VMD Installation Guide

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Description

This document describes how to install one of the precompiled releases of VMD and contains instructions on how to compile VMD from the source code release.

[1] http://www.ks.uiuc.edu/

1 Registering VMD

VMD is made available free of charge for all interested end-users of the software (but please see the Copyright and Disclaimer notices). Please check the current VMD license agreement for details. Registration is part of our software download procedure. Once you've filled out the forms on the VMD download area and have read and agreed to the license, you are finished with the registration process.

2 Citation Reference

The authors request that any published work or images created using VMD include the following reference:

Humphrey, W., Dalke, A. and Schulten, K., "VMD - Visual Molecular Dynamics" *J. Molec. Graphics* **1996**, *14.1*, 33-38.

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3 Acknowledgments

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Many external libraries and packages are used in VMD, and the program would not be as capable without them. The authors of VMDwish to thank the authors of FLTK; the authors of Tcl and Tk; the authors of Python; the authors of VRPN; Jon Leech for uniform point distributions; Amitabh Varshney for SURF; Dmitrij Frishman for developing STRIDE; Jack Lund for the url_get perl script; Brad Grantham for the ACTC triangle consolidation library; John E. Stone for the Tachyon ray tracer and Spaceball drivers; and Ethan Merrit for one of the ribbon drawing algorithms.

4 Copyright and Disclaimer Notices

VMD is Copyright © 1995-2006 Theoretical and Computational Biophysics Group and the

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Portions of this code are copyright © 1997-1998 Andrew Dalke.

The terms for using, copying, modifying, and distributing VMD are specified by the VMD License. The license agreement is distributed with VMD in the file LICENSE. If for any reason you do not have this file in your distribution, it can be downloaded from:
`http://www.ks.uiuc.edu/Research/vmd/current/LICENSE.html`
Some of the code and executables used by VMD have their own usage restrictions:

- ACTC
  ACTC, the triangle consolidation library used in some versions of VMD, is Copyright (C) 2000, Brad Grantham and Applied Conjecture, all rights reserved.

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- Python
  Python is made available subject to the terms and conditions in CNRI's License Agreement. This Agreement together with Python may be obtained from a proxy server on the Internet using the following URL: `http://hdl.handle.net/1895.22/1012`

- PCRE
  The Perl Compatible Regular Expressions (PCRE) library used in VMD was written by Philip Hazel and is Copyright (c) 1997-1999 University of Cambridge.
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  3. Altered versions must be plainly marked as such, and must not be misrepresented as being the original software.
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License (GPL), then the terms of that license shall supersede any condition above with which it is incompatible.

- STRIDE
  STRIDE, the program used for secondary structure calculation, is free to both academic and commercial sites provided that STRIDE will not be a part of a package sold for money. The use of STRIDE in commercial packages is not allowed without a prior written commercial license agreement. See `http://www.embl-heidelberg.de/argos/stride/stride_info.html`

- SURF
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  This software was developed and is made available for public use with the support of the National Institutes of Health, National Center for Research Resources under grant RR02170.

- Tachyon
  The Tachyon multiprocessor ray tracing system and derivative code built into VMD is Copyright (c) 1994-2006 by John E. Stone. See the Tachyon distribution for redistribution and licensing information.

5 Obtaining VMD Source and Binary Distributions

The VMD source code and binary distributions can be obtained after registering at the VMD web page. Download the appropriate distribution file with your web browser. Windows binary distributions are self extracting, so once the distribution file is downloaded, proceed to the installation directions below.

For source distributions and Unix binary distributions, uncompress and untar the file. This will produce a subdirectory named `vmd-1.8.4`. Unless otherwise specified, all references to VMD code will be from this subdirectory, so `cd` there.

6 Installing a Pre-Compiled Version of VMD

To install the pre-compiled Windows version of VMD, simply run the self-extracting executable, and it will start the VMD Windows installer program, which includes built-in help. This process is automated and should be familiar to most Windows users. When installing VMD be sure that you have administrator privileges.

To install the pre-compiled MacOS X bundle version of VMD, open the VMD disk image and drag the VMD application into an appropriate directory. Once the VMD application has been placed appropriately it should be ready for immediate use as no other installation steps are required.

To install the pre-compiled Unix version of VMD, then only three steps remain to be done after you uncompress and untar the distribution.

- Edit the `configure` script. If necessary, change the following values:

```
   $install_bin_dir

This is the location of the startup script 'vmd'.  It should
be located in the path of users interested in running VMD.

   $install_library_dir

This is the location of all other VMD files.  This includes
the binary and helper scripts.  It should not be in the path.
```

- Next generate the Makefile based on these configuration variables. This is done by running `./configure` .
- After configuration is complete, `cd` to the `src` directory and type `make install`. This will put the code in the two directories listed above. After this, you just type `vmd` to begin, provided that `vmd` is in your path.

7 Customizing VMD Startup

The Unix version of VMD reads in several data files (if they exist) when it starts up. These files control the initial appearance and behavior of VMD at the start, and may be customized to

suit each users particular tastes. Default versions of these files are placed in the INSTALLLIBDIR directory (usually /usr/local/lib/vmd). While each user may specify to use different versions of these files, unless this is done the commands and values in the default files are used. In this way, an administrator may customize the default behavior of VMD for all users, while allowing each user the option to change the default behavior however they choose. This chapter describes each of these data files.

Several configurable parameters may also be set in a number of ways, including by command-line options or by environment variables. The order of precedence of these methods is as follows (highest precedence to lowest):

1. Command-line options (see the Users Guide).
2. Environment variable settings (see the Users Guide).
3. Built-in defaults, as specified by compilation configurable parameters. These are used only if no other values are specified by the other methods mentioned in this list.

8 The .vmdrc and vmd.rc files

After initialization is complete, VMD reads the *startup* file. This file contains text commands for VMD to execute, just as if they had been entered at the VMD text console command prompt. The file can contain any number of commands, including blank lines and comment lines (which begin with the # character). If an error is encountered while reading this file, the command in error is skipped and processing of the file continues.

The base filename for this startup file is .vmdrc by default on Unix systems and vmd.rc on Windows; this is determined by the configuration parameter STARTUPFILENAME. VMD searches for this file in a number of locations, and reads in the *first* version of the file it finds. The order of searching for the file is:

1. ./STARTUPFILENAME
2. $HOME/STARTUPFILENAME
3. INSTALLLIBDIR/STARTUPFILENAME

See the Users Guide for a list of all VMD text commands.

9 The .vmdsensors file

If VMD is compiled with the VRPN option, it will look for files that specify how to access the external spatial tracking devices. These files are read whenever VMD is told to initialize a specific external device. The Tracker library will load the first file it finds in the following search order:

1. $HOME/.vmdsensors
2. The $VMDSENSOR environment variable.
3. INSTALLLIBDIR/.vmdsensors

This last file (INSTALLLIBDIR/.vmdsensors) contains extensive comments on how to configure the sensor description files properly. If the VRPN option is omitted when compiling VMD, this file is not used.

10 What to Do If It Doesn't Work

If you are running a VMD binary which has been built with a native OpenGL implementation (i.e. not Mesa), you should make sure that you have the vendor provided OpenGL runtime libraries and the X server extensions correctly installed. SGI systems normally have the OpenGL runtime support installed on them. Sun, HP, and IBM systems often do not come with OpenGL support by default. If you don't have the OpenGL runtime libraries for these systems, they can be downloaded for free from the Sun, HP, and IBM web sites respectively. Each of the vendor's OpenGL implementations generally include "install check" programs which verify the correct installation and operation of the OpenGL libraries.

- Sun's OpenGL site is at `http://www.sun.com/software/graphics/opengl/`
- HP's OpenGL site is at `http://www.hp.com/unixwork/products/opengl.html`
- IBM's OpenGL site is at `http://www.austin.ibm.com/software/OpenGL/`

We suggest that you check that you are doing everything correctly, and if it still doesn't work, report the problem by e-mail to `vmd@ks.uiuc.edu`. We'll try to help you.

11 Compiling Your Own Version of VMD

If for some reason you want to recompile VMD, then you will need to read the rest of this document. Most users will want to use the binary distributions we provide since they have been thorougly tested prior to release. It may be necessary for you to compile your own version of VMD in cases where we do not provide a binary for your platform, or when the provided binaries will not run correctly with a particular version of your operating system. Full compilation instructions for VMD are found in the online VMD Programmer's Guide: `http://www.ks.uiuc.edu/Research/vmd/doxygen/`