VMD Installation Guide

J. Cohen, J. Stone

Version 1.8.6

April 3, 2007

Theoretical Biophysics Group[1]
University of Illinois and Beckman Institute
405 N. Mathews
Urbana, IL 61801
VMD home page: `http://www.ks.uiuc.edu/Research/vmd/`

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.

3 Acknowledgments

4 Copyright and Disclaimer Notices

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.

  Redistribution and use in source and binary forms, with or without modification, are permitted provided that the following conditions are met:
  1. Redistributions of source code must retain the above copyright notice, this list of conditions and the following disclaimer.
  2. Redistributions in binary form must reproduce the above copyright notice, this list of conditions and the following disclaimer in the documentation and/or other materials provided with the distribution.
  3. All advertising materials mentioning features or use of this software must display the following acknowledgment: This product includes software developed by Brad Grantham and Applied Conjecture.
  4. Neither the name Brad Grantham nor Applied Conjecture may be used to endorse or promote products derived from this software without specific prior written permission.
  5. Notification must be made to Brad Grantham about inclusion of this software in a product including the author of the product and the name and purpose of the product. Notification can be made using email to Brad Grantham's current address (grantham@plunk.org as of September 20th, 2000) or current U.S. mail address.

- 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.
  Permission is granted to anyone to use this software for any purpose on any computer system, and to redistribute it freely, subject to the following restrictions:
  1. This software is distributed in the hope that it will be useful, but WITHOUT ANY WARRANTY; without even the implied warranty of MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE.
  2. The origin of this software must not be misrepresented, either by explicit claim or by omission.
  3. Altered versions must be plainly marked as such, and must not be misrepresented as being the original software.
  4. If PCRE is embedded in any software that is released under the GNU General Purpose

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
  The source code for SURF is copyrighted by the original author, Amitabh Varshney, and the University of North Carolina at Chapel Hill. Permission to use, copy, modify, and distribute this software and its documentation for educational, research, and non-profit purposes is hereby granted, provided this notice, all the source files, and the name(s) of the original author(s) appear in all such copies.
  BECAUSE THE CODE IS PROVIDED FREE OF CHARGE, IT IS PROVIDED "AS IS" AND WITHOUT WARRANTY OF ANY KIND, EITHER EXPRESSED OR IMPLIED.
  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) 1994-2007 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-1.8.6`. 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

5

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 thoroughly 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/`