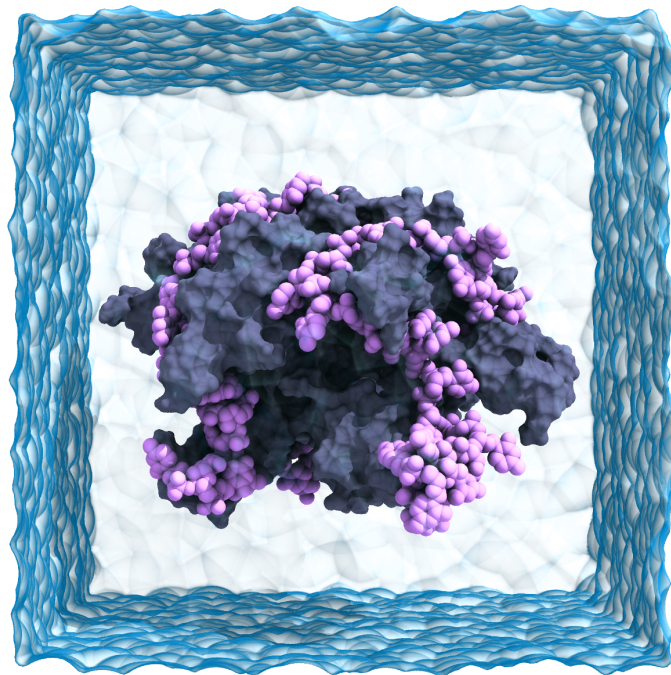**Aksimentiev Group**
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Rendering with Tachyon: a practical guide

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Contents

1 Introduction

In this tutorial, you will be shown how to make an looking image using Tachyon through VMD's graphical interface. Tachyon is a ray-tracing program written to run very quickly, taking advantage of multiple computer cores. In general, ray-tracing renderers use a realistic lighting model that can properly model shadows, yielding a sense depth to the final image. Tachyon takes advantage of multiple CPU cores to quickly produce high quality images.

    This tutorial focuses on features recently added to VMD that affect Tachyon renderings, and does not attempt to be a comprehensive guide to image making with VMD. We assume you have a working knowledge of VMD and refer inexperienced readers to the VMD tutorial. Furthermore, we assume the reader has VMD, Tachyon, and MSMS installed.

2 Create representations of your atoms

We have included a structure (ssbFigure.psf) and coordinate (ssbFigure.pdb) file that contains both DNA and protein, but feel free to use your own atomic model (e.g. a pdb obtained from RCSB). Load the files into VMD. Open the **graphical representations** window from the **Graphics** menu of the **VMD Main** window.

2.1 Create selections for different atoms

Each representation you use begins with a selection of a subset of the atoms present in your system. Try creating and modifying separate representations for:

    1. "protein"

2. "nucleic"

3. "same residue as water and {within 4 of protein} and {within 4 of nucleic}"

4. "ion and x*x+y*y+z*z < 35*35"

A figure rendered with all these representation would most likely appear very busy, but these are some common atom selections that demonstrate some of VMD's capabilities. For more information about atom selections, see the Selection Methods section of the VMD user guide (pdf or html). For the image on the cover of this tutorial, we retained only the first two atom selections ("protein" and "nucleic").

2.2   Choose a draw style

A **Drawing Method** is associated with each selection that you create, and these can radically affect the appearance of a selection. Choose one for a given representation from the **Drawing Method** pull-down menu of the **Draw style** tab.

Because Tachyon handles shadows realistically, representations that have cracks and crevices appear to have three-dimensional depth, making "**vdW**", "**Surf**" and "**MSMS**" good choices (see Fig. 1). In general, we recommend the "**MSMS**" representation over "**Surf**" since it draws more quickly and produces very similar output. Other frequently used representation include, "**NewCartoon**", which emphasizes the secondary structure of a protein, and "**Licorice**", which represents atomic detail nicely without the bulk of the "**vdW**" representation.
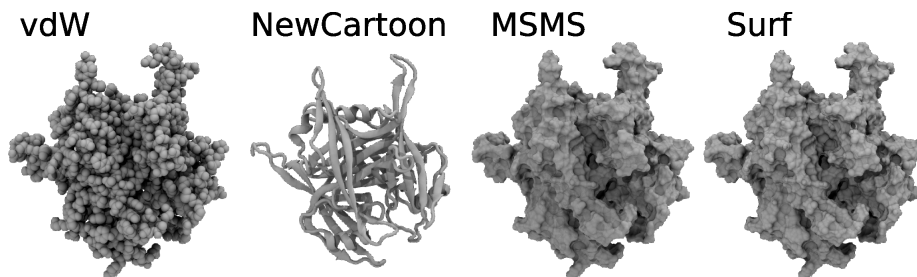

vdW   NewCartoon   MSMS   Surf

Figure 1: Examples of SSB rendered using different draw styles.

2.3   Material

The VMD materials—which specify how light interacts with each representation—that look best with Tachyon are typically very diffuse. There are a number of

predefined materials that are suitable for most tasks. Several materials (prefixed by "AO") were added to VMD to work well with the ambient occlusion lighting model that we will be using with Tachyon. This lighting model does a good job of mimicking a bright sky and represents shadows realistically, giving the representations a sense of depth. We recommend using these materials or modifying them slightly when rendering with Tachyon. The example figure was produced using AOChalky for both the DNA and protein. However, several parameters can be adjusted to create different appearances from the **Materials** window (accessible from the **Graphics** menu of the **VMD Main** window), and we recommend that the curious reader experiment with each of these.
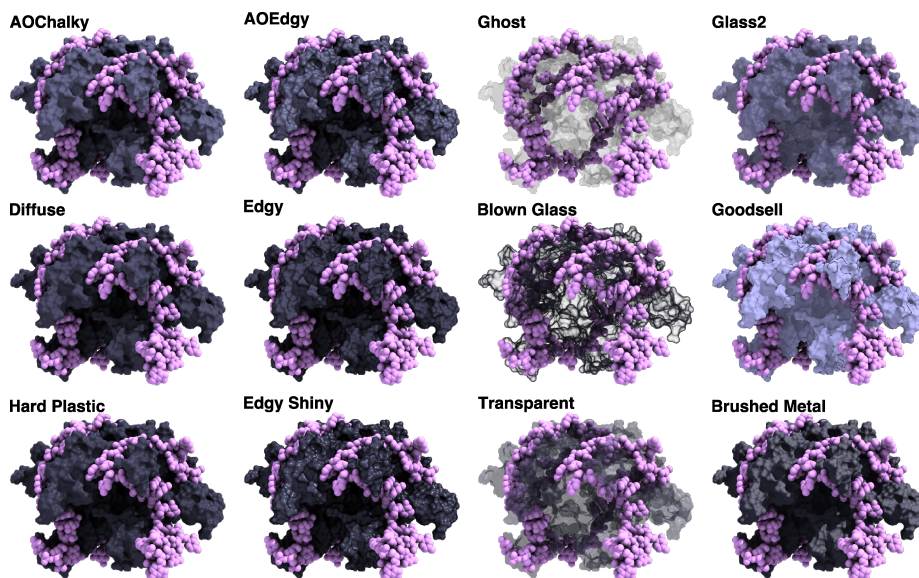

Figure 2: SSB with DNA rendered using different materials for the protein. The protein color and the lighting was identical across all renderings. Note the effect that the choice of material on the brightness of the final rendering.

For images displaying a system of a biomolecule in solvent, the solvent can be shown nicely by representing outer surface of the solution using a coarse (large probe radius), semi-transparent "**MSMS**" surface. However, rendering such a material can take a while and should be considered only once a good rendering of the solute had been obtained.

To make such a representation, select the "AOChalky" material from the **Materials** window and click the **Create New** button to create a new material based on the selected material. Change the name of this new material to "WaterBox", check the **Angle-Modulated Transparency**, and bring the **Opacity**

slide down to 0.2. Now return to the **Graphical Representations** window, and create a representation with the selection "water and noh" to select only the oxygen atoms of the water molecule. Select the "**MSMS**" draw style and change the **Probe Radius** to 6.5 (unchecking **Apply Changes Automatically** will hasten this process, but don't forget to click the **Apply** button), and wait a moment for the representation to be created. Finally, change the **Material** to "WaterBox".

2.4   Color

In addition to a drawing method, you may specify a coloring method for each representation. In the authors' experience, images often look best when using a single color for each representation chosen using the ColorID option from the **Coloring Method** pull-down menu of the **Graphical Representations** window. This usually results in the best contrast between different molecule in the system. The color of a given ColorID may be modified by adjusting the sliders in the **Color Definitions** tab of the **Color Controls** window, accessible from the Graphics menu item of the **VMD Main** window. In our example figure, a modified, lightened magenta was chosen for the DNA, and a modified, darker IceBlue was used for the protein. Cyan was chosen for the water box. Note that your choice of material, and the strength of your lights will both affect the brightness of the color when rendered, and some experimentation is necessary.

> **Color Scale.** The **Color Scale** tab of the **Color Controls** window gives control over the appearance of coloring methods utilizing a range of colors (e.g. Beta, User, or Position).

We encourage you to select colors that will provide good contrast between the protein and DNA molecules when viewed in grayscale, since figures are often printed in black and white. Additionally, you may want to consider how your image will appear to people who are red-green color blind, the most common form of color blindness.

3   Setting display options

The **Display Settings** window can be accessed from the bottom of the **Display** menu of the **VMD Main** window.

The first set of options in the **Display Settings** window has little impact on the rendered output, but feel free to play around with these settings

The next set of options (Screen Hgt and Screen Dist) are only important when perspective projection is in use.
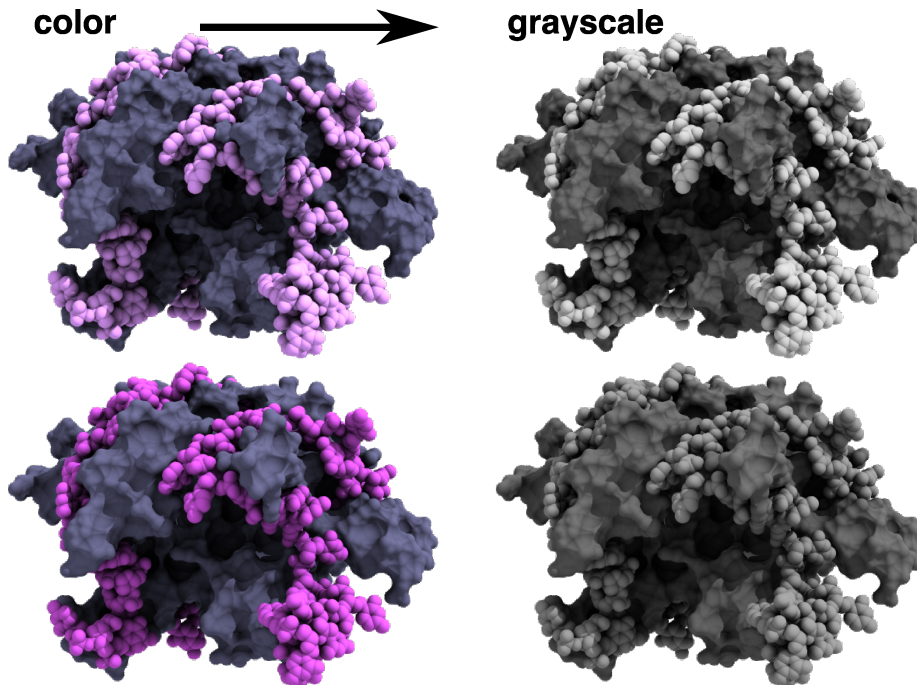
color ⟶ **grayscale**

Figure 3:   SSB with DNA rendered using two different shades of the same color. Both images were converted to grayscale to emphasize the importance and challenge of choosing colors with good contrast.

Perspective and orthographic projections..   VMD supports both perspective and orthographic projections, and these can be toggled from the **Display** menu of the **VMD Main** window. A perspective projection makes further objects appear smaller. An orthographic projection makes objects that are the same physical size appear the same size regardless of how far away it is. The example image was rendered using the perspective projection.

The exaggerated default perspective looks better when **Screen Hgt** is set to 1.0 and **Screen Dist** is set to -1.0, but you'll have to change the zoom a lot every time the view in VMD is reset (e.g. when the = key is pressed).

The third set of options control the fog, but only affect the output when Depth Cueing is turned on in the **Display** menu of the **VMD main** window. At the time of writing, the only **Cue Mode** for which VMD and Tachyon have similar behavior is **Exp2**.

For our purposes, the fourth section of this window, **External Renderer Options**, is the most important section of the **Display Settings** window. For

high quality renderings with Tachyon, turn on **Shadows** and **Amb Occl**. The values of **AO Ambient** and **AO Direct** will depend on the number of lights you are using, how strong you want your point light sources (AO Direct) to appear compared the ambient light (AO Ambient), as well as your personal preference for washed out images. A good rule of thumb is "AODirect × num.Lights + AOAmbient ≈ 1.8". For the final image, a single point light source was used with **AO Ambient** set to 1.0 and **AO Direct** set to 0.8. You turn lights on and off from the **Display** menu and use the mouse to set their positions from the Move Lights item of the **Mouse** menu of the **VMD Main** window. The light in the example figure was moved in front of the solute, a little to the right and above.

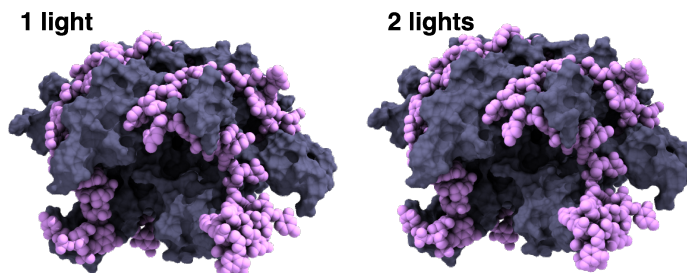**1 light**   **2 lights**

Figure 4: SSB with DNA rendered using 1 and 2 lights. The intensity of the each light was reduced by half for the figure on the right so that the balance between ambient and direct light is constant across the figures.

4 Rendering your image

Select "Render" from the **File** menu of the **VMD Main** window to open the **File Render Controls** window. Select TachyonInternal from the **Render using** drop menu. Select a name for your file. Finally, press the **Start Rendering** button and wait.

You can also use the "Tachyon" render mode, which gives specific control over command-line options. This render mode writes a Tachyon configuration file before rendering that file to a bitmap image. This can be useful when you may want to recreate an image at a different resolution (typically much higher, e.g. for a poster) at some later date. To do so, you could run Tachyon directly from the command-line (at least on Unix systems) without even opening VMD. For more information about the options you can give to Tachyon, execute Tachyon from the command line.
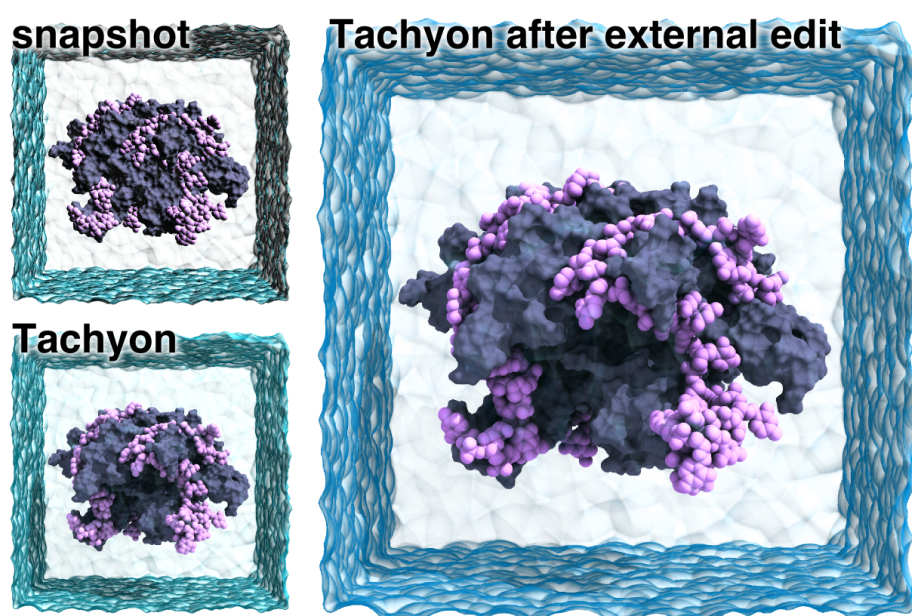
Figure 5: DNA bound to SSB. A VMD snapshot (upper left) was taken before rendering the scene with Tachyon (lower left). The levels, saturation, and the hue of the water were adjusted using the Gimp (open source image editing software) to produce the final image (right).