, we will be examining a script. Let's see what it does. Type the following in the Tk Console window:

```
source pore.tcl
enabletrace
```

- 3** Start the animation. The blue cylinder is drawn at the radius of the potential used in the simulation. (See Fig. 13.)

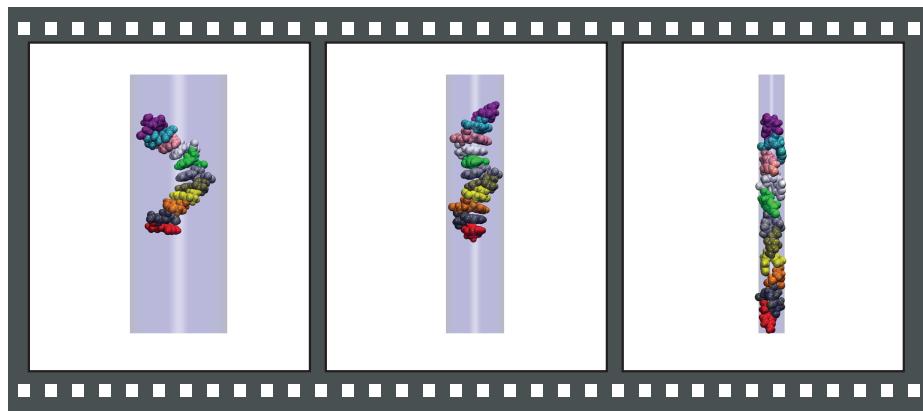


Figure 13: Movie `pore.mpg`.

- 4** Now hide your DNA representation, and type the command `enablearrows`.
- 5** Restart the animation. The DNA is now drawn by the script as well, represented as arrows. You should see something like Fig. 14. The command `disablearrows` will turn this off. `disabletrace` will turn off everything done by this script.
- 6** Now that we see what it does, let's look at the script. Open the file `pore.tcl` in a text editor.

- 7** The first few lines defines the procs for enabling and disabling the script:

```
proc enabletrace {} {
    global vmd_frame
    trace variable vmd_frame([molinfo top]) w drawcounter
}
```

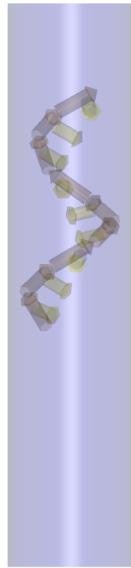


Figure 14: DNA represented as arrows.

```
proc disabletrace {} {
    global vmd_frame
    trace vdelete vmd_frame([molinfo top]) w drawcounter
}
```

These procs use the `trace` feature of Tcl, which is a mechanism for setting up some action when some variable changes. The command

```
trace variable vmd_frame([molinfo top]) w drawcounter
```

says to call the command `drawcounter` everytime the variable `vmd_frame ([molinfo top])` is written (`w` above is short for `write`). See the VMD User's Guide at <http://www.ks.uiuc.edu/Research/vmd/current/ug/ug.html> for a list of VMD variables that `trace` can be used with.

- 8 The next few lines set up the procs to turn the arrows on and off:

```
set pore_draw_arrows 0

proc enablearrows {} {
    global pore_draw_arrows
    set pore_draw_arrows 1
}
```

```
proc disablearrows {} {
    global pore_draw_arrows
    set pore_draw_arrows 0
}
```

- 9** Next we have procs which draw the arrows:

```
proc vmd_draw_arrow_BASE {mol start end} {
    set coneEnd [vecadd $end [veccscale 0.25 [vecsub $end $start]]]
    graphics $mol cylinder $start $end radius 1.0
    graphics $mol cone $end $coneEnd radius 1.5
}

proc vmd_draw_arrow {mol start end} {
    set middle [vecadd $start [veccscale 0.8 [vecsub $end $start]]]
    graphics $mol cylinder $start $middle radius 1.0
    graphics $mol cone $middle $end radius 1.5
}
```

These simply draw the arrows by using built-in procs for drawing cylinders and cones.

- 10** Next, the script sets some parameters defining the size of the pore cylinder and how it changes through the trajectory:

```
set Rstart      14
set Rrate       0.00001
set Rtarget     4.0
set frameRate   10000
set Center      0.0
```

Obviously, these should coincide with those used in the original simulation.

- 11** Now we make note of the DNA residues:

```
set sel [atomselect top "segid ADNA and name P"]
set residList [lsort -integer [$sel get resid] ]
set residStart [lindex $residList 0]
set residEnd [lindex $residList end]
```

- 12** Now we get to the real meat of the script: the `drawcounter` proc. This is the procedure called every time the frame changes.

```
proc drawcounter { name element op } {
    ...
}
```

`trace` calls the callback proc with three arguments, which are basically just the arguments we provided `trace` to begin with, and which we don't use.

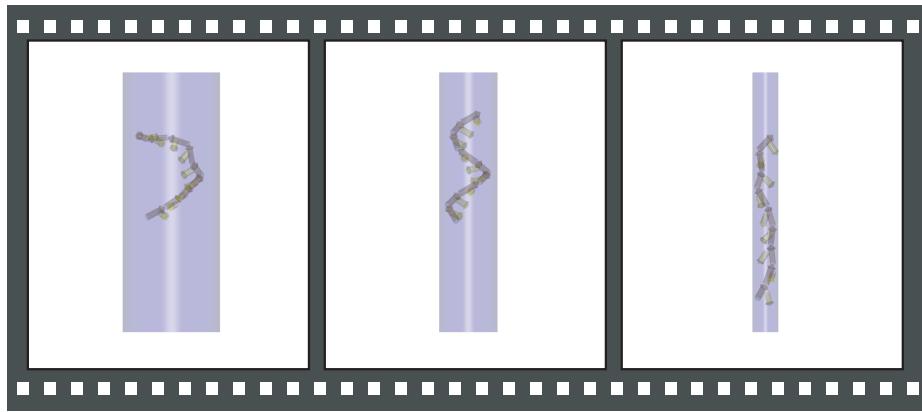


Figure 15: Movie `arrows.mpg`.

- 13** Now let's look at the `drawcounter` proc itself. First, it sets some global variables, which we won't reproduce here. Then it calculates the proper radius of the cylinder for the current timestep:

```
set R [expr $Rstart - $Rrate*$frameRate \
        *$vmd_frame([molinfo top]) + 1.0]
if {$R < $Rtarget} {
    set R $Rtarget
}
```

- 14** Next is the code which actually draws the cylinder:

```
draw delete all
draw color blue
draw material Transparent
set start_pt [list 0 0 [expr $Center - 30]]
set stop_pt [list 0 0 [expr $Center + 50]]
draw cylinder $start_pt $stop_pt radius $R resolution 32
```

Here we use VMD's `draw` command to set the drawing parameters and draw the cylinder.

- 15** Finally, we draw the DNA arrows, if it's enabled:

```
if { $pore_draw_arrows } {
    for {set resid [expr $residStart]} {$resid < $residEnd} {incr resid} {
        set residONE [expr $resid + 1]
        set tmpSel1 [atomselect top "resid $resid and name N1 C3'"]
        frame $vmd_frame([molinfo top])
        foreach {coordN1 coordC1} [$tmpSel1 get "x y z"] { break }
```

```

draw color yellow
vmd_draw_arrow_BASE top $coordC1 $coordN1
set tmpSel2 [atomselect top "(resid $resid and name P)
    or (resid $residONE and name P)" frame $vmd_frame([molinfo top])]
foreach {coordP1 coordP2} [$tmpSel2 get "x y z"] { break }

draw color 14
vmd_draw_arrow top $coordP1 $coordP2

$tmpSel1 delete
$tmpSel2 delete
}
}

```

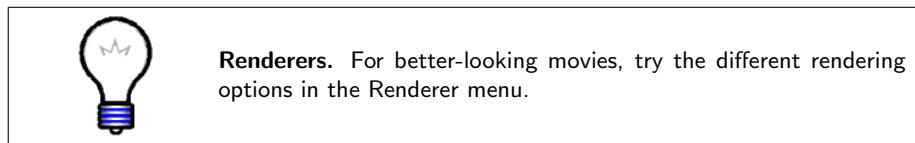
The script simply uses the atomic coordinates of three of the atoms of each base to define where the arrow should be drawn, then the appropriate drawing command, defined above, is called.

You now have some powerful techniques for working with trajectories. The last section of this tutorial will show you how to take everything you've learned to produce movies of your system.

2.3 Making Movies

In this final section, you'll first learn how to make a basic movie. Then we'll see how to do more advanced animations, again using Tcl's callback functionality.

- 1** Leave everything loaded in VMD from the last section, or start a fresh VMD session and type `source makingmovies-restart.tcl` in the Tk Console window to load everything you need for this section. To make our movies, we will use the VMD Movie Maker plugin. Go to **Extensions → Visualization → Movie Maker**.
- 2** First, let's look at some of the options for our movie. Click on the **Movie Settings** menu. In addition to a trajectory movie, Movie Maker can also take still frames and animate camera motion.
- 3** Set up your representations and angle to something you like.
- 4** Select **Rock and Roll**, set the working directory to something convenient, give your movie a name, and click **Make Movie**. You will see the VMD display update as the movie is made.
- 5** Once VMD is finished, open the movie. This movie setting is good for showing one side of your system primarily.
- 6** Now, try a trajectory movie. Select **Movie Settings → Trajectory**, give this one a different name, and click **Make Movie**.



- 7 It is possible to show multiple views of your molecule at once, which can be very helpful in some cases. Load the files `pore.psf` and `pore.dcd` again, creating a new molecule. (You may want to rename it by double-clicking its name.)
- 8 Fix the original molecule by double-clicking the “F” next to its name in the VMD Main window. Now you can manipulate the view of the second copy without affecting the first. Make your window wider, and use the Translate mouse mode to shift your second view to the left of the first.

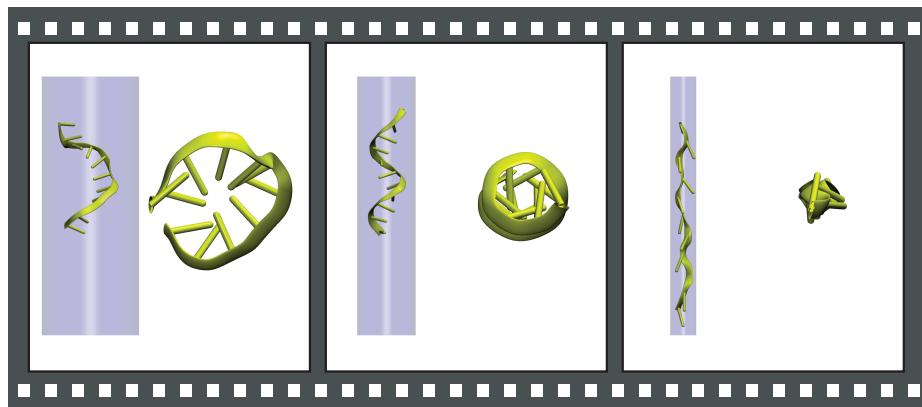


Figure 16: Movie `2views.mpg`.

- 9 Since the new copy is its own molecule, you have complete control of how it is displayed, independent of the original copy. When you play the trajectory or make a movie, VMD will keep the two views synchronized. The file `2views.mpg` shows an example of this technique, as does Fig. 17.
- 10 Finally, we’ll look at how to use user-defined scripts to dictate the animation. Type the following commands in the Tk Console:

```
source usermovie.tcl
enablemoviecallback
```

Now select **Movie Settings → User Defined Procedure**, and click **Make Movie**. Now, in addition to simply going through the trajectory, the camera starts above the DNA and rotates down and around it. An example movie is provided, and shown in Fig. 18

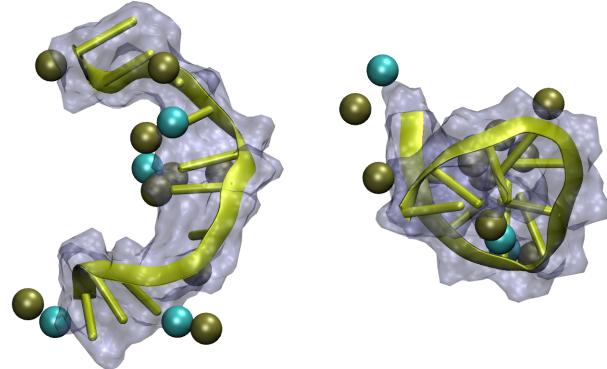


Figure 17: Example of showing the same object from multiple perspectives.



Figure 18: Movie `usermovie.mpg`

11 Let's see how it works. Its contents are reproduced here:

```
set trajectory_frames [molinfo top get numframes]

proc moviecallback { args } {
    global trajectory_frames
    set frac [expr double($::MovieMaker::userframe)/$::MovieMaker::numframes]
    rotate z to [expr $frac*360.0]
    rotate x by [expr -90.0*$frac]
    set frac [expr double($::MovieMaker::userframe)/$::MovieMaker::numframes]
    animate goto [expr $frac * $trajectory_frames]
}
```

```
proc enablemoviecallback { } {
    animate goto 0
    trace add variable ::MovieMaker::userframe write moviecallback
}
proc disablemoviecallback { } {
    trace remove variable ::MovieMaker::userframe write moviecallback
}
```

This should look familiar. We are again using the `trace` feature of Tcl. The Movie Maker plugin sets the writes the variable `::MovieMaker::userframe` each time it changes frames for animation, and when that happens, our proc `moviecallback` is called. This proc rotates the scene, and advances the animation frame.

You've now completed the tutorial. We've seen a number of techniques for representing molecular systems clearly and effectively, and gotten a taste of VMD's capabilities. The VMD website, listed at the beginning of this tutorial, has many other tutorials and resources for VMD users.