VMD User's Guide

Version 1.9.3

November 27, 2016

NIH Biomedical Research Center for Macromolecular Modeling and Bioinformatics

Theoretical and Computational Biophysics Group[1]
Beckman Institute for Advanced Science and Technology
University of Illinois at Urbana-Champaign
405 N. Mathews
Urbana, IL 61801

`http://www.ks.uiuc.edu/Research/vmd/`

Description

The VMD User's Guide describes how to run and use the molecular visualization and analysis program VMD. This guide documents the user interfaces displaying and grapically manipulating molecules, and describes how to use the scripting interfaces for analysis and to customize the behavior of VMD.

VMD development is supported by the National Institutes of Health grant numbers NIH 9P41GM104601 and 5R01GM098243-02.

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

Contents

1 Introduction **10**
- 1.1 Contacting the authors . . . 11
- 1.2 Registering VMD . . . 11
- 1.3 Citation Reference . . . 11
- 1.4 Acknowledgments . . . 12
- 1.5 Copyright and Disclaimer Notices . . . 12
- 1.6 For information on our other software . . . 14

2 Hardware and Software Requirements **16**
- 2.1 Basic Hardware and Software Requirements . . . 16
- 2.2 Multi-core CPUs and GPU Acceleration . . . 16
- 2.3 Parallel Computing on Clusters and Supercomputers . . . 17

3 Tutorials **18**
- 3.1 Rapid Introduction to VMD . . . 18
- 3.2 Viewing a molecule: Myoglobin . . . 18
- 3.3 Rendering an Image . . . 20
- 3.4 A Quick Animation . . . 20
- 3.5 An Introduction to Atom Selection . . . 21
- 3.6 Comparing Two Structures . . . 21
- 3.7 Some Nice Represenations . . . 22
- 3.8 Saving your work . . . 23
- 3.9 Tracking Script Command Versions of the GUI Actions . . . 23

4 Loading A Molecule **25**
- 4.1 Notes on common molecular file formats . . . 25
- 4.2 What happens when a file is loaded? . . . 26
- 4.3 Babel interface . . . 26
- 4.4 Raster3D file format . . . 27

5 User Interface Components **28**
- 5.1 Using the Mouse in the Graphics Window . . . 28
  - 5.1.1 Mouse Modes . . . 28
  - 5.1.2 Pick Modes . . . 29
  - 5.1.3 Hot Keys . . . 31
- 5.2 Using the Spaceball in the Graphics Window . . . 32
  - 5.2.1 Spaceball Driver . . . 32

5.3 Using the Joystick in the Graphics Window . . . 34
5.4 Description of each VMD window . . . 35
5.4.1 Main Window . . . 35
5.4.2 Main Window Molecule List browser . . . 35
5.4.3 Main Window Animation Controls . . . 37
5.4.4 Molecule File Browser Window . . . 38
5.4.5 Mouse Menu . . . 39
5.4.6 Display Menu and Display Settings Window . . . 41
5.4.7 Graphics Window . . . 44
5.4.8 Labels Window . . . 48
5.4.9 Color Window . . . 50
5.4.10 Material Window . . . 52
5.4.11 Render Window . . . 53
5.4.12 Tool Window . . . 53
5.4.13 IMD Connect Simulation Window . . . 56
5.4.14 Sequence Window . . . 58
5.4.15 RamaPlot . . . 60

6 Molecular Drawing Methods 62
6.1 Rendering methods . . . 62
6.1.1 Lines . . . 63
6.1.2 Bonds . . . 63
6.1.3 DynamicBonds . . . 64
6.1.4 HBonds . . . 64
6.1.5 Points . . . 64
6.1.6 VDW . . . 65
6.1.7 CPK . . . 65
6.1.8 Licorice . . . 65
6.1.9 Polyhedra . . . 65
6.1.10 Trace . . . 66
6.1.11 Tube . . . 66
6.1.12 Ribbons . . . 66
6.1.13 NewRibbons . . . 67
6.1.14 Cartoon . . . 67
6.1.15 NewCartoon . . . 68
6.1.16 PaperChain . . . 68
6.1.17 Twister . . . 68
6.1.18 QuickSurf . . . 68
6.1.19 Surf . . . 69
6.1.20 MSMS . . . 70
6.1.21 VolumeSlice . . . 70
6.1.22 Isosurface . . . 71
6.1.23 FieldLines . . . 71
6.1.24 Orbital . . . 72
6.1.25 Beads . . . 72
6.1.26 Dotted . . . 72
6.1.27 Solvent . . . 72

6.2 Coloring Methods . . . 73
6.2.1 Color categories . . . 73
6.2.2 Coloring Methods . . . 73
6.2.3 Coloring by color categories . . . 73
6.2.4 Color scale . . . 74
6.2.5 Materials . . . 75
6.3 Selection Methods . . . 77
6.3.1 Definition of Keywords and Functions . . . 79
6.3.2 Boolean Keywords . . . 80
6.3.3 Short Circuiting . . . 80
6.3.4 Quoting with Single Quotes . . . 80
6.3.5 Double Quotes and Regular Expressions . . . 81
6.3.6 Comparison selections . . . 82
6.3.7 Comparison Operators . . . 82
6.3.8 Other selections . . . 83

7 Viewing Modes **89**
7.1 Perspective/Orthographic views . . . 89
7.2 Monoscopic Modes . . . 89
7.3 Stereoscopic Modes . . . 89
7.3.1 Quad-buffered Stereo . . . 90
7.3.2 Side-By-Side and Cross-Eyed Stereo . . . 90
7.3.3 HDTV Side-by-side Stereo . . . 91
7.3.4 Checkerboard Stereo . . . 91
7.3.5 Column Interleaved Stereo . . . 91
7.3.6 Row Interleaved Stereo . . . 91
7.3.7 Anaglyph Stereo . . . 91
7.3.8 Stereo Parameters . . . 92

8 Scene Export and Rendering **93**
8.1 Screen Capture Using Snapshot . . . 93
8.2 Higher Quality Rendering . . . 93
8.3 Caveats . . . 94
8.4 One Step Printing . . . 95
8.5 Making Stereo Images . . . 95
8.6 Making a Movie . . . 96

9 Tcl Text Interface **98**
9.1 Using text commands . . . 98
9.2 Tcl/Tk . . . 99
9.3 Tcl Text Commands . . . 99
9.3.1 animate . . . 99
9.3.2 atomselect . . . 101
9.3.3 axes . . . 104
9.3.4 color . . . 104
9.3.5 colorinfo . . . 105
9.3.6 display . . . 106

9.3.7 draw . . . 108
9.3.8 exit . . . 109
9.3.9 graphics . . . 109
9.3.10 gettimestep . . . 111
9.3.11 help . . . 111
9.3.12 imd . . . 111
9.3.13 label . . . 112
9.3.14 light . . . 113
9.3.15 logfile . . . 114
9.3.16 material . . . 114
9.3.17 mdffi . . . 115
9.3.18 measure . . . 115
9.3.19 menu . . . 123
9.3.20 mol . . . 123
9.3.21 molecule . . . 127
9.3.22 molinfo . . . 127
9.3.23 mouse . . . 129
9.3.24 parallel . . . 129
9.3.25 play . . . 130
9.3.26 quit . . . 130
9.3.27 render . . . 130
9.3.28 rock . . . 131
9.3.29 rotate . . . 132
9.3.30 scale . . . 132
9.3.31 stage . . . 132
9.3.32 tool . . . 132
9.3.33 translate . . . 133
9.3.34 user . . . 133
9.3.35 vmdinfo . . . 133
9.3.36 volmap . . . 134
9.3.37 wait . . . 139
9.3.38 sleep . . . 139
9.4 Tcl callbacks . . . 140

10 Python Text Interface **142**
10.1 Using the Python interpreter within VMD . . . 142
10.2 Python modules within VMD . . . 142
10.3 Atom selections in Python . . . 143
10.3.1 The built-in atomsel type . . . 143
10.3.2 The AtomSel class (DEPRECATED) . . . 143
10.3.3 An atom selection example . . . 145
10.3.4 Changing the selection and the frame . . . 146
10.3.5 Combining atom selections . . . 147
10.3.6 RMS example . . . 148
10.4 Python callbacks . . . 150
10.4.1 Using Tkinter menus in VMD . . . 151
10.5 Controlling VMD from Python . . . 151

10.5.1 animate . . . 151
10.5.2 axes . . . 152
10.5.3 color . . . 152
10.5.4 display . . . 153
10.5.5 evaltcl . . . 153
10.5.6 graphics . . . 153
10.5.7 imd . . . 154
10.5.8 label . . . 155
10.5.9 material . . . 156
10.5.10 molecule . . . 156
10.5.11 molrep . . . 158
10.5.12 render . . . 159
10.5.13 trans . . . 160
10.5.14 vmdnumpy . . . 160
10.6 High-level Python Interface . . . 161
10.6.1 Molecule . . . 161
10.6.2 MoleculeRep . . . 163
10.6.3 Draw Style Methods . . . 164
10.6.4 Saving and Restoring Molecule State . . . 164

11 Vectors and Matrices **165**
11.1 Vectors . . . 165
11.2 Matrix routines . . . 168
11.3 Multiplying vectors and matrices . . . 171
11.4 Misc. functions and values . . . 171

12 Molecular Analysis **173**
12.1 Using the `molinfo` command . . . 173
12.2 Using the `atomselect` command . . . 174
12.3 Analysis scripts . . . 179
12.4 RMS Fit and Alignment . . . 182
12.4.1 RMS Fit and Alignment Extension . . . 183
12.4.2 RMS and scripting . . . 184
12.5 VMD Script Commands for Colors . . . 186
12.5.1 Changing the color scale definitions . . . 186
12.5.2 Creating a set of black-and-white color definitions . . . 187
12.5.3 Revert all RGB values to defaults . . . 187
12.5.4 Coloring Trick - Override a Coloring Category . . . 188

13 Collective Variables Interface (Colvars) **189**
13.1 General parameters and input/output files . . . 190
13.1.1 Using the `cv` command . . . 190
13.1.2 Configuration syntax for the Colvars module . . . 192
13.1.3 Input state file (optional) . . . 195
13.1.4 Output files . . . 195
13.2 Defining collective variables and their properties . . . 195
13.2.1 General options for a collective variable . . . 196

13.2.2 Artificial boundary potentials (walls) . . . 197
13.2.3 Trajectory output . . . 198
13.2.4 Extended Lagrangian. . . . 199
13.2.5 Statistical analysis of collective variables . . . 200
13.3 Selecting atoms for colvars: defining atom groups . . . 202
13.3.1 Selection keywords . . . 202
13.3.2 Moving frame of reference. . . . 204
13.3.3 Treatment of periodic boundary conditions. . . . 207
13.3.4 Performance a Colvars calculation based on group size. . . . 207
13.4 Collective variable components (basis functions) . . . 208
13.4.1 List of available colvar components . . . 209
13.4.2 Configuration keywords shared by all components . . . 225
13.4.3 Advanced usage and special considerations . . . 225
13.4.4 Linear and polynomial combinations of components . . . 227
13.4.5 Colvars as scripted functions of components . . . 227
13.5 Biasing and analysis methods . . . 228
13.5.1 Adaptive Biasing Force . . . 229
13.5.2 Extended-system Adaptive Biasing Force (eABF) . . . 234
13.5.3 Metadynamics . . . 235
13.5.4 Harmonic restraints . . . 240
13.5.5 Linear restraints . . . 244
13.5.6 Adaptive Linear Bias/Experiment Directed Simulation . . . 245
13.5.7 Multidimensional histograms . . . 246
13.5.8 Probability distribution-restraints . . . 247
13.5.9 Scripted biases . . . 249

14 Customizing VMD Sessions **250**
14.1 VMD Command-Line Options . . . 250
14.2 Environment Variables . . . 252
14.3 Startup Files . . . 257
14.3.1 Core Script Files . . . 257
14.3.2 User Script Files . . . 257
14.3.3 `.vmdrc` and `vmd.rc` Files . . . 257
14.4 Using VMD as a WWW Client (for chemical/* documents) . . . 258
14.4.1 MIME types . . . 258
14.4.2 Setting up your `.mailcap` . . . 258
14.4.3 Example sites . . . 259

References **260**

List of Figures

3.1 Sample VMD session displaying myoglobin. 19

5.1 The Main window 35
5.2 The Main window animation controls 37
5.3 The Molecule File Browser window 38
5.4 The Display menu 41
5.5 Relationship between screen height, distance to origin, and the viewer 44
5.6 The Graphics window (in Draw Style mode) 45
5.7 The Graphics window (in Selections mode) 47
5.8 The Labels window 49
5.9 The Color window 51
5.10 The Material Window 52
5.11 The Render window 53
5.12 The Tool window 54
5.13 The Sequence window 58
5.14 The RamaPlot Window 60

6.1 Example showing red/green/blue gradients summed to produce the color scale. . . . 77
6.2 The shift to the red component of the RGB scale caused by the value of "min". . . . 77

12.1 RMS calculation and alignment extension 183

13.1 Graphical representation of a Colvars configuration. 190

List of Tables

5.1 Mouse control hot keys. 32
5.2 Rotation & scaling hot keys. 33
5.3 Menu control hot keys. 33
5.4 Animation hot keys. 34
5.5 Description of secondary structure codes in the Sequence window. 58

6.1 Molecular view representation styles. 63
6.2 Color categories used in VMD. 74
6.3 Molecular coloring methods. 75
6.4 Available Color Scale Gradations. 76
6.5 Atom selection keywords. 85
6.6 Atom selection keywords (continued). 86
6.7 Atom selection functions. 87
6.8 Read-only atom selection keywords for volumetric map queries 87
6.9 Regular expression methods. 87
6.10 Regular expression conversions. 88

8.1 Miscellaneous Rendering Options 97

9.1 Summary of core text commands in VMD. 100
9.2 On-line Help Sources 112
9.3 `molinfo set/get` keywords 128
9.4 Description of Tcl callback variables in VMD. 141

10.1 Description of callbacks available to Python scripts running in VMD. 150

Chapter 1

Introduction

VMD [1] is a molecular graphics program designed for the interactive visualization and analysis of biopolymers such as proteins, nucleic acids, lipids, and membranes. VMD runs on all major Unix workstations, Apple MacOS X, and Microsoft Windows. Online information about VMD is available from:
`http://www.ks.uiuc.edu/Research/vmd/`

List of key VMD features:

- **General molecular visualization**
  At its heart, VMD is a general application for displaying molecules containing any number of atoms and is similar to other molecular visualization programs in its basic capabilities. VMD reads data files using an extensible plugin system, and supports Babel for conversion of other formats. User-defined atom selections can be displayed in any of the standard molecular representations. Displayed graphics can be exported to an image file, to a scene file usable by ray tracing programs, or to a geometry description file suitable for use with 3-D printers.

- **Visualization of dynamic molecular data**
  VMD can load atomic coordinate trajectories from AMBER, Charmm, DLPOLY, Gromacs, MMTK, NAMD, X-PLOR, and many other simulation packages. The data can be used to animate the molecule or to plot the change in molecular properties such as angles, dihedrals, interatomic distances, or energies over time.

- **Visualization of volumetric data**
  VMD can load, generate, and display, volumetric maps. Supported map formats include CryoEM maps, electrostatic potential maps, electron density maps, and many other map file formats.

- **Interactive molecular dynamics simulations**
  VMD can be used as a graphical front-end to a live molecular dynamics program running on a remote supercomputer or high-performance workstation. VMD can interactively apply and visualize forces in an MD simulation as it runs.

- **Molecular analysis commands**
  Many commands are provided for molecular analysis. These include commands to extract information on sets of atoms and molecules, vector and matrix routines for coordinate manipulation, and functions for computing values such as center of mass and radius of gyration.

- **Tcl and Python scripting languages**
  VMD uses the freely available Python and Tcl scripting languages for processing text commands. These popular languages which contain variables, loops, subroutines, and much more. VMD also uses the Tk Toolkit - a simple user interface toolkit that interfaces with Tcl.

- **Easy to extend**
  VMD is written in C and C++ and employs object-oriented design. VMD implements a plugin interface for extending its file format support and for general purpose extensions in functionality.

- **Support for multimodal input and various display systems**
  A number of different visual display and control systems are supported in addition to the usual monitor, keyboard, and mouse. The VRPN library is used to get position and orientation information from a wide variety of spatial input devices, including magnetic trackers, haptic (force feedback) devices, Spaceballs, etc. VMD works with WireGL and Chromium on tiled display walls, and immersive VR environments via compiled-in CAVE and FreeVR support.

1.1 Contacting the authors

The current developer of VMD is John E. Stone. The list of individuals that made signficant contributions to this version of VMD in the form of patches, bug fixes, and completely new plugins includes Anton Arkhipov, Michael Bach, Robert Brunner, Jordi Cohen, Simon Cross, Markus Dittrich, John Eargle, Peter Freddolino, Luis Gracia, Justin Gullingsrud, David Hardy, Konrad Hinsen, James Gumbart, Robert Johnson, Axel Kohlmeyer, Michell Kuttel, John Mongan, Jim Phillips, Elijah Roberts, Jan Saam, Alexander Spaar, Marcos Sotomayor, Leonardo Trabuco, Dan Wright, and Kirby Vandivort.

We are very interested in and grateful for any user comments and reports of program bugs or inaccuracies. If you have any suggestions, bug reports, or general comments about VMD, please send them to us at `vmd@ks.uiuc.edu`.

1.2 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.

1.3 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.

VMD has been developed by the Theoretical and Computational Biophysics Group at the Beckman Institute for Advanced Science and Technology of the University of Illinois at Urbana-Champaign. This work is supported by the National Institutes of Health under grant numbers NIH 9P41GM104601 and 5R01GM098243-02.

1.4 Acknowledgments

The authors would particularly like to thank those individuals who have contributed suggestions and improvements, particularly those contributing new features. Special thanks go to Joshua Anderson, Anton Arkhipov, Andrew Dalke, Michael Bach, Alexander Balaeff, Ilya Balabin, Robert Brunner, Eamon Caddigan, Jordi Cohen, Simon Cross, Markus Dittrich, John Eargle, Peter Freddolino, Todd Furlong, Luis Gracia, Paul Grayson, Justin Gullingsrud, James Gumbart, David Hardy, Konrad Hinsen, Barry Isralewitz, Sergei Izrailev, Robert Johnson, Axel Kohlmeyer, Michael Krone, Michelle Kuttell, Benjamin Levine, John Mongan, Jim Phillips, Elijah Roberts, Jan Saam, Charles Schwieters, Marcos Sotomayor, Alexander Spaar, John E. Stone, Johan Strumpfer, Alexey Titov, Leonardo Trabuco, Dan Wright, and Kirby Vandivort. The entire VMD user community now benefits from your contributions.

The authors would like to thank individuals who have indirectly helped with development by making suggestions, pushing for new features, and trying out buggy code. Thanks go to Aleksei Aksimentiev, Daniel Barsky, Axel Berg, Tom Bishop, Robert Brunner, Ivo Hofacker, Mu Gao, James Gumbart, Xiche Hu, Tim Isgro, Dorina Kosztin, Ioan Kosztin, Joe Landman, Ilya Logunov, Clare Macrae, Amy Shih, Lukasz Salwinski, Stephen Searle, Charles Schwieters, Ari Shinozaki, Svilen Tzonev, Emad Tajkhorshid, Michael Tiemann, Elizabeth Villa, Raymond de Vries, Simon Warfield, Willy Wriggers, Dong Xu, and Feng Zhou.

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, WorkForce threading and timer routines, hash table code, and Spaceball drivers; and Ethan Merrit for one of the ribbon drawing algorithms.

1.5 Copyright and Disclaimer Notices

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) 1994-2016 by John E. Stone. See the Tachyon distribution for redistribution and licensing information.

- Desmond and Maestro plugins by D. E. Shaw Research
  Copyright 2009, D. E. Shaw Research, LLC All rights reserved.
  Redistribution and use in source and binary forms, with or without modification, are permitted provided that the following conditions are met:
  Redistributions of source code must retain the above copyright notice, this list of conditions, and the following disclaimer.
  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.
  Neither the name of D. E. Shaw Research, LLC nor the names of its contributors may be used to endorse or promote products derived from this software without specific prior written permission.
  THIS SOFTWARE IS PROVIDED BY THE COPYRIGHT HOLDERS AND CONTRIBUTORS "AS IS" AND ANY EXPRESS OR IMPLIED WARRANTIES, INCLUDING, BUT NOT LIMITED TO, THE IMPLIED WARRANTIES OF MERCHANTABILITY AND FITNESS FOR A PARTICULAR PURPOSE ARE DISCLAIMED. IN NO EVENT SHALL THE COPYRIGHT OWNER OR CONTRIBUTORS BE LIABLE FOR ANY DIRECT, INDIRECT, INCIDENTAL, SPECIAL, EXEMPLARY, OR CONSEQUENTIAL DAMAGES (INCLUDING, BUT NOT LIMITED TO, PROCUREMENT OF SUBSTITUTE GOODS OR SERVICES; LOSS OF USE, DATA, OR PROFITS; OR BUSINESS INTERRUPTION) HOWEVER CAUSED AND ON ANY THEORY OF LIABILITY, WHETHER IN CONTRACT, STRICT LIABILITY, OR TORT (INCLUDING NEGLIGENCE OR OTHERWISE) ARISING IN ANY WAY OUT OF THE USE OF THIS SOFTWARE, EVEN IF ADVISED OF THE POSSIBILITY OF SUCH DAMAGE.

1.6 For information on our other software

VMD is part of a suite of tools developed by the Theoretical and Computational Biophysics group at the University of Illinois.

- BioCoRE
  BioCoRE is a web-based collaborative environment for structural biology which provides tools to allow collaboration between researchers down the hall or around the world. Anyone with access to the internet and a standard web browser can join BioCoRE and create or be

added to research projects, and information about a particular project is shared among all members of that project. More information is available at the BioCoRE home page[1]

- NAMD
  A parallel, object-oriented molecular dynamics code designed for high-performance simulation of large biomolecular systems. NAMD uses the CHARMM force field and file formats compatible with both CHARMM and X-PLOR. NAMD supports both periodic and non-periodic boundaries with efficient full electrostatics, multiple timestepping, constant pressure and temperature ensemble simulation methods. More information is available at the NAMD home page[2]

- MDTools
  MDTools is a collection of programs, scripts, and utilities provided for researchers to make various modeling and simulation tasks easier. More information is available at the MDTools home page[3]

For more information on our software efforts, see the Theoretical and Computational Biophysics Group home page[4].

[1] http://www.ks.uiuc.edu/Research/biocore
[2] http://www.ks.uiuc.edu/Researach/namd
[3] http://www.ks.uiuc.edu/Development/MDTools
[4] http://www.ks.uiuc.edu/

Chapter 2

Hardware and Software Requirements

2.1 Basic Hardware and Software Requirements

The basic hardware requirements for running VMD vary depending on how it was compiled and how it will be used. VMD has two primary modes of operation, the typical full-featured graphics-enabled mode, and a purely text-based mode of operation suited for remote analysis on supercomputers, embedded use in other packages, and similar batch-oriented analytical uses.

The full-featured graphics-enabled mode of VMD is the most demanding, and requires an OpenGL-capable graphics accelerator with up-to-date drivers. Some graphics chipsets or GPUs come with drivers that are below-spec and will not be able to run VMD with full graphics capability. These will either automatically, or as the result of user-defined environment variables (e.g. VMDSIMPLEGRAPHICS), use a reduced functionality graphics mode within VMD. Since the choice of the GPU chipset or card has the biggest impact on the visualization capabilities and performance of VMD, this is the hardware component that is worth spending money on if one's intended use of VMD is primarily focused on visualization related tasks. VMD implements a variety of advanced rendering features that hinge upon the availability of GPU hardware and driver support. When available, these features enable VMD to interactively display very large or complex structures and support a variety of special stereoscopic 3-D displays [1, 2, 3, 4, 5, 6, 7]. As an added bonus, recent GPUs are now also capable of accelerating some of the computationally demanding tasks within VMD, discussed in more detail below.

Following the choice of graphics accelerator, the amount of available system memory tends to have the next most significant impact on the performance and capability of VMD. The more memory a machine has, the more frames can be loaded at once from large molecular dynamics trajectory files. For batch-mode analysis tasks that consist primarily of scripting, system memory is frequently the resource that limits feasability of many analysis tasks.

2.2 Multi-core CPUs and GPU Acceleration

VMD makes full use of multi-core processors and multiple GPUs for acceleration of the most computationally demanding visualization and analysis tasks. Multi-core CPUs accelerate features including interactive molecular dynamics [8, 9], bond determination, "within" atom selections and derivatives, so-called streamline or field line visualizations [10], radial distribution functions [11], and high quality renderings using the built-in Tachyon [12, 13, 14] and OSPRay [15] ray tracing engines. VMD also supports GPU acceleration using CUDA, and takes advantage of both multi-

core CPUs and GPUs for acceleration of electrostatics (i.e. "volmap coulomb", and "volmap coulombmsm") [16, 17, 18, 19, 20, 21, 22, 23, 24, 25], implicit ligand sampling (i.e. "volmap ils"), computation of radial distribution functions [11], quality-of-fit cross correlation calculation for hybrid fitting methods [26, 27], trajectory clustering analyses [28], and computation and rendering of molecular orbitals [29, 5, 30, 31, 32] and molecular surfaces [33, 34, 14, 35, 36], The latest versions of VMD also incorporate a GPU-accelerated batch and interactive versions of the Tachyon ray tracing engine [35, 36, 37, 38, 7] based on NVIDIA OptiX and CUDA [39].

2.3 Parallel Computing on Clusters and Supercomputers

VMD supports large scale batch mode parallel analysis and visualization on clusters and supercomputers when it has been compiled with MPI support [14, 35, 26, 40, 41, 36, 37, 38, 42]. When running VMD on clusters and parallel computers it is possible to run one MPI rank per CPU core, or more likely, one MPI rank for several CPU cores, or one MPI rank for an entire compute node. If running more than one VMD instance per compute node, it is typically necessary to set environment variables to limit which CPU cores and/or GPUs each VMD instance attempts to use to prevent performance anomalies from arising due to resource contention [20].

Chapter 3

Tutorials

3.1 Rapid Introduction to VMD

For those of you who don't like reading manuals, here is a quick introduction to VMD. The molecules and data files used in this tutorial can be downloaded from the VMD home page from the documentation area associated with this version and is clearly labeled as User's Guide tutorial data. The rest of this tutorial assumes that you have downloaded and unpacked this data set.

To start VMD type `vmd` on the command line of your shell (Unix), or start it by clicking the VMD icon in your desktop or Start menu (Apple MacOS X and Microsoft Windows). VMD should start up with a window titled vmd console, a display window entitled VMD OpenGL Display, and a main menu entitled VMD. Text commands are typed in the console window, molecules are displayed and manipulated in the graphics window, and other interfaces and extensions are available from the menu interface. All of the windows can be closed or minimized, using your computer's standard windowing controls or the `menu` command [§9.3.19] in text console. Most functions can be performed with both the menu interface and the text console, though some of the more sophisticated scripting features are only available as text commands.

3.2 Viewing a molecule: Myoglobin

In our quick tour of VMD, we'll start out by demonstrating a few of its visualization features. To load a new molecule, select New Molecule... from the File menu in the Main window, this will open the Files window [§5.4.4]. We will load a PDB (Protein Data Bank) file containing the coordinates of the atoms in myoglobin (compliments of Joel Berendzen of Los Alamos National Laboratory). Select the Browse... button in the files window to bring up a file browser. Go into the `proteins/` directory of the tutorial data set that you have downloaded from the VMD web site. Once there, select the file `mbco.pdb` in the file browser, and press the Load button in the molecule file browser. button in the Files window. Figure 3.1 shows an example of VMD displaying this protein.

You can use the mouse to manipulate the structure in the display window. There are three basic mouse modes [§5.1.1]: rotation, translation, and scaling. The mode can be changed from the Mouse menu in the main window, or by pressing `r`, `t`, or `s` on the keyboard while the mouse is in the graphics window. While experimenting, note how the cursor changes to indicate the mouse mode. In rotation mode, the left mouse button controls rotation about axes parallel to the screen, and the middle button controls rotation about the axis perpendicular to the screen. In translation mode, the left mouse button controls translation parallel to the screen, while the middle button

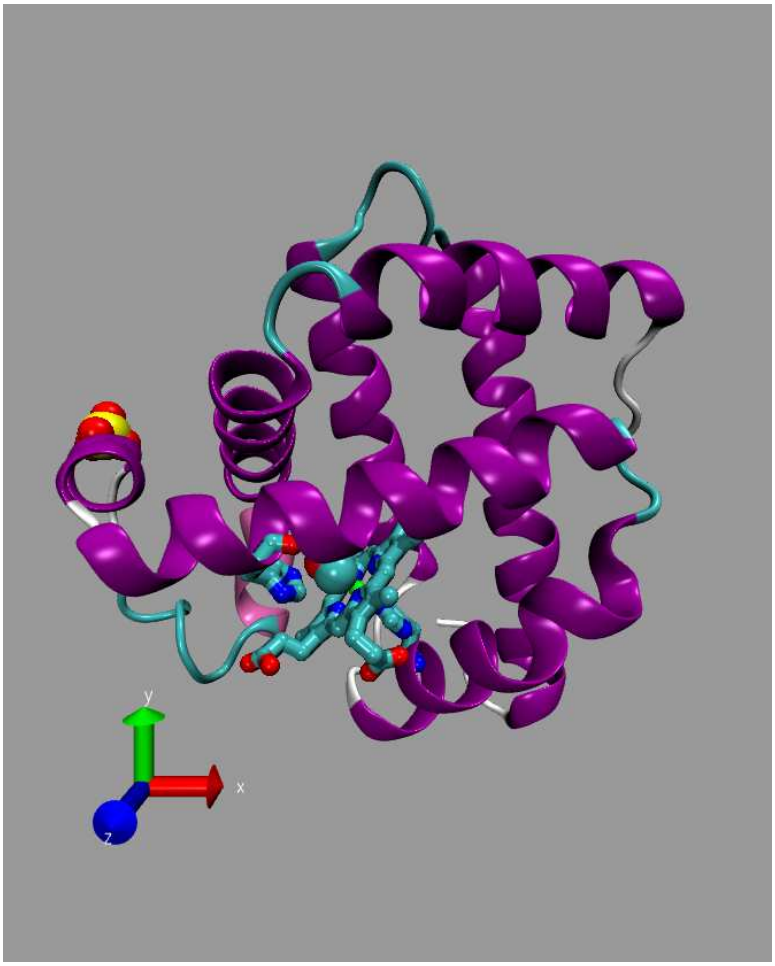


Figure 3.1: Sample VMD session displaying myoglobin.

controls translation in and out of the screen. Finally, in scaling mode, both the left and middle buttons control global scaling when the mouse is moved left or right, but the middle button causes larger changes.

By default molecules are displayed in a "lines" representation, colored by atom type. Suppose you would like to view the myoglobin structure with its protein backbone represented as a tube, the heme represented as licorice, the SO_4 ion and CO molecule represented as van der Waals spheres, and histidines 64 and 93 represented as CPK models. First, open the Graphics window [§5.4.7] by selecting the Representations item in the the graphics menu of the VMD Main window. Type `backbone` in the Selected Atoms text entry area and press 'enter' to select the myoglobin backbone. All of the protein except for the backbone will disappear. Choose NewCartoon in the drawing method chooser to display the backbone as a tube, and choose Structure in the coloring method chooser to color the tube with the predefined secondary structure color. Press the Create Rep button. This creates a new representation in the browser, identical to the original one. The new representation can be changed without affecting others, so clear the atom selection text area and enter `resname HEM` to select the heme. At this point the heme isn't visible because it cannot be drawn as a cartoon, so choose the 'Licorice' drawing method to make it appear. Click on

Create New again to make a new view, and enter `resname SO4 CO` to select the SO_4 ion and the CO molecule, and choose the drawing method 'VDW' to render them as Van der Waal spheres. Once again, press the Create Rep button and enter `resid 93 64` to select the two histidines, and render them as 'CPK'. If you followed all that, then congratulations, you have made a nice image of myoglobin! With further experimentation you should be well on your way to learning how to use VMD.

3.3 Rendering an Image

Find an interesting view of the molecule from the previous tutorial. Suppose you want to publish this view in a journal and want a high quality image, or you want to make a large poster. Taking the image from a screen capture often results in a rather grainy image as the size of the pixels becomes apparent, so you want something with more resolution. There are several programs available which can render a high-quality raster image, based on an input script. VMD has the option to create input scripts for many of these image processing programs, which may then be processed to create a higher quality image of the scene displayed by VMD at the time the script was created. See Chapter 8 on rendering for a further description of how this works.

Open the Render window [§ 5.4.11] and select 'Tachyon' from the Render Using menu. Both of the text boxes will be filled with default values which should not need to be changed for the purposes of this tutorial. Press the Start Rendering button. After a few moments of processing, you sould see the message

```
Info) Rendering complete.
```

in the VMD text console. If everything worked correctly, you will end up with an image file named plot.dat.tga (on MacOS X or Unix) or plot.dat.bmp (on Windows) in your current working directory. This image is in either Windows BMP or Targa graphics format, and can be read by many programs (such as `display`, `ipaste`, `xv`, Gimp or Photoshop).

3.4 A Quick Animation

Another strength of VMD lies in its ability to playback trajectories resulting from molecular dynamics simulations. A sample trajectory, `alanin.dcd` is provided in the `proteins` directory included with VMD. To load it, open the molecule file browser as described previously. Next click on the Browse button and select the `alanin.psf` file in the file browser. Once selected, press the Load button to load the structure file. Next, select the `alanin.dcd` file and load it as well. This will read the DCD trajectory frames into the same molecule with the previously loaded `alanin.psf` file.

In the display window you should see a simulation of an alanin residue in vacuo. It isn't particularly informative, but you can easily see that the structure is quite unstable in an isolated environment. After the DCD file has loaded, animation will stop. To see it again or to fine- tune playback, use the animation controls [§5.4.3] found at the bottom of the main VMD window. Press the button that looks like > to play the animation. Use the Speed slider at the bottom of the window to change the speed of playback. By rotating the molecule around, etc. you should get an idea about how the system destabilizes over the course of the simulation. The animation controls are generally similar to what you'd find on a DVD or CD player.

3.5 An Introduction to Atom Selection

In this section it is assumed that you have the myoglobin structure `mbco.pdb` loaded and the views discussed in section 3.2 created. If this is not true, go back and repeat the process described there.

VMD has a powerful atom selection method which is very helpful when generating attractive, informative, and complex graphics. In the previous section you used a few of these atom selection tools. This tutorial assumes that you have already loaded the myoglobin molecule, but it isn't necessary to recreate all the graphical representations.

To change which atoms are used to display each representation of the molecule shown in the display window, open the Graphics window [§ 5.4.7] and select the representation you want to change. You can then either edit the different fields (selection, coloring method, or drawing method) or use the Delete button to delete the view entirely. Try changing or deleting some of the views. When finished, delete all representations for the myoglobin structure. To get the basic line drawing view back, clear the atom selection text entry area, enter `all` and press the Create Rep button.

Atoms may be selected on the basis of a property, i.e. `protein` or `not protein`, `water`, or `nucleic backbone`. They may also be selected by atom name, such as `atom C`, by residue name, such as `resname HEM`, or by many other identifiers. Multiple atoms may be specified with one keyword. For example, the selection `name C CA N O` will select the backbone atoms. (A similar effect may be obtained with the command `protein backbone`.) VMD can handle regular expressions, so that `name "C.*"` will select all atoms with names starting with C. VMD also understands the boolean operators `and`, `or`, and `not`, so the selection `resname HEM and not name "N.*"` selects all non-nitrogen atoms in the heme group of myoglobin.

Several more abstract selection criteria are available. For instance, the selection `x > 5` finds all atoms with an x coordinate greater than 5, while `mass >12 and mass < 14` selects all atoms with mass greater than 12 and less than 14 atomic mass units. Many math functions [§ 6.7] are also provided, so the selection `sqrt( sqr(x) + sqr(y) + sqr(z) ) < 10` will select atoms in a spherical region of radius 10 Å centered about the origin of the coordinate space. You can pick atoms nearby a selection with the phrase "within <distance> of <selection>" and all residues with the same property as a given selection as "same <property> as <selection>".

See section 6.3 for a full description of the selection command.

3.6 Comparing Two Structures

Let's start from scratch by deleting everything: use the text console and tye the command `mol delete all` and press enter. This deletes all loaded molecules and is often more convenient then selecting them and deleting them all one by one. Alternatively, you could highlight each molecule in the molecule browser, and use the Delete Molecule item in the Molecule menu to remove them one by one.

Begin by loading the `mbco.pdb` structure with the Files window. Turn on just the heme, CO, and histidines by using the selection commands `resname HEM CO or resid 64 93`. The dot (probably green) in the middle is the iron and you can verify that by picking it with the mouse. Do this by changing the "Object Mode" pull-down to "Pick", and selecting "Atoms" for the pick mode in the Mouse menu. The label `HEM154:FE` should appear both on the display and in the text console.

Change the pick mode in the Mouse menu to "Bonds". To get the distance between the iron and the oxygen of the CO, click with the left mouse button first on the iron and then on the oxygen. The first click turned the FE label on and the second turned the O label on and drew

a line between the two atoms with the distance drawn in the middle and a bit to the right. The distance between the two atoms is 2.94 Å, as compared to 2.93 Å in the paper; not bad. However, picking the distance between the FE and the C of the CO reveals a distance of 1.91 Å as compared to 1.85 Å in the paper. The difference is that the structures in the VMD distribution are actually preliminary structures obtained before the final coordinates were determined.

In order to experiment with more complex picking modes, consider the angle made by the O of the CO with the FE of the heme and the NE2 of residue 93 (you can click on the atoms to find which ones are which). Using the Mouse menu, change the pick mode to "Angles". This should cause the cursor to become a red crosshair. Click on each of the three atoms using the left mouse button. After the third pick, a shallow angle will appear indicating an 8.71 degree angle between the three atoms.

Now load the intermediate `star.pdb` file which can also be found in the `proteins` directory of your distribution. Again use the Files window to do this. Both of the molecules will be loaded side by side. Go to the Graphics window and change the selection so it the same as the first, i.e. `resname HEM CO or resid 64 93`. The two molecules are almost atop each other, making it hard to distinguish the two, so change the colors to simplify things.

First, in the Graphics window, change the Coloring method to 'Molecule'. Use the Selected Molecule chooser to change the `mbco.pdb` Coloring method to 'Molecule' as well. Open the Color window [§5.4.9] and scroll the Category browser down until the line 'Molecule' is visible. Click on it then click on the line which says `mbco.pdb`. (There may be two `mbco` lines if the file had been loaded before in this session.) Scroll the Colors browser up to click on 'blue'. This should change one of the molecules in the display to blue.

Next, click on the last line in the Names chooser, which says `star.pdb`. This time, choose 'red' from the Colors chooser. The display should be much easier to understand. The myoglobin with the bound CO is in blue and the intermediate state is in red. At this point it is easy to measure the change in position between the two different states by using the middle mouse button to pick the same atom in the two conformations.

Once that is done, it is easy to point out one interesting aspect of the way VMD handles the graphics. Go to the main window, select one of the two molecules, and press Toggle Fixed. Enter translation mode and move the other molecule around. Notice that the number which lists the distance between the two atoms never changes. That's because the mouse only affects the way the coordinates are translated to the screen image. It does not affect the real coordinates at all. It is possible to change the coordinates in a molecule using the text command interface, or by using the atom move pick modes [§5.1.2]).

By the way, unfix the molecules and do a 'Reset View' from the Display menu to reset everything. Load up the third structure, `deoxy.pdb` and give it the same selection as the other two molecules. However, color this one green. Pull out Nature v. 371, Oct. 27, 1994 and turn to page 740. With a bit of manipulation you should be able to recreate the image that appears there.

3.7 Some Nice Represenations

The following views are quite nice for displaying proteins and nucleic acids:

```
selection: all
drawing method: tube
coloring method: segname (or chain)
why?  This show the backbone of the protein and nucleic acid strands
```

```
selection: protein and (name CA or not backbone)
drawing method: lines
coloring method: segname (or chain)
why? shows where the side chains are located, but they are thin so the
  backbone is still visible and the scene is quickly drawn

selection: (numbonds = 0) and not waters
drawing method: vdw
coloring method: name
why? shows ions.  The "not waters" omits cases where a water's oxygen is
  known but not the hydrogen.

selection: not (waters or protein or nucleic)
drawing method: lines
coloring method: name
why? shows whatever is left; usually ligands and crystallizing agents
```

3.8 Saving your work

After creating a set of attractive and informative representations of your molecule, you may want to save your work so that you can regenerate the scene later. There are two ways to do this in VMD:

- In the main menu, press the Save State button found in the File menu; this will bring up a browser window where you can enter a file name in which to save your work.
- In the text console, type `save_state` *filename*, where *filename* is the name of the file in which to save your work.

To restore your scene, you also have three choices:

- Use the Load State item in the File manu to select and load a previously saved VMD session.
- From the command line, start VMD with the options `vmd -e` *filename*, where *filename* was the name of the file you saved before.
- After starting VMD, from the text console, type `play` *filename*.

The most common source of problems is when VMD can't find the files you used to load the molecule. If this happens, try changing to the directory you were in when you first loaded the molecule, or edit the state file and use the full path names where you see `mol new`, `mol addfile`, or `mol load` commands.

3.9 Tracking Script Command Versions of the GUI Actions

For most actions performed from the VMDGUI, there is an equivalent script command. VMDcan print these commands to a log file or the console. This is a convenient way to automate file

processing by first doing all steps interactively while logging to a file and then editing the logfile to turn it into a Tcl script operating on multiple files. There are two ways to do this in VMD:

- In the main menu, press the Log TCL Commands to File button found in the File menu; this will bring up a browser window where you can enter a file name in which you can save the resulting script code.
- In the text console, type `logfile` *filename*, where *filename* is the name of the log file.

The resulting file will contain Tcl script code that can be executed from the VMDcommand prompt. The Log TCL Commands to Console button or the command `logfile console` will print the Tcl commands to the console window instead. This is most useful, if you just want to find out, which VMDcommand is used to perform a specific action.

Finally, the `logfile off` command or clicking on the Turn Off Logging button will stop the log and close the log file, if needed.

Chapter 4

Loading A Molecule

The File menu is the primary means for loading molecules and other data into VMD. The built-in file readers will load molecular structures from combinations of topology files, coordinate files, and trajectory files. Readers are also included for data such as potential maps, electron density maps, Grasp surface data, and arbitrary 3-D geometric data from Raster3D scene files. VMD can load structures directly from Protein Data Bank over the internet, provided that a network connection is present. Entering the four-character PDB accession code in the molecule file broswer form will retrieve and load the structure over the network.

4.1 Notes on common molecular file formats

VMD natively understands several popular molecular data file formats: PDB coordinate files, CHARMM, NAMD, and X-PLOR style PSF topology files, CHARMM, NAMD, and X-PLOR style DCD trajectory files, NAMD binary restart (coordinate) files, AMBER structure (PARM) and trajectory (CRD) files including both the old format and the new formats used by AMBER 7.0, and Gromacs (e.g. GRO, G96, XTC, TRR) structure and trajectory files. These files may contain some redundant information and can be loaded in different combinations.

PDB files contains data about atoms, residues, segment names, occupancy and beta factor, and one coordinate set. PSF and PARM files contain atoms, residues, segment names, residue types, atomic mass and charge, and the bond connectivity. VMD supports four file formats used by Gromacs: GRO, G96, TRR and XTC. GRO and G96 files contain structure information including atoms, residue and segment data, and one coordinate set. CRD, DCD, TRR and XTC files contain only coordinate data (frames). It should be noted that while PDB, GRO and G96 files were designed to contain only one coordinate set, multiple files can be concatenated into one larger file to create a makeshift trajectory file which can be loaded by VMD.

When VMD loads a file it requires information about atom names and coordinates and tries to fill in the rest. Since the PDB file contains all this information, it does not need to be loaded with any other data files. However, the PDB file doesn't contain the atom types, masses, and charges, so these are guessed or assigned default values. In particular, charges will be assigned a value of 0.0 if the file does not contain explicit charge information.

A PSF file does not contain coordinate information so it must be loaded along with a PDB or DCD file. If a PDB and PSF are given there is no missing data and VMD makes no assumptions. If a PSF and DCD are given then only the chain identifier and occupancy and beta values are missing so they are given a default value. A PARM file is similar to a PSF in that it too contains

no coordinate information. It must be loaded along with a CRD trajectory file. If a PARM and CRD file are loaded together, then only the segname and chain ID for the atoms are left blank. A CRD or DCD file can be specified along with the PDB, in which case the PDB file will be read as normal, and then coordinate sets are read from the DCD or CRD until the end of the file is reached. Gromacs GRO and G96 files can be loaded on their own since they contain the necessary atom data and coordinates. They can also be loaded along with TRR and XTC files to obtain trajectory data. Additional coordinates from a PDB, CRD, or DCD file can be appended to the current coordinate set using the Molecule File Browser form.

4.2 What happens when a file is loaded?

When a coordinate file is loaded by itself (i.e. just a PDB, no PSF), VMD uses heuristics to replace missing values that would normally be provided by a structure file. If necessary, VMD does a distance-based bond search to determine connectivity. A bond is formed whenever two atoms are within $(R_1 + R_2) * 0.6$ of each other, where R_1 and R_2 are the respective radii of candidate atoms. If both structure and coordinate files are loaded, no approximations or guesses are made.

After the molecule is read in, new names are added to the coloring categories [§6.2.3], and assigned colors. Next, bond connectivity is established and the molecule is analyzed to identify its components, i.e., to determine which residues are protein, nucleic acids, and waters, etc. A search is then made to connect these into larger fragments of the same type, and summary information is printed to the screen. An example output for BPTI is:

```
Info 1) Analyzing structure ...
Info 1)    Atoms: 898   Bonds: 909
Info 1)    Backbone bonds: Protein: 231  DNA: 0
Info 1)    Residues: 58
Info 1)    Waters: 0
Info 1)    Segments: 1
Info 1)    Fragments: 1   Protein: 1   Nucleic: 0
```

There are several types of fragments. Protein and nucleic fragments are homogeneous; either all proteins, or all nucleic acids. However, it is possible for a protein to be connected to a nucleic acid or some other non-protein. When this occurs, a warning message is printed, as in:

```
Warning 1) Unusual bond between residues 1 and 2
```

These warnings will occur with terminal amino acids, zinc fingers, myristolated residues, and poorly defined structures.

4.3 Babel interface

VMD can use the program Babel, if installed, to translate a wide variety of different molecular data files into the PDB format. Not all of these have been tested for use with VMD, so your results may vary. VMD only uses Babel to read files and does not allow the use of Babel to save files to other formats. The `VMDBABELBIN` environment variable [§14.2] is used to specify the absolute path to the the Babel executable (including the executable name). For more information about Babel, see `http://smog.com/chem/babel/`. VMD currently supports version 1.6 of Babel.

4.4 Raster3D file format

In addition to the molecular file formats, VMD can read the input file for Raster3D. (Raster3D converts an input file into a shaded raster image for use in making high quality pictures. It is often used with MolScript.) The ability to read Raster3D allows users to view MolScript files in 3D and incorporate special images into the display without having to edit the VMD code. The file format, which is part of the Raster3D documentation, describes a simple collection of triangles, spheres, and cylinders with either flat or spherical ends. Each shape is colored by an RGB triplet.

Certain newer Raster3D objects are ignored, such as quadrics. Also, nearly all of the header information is ignored—most notably, the viewing matrix. Raster3D uses many cylinders with spherical (rounded) ends. VMD deliberately omits these rounded ends since the resultant image would be very slow to render interactively. VMD uses a fixed size palette of colors, each triplet is converted into its "nearest" indexed color. This may cause images to be colored slightly differently than expected.

Chapter 5

User Interface Components

VMD provides several methods for the user to control and interact with the molecular display. The primary methods are by using the mouse, either in the graphics window or in the different graphical user interface (GUI) *forms* provided by the program. In addition to the mouse, VMD also supports a number of more advanced input devices such as the Spaceball, Magellan, and Phantom, which provide the ability to manipulate molecules with six degrees of freedom. Some devices such as the Phantom can also provide haptic (sense of touch) force feedback. VMD also provides a text console interface for executing built-in commands or running scripts. This chapter describes how to use the mouse-based user interfaces, and some of the advanced input devices supported in VMD. The the text and scripting interface is described fully in chapter 9.

5.1 Using the Mouse in the Graphics Window

The graphics window is labeled VMD OpenGL Display and contains a view of the molecules and other objects which make up the scene. When the mouse is in the graphics display window, it may be used to perform the following actions such as:

- Rotate, translate, or scale the displayed molecules
- Select, or 'pick' atoms or other objects in order to move them, or label them
- Translate and rotate a set of atoms
- Apply a force (acceleration) to a set of atoms
- Move the lights

User-defined keyboard accelerators, or *hot keys*, are also available when the mouse is in the graphics display window. These keys are bound to VMD text commands, which are executed when the key is pressed. VMD has many built-in default hot key commands (see Tables 5.1, 5.2, 5.3 and 5.4). Users can add new hot keys, overriding default settings if desired.

5.1.1 Mouse Modes

The mouse is in one of several *modes* at any time; the current mouse mode determines the effect of pressing and releasing mouse buttons or the mouse wheel while the mouse is in the graphics window.

Each mouse mode, except the lights mode (see below), sets the mouse cursor to a characteristic shape. The mouse mode is selected via the Mouse menu.

The available mouse modes are as follows:

- **Rotate Mode** (hot key 'r')
  When the mouse is in rotate mode, holding the left mouse button down and moving the mouse rotates the molecules about axes parallel to the screen, in a 'virtual trackball' behavior. To get a rotation around the axes coming out of the screen (the 'z' axis), hold the middle button down and move the mouse left or right.

  You can leave molecules rotating without continuously moving the mouse. Start the molecule moving with the mouse, as above, then release the mouse button before you stop moving the mouse. With some practice it becomes easy to impart a slight spin on the molecule, or whirl it about madly. To stop the rotation, either press and hold the left mouse button down until the molecule stops moving, or select 'Stop Rotation' in the Mouse menu. Also, pressing the rotation hot key `r` or any of the other mouse mode hot keys causes rotation to stop.

- **Translate Mode** (hot key 't')
  When the mouse is in translate mode, holding the left button down allows you to move the molecules parallel to the screen plane (left, right, up, and down). To move the molecule towards or away from you, hold the middle button down and move the mouse right or left, respectively.

- **Scale Mode** (hot key 's')
  Pressing either the left or middle button down and moving to the right enlarges the molecules, and moving the mouse left shrinks them. The difference is that the middle button scales faster than the left button. Scaling can also be accomplished with the mouse wheel (irrespective of the current mode setting) on computers equipped with an appropriate mouse.

- **Move Light**
  VMD provides four directional lights to illuminate the molecular scene. The lights provide diffuse lighting and specular highlights and help the user perceive surface shape in rendered objects. You can use the mouse to rotate each of the light source directions to a new position. If the light isn't on, moving it will not affect the displayed image. To turn a light on or off, use the Lights item within the Mouse menu.

- **Add/Remove Bonds**
  When the mouse is in add/remove bonds mode, clicking on atoms in a molecule will add a bond between those atoms if one is not already present, or remove the bond between those atoms if there is already a bond. The two atoms must belong to the same molecule.

5.1.2 Pick Modes

Mouse picking can be used to turn on or off various types of labels, to query for information about an object, or to move items around on the screen. You can label an atom (and display the atom name), or you can label geometric values such as the distance between two atoms (a *bond* label), an angle between three atoms (an *angle* label), or the dihedral angle formed by four atoms (a *dihedral* label). This is done by setting the mouse into the proper picking mode and then selecting the relevant atoms with the mouse. Picking modes are selected from the Mouse menu.

The available pick mode actions are:

- **Center** (hot key 'c')
  This mode is used to change the point about which a molecule rotates when the molecule is rotated. To cause a molecule to rotate about a specific atom, select this mode and then click on that atom. The rotation point may be restored to its default position (the center of volume of the molecule) by executing the 'Reset View' option from the Mouse menu.

- **Query** (hot key '0')
  Clicking on an item will print out the name of the item (e.g. the atom name) to the text console window.

- **Label → Atom** (hot key '1')
  Clicking on an atom will toggle on/off a label for the atom.

- **Label → Bond** (hot key '2')
  Clicking on two atoms in a row will toggle on/off a bond distance label between the two atoms (a dotted line with the distance printed at the midpoint).

- **Label → Angle** (hot key '3')
  Clicking on three atoms in a row will toggle on/off a label showing the angle formed by the three atoms.

- **Label → Dihedral** (hot key '4')
  Clicking on four atoms in a row toggles on/off a label showing the dihedral angle formed by the four atoms.

- **Move → Atom** (hot key '5')
  In this mode, the position of an atom can be changed by clicking on the desired atom, and dragging with the mouse while the button is still pressed. This will change the atom coordinates.

- **Move → Residue** (hot key '6')
  This mode may be used to move all the atoms in a selected residue at the same time. Select an atom in a residue, and move it to a new position while keeping the mouse button pressed. All the atoms in the same residue as the selected one will be moved the same amount. Holding down the ¡shift¿ key and the left mouse button while moving the mouse will rotate the atoms in the residue about the selected atom. If the middle mouse button is held down instead, the atoms in the residue will rotate about a line drawn through the picked atom and parallel to a line coming directly out of the screen. This behavior is similar to the usual Rotate mode, except that coordinates of atoms are changed.

- **Move → Fragment** (hot key '7')
  A *fragment* is a set of atoms all connected by a series of covalent bonds. This mode acts just like MoveResidue, except that the atoms which are moved are all in the selected fragment rather than in the selected residue. This will change the atom coordinates. Holding down the ¡shift¿ key and the left mouse button while moving the mouse will rotate the atoms in the fragment about the selected atom. If the middle mouse button is held down instead, the atoms in the fragment will rotate about a line drawn through the picked atom and parallel to a line coming directly out of the screen. This behavior is similar to the usual Rotate mode, except that coordinates of atoms are changed.

- **Move → Molecule** (hot key '8')
  This mode may be used to move all the atoms in a selected molecule at the same time. Select an atom in a molecule, and move it to a new position while keeping the mouse button pressed. All the atoms in the same molecule as the selected one will be moved the same amount. Holding down the ¡shift¿ key and the left mouse button while moving the mouse will rotate the atoms in the molecule about the selected atom. If the middle mouse button is held down instead, the atoms in the molecule will rotate about a line drawn through the picked atom and parallel to a line coming directly out of the screen. This behavior is similar to the usual Rotate mode, except that coordinates of atoms are changed.

- **Move → Rep** (hot key '9')
  This mode may be used to move all the atoms in a selected representation at the same time. You select a representation by clicking on one of the reps in the browser window of the Graphics window. In order to move the atoms in this rep, the atom you pick with the mouse must be selected by that rep.

  When you have clicked on an atom in the rep, move the mouse to a new position while keeping the mouse button pressed. All the atoms selected by the highlighted rep will be moved the same amount. Holding down the ¡shift¿ key and the left mouse button while moving the mouse will rotate the atoms in the rep about the selected atom. If the middle mouse button is held down instead, the atoms in the rep will rotate about a line drawn through the picked atom and parallel to a line coming directly out of the screen. This behavior is similar to the usual Rotate mode, except that coordinates of atoms are changed.

5.1.3 Hot Keys

When the mouse is in the graphics window, many commands are accessible via programmable hot keys. Hot keys allow you to do things like change mouse modes or advance the animation by a frame by simply pressing a key. There are a number of predefined hot keys, as listed in tables 5.1, 5.2, 5.3, and 5.4. They can be printed out with the command `user print keys`. The commands listed are the text commands which are executed when the hot key is pressed; these text commands are explained in section 9.3.

To add or modify a hot key, use the command `user add key` *key command*. The *key* parameter must be a single character. If *command* contains more than one word, it must be enclosed in braces so that the subsequent command words are not ignored. When that key is pressed while the mouse cursor is in the graphics display window, the associated command will be executed. Once you have a set of commands which are particularly useful and familiar for you, you will want these hot key commands automatically available every time you run VMD. This can be done by placing the commands to add these items in your `.vmdrc` file, which is a file containing VMD text commands that is executed every time VMD starts up. The basic method for setting up this file is described in section 14.3.3. Once you have such a file, put the `user add` commands in it.

Hot Key	Command	Purpose
r, R	mouse mode 0 0	enter rotate mode; stop rotation
t, T	mouse mode 1 0	enter translate mode
s, S	mouse mode 2 0	enter scaling mode
0	mouse mode 4 0	query item
c	mouse mode 4 1	assign rotation center
1	mouse mode 4 2	pick atom
2	mouse mode 4 3	pick bond (2 atoms)
3	mouse mode 4 4	pick angle (3 atoms)
4	mouse mode 4 5	pick dihedral (4 atoms)
5	mouse mode 4 6	move atom
6	mouse mode 4 7	move residue
7	mouse mode 4 8	move fragment
8	mouse mode 4 9	move molecule
9	mouse mode 4 13	move highlighted rep
%	mouse mode 4 10	apply force on atom
^	mouse mode 4 11	apply force on residue
&	mouse mode 4 12	apply force on fragment

Table 5.1: Mouse control hot keys.

5.2 Using the Spaceball in the Graphics Window

VMD provides optional support for SpaceNavigator, Magellan, and Spaceball six-degree-of-freedom input devices. The Spaceball may be used to rotate, translate, and scale molecules, using up to 6 control axes simultaneously (3 axes in translation, 3 in rotation). The Spaceball can be used independently and simultaneously with the mouse. With the spaceball in one hand and the mouse in the other, a user can perform complex picking and identification operations more efficiently, since the mouse can be left in pick mode (for example) while the Spaceball is used to perform rotations, translations, and scaling operations with the other hand.

The Spaceball can be run in one of several modes within VMD. The Spaceball interface currently provides two methods of rotation and translation, and a scaling mode. The Spaceball interface currently uses *Button 1* (known as *Function 1* in the SpaceWare driver) to reset the view, and *Button 2* to cycle through the available Spaceball interface modes.

5.2.1 Spaceball Driver

VMD interfaces to the Spaceball in one of two ways; either by communicating directly with the Spaceball using built-in serial interface software, or vendor provided drivers. Unix and Mac OS X versions of VMD use the built-in serial Spaceball driver. At startup, VMD checks for the existence of an environment variable *VMDSPACEBALLPORT*. This environment variable must be set to the Unix device name of the serial port to which the Spaceball is attached. The serial port device permissions must be set to allow the VMD user to open the device for reading and writing. In typical usage, this usually requires performing a `chmod 666 /dev/somettyname` on the appropriate device as root. One restriction with the use of the built-in Spaceball driver is that only one VMD process may safely use the Spaceball at a time. If multiple VMD sessions are started on the same machine and all are set to open the Spaceball, it will behave very erratically.

Hot Key	Command	Purpose
x	`rock x by 1 -1`	spin about x axis
X	`rock x by 1 70`	rock about x axis
y	`rock y by 1 -1`	spin about y axis
Y	`rock y by 1 70`	rock about y axis
z	`rock z by 1 -1`	spin about z axis
Z	`rock z by 1 70`	rock about z axis
j, Cntl-n	`rotate x by 2`	rotate 2° about x
k, Cntl-p	`rotate x by -2`	rotate −2° about x
l, Cntl-f	`rotate y by 2`	rotate 2° about y
h, Cntl-b	`rotate y by -2`	rotate −2° about y
g	`rotate z by 2`	rotate 2° about z
G	`rotate z by -2`	rotate −2° about z
Cntl-a	`scale by 1.1`	enlarge 10 percent
Cntl-z	`scale by 0.9`	shrink 10 percent

Table 5.2: Rotation & scaling hot keys.

Hot Key	Command	Purpose
Alt-M	`menu main off;menu main on`	Show main menu
Alt-f	`menu files off;menu files on`	Show files menu
Alt-g	`menu graphics off;menu graphics on`	Show graphics menu
Alt-l	`menu labels off;menu labels on`	Show labels menu
Alt-r	`menu render off;menu render on`	Show render menu
Alt-d	`menu display off;menu display on`	Show display menu
Alt-c	`menu color off;menu color on`	Show color menu
Cntl-r	`display resetview`	Reset display
Alt-q	`quit confirm`	Quit VMD with confirmation
Alt-Q	`quit`	Quit VMD
Alt-h	`hyperref invert`	Invert hyper text mode (NOT help)

Table 5.3: Menu control hot keys.

The Linux and Windows version of VMD can use open source (e.g. spacenavd) or vendor-provided (SpaceWare) driver to communicate with SpaceNavigator, Magellan, or Spaceball devices via windowing system events. The window system drivers operate somewhat differently from the serial driver built into VMD. The window system driver software runs as a separate process from VMD and must be started and fully operational before VMD is run. At startup time VMD attempts to open the windowing system driver interface, displaying the success or failure of initialization as it occurs, with applicable diagnostic information. The windowing system driver provides detailed control over the sensitivity and configuration of the Spaceball, Magellan, or SpaceNavigator device. In order to use the Spaceball function keys with VMD the windowing system driver must be set to send button events as *Function 1* and *Function 2* at a minimum. Once set, it should be possible to cycle through the various VMD Spaceball operational modes as described below.

Hot Key	Command	Purpose
+,f,F	`animate next`	move to next frame
-,b,B	`animate prev`	move to previous frame
.,>	`animate forward`	play animation forward
,	`animate reverse`	play animation reverse
<	`animate reverse`	play animation reverse
/, ?	`animate pause`	stop animation

Table 5.4: Animation hot keys.

5.3 Using the Joystick in the Graphics Window

The Windows version of VMD provides support for the Windows joystick driver, and will enumerate all available joystick devices at startup time. The joystick interface employed in VMD is quite simple, allowing the use of three control axes to translate, rotate, and scale the molecule. The joystick interface assumes a device with at least two buttons. The first joystick button resets the view in the display window, and the second button cycles through each of the available joystick modes. When VMD first attaches to each of the joysticks, they are initially disabled so that miscalibrated joysticks do not adversely affect the VMD session. Each joystick is initially enabled by pressing its second button to switch modes. All joysticks are independently controlled such that multiple joysticks can control different control axes, and multiple users could interact with the program with separate controls.

5.4 Description of each VMD window

VMD uses several different GUI windows, each designed to control a specific aspect of the molecular display (e.g., to control the appearance of the graphics display window, or to change the colors of displayed objects). The following sections give a brief description of the windows available in VMD; the remaining chapters in this manual describe the actions which these windows make available in greater detail.

5.4.1 Main Window

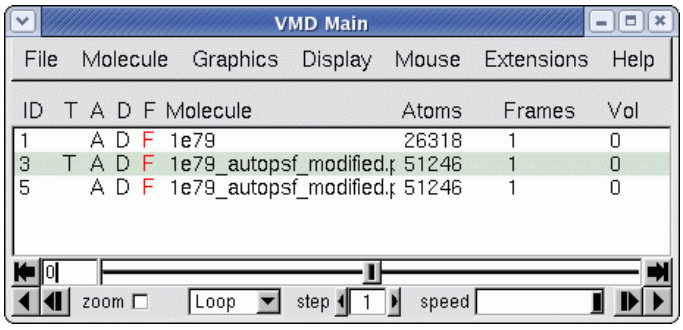


Figure 5.1: The Main window

The Main window is the main way to access other windows, load and save files, control trajectory playback, change various global program settings, access help, and to quit the program. Many of these actions can also be performed with the menu shortcut keys described in Table 5.3.

The Quit menu item exits VMD. This will bring up another window which verifies that you do indeed wish to exit. Press Yes to quit, or No to return to VMD.

Help

The Help menu items each start a web browser to display on-line VMD help documents. The browser is designated by the environment variable `VMDHTMLVIEWER` [§ 14.2]. Selecting a help item multiple times may start multiple browsers. The default web browser is Mozilla for Unix systems, and the built-in Explorer shell for Windows systems. The menu contains items for the VMD Quick Help page, as well as the current User's Guide, FAQ, and links to various helpful information and programs.

5.4.2 Main Window Molecule List browser

The Main window shows the global status of the loaded molecules. Any number of molecules may be displayed by VMD simultaneously. Each molecule can separately be hidden from view or fixed in place (e.g., prevented from being affected by mouse rotation commands). The window contains controls to change the status of the molecules individually or in groups.

The browser displays information about each molecule. A unique integer ID is assigned to each molecule by VMD when it is loaded. The Molecule is the file name which contained the topology information. Atoms shows the number of atoms in the molecule, and Frames gives the number of frames associated with the file.

Next to each molecule is a set of status flags, which indicate the current Status of each molecule. Each molecule has the following characteristics, which can be *on* or *off*:

- **Top (T)**
  Top indicates the default molecule used in the text commands when nothing is specified for the `mol` text command. It is also used in some forms (like Graphics and Animate) to determine certain values. There can be only one top molecule at a time.

- **Active (A)**
  Several commands and actions in VMD operate on many molecules. These commands, unless specifically specified otherwise, will do their action for all the *active* molecules. The primary use for this control is to prevent some molecules from being animated. Inactive molecules will not animate when the play button is pressed.

- **Drawn (D)**
  If a molecule is *Drawn* then it is being displayed in the graphics display window. This is useful for temporarily hiding a molecule from view without deleting it.

- **Fixed (F)**
  Fixed molecules do not undergo rotation, translation, or scaling. Note that while it may seem that one molecule has been moved relative to another, the difference is only apparent. The internal coordinates do not change when a standard rotation is applied by using, for example, the mouse. It is possible, however, to change the coordinates of atoms in a molecule, using the text command interface, and by using the atom move picking modes.

Changing the Molecule's Status

The status of a given molecule can be changed by selecting the molecule in the browser and double-clicking the appropriate flag. Only one molecule can be top at any one time, so the previous top molecule will change status when another is toggled.

Saving Trajectory Frames

Using the Save Coordinates... menu item, you can write trajectory frames to a file in one of several file formats including PDB, DCD, Amber CRD, etc. This feature may be used to write out a new trajectory in a single file after assembling many frames from different sources (such as PDB CRD, DCD or Gromacs files, or even from a remote simulation). You can also use this, in combination with the molecule file browser as a way to make PDB files from a DCD/CRD trajectory.

You can either save the entire stored trajectory, or a slice of the data by using the Amount chooser [§ 5.4.4]. Then select the appropriate output file type in the File Type chooser, and press the Save button in the bottom right corner. This brings up the file browser, which you can use to enter the new filename. Once you press the Save button in the browser, the file will be written without further confirmation. See the section on the `atomselect writexxx` [§ 9.3.2] command for information on how to write atom coordinates for an atom selection in a PDB file.

Deleting Trajectory Frames

You can delete frames from memory through a dialog box. To bring it up, start by selecting a molecule and choosing the Delete Frames... from the Molecule menu, or by double-clicking on the

Frames column for that molecule in the Molecule Browser. On this is done, choose the range of frames you wish to delete with the First and Last controls, and then press the Delete button. There is no confirmation of deletions.

The Stride control allows you to keep some frames in the range using the specified interval. For example, if your range contains 10 frames labeled 0 through 9, and you use a stride of 4, the frames numbered 0, 4 and 8 will be kept. A stride of 0 (zero) implies that all frames will be deleted.

Deleting a Molecule

The Delete Molecule menu item deletes all the selected molecules. There is no prompt verifying the deletion, so take some care. If a deleted molecule was the top molecule, a new top molecule will be set from the remaining structures.

GUI Shortcuts

There are a few useful mouse-based shortcuts that can be used in the Molecule List browser. Here is a list:

- Double-clicking on a molecule's name brings up the Rename Molecule dialog box.
- Double-clicking on a molecule's number of frames brings up the Delete Frames dialog box.
- Triple-clicking on the T (top) in front of a molecule focusses on that molecule by making it the only molecule to be displayed (D) and active (A). Furthermore, the view is reset and the molecule gets selected in the Representations window.

5.4.3 Main Window Animation Controls

Figure 5.2: The Main window animation controls

Each molecule in VMD can contain multiple sets of atomic coordinates, which may be animated to show its motion over time. The coordinate sets can come from a molecular dynamics simulation, or simply multiple versions of the same molecular structure. The Main window contains controls for animated playback of these trajectories. The controls contains several buttons which act like the buttons on a VCR or DVD player. The buttons provide a way to play the trajectory, step forward, stop, go to a specific frame, and go to the beginning or end. The status and frame counters shown in the animation control reflects the state of the *top* molecule. Commands entered via this control, however, affect all active molecules [§5.4.2], not just the top molecule, allowing concurrent animation of multiple molecules.

Animation Speed

The rate of playback can be controlled in two ways. The Step control changes the animation step size. By default, the frame step is 1, so each step of the playback increases (or decreases) the

animation frame number by one. If the frame step is 5 then the animation proceeds five times faster because only a fifth of the frames are shown. The Speed slider at the bottom of the window also affects the playback speed. Internally, this controls how many screen updates are needed between each step. By default, the slider is at the far right indicating that one step is performed for each screen redraw. Moving the slider to the left increases the minimum time required between updates.

Jumping to Specific Frames

The start and end buttons are used to simplify the comparison between the initial and final structures. The start button resets the current animation to the first frame, and end jumps to the last frame. If you need to jump to a specific frame, enter the frame number in the frame counter text area next to the start button and press enter. One thing to bear in mind is that the frame number starts at 0, so to jump to the 5th frame, you must actually enter 4 here. The animation controls are all relative to the top molecule [§5.4.2].

Looping Styles

When the animation is playing forward and reaches the end of the data available for the top molecule, one of three possible actions takes place, as specified in the style chooser. The default is 'Loop', which will reset the active molecules to the first frame and continue playing forward. 'Once' will stop the animation when it reaches the last frame, and 'Rock' reverses the direction of animation. The actions are symmetrical when the animation is playing in reverse.

5.4.4 Molecule File Browser Window

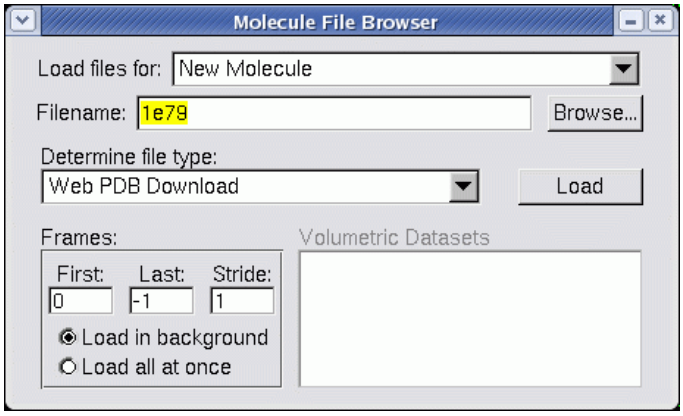


Figure 5.3: The Molecule File Browser window

The Files window is used to load a file from disk into a new or existing VMD molecule. It can be brought up by choosing New Molecule... from the File menu, or by hilighting a molecule in the Main window5.4.1 and choosing the Load Data Into Molecule... menu item. Once the window appears, select the file you want by using the file browser or by typing the filename into the text entry area. By default VMD will try to guess the type of file you are loading by matching the filename extension with one of the file reader plugins in the file type list (the available file types are

described in Chapter 4). If VMD is unable to guess the appropriate file type or guesses incorrectly, you must select it from the list manually.

You can control into which VMD molecule you want to load your data by selecting it from the Load files for: popup menu at the top of the window. If the file being loaded is intended for a new molecule, select New Molecule instead. If the file being loaded contains additional coordinate frames, electron density map, or other ancillary data for an existing molecule, choose the appropriate molecule from the selection list at the top of the window. If the file being loaded contains trajectory frames , you have the option of loading a subset of the trajectory skipping ranges or strides of frames rather than the whole thing. You can also select for VMD to load all frames before continuing on, or to load them in the background so that you may continue to interact with the menus and windows while it loads additional frames . If the file being loaded contains multiple volumetric data, you may select which data sets you would like to load.

Once you have selected the file to be loaded, the appropriate file type, and the way it will be loaded, press the Load button and VMD will being loading the selected file. Any informational messages, errors or warnings which occur while loading the file will appear in the text window.

Reading Trajectory Frames

VMD can read in new coordinate sets from one of several file formats such as PDB, CRD, DCD, or Gromacs files. The new coordinate sets are appended to the end of the stored frames for the selected molecule. Loading coordinate data is like loading any other file, select it with the file browser make sure the file type is set correctly for the file being loaded, and then press the Load button.

By default, VMD will load all of the frames contained in a coordinate or trajectory file.

Sometimes you may not want to read in a whole coordinate or trajectory file. For example, you may only want the last frame, or every tenth frame. You can do this by changing the options in the Frames control of Files window. The Frames controls consist of three numeric input fields labeled First, Last, and Stride. These make it possible to use a subset of the frames, starting at frame First and selecting every Stride frames until the Last is reached. For instance, to select every fifth frame between frames 14 and 98, set:

- First to 14
- Last to 98
- Stride to 5

(Remember that frame numbers in VMD start at 0, so frame 0 is the first frame.) The value '-1' is a special number; setting First to -1 is the same as starting at the first frame, Last = -1 is the same as ending at the last frame, and Stride = -1 is the same as taking one step.

5.4.5 Mouse Menu

The Mouse menu indicates and controls the behavior of the mouse when the mouse moves and clicks within the graphics window. Mouse clicks and drags can affect VMD in one of two ways. It can change the *view* of the scene, either by rotating, translating, or scaling. It can also *pick* objects in the scene, causing some further action to be taken. These behaviors are all reflected in the state of the Mouse menu.

Below, we describe the main parts of the Mouse menu.

Mouse modes

The top three menu items select whether the mouse will rotate, translate, or scale the scene when the user clicks and drags with the left mouse button.

Pick modes

These modes, located right below the mouse modes in the Mouse menu, control how the mouse affects objects in the scene (as opposed to how the mouse changes the *view* of these objects). Note that any time you choose a new pick mode, the current mouse mode changes to "Rotate".

- **Center** changes how VMD rotates and scales the scene. To get a feel for how this works, select "Center" from the Mouse menu, then click on an atom in the scene. If you now rotate the scene by clicking and dragging with the left mouse button, the scene should rotate about the picked atom. If you change the view mode to "Scale" using the "View Mode" pulldown menu, the scene will expand while keeping the picked atom in view. The picked atom will remain the center atom until a new atom is selected as "Center", the "Reset View" button is pressed, or a new molecule is loaded.
- **Query** prints information about the item (e.g. the atom name) on the text console window.
- **Label** adds labels to atoms in the scene. Labels include atoms, bonds, angles, and dihedrals. These labels require, respectively, one, two, three, and four atoms to be picked. For the latter three label types, the numerical value of the geometric label is displayed, along with a stippled line connecting the picked atoms. The units for "Bonds" corresponds to whatever units the coordinate file is written in. "Angles" and "Dihedrals" are measure in degrees.

  Labels can then be manipulated through the Labels window.
- **Move** changes the actual coordinates of atoms in the scene. Note that this is different from simply changing the view. Clicking on one of the buttons in the Mode Mode menu selects what group of atoms to move. "Atom" moves only the selected atom. "Residue" moves all atoms in the same residue (e.g., amino acid or nucleotide) as the selected atom. "Fragment" moves all atoms connected by a bond to the picked atom. "Molecule" moves every atom in the molecular structure. "Highlighted Rep" is the most flexible; it moves all atoms in the highlighted representation in the browser window of the Graphics window.

  Atoms are moved by clicking and dragging with the left mouse button. If the shift key is held while the mouse is moved, the affected atoms are *rotated* about the selected atom. Rotating atoms with the left button rotates about the x or y axis of the screen; rotating with the middle or right button rotates about an axis perpendicular to the screen.

  Note that there is currently no way to undo Move operations, so the atom coordinates should first be saved to a file.
- **Force** applies a force to selected atoms in a running simualtion. These forces will be visible only if an IMD connection has been established. Clicking and dragging with the left mouse button will apply a force to the selected Atom, Residue, or Fragment, as in Move Mode. Clicking with the middle or right button will cancel the force on the selected atoms.
- **Move Light** allows the lights to be positioned around the scene. Individual lights are turned on or off in the Display window. Selecting one of the lights in the Move Light menu rotates

the selected light about the origin. The Move Light Mode can also be cancelled by changing into any other pick mode or mouse mode.

- **Add/Remove Bonds** adds a bond between two clicked atoms if there is not one present, and removes the bond otherwise. Both atoms must belong to the same molecule.

5.4.6 Display Menu and Display Settings Window

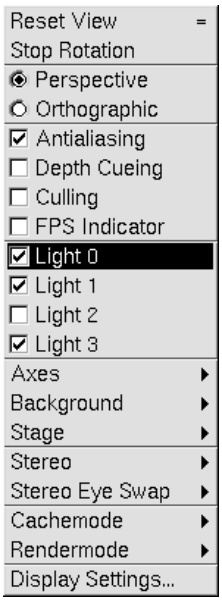


Figure 5.4: The Display menu

The Display menu controls many of the characteristics of the graphics display window. The characteristics which may be modified include:

- **Reset View** – This menu item can be used to force VMD to reset the scene back to the default viewing orientation and scale as is done when a molecule is first loaded.

- **Stop Rotation** – This menu item stops autorotation of the scene. The scene can be autorotated by quickly dragging the mouse while briefly depressing and releaseing the mouse button, leaving the scene spinning until it is stopped either by this menu item or by further mouse interactions.

- **Perspective** – The view of the scene can be Perspective or Orthographic. In the perspective view (the default), objects which are far away are smaller than those near by. In the orthographic view, both objects appear at the same scale. Note that several of the supported external rendering programs do not support orthographic rendering. As such, it may be necessary to "fake it" by translating the scene far away from the camera, and apply a zoom factor. This has the effect of significantly reducing the perspective, while not truly an orthographic view.

- **Antialiasing** – Turns antialiasing on or off. Antialiasing helps smooth out the jagged appearance of displayed geometry resulting from the inherently discrete pixels on the display device. The antialiasing feature is only available on platforms which support full-screen antialiasing, sometimes known as "multisample antialiasing". On platforms lacking the multisample capability, there may be alternate ways to perform full-screen antialiasing by selecting an option in the display driver setup. Windows machines most commonly place these controls in the display driver configuration panel.

- **Depth Cueing** – Turns depth cueing on or off. Depth cueing causes distant objects to blend into the background color, in order to aid in 3-D depth perception. The depth cueing settings controlled in the Display Settings window. The **Cue Mode** parameter controls which type of fog equation is used. The **Linear** depth cueing mode provides a simple depth gradient with a defined starting point and endpoint. The **Exp** and **Exp2** depth cueing modes take a density parameter, and generally blend into the background color much more sharply than the linear depth cueing mode. Scaling up the molecule will increase the amount of depth cueing effect that is visible, since it will occupy a larger depth range. Scaling the molecule size down decreases the depth cueing effect. Translating the molecule into and out of the screen will cause it to blend into and out of the background color.

- **Culling** – Turns backface culling on or off. This feature is primarily used to accelerate rendering performance on software based implementations of OpenGL, such as Mesa. Backface culling actually reduces performance on some hardware renderers, so you'll have to use your own best judgement on whether or not it is helpful to use on your specific computer system.

- **FPS** – This option enables or disables on-the-fly display of the achieved VMD rendering frame rate. The frame rate is displayed in the upper right hand corner of the graphics window when it is enabled.

- **Lights** – The graphics display window can use up to four separate light sources to add a realistic effect to displayed graphical objects. The Lights On browser turns these light sources on or off. If the number is highlighted, the light is on, and clicking on it turns the light off. See section 5.1.1 for more discussion regarding lights.

- **Axes** – A set of XYZ axes may be displayed at any one of five places on the screen (each of the corners or the center) or turned off. This is controlled by the Axes chooser.

- **Background** – The display background can either be set to a uniform color over the entire scene, or a vertical gradient can be set with a linearly changing color from the top of the viewport to the bottom.

- **Stage** – The Stage browser controls the stage, which is a checkerboard plane that can be located in any one of six places or turned off.

- **Stereo, Eye Sep, and Focal Length** – These controls are found in the Display Settings window. These controls set the stereo mode and parameters; stereo is discussed fully in chapter 7. The Stereo chooser changes the stereo mode, while the Eye Sep and Focal Length controls change the eye separation distance and the focal length, respectively. The Stereo Eye Swap control optionally reverses the left/right eyes when displaying on projectors or other devices that for one reason or another don't preserve the correct left/right eye assignments.

- **Cachemode** – The Cachemode toggle controls whether or not VMD uses a display list caching mechanism to accelerate rendering of static geometry. This feature can be extremely beneficial for achieving good interactive display performance on tiled display walls, and for remote display over a network. Caching cannot be performed while animating trajectories, so the performance benefit is only possible interactive rotation and zooming of static molecular structures.

- **Rendermode** – The Rendermode chooser controls which low-level rendering method VMD uses. The **Normal** rendering mode is the default VMD rendering algorithm based on standard fixed-function OpenGL. The **GLSL** rendering mode uses OpenGL Programmable Shading Language to implement real-time ray tracing of spheres, alpha-blended transparency, and high-quality per-pixel lighting for all geometry. On machines with high performance graphics boards supporting programmable shading, the **GLSL** rendering mode provides quality on par with many of the external software renderers supported by VMD but at interactive display rates.

- **Clipping Planes (Near Clip and Far Clip)** – These controls are found in the Display Settings window. Only those parts of the scene between the near and far clipping planes are drawn. The display clipping planes also set the depth cueing start and endpoints. Objects at the near clipping plane are distinct and crisp, objects at the far clipping plane will be blended into the background. Clipping planes positions are changed with the Near Clip and Far Clip controls. It is not possible for the near clip to be farther away than the far clip. When using stereo, it may be useful to set the near clip plane much lower than the default value. This makes the geometry "pop out of the screen" a bit more, and can be used for greater dramatic effect.

- **Screen Height (Hgt) and Distance (Dist)** – These controls are found in the Display Settings window. The screen height, along with the screen distance, defines the geometry and position of the display screen relative to the viewer. The screen height is the vertical size of the display screen, in 'world' coordinates. Each molecule is initially scaled and translated to fit within a 2 x 2 x 2 box centered at the origin; so the screen height helps determine how large the molecule appears initially to the viewer.

  The screen distance parameter determines the distance, in 'world' coordinates, from the origin to the display screen. If this is zero, the origin of the coordinate system in which molecules (and all other graphical objects) are drawn coincides with the center of the display. If distance is negative the origin is located between the viewer and the screen, if it is positive, the screen is closer to the viewer than the origin. A negative value puts any stereo image in front of the screen, aiding the three-dimensional effect; a positive value results in a stereo image that is behind the screen, a less dramatic effect (but easier to see, for some people) stereo effect.

  Figure 5.5 describes the relationship between the screen height, the screen distance, and the world coordinate space.

- **Shadows** – The shadows control enables and disables direct lighting shadowing when using the built-in Tachyon CPU or GPU renderers or when exporting the VMD molecular scene to external renderers that implement shadowing algorithms. The simple direct lighting model implemented in most renderers yields shadows that are completely dark, producing a somewhat harsh lighting quality akin to what would be expected in a desert under full sunlight with no clouds.

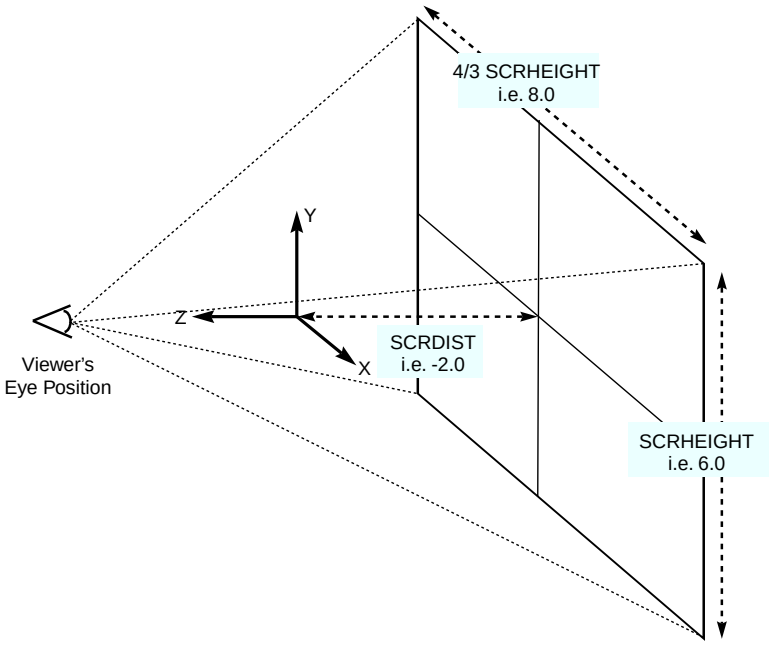


Figure 5.5: Relationship between screen height (SCRHEIGHT), screen distance to origin (SCRDIST), and the viewer

- **Ambient Occlusion** – The ambient occlusion (AO) lighting control enables the use of so-called ambient occlusion indirect lighting when using the built-in Tachyon CPU or GPU renderers, or external renderers that implement AO. Images with much higher quality shading can be produced by augmenting direct lighting with ambient occlusion or broad angle or indirect lighting techniques. Ambient occlusion lighting emulates the broad lighting effects similar to what would be experienced on a cloudy or overcast day with omnidirectional light arriving on all surfaces. The AO ambient coefficient controls the strength of the omnidirectional lighting components. The AO direct coefficient scales the direct lighting contribution associated with the directional and positional lights.

- **Depth of Field (DoF)** – The depth of field (DoF) control enables or disables emulation of depth of field focal blur effects associated with fast focal ratio camera optics and close focus distances. The depth of field implementation provided by the built-in Tachyon ray tracer and most other renderers yields a plane of perfect focus at a specified distance from the camera. The degree of focal blurring with increasing distance from the plane of perfect focus depends on both the simulated f/stop and the distance between the plane of perfect focus and the camera.

5.4.7 Graphics Window

The Graphical Representations or "Graphics" window controls how molecules are drawn. Molecules are represented by *reps*, which are defined by four main parameters: the selection [§ 6.3], the drawing method [§ 6], the coloring method [§ 6.2], and the material [§ 6.2.5]. The selection determines which part of the molecule is drawn, the drawing method defines which graphical representation is

used, the coloring method gives the the color of each part of the representation, and the material determines the effects of lighting, shading, and transparency on the representation.

Draw Style Tab

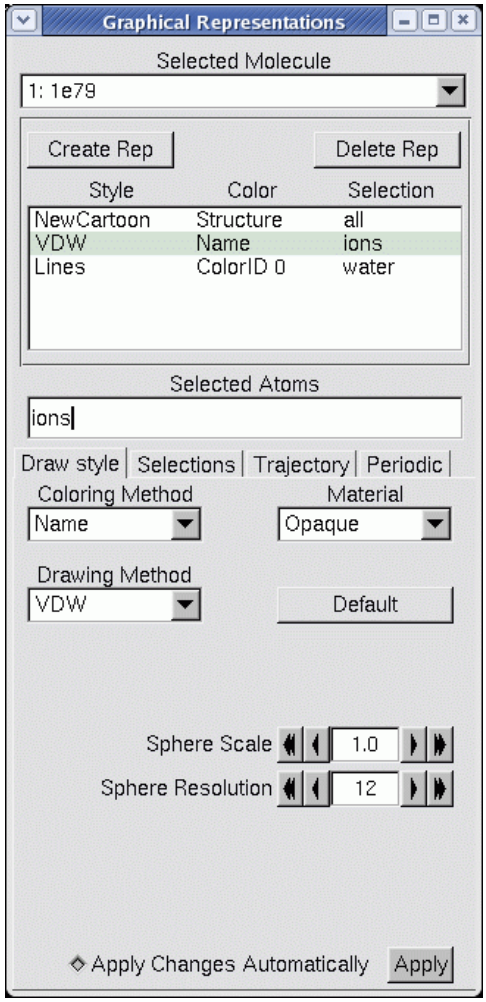


Figure 5.6: The Graphics window (in Draw Style mode)

Select a molecule for editing using the 'Selected Molecule' chooser at the top of the window. The browser below this chooser lists the reps available for the molecule. Each line of the browser summarizes information about the drawing method, the coloring method, and the selection. Below this browser, choosers and a text input filed reflect the current state of the rep, and provide controls for changing the properties of the rep. Each drawing method has specific controls which will appear when it is selected. When the 'ColorID' coloring method is selected, a text entry box is shown allowing you to specify the index of a color to use for the selection, which may be a number from 0 to 16.

Changing a rep. To change a representation, select it in the representation browser. The atom selection for that rep will appear in the Selected Atoms text area and the controls will update to reflect the current settings. Changing the settings will immediately affect the displayed representation if the Apply Changes Automatically check box is selected. When it is disabled updates will only occur when the Apply button is pressed. Changing the drawing method brings up method-specific controls and defaults. If you go back to the previous draw style, VMD restores any changes that you may have made to the settings. Pressing the Default button will restore the default settings. The display will be updated after every change.

Adding a rep. To add a new representation of the molecule, enter the selection into the Atom Selection text area (or keep what is there) and press Create Rep. This adds the representation to the currently selected molecule.

Deleting a rep. To delete a representation, select the representation in the browser and press the Delete button. Bear in mind that this does not delete the molecule, it only deletes one of its graphical representations.

Hiding a rep. To hide a rep, double-click its entry in the browser. The text will turn pink to indicate that the rep is hidden. Turn the rep back on by double-clicking again on the same line. Hidden reps will not recalculate their geometry if the animation frame changes until the rep is turned back on.

Selections Tab

The Selections tab provides access to browsers which display the lists of atom names, residue names, and so forth for the selected molecule. When the Selections tab is pressed, several browsers appear in place of the drawing and coloring method controls. These are used to list the available keywords, macros, and values for use in selecting atoms for the associated representation. The top browser lists singlewords and macros such as `all`, `water`, and `hydrophobic`. The botton left browser contains a list of the keywords and functions understood by the selection command [§6.3]. If a keyword is selected which can take on a value (for instance, `name` and `index`), then the possible names will be displayed in the bottom-rightmost browser. The functions can be identified by the `(` to the right of the name. After selecting a keyword, the right browser will display all the names associated with the keyword. For example, selecting resname in the left browser will show all the three-letter residue names known for the selected molecule.

Clicking on a field in the value browser will add it to the selection text field. *Double* clicking a keyword field adds the keyword to the text field. Press Apply to actually change the atom selection for the current rep. Press Reset to restore the atom selection to its original value.

The Selections tab also shows the atom selection macros that have been defined. These macros let you define a commonly used atom selection as a single word so that it can be inserted into a rep more conveniently. Atom selection macros can currently be defined only through the Tcl [§9.3.2] or Python [§10.3] text interfaces; see these sections for details.

Trajectory Tab

Selection and Color auto-update. When an atom selection such as `water within 3 of protein` is made, the atoms in the selection are computed for the current animation frame. When

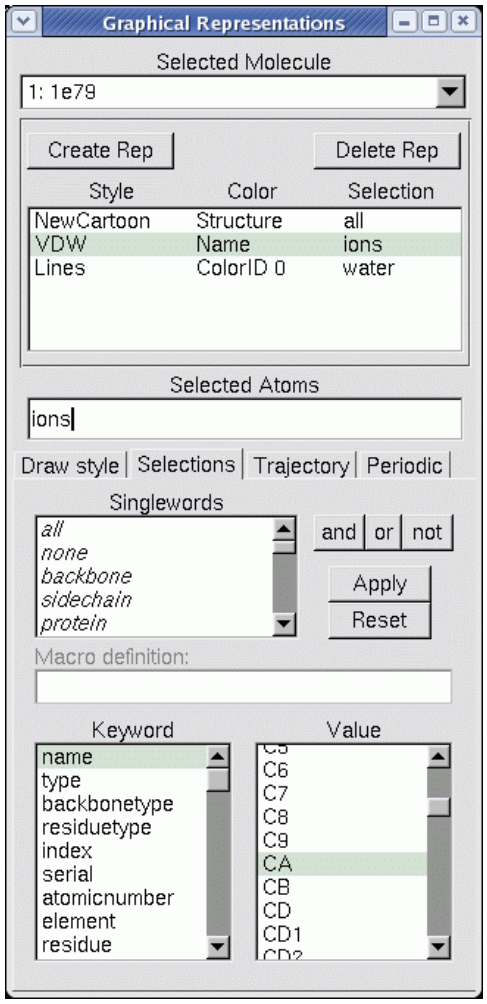


Figure 5.7: The Graphics window (in Selections mode)

the animation frame changes, the selection is not normally recalculated; thus the displayed atoms may not correspond to those that would be selected if the atom selection were performed for the new animation frame. If the Update Selection Every Frame checkbox is highlighted by clicking on the checkbox, then the atom selection for the current rep will be recalculated every time the animation frame changes. Similarly, if the Update Color Every Frame checkbox is activated, the color will be recalculated for every frame.

Color Scale Data Range. Several of the coloring methods available in Draw Style tab operate over data fields that have no specifically implied range of values. It is often useful to highlight a very specific range of data values, in order to accomplish this the color scale range can be manually set to a specific starting and ending values, overriding the default behavior which is to autoscale from the minimum value to the maximum value. This feature is particularly useful when displaying trajectories, since the range of values of interest may be quite different from the autoscaled range for a single frame or all frames.

Draw Multiple Frames. Draw multiple trajectory frames or coordinate sets simultaneously. This setting allows the user to select one or more ranges of frames to display simultaneously. The frame specification takes one of the following forms **now**, *frame_number*, *start:end*, or *start:step:end*.

Trajectory Smoothing. The Trajectory Smoothing Window Size is used to control the application of a per-representation windowed-averaging smoothing function. This simple smoothing feature can be used to eliminate much of the thermal noise inherent in a molecular dynamics trajectory so that one can more easily see structural changes occuring over a wider time scale. The window size parameter controls how many frames are averaged together to produce the coordinates which are actually displayed. One important consideration when using the trajectory smoothing feature is that VMD does not take periodic boundary conditions into consideration when smoothing trajectory coordinates, so any atoms which wrap around within the span of the window will cause erratic motions in the displayed representation. This can be avoided by unwrapping trajectory coordinates prior to loading into VMD or by using atom selections to eliminate atoms which wrap around.

Periodic Tab

The Periodic tab controls the display of periodic images of a molecule. In order to display periodic images, a molecule must have unit cell information set for `a`, `b`, `c`, `alpha`, `beta`, and `gamma`, which are discussed in section 9.3.22. When the proper unit cell information is present, the periodic display feature can show periodic images of the unit cell by transforming and rendering additional copies of the structure. The current implementation of this feature doesn't provide for complex crystallographic symmetry operations. Unit cells that can be replicated by translation along the three unit cell axes are the only ones supported presently. The periodic images to be drawn are selected by enabling images in one or more of the six faces of the unit cell. The Self image selects the untranslated unit cell itself, so that one my render a representation consisting of only replica images. This feature allows the unit cell and its periodic images to be displayed using different materials, for cases where it is desirable to draw more attention to the original unit cell or to one ore more of the replicas. The Number of Images counter controls how many replicas are made in each of the six directions. Some file formats read by VMD may not include unit cell information, in such cases you can use the scripting interface to set the unit cell information manually. PDB files containing CRYST1 records are an example of a file format that provides unit cell information.

5.4.8 Labels Window

The Labels window is used to manipulate the labels which may be placed on atoms, and the geometry monitors which may be placed between atoms. Labels are selected with a mouse, as discussed in section 5.1.2. Once selected, the Labels window can be used to turn different labels on or off or to delete them entirely. Also, labels displaying geometrical data such as bond lengths may be graphically displayed using this window.

Label categories

The Category chooser (in the upper left) is used to select which category of labels to manipulate. The different label categories include:

- Atoms, which are shown as a text string next to the atom listing the name and residue of the atom;

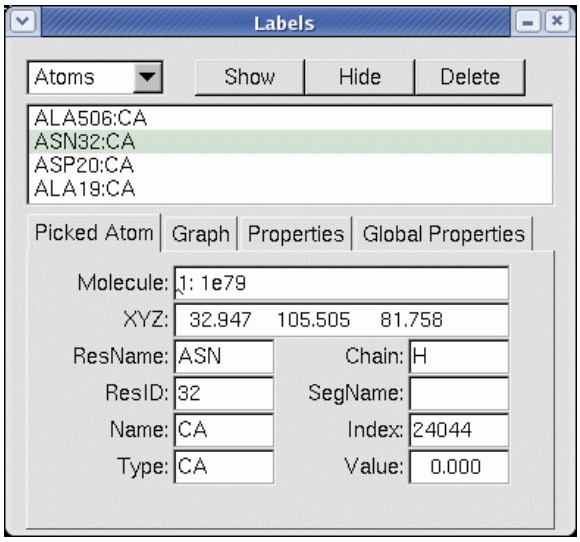


Figure 5.8: The Labels window

- Bonds, which are shown as dotted lines between the atoms with the bond length displayed at the bond midpoint;
- Angles, which are shown as dotted lines between the three atoms with the angle displayed at the center of the defined triangle;
- Dihedrals, which are shown as dotted lines between the four atoms with the dihedral angle (the angle between the planes formed by the first three atoms and the last three atoms) shown at the midpoint of the torsional bond.
- Springs, which are shown as dotted lines between the atoms with the bond length displayed at the bond midpoint;

All the labels for the selected category which have been previously added are displayed in the browser in the center of the window. The line itself contains from 1 to 4 atom names, depending on the category; the atom names have the form `<residue name><residue id>:<atom name>` followed by either `(on)` or `(off)`. The last word indicates if the label is turned on or off.

Modifying or deleting a label

A label can be turned on or off without deleting it, by selecting the label in the central browser and pressing the Hide button. To turn it back on, select it again then press the Show button. Press the Delete button to delete it. This browser allows multiple selections, which, for example, allows you to delete several labels at once. To select everything in the current category, press Select All; to unselect them, press Unselect All. If nothing is selected, the action is applied to everything. Thus, one way to turn everything off is to press Unselect All then press Hide. (It may seem counterintuitive, but it was done this way so all the labels could be deleted by just pressing Delete.)

Pick information

The Picked Atom tab displays information about the last atom picked by the mouse. This information is also echoed to the vmd console. The data in the will remain in until a new label is selected by the mouse. Information about the following fields is identified:

- Molecule - the name of the molecule referenced
- XYZ - the position of the atom in 3D space
- Resname - the type of the amino or nucleic acid to which this atom belongs
- ResID - the internal VMD ID number of the entire residue to which the particular atom belongs. E.g., ResId for an atom of a protein is the same as the residue number of that atom as listed in its PDB file.
- Name - the name of the atom as it appeared in the coordinate file
- Type - the type of the atom, as determined by an internal VMD match-up of the given name to a likely atom type associated with that name
- Chain - if the coordinate file contained data in the "Chain" field for this atom, then that data is given here.
- Segname - the name of the segment to which this atom belongs
- Index - the internal VMD index used to identify the atom; this is useful for specifying selection syntax to generate different representation styles for particular atoms. For PDB files Index corresponds to the atom number listed in the file minus 1 (so that the index starts with 0).
- Value - the calculated length of bonds, angles, or geometric measurements performed by the selected label

Plotting a label's value

If the label has a numeric value (such as a bond length geometry monitor), it is easy to graph the change of the value over time (for multiple frames in an animation). The Graph button calls a Tcl script to plot the data for the selected labels. You can create your own script to handle label plotting simply by creating a Tcl proc named `vmd_labelcb_user`. The proc should accept three arguments. Have a look at the default scripts in the VMD scripts directory, found in the VMD installation directory under `scripts/vmd/graphlabels.tcl`. If no supported graphing program is available, a dialog box will be presented which will allow you to save the values of the labels to a file.

5.4.9 Color Window

VMD maintains a database of the colors used for the molecules and the other graphical objects in the display window. The database consists of several color *categories*; each color category contains a list of names, and each name is assigned a color. The assignment of colors to names can be changed with this window. There are 16 colors, as well as black (the VMD color *map*), and this

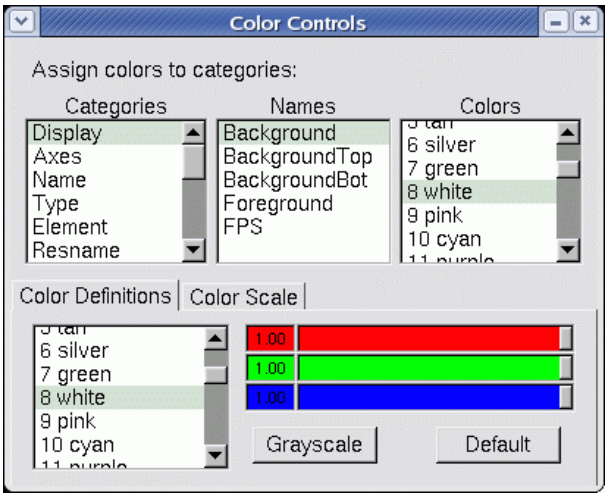


Figure 5.9: The Color window

window can also be used to modify the definitions of these 17 colors. For more about colors, see the chapter on Coloring [§6.2].

To see the names associated with a color category, click on the category in the Category browser located on the left side of the window. Click on the name to see the color to which it is mapped. To change the mapping, click on a new color in the browser to the right of the Category browser. For instance, to change the background to white, pick 'Display' in the left browser and 'Background' in the center one. The right browser will indicate the current color (which is initially `black` for the background). Scroll through the right browser and select `white` to change the background.

Changing the RGB Value of a Color

The Color Definitions tab at the bottom of the Color menu lets you change the RGB definition of the 17 palette colors. Select a color to edit using the browser at the bottom left corner of the menu, then slide the three sliders to set the amount of each red, green and blue component. Default restores the original color definition, and Grayscale toggles whether or not the three sliders will move together as a unit. Color definitions are immediately updated in the graphics window, so you can see the result of your editing right away.

Color Scale

Several of the coloring methods in the graphics window (e.g., Beta, Index, Position) are used to color a range of values, as opposed to a list of names. The actual coloring is determined by the color scale [§6.2.4].

The color scale used to assign these colors is set in the Color Scale tab of the color menu. Choose one of the ten color scales from the chooser, and adjust the Offset and Midpoint sliders until the color scale shown at the bottom of the tab is as desired.

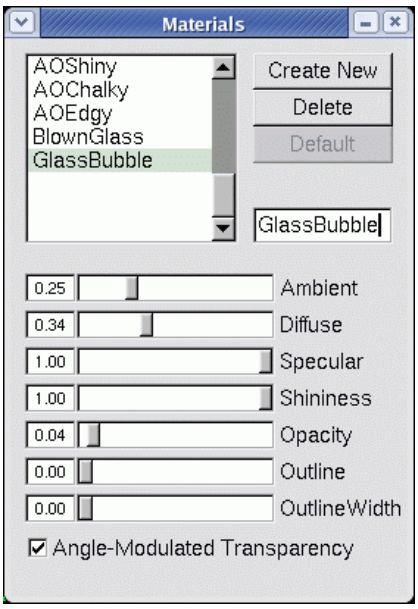


Figure 5.10: The Material Window

5.4.10 Material Window

This window is used to create and modify material definitions. The material definitions created here will show up in the pulldown menu in the Graphics window, allowing you to apply a material to a given representation.

The upper left corner of the Materials window contains a browser listing all the currently defined materials. Below this browser is a set of five sliders which indicate the current materials settings for the material highlighted in the browser. Highlighting a different material in the browser by clicking with the mouse will update the settings of the sliders. Conversely, moving the sliders will change the definition of the the currently highlighted material in the browser. Pressing the "Default" button will restore either of the first two materials, "Opaque" and "Transparent", to their original settings.

To create a new material, press the "Create New" button in the upper right corner of the window. A new material with a default name will be created and displayed in the browser window. This name can be changed at any time to something more descriptive by typing in the input box to the right of the material browser and pressing "enter" (note that the names of "Opaque" and "Transparent" cannot be changed). You can now edit the properties of this material using the sliders at the bottom of the window. All materials in the materials browser, including those you create, will appear in the Material pulldown menu in the Graphics window.

To experiment with the material settings, first create a new material so that you can edit its values. Next, load any molecule, change its drawing method to VDW representation, and using the Material pulldown menu in the Graphics window, change the representation's material to the material you just created. Now, go back to the Materials window, highlight the new material in the browser, and change some of the values in the sliders. The effect of changing shininess should be especially dramatic.

5.4.11 Render Window

The Render window is used to export the currently displayed graphics scene to an image file or to a geometric scene description file suitable for use by one of several external renderers, which can produce a final image. The supported rendering packages are listed in table 8.1. See Chapter 8 for detailed information on how rendering is performed using external programs, as well as information on 3-D printing and other uses of the exported scene description files.

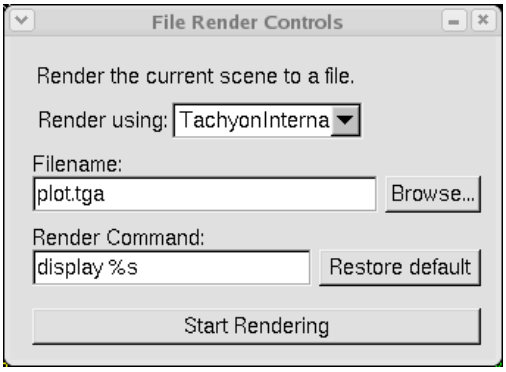


Figure 5.11: The Render window

The rendering process works in two stages. The first stage exports the displayed VMD scene to a text or image file in the selected format. The second (optional) stage renders the exported file, potentially displaying the results when complete. The exported file is named in the Filename field; a default name is given when a new format is selected, so it is best to hold off entering the filename until after the file format is selected. Another way to select the filename is available by pressing the Browse button, which opens up a file browser. Pressing the Start Rendering button writes the data file. After that, the Render Command is executed. The default command should start the appropriate rendering program if it is available.

Some of the rendering commands have been set to call a display program on the rendered image when it is completed. VMD will wait for the display program to finish, which causes VMD to freeze until the display program closes, so you may want to run the job in the background. This can be done (on Unix) by enclosing the existing text with `()`'s and putting an `&` at the end. For example, the way to make the Raster3D render command run in the background is:

```
(render < %s -sgi %s.rgb; ipaste %s.rgb)&
```

5.4.12 Tool Window

The Tool window is used to set up external 3D pointers, buttons, force-feedback devices, and the VMD "tools" that they control. VMD communicates with input devices through CAVElib, FreeVR, or via Virtual Reality Peripheral Network (VRPN), or with direct operating system interfaces. Since VRPN provides networked device abstraction, VMD doesn't have to be running on the same computer that VRPN devices are attached to. With VRPN, you may use buttons, trackers, and also force-feedback (haptic) devices such as the PHANToM. In the CAVE or FreeVR, VMD recognizes two types of devices: buttons and trackers. The built-in Spaceball driver can also be used to control tools.

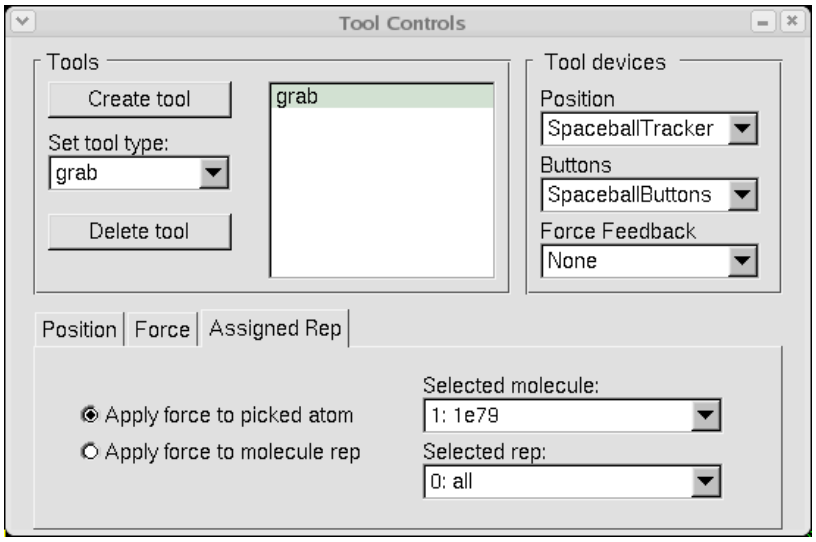


Figure 5.12: The Tool window

Configuring input devices

To use input devices with VMD "tools", you need a *sensor configuration file*, in your home directory called `.vmdsensors` (see the VMD Installer Guide). In this file, any number of devices can be specified, using a *universal sensor locator* (USL). The format for a USL is as follows:
USL – type`://`*place/name*`:`*nums*

- *type* – the type of sensor (`vrpntracker`, `vrpnbuttons`, `vrpnfeedback`, `cavetracker`, `cavebuttons`, or `sballtracker`)
- *place* – the machine that controls it. Devices that cannot yet be used on arbitrary computers over the network must have the keyword `local` here to be compatible with future versions.
- *name* – the name of the device within that machine. If multiple devices can't currently exist, such as with the CAVE, then a standard name should be used, such as `cave`, so that the same USL will make sense in the future, when multiple devices are allowed.
- *nums* – a comma-separated list of numbers of devices belonging to that names (optional, defaults to zero). Some devices demand only one number or a specific number but button devices should work correctly now.

The lines of a sensor configuration file come in four flavors:

- *Comments* begin with `#` and are ignored.
- *Empty lines* are also ignored.
- *Device lines* have the form `device` *name USL*, where *name* is the name that VMD will use to refer to the device, and *USL* is the device's USL.
- *Options* tell VMD how to use the most recently listed device. Currently, there are four supported options:

– "`scale` x" scales the position of a tracker by a factor x.

– "`offset` x y z" adds a constant vector to the position of a tracker.

– "`rot right`—`left` A_{00} $A_{01} \ldots A_{33}$" multiplies the orientation matrix returned by a tracker on either the right or the left by the matrix A.

– "`forcescale` x" multiplies the force applied to a force-feedback device by the amount x.

Here is a simple example, showing some of the things you can do with a sensor configuration file, for a more complete example, please refer to the .vmdsensors file that came with your VMD distribution:

```
### Sensable PHANTOM via VRPN
### http://www.sensable.com/
### The Phantom haptic device connected to the computer "odessa"
device phantomtracker   vrpntracker://odessa/Phantom0
scale 10
rot left 0 0 -1 0 1 0 1 0 0
device phantombuttons   vrpnbuttons://odessa/Phantom0
device phantomfeedback vrpnfeedback://odessa/Phantom0
```

Using Tools

There are several different "tools", each of which can be used with any of the input devices[1]:

- The **Grab Tool** mimics a pair of tweezers, and can be used to move molecules around on the screen without any keyboard or mouse commands. Pressing a button connects the 3d cursor to the nearest molecule. Then, moving or rotating the tracker will cause the molecule to move or rotate around on the screen.

- The **Rotate Tool** is a tool for precisely rotating molecules with haptic devices. When a button is pressed and released, the cursor is again connected to the molecule. With this tool, however, the center of the molecule is fixed, and the end of the haptic pointer is forced to lie on the surface of a sphere about this center. Moving the device around the surface of the sphere rotates the molecule, and another button click releases the molecule. There are detentes — like the clicks commonly felt in a 2d dial — on the surface of the sphere, arranged so that the user can rotate the molecule to precise 90-degree points. If the user holds down the button for a while initially, he can feel the sphere and the detentes, but do not affect the molecule. This "preview mode" allows the user to find a good point from which to start the rotation.

- The **Joystick Tool** is the three-dimensional equivalent of a Joystick, for haptic devices. Pressing the button creates a virtual "spring," holding the device to its current location. If it is pushed away from this point in some direction, the selected molecule starts sliding in that direction, with a velocity that is proportional to the displacement of the device. The joystick tool shows how a three dimensional input device can be used to supply relative (differential) coordinates instead of absolute coordinates.

[1]The tools have been designed to allow VMD to use haptic devices. Most of the tools can give force-feedback to the user, but none of them require haptic devices in order to operate.

- The **Tug Tool** is a tool that allows interaction with running molecular dynamics simulations. Pressing the button connects the device with a simulated spring to the nearest atom, and pulling on it adds a force to the simulation. If a haptic device is being used, the user will feel a force on his hand that is proportional to this force. In this way, the tug tool implements something like the click-and-drag that is commonly used with windowing systems.

  If an atom selection is assigned to the Tools, the the Tug Tool will apply a force to all the atoms in the selection. The force applied will be proportional to the masses of the atoms in the selection, so that all atoms experience the same acceleration. When a Tool Selection has been assigned, the Tug Tool will always affect that selection, even if the button is pressed far from any atoms in the selection; this is intended to make it easier for the user to apply forces only on those atoms he/she intends to steer.

- The **Spring Tool** also allows interaction with running molecular dynamics simulations. It works like the Tug Tool *except* that when the button on the tracker is released near an atom, the simulated spring is connected to it. See section 5.4.8 for information on viewing and modifying the list of active springs.

- The **Pinch Tool** is similar to the Tug Tool, except that force is applied only along the axis defined by the orientation of the tracker.

- The **Print Tool** is meant to be used as a debugging aid when one first sets up VMD for use with VRPN, the CAVE, or other 3-D input devices. When enabled, this tool prints text messages to the VMD console indicating the current position of the tool in question. This tool is useful when calibrating the various transformation matrices that operate on tracker position and orientation data (whether in VMD or in VRPN, CAVElib, etc).

To add a new tool to a VMD session, open the Tool window and click the **Create Tool** button. The tool's number and type are displayed in the list to the left. Devices can be added to the tool by selecting them from the **Add Device** menu, or removed with the **Delete Device** button. Some of the options that can be specified in the sensor configuration file can be edited in using the controls below, and the tool's type can be changed with the **Type** menu.

5.4.13 IMD Connect Simulation Window

VMD has the ability to work with a molecular dynamics program running on another computer, to interact with and display the results of a simulation as they are calculated. A major feature in VMD is the ability to add perturbative steering forces to a running simulation, which are incorporated directly into the dynamics calculation; we refer to this capability as Interactive Molecular Dynamics (IMD). In order to run and IMD simulation it is necessary to have a molecular dynamics program that supports the IMD communication protocol. To date, two such programs exist; NAMD, developed at University of Illinois, and Protomol, developed at Notre Dame. The rest of the discussion in this chapter assumes you are using NAMD. See the NAMD home page[2] for information on obtaining NAMD.

Interactive Molecular Dynamics

IMD works by establishing a TCP connection between VMD and the molecular dynamics simulation program. NAMD, or whichever MD program is being used, acts as the server. In order to

[2] http://www.ks.uiuc.edu/Research/namd/

prepare NAMDto accept VMD's IMD connection request, NAMDmust be configured to listen for incoming connections on a network port. Once NAMD has started up, may wait for the user to connect through that port. When VMDconnects to NAMDsuccesfully, the simulation commences. Before connecting to the remote simulation, the VMDuser must first load a molecule corresponding to the system being simulated. The structure file should correspond to the same structure file used by NAMD. Once the molecule is loaded and NAMD has been started and is listening for a connection, you are ready to connect to the simulation and start receiving coordinates. To establish a connection, open the Simulation window, enter the hostname on which NAMD is running and the port on which NAMD is listening for incoming connections, then press the Connect button to establish the connection. If NAMD is running on several distributed nodes, VMD must connect to the root node on which NAMD initially started out.

IMD Using the Simulation window

The Simulation window allows you to control the behavior of a molecular dynamics simulations which has been previously connected to through use of the Remote window. This window contains controls to change parameters for the simulation and to affect how VMD displays the results of the simulation. The window also contains informative displays, which show the current status of the simulation connection, and such things as the current energy, temperature, and timestep of the molecular system being simulated.

At the top of the window are two entry fields and a button for establishing a connection to a running MD simulation. Enter both the hostname on which the simulation is running, and the port on which the simulation is listening, then press the Connect button to establish the connection. See the text console for possible error messages and status updates. Below the connection display is a browser used to set some connection parameters. These include:

- **Transfer Rate**: How often a timestep is transferred from the remote simulation program to VMD. By default, this is 1, which means every calculated timestep is sent. If this is set to some value N, then only every Nth step will send from the remote computer, thereby decreasing the amount of network processing and rendering that needs to be done.

- **Keep Rate**: How often VMD saves the timestep in its animation list, instead of just discarding it after displaying it. By default, this is 0, which means that VMD does not save any timesteps. When this is 0, then when VMD receives a new timestep it *replaces* the last timestep in the animation list with the new timestep, instead of *appending* it. When it is set to some number N larger than 0, then every Nth timestep received from the remote simulation will be appended to the molecule.

Parameters may be changed by entering text into the appropriate entry field and pressing `<return>`. When a new value is entered, a command is sent to the remote simulation to change it. There may be some delay between when the simulation gets commands, acts on them, and the results propagate back to VMD. Connection state is shown in the center of the window. The simulation status text area displays energy values for the system being simulated (kinetic, electrostatic, etc.), as well as the current timestep and the temperature. It is updated each time a new coordinate set (timestep) is received by VMD. The Stop Sim button will terminate the remote simulation, but will not delete the molecule in VMD. The Detach Sim button will sever the connection between VMD and NAMD, but will allow the simulation to continue running.

5.4.14 Sequence Window

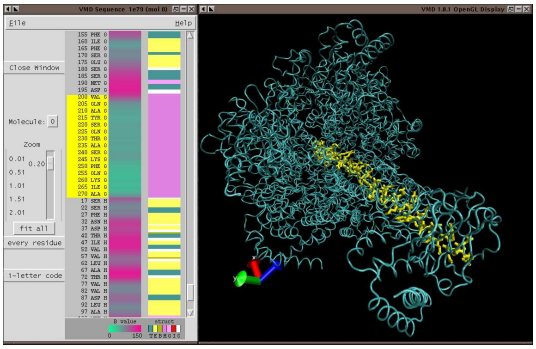


Figure 5.13: The Sequence window

The Sequence window is used to list the residue sequences of proteins and the base sequences of nucleic acids, and to select residues/bases from the sequence list for highlighting in the 3-D structure in the main VMD window. When residues are selected in the main VMD window, the corresponding residue is highlighted in the sequence list in this window. Color-coded protein structure information is displayed for amino-acid residues, and B-factor information is displayed for all residues. In this section, "residues" refers both to amino acid residues in proteins, and to nucleotide bases with associated backbone in DNA and RNA molecules.

Sequence information

The Sequence window contains a vertical listing of the residue sequence of a loaded molecule. The Molecule pop-up menu control chooses which molecule to display the sequence of, the current 'top' molecule is displayed the first time the Sequence window is opened. The name and molecule number of the sequence displayed is shown in the title frame of the Sequence window.

For each residue displayed, the window lists: residue number, residue name/code, and chain letter. If no chain is specified, chain letter is set to "X". To the right of this are two color coded columns, "B value" and "struct". "B-value" shows the contents of the B-value (temperature factor) field. The "struct" field shows protein secondary structure; select Help:Structure Codes from the window menu, or see Table 5.5, for an explanation of the single letter codes in the color key.

Code	Description
T	Turn
E	Extended conformation
B	Isolated bridge
H	Alpha helix
G	3-10 helix
I	Pi-helix
C	Coil

Table 5.5: Description of secondary structure codes in the Sequence window.

Selecting residues from the Sequence window listing

Click anywhere in the vertical listing with the left mouse button to highlight one residue. Click and drag with the left mouse button to highlight multiple residues, shift-click to add a single residue to the current selection, shift-click and drag to add multiple residues to your selection, right-click to de-select a residue. Highlights appear as thick yellow "Bonds" representations, these can be changed or turned off[§ 5.4.14].

Selecting residues by clicking on the 3-D structure

Use the Mouse menu to enter "Pick Atom" mode (or press "1", the standard keyboard shortcut). Click on any protein atom or nucleic acid atom, and its residue will highlight, and the sequence list will scroll to display this residue. Shift-click works the same way, but adds to the current selection. Note that if the zoom factor is smaller than 1.0, the single-residue sequence highlight will be shorter in height than a full line of text. Once the Sequence window has been opened, any "Pick" will create or add to selections, until highlighting is turned off[§ 5.4.14].

Sequence Zooming

Larger molecules contain thousands of residues, too many to display in a linear text list all at once. The sequence window can only list about 40 text lines; to work with a molecule of more than 40 residues use the scroll bars to scroll through the long list, or use the Zoom controls to fit the data from a long list into a small space.

The Zoom slider, and the Fit all, Every Residue buttons, zoom in and out of a long sequence list to allow viewing and selecting from the entire list all at once. To represent more than 40 residues on the window, the text list seems to "skip" residues, but selections, highlights and color-coded data are still active for all residues.

By setting the Zoom slider to a value smaller than 1.0, or by pressing the Fit all button, more or all of the sequence information for a large molecule can be seen at once. To show a text line for every residue in the sequence (zoom factor = 1.0), click on the Every Residue button. The Zoom slider can be dragged with the left mouse button (to re-scale sequence smoothly) or it can jump to a given value by clicking along the slider track with the middle button (this is useful to work more quickly with very long sequences).

For a multi-thousand residue protein with Fit all selected, hundreds of residues can be selected at once, and trends in B-value and structure across the entire protein sequence can be detected. In the screen-shot above, a section of 70 residues with lower B-values than surrounding sequence is selected, by dragging a rectangle around the green stretch in the B-value column.

Other controls include:

- **Toggle display of 3-letter and 1-letter codes** – Click on 1-letter code to switch from 3-letter to 1-letter amino acid codes. The same button then reads 3-letter code, click it to switch back from 1-letter to 3-letter codes.

- **Print contents of sequence window** – Select File:Print to File to create a postscript file containing the current sequence listing and highlighting.

Turn off highlighting / Change highlight style

To clear all highlights, reselect the current molecule from the Molecule pop-up menu. To turn the highlight representation off completely for a given molecule, find the representation in the Graphics window which the Sequence window has created (appears with "Bonds ColorID 4") and set the style to "none". To change highlighting style, set this same representation to your preferred style and coloring. The selection for this representation will still change whenever the sequence window selection changes. Example application: specify Multiple Frames in the Trajectory tab of the highlight representation. This will display the trajectory motions of the residues clicked on in the main VMD window, or in the Sequence window.

Caveats

- Pause on first use: Since the sequence window displays secondary structure of loaded molecules, there may be a pause for structure calculation the first time the sequence for a protein is displayed.
- Selections by chain: When there are multiple segments in a chain, it is possible for several residues to have the same residue number and chain name. These residues will be highlighted/selected/deselected together.
- B-values can be user assigned: To use the B-value column to view arbitrary data, use the selection `set beta` commands to change B-values. To refresh the displayed B-value data, re-select the currently displayed molecule from the Molecule pop-up menu.

5.4.15 RamaPlot

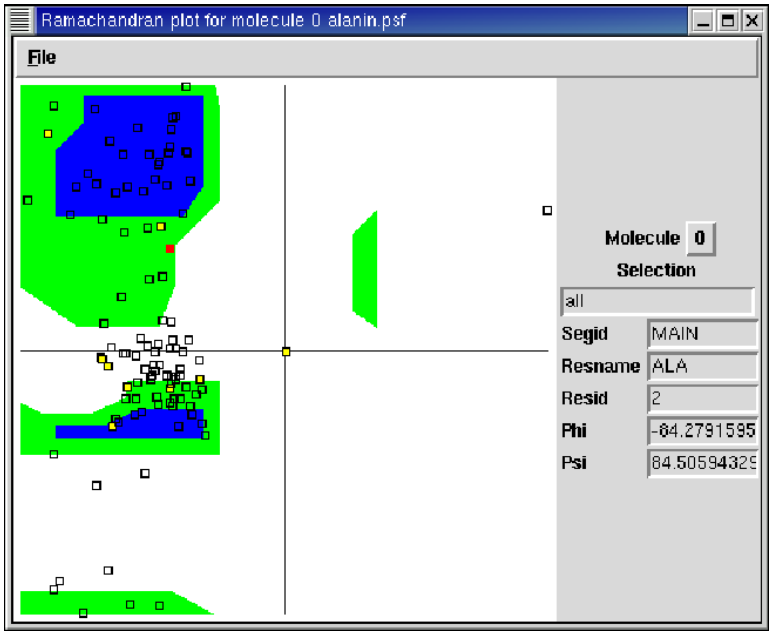


Figure 5.14: The RamaPlot Window

The RamaPlot window displays a Ramachandran plot for a selected molecule. If you animate your molecule over a range of frames , RamaPlot will update the Ramachandran plot automatically. You can select a range of residues to be displayed in the plot. Clicking on a point in the Ramachandran plot will show the trajectory of the selected residue in Ramachandran space over all frames . Fields on the right of the window show the computed value of phi and psi for the most recently selected residue. Finally, you can create a PostScript image of the current Ramachandran plot. RamaPlot functionality is summarized in Fig. 5.14.

Using RamaPlot

Start RamaPlot by typing "`ramaplot`" in the VMD text console, or by selecting the ramaplot menu item in the Extensions menu. The main window contains a Ramachandran graph, with phi and psi running along the horizontal and vertical axis, respectively, from -180 to 180 degrees. The most allowed region of Ramachandran space is colored blue; partially allowed regions are colored green.

After loading a molecule, using the pulldown menu in the upper right part of the window to choose a molecule. Protein residues in the current molecule are mapped to the Ramachandran diagram with yellow squares. Clicking on a square causes the square to turn red, displays residue information in the fields on the right side of the window, and, if trajectory data is present, draws the location of the selected residue in Ramachandran space for all frames in the trajectory as empty black squares. Clicking one of the empty squares causes VMD to redraw the graphics display window with coordinates from the timestep corresponding to that square. Clicking a second time on a red highlighted residue switches off the trajectory information in the RamaPlot window.

When a protein contains many residues, it may be inconvenient to display all residues at once. Enter an atom selection in the Selection input to choose which residues to display. Note that the selection must contain the alpha carbons (name CA) of the residues you want to show. Note also that, just like the Graphics window, the selection will not be recomputed if you change the animation frame.

To print the contents of the white Ramachandran plot, select "Print to file..." from the RamaPlot File pulldown menu. Enter a filename to save the contents of the window.

Chapter 6

Molecular Drawing Methods

Each molecule in VMD is drawn as a collection of several *representations*, of the molecule. A representation is just one particular way of drawing the molecule, and consists of several characteristics:

- An *atom selection*, which determines which of the atoms in the molecule will be included in the view. This selection is entered in the text input field at the bottom of the Graphics window. Atom selections don't apply when drawing volumetric data such as an electron density map, electrostatic potential map, etc. Section 6.3 describes the syntax used to select atoms.
- A *drawing method* (representation *style*), which determines what shape to draw the atoms, bonds, and other components of the molecule. Section 6.1 describes the rendering methods available in VMD.
- A *coloring method*, which determines how to color each of the atoms and bonds included in the view. The Graphics window contains controls to set the coloring method at the right of the window. Section 6.2 describes VMD's coloring methods.
- A *material*, which determines the shininess, opacity, and other lighting and shading characteristics used when rendering the molecule.

A molecule can contain any number of different representations, and complex pictures of the molecule can be generated by creating views with different selections, coloring schemes, and rendering methods. For example, the protein backbone can be drawn as a smooth tube in one view, and important residues in the protein can be drawn as spheres or licorice bonds in other views. When a molecule is first loaded, it is given a 'default' view, which will draw all the atoms as lines and points, coloring each atom by what kind of element it is.

6.1 Rendering methods

All of the different rendering methods have various parameters which determine how they are drawn. For each method, there are controls in the Graphics window which modify the associated parameters, such as the line width and sphere resolution (the graphical controls are described in section 5.4.7). Table 6.1 lists the available rendering methods, and the following sections describe these methods and the parameters which modify their appearance.

Representation styles	Description
Lines	simple lines for bonds, points for atoms
Bonds	lighted cylinders for bonds
DynamicBonds	dynamically calculated distance-based bonds
HBonds	display hydrogen bonds
Points	just points for atoms, no bonds
VDW	solid van der Waal spheres for atoms, no bonds
CPK	scaled VDW spheres, with cylinders for bonds
Licorice	spheres for atoms, cylinders for bonds, same radius
Polyhedra	polyhedra connecting atoms within a cutoff radius
Trace	connected cylindrical segments through C_α atoms
Tube	smooth cylindrical tube through the C_α atoms
Ribbons	flat ribbon through the C_α atoms
NewRibbons	smooth ribbon through the C_α atoms
Cartoon	cartoon diagram (cylinders and ribbons) based on secondary structure
NewCartoon	smooth cartoon diagram (smooth ribbons) based on secondary structure
PaperChain	display ring structures as polygons, colored by ring pucker
Twister	flat ribbon tracing glycosidic bonds, with twists oriented by sugar residues
QuickSurf	molecular surface (Gaussian density surface)
MSMS	molecular surface as determined by the program MSMS
Surf	molecular surface as determined by SURF
VolumeSlice	display a texture mapped slice from a volumetric data set
Isosurface	display an isovalue surface from a volumetric data set
FieldLines	field lines generated by integrating particles by volume gradient vectors
Orbital	molecular orbital selected by wavefunction type, spin, excitation, and orbital ID
Beads	per-residue approximate bounding spheres
Dotted	dotted van der Waals spheres for atoms, no bonds
Solvent	dotted representation of the solvent accessible surface

Table 6.1: Molecular view representation styles.

6.1.1 Lines

The default representation is 'Lines', which is also known as 'wireframe'. It draws a line between each atom and the atoms to which it is bonded. Both atoms have to be selected before the bond will be drawn. The first half of each bond is colored appropriately for the first atom, while the color of the final half corresponds to the second atom. The only parameter for the lines representation is the line Thickness.

6.1.2 Bonds

Nearly everything about this option is the same as 'Lines' [§ 6.1.1] except that instead of drawing a bond as a line between two atoms, a cylinder is drawn instead. To be more specific, it draws an n-sided prism, where the number of sides is determined in the Graphics window [§5.4.7] by the Bond Resolution control and the radius is given by the value of Bond Radius, in Angstroms. If the radius or number of sides gets too small, the bonds are drawn as lines.

In order to fine tune the bond representation, VMD does a small amount of trickery to the

prisms. That is, imagine two hollow cylinders coming together so that the center of the face of one cylinder is in the same position as the center of the face of the other cylinder. Also suppose these two cylinders come together at 90 degrees. Although most of these two cylinders will overlap, there will appear to be a gap at their intersection.

To correct for this problem, VMD extends both cylinders somewhat so that the far ends touch. If one looks closely, this produces more of an overlap, but it is much nicer looking than the gap. When three or more bonds join at one atom, VMD chooses the lowest numbered bond and extends all other bonds to meet with that one. It then extends that lowest numbered bond to meet with the second lowest numbered one.

6.1.3 DynamicBonds

The 'DynamicBonds' representation will automatically perform a distanced-based bond search for the active atom selection and active trajectory frame. This representation does not perform the endpoint fixup procedure described above for the regular 'Bonds' [§ 6.1.2] representation. Instead, it is intended to be used in concert with the 'VDW' [§ 6.1.6] representation to show bonds that are being created and destroyed during the course of a trajectory. A bond is drawn if the atoms are within Distance Cutoff of eachother.

6.1.4 HBonds

The 'HBonds' representation will draw a dotted line between two atoms if there is a possible hydrogen bond between them. A possible hydrogen bond is defined by the following criteria:

```
Given an atom D with a hydrogen H bonded to it and an atom
A which is not bonded to D, a hydrogen bond exists between
A and H iff the distance ||D-A|| < dist and the angle D-H-A < ang,
where ang and dist are user defined.
```

Only the selected atoms are searched, so both the donor and acceptor must be selected for the bond to be drawn. Also, you'll note that the above doesn't check the atom type of the donor or acceptor; the only criterion is if it already has or doesn't have a hydrogen.

One downfall of the current implementation is that it does an n^2 search of the selected atoms so you probably don't want to show all the HBonds of a very large structure. Look for performance improvements in future versions of VMD.

If you choose an HBonds representation but fail to see any hydrogen bonds, it may be because the default Angle Cutoff and Distance Cutoff criterion in VMD are too small, so you might want to try increasing the angle value from 20 to 30 degrees and the distance value from 3 to 4.

The HBonds are drawn as dotted lines of a given width. The default Line Thickness is 1 but you should probably increase that to 2. On most SGIs you can't make it any wider than that, as described in the man page for linewidth. The bond is colored by the color associated with the acceptor.

6.1.5 Points

'Points' draws each atom as a point, and does not draw any of the bonds. This option is useful when rendering very large molecules containing millions of atoms, particularly for rendering water or other structures for which geometric detail may not be necessary. The Size of the points can

be changed. When the VMD rendering mode is set to GLSL, the Points representation will render space filling spheres with a size proportional to the Size parameter, and with performance on par with the non-shaded points drawn in other rendering modes.

6.1.6 VDW

'VDW' draws the atoms as spheres. The Sphere Scale used is the van der Waals radius multiplied by a user-selectable scaling factor.

The Sphere Resolution determines how finely to tessellate the spheres that are drawn, when using rendering modes and external rendering tools that can only draw polygonal geometry. The performance of polygonal sphere rendering varies inversely with the number of triangles produced by tessellation into triangles. The number of triangles per sphere varies proportionally with the Sphere Resolution parameter value squared. For rendering modes such as GLSL, and for external rendering tools that can directly represent spheres and other quadric surfaces, the Sphere Resolution parameter has no effect.

Note: Due to variations in atom naming conventions, in rare instances VMD may improperly assign VDW radii to specific atoms, since VMD determines each atom type based on the first letter forming its name. For example, VMD would assume an atom named "HG" to be a hydrogen rather than a mercury. If this happens, you are always free to redefine the radii, using a syntax much like that below:

```
set sel [atomselect top ‘‘name HG’’]
$sel set radius 1.9
```

6.1.7 CPK

'CPK' is a combination of both 'Bonds'[§ 6.1.2] and 'VDW'[§ 6.1.6] in that it draws the atoms as spheres and the bonds as cylinders. The resolution and radius can be modified independently. The size of the sphere drawn in CPK mode is by default the scaled-down VDW radius, but this scaling-factor can be changed by adjusting the Sphere Scale parameter. Since a sphere is drawn for each atom, it will always be slower than the 'VDW' option. If the radii for a sphere or bond are too small, they will not be drawn.

6.1.8 Licorice

'Licorice' draws the atoms as spheres and the bonds as cylinders. The difference between this and 'CPK' [§ 6.1.7] is that the sphere radius is not controllable; instead, it is made the same size as the bond. This makes for a nice, smooth transition and is one of the most often used representations. It can be rather slow for large molecules.

6.1.9 Polyhedra

'Polyhedra' draws a collection of triangles that connect all triplets of groups of atoms within a user-defined radius. This is commonly used in conjunction with specific atom selections for visualization of amorphous silicon nanodevice structures and the like. At present, a single atom selection is used for all candidate atoms, and only the radius parameter can be modified.

6.1.10 Trace

This representation applies much of the procedure used to construct the 'Tube' [§ 6.1.11]. In the end, it connects the alpha-carbon atoms of successive residues by cylindrical segments with adjustable width. In the case of nucleic acids, it is the P backbone atoms which are connected. As always, the segment pieces are colored according to the atom they are associated with. If the cylinder radius is made 0.00, then the cylinder segments are replaced with lines.

Note: the Trace option is useful for people doing threading or protein folding work who only look at the C_α coordinates and residue names, for then they don't have to build the sidechains necessary to see their structure. Also, people working on polymers can fake their structure by naming everything "CA." in the PDB file and then using Trace.

6.1.11 Tube

There are two ways to draw a 'Tube' representation, one for proteins and the other for nucleic acids. The protein tube is a smooth curve through the selected C_α positions, and the nucleic acid tube is a smooth curve through the backbone phosphates.

The protein tube is a spline curve that passes through all the C_α atoms in a protein fragment. Five evenly spaced interpolation points are found along the curve to break the curve connecting the two C_α atoms into six line segments. If the first C_α is selected, the first three segments are colored by the color assigned to that C_α. If the second C_α is selected, the last three segments are colored by the color of the second C_α. The nucleic acid tube is constructed in the same manner except that the phosphate atoms are used.

The two controls set the spline radius and resolution and have the same meaning as they did in the 'Bond' [§ 6.1.2] control. However, if the bond's Radius becomes 0 or Resolution is 2 or less then the spline is drawn as a simple line. This make moving and rotation the image much faster.

It is possible to pick with the mouse the C_α which defines the tube by clicking near the middle of the six tube segments which are associated with that atom.

6.1.12 Ribbons

The 'Ribbons' representation is similar to 'Tube' [§ 6.1.11] in that it follows the same spline curve for both the protein and nucleic acids. However, it uses additional information (the O of the protein backbone or some of the phosphate oxygens for nucleic acids) to find a normal for drawing the oriented ribbon. (There may be some problems with the ribbon definition for nucleic acids as it is possible for the nucleic acid detection routine to label a residue as a nucleic acid even though it does not have phosphate oxygens.)

Given the coordinates of each atom and the offset vector for the ribbon vector, the drawing code finds the spline curves for the top and bottom of the ribbon. The two splines are connected by triangles and both splines are drawn as small tubes. As with the 'Tube' representation, the six ribbon segments nearest the given atom are drawn with the color assigned to that atom and the atom can be selected by clicking near the center of those six elements.

Bond Radius and Resolution modify the tubes that make up the top and bottom of the ribbon. If the radius or resolution get too small, the tubes are not drawn (this speeds up drawing time by an appreciable amount). The Width controls the width of the ribbon and make it look like everything from vermicelli to lasagna. Additionally, the sugars are drawn filled in with triangles. This helps highlight the pucker.

Thanks to Ethan Merrit for the ribbon drawing algorithm taken from Raster3D.

6.1.13 NewRibbons

The 'NewRibbons' representation is similar to 'Tube' [§ 6.1.11] in that it follows the a spline curve for both the protein and nucleic acids. However, it uses additional information (the O of the protein backbone or some of the phosphate oxygens for nucleic acids) to find a normal for drawing an oriented ribbon. (There may be some problems with the ribbon definition for nucleic acids as it is possible for the nucleic acid detection routine to label a residue as a nucleic acid even though it does not have phosphate oxygens.)

The NewRibbons representation uses the alpha Carbons as control points for a spline which defines the ribbon backbone. The ribbon is drawn by extruding a two-dimensional cross section along the length of the spline orienting it by referencing the positions of the Oxygens on the protein backbone. As with the 'Tube' representation, the six ribbon segments nearest the given atom are drawn with the color assigned to that atom and the atom can be selected by clicking near the center of those six elements.

The Aspect Ratio parameter controls the width of the ribbon relative to the thickness value, as a multiplicative factor. An aspect ratio of 1.0 yields a Tube-like representation. The Resolution parameter controls the degree to which the ribbon surface is tesselated with triangles. Higher settings yield nicer looking images at the expense of interactive rendering performance. Points can be interpolated with either a Catmull Rom or B-Spline by changing the value of Spline Style. Note that the B-Spline does not always pass through the C_α positions, as it is a smoother spline.

6.1.14 Cartoon

The 'Cartoon' option produces a simplified representation of a protein based on its secondary structure. Helices are drawn as cylinders, beta sheets as solid ribbons, and all other structures (coils and turns) as a tube. If the secondary structure has not yet been determined, it will be calculated automatically by the program STRIDE.

A helix cylinder is constructed by finding the least squares linear fit along the coordinates of the helix's C_α atoms. If a given residue's C_α is selected, the small cylinder (found by linear interpolation along the line of best fit) is drawn with radius determined by the radius parameter. Because this method computes a best fit, a helix must have at least 3 residues before it is drawn (those helicies with one or two residues are drawn as a coil). It is possible to pick the C_α for each cylinder segment, but they are at the location of the C_α, which is not near the axis cylinder. Interesting results occur when the whole protein is defined to be a helix and drawn as a cartoon.

The solid beta ribbon is constructed by building a spline along the center points between each beta sheet residue. Again, the spline is linearly interpolated to find the start and end points for each residue. Those are extended to construct the corners for a ribbon with rectangular cross section (the amount of extension is determined with the thickness parameter). A ribbon segment is used if the corresponding C_α atom is selected. Note that since this method assumes the protein is in a beta conformation, it draws a much smoother ribbon than the standard 'Ribbons' [§ 6.1.12] option, which draw the ribbon with an oscillation along the sheet.

The other conformations are drawn as a tube. Since the endpoints of the helix cylinder and cartoon sheet are not at the C_α coordinate, the tube method was slightly changed to make the tube go to the new locations. This does not always work, resulting in a tube which does not quite connect to a cylinder.

6.1.15 NewCartoon

The 'NewCartoon' representation is a variation of the original 'Cartoon' combined with the 'NewRibbons' representation look and features. The main difference between the original 'Cartoon' representation and 'NewCartoon' is that helices are left in a ribbon representation which follows curved structures much more accurately than the straight cylinders used in the original 'Cartoon' did.

The Aspect Ratio parameter controls the width of the ribbon relative to the thickness value, as a multiplicative factor. An aspect ratio of 1.0 yields a Tube-like representation. The Resolution parameter controls the degree to which the ribbon surface is tesselated with triangles. Higher settings yield nicer looking images at the expense of interactive rendering performance. Points can be interpolated with either a Catmull Rom or B-Spline by changing the value of Spline Style. Note that the B-Spline does not always pass through the C_α positions, as it is a smoother spline.

6.1.16 PaperChain

The 'PaperChain' representation finds all rings up to a user-defined maximum size by walking the molecular topology, then proceeds to render each ring by fitting a polyhedron to the involved atoms and the ring centroid. The rings are drawn as bipyramids with a user-controlled height. The rings are colored by pucker, using the Cremer-Pople pucker amplitude, which is defined for all rings of three atoms or greater.

6.1.17 Twister

The 'Twister' representation traces glycosidic bonds with a flat ribbon that twists according to the relative orientation of successive sugar residues. The concept is similar to the familiar ribbon representations VMD uses for proteins. The paths connecting oriented rings are connected by thin ribbons with user-adjustable width and thickness, and with adjustable geometric resolution, and the representation handles branched structures.

6.1.18 QuickSurf

The 'QuickSurf' representation computes an isosurface extracted from a volumetric Gaussian density map computed from atoms or particles in the neighborhood of each lattice point [33, 34, 14, 35, 43, 26, 36]. The density map generation algorithm accumulates Gaussian densities on a uniformly-spaced 3-D lattice defined within a bounding box large enough to contain all of the atoms or particles that are selected as part of the rendered surface; sufficient padding at the edges of the volume ensures that the extracted surface is not clipped off. The density map generation algorithm satisfies

$$\rho(\vec{r};\, \vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N) = \sum_{i=1}^{N} e^{\frac{-|\vec{r}-\vec{r}_i|^2}{2\alpha^2}}, \tag{6.1}$$

where the density ρ is evaluated at a position $\vec{r}$ by summing over all N atoms. Each atom i is located at position $\vec{r}_i$ and has an associated weighting factor α which is determined by multiplying its radius with user-defined weighting and scaling factors that customize the visualization to produce a surface with an appropriate user-defined level of detail.

The QuickSurf representation includes several controls which modify the parameters of Eq. 6.1 to produce a surface that meets the required spatial fidelity and interactive rendering performance.

- Resolution – An overall spatial resolution approximation slider, which automatically sets the values of the detailed parameters below
- Radius Scale – A radius scaling factor applied to all atoms prior to computing their density map contributions
- Density Isovalue – The density isovalue to use when extracting the generated isosurface
- Grid Spacing – The density map uniform lattice spacing parameter.
- Surface Quality – The maximum cutoff distance to use when gathering Gaussian density contributions from atoms or particles in the neighborhood of each lattice point

Several factors influence the interactive calculation and display performance of the QuickSurf representation. The CPU version of the QuickSurf algorithm is multithreaded, but due to the potential for significant memory usage associated with CPU core, the number of CPU cores used by the algorithm may be clamped to a maximum of eight, and for density map volumes approaching 1 GB in size, or larger, the algorithm may reduce the number of CPU cores used to four or less to prevent out-of-memory conditions from occuring at runtime.

On machines equipped with appropriate GPU hardware, the QuickSurf representation will use a GPU-accelerated implementation that runs one to two orders of magnitude faster than the CPU version. The speed of the GPU algorithm is somewhat dependent on the memory capacity of the target GPUs, since density maps larger than the capacity of the GPU must be computed in multiple passes.

6.1.19 Surf

This option uses the molecular surface solver written by Amitabh Varshney when he was at the University of North Carolina. When this option is used, the radii and coordinates are written to a temporary file and the 'surf' executable is run with the Probe Radius as a parameter. When finished, the output is written to another temporary file which is then read by VMD and colored and displayed. The value of the probe radius is controlled by the sphere radius, and this is identical to the probe size in Å.

- Probe Radius – Probe radius used to construct the molecular surface
- Representation Method – The surface can optionally be drawn using lines rather than solid triangles

This surface is rather slow in both generation and display for systems over several hundred atoms. The SURF calculation is quite exact and will show complete detail even when it isn't needed. The use of disk space as an interprocess communications medium takes up about half of the run time.

There is an environment variable [§ 14.2] which can affect the Surf display option:

- `SURF_BIN` – location of the SURF binary (defaults to `SURF_$ARCH` as defined in the vmd startup script)

A helpful trick when constructing surfaces is to use the Apply Changes Automatically toggle button on the graphics window wisely. That is, since surfaces often take a long time to build, changing viewing parameters such as the probe radius can cause long delays. By default, each time you hit the probe radius button, VMD rebuilds the surface. If you want to reduce or enlarge the probe radius by several increments, then you would end up rebuilding the surface multiple times. By toggling the afore-mentioned button, you can force VMD to update on your command only. This trick is sometimes helpful with other representations as well.

For a much faster surface rendering method, see the descriptions of 'MSMS' [§ 6.1.20]. 'QuickSurf' [§ 6.1.18].

6.1.20 MSMS

Another molecular surface renderer is 'MSMS', a program written by Michael Sanner of Olsen's lab at Scripps. This program is much faster than Surf, and can be a better choice depending on how it is used. See the web page `http://www.scripps.edu/pub/olson-web/people/sanner/html/msms_home.html` for more details. Available options include

- Which Atoms – should the surface be of the selection (0) or of the contribution of this selection to the surface of all the atoms? (1)
- Sample Density – triangle density on the surface (typical values are 1.0 for molecules with more than one thousand atoms and 3.0 for smaller molecules)
- Probe Radius – Probe radius used to construct the molecular surface
- Representation Method – The surface can optionally be drawn using lines rather than solid triangles

There is an environment variable [§ 14.2] which can affect the MSMS display option:

- `MSMSSERVER` – location of the MSMS binary (defaults to `msms` which is assumed to be in the user's path) On Windows machines, sets this as a systemwide environment variable in the environment variables window found in the system properties control panel.

6.1.21 VolumeSlice

The 'VolumeSlice' representation draws a texture mapped two-dimensional slice from a volumetric data set already loaded into VMD using the `mol volume` [§ 9.3.20] text command, or by other means. The colors span the scalar value range of the data set, with red indicating low values and blue indicating high values in the data. The slice is drawn as a plane perpendicular to the X, Y, or Z axis, and can be positioned anywhere within the coordinate system of the volumetric data set. This feature is currently only available on machines that have full support for hardware 3-D texture mapping. On machines lacking 3-D texturing, nothing will be displayed. Future versions of VMD will greatly enhance the user interfaces and capabilities of this feature.

The following selectors control the VolumeSlice representation:

- Data Set – This controls which volume data set is referenced in the representation, since multiple volumetric data sets can be loaded for a single molecule.
- Slice Offset – The slice setting indicates the position of the volume slice along the chosen axis, in the coordinate system of the volumetric data, range 0 to 1.

- Slice Axis – The orthogonal axis along which the slice plane moves, can be X, Y, or Z.
- Render Quality – The quality can be set to either Low, or Medium. The Low setting causes the slice texture map to be rendered using the color nearest the sample point. A quality level of Medium indicates that the slice texture map will be rendered using bilinear interpolation.

6.1.22 Isosurface

The 'Isosurface' representation computes and draws a surface within a volumetric data field, on a 3-D surface corresponding to points with a single scalar value.

There are several settings which control how the isosurface is displayed.

- Data Set – This control selects which volume dataset is used for the isosurface calculation, since a given molecule can contain multiple volumetric data sets.
- Isovalue – The Isovalue control selects the value for which the isosurface will be computed. In the GUI, when dragging the isovalue slider, the drawn isosurfaces are temporarily calculated at a lower resolution to improve interactivity; to prevent this behavior, you can use the middle or right button (or the control/shift/alt modifier keys) while dragging the slider.
- Draw – This can be set to Points, Shaded Points, Wireframe, or Solid Surface. The default drawing mode is Points. When viewing very dense isosurfaces of huge volumetric maps, the Shaded Points drawing method can be an excellent compromise between the speed of the Points method and the quality of the Solid Surface method.
- Boundary – Setting the boundary to Box causes the volume data bounding box and coordinate axes to be drawn rather than the isosurface for the data. This is often useful when first working with volumetric data, and checking that the coordinate systems of the volume data and the molecule match.
- Step – This setting can be used to greatly reduce the resolution of the generated isosurface, by skipping voxels.
- Size – This sets the thickness of the point and line based isosurface representations.

This and other volumetric display features will be greatly expanded in forthcoming releases of VMD.

6.1.23 FieldLines

The 'FieldLines' representation computes lines that trace the result of integrating the motions of massless particles advected by the volume gradient vectors associated with each location in a volumetric dataset. VMD computes the volume gradient map when a volumetric dataset is initially loaded, and the particle advection routines use a simple trilinear interpolation of the volume gradients are along with a fast (but simple) application of Euler's method to advect the particles at each integration step. The user-adjustable gradient magnitude control affects which points within the volumetric dataset are considered candidates for field line seeds. The resulting set of seed points are the initial points from which particles begin advection/integration. The min and max length controls affect the minimum and maximum length of the resulting field lines that will be selected for display. Field lines shorter than the minimum or longer than the maximum are not displayed. Similarly, field lines that collide with a critical point in the dataset early in their integration are discarded.

6.1.24 Orbital

The 'Orbital' representation draws a molecular orbital isosurface corresponding to a user-defined wavefunction amplitude computed on a regularly spaced grid, resulting from the selected wavefunction type, spin, excitation, and orbital index [29, 30]. The size parameter controls the thickness of points and line isosurface representations, and the grid spacing parameter controls the density of the regular grid upon which the wavefunction amplitude is computed.

6.1.25 Beads

A bounding sphere is drawn in place of each residue in the atom selection. This representation can be used as a crude means of drawing very large structures in a space filling representation and can be particularly useful for animating trajectories.

6.1.26 Dotted

Same as 'VDW' [§ 6.1.6] except that the spheres are drawn dotted instead of solid. That is, a dot is placed at each of the vertices of the triangle making up each sphere. This can be used, for instance, to imitate a surface representation.

6.1.27 Solvent

This method is similar in spirit to the 'Dotted' [§ 6.1.26] representation in that it gives a quick estimate of the molecular surface with a collection of dots. However, it goes above and beyond the Dotted option by giving a more uniform coverage of the surface. The method that VMD uses to check for overlaps isn't technically correct, but it is fast and works quite well. A technical description of the algorithm is as follows:

For each point of the surface distribution (of radius r = atom radius + probe radius) of atom i, check each of the atoms j to which it is covalently bound. If the point is too close to j, don't display it. Also, if the point is too close to any neighbor k of j ($k \neq i$) then don't draw it. This is fast since there aren't that many neighbors to check, but it doesn't omit parts of the surface in contact with atoms which aren't one or two bonds away. This can be considered a good thing since you might get a better idea of the contact surface.

There are three parameters for this option. One is the Probe Radius, which was mentioned in the description. If the probe radius is too large, the problem of over-lapping surfaces between non-connected atoms becomes more apparent. The second is Detail Level, which should probably be renamed "Density" as it determines the surface density of the distributions. The higher the detail, the higher the density. The final option is the Representation Method. By default the surface is drawn as a collection of points, but a point is a pixel in size regardless of the scale of the molecule, so when scaled small the surface density appears high, and when scaled large, the density appears low. Method 2 draws little plus signs instead of points, which does scale better so the density appears more contant. Method 3 draw lines between the surface points that are on the same atom, but makes no attempt to connect the two spheres.

Thanks to Jan Hermans for implementation pointers and thanks again to Jon Leech for the code to compute the uniform point distributions. That code was included as part of the 1.x distribution.

6.2 Coloring Methods

VMD maintains a database of the colors used for the molecules and other graphical objects which are visible in the display window. It keeps track of

- color name definitions - its RGB value;
- mappings from a color category to color name - so residue name MET is colored yellow
- the current color scale - red to white to blue, and several related parameters

There are 1057 colors available in VMD, with color ids ranging from 0 to 1056. The first 33 are, in order: blue, red, gray, orange, yellow, tan, silver, green, white, pink, cyan, purple, lime, mauve, ochre, iceblue, black, yellow2, yellow3, green2, green3, cyan2, cyan3, blue2, blue3, violet, violet2, magenta, magenta2, red2, red3, orange2, and orange3.

The next group of 1024 colors (from 33 to 1056) are colors used in the color map, These can be set to one of several ranges with the Color window or the `color` text command: red→green→blue, red→white→blue, or black→white, etc. There are no names for the specific colors. The color map will be discussed in more detail in a section to follow.

6.2.1 Color categories

VMD maintains a database of the colors used for the molecules and the other graphical objects in the display window. The database consists of several color *categories*; each color category contains a list of names, and each name is assigned a color. For example, there is a Resname color category, and within this category there are many names; one for each of the available residue names. Some of these are `ALA`, `CYS`, and `PRO`. Each name can be assigned a color from a list of 33 available colors called the *color map*. The RGB value of each color can be modified directly in the Color window [§5.4.9]. To color items in a gradation manner, there are additional 1024 colors used in the color scale [§6.2.4].

The different color categories in VMD are listed in table 6.2. The Color window can be used to change the assignment of colors to the names in each of these categories. For example, to change the color used to draw Arginine residues when molecules are colored by residue, you would use the Color window, select the 'Resname' category, select the 'Arg' name there, and then pick the color to use for Arginine's from the list of colors next to the names.

6.2.2 Coloring Methods

As described in chapter 6, each representation for a molecule has a specific *coloring method*. The coloring method determines how the color for each atom in the representation (view) is determined. These different methods use the colors assigned to the names in the categories listed above, and use those names to color the atoms. Molecular drawing methods which also draw the bonds between atoms will always color each half of the bond separately, using the color of the nearest atom for each half. Table 6.3 lists the different coloring methods available. The description for each method explains the source of the information used to determine the color.

6.2.3 Coloring by color categories

The default method is to color by the atom name. The way it works is that there is a color category called 'Name' which contains a list of all the atom names (e.g., CA, N, O5', and H) that have been

Category	Contents
Display	Color of background, gradient, depth cueing, text
Axes	The components of the axes
Name	The available atom names (color by Name)
Type	The available atom types (color by Type)
Element	Atomic elements (color by Element), with "X" for unknown
Resname	The residue names (color by ResName)
Restype	The residue types (color by ResType)
Chain	The one-character chain identifier.
Segname	The segment names (color by SegName)
Conformation	The available conformation codes (color by Conformation)
Molecule	The names assigned to each molecule (color by Molecule)
Highlight	The protein, nucleic, and non-backbone colors
Structure	The secondary structure type (helix, sheet, coil) (color by Structure)
Surface	The surface types
Labels	The different labels (atoms, bonds, etc.)
Stage	The colors for the checkboard stage

Table 6.2: Color categories used in VMD.

loaded into VMD. Each name is assigned one of the 16 main colors (e.g., cyan, blue, red, and white). When the drawing representation needs a color for a specific atom, it looks in the appropriate color category and finds that CA is colored cyan, N is blue, and so on.

Most of the coloring methods are based on color categories, so coloring by 'ResName' colors each residue name differently, 'SegName' colors each segment differently, and so on. The mapping between a given item in a color category and a color can be changed using the Color window [§5.4.9]. This allows users to make atoms with the name CA be black and the residue CYS be yellow. Some attention was given to making the colors reasonable, so that oxygens are red, nitrogens blue, sulphur and cysteines yellow, etc.

6.2.4 Color scale

Several of the coloring methods, including 'Beta', 'Charge', and 'Occupancy', describe a range of floating point values rather than a set of names. These are colored via the *color scale*, which is a list of 1024 smoothly changing colors. There are many color gradations available. All of them consist of transformations of three colors. For instance, "RGB" colors the smallest value red, values near the middle of the scale are green, and the largest values are blue. Colors in-between are linear mixes of the two colors. The list of available gradations is given below.

The minimum of the range of values is linearly scaled and shifted to start at 0 and end at 1. Assume the color scale is RGB. For a given value of x in the scale range [0..1], the RGB value is found first from a linear scaling based on the midpoint. If x = 0, R is 1 (for maximum red). This continues linearly until x = midpoint, at which point, R is 0 and stays 0. The green component is 0 at both x = 0 and x = 1 and is 1 at the midpoint. Linear scaling occurs in between. The blue component is 0 for x <= midpoint, and 1 for x = 1.

An additional term, "min", is added to each of the component terms before they are merged. This shifts the final colors more towards white or black. Min can take on values from -1 to 1.

Method	Description
Name	Atom name, using the Name category
Type	Atom type, using the Type category
Element	Atomic element, using the Element category
ResName	Residue name, using the Resname category
ResType	Residue type, using the Restype category
ResID	Residue identifier, using the resid mod 16 for the color
Chain	The one-character chain identifier, using the Chain category
SegName	Segment name, using the Segname category
Conformation	Conformation, e.g. PDB alternate location identifier
Molecule	Molecule all one color, using the Molecule category
Structure	Helix, sheet, and coils are colored differently
ColorID	Use a user-specified color index (from 0 to 15)
Beta	Color scale based on beta value of the PDB file
Occupancy	Color scale based on the occupancy field of the PDB file
Mass	Color scale based on the atomic mass
Charge	Color scale based on the atomic charge
Pos	Color scale based on radial distance from the molecule center
PosX, PosY, PosZ	Color scale based on axial distance from the molecule center
User, User2, User3, User4	Color scale assigned by per-atom values for each timestep
PhysicalTime, Timestep	Color scale based on the physical (simulation) time or timestep index associated with the displayed trajectory frame
Velocity	Color scale based on the per-atom velocity value associated with the displayed trajectory frame
Fragment	Color scale based on the VMD fragment index
Index	Color scale based on the VMD atom index
Backbone	Backbone atoms green, everything else is blue
Throb	Color scale animated by the current wall clock time
Volume	Surfaces are colored by the linked volumetric data set

Table 6.3: Molecular coloring methods.

There is only one color scale used at a time so it is impossible to display objects colored by multiple different color scales.

6.2.5 Materials

VMD allows users to apply a materials property to the molecular models they create. The material determines such things as how transparent an object is, or how shiny, or how large the specular reflections are. Making objects semi-transparent is a potentially powerful means of viewing multiple layers of the molecule simultaneously. Imagine a protein on the surface of, and extending part way into, a membrane. One way to visualize the extent of the penetration is to represent the lipids as 'Bonds' and make them transparent. That will show the membrane without completely obstructing the view of the protein.

VMD maintains a database of materials which can be applied to any representation in the system, much like the database for colors. There are two default materials, "Opaque" and "Transparent", which cannot be modified. Each material is defined by five settings, as follows:

Method	Description
RWB	small=red, middle=white, large=blue
BWR	small=blue, middle=white, large=red
RGryB	small=red, middle=gray, large=blue
BGryR	small=blue, middle=gray, large=red
RGB	small=red, middle=green, large=blue
BGR	small=blue, middle=green, large=red
RWG	small=red, middle=white, large=green
GWR	small=green, middle=white, large=red
GWB	small=green, middle=white, large=blue
BWG	small=blue, middle=white, large=green
BlkW	small=black, large=white
WBlk	small=white, large=black

Table 6.4: Available Color Scale Gradations.

- Ambient: The ambient coefficient describes how strongly the material reflects ambient light. Ambient light provides a uniform illumination of objects with a background lighting of the object color. The ambient light factor is generally used to moderate the effects of shadows from direct lighting, making shadows less dark than they otherwise would be.
- Diffuse: Diffuse reflections are independent of the viewing direction, but depend on the direction of the light source with respect to the surface of the displayed object.
- Specular: The specular coefficient describes the intensity of specular highlights. The higher the specular value, the brighter the resulting highlights.
- Shininess: The shininess coefficient describes the breadth of the angle of specular reflection. The smaller the number the broader the angle and the rougher objects appear. The larger the value of shininess, the narrower the angle of specular reflection, and the smoother the surface. Default corresponds to a Phong exponent of 40.
- Mirror: The mirror coefficient describes the mirror reflectivity of a surface. When the scene is rendered using ray tracing, surfaces with mirror reflectivity will show reflections much like a mirror-polished metal surface.
- Opacity: The opacity coefficient describes how opaque the surface is; 1 is solid, 0 is transparent. By default, transparent objects are drawn with Opacity set to 0.3.
- Outline: The outline coefficient controls shading of sillhouette edges, darkening the visible edges of surfaces where they are nearly perpendicular to the camera view direction. The outline parameter scales the degree of edge shading (darkening).
- OutlineWidth: The outlinewidth coefficient controls the angular width of nearly perpendicular sillhouette edge that is shaded.

For details regarding these material properties, consult an elementary graphics book such as Foley & Van Dam (Computer Graphics).

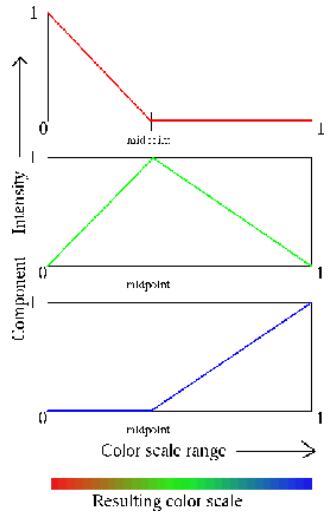


Figure 6.1: Example showing red/green/blue gradients summed to produce the color scale.

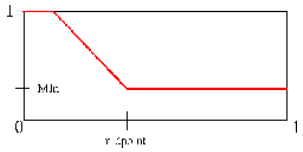


Figure 6.2: The shift to the red component of the RGB scale caused by the value of "min".

6.3 Selection Methods

VMD has a rather powerful atom selection language available. It is based around the assumption that every atom has a set of associated with it values which can be accessed through keywords. These values could be boolean (is this a protein atom?), numeric (as in the atom index or atomic mass), or string (the atom name). The values can even be referenced via a Tcl array.

To start off, here are some examples of valid selection commands in VMD. Following these will be a more in depth description of how selections work.

```
name CA
resid 35
name CA and resname ALA
backbone
not protein
protein (backbone or name H)
name 'A 1'
name 'A *'
name "C.*"
mass < 5
numbonds = 2
```

```
abs(charge) > 1
x < 6 and x > 3
sqr(x-5)+sqr(y+4)+sqr(z) > sqr(5)
within 5 of name FE
exwithin 3 of protein
protein within 5 of nucleic
same resname as (protein within 5 of nucleic)
protein sequence "C..C"
name eq $atomname
```

There are two types of selection modes. The first is a keyword followed by a list of either values or a range of values. For example,

```
name CA
```

selects all atoms with the name CA (which could be a C_α or a calcium);

```
resname ALA PHE ASP
```

selects all atoms in either alanine, phenylalanine, or asparagine;

```
index 5
```

selects the 6th atom (in the internal VMD numbering scheme).

VMD can also do range selections, similar to X-PLOR's ':' notation:

```
mass 5 to 11.5
```

selects atoms with mass between 5 and 11.5 inclusive,

```
resname ALA to CYS TYR
```

selects atoms in alanine, arginine, asparagine, aspartic acid, cystine, and also tyrosine.

The keyword selection works by checking each term on the list following the keyword. The term is either a single word (eg, `name CA`) or a range (eg `resid 35 to 90`).

The method for determining the range checking is determined from the keyword data type; numeric comparisons are different than string comparisons. The comparison should work as expected so that "8" is between "1" and "11" in a numeric context but not in a string one. This may lead to some peculiar problems. Some keywords, such as `segname`, can take on string values but can also be used by some people as a number field. Suppose someone labeled the `segname` field with the numbers 1 through 12 on the assumption that they are numbers. That person would be rather confused to find that `segname 1 to 11` only returns two segments. Also, strings will be converted (via `atof()`) to a number so if the string isn't a number, it will be given the value of 0. It is possible to force a search to be done in either a string or numeric context using the relational operator discussed in §6.3.6

Selections can be combined with the boolean operators `and` and `or`, collected inside of parenthesis, and modified by `not`, as in

```
(name CA or name CB) and mass 12 to 17
```

which selects all atoms name CA or CB and have masses between 12 and 17 amu (this could be used to distinguish a C-alpha from a calcium). VMD has operator precedence similar to C so leaving the parentheis out of the previous expression, as in:

```
name CA or name CB and mass 12 to 17
```

actually selects all atoms named CA or those that are named CB and have the appropriate mass.

6.3.1 Definition of Keywords and Functions

The keywords available for selecting atoms in VMD are listed in tables 6.5 and 6.6 at the end of this chapter. If a keyword definition is followed by *bool*, it is either on or off. If followed by *str* it takes a value in the string context. If followed by *num* it takes a value in the number context.

Table 6.7 lists the built-in functions which may be used in atom selection expressions with keywords which take on a numeric value.

Table 6.8 lists the built-in atom selection keywords which may be used in atom selection expressions to query the values of an underlying volumetric map in the same molecule. These are read-only.

6.3.2 Boolean Keywords

Some selections take no values. For example, `backbone` selects the backbone atoms of the protein and nucleic acids and `protein` selects protein atoms. Giving options to these selections is an error. The selections can be used in the same way as other selections, as in:

```
protein and backbone
nucleic or protein
```

In addition, if neither `and` nor `or` are located after a boolean keyword, then an implicit `and` is inserted, so that the following are valid:

```
protein name CA          (same as: protein and name CA)
nucleic backbone
```

6.3.3 Short Circuiting

The boolean logic in VMD does *short circuit* evaluation on an element-wise basis. For instance, given one atom, if `X` is true then `X or Y` will be true regradless of the value of `Y`, so there is no need to evaluate it. Similarly, if `X` is false, then `X and Y` will also be false, so `Y` again need not be evaluated.

Knowing how short circuit selections work can speed up several types of selections. Consider a system with a large number of waters and a protein. The expression `protein and segname < 10` is faster than `segname < 10 and protein` since in the first selection only the atoms which are proteins have the `segname` converted to a number, while in the second selection, all the segment names are converted.

The `within` selection has its own form of short circuiting. The command can be interpreted as "find the atoms of A which are withing a given distance from B," and if A isn't given, search all the atoms. The search done in VMD takes a time roughly proportional to the number of atoms in A multiplied by the number of atoms in B, so reducing the number of atoms in A (i.e., by not testing every atoms) make the search faster.

Using the system with a lot of water and a protein, compare the selection
`protein within 5 of resid 1`
to `(within 5 of resid 1) and protein`.
The first is very fast as it does a distance search between all the protein atoms and all the atoms in resid 1. However, the second selection searches through all the atoms for those which are within 5 Å of resid and then finds which of those are protein atoms.

6.3.4 Quoting with Single Quotes

VMD allows two types of quoting mechanisms, single and double quotes. Single quotes are used to include spaces and other non-alphanumeric characters. Believe it or not, there are some residue names with a space in them, so they can be referenced as, for example,

```
resname 'A 1'
```

More importantly, ribose atoms can be given names like `C5'` or `C5*` (depending on the age of the PDB record). The lexer in VMD has been modified so that `C5'`, `O"`, and `N''` can be used without quotes, but it cannot handle an unquoted asterisk (`*` conflicts with multiplication and the parser is not able to resolve the difference). Some examples are:

```
name 'O5*'
segname 'A *'
name O5'
```

Quotes may also be used to get around a reserved selection word, like `x`. The selection command `segname x` will give an error because `x` is another keyword. Instead, use `segname 'x'`. There is an escape mechanism for including single quotes inside a single quoted string which uses a backslash ('\') before the single quote. This allows unusual names like `C '` to be quoted as `'C \''`.

```
segname x      <---- error; conflicts with the 'x' keyword
segname 'x'
name 'O5\''
```

Also, double quotes (discussed in the next section) can be used, as in `"C '"` or `"C \*"`.

6.3.5 Double Quotes and Regular Expressions

Double quotes around a string are used to specify a regular expression search (compatible with Perl 5.005, using the Perl-compatible regular expressions library written by Philip Hazel). If you don't know how to use them, try consulting the man pages for `ed`, `egrep`, `vi`, or `regex`. If not, read the Perl docs, or get any one of a number of books including the O'Reilly and Associates Sed and Awk book. The following examples show just a few ways that regular expressions can be used within VMD.
Selection of all atoms with a name starting with `C`:

```
name "C.*"
```

Segment names containing a number:

```
segname ".*[0-9]+.*"
```

Multiple terms can be provided on the list of matching keywords. This example selects residues starting with an `A`, the glycine residues, and residues ending with a `T`. As with a string, a regular expression in a numeric context gets converted to an integer, which will always be zero:

```
resname "A.*" GLY ".*T"
```

Selections containing special characters such as +, −, or ∗, must be escaped with the `\` character. In order to select atoms named `Na+`, one would use the selection:

```
name "Na\+"
```

In brief, a regular selection allows matching to multiple possibilities, instead of just one character. Table 6.9 shows some of the methods that can be used.

There are many ways to do some selections. For example, choosing atoms with a name of either CA or CB can be done in the following ways:

```
name CA CB
name "CA|CB"
name "C[AB]"
name "C(A|B)"
```

Several caveats for those who already understand regular expressions. VMD automatically prepends "`^(`" and appends "`)$`" to the selection string. This makes the selection `O` match only `O` and not `OG` or `PRO`. On the other hand, putting `^` and `$` into the command won't really affect anything, selections that match on a substring must be preceded and followed by ".*", as in `.*O.*`, and some illegal selections could be accepted as correct, but strange, as in `C)|(O` , which gets converted to `^(C)|(O)$` and matches anything starting with a C or ending with an O.

A regular expression is similar to wildcard matching in X-PLOR. Table 6.10 is a list of conversions from X-PLOR style wildcards to the matching regular expression.

6.3.6 Comparison selections

Comparisons can be used in VMD to do atom selections like `mass < 5`, which selects atoms with mass less than 5 amu, and `name eq CA`, which is another way of choosing the CA atoms. The underlying idea for the comparison selection is also based on the concept that every atom has a property as specified by a keyword. When the keyword is given in the expression, the array (or vector) of the corresponding values is constructed, and the size of the array is the same as the number of atoms in the molecule. (If a single number or string is given instead of a keyword, the array consists of copies of that given value.) The operations, like addition, multiplication, string matching, and comparison, are then applied element-wise along the array. This type of selection is similar to the vector statement in X-PLOR.

Take the example `mass < 5` when applied on water, which has an oxygen of mass 15.9994 and two hydrogens of mass 1.008. VMD sees the keyword **mass** and constructs the array [15.9994, 1.008, 1.008], then sees the "5" and makes the array [5, 5, 5]. It then compares each term of the array and returns with the boolean array [False, True, True] (since 15.9994 is not less than 5, but 1.008 is). This final boolean array is then used to determine which atoms are selected; in this case, the hydrogens.

More complicated comparison selections can be constructed, either from arithmetic operations or by using some of the standard math functions (the functions are listed in Table 6.7). Probably the most often used function will be `sqr`, which squares each element of the array. Thus, the command to select all atoms within 5 Å of a point (x,y,z) = (3,4,-5) in space is:

```
sqr(x-3)+sqr(y-4)+sqr(z+5) <= sqr(5)
```

6.3.7 Comparison Operators

There are two types of comparison operators — numeric and string — which allow the user to specify the appropriate comparison function. Suppose the segment name, which takes on a string value, contains the names '11', and '8'. VMD cannot figure out if '8' should be less than '11' (in

the numeric sense) or greater than '11' (in the lexographical sense). Instead of trying to resolve this problem through some sort of internal heuristics, VMD leaves it up to the user so that `8 < 11` but `11 lt 8`. (Perl users should recognize this solution.)

The numeric comparisons are the standard ones: `<`, `<=`, `=` or `==`, `>=`, `>`, and `!=`. The corresponding string comparisons are: `lt`, `le`, `eq`, `ge`, `gt`, and `ne`. As in perl there is a "match" operator, `=~`, so that

```
'CA' =~ "C.*"
segname =~ "VP[1-4]" (matches VP1, VP2, VP3, and VP4, present in some
                      virus structures)
```

are valid. No distinction is made between single and double quotes.

6.3.8 Other selections

sequence

VMD supports selection based on the one-letter amino acid sequence with the `sequence` selection keyword. This allows selections of the form

```
sequence APD
sequence "C..C"       (might be used to pick out zinc fingers)
sequence AATCGGAT
```

Unlike the other string selection commands which take one of three types of strings, all the strings for `sequence` are taken as regular expressions (though strings with non-alphanumerics must still be quoted to get past the input parser). The method works by taking each of the protein and nucleic acid fragments (pfrag and nfrag) in turn and constructing the one-letter amino acid sequence. If a regular expression matches any of the sequence, the atoms in the matching residues are selected. Multiple matches are allowed, though they cannot overlap. As is usual with regular expressions, the largest possible match is made, so take care with expressions like `C.*C`.

within and same

Two useful types of selection mechanisms available in VMDare: `within <number> of <selection>` and `same <keyword> as <selection>`. The first selects all atoms within the specified distance (in Å) from a selection, including the selection itself. Therefore, the command:

```
within 5 of name FE
```

selects all atoms within 5 Å of atoms named FE. One common use for this command is to limit the region of atoms shown on the screen. Another is to find atoms that may be involved in interactions. For instance:

```
protein within 5 of nucleic
```

finds the protein atoms that are nearby nucleic acids. Some selections may be sped up by short circuiting [§6.3.3].

A related atom selection construct is `exwithin`, short for 'exclusive within'. The atom selection `(within 3 of protein) and not protein` is equivalent to `exwithin 3 of protein`.

The `same <keyword> as <selection>` finds all the atoms which have the same 'keyword' as the atoms in the selection. This can be used for selections like

```
same fragment as resid 35
```

which finds all the atoms attached to residue id 35. Any keyword can be used, so selections like

```
same resname as (protein within 5 of nucleic)
```

are fine, although weird. The perhaps the most useful keyword for this command is `residue`, so you can say `same residue as ...`.

Finding contact residues

Suppose you want to view the atoms in "A" which are in contact with "B". Use the `within <distance> of <selection>` selection command. For purposes of demonstration, let A be protein, B be nucleic, and define contact as an atom in A which is within 2 Å of an atom in B. Then the selection command is

```
protein within 2 of nucleic
```

If you want to see all the residues of A which have at least one atom in contact with B, use

```
same residue as (protein within 2 of nucleic)
```

Keyword	Arg	Description
all	*bool*	everything
none	*bool*	nothing
name	*str*	atom name
type	*str*	atom type
index	*num*	the atom number, starting at 0
serial	*num*	the atom number, starting at 1
atomicnumber	*num*	atomic number (0 if undefined)
element	*str*	atomic element symbol string ('X' if undefined)
altloc	*str*	alternate location/conformation identifier
chain	*str*	the one-character chain identifier
residue	*num*	a set of connected atoms with the same residue number
protein	*bool*	a residue with atoms named `C, N, CA,` and `O`
nucleic	*bool*	a residue with atoms named `P, O1P, O2P` and either `O3', C3', C4', C5', O5'` or `O3*, C3*, C4*, C5*, O5*`. This definition assumes that the base is phosphorylated, an assumption which will be corrected in the future.
backbone	*bool*	the `C`, `N`, `CA`, and `O` atoms of a protein and the equivalent atoms in a nucleic acid.
sidechain	*bool*	non-backbone atoms and bonds
water, waters	*bool*	all atoms with the resname `H2O, HHO, OHH, HOH, OH2, SOL, WAT, TIP, TIP2, TIP3` or `TIP4`
fragment	*num*	a set of connected residues
pfrag	*num*	a set of connected protein residues
nfrag	*num*	a set of connected nucleic residues
sequence	*str*	a sequence given by one letter names
numbonds	*num*	number of bonds
resname	*str*	residue name
resid	*num*	residue id
segname	*str*	segment name
x, y, z	*float*	x, y, or z coordinates
radius	*float*	atomic radius
mass	*float*	atomic mass
charge	*float*	atomic charge
beta	*float*	temperature factor
occupancy	*float*	occupancy
user	*float*	time-varying user-specified value
at	*bool*	residues named `ADA A THY T`
acidic	*bool*	residues named `ASP GLU`
acyclic	*bool*	"protein and not cyclic"
aliphatic	*bool*	residues named `ALA GLY ILE LEU VAL`
alpha	*bool*	atom's residue is an alpha helix
amino	*bool*	a residue with atoms named `C, N, CA`, and `O`
aromatic	*bool*	residues named `HIS PHE TRP TYR`
basic	*bool*	residues named `ARG HIS LYS`
bonded	*bool*	atoms for which numbonds > 0
buried	*bool*	residues named `ALA LEU VAL ILE PHE CYS MET TRP`
cg	*bool*	residues named `CYT C GUA G`
charged	*bool*	"basic or acidic" 85
cyclic	*bool*	residues named `HIS PHE PRO TRP TYR`

Table 6.5: Atom selection keywords.

Keyword	Arg	Description
hetero	*bool*	"not (protein or nucleic)"
hydrogen	*bool*	name "[0-9]?H.*"
large	*bool*	"protein and not (small or medium)"
medium	*bool*	residues named `VAL THR ASP ASN PRO CYS ASX PCA HYP`
neutral	*bool*	residues named `VAL PHE GLN TYR HIS CYS MET TRP ASX GLX PCA HYP`
polar	*bool*	"protein and not hydrophobic"
purine	*bool*	residues named `ADE A GUA G`
pyrimidine	*bool*	residues named `CYT C THY T URI U`
small	*bool*	residues named `ALA GLY SER`
surface	*bool*	"protein and not buried"
rasmol	*str*	translates Rasmol selection string to VMD
alpha_helix	*bool*	atom's residue is in an alpha helix
pi_helix	*bool*	atom's residue is in a pi helix
helix_3_10	*bool*	atom's residue is in a 3-10 helix
helix	*bool*	atom's residue is in an alpha or pi or 3-10 helix
extended_beta	*bool*	atom's residue is a beta sheet
bridge_beta	*bool*	atom's residue is a beta sheet
sheet	*bool*	atom's residue is a beta sheet
turn	*bool*	atom's residue is in a turn conformation
coil	*bool*	atom's residue is in a coil conformation
structure	*str*	single letter name for the secondary structure
phi, psi	*float*	backbone conformational angles
within	*str*	selects atoms within a specified distance of a selection (i.e `within 5 of name FE`).
exwithin	*str*	exclusive within, equivalent to `(within 3 of X) and not X`.
same	*str*	selects atoms which have the same keyword as the atoms in a given selection (i.e. `same segname as resid 35`)
ufx, ufy, ufz	*num*	force to apply in the x, y, or z coordinates

Table 6.6: Atom selection keywords (continued).

Function	Description
sqr(x)	square of x
sqrt(x)	square root of x
abs(x)	absolute value of x
floor(x)	largest integer not greater than x
ceil(x)	smallest integer not less than x
sin(x)	sine of x
cos(x)	cosine of x
tan(x)	tangent of x
atan(x)	arctangent of x
asin(x)	arcsin of x
acos(x)	arccos of x
sinh(x)	hyperbolic sine of x
cosh(x)	hyperbolic cosine of x
tanh(x)	hyperbolic tangent of x
exp(x)	"e to the power x"
log(x)	natural log of x
log10(x)	log base 10 of x

Table 6.7: Atom selection functions.

Function	Arg	Description
vol$N$	*float*	value of the voxel of the volumetric data of ID N nearest to the atom
interpvol$N$	*float*	interpolated value of the voxels of the volumetric data of ID N around the atom

Table 6.8: Read-only atom selection keywords which may be used to query the values of an underlying volumetric map in the same molecule. The value of N, which can be 0 to 7 inclusively, refers to the volID of the underlying volumetric data (*e.g.*, you could type `interpvol2`).
Read-only atom selection keywords for querying volumetric data

Symbol	Example	Definition
.	`. , A.C`	match any character
[]	`[ABCabc] , [A-Ca-c]`	match any char in the list
[~]	`[~Z] , [~XYZ] , [^x-z]`	match all except the chars in the list
^	`^C , ^A.*`	next token must be the first part of string
$	`[CO]G$`	prev token must be the last part of string
*	`C* , [ab]*`	match 0 or more copies of prev char or regular expression token
+	`C+ , [ab]+`	match 1 or more copies of the prev token
|	`C|O`	match either the 1st token or the 2nd
\(\)	`\(CA\)+`	combines multiple tokens into one

Table 6.9: Regular expression methods.

X-PLOR Wildcard	Description	Regular Expression
*	matches any string	.*
%	matches a single character	.
+	matches any digit	[0-9]
#	matches any number	[0-9]+

Table 6.10: Regular expression conversions.

Chapter 7

Viewing Modes

There are many different viewing modes available. These show the scene in orthographic or perspective views, and in several mono- and stereo- graphic displays. The stereo mode can be changed using the `stereo` entry in the Display menu or the text command `display stereo` *`mode`*.

7.1 Perspective/Orthographic views

In the perspective view (the default), objects which are far away are smaller than those nearby. In the orthographic view, all objects appear at the same scale. Since some prefer one over the other, both options are available. Perspective viewpoints give more information about depth and are often easier to view because you use perspective views in real life. Orthographic viewpoints make it much easier to compare two parts of the molecule, as there is no question about how the viewpoint may affect the perception of distance.

7.2 Monoscopic Modes

When you normally look at objects, your two eyes see slightly different images (because they are located at different viewpoints). Your brain puts the images together to generate a stereoscopic viewpoint. When generating a single image for the computer display, the default calculations (mode Stereo Off) assume there is one eye centered between where two eyes would be. For stereo, the left and right eye views need to be generated independently. Choosing mode Left produces the left eye viewpoint, while Right produces the right eye viewpoint. The left and right monoscopic modes are most useful when exporting scenes to external ray tracers.

7.3 Stereoscopic Modes

Molecules may be rendered in stereo, which can greatly enhance the appearance and visual content of the displayed systems. There are several stereo formats available:

1. Quad-buffered stereo, (aka CrystalEyes in older versions), which requires a stereo-capable monitor, quad-buffered stereo video board or GPU, stereo emitters and stereo glasses equipped with liquid crystal or polarized lenses.

2. Above/Below stereo;

3. Side-by-side stereo for paper-printed images;
4. HDTV Side-by-side stereo for stereo flat panel displays and TVs
5. Anaglyph stereo (requires stereo-capable monitor, quad-buffered stereo video board, and red-blue horror-movie-style stereo glasses).
6. Checkerboard, also known as line blanking stereo, works with compatible shutter glasses and DLP projectors.
7. Column-interleaved, works with compatible shutter glasses and LCD panel displays.
8. Row-interleaved, also known as line blanking stereo, works with compatible shutter glasses and LCD panel displays.

7.3.1 Quad-buffered Stereo

Quad-buffered (aka CrystalEyes) stereo is the name used within VMD for the quad-buffered frame-sequential stereo display mode found on professional graphics workstations. Quad-buffered stereo generally yields the highest quality output, and is therefore the most desirable stereo mode to use when available. Since quad-buffered stereo requires more video memory, and special display synchronization circuitry, this mode is usually only available on professional-grade GPUs such as AMD FireGL, NVidia Quadro, and similar products. Typically this mode is used to drive LCD shutter glasses with a CRT display, 120Hz LCD panels, or various high-end stereo-capable projection systems.

Quad-buffered stereo mode provides separate left and right eye frame buffers. It allows the a window display in stereo, while all other windows appear as normal. The display must be set in a stereo-capable mode before starting VMD, using the appropriate operating system-specific utilities to set the video mode prior to launching VMD.

Once set in the proper display mode, start VMD as normal, and select 'QuadBuffered stereo' from the Display menu. The image should switch to two images nearly superimposed, but slightly offset.

7.3.2 Side-By-Side and Cross-Eyed Stereo

Side-by-side stereo means that the normal display is divided into two halves, a left view and a right view, each occupying one-half of the original display area. Each view displays the current molecules from a slightly different perspective, corresponding to the left and right eye of the viewer. The images are separated, however, so to actually see a 3D object you must direct your eyes until the two images are on top of each other, and then focus on the resulting image until you can see it as three-dimensional.

There are two ways of placing the images. In wall-eyed stereo, the left eye's image is located on the left side of the display, and the right eye's image is on the right. This is the standard method for displaying stereo images in publications as it works well when the display (in this case, the piece of paper) is close to the eyes. It is called wall-eyed because your eyes are directed the same way they would be if looking at a distant wall. In VMD, this method is referred to as "SideBySide" stereo.

In cross-eyed stereo, the left eye's image is located on the right side of the display, and the right eye's image is on the left, and hence the name cross-eyed. This is mostly used for distant displays

(such as overhead projections) as it is much easier to cross eyes at that range than use the wall-eyed method – you are already looking at the wall. In VMD, this method is referred to as "CrossEyes" stereo. This mode is supported by all GPUs.

7.3.3 HDTV Side-by-side Stereo

This stereo mode is the same as the regular side-by-side stereo mode except that the aspect ratio of the displayed image is adjusted to work correctly on HDTVs and stereo flat panel displays such as DTI autostereoscopic LCD displays. This mode is supported by all GPUs.

7.3.4 Checkerboard Stereo

Checkerboard stereo works by interleaving the left and right eye views on every other pixel in the display, in a checkerboard pattern. This type of stereoscopic display mode is compatible with a range of DLP projectors and TV's, in combination with shutter glasses. The only special requirements for the graphics accelerator are that it provide a stencil buffer which is used to generate the alternating columns in the final image. This mode is generally supported by low-cost gaming GPUs.

7.3.5 Column Interleaved Stereo

Column-interleaved stereo works by interleaving the left and right eye views on every other vertical column in the display. The stereo hardware either separates them into two separate displays or blanks the even or odd columns in sync with shutter glasses, or otherwise makes them visible only to one or the other eye, in the case of autostereoscopic displays. The only special requirements for the graphics accelerator are that it provide a stencil buffer which is used to generate the alternating columns in the final image. This mode is generally supported by low-cost gaming GPUs.

7.3.6 Row Interleaved Stereo

Row-interleaved stereo, also referred to as scanline-interleaved, or line blanking stereo, works by interleaving the left and right eye views every other scanline in the display. The stereo hardware then decodes the interlaced signal and either separates them into two separate displays or blanks the even or odd scanlines to display only the left or right eye image at the same time that shutter glasses are polarized in the appropriate way. The only special requirements for the graphics accelerator are that it provide a stencil buffer which is used to generate the alternating scanlines in the final image. This mode is generally supported by low-cost gaming GPUs.

7.3.7 Anaglyph Stereo

Anaglyph stereo refers to the use of colors to separate the left and right eye views from each other. The user must wear glasses with colored lenses, such as the red-blue glasses one finds at some sci-fi and horror movie showings. Anaglyph stereo has one major disadvantage when compared with quad-buffered stereo, which is that its color rendition is severely constrained. This is an unavoidable limitation of anaglyph stereo, and it is up to the user to use color schemes for their molecules that still look visually pleasing in this mode. This mode is supported by all GPUs.

7.3.8 Stereo Parameters

A stereo image is generated by drawing two images from two different perspectives, one from the left eye and one from the right. The images are made by finding the view that would be seen by someone located inside the scene. The method uses two parameters to find the view; the *eye separation* and the *focal length*. The first defines the distance between the eyes and gives the parallax effect. Setting the separation to 0 will result in a flat 2D image, while setting it too large will give most people a headache.

The graphics model used by VMD assumes the eyes looking in front of the viewer and focusing at the same point the focal length away. If the focal length is 0, the viewer's eyes are crossed and looking at each other. A larger focal length will often help in creating a viewable image.

The two parameters can be changed with the text commands `display focallength` and `display eyesep`, or using the Display Settings window [§5.4.6].

In general, try to make the eye separation as large as possible without giving the viewer a migrane, and try to vary the focal length to cut down on double images. It may often help to translate the molecule forward or backward and also adjust the scaling, since there is typically an optimum position for a molecule for a given set of stereo parameters.

Chapter 8

Scene Export and Rendering

One of the most common tasks performed by users of VMD is producing images which can be loaded into other programs or used in printed documents, posters, slides, and transparencies. The Render window provides a simple mechanism for generating image files from snapshots of the VMD graphics window and through the use of external rendering and ray tracing programs.

8.1 Screen Capture Using Snapshot

The simplest way to produce raster image files in VMD is to use the "Snapshot" feature. The snapshot feature captures the contents of the VMD graphics window, and saves them to a raster image file. On Unix systems, the captured image is written to a 24-bit color Truevision "Targa" file. On Windows systems, the captured image is written to a 24-bit color Windows Bitmap, or "BMP" file. To use the `snapshot` feature, simply open the Render[§ 5.4.11] window and choose the `snapshot` option. VMD will capture the contents of the graphics window, and attempt to save the resulting image to the filename given in the Render window. You may find that it is important not to have other windows or cursors in front of the VMD graphics display when using snapshot, since the resulting images may include obscuring windows or cursors. This is a platform-dependent behavior, so you will need to determine if your system does this or not.

8.2 Higher Quality Rendering

Sometimes images produced by screen capture aren't good enough; you may want a very large, high quality picture, or a picture with shadows, reflections, or high quality rendering of transparent surfaces. While VMD generally produces nice looking images in its graphics window, it was designed to generate its images very rapidly to maximize interactivity, which precludes the use of photorealistic rendering techniques that would slow down the operation of whole program. Instead of producing high quality images directly, VMD writes scene description files which can be used as input to several popular scanline rendering and ray tracing programs. Tables 8.1 lists the currently supported output formats, and where appropriate rendering software may be obtained.

Making a raster image is usually a two step process, e.g. with the exception of the built-in renderers such as TachyonInternal, TachyonLOptiXInternal, and TachyonLOSPRayInternal, or their respective interactive variants. First you must make a scene description file suitable for the chosen rendering program, and then execute the program using the new file as input to produce the raster image output. The external rendering programs typically support different output file

formats, which may need to be converted to something more appropriate for you. It is impossible to predict what that might be, so we'll describe how to convert the different file types to Targa and let you use the tools listed in Table 8.1 to get what you need. Raster3D, Tachyon, and POV-Ray can produce Targa files, so you don't need to do anything but specify this output format. Rayshade creates RLE image files, which can be converted using ImageMagick. Radiance generates an .oct file, which can be converted with the `rview` and `rpict` commands included in the Radiance distribution.

The free program `display` from ImageMagick – see `http://www.imagemagick.org/` – should be able to read and convert between all of these formats.

We suggest using Tachyon or Raster3D as they are generally the fastest programs. These programs are easy to understand, and are fast even when rendering very complex molecules.

The generated scene files are plain text so they are very easy to modify. This is most often done to create a larger raster file, though some have other global options which you may wish to change. For instance, by default the Raster3D file turns shadows on. We suggest you consult the relevant renderer's documentation to determine what can be modified in the file.

To actually render the current image into an output file, first set up the graphics in VMD just as you wish the output to appear. Then, either use the Render window [§ 5.4.11], or the following text command, to create the input file and start the rendering program going:

render *method filename* [*render command*]

method is one of the names listed in the first column of table 8.1, and *filename* is the name of the file which will contain the resulting image processing program script. Any text following this will be used as a command to be run to process the file. If `%s` appear in the command string, they will be replaced with the name of the script file.

8.3 Caveats

When VMD creates the output file it will try to match the current view and screen size. For the most part it does a good a job but there can be some problems. The colors in the final raster image can sometimes look different from what is seen in the VMD graphics window. This is because the external rendering programs use different shading equations and algorithms from what VMD uses. Potential rendering discrepencies include:

- Geometry may look slightly different; in VMD curved surfaces are polygonalized and drawn using a number of polygonal facets, curved surfaces may be rendered entirely smoothly in the final output (which is generally looked upon as an improvement!)
- The rendered object colors or intensities may be slightly different due to different colormaps, gamma values, or lighting models; This is particularly true with the material properties used for performing complex shading. VMD's real-time rendering of these material properties is often simplistic or limited compared to full-fledged photorealistic renderers, so there can potentially be big differences between implementations of transparency, specular highlights, etc.
- Many of the external renderers do not support true orthographic rendering. This can be "faked" by translating the camera very far away from the molecule, followed by zooming the camera so that the image size is acceptable again. This will significantly decrease the perspective effect, but is not a true orthographic projection.

- The rendering commands do not currently support stereo output, so even if the display is currently in stereo mode, a non-stereo perspective will be used for the rendering program input script; Rendering in stereo is accomplished by setting the display mode to "left", then rendering an image, followed by "right", and rendering again. This will yield a stereo pair to the best of VMD's ability with the external rendering program.
- The near and far clipping planes are ignored by all external renderers;
- Text is generally not available as a graphics primitive in the renderer scene languages, so label text will not appear, although the lines of bond, angle, etc. labels will be drawn. The only exception is in Postscript output, which supports text output.
- Dotted spheres are not drawn with dots.
- The background color may be black, as not all output formats support a background color other than black;

8.4 One Step Printing

A frequently asked question is "How can I quickly get a printout of the VMD Display?" There are several one step solutions to this problem, a few are listed below:

- Choose the `snapshot` option and convert the resulting image to your desired image format using ImageMagick or similar tools.
- Choose the `TachyonInternal` option and convert the resulting image to your desired image format using ImageMagick or similar tools.

8.5 Making Stereo Images

Stereoscopic images can be rendered with a simple sequence of text commands, cycling between the left and right monoscopic stereo modes and exporting one scene for each eye:

```
display stereo left
render TachyonInternal left.tga
display stereo right
render TachyonInternal right.tga
```

External renderers don't always support the ability to draw stereo images. In principle, it is possible to write the scene to the file twice with the appropriate transformations applied to make the view correct for each eye, but then the shadows would be incorrect. Instead, we suggest making one image of the current scene, then shift the molecules to the left (or right) to make the other image. The text commands for this are something like:

```
display stereo off
render Raster3D left.r3d
trans by -.1 0 0
render Raster3D right.r3d
```

The two files must then be rendered to produce the rgb file. As it turns out, this method makes it easy to produce stereo images of ordinary Raster3D files. Since VMD can read the Raster3D format, all you have to do is read the file and then execute the commands listed above. The text commands for generating left or right views also have equivalents in the GUI under the `Stereo` option of the Display window.

8.6 Making a Movie

It is possible to make movies with VMD, through the use of Tcl or Python scripts, or with the "vmdmovie" extension included with VMD. Several movie making scripts are provided in the VMD script library on the VMD home page. These scripts can be used as-is, or they can be customized to perform complex animation tasks beyond the scope of this user guide. In general, movies are created by driving render commands with a script, producing a sequence of individual image files. When the script has completed rendering all of the individual frames, the images are ready for import into an animation package, or can be converted to one of several popular compressed movie formats by further processing. The "vmdmovie" extension provided with VMD completely automates the movie creation process, though it requires a number of software packages be installed in order to do the job. Please see the separate documentation on the movie scripts and "vmdmovie" in the VMD script library.

Name	Description
ART[1]	Simple VORT ray tracer
Gelato	NVIDIA Gelato PYG Format
PostScript	Simple Vector PostScript Output
POV3[2]	POV-Ray 3.x ray tracer
Radiance[3]	Radiosity ray tracer
Raster3D[4]	Fast raster file generator
Rayshade[5]	Rayshade ray tracer
RenderMan	PIXAR RenderMan RIB Format, render with Aqsis, Pixie, PRMan, RenderDotC
STL	Stereolithography format, triangles only
Tachyon[6]	High quality parallel ray tracer
TachyonInternal[6]	Fast, built-in Tachyon engine that generates images directly from VMD internal data structures with no intermediate step
TachyonLOptiXInternal	Fast, built-in GPU-accelerated Tachyon for NVIDIA GPUs (available on supported platforms)
TachyonLOptiXInteractive	Interactive, built-in, GPU-accelerated version of Tachyon for NVIDIA GPUs (available on supported platforms)
TachyonLOSPRayInternal	Fast, built-in OSPRay ray tracer for Intel CPUs (available on supported platforms)
TachyonLOSPRayInteractive	Interactive, built-in, OSPRay ray tracer for Intel CPUs (available on supported platforms)
VRML-1	Virtual Reality Markup Language V1.0
VRML-2	Virtual Reality Markup Language V2.0
Wavefront	Wavefront .OBJ/.MTL scene format, loads into 3DS Max, Blender, Maya, and others
X3D[7]	X3D declarative scene format
X3DOM[8]	Open source HTML5-based X3D viewing system

[1]Available from `http://bund.com.au/~dgh/eric/` along with the rest of VORT package
[2]See `http://www.povray.org/`
[3]See `http://radsite.lbl.gov/radiance/HOME.html`
[4]See `http://www.bmsc.washington.edu/raster3d/`
[5]See `http://graphics.stanford.edu/~cek/rayshade/rayshade.html`
[6]See `http://www.photonlimited.com/~johns/tachyon/`
[7]See `http://www.web3d.org/x3d/`
[8]See `http://www.x3dom.org/`

Table 8.1: Miscellaneous Rendering Options

Chapter 9

Tcl Text Interface

The Tcl text interface provides complete access to all the VMD commands. Anything that can be done from the menus can be done with VMD text commands.

9.1 Using text commands

Text commands can be entered into VMD in several ways:

- Commands can be entered by typing them at the VMD prompt in the text console window. This window normally contains the prompt `vmd >` . When other text (e.g., from a mouse pick) is displayed to the screen, it will scroll the screen up so the prompt is not at the last line of the screen. To make it reappear, press enter. When entering multi-line commands, an alternate prompt appears, `?` , and will not disappear until the command is finished. Sometimes it is waiting for a close to a double quote, open brace, or open bracket, while at other times it is waiting for a line that doesn't end in a backslash.

- Since you may not want to retype all the data in every time, there are two ways to read the data in from a text file. One is the `play` command. This reads a line from the file, executes it, then updates the screen and checks for any changes in the mouse or window input, so that VMD stays interactive during execution of the script. The second way is the Tcl command `source`. This reads the whole file before allowing the mouse and windows to respond to new input. This is often more efficient when your script contains many lines.

- On Unix/Linux platforms, if the file `.vmdrc` (see section 14.3.3) exists in your home directory, it is played at VMD startup. If you don't have a `.vmdrc` file, VMD uses a default script in the VMD installation directory. Similarly, at startup the `-e` command line flag can be used to specify an input file to be played after reading the `.vmdrc` file. The Windows version of VMD works similarly, though the startup file is named `vmd.rc`.

  A good use of the `.vmdrc file` is to specify which VMD menus you would like to have open when you start VMD and where they should be placed; see section 9.3.19) for information on usage.

9.2 Tcl/Tk

The standard distribution is compiled with Tcl, which add a complete scripting language including variables, loops, and conditionals along with a standard method for communicating with other programs via standard TCP/IP sockets. Versions 1.2 and later also include the Tk toolkit, for creating menus with buttons bound to one's favorite actions.

Tcl (short for Tool Command Language, developed by John Ousterhout) is an embeddable and extensible scripting language. In other words, Tcl sits inside VMD as a language interpreter where it can execute its standard language commands or the various VMD specific extensions.

VMD uses Tcl and Tk version 8.4.1. We refer you to `http://www.tcl.tk/` for more information about Tcl.

9.3 Tcl Text Commands

All Tcl commands in VMD are composed of one or more words or phrases separated by white space, and terminated by a newline. In Tcl, a "phrase" is text surrounded by double quotes or by a matching set of open and close braces. The first word of each command indicates the general purpose for the command, and the following words specify the exact type of command to execute. Table 9.1 summarizes the text commands in VMD by listing the first words, and describing the general purpose for commands starting with those words.

The commands described in the following sections are listed by name, and followed by a list of the available arguments. If an argument is optional, it is enclosed in `[]`s. If only one of a list of arguments is needed, the list is enclosed in `<>`s and the items are separated by `|`. Words in italics indicate a string or value to be specified by the user.

9.3.1 animate

These commands control the animation of a molecular trajectory and are used to read and write animation frames to/from a file or Play/Pause/Rewind a molecular trajectory.

- **dup** `[` **frame** *frame_number* `]` *molId*: Duplicate the given frame (default "now") of molecule *molId* and add the new frame to this molecule.
- **forward**: Play animation forward.
- **for**: Same as forward.
- **reverse**: Play animation backward.
- **rev**: Same as reverse.
- **pause**: Pause animation.
- **prev**: Go to previous frame.
- **next**: Go to next frame.
- **skip** *n*: Set stride to n+1 frames.
- **delete all**: Delete all frames from memory.

First Word	Description
animate	Play/Pause/Rewind a molecular trajectory.
atomselect	Create atom selection objects for analysis.
axes	Position a set of XYZ axes on the screen.
color	Change the color assigned to molecules, or edit the colormap.
colorinfo	(Tcl) Obtain color properties for various objects
display	Change various aspects of the graphical display window.
exit, quit	Quit VMD.
gettimestep	Retrieve a timestep as a binary Tcl array (use for plugins)
help	Display an on-line help file with an HTML viewer.
imd	Control the connection to a remote simulation.
label	Turn on/off labels for atoms, bonds, angles, dihedral angles, or springs.
light	Control the light sources used to illuminate graphical objects.
logfile	Turn on/off logging a VMD session to a file or the console.
material	Create new material definitions and modify their settings.
mdffi	MDFF density map synthesis and cross correlation commands
measure	Measure properties of moleculear structures.
menu	Control or query the on-screen GUI windows.
molecule or mol	Load, modify, or delete a molecule.
molinfo	Get information about a molecule or loaded file.
mouse	Change the current state (mode) of the mouse.
parallel	Execute commands in parallel on clusters or supercomputers.
play	Start executing text commands from a specified file.
render	Output the currently displayed image (scene) to a file.
rock	Rotate the current scene continually at a specified rate.
rotate	Rotate the current scene around a given axis by a certain angle.
scale	Scale the current scene up or down.
stage	Position a checkerboard stage on the screen.
tool	Initialize and control external spatial tracking devices.
translate	Translate the objects in the current scene.
user	Add new keyboard commands.
vmdinfo	(Tcl) Get information about this version of VMD
volmap	Create volumetric data based on molecular information
wait	Wait a number of seconds before reading another command. Animation continues.
sleep	Sleep a number of seconds before reading another command. Animation is frozen.

Table 9.1: Summary of core text commands in VMD.

- **speed** *n*: Set animation speed to *n*.
- **style once**: Set to play animation once.
- **style loop**: Set to loop through animation continuously.
- **style rock**: Set to play animation forward and back continuously.
- **styles**: Return a list of the available styles.
- **goto start**: Go to first frame.
- **goto end**: Go to last frame.
- **goto** *n*: Go to frame *n*.
- **read** *file_type filename* **[beg** *nb*] **[end** *ne*] **[skip** *ns*] **[waitfor** *nw*] [*molecule_number*]:

  Read data for *molecule_number* from *filename* of type *file_type*, beginning with frame *nb*, ending with frame *ne*, with a stride of *ns*. Return the number of frames read from this file; if the file contains more than this number, the remaining frames will be loaded during subsequent VMD display updates. By default, one frame will be loaded before the command returns. The `waitfor` option allows you to specify how many frames to load before returning. The `waitfor` parameter *nw* can be any integer, or `all`; choosing *nw* less than zero is the same as choosing `all`. If frames from other files are still being loaded when the animate command is issued, these frames will be loaded first.
- **write** *file_type filename* **[beg** *nb*] **[end** *ne*] **[skip** *ns*] **[waitfor** *nw*] **[sel** *selection*] [*molecule_number*]: Write data from *molecule_number* to *filename* of type *file_type*, beginning with frame *nb*, ending with frame *ne*, with a stride of *ns*. Return the number of frames written to this file; if more frames have been specified than this number, the remaining frames will be written during subsequent VMD display updates. By default, one frame will be written before the command returns. The `waitfor` option allows you to specify how many frames to write before returning. The `waitfor` parameter *nw* can be any integer, or `all`; choosing *nw* less than zero is the same as choosing `all`. Pass the name of an atom selection as *selection* to write only the selected atoms to the file.
- **delete [beg** *nb*] **[end** *ne*] **[skip** *ns*] [*molecule_number*]: Delete data for *molecule_number*, beginning with frame *nb*, ending with frame *ne*, and keep frames with a stride of *ns* (a stride of -1 implies to keep all frames).

9.3.2 atomselect

Atom selection is the primary method to access information about the atoms in a molecule. It works in two steps. The first step is to create a selection given the selection text, molecule id, and optional frame number. This is done by a function called `atomselect`, which returns the name of the new atom selection. the second step is to use the created selection to access the information about the atoms in the selections.

- **list**: Return a list of all undeleted atom selections.

- **keywords**: Return a list of all recognized keywords in an atom selection text.
- **macro** *name selection*: Create a new singleword atom selection out of existing atom selections. *name* must be a single word starting with a non-numeric character and contain no spaces or special characters. *selection* can be any valid atom selection, and can even contain other macros. You should ensure that your macros do not contain themselves, either directly or through a chain of other macros. If VMD detects this situation, it will abort the evaluation of the atom selection.

  If no selection is given, the macro for the given name is returned.

  If no name is given, a list of all macro names is returned.

  If a macro already exists for the given name, the old selection will be replaced with the new selection. Singlewords that are not defined as macros, like `protein` and `water`, cannot be redefined with the macro command.
- **delmacro** *name*: Delete the macro corresponding to *name*. Singlewords that are not defined as macros cannot be deleted.
- *molecule_id selection_text* [**frame** *frame_number*] Creates a new atom selection and returns its name. The returned name can be used as a Tcl proc in order to access the atom selection. The *selection text* is the same language used in the Graphics window [§ 5.4.7] and described in Chapter 6.3. It is used to pick a given subset of the atom. The text cannot be changed once a selection is made. Some of the terms in the selection depend on data that change during a trajectory (so far only the keywords 'x', 'y', and 'z' can change over time). For these, the optional 'frame value' is used to determine which specific frame to use. The frame number can be a non-negative integer, the word `now` (the current frame), the word `first` (for frame 0) and `last` (for the last frame).

  Some examples are:

```
vmd> atomselect top "name CA"
atomselect0
vmd> atomselect 3 "resid 25" frame last
atomselect1
vmd> atomselect top "within 5 of resname LYR" frame 23
atomselect2
```

  The newly created atom selection is a Tcl proc, which takes the following options:

  - **num**: Return the number of atoms in the selection.
  - **list**: Return a list of the atom indices in the selection (BTW, this is the same as `get index`).
  - **text**: Return the text used to create this selection.
  - **molid**: Returns the molecule id used to create this selection.
  - **frame**: Returns the animation frame associated with this selection. The result will be either `now`, `last`, or an integer corresponding to the frame. When the frame is `now`, the atom selection will use atomic coordinates from the current frame for its associated molecule. If the frame is `last`, the atom selection will always use coordinates from the

last frame. If the frame is a specific integer, the selection will always use coordinates from that frame, even if the current animation frame changes. Note that if a nonexistent frame is specified, the atomic coordinates will reference the last frame.

- **frame** *frame*: Set the frame for the selection. *frame* should be either `now`, `last`, or an integer.
- **delete**: Delete this object (removes the function).
- **global**: Moves the object into the global namespace. Atom selections created within a Tcl proc that are not made global are deleted when the proc exits.
- **uplevel** *level*: Moves the object to a new level in the namespace stack. Works the same as the Tcl function `uplevel`.
- **get** *attribute_list*: Given an attribute or a list of attributes, returns the attribute values. If only a single attribute is given, a list of corresponding attributes values will be returned. If a list of attributes is given, then a list of sublists will be returned; each sublist will contain the values for the corresponding attributes. See Tables 6.5, 6.6, and 6.8 for the recognized attribute keywords.
- **set** *attribute_list values_lists*: Set the attributes in the attribute list with the values gven in the values lists. If there is only one attribute, then *values_lists* can be either a single value or a list of values, one for each selected atom. If there is more than one attribute, then *values_lists* must be a list of sublists; the number of sublists must equal the number of selected atoms, and the number of items in each sublist must equal the number of attributes.

  Example:

```
set sel [atomselect top all]
set mass [$sel get mass]
set xyz [$sel get {x y z}]
$sel set beta 0      # all values are set to zero
$sel set beta $mass  # copy mass to beta
# set occupancy to x, mass to y, beta to z
$sel set {occupancy mass beta} $xyz
```

  It is an error to set integer or floating point keywords using non-numeric values. If floating point values are passed to integer keywords, they will be converted to integers, and vice versa.

  The set command immediately updates all representations of the selected molecule. If speed is an issue, delete all representations of the molecule before setting the values.
- **getbonds**: returns a list of bondlists; each bondlist contains the id's of the atoms bonded to the corresponding atom in the selection.
- **setbonds**: Set the bonds for the atoms in the selection; the second argument should be a list of bondlists, one bondlist for each selected atom.
- **move** *4x4 matrix*: Applies the given transformation matrix to the coordinates of each atom in the selection.
- **moveby** *offset*: move all the atoms by a given offset.
- **lmoveby** *offset_list*: move each atom by an offset given in the list.

- **moveto** *position*: move all the atoms to a given location.
- **lmoveto** *position_list*: move each atom to a point given by the appropriate list element.
- **writeXXX** *filename*: write the selected atoms to a file of type XXX; e.g., pdb, dcd. **New in VMD 1.8**: writepdb requires a filename; omitting the filename no longer returns the PDB data as a string. To get the PDB data as a string, first write to a file, then enter the following commands: `set fd [open` *filename* `r]; set s [read $fd]; close $fd`. The text will be contained in the variable `s`.
- **update**: Update the atom selection based on the frame for the selection (the frame can be specified using the **frame** option as described above).

See section 12.2 for more on using atom selections for fun and profit, as well as issues relating to speed of analysis scripts.

9.3.3 axes

The axes (orthogonal vectors pointing along the x, y, and z directions) can be placed in any of 5 locations on the screen, or turned off.

- **locations**: Return a list of possible locations.
- **location**: Get the current location.
- **location < off | origin | lowerleft | lowerright | upperleft | upperright >**: Position axes.

Also, though this may seem like a likely command for changing the color of the axes, this function can only be performed from the Colors window or by the `color` command (see below). Future implementations of VMD may change this.

9.3.4 color

Change the color assigned to molecules, or edit the color scale. All color values are in the range 0 ... 1. Please see the section on coloring [§ 6.2] for a full description of the various options.

- *category name color*: Set the color of the object specified by *category* and *name* to *color*.
- *category name*: Get the color of the object specified by *category* and *name*.
- **scale method <** *scale_name* **>**: Set type of scale to use for coloring objects by values. They are:
  - RGB – Red to green to blue.
  - BGR – Blue to green to red.
  - RWB – Red to white to blue.
  - BWR – Blue to white to red.
  - RWG – Red to white to green.
  - GWR – Green to white to red.

  - GWB – Green to white to blue.
  - BWG – Blue to white to green.
  - BlkW – Black to white.
  - WBlk – White to black.

- **scale midpoint** *x*: Set midpoint of color scale to *x*, in the range 0 ... 1.
- **scale min** *x*: Set minimum of color scale to *x*, in the range 0 ... 1.
- **scale max** *x*: Set maximum of color scale to *x*, in the range 0 ... 1.
- **change rgb** *color*: Reset rgb of *color* to default value.
- **change rgb** *color r g b*: Set the RGB of *color* to *r g b*.
- **restype** *resname* `[` *restype* `]`: Set the residue type for *resname* to *restype*. If the *restype* parameter is omitted, the current residue type is returned.
- **add item** *category name colorname*: Adds colors for the named color category, item name, using the colorname color.

See the colorinfo § 9.3.5 command for additional ways to query VMD's color settings. See the graphics § 9.3.9 command for how to change color of a user-defined graphics object.

9.3.5 colorinfo

(Tcl) This command provides access to the color definitions. For information on the color properties see the chapter on Coloring [§6.2].

- **colorinfo categories**: returns a list of available categories
- **colorinfo category** *category*: returns a list of names for the given category
- **colorinfo num**: returns the number of base solid colors (33)
- **colorinfo max**: returns the total number of colors available (1057)
- **colorinfo colors**: returns a list of the named solid colors
- **colorinfo** `[` **index | rgb** `]` `<` **name | value** `>` : returns the index or rgb of the given name or color id.
- **colorinfo scale** `<` **method | methods | midpoint | min | max** `>`: returns the information about the color scales

Examples:

```
# find out what color corresponds to which id:
set i 0
foreach color [colorinfo colors] {
  puts "$i $color"
```

```
  incr i
}


# also get a list of RGB values
set i 0
foreach color [colorinfo colors] {
  lassign [colorinfo rgb $color] r g b
  puts "$i $color   \{$r $g $b\}"
  incr i
}
```

9.3.6 display

Change various aspects of the graphical display window. For information about the options, see the section describing the Display window [§5.4.6].

- **get < backgroundgradient | eyesep | focallength | height | distance | antialias | depthcue | culling | rendermode | size | stereo | projection | nearclip | farclip | cuestart | cueend | cuedensity | cuemode shadows | ambientocclusion | aoambient | aodirect | dof | dof_fnumber | dof_focaldist | backgroundgradient >**: Return the current value of the requested option.
- **get < rendermodes | stereomodes | projections |**: Return a list of the available values for the given options. (See section 5.4.6 and chapter 7 for more information.)
- **antialias < on | off >**: Turn antialiasing on or off.
- **ambientocclusion < on | off >**: Turn ambient occlusion lighting on or off. This only affects renderers that support ambient occlusion lighting. It will have no visible effect on the interactive VMD display or on renderers that don't support it. At present, only the Tachyon and TachyonInternal renderers are capable of ambient occlusion lighting.
- **aoambient** *value*: Set ambient occlusion lighting factor to *value*. Useful values tend to range from 0.7 to 1.0. At present, only the Tachyon and TachyonInternal renderers are capable of ambient occlusion lighting.
- **aodirect** *value*: Set ambient occlusion direct lighting rescaling factor to *value*. Useful values tend to range from 0.0 to 0.4. At present, only the Tachyon and TachyonInternal renderers are capable of ambient occlusion lighting.
- **dof < on | off >**: Turn depth of field focal blur on or off. This only affects renderers that support depth of field. It will have no visible effect on the interactive VMD display or on renderers that don't support it. At present, only the various Tachyon and POV-Ray renderers are capable of depth of field.
- **dof_fnumber** *value*: Set depth of field aperture f/stop number to *value*. Useful values fall over a broad range from f/30 to f/1000 due to the reciprocal relationship between the f/stop number and the resulting the size of the blur aperture. The blur aperture relates directly to

the size of out of focus bokeh effects in the final rendered image. At present, only the various Tachyon and POV-Ray renderers are capable of depth of field.

- **dof_focaldist** *value*: Set depth of field focal plane distance to *value*. Useful values fall over a broad range from f/30 to f/1000. At present, only the various Tachyon and POV-Ray renderers are capable of depth of field.
- **backgroundgradient < on | off >**: Enable or disable the gradient background.
- **culling < on | off >**: Turn backface culling on or off.
- **depthcue < on | off >**: Turn depth cueing on or off.
- **eyesep** *value*: Set the eye separation to *value*.
- **fps < on | off >**: Turn frames-per-second indicator on or off.
- **focallength** *value*: Set the focal length to *value*.
- **height** *value*: Set the screen height to *value*.
- **distance** *value*: Set the screen distance to *value*.
- **nearclip < set | add >** *value*: Add or set near clipping plane position to it value.
- **farclip < set | add >** *value*: Add or set far clipping plane position to *value*.
- **projection < perspective | orthographic >**: Set the projection mode to *mode*.
- **rendermode < Normal | GLSL | Acrobat3D >**: Set the rendering mode to *mode*. This parameter allows the use of various OpenGL extensions to implement alpha-blended transparency, or programmable shading for higher quality molecular graphics. The default rendering mode does not enable these features since they significantly alter the rendering and performance characteristics of VMD when they are enabled. The Acrobat3D mode is used to allow successful capture of molecular geometry into Acrobat3D.
- **resetview**: Reset the view.
- **resize** *valueX valueY*: Set the size of the display window to *valueX* × *valueY*.
- **reposition** *valueX valueY*: Set the position of the upper-left corner of the display window to *valueX* × *valueY* pixels from the lower-left corner of the screen.
- **shadows < on | off >**: Turn shadow rendering on or off. This only affects renderers that support control of shadow rendering. It will have no visible effect on the interactive VMD display or on renderers that don't support it. At present, only the Tachyon and TachyonInternal renderers are capable of controlling the shadow rendering mode.
- **stereo** *mode*: Set the stereo mode to *mode*.
- **update**: Force a display update. Used if the display update is off or to force a redraw. This does not necessarily take care of resizing the display window or using the GUI while the display update is turned off.

- **update on**: Turn display update on.
- **update off**: Turn display update off. By default VMD does the display updates constantly. Sometimes it is beneficial to turn the turn the display updates off. This prevents VMD from redrawing the scene as a response to every change, thus saving time while doing changes of representations. See the VMD script library for examples of use.
- **update status**: Return the display update status (on or off).
- **update ui**: Similar to `display update`, but also forces updates of the GUI windows. The windowed interface is subject to the following behavior: if the display update is set to `off` and actions (such as, e.g., iconify/deiconify) have been performed to the windows, the windows do not get updated by just `display update` command, whereas `display update ui` forces both updates to happen. Tk does not seem to have this problem, so this option will become obsolete after switching to Tk graphics user interface.

9.3.7 draw

VMD offers a way to display user-defined objects built from graphics primitives such as points, lines, cylinders, cones, spheres, triangles, and text. Since these are displayed in the scene just like all other graphics, they can also be exported to the various ray tracing formats, 3-D printers, etc. User-defined graphics can be used to draw a box around a molecule, draw an arrow between two atoms, place a text label somewhere in space, or to test a new method for visualizing a molecule.

The `draw` command is a straight Tcl function which is meant to simplify the interface to the `graphics` command as well as provide a base for extensions to the standard graphics primitives. The format of the `draw` command is:

- **draw** *command* [*arguments*]

The draw command is equivalent (in most cases) to `graphics top` *command* `[`*arguments*`]`, in that it simply adds graphics primitives to the top molecule, saving you the trouble of typing an extra argument. However, `draw` extends graphics in two ways. First, if no molecule exists, `draw` creates one for you automatically. Second, `draw` can be extended with user-defined drawing commands. This is done by defining for a function of the form `vmd_draw_$command`. If the function exists, it is called with the first parameter as the molecule index and the rest as the arguments from the original `draw` call. Here's an example which extends the draw command to include an "arrow" primitive.

```
proc vmd_draw_arrow {mol start end} {
    # an arrow is made of a cylinder and a cone
    set middle [vecadd $start [vecscale 0.9 [vecsub $end $start]]]
    graphics $mol cylinder $start $middle radius 0.15
    graphics $mol cone $middle $end radius 0.25
}
```

After entering this command into VMD, you can use a command such as `draw arrow {0 0 0} {1 1 1}` to draw an arrow. In addition to defining new commands, user-defined drawing commands can also be used to override existing commands. For example, if you define `vmd_draw_sphere`, then `draw sphere {0 0 0}` will call your sphere routine, not the one from `graphics`.

Here's a quick way to add your own label to an atom selection [§6.3]. This function take the selection text and the labels that atom (in the top molecule) with the given string. It returns with an error if more anything other than one atom is selected.

```
proc label_atom {selection_string label_string} {
    set sel [atomselect top $selection_string]
    if {[$sel num] != 1} {
        error "label_atom: '$selection_string' must select 1 atom"
    }
    # get the coordinates of the atom
    lassign [$sel get {x y z}] coord
    # and draw the text
    draw text $coord $label_string
}
```

9.3.8 exit

Quit VMD.

9.3.9 graphics

The `graphics` command draws low-level graphics primitives. These primitives can be used to draw a box around a molecule, or an arrow between two atoms, or place a text label somewhere in space. The command syntax is `graphics <molid> <cmd>`, where `<molid>` is a valid molecule id and `<cmd>` is one of the commands listed below. To create a "blank" molecule, use the Tcl command `mol new`. See the draw [§ 9.3.7] command for a possibly more convenient interface. Also refer to the VMD script library[1] for some examples of user-defined graphics scripts.

As graphical primitives are added to the list they are assigned a unique, increasing `id`. The first object added is assigned 0, the second is assigned 1, etc. The commands which add an item return its value.

- **point {***x y z***}**: Draws a point at the given position.
- **line {***x1 y1 z1***} {***x2 y2 z2***}** [**width** *w*] [**style** <**solid**|**dashed**>] :

  Draws either a solid or dashed line of the given width from the first point to the second. By default, this is a solid line of width 1.
- **cylinder {***x1 y1 z1***} {***x2 y2 z2***}** [**radius** *r*] [**resolution** *n*] [**filled** <**yes**|**no**>]:

  Draws a cylinder of the given radius (default `r`=1) from the first point to the second. The cylinder is actually drawn as an `n` sided polygon. If the `filled` option is true, the ends are capped with flat disks, otherwise the cylinder is hollow (default). width of the base. The resolution parameter (default `n`=6) determines the number of polygons used in the approximation.
- **cone {***basex basey basez***} {***tipz tipy tipz***}** [**radius** *r*] [**resolution** *n*]:

[1] http://www.ks.uiuc.edu/Research/vmd/script_library

Draw a cone with the center of the base at the first point and the tip at the second. The radius(default `r`=1) determines the width of the base. As with `cylinder`, the resolution (default `n`=6) determines the number of polygons used in the approximation.

- **triangle** {*x1 y1 z1*} {*x2 y2 z3*} {*x3 y3 z3*}:

  Draws a triangle with endpoints at each of the three vertices

- **trinorm** {*x1 y1 z1*} {*x2 y2 z3*} {*x3 y3 z3*} {*nx1 y1 z1*} {*nx2 ny2 nz3*} {*nx3 ny3 nz3*}:

  Draws a triangle with endpoints at each of the first three points. The second group of three values specify the normals for the three points. This is used for making a smooth shading across the triangle. The normals must be normalized to unit-length for proper display.

- **tricolor** {*x1 y1 z1*} {*x2 y2 z3*} {*x3 y3 z3*} {*nx1 y1 z1*} {*nx2 ny2 nz3*} {*nx3 ny3 nz3*} *c1 c2 c3*:

  Draws a triangle with endpoints at each of the first three points. The second group of three values specify the normals for the three points. The last three integers indicate the colors to apply to each vertex. This is used for making a smooth shading across the triangle. The normals must be normalized to unit-length for proper display.

- **sphere** {*x y z*} [**radius** *r*] [**resolution** *n*]:

  Draws a sphere of the given radius (default `r`=1) centered at the vertex. The resolution (default `n`=6) determines how many polygons are used in the approximation of a sphere.

- **text** {*x y z*} "*text string*" [**size** *s*] [**thickness** *t*]:

  Displays the text string with the bottom left of the string starting at the given coordinates, with the font size scaled by the optional size parameter, and drawn with line thickness determined by the optional thickness parameter.

- **color** *colorId*

- **color** *name*

- **color** *trans_name*: Each of the above geometrical objects are drawn using the current color. Initially, that color is blue, which has the colorid of 0. The `color` command changes the current color, and stays info effect until the next `color` command. Thus, to draw a red cylinder then a red sphere, first use the command `color red` command to change the color, then use the `cylinder` and `sphere` commands.

- **materials** <**on**|**off**>: Material properties are used to make the graphical objects (lines, cylinders, etc.) be affected by the light sources. These make the objects look more realistic, but are slower on machines which don't implement materials in hardware (see chapter 6.2 and sections on color [§ 9.3.4] and colorinfo [§ 9.3.5] commands for the information on how to turn off material characteristics for all objects in VMD). One surprising effect of material characteristics is that lines are affected. In some lighting situations, the lines can even appear to disappear. Thus, you may want to turn off materials before drawing lines.

- **material** <**name**>: Sets the material to use for the corresponding graphics molecule. `name` must be a valid material name, as displayed in the Materials menu.

- **delete** *id*: Deletes the graphics primitive with the given id.
- **delete all**: Deletes all graphics primitives.
- **replace** *id*: Causes the next graphics primitive to replace the one with the given id. Subsequent graphics primitives will be added to the end of the list as usual.
- **exists** *id*: Returns whether the primitive with the given id exists.
- **list**: Returns a list of valid graphics id's.
- **info** *id*: Returns the text of a Tcl command which will recreate the graphics primitive with the given *id*.

9.3.10 gettimestep

Retrieve the specified molecule's timestep as a Tcl byte array which can be used for high-efficiency analysis calculations by compiled Tcl plugins.

- < *molid*> < *timestep* >: retrieve timestep as a Tcl byte array for use in compiled analysis plugins.

9.3.11 help

Display the on-line help file with an HTML viewer. See Chapter 14 for information on how to change the default viewer (which is Netscape).

- [*subject*]: Jump to help corresponding to *subject*.

Presently, "subject" can be any one of the following words, which launches the associated URL. To guarantee that the help system will work correctly, you will probably want to start up your web browser before choosing one of these options. After you do this, VMD will properly direct the browser to the pages mentioned below.

9.3.12 imd

Controls the connection to a remote simulation.

- **connect** *host port*: connect to an MD simulation running on the machine named *host* and listening on port *port*. This command will fail if a previously-established connection has not yet been disconnected.
- **detach**: Disconnect from the simulation; the simulation will continue to run.
- **kill**: Disconnect from the simulation and also cause it to halt.
- **pause < on | off | toggle >**: Pause, unpause or toggle the paused state of the remote simulation.
- **transfer** *rate*: Set the rate at which new coordinates are sent by the remote simulation to VMD to the specified value.

Source	Associated URL
raster3d	http://www.bmsc.washington.edu/raster3d/
msms	http://www.scripps.edu/pub/olson-web/people/sanner/html/msms_home.html
faq	http://www.ks.uiuc.edu/Research/vmd/allversions/vmd_faq.html
biocore	http://www.ks.uiuc.edu/Research/biocore/
tachyon	http://www.photonlimited.com/~johns/tachyon/
babel	http://www.eyesopen.com/babel/
homepage	http://www.ks.uiuc.edu/Research/vmd/
quickhelp	http://www.ks.uiuc.edu/Research/vmd/vmd_help.html
radiance	http://radsite.lbl.gov/radiance/HOME.html
maillist	http://www.ks.uiuc.edu/Research/vmd/mailing_list/
scripts	http://www.ks.uiuc.edu/Research/vmd/script_library/
namd	http://www.ks.uiuc.edu/Research/namd/
vrml	http://www.web3d.org/
rayshade	http://www-graphics.stanford.edu/~cek/rayshade/rayshade.html
povray	http://www.povray.org/
plugins	http://www.ks.uiuc.edu/Research/vmd/plugins/
python	http://www.python.org/
software	http://www.ks.uiuc.edu/Research/vmd/allversions/related_programs.html
tcl	http://www.tcl.tk/
userguide	http://www.ks.uiuc.edu/Research/vmd/vmd-1.8.1/ug/ug.html

Table 9.2: On-line Help Sources

- **keep** *rate*: Set the keep rate, i.e. the frequency at which VMD saves simulation frames to memory, to the specified value.
- **copyunitcell < on | off >**: Enable or disable copying unit cell information from the previous frame when updating or saving frames through IMD. This can be useful when using periodic display with IMD since the IMD protocol currently doesn't support communicating the unitcell information, or when using a IMD client that does not provide this information after the protocol has been extended.
  WARNING: when using **imd copyunitcell on** with simulations in NPT ensemble, the resulting unit cell information will be incorrect.
  The default setting is **off**.

9.3.13 label

Turn on or off labels for the four categories: atoms, bonds, angles, or dihedral angles; create and destroy simulated springs. Once a label is created (given the list of associated atoms) it can be turned on or off until it is deleted. Also, the value of the label over the trajectory can be saved to a file and viewed with an external program such as `xmgrace`. In the following, *category* implies one of `[`Atoms—Bonds—Angles—Dihedrals`]`.

- **list**: Return a list of available categories.
- **list** *category*: List all labels in the given category.

- **add** *category molID1/atomID1* `[` *molID2/atomID2...* `]`: Add a label involving the atom(s) *atomID* of the molecule *molID* to the given category.
- **show** *category* `<` **all** `|` *label_number* `>`: Turn on labels in the given category.
- **hide** *category* `<` **all** `|` *label_number* `>`: Turn off labels in the given category.
- **delete** *category* `<` **all** `|`*label_number*`>`: Delete labels in the given category.
- **graph** *category label_number* `[`*filename*`]`: Retrieve the values of the labels for all timesteps. If the optional `filename` is given, the data will be written to that file; otherwise it will be returned as a list. You can use the Tcl `exec` command to launch an external graphing program to plot the data if you wish.
- **addspring** *molID1 atomID1 atomID2* `k`: Add a spring connecting the atom(s) *atomID* and *atomID2* of the molecule *molID*. The spring will have spring constant *k*.
- **textsize** [*newsize*]: Get/set the text size for all labels, which is 1.0 by default. *newsize* should be a decimal value greater than zero.
- **textthickness** [*newthickness*]: Get/set the text line thickness for all labels, which is 1.0 by default. *newthickness* should be a decimal value greater than zero.

9.3.14 light

There are four light sources, numbered 0 to 3, which are used to illuminate graphical objects. They are point sources located at infinity, so setting their positions places them along a ray from the origin through the given point.

- **num**: Return the number of lights available.
- *light_number* **on**: Turn a light on.
- *light_number* **off**: Turn a light off.
- *light_number* **status**: Return the pair on/off highlight/unhighlight
- *light_number* **rot** `<` **x** `|` **y** `|` **z** `>` *angle*: Rotate a light (at infinity) *angle* degrees about a given axis.
- *light _numer* **pos**: Return current position.
- *light _numer* **pos default**: Return default position.
- *light _numer* **pos** `{ x y z}`: Set light position.

9.3.15 logfile

Turn on/off logging a VMD session to a log file. This will create a log file with commands for all the actions taken during the session. The log file may be played back later by using the 'play' command or the Tcl 'source' command. The only actions recorded are those which change the state of the VMD display, so straight Tcl commands are not saved. All of the core VMD commands will write to the log.

- *filename*: Turn on logging to *filename*.
- **console**: Turn on logging and direct it to the VMD text console window.
- **off**: Turn off logging.

To write log information to the file 'off', use the file name './off'.

9.3.16 material

This set of commands is used to create new material definitions and modify existing ones.

- **list**: Return a list of the available materials
- **settings** *name*: Return a list of the five material settings for the material of the given name. These settings take on floating point values between 0 and 1. The values are returned in the following order: ambient, specular, diffuse, shininess, mirror, opacity. If the specified material has not been defined, nothing is returned.
- **add** *name*: create a new material with the given name. The new material will start with the settings for Opaque. If the name already exists, no new material is created.
- **add copy** *name*: create a new material copied from the selected material name.
- **rename** *oldname newname*: rename the given material. The command will fail if the name is already used.
- **change** *property name value*: Change a material property of the material named *name* to the value *value*. *property* must be one of the following:
  - ambient
  - specular
  - diffuse
  - shininess
  - mirror
  - opacity
- **delete** *name*: Delete the given material.

9.3.17 mdffi

The mdffi command provides fast internal implementations of key cross correlation and density map synthesis algorithms used for molecular dynamics flexible fitting (MDFF) simulation, analysis, and visualization [26].

- **cc** *selection* [–**allframes**] [**-i** *input density map*] [**-mol** *molid* | **-vol** *volume ID*] [**-thresholddensity** *threshold value*] : Computes the MDFF cross correlation between an selection from an all-atom molecular structure, and a density map.
- **sim** *selection* [**-o** *output density map*] [**-res** *target resolution in Å*] [**-spacing** *grid spacing*] : Compute a simulated density map from an atom selection on an all-atom molecular structure.

9.3.18 measure

The measure command supplies several algorithms for analyzing molecular structures. In the following options, *selection* refers to an atom selection, as returned by the `atomselect` command described in section 9.3.2. The optional *weight* must be either `none`, an atom selection keyword such as `mass`, or a list of values, one for each atom in the selection, to be used as weights. If *weight* is missing or is `none`, then all weights are taken to be 1. When an atom selection keyword is used, the weights are taken from *selection1*.

- **avpos** *selection* [**first** *first*] [**last** *last*] [**step** *step*]: Returns the average position of each of the selected atoms, for the selected frames. If no first, last, or step values are provided the calculation will be done for all frames.
- **center** *selection* [**weight** *weight*]: Returns the geometric center of atoms in *selection* using the given `weight`.
- **cluster** *selection* [**num** *numclusters*] [**distfunc** *flag*] [**cutoff** *cutoff*] [**first** *first*] [**last** *last*] [**step** *step*] [**selupdate** *bool*] [**weight** *weight*]: Performs a cluster analysis (find clusters of timesteps that are similar with respect to a given distance function) for the atoms in *selection* using the given `weight`. The implementation is based on the *quality threshold* (QT) algorithm. See `http://dx.doi.org/10.1101/gr.9.11.1106` and Cluster Analysis on Wikipedia for more details on the algorithm. Typically, only a small number of the largest clusters are of interest. This implementation takes this into account and trades low memory consumption on data sets with many frames for fast determination of multiple clusters. Use the `num` keyword to adjust how many clusters to determine (default is 5). The `distfunc` flag selects the "distance function"; available options are 'rmsd' (root mean squared atom–to–atom distance), 'fitrmsd' (root mean squared atom–to–atom distance after alignment), and 'rgyrd' (difference in radius of gyration). The `cutoff` flag defines the maximal distance value between two frames that are considered similar (default value is 1.0). The `weight` flag allows to use an atom property, e.g. mass or radius, to be used as weighting factor (default is no weighting). The command returns a list of *numcluster + 1* lists, each containing the list of trajectory frame indices belonging to a cluster of decreasing size. The last list contains the remaining, yet unclustered frame indices.
- **contacts** *cutoff selection1* [*selection2*]: Find all atoms in *selection1* that are within *cutoff* of any atom in *selection2* and not bonded to it. If *selection2* is omitted, it is taken to be the

same as *selection1*. *selection2* and *selection1* can either be from the same of from different molecules. Returns two lists of atom indices, the first containing the first index of each pair (taken from *selection1*) and the second containing the second index (taken from *selection2*). Note that the index is the global index of the atom with respect to its parent molecule, as opposed to the index within the given atom selection that contains it.

- **dipole** *selection* [**-elementary**—**-debye**] [**-geocenter**—**-masscenter**—**-origincenter**]: Compute the dipole moment vector of the atoms in *selection* from their respective positions and `charge` values. The result by default assumes charges given in units of an elementary charge and distances in angstrom. By default the result is given in the same units (same as using the *-elementary* flag), setting the *-debye* flag will convert the output to units of Debye. For selections that have a residual charge after summing up all individual charges, the resulting dipole vector depends on the choice of center of the charge distribution. By default, the center will be the geometrical center of the selection (sames as using the *-geocenter* flag), but using the selection's center of mass through the *-masscenter* flag is available, as well as using the origin via the *-origincenter* flag. Using *-masscenter* is recommended, but not made default as it depends on the `mass` value to be correctly set for all atoms.

- **fit** *selection1 selection2* [**weight** *weight*] [**order** *index list*]: Returns a 4x4 transformation matrix which, when applied to the atoms in *selection1*, minimizes the weighted RMSD between *selection1* and *selection2*. See section 12.4.2 for more on RMSD alignment. The optional flag *order* takes as argument a list of 0-based indices specifying how to reorder the atoms in *selection2* (Example: To reverse the order of atoms in a selection containing 10 atoms one would use `order` {`9 8 7 6 5 4 3 2 1 0`}).

- **gofr** *selection1 selection2* [**delta** *value*] [**rmax** *value*] [**usepbc** *boolean*] [**selupdate** *boolean*] [**first** *first*] [**last** *last*] [**step** *step*]: Calculates the atomic radial pair distribution function $g(r)$ and the number integral $\int_0^r \rho g(r) r^2 \mathrm{d}r$ for all pairs of atoms in the two selections. Both selections have to reference the same molecule and may be identical. In case one of the selections resolves to an empty list for a given time step, and empty array is added to the histograms. The command returns a list of five lists containing r, $g(r)$, $\int_0^r \rho g(r) r^2 \mathrm{d}r$, the unnormalized histogram, and a list of frame counters containing currently 3 elements: total number of frames processed, the number of skipped frames and the number of frames handled with the orthogonal cell algorithm (Further algorithm and corresponding list entris will be added in the future). With the optional arguments *delta* (default 0.1) and *rmax* (default 10.0) one can set the resolution and the maximum r value. With the *usepbc* flag processing of periodic boundary conditions can be turned on. With the *selupdate* flag enabled, both atom selections are updated as each frame is processed, allowing productive use of "within" selections. The size of the unitcell has to be stored in the trajectory file or has to be set manually for all frames with the *molinfo* command. The command uses by default only the current active frame for both selections. Using an explicite frame range via *first*, *last*, and *step* is recommended for most cases.

- **hbonds** *cutoff angle selection1* [*selection2*]: Find all hydrogen bonds in the given selection(s), using simple geometric criteria. Donor and acceptor must be within the *cutoff* distance, and the angle formed by the donor, hydrogen, and acceptor must be less than *angle* from 180 degrees. Only non-hydrogen atoms are considered in either selection. If both *selection1* and *selection2* are given, the *selection1* is considered the donor and *selection2* is considered the

acceptor. If only one selection is given, all non-hydrogen atoms in the selection are considered as both donors and acceptors. The two selections must be from the same molecule. The function returns three lists; each element in each list corresponds to one hydrogen bond. The first list contains the indices of the donors, the second contains the indices of the acceptors, and the third contains the index of the hydrogen atom in the hydrogen bond.

Known Issue: The output of hbonds cannot be considered 100% accurate if the donor and acceptor selection share a common set of atoms.

- **inverse** *matrix*: Returns the inverse of the given 4x4 matrix.
- **minmax** *selection*: Returns two vectors, the first containing the minimum x, y, and z coordinates of all atoms in *selection*, and the second containing the corresponding maxima.
- **rgyr** *selection* [**weight** *weights*]: Returns the radius of gyration of atoms in *selection* using the given `weight`. The radius of gyration is computed as

$$r_{gyr}^2 = \left(\sum_{i=1}^{n} w(i)(r(i) - \bar{r})^2 \right) / \left(\sum_{i=1}^{n} w(i) \right) \tag{9.1}$$

  where $r(i)$ is the position of the ith atom and $\bar{r}$ is the weighted center as computer by `measure center`.
- **rmsd** *selection1 selection2* [**weight** *weights*]: Returns the root mean square distance between corresponding atoms in the two selections, weighted by the given *weight*. *selection1* and *selection2* must contain the same number of atoms (the selections may be from different molecules that have different numbers of atoms).
- **rmsf** *selection* [**first** *first*] [**last** *last*] [**step** *step*]: Returns the root mean square position fluctuation for each selected atom in the selected frames. If no first, last, or step values are provided the calculation will be done for all frames.
- **sasa** *srad selection* [**-points** *varname*] [**-restrict** *restrictedsel*] [**-samples** *numsamples*]: Returns the solvent-accessible surface area of atoms in the *selection* using the assigned radius for each atom, extending each radius by `srad` to find the points on a sphere that are exposed to solvent. If the *restrictedsel* selection is used, only solvent-accessible points near that selection will be considered. The restrict option can be used to prevent internal protein voids or pockets from affecting the surface area results. The points option can be used to see where the area contributions are coming from, and then the restrict flag can be used to eliminate any unwanted contributions after visualizing them. The *varname* parameter can be used to collect the points which are determined to be solvent-accessible.
- **sumweights** *selection* **weight** *weights*: Returns the sum of the list of weights (or data field to use for the weights) for all of the atoms in the selection.
- **bond** *atom_list* [*options*]: Returns the distance of the two specified atoms. The atoms are specified in form of a list of atom indexes. Unless you specify a certain molecule through 'molid *molecule_number*' these indices refer to the current top molecule. If the atoms are in different molecules you can use the form {{*atomid1* [*molid1*]} {*atomid2* [*molid2*]} ... } where you can set the molecule ID for the individual atoms. Note that `measure bond` does not care

about the bond that are specified in a psf file or that are drawn in VMD it just returns the distance! Similar things are true for `measure angle`, `dihed` and `imprp`.
The following options can be specified:

- `molid <default molid>`: The default molecule to which an atom belongs unless a molecule number was explicitely specified for this atom in the atom list. Further, all frame specifications refer to this molecule. (Default is the current top molecule.)
- `frame <frame>`: By default the value for the current frame will be returned but a specific frame can be chosen through this option. One can also specify *all* or *last* instead of a frame number in order to get a list of values for all frames or just the last frame respectively.
- `first <frame>`: Use this option to specify the first frame of a frame range. (Default is the current frame.)
- `last <frame>`: Use this option to specify the last frame of a frame range. (Default is the last frame of the molecule).

In case you specified the molecule IDs in the atom list then all frames specifications will refer to the current top molecule unless a default molecule was set using the 'molid' option. Since the top molecule can be different from the molecules involved in the selected atoms, it is generally a good idea to specify a default molecule.

Here are a few examples of usage:
`measure bond {3 5}` – Returns the distance between atoms 3 and 5 of the current frame of the top molecule. `measure bond {3 5} molid 1 frame all` – Returns the distance between atoms 3 and 5 of molecule 1 for all frames.
`measure bond {3 {5 1}} molid 0 first 7` – Returns the distance between atoms 3 of molecule 0 and atom 5 of molecule 1. The value is computed for all frames between the seventh and the last frame of molecule 0.

- **angle** *atom_list* [*options*]: Returns the angle spanned by three atoms. Same input format as the `measure bond` command.
- **dihed** *atom_list* [*options*]: Returns the dihedral angle defined by four atoms. Same input format as the `measure bond` command.
- **imprp** *atom_list* [*options*]: Returns the improper dihedral angle defined by four atoms. Same input format as the `measure bond` command.
- **energy** *energy_term atom_list* [parameters] [options]: Returns the specified energy term for a given set of atoms. The energy term must be one of **bond**, **angle**, **dihed**, **imprp**, **vdw** or **elect** where vdw stands for 'van der Waals' and elect for electrostatic energy. The energy is computed based on the CHARMM force field functions, the given parameters and the current coordinates. All options for the `measure bond` command work for `measure energy`, too. Thus, you can for instance request energies for a range of frames of a trajectory. Also the format of the atom list is the same. The following parameters can be specified:
  - `k <value>`: force constant for bond, angle, dihed and imprp energies in kcal/mol/A^2 or kcal/mol/rad^2 respectively.

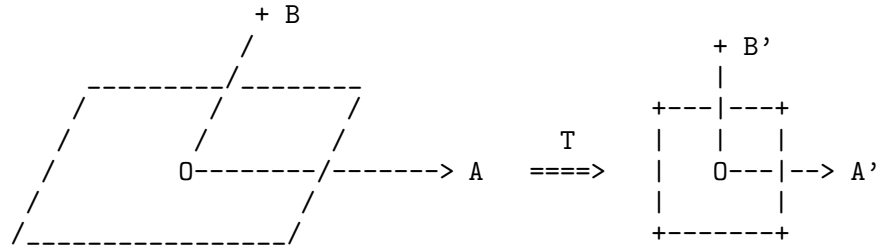
- `x0 <value>`: equilibrium value for bond length, angle, dihedral angles and improper dihedrals in Angstrom or degree.
- `kub <value>`: Urey-Bradley force constant for angles in kcal/mol/A^2.
- `s0 <value>`: Urey-Bradley equilibrium distance for angles in Angstrom.
- `n <value>`: dihedral periodicity.
- `delta <value>`: dihedral phase shift in degree (usually 0.0 or 180.0).
- `rmin1 <value>`: VDW equilibrium distance for atom 1 in Angstrom.
- `rmin2 <value>`: VDW equilibrium distance for atom 2 in Angstrom.
- `eps1 <value>`: VDW energy well depth (epsilon) for atom 1 in kcal/mol.
- `eps2 <value>`: VDW energy well depth (epsilon) for atom 2 in kcal/mol.
- `q1 <value>`: charge for atom 1.
- `q2 <value>`: charge for atom 2.
- `cutoff <value>`: nonbonded cutoff distance.
- `switchdist <value>`: nonbonded switching distance.

For all omitted parameters a default value of 0.0 is assumed. For the electrostatic energy the default charges are taken from the according atom based field of the molecule. If the cutoff is not set or zero then no cutoff function will be used.

- **surface** *selection gridsize radius depth*: Returns a list of atom indices comprising the surface of the selected atoms. The method for determining the surface is to construct a grid with a spacing approximately equal to *gridsize*, where each grid point is either marked full or empty, depending on whether any atoms from the *selection* are within *radius* distance of the grid point. If the periodic cell parameters are defined in VMD, the molecule is considered periodic and the grid reflects the coordinates of periodic images of the selection. The grid size may be modified from that passed to the routine so that an integer grid dimension fits the dimensions of the box containing the molecule. Finally, each atom that falls within *depth* distance of an empty grid point is considered a surface atom, and the command returns a list of atom indices for all such atoms.

- **pbc2onc** *center* [frame *frame*|*last*]: Computes the transformation matrix that transforms coordinates from an arbitrary PBC cell into an orthonormal unitcell. Since the cell center is not stored by VMD you have to specify it.

  Here is a 2D example of a nonorthogonal PBC cell: A and B are the are the displacement vectors which are needed to create the neighboring images. The parallelogram denotes the PBC cell with the origin O at its center. The square to the right indicates the orthonormal unit cell i.e. the area into which the atoms will be wrapped by transformation T.




```
A  = displacement vector along X-axis with length a
B  = displacement vector in XY-plane with length b
A' = displacement vector along X-axis with length 1
B' = displacement vector along Y-axis with length 1
O  = origin of the PBC cell
```

- **pbcneighbors** *center cutoff* [*options*]: Returns all image atoms that are within *cutoff* Å of the PBC unitcell in form of two lists. The first list holds the atom coordinates while the second one is an indexlist mapping the image atoms to the atoms in the unitcell. Since the PBC cell center is not stored in DCDs and cannot be set in VMD it must be provided by the user as the first argument.

  The second argument (*cutoff*) is the maximum distance (in Å) from the PBC unit cell for atoms to be considered. In other words the cutoff vector defines the region surrounding the pbc cell for which image atoms shall be constructed (i.e. {6 8 0} means 6 Å for the direction of A, 8 Å for B and no images in the C-direction).

  The following options can be specified:

  - `molid <molecule_number>`: The default molecule to which an atom belongs unless a molecule number was explicitely specified for this atom in the atom list. Further, all frame specifications refer to this molecule. (Default is the current top molecule.)
  - `frame <frame>`: By default the value for the current frame will be returned but a specific frame can be chosen through this option. One can also specify *all* or *last* instead of a frame number in order to get a list of values for all frames or just the last frame respectively.
  - `sel <selection>`: If an atomselection is provided then only those image atoms are returned that are within cutoff of the selected atoms of the main cell. In case cutoff is a vector the largest value will be used.
  - `align <matrix>`: In case the molecule was aligned you can supply the alignment matrix which is then used to correct for the rotation and shift of the pbc cell.
  - `boundingbox PBC|{<mincoord> <maxcoord>}`: With this option the atoms are wrapped into a rectangular bounding box. If you provide "PBC" as an argument then the bounding box encloses the PBC box but then the cutoff is added to the bounding box. Negative values for the cutoff dimensions are allowed and lead to a smaller box. Instead you can also provide a custom bounding box in form of the minmax coordinates (list containing two coordinate vectors such as returned by the measure minmax command). Here, again, the cutoff is added to the bounding box.

- **inertia** *selection* [**moments**] [**eigenvals**]: Returns the center of mass and the principles axes of inertia for the selected atoms. If `moments` is set then the moments of inertia tensor are

also returned. With option `eigenvals` the corresponding eigenvalues will be returned, too. If both flags are set then the eigenvalues will be listed after the moments.

- **symmetry** *selection* [**plane**|**I**|**C***n*|**S***n* [*vector*]] [**tol** *value*] [**nobonds**] [**verbose** *level*]: This function evaluates the molecular symmetry of an atom selection. The underlying algorithm finds the symmetry elements such as inversion center, mirror planes, rotary axes and rotary reflections. Based on the found symmetry elements it guesses the underlying point group. The guess is fairly robust and can handle molecules whose coordinates deviate to a certain extent from the ideal symmetry. The closest match with the highest symmetry will be returned.

  Options:

  - `tol <value>`: Allows one to control tolerance of the algorithm when considering wether something is symmetric or not. A smaller value signifies a lower tolerance, the default is 0.1.
  - `nobonds`: If this flag is set then the bond order and orientation are not considered when comparing structures.
  - `verbose <level>`: Controls the amount of console output. A level of 0 means no output, 1 gives some statistics at the end of the search (default). Level 2 gives additional info about each stage, and 2, 3, 4 yield even more info for each iteration.
  - `idealsel <selection>`: The symmetry search will be performed on the regular selection but then the found symmetry elements will be imposed on the selection given with this option an the search is repeated with this second selection. This method allows, for example, to perform the symmetry guess on a selection without hydrogens (which might point in random directions for rotable groups) but still get the ideal coordinates and unique atoms for the entire structure. The selection specified here must be a superset of the selection used for the symmetry search.
  - `I`: Instead of guessing the symmetry pointgroup of the selection determine if the selection's center off mass represents an inversion center. The returned value is a score between 0 and 1 where 1 denotes a perfect match.
  - `plane <vector>`: Instead of guessing the symmetry pointgroup of the selection determine if the plane with the defined by its normal *vector* is a mirror plane of the selection. The returned value is a score between 0 and 1 where 1 denotes a perfect match.
  - `C`*n*|`S`*n* `<vector>`: Instead of guessing the symmetry pointgroup of the selection determine if the rotation or rotary reflection axis Cn/Sn with order *n* defined by *vector* exists for the selection. E.g., if you want to query wether the Y-axis has a C3 rotational symmetry you specify `C3 {0 1 0}`. The returned value is a score between 0 and 1 where 1 denotes a perfect match.
  - `imposeinversion`: Impose an inversion center on the structure.
  - `imposeplanes {<vector> [<vector> ...]}`: Impose the planes given by a list of normal vectors on the structure.
  - `imposeaxes|imposerotref {<vector> order [<vector> order ...]}`:
    Impose rotary axes or rotary reflections on the structure specified by a list of pairs of a vector and an integer. Each pair defines an axis and its order.

The scores for the individual symmetry elements depend on the specified tolerance. Imposing symmetry elements on a structure will wrap the atoms around these elements and average the coordinates of the atoms and its images. Atoms for which no image is found (with respect to that transformation) will not be wrapped. I.e. if you, for instance, impose an axis on a molecule that has no such rotary symmetry within the given tolerance then nothing will happen.

Result:

The return value is a TCL list of pairs consisting of a label string and a value or list. For each label the data following it are described below:

pointgroup The guessed point group. For point groups that have an order associated with it, like C3v or D2, the order is replaced by 'n' and we have Cnv or Dn. The order is given separately (see below).

order Point group order, i.e. order of highest axis (0 if not applicable).

elements Summary of found symmetry elements, i.e. inversion center, rotary axes, rotary reflections, mirror planes. Example: "(i) (C3) 3*(C2) (S6) 3*(sigma)" for point group D3d.

missing Elements missing with respect to ideal set of elements (same format as above). If this is not an empty list then something has gone awfully wrong with the symmetry finding algorithm.

additional Additional elements that would not be expected for this point group (same format as above). If this is not an empty list then something has gone awfully wrong with the symmetry finding algorithm.

com Center of mass of the selection based on the idealized coordinates (see 'ideal' below).

inertia List of the three axes of inertia, the eigenvalues of the moments of inertia tensor and a list of three 0/1 flags specifying for each axis wether it is unique or not.

inversion Flag 0/1 signifying if there is an inversion center.

axes Normalized vectors defining rotary axes

rotreflect Normalized vectors defining rotary reflections

planes Normalized vectors defining mirror planes.

ideal Idealized symmetric coordinates for all atoms of the selection. The coordinates are listed in the order of increasing atom indices (same order asa returned by the atomselect command "get x y z"). Thus you can use the list to set the atoms of your selection to the ideal coordinates (see example below).

unique Index list defining a set of atoms with unique coordinates.

orient Matrix that aligns molecule with GAMESS standard orientation.

If a certain item is not present (e.g. no planes or no axes) then the corresponding value is an empty list. The pair format allows to use the result as a TCL array for convenient access of the different return items.

Example:

```
set sel [atomselect top all]
# Determine the symmetry
set result [measure symmetry $sel]
# Create array 'symm' containing the results
array set symm $result
# Print selected elements of the array
puts $symm(pointgroup)
puts $symm(order)
puts $symm(elements)
puts $symm(axes)
# Set atoms of selection to ideally symmetric coordinates
$sel set {x y z} $symm(ideal)
```

9.3.19 menu

The menu command controls or queries the on-screen GUI windows.

- **list**: Return a list of the available menus
- *menu_name* **on**: Turn a menu on.
- *menu_name* **off**: Turn a menu off.
- *menu_name* **status**: Return `on` if on, `off` if off.
- *menu_name* **loc**: Return the x y location.
- *menu_name* **move** x y: Move a menu to the given (x, y) location

The parameter *menu_name* is one of the following menu names: color, display, files, graphics, labels, main, material, ramaplot. render, save, sequence, simulation, or tool.

9.3.20 mol

Load, modify, or delete a molecule in VMD. In the following, *molecule_number* is a string describing which molecules are to be affected by the command. It is one of the following: `all`, `top`, `active`, `inactive`, `displayed`, `on`, `off`, `fixed`, `free`, or one of the unique integer ID codes assigned to the molecules when they are loaded (starting with 0). The codes (molIDs) are not reused after a molecule is deleted, so if you, for example, have three molecules loaded (numbered 0, 1, 2), delete molecule with molID equal to 0, and then load another molecule, the new molecule will have molID 3. Thus, the list of available molecule IDs becomes (1 2 3). The index of the molecule on this list is, among many other things, accessible through the `molinfo` command [§9.3.22]. In the above case, for example, molecule that was loaded the last has molID equal to 3, however, it is the third on the list of molecules, so it has the index equal to 2 (since we start countin from 0).

The molecule representations (views) are assigned integer number (starting with 0 for each molecule), which appear in the list on the Graphics window [§5.4.7]. The representations can be added, deleted or changed with the `mol` command. See also sections on `molinfo` command [§ 9.3.22] for more ways of retrieving information about the representations.

- **new** [*filename*] [*options*]:
- **addfile** < *filename* > [*options*]:

  `mol new` is used to create a new molecule from a file; if the optional *filename* parameter is omitted, a plain, "blank" molecule is created with no atoms (this can be used to create a canvas for drawing user-defined geometry). `mol addfile` is like `mol new` except that the structure and coordinate data are loaded into the top molecule (whichever molecule was loaded last) instead of creating a new one. Both `mol new` and `mol addfile` accept the following set of options:

  - `type <type>`: Specifies the file type (psf, pdb, etc.) If this option is omitted, the filename extension is used to guess the filetype; otherwise, it overrides what would be guessed from the filename.
  - `first <frame>`:
  - `last <frame>`:
  - `step <frame>`: For files containing coordinate frames , specifies which frames to load. Frames are indexed starting at 0. A step of 1 means all frames in the range will be loaded; a step of 2 means load every other frame.
  - `waitfor <frames>`: For files containing coordinate frames , specifies how many frames to load before returning; the default is 1. If `frames` is less than the number of frames in the file, the rest of the frames will be loaded in the background on subsequent VMD display updates. If `frames` is `-1` or `all`, then all frames in all files still in progress will be loaded at once before the command returns. Frames loaded this way will load faster than if they are loaded in the background. If files are still being loaded in the background when the addfile command is issued, frames from the files in progress will be loaded first.
  - `volsets <set ids>`: For files containing volumetric data, specifies which data sets to load. `<set ids>` should be a list of zero-based indices.
  - `autobonds <on|off>`: Turn automatic bond calculation on/off. This can be useful for loading unusual non-molecular coordinates for which VMD's bond-finding algorithm is too slow (e.g., if the point density is very high). Default is on.
  - `molid`: For addfile only. The molecule id of the molecule into which the file should be loaded may be specified. It must be the last option specified. If omitted, the default is the top molecule.

- **load** *structure_file_type structure_file* [*coordinate_file_type coordinate_file*] : Load a new molecule from *filename(s)* using the given *format*. If an additional coordinate file is specified, load this file as well. **New in VMD 1.8:** All frames from the coordinate file will be loaded before the command returns. If this is not desirable, use the `animate read` command for more fine-grained control over how coordinate files are loaded. Previous version of VMD loaded only one frame before returning. The function will return the id of the newly created molecule, or return an error if unsuccessful.
- **urlload <file_type> <URL>**: Load a molecule of *file_type* from a given URL address. Return the id of the newly created molecule, or an error if unsuccessful.

- **pdbload <four_letter_accession_id>**: Retrieve the PDB file with the specified accession code from the RCSB web site. Returns the id of the newly created molecule, or an error if unsuccessful.
- **list**: Print a one-line status summary for each molecule.
- **list** *molecule_number*: Print a one-line status summary for each molecule matching the *molecule_number*. If only one molecule matches the *molecule_number*, also print the representation status for this molecule, i.e., number of representations as well as the representation number, coloring method , representation style and the selection string for each of the representations.
- **color** *coloring_method*: Change the default atom coloring method setting.
- **material** *material_name*: Change the default material setting.
- **representation** *rep_style*: Change the default rendering method setting.
- **selection** *select_method*: Change the default atom selection setting.
- **clipplane center** *clipplane_id rep_number molecule_number* `[` *vector* `]`
- **clipplane color** *clipplane_id rep_number molecule_number* `[` *vector* `]`
- **clipplane normal** *clipplane_id rep_number molecule_number* `[` *vector* `]`
- **clipplane status** *clipplane_id rep_number molecule_number* `[` *boolean* `]`
- **modcolor** *rep_number molecule_number coloring_method*: Change the current coloring method for the given representation in the specified molecule.
- **modmaterial** *rep_number molecule_number material_name*: Change the current material for the given representation in the specified molecule.
- **modstyle** *rep_number molecule_number rep_style*: Change the current rendering method (style) for the given representation in the specified molecule.
- **modselect** *rep_number molecule_number select_method*: Change the current selection for the given representation in the specified molecule.
- **addrep** *molecule_number*: Using the current default settings for the atom selection, coloring, and rendering methods, add a new representation to the specified molecule.
- **default** *category value*: Set the default settings for color, style, selection, or material to the supplied value.
- **delrep** *rep_number molecule_number*: Deletes the given representation from the specified molecule.
- **modrep** *rep_number molecule_number*: Using the current default settings for the atom selection, coloring, and rendering methods, changes the given representation to the current defaults.
- **delete** *molecule_number*: Delete molecule(s).

- **active** *molecule_number*: Make molecule(s) active.
- **inactive** *molecule_number*: Make molecule(s) inactive.
- **on** *molecule_number*: Turn molecule(s) on (make drawn).
- **off** *molecule_number* : Turn molecule(s) off (hide).
- **fix** *molecule_number*: Fix molecule(s).
- **free** *molecule_number*: Unfix molecule(s).
- **top** *molecule_number*: Set the top molecule.
- **cancel** *molecule_number*: Cancel loading trajectories.
- **reanalyze** *molecule_number*: Re-analyze structure after bonding and atom name changes.
- **bondsrecalc** *molecule_number*: Recalculate bonds from distances for current timestep.
- **ssrecalc** *molecule_number*: Recalculate secondary structure.
- **rename** *molecule_number newname*: Rename the specified molecule.
- **repname** *molecule_number rep_number*: Returns the name of the given rep. This name is guaranteed to be unique for all reps in the molecule, and will stay with the rep even if the rep_number changes.
- **repindex** *molecule_number name*: Return the *rep_number* for the rep with the given name, or -1 if no rep with that name exists in that molecule.
- **selupdate** *rep_number molecule_number [onoff]*: Update the selection for the specified rep each time the molecule's timestep changes. If *onoff* is not specified, returns the current update state.
- **colupdate** *rep_number molecule_number [onoff]*: Update the calculated color for the specified rep each time the molecule's timestep changes. If *onoff* is not specified, returns the current update state.
- **drawframes** *molecule_number rep_number [frame_specification]*: Draw multiple trajectory frames or coordinate sets simultaneously. This setting allows the user to select one or more ranges of frames to display simultaneously. The frame specification takes one of the following forms **now**, *frame_number*, *start:end*, or *start:step:end*. If the *frame_specification* is not specified, the command returns the currently active frame selection text.
- **smoothrep** *molecule_number rep_number [n]*: Get/set the window size for on-the-fly smoothing of trajectories. Instead of drawing the specified rep from the current coordinates, VMD will calculate the average of the coordinates from the n previous and subsequent timesteps. If n is zero then no smoothing is performed. Note that this smoothing does not affect any label measurements, and does not change the values of the coordinates returned by atom selections or written to files; it only affects how the rep is drawn. Smoothing can be especially useful in visualizing rapidly fluctuating molecules or making movies.

- **scaleminmax** *molecule_number rep_number [min max | auto]*: Get/set the color scale range for this rep. Normally the color scale is automatically scaled to the minimum and maximum of the corresponding range of data. This command overrides the autoscaled values with the values you specify. Omit the *min* and *max* arguments to get the current values. Use "auto" instead of a min and max to rescale the color scale to the maximum range again.
- **showrep** *molecule_number rep_number [on | off]*: Get/set whether the given rep is shown or hidden. Hidden reps cannot be picked and do not show any graphics.
- **volume** *molecule_number* <*volumeset_name*> <*Origin*> <*a*> <*b*> <*c*> *#a #b #c* <*Data*> Add a volumetric data set to the current molecule. Origin, a, b, and c are vectors setting the origin and the three cell vectors. #a, #b, and #c are the number of grid points in the respective cell vector directions and finally the data has to be provided as one list with the data following the grid points along the c-axis fastest, then the b-axis and finally the a-axis.

9.3.21 molecule

Same as mol.

9.3.22 molinfo

The `molinfo` command is used to get information about a molecule (or loaded file) including the number of loaded atoms, the filename, the graphics selections, and the viewing matrices. It can also be used to return information about the list of loaded molecules.

Each molecule has a unique id, which is assigned to it when it is first loaded. These start at zero and increase by 1 for each new molecule. When a molecule is deleted, the number is not used again. There is one unique molecule, called the `top` molecule [§5.4.2], which is used to determine some parameters, such as the center of view, the data in the animation controls, etc.

- **list**: Returns a list of all current molecule id's.
- **num**: Returns the number of loaded molecules.
- **top**: Returns the id of the top molecule.
- **index** *n*: Returns the id of the *n*'th molecule.
- *molecule_id* **get** {*list of keywords*}
- *molecule_id* **set** {*list of keywords*} {*list of values*} Access and, in some cases, modify information about a given molecule. The list of recognized keywords is given in Table 9.3.

```
Examples:
vmd > molinfo top get numatoms
568
molinfo 0 get {filetype filename}
pdb /home/dalke/pdb/bpti.pdb
vmd > molinfo 0 get { {rep 0} {color 0} {rep 1} {color 1} }
{VDW 1.000000 8.000000} {ColorID 5} Lines 1.0000 SegName
```

Keyword	Aliases	Arg	Set	Description
id		*int*	N	molecular id
index		*int*	N	index on the molecule list
numatoms		*int*	N	number of atoms
name		*str*	N	the name of the molecule (usually the name of the file)
filename		*str*	N	list of filenames for all files loaded for this molecule
filetype		*str*	N	list of file types for this molecule
database		*str*	N	list of databases for this molecule
accession		*str*	N	list of database accession codes for this molecule
remarks		*str*	N	list of freeform remarks for this molecule
active		*bool*	Y	is/make the molecule active
drawn	displayed	*bool*	Y	is/make the molecule drawn
fixed		*bool*	Y	is/make the molecule fixed
top		*bool*	Y	is/make the molecule top
center		*vector*	Y	get/set the coordinate used as the center
center_matrix		*matrix*	Y	get/set the centering matrix
rotate_matrix		*matrix*	Y	get/set the rotation matrix
scale_matrix		*matrix*	Y	get/set the scaling matrix
global_matrix		*matrix*	Y	get/set the global (rotation/scaling) matrix
view_matrix		*matrix*	N	get/set the overall viewing matrix
numreps		*int*	N	the number of representations
selection *i*		*string*	N	the string for the i'th selection
rep *i*		*string*	N	the string for the i'th representation
color *i*	colour	*string*	N	the string for the i'th coloring method
numframes		*int*	N	number of animation frames
numvolumedata		*int*	N	number of volumetric data sets
frame		*int*	Y	current frame number
timesteps		*int*	Y	number of elapsed timesteps in an interactive simulation
angles		*list*	Y	topology angle types and definitions {type a1 a2 a3}
dihedrals		*list*	Y	topology dihedral types and definitions {type a1 a2 a3 a4}
impropers		*list*	Y	topology improper types and definitions {type a1 a2 a3 a4}
bond		*float*	N	the bond energy (for the current frame)
angle		*float*	N	the angle energy
dihedral		*float*	N	the dihedral energy
improper		*float*	N	the improper energy
vdw		*float*	N	the van der Waal energy
electrostatic	elec	*float*	N	the electrostatic energy
hbond		*float*	N	the hydrogen bond energy
kinetic		*float*	N	the total kinetic energy
potential		*float*	N	the total potential energy
energy		*float*	N	the total energy
temperature	temp	*float*	N	the overall temperature
pressure		*float*	Y	the simulation pressure
volume		*float*	Y	the simulation volume
efield		*float*	Y	efield
alpha		*float*	Y	unit cell angle alpha in degrees (for the current frame)
beta		*float*	Y	unit cell angle beta in degrees (for the current frame)
gamma		*float*	Y	unit cell angle gamma in degrees (for the current frame)
a		*float*	Y	unit cell length a in Angstroms (for the current frame)
b		*float*	Y	unit cell length b in Angstroms (for the current frame)
c		*float*	Y	unit cell length c in Angstroms (for the current frame)

Table 9.3: `molinfo set/get` keywords

9.3.23 mouse

Change the current state (mode) of the mouse, optionally active TCL callbacks.

- **mode 0**: Set mouse mode to rotation.
- **mode 1**: Set mouse mode to translation.
- **mode 2**: Set mouse mode to scaling.
- **mode 3** *N*: Set mouse mode to rotate light *N*.
- **mode 4** *N*: Set mouse mode to picking mode *N*, where *N* is one of the following:
  - 0: query item
  - 1: pick center
  - 2: pick atom
  - 3: pick bond
  - 4: pick angle
  - 5: pick dihedral
  - 6: move atom
  - 7: move residue
  - 8: move fragment
  - 9: move molecule
  - 10: force on atom
  - 11: force on residue
  - 12: force on fragment

- **callback on/off**: Turn the callbacks on or off. To use the callbacks, trace the variable `vmd_pick_atom_silent`. See below for information on tracing.
- **rocking on/off**: Enable/disable persistent rotation of the scene with the mouse.
- **stoprotation**: Stop any mouse-initiated scene rotation as well as any rocking initiated with the "rock" command.

9.3.24 parallel

The parallel command enables large scale parallel scripting when VMD has been compiled with MPI support. In absence of MPI support, the parallel command is still available, but it operates the same way it would if an MPI-enabled VMD would when run on only a single node. The parallel command enables large analysis scripts to be easily adapted for execution on large clusters and supercomputers to support simulation, analysis, and visualization operations that would otherwise be too computationally demanding for conventional workstations [14, 35, 26, 40].

- **nodename**: Return the hostname of the current compute node.

- **noderank**: Return the MPI rank of the current compute node.
- **nodecount**: Return the total number of MPI ranks in the currently running VMD job.
- **allgather** *object*: Perform a parallel allgather operation across all MPI ranks, taking the user defined object as input to each caller. All VMD MPI ranks must participate in the allgather operation.
- **allreduce** *user_reduction_procedure object*: Perform a parallel reduction across all MPI ranks by calling the user-supplied reduction procedure, passing in a user defined object. All VMD MPI ranks must participate in the allreduce operation.
- **barrier**: Perform a barrier synchronization across all MPI ranks in the running VMD job.
- **for** *startcount endcount user_worker_procedure object*: Invoke VMD parallel work scheduler to run a computation over all MPI ranks. The VMD work scheduler uses dynamic load balancing to assign work indices to workers, calling the user-defined worker callback procedure for each work item.

9.3.25 play

Start executing text commands from a specified file, instead of from the console. When the end of the file is reached, VMD will resume reading commands from the previous source. This command may be nested, so commands being read from one file can include commands to read other files.

- *filename*: Execute commands from *filename*.

9.3.26 quit

Same as exit.

9.3.27 render

Output the currently displayed image (scene) to a file using the global VMD display settings and any renderer-specific settings.

- **list**: List the available rendering methods.
- **hasaa** *method*: Query whether or not a renderer has controllable antialiasing feature.
- **aasamples** *method samples*: Query or set the number of antialiasing samples to be used by this renderer, if supported.
- **aosamples** *method samples*: Query or set the number of ambient occlusion lighting samples to be used by this renderer, if supported.
- **formats** *method*: List a renderer's available image output formats/modes.
- **format** *method format*: Set a renderer's active image output format/mode.

- *method filename*: Render the global scene to *filename* using *method* and execute the default command, where *method* can be one of the following:
  - ART
  - Gelato
  - POV3
  - PostScript
  - Radiance
  - Raster3D
  - Rayshade
  - Renderman
  - snapshot
  - STL
  - Tachyon
  - TachyonInternal
  - VRML-1
  - VRML-2
  - Wavefront
- *method filename command*: Render the global scene to *filename*, then execute '*command*'. Any %s in '*command*' are replaced by the filename (up to 5).
- **options** *method*: Get the default command string.
- **options** *method command*: Set new default command.
- **default** *method*: Get the original default command.

9.3.28 rock

Rotate the current scene continually at a specified rate.

- **off**: Stops rocking.
- **< x | y | z > by** *step*: Rock around the given axis at a rate of *step* degrees per redraw.
- **< x | y | z > by** *step n*: Rock around the given axis at a rate of *step* degrees per redraw for *n* steps, reverse, and repeat.

9.3.29 rotate

Rotate the current scene around a given axis by a certain angle. This does not change atom coordinates.

- **stop**: Stop all rotation, similar to rock off, but it also stops mouse rotations as well.
- **< x | y | z > by** *angle*: Rotate around the given axis *angle* degrees.
- **< x | y | z > to** *angle*: Rotate the given axis to the absolute position *angle*.
- **< x | y | z > < by | to >** *angle step*: Rotate at a rate of *step* degrees per redraw.

9.3.30 scale

Scale the current scene up or down. This does not change atom coordinates.

- **by** *f*: Multiply scene scaling factor by *f*.
- **to** *f*: Set scene scaling factor to *f*.

9.3.31 stage

Position a checkerboard stage on the screen.

- **location < off | origin | bottom | top | left | right | behind >**: Set the location.
- **location**: Get the current location.
- **locations**: Get a list of possible locations.
- **panels** *n*: Set number of panels in stage, up to 30.
- **panels**: Get the number of panels in use

9.3.32 tool

Initialize and control the tools that are controlled by external tracking devices.

- **create**: Create a new tool
- **change** *type* `[` *toolid* `]`: Change the type of a tool.
- **scale** *scale* `[` *toolid* `]`: Change the scale of the coordinates reported by a tool.
- **scaleforce** *scale* `[` *toolid* `]`: Increase or decrease the force on a force-feedback device.
- **offset** *x y z* `[` *toolid* `]`: Add a vector to a tool's position.
- **delete** `[` *toolid* `]`: Remove a tool.

- **rep** *molid repid*: Choose only a single representation for tugging or SMD.
- **adddevice** *name* `[` *toolid* `]` : Add a device to a tool, using a name found in the sensor configuration file.
- **removedevice** *name* `[` *toolid* `]` : Remove a device from a tool, using a name found in the sensor configuration file.
- **callback** `on/off` : Enable callbacks for the tools.

9.3.33 translate

Translate the objects in the current scene. This does not change the atom coordinates.

- **by** *x y z*: Translate by vector (*x*, *y*, *z*) in screen units (note, that this does not change the atom coordinates).
- **to** *x y z*: Translate to the absolute position (*x*, *y*, *z*) in screen units.

9.3.34 user

Add user-customized commands.

- **add key** *key command*: Assign the given text command to the hot key *key*. When *key* is pressed while the mouse is in the display window, the specified command will be executed.
- **print keys** : Print out the current definition of the hot keys.

See section 5.1.3 for examples of the use of the `user` command.

9.3.35 vmdinfo

(Tcl) Returns information about this version of VMD.

- **version**: Returns the version number;
- **versionmsg**: Full information about this version;
- **authors**: List of authors;
- **arch**: architecture type (in case you couldn't tell);
- **options**: options used to compile VMD;
- **www**: VMD home page;
- **wwwhelp**: VMD help page.

This function is available without Tcl and the information is displayed to the screen.

9.3.36 volmap

The `volmap` command creates volumetric maps (3D grids containing a value at each grid point) based on the molecular data, which can then be visualized in VMD using the Isosurface and VolumeSlice representations or using the Volume coloring mode. Also note that the VolMap plugin, accessible from the VMD Extension menu, provides a graphical front-end to many of the `volmap` command's capabilities.

To create a volumetric map, the `volmap` command is run in the following way, where the atom selection specifies the atoms and molecule to include in the calculation, and where the maptype specifies the type of volumetric data to create:

```
volmap <maptype> <atom selection> [optional arguments]
```

For example, to create a mass density map with a cell side of 0.5 Å, averaged over all frames of the top molecule, and add the volumetric data to the top molecule, on would use:

```
volmap density [atomselect top "all"] -res 0.5 -weight mass -allframes \
                                                  -combine avg -mol top
```

The various volumetric data map types currently supported by `volmap` are listed as follows. Please note that when a map type description refers to an atoms radius or beta field, *etc.*, that these values will be read directly from VMD's associated fields for that atom. In certain cases, you may want to adjust the atom selections fields (such as radius, beta, *etc.*) before performing the volmap analysis.

- **density**: creates a map of the weighted atomic density at each gridpoint. This is done by replacing each atom in the selection with a normalized gaussian distribution of width (standard deviation) equal to its atomic radius. The gaussian distribution for each atom is then weighted using an optional weight (see the `-weight` argument), and defaults to a weight of one (*i.e*, the number density). The various gaussians are then additively distributed on a grid.

- **interp**: creates a map with the atomic weights interpolated onto a grid. For each atom, its weight is distributed to the 8 nearest voxels via a trilinear interpolation. The optional weight (see the `-weight` argument) defaults to a weight of one.

- **distance**: creates a map for which each gridpoint contains the distance between that point and the edge of the nearest atom. In other words, each gridpoint specifies the maximum radius of a sphere cnetered at that point which does not intersect with the spheres of any other atoms. All atoms are treated as spheres using the atoms' VMD radii.

- **coulomb**, **coulombmsm**: Creates a map of the electrostatic field of the atom selection, made by computing the non-bonded Coulomb potential from each atom in the selection (in units of k_BT/e). The coulomb map generation is optimized to take advantage of multi-core CPUs and programmable GPUs if they are available [16, 17, 18, 19, 20, 21, 22, 23, 24].

- **ils**: Creates a free energy map of the distribution of a weakly-interacting monoatomic or diatomic gas ligand throughout the system using the Implicit Ligand Sampling (ILS) technique. See additional information about ILS below.

- **mask**: Creates a map which is set to 0 or 1 depending on whether they are within a specified cutoff distance (use the `-cutoff` argument) of any atoms in the selection. The mask map is typically used in combination with other maps in order to hide/mask data that is far from a region of interest.

- **occupancy**: Each grid point is set to either 0 or 1, depending on whether it contains onbe or more atoms or not. When averaged over many frames, this will provide the fractional occupancy of that grid point. By default, atoms are treated as spheres using the atomic radii and a gridpoint is considered to be "occupied" if it lies inside that sphere. Use the `-points` argument to treat atoms as points (a grid point is "occupied" if its grid cube contains an atom's center).

The following optional arguments are universally understood by every volmap map types:

- **-allframes**: Use every frame in the molecule instead of just the current one to compute the volumetric map. The method used to combine the various trajectory frame maps can be specified using the `-combine` argument. By default, volmap only uses the current frame.

- **-combine < avg | max | min | stdev | pmf >**: Specifies the rule to use to combine frames when using the `-allframes` argument. These correspond to keeping the average, maximum or minimum values from the range of calculated frames. `stdev` will return the standard deviation for each point over the range of frames, and `pmf` uses a thermal average $-\ln \sum_i^N e^{-value_i}/N$ for each point. The default is `avg` except for ligand maps where the default is `pmf`.

- **-res** *resolution*: Sets the resolution of the map. This means that the volume will be subdivided into many small cubes whose side have a length of *resolution*.

- **-minmax** $\{\{x_{min}\ y_{min}\ z_{min}\}\ \{x_{max}\ y_{max}\ z_{max}\}\}$: Allows the user to specify the min-max boundaries of the grid in which the volumetric map will be computed. The argument to -minmax is a list of two 3-vectors specifying the minimum and maximum coordinates of the desired volumetric data grid.

- **-checkpoint** *frequency*: For the analysis of long trajectories, it can be desirable to have intermediate outputs of the volmap computation. The checkpoint option forces the volmap computation to output a map of what has been computed so far, at every *frequency* frames. The default *frequency* is 500; setting the *frequency* to zero disables the checkpointing feature.

- **-mol <** *molid* **| top >**: Exports the final volumetric data into the VMD molecule specified by *molid*. By default, all maps are exported to a file or name *maptype*_out.dx; using the `-mol` option overrides this.

- **-o** *filename*: Exports the final volumetric data into a DX file (.dx extension is added if missing). By default, all maps are exported to a file or name *maptype*_out.dx.

The following optional arguments are special arguments understood only by some volmap map types. Some arguments may only apply to certain map types or may have different meaning for different map types:

- **-cutoff** *cutoff*: Specifies a cutoff distance. For the distance maps, specifies the largest distance that will be considered (large number is better but slower). For the mask maps, specifies the distance from each atom which will be considered part of the mask.
- **-points**: For the occupancy map type. Treat atoms as point particles instead of as spheres.
- **-radscale** *factor*: For the density map type. Sets a multiplication factor that multiplies all the VMD atomic radii for the purpose of the calculation.
- **-weight** `<` *field name* `|` *value list* `>`: For the density map type. Sets a per-atom weight to be used when computing the density. This can be the name of any VMD numerical atomic field (such as mass, charge, beta, occupancy, user, radius, *etc.*) or else a Tcl list of numbers of the same length as the number of atoms.

Implicit Ligand Sampling (`volmap ils` command)

This command computes a map of the estimated potential of mean force (in units of k_BT at 300 K) of placing a weakly-interacting gas monoatomic or multiatomic ligand at every gridpoint. These results will only be valid when averaging over a large set of frames. Note that if you have a CUDA enabled GPU then your ILS calculation will run about 20 times faster than on a CPU.

Please refer to and cite:
Cohen, J., A. Arkhipov, R. Braun and K. Schulten, *"Imaging the migration pathways for O_2, CO, NO, and Xe inside myoglobin"*, Biophysical Journal **91**, 1844–1857, 2006.

The command syntax differs from the other volmap commands and it has its own set of options:

`volmap ils` *molid* `<` *minmax* `|` `pbcbox` `>` `[options]`

Here *minmax* denotes the boundaries of the grid in which the volumetric map will be computed. It is given as a list of two 3-vectors specifying the minimum and maximum coordinates of the desired volumetric data grid $\{\{x_{min}\ y_{min}\ z_{min}\}\ \{x_{max}\ y_{max}\ z_{max}\}\}$. If you provide the keyword **pbcbox** instead of the *minmax* coordinates then the target grid will be set to the rectangular box that encloses the PBC cell. A typical choice for the minmax parameters would be the minmax box of a subset of your system (for instance the just protein) as returned by the `measure minmax` command.

Based on the grid dimensions a selection that includes all atoms within the interaction cutoff distance (specified by `-cutoff`) is automatically chosen for the computation of the interactions.

In case your minmax box exceeds the periodic bounday box the non-overlapping parts of your map will be ill defined and a warning is printed. In this case you should consider wrapping the coordinates so that the requested grid lies in the center of the box. You can use the `pbc wrap` command from the PBCtool plugin for this.

In case the nonbonded interaction margin exceeds the periodic boundaries regions of your map will be based on incomplete interactions and a warning is printed. If this happens you should use the `-pbc` flag which automatically takes atoms of the neighboring cells into account.

Before starting the computation, the atomic radii of each atom in the molecule should be set to the corresponding CHARMM Lennard-Jones $R_{\min}/2$ parameter (in Ångström), and the *beta* value of each atom should be set to the CHARMM Lennard-Jones ϵ (energy well depth in kcal/mol) parameter. This can be done using VMD's VolMap plugin. Simply call in succession the following

commands within the VMD console environment to use default CHARMM values for the various atoms of a molecule:

```
package require ilstools
ILStools::readcharmmparams [list of CHARMM parameter files]
ILStools::assigncharmmparams <molid>
```

The following optional arguments are understood:

- **-first** *frame*: First frame to process. (default: frame 0)
- **-last** *frame*: Last frame to process. (default: last frame of molecule)
- **-o** *filename*: Exports the final volumetric data into a DX file (.dx extension is added if missing). By default, all maps are exported to a file or name *maptype*_out.dx.
- **-res** *resolution*: Sets the resolution of the final map. This means that the volume will be subdivided into many small cubes whose side have a length of *resolution*. The computation should be performed on a finer grid (see `-subres` option) but at the end the map is downsampled to this resolution. A good choice for the grid resolution 1 Å (argument `-res`). Lower resolutions make it difficult to see features, higher ones will be very costly in terms of computation time. Also, since the fluctuation of the protein backbone is on the order of 1-2 Angstrom a higher grid resolution doesn't make much sense.
- **-subres** *num*: Number of points in each dimension of the subsampling grid, e.g. 2 for a 2x2x2 subgrid or 3 for a 3x3x3 subgrid. A value of 1 means is no subsampling, the default is (`-subres 3`). Without subsampling the probe is placed at each grid cell center (for diatomic probes in *numconf* different random orientations, see argument `-orient`). This position is assumed to be representative for the interaction of the probe in this voxel with the system. However, for a typical voxel size of 1x1x1 Å the energy value can differ significantly within the voxel and the value at the center might not be close to the average. Subsampling averages over the interaction on a regular subgrid in each voxel thus producing a more accurate free energy value for placing the probe into each voxel. Even though this severely increases the computational cost it is highly recommended that you use subsampling! A 3x3x3 subgrid for a 1 Å resolution map is a good choice.
- **-T** *temperature*: The temperature in Kelvin at which the MD simulation was performed. (default: 300)
- **-probesel** *selection*: Atom selection that defines the probe molecule. The radius and occupancy fields should be populated with the VDW radii and VDW epsilon parameters from the force field (see option `-probevdw`). Alternatively, you can specify the probe coordinates and VDW parameters probe atoms directly using the `-probecoor` and `-probevdw` options.
- **-probecoor** *atomcoords*: Set the coordinates of the probe atoms in form of a list of triples $\{\{x_0\ y_0\ z_0\} \ldots \{x_N\ y_N\ z_N\}\}$.
- **-probevdw** *parameterlist*: Set the tuple of van der Waals parameters for each probe atom in the form $\{\{\epsilon_0\ R_{\min,0}/2\} \ldots \{\epsilon_N\ R_{\min,N}/2\}\}$. They define the nonbonded interactions of

the probe evaluated by the Lennard-Jones potential

$$U_{\mathrm{VDW}} = \sum_{\text{atoms } i,j} \epsilon_{ij} \left(\left(\frac{R_{ij}}{r_{ij}} \right)^{12} - 2 \left(\frac{R_{ij}}{r_{ij}} \right)^{6} \right) \tag{9.2}$$

where $R_{ij} = (R_{\mathrm{min},i} + R_{\mathrm{min},j})/2$ and $\epsilon_{ij} = \sqrt{\epsilon_i \cdot \epsilon_j}$. (That's the same form as in CHARMM and AMBER parameter files). Units of ϵ are kcal/mol, and of $R_{\mathrm{min}}/2$ are Ångström.

- **-orient** *n*: Control the number of samples of different probe orientations for multiatom probes at each grid point. The number n determines the angular spacing of probe orientation vectors and of the rotations around each of these vectors.

  $n = 1$: use 1 orientation only
  $n = 2$: use 6 orientations (vertices of a octahedron)
  $n = 3$: use 8 orientations (vertices of a hexahedron)
  $n = 4$: use 12 orientations (faces of a dodecahedron)
  $n = 5$: use 20 orientations (vertices of a dodecahedron)
  $n = 6$: use 32 orientations (faces+vertices of a dodecahedron)
  $n > 6$: geodesic subdivisions of icosahedral faces with frequency 1, 2, ... $n - 6$

  For each orientation a number of rotamers will be generated. The angular spacing of the rotations around the orientation vectors is chosen to be about the same as the angular spacing of the orientation vector itself. If the probe has at least one symmetry axis then the rotations around the orientation vectors are reduced accordingly. If there is an infinite oder axis (linear molecule) the rotation will be omitted. In case there is an additional perpendicular C2 axis the half of the orientations will be ignored so that there are no antiparallel pairs.

  Probes with tetrahedral symmetry:
  Here n denotes the number of rotamers for each of the 8 orientations defined by the vertices of the tetrahedron and its dual tetrahedron.

- **-cutoff** *cutoff*: Set the CHARMM van der Waals cutoff beyond which the interaction between the probe and protein atoms is set to zero.

- **-maxenergy** *energy*: Cutoff energy above which the occupancy of a grid cell is regarded zero. For GPUs energies of more than 87 always correspond to floating point values of zero for the occupancy. Hence there is no point going higher than that. For CPUs that number is higher, however, the lower the occupancy the more severely these points will be undersampled and the according error will be very high. Thus, in the final map it probably does not make sense to look at values higher than 10kT which not a big loss since the low energy regions are the ones we are interested in. So you probably want to set this to a value between 10 and 87 (we are in thye process of testing this but I suppose 20 kT would be a safe number).

- **-alignsel** *selection*: Use the provided selection to align all trajectory frames to the first frame. If you don't use this option you should make sure that you aligned all frames yourself before running volmap ils.

- **-transform** *matrix*: Suppose you want to align your trajectory to a reference frame from a different molecule. In this case you should align the first frame of your trajectory to the reference and provide the according alignment matrix as returned by "`measure fit`") using the -transform option. `volmap ils` will take care of the rest.

- **-pbc**: This flag signals that you want a periodic boundary aware ILS calculation. Depending on the desired target grid size image atoms from neighboring PBC cells are taken into account for the computation. The atoms used for the calculation are chosen from a box that exceeds the target grid size by the interaction cutoff in each direction.
  Note: If your molecule rotated or drifted from the PBC center during your MD simulation then the structure alignment will rotate or shift the PBC cell so that your map might not lie entirely inside the PBC cell anymore. This will lead to ill-defined fringes of the map and you might want to consider rewrapping the coordinates. Rewrapping cannot undo the rotation but unless you have a very oblonged PBC cell removing the shift by rewrapping will in most cases yield a map without or with little boundary effects. See the `pbc wrap` command from the PBCtool plugin.
  Warning: If you use `-pbc` DO NOT ALIGN the frames of the structure yourself prior to the calculation! It will totally mess up the definition of your PBC cells. Instead you should use the `-alignsel` option and let volmap handle the alignment. However, you CAN align the sturcture globally (i.e. align all frames using the SAME transformation matrix) to a reference frame. In this case you have to provide the transformation matrix you used via -transform.

- **-pbccenter** *vector*: Since the PBC cell origin is stored neither in DCD files nor in VMD you have to specify it in case it is different than the default {0 0 0}.

- **-maskonly**: This flag requests to compute only a mask map telling for which gridpoints we expect valid energies, i.e. the points for which the maps overlap for all frames will contain 1, all other points will be 0. This is useful if you don't use periodic boundary conditions where it can happen that due to the choice of the grid and/or the rotation of the protein the box including your grid plus the interaction cutoff will lie partially outside your system which means you would miss some of the interactions. The map produced by the `-maskonly` mode will tell where are these ill defined regions.

9.3.37 wait

Specify a number of seconds to wait before reading another command. Animation *continues* during this time. The wait command will not behave as expected if called within a complex Tcl proc or loop structures. The wait command doesn't actually run until the next complete Tcl code block due to the way VMD processes its commands.

- *time*: wait *time* seconds.

9.3.38 sleep

Specify a number of seconds to sleep before reading another command. Animation *stops* during this time.

- *time*: sleep *time* seconds.

9.4 Tcl callbacks

When certain events occur, VMD notifies the Tcl interpreter by setting certain Tcl variables to new values. You can use this feature to customize VMD, for instance, by causing new graphics to appear when the user picks an atom, or recalculating secondary structure on the fly.

To make these new feature happen at the right time, you need to write a script that takes a certain set of arguments, and register this script with the variable you are interested. Registering scripts is done with the built-in Tcl command `trace`; see `http://www.tcl.tk/man/tcl8.4/TclCmd/trace.htm` for documentation on how to use this command. The idea is that after you register your callback, when VMD changes the value of the variable, your script will immediately be called with the new value of the variable as arguments. Table 9.4 summarizes the callback variables available in VMD.

In the VMD script library at `http://www.ks.uiuc.edu/Research/vmd/script_library/`, you can find a number of scripts that take advantage of Tcl variable tracing. Below, we give a simple example. The following procedure takes the picked atom and finds the molecular weight of residue it is on.

```
proc mol_weight {args} {
  # use the picked atom's index and molecule id
  global vmd_pick_atom vmd_pick_mol
  set sel [atomselect $vmd_pick_mol "same residue as index $vmd_pick_atom"]
  set mass 0
  foreach m [$sel get mass] {
    set mass [expr $mass + $m]
  }
  # get residue name and id
  set atom [atomselect $vmd_pick_mol "index $vmd_pick_atom"]
  lassign [$atom get {resname resid}] resname resid
  # print the result
  puts "Mass of $resname $resid = $mass"
}
```

Once an atom has been picked, run the command `mol_weight` to get output like:

```
Mass of ALA 7 : 67.047
```

Since VMD sets the vmd_pick_event, it can be traced. The trace function is registered as:

```
trace add variable ::vmd_pick_event write mol_weight
```

And now the residue masses will be printed automatically when an atom is picked. Make sure to turn off the trace when you are done with it (*e.g.* your plugin's window gets closed):

```
trace remove variable ::vmd_pick_event write mol_weight
```

Table 9.4: Description of Tcl callback variables in VMD.

When called	Name	Description
Molecule `molid` was deleted	`vmd_molecule(molid)`	0
Molecule `molid` was created (data may not have been loaded yet)	`vmd_molecule(molid)`	1
Molecule `molid` was renamed	`vmd_molecule(molid)`	2
Structure file loaded	`vmd_initialize_structure(molid)`	1
Coordinate file loaded	`vmd_trajectory_read(molid)`	*name of coordinate file*
Molecule `molid` changed animation frames	`vmd_frame(molid)`	*new animation frame*
Any VMD command executed	`vmd_logfile`	Tcl text equivalent of command
An atom has been picked using the "Pick" mouse mode	`vmd_pick_event`	When receiving this event, the following global variables are also set: vmd_pick_atom (id of picked atom), vmd_pick_mol (id of picked molecule)
Pointer moved.	`vmd_pick_client`	name of pointer
Pointer moved.	`vmd_pick_mol_silent`	id of nearby mol
Pointer moved.	`vmd_pick_atom_silent`	id of nearby atom
Atom picked	`vmd_pick_shift_state`	1 if shift key down during pick, 0 otherwise
IMD coordinate set received	`vmd_timestep(molid)`	frame containing new coordinates
Set of labels to be graphed	`vmd_graph_label`	{labeltype labelid} {labeltype labelid} ...
Tcl interpreter is shutting down	`vmd_quit`	1

Chapter 10

Python Text Interface

VMD 1.6 and later contain an embedded, fully-functional Python interpreter. The interpreter acts just like the Python command line: you can import your own modules and run them from with the text console of VMD. In addition, VMD provides a number of modules for loading molecules and controlling their display.

Pre-compiled VMD binaries currently use Python version 2.5. The current VMD source code has been tested to compile with Python versions 2.4 to 2.6 on a few platforms. User contributed VMD rpm or deb packages can be thus be compiled against any of those versions.

10.1 Using the Python interpreter within VMD

When you start VMD, the VMD text console normally uses the Tcl command interpreter to process what you type. In order to use the Python interpreter, you have to tell VMD to switch to 'Python mode'. There are three ways to do this: (1) Type `gopython` in the console window; (2) pass `-python` as a command line option; or (3) put `gopython` on the last line of your `.vmdrc` file. If VMD prints an error message reporting that the Python interpreter is not available, your version of VMD was not compiled with Python support; contact the VMD developers for help. If all goes well, you should see Python command prompt '>>> ' in the console window. To switch back to the Tcl interpreter, press Ctrl-D as though you were exiting Python. Switching back and forth between Python and Tcl does not destroy any of your work; all variables and modules will still be defined until you exit VMD.

Typing 'gopython <filename>', where <filename> is the name of a file containing Python code will cause VMD to switch to Python mode, process the file, then switch back to Tcl. In this way, you can embed Python functions inside your Tcl scripts!

You can also type 'gopython -command "*your code here*" to run an arbitrary line of python code.

10.2 Python modules within VMD

Once you enter the VMD Python environment, you will find a module called "VMD" already loaded. This module contains all the other built-in modules for writing VMD Python scripts.

VMD is not distributed with an entire Python environment. In order to use the set of libraries that normally come with a Python distribution, you must tell Python where to find the libraries. There are two primary means of doing this. The `PYTHONHOME` environment variable points to

the location where Python is installed; the version installed at this point must match VMD's version (2.5). Thus if you have Python libraries in /usr/local/lib/python2.5, adding the line `set env(PYTHONHOME) /usr/local` to your startup script or .vmdrc file will do the trick.

If you have additional modules that you want to use within VMD, use the `PYTHONPATH` environment variable to tell Python where to find them. Please note that any of these modules have to be compiled against matching versions of the Python package and its subpackages that are distributed with the pre-compiled VMD binaries. If you want to use the *native* Python and its packages, you will have to compile VMD from source code or install a user contributed package that matches your OS. See any Python book and the instructions for compiling VMD from source code for more information.

if the Tkinter module is found in the Python installation, VMD will load it at Python startup in order to make Tkinter windows work in harmony with windows created from within Tk. In addition, if you have Numeric Python installed in your system, a submodule called vmdnumpy will become available within the VMD module; see below for details.

10.3 Atom selections in Python

10.3.1 The built-in atomsel type

NEW IN VMD 1.8.6: The AtomSel class has been deprecated, in favor of a new built-in type called `atomsel`. The atomsel type functions much the same way as the old AtomSel class, but also provides methods similar to the Tcl interface for returning RMS fit matrices and applying those transformations to coordinates.

The new `atomsel` type is found in a new built-in module, also called `atomsel`. Use `help(atomsel)` to get the complete documentation.

10.3.2 The AtomSel class (DEPRECATED)

VMD provides an atom selection class for use in the Python interpreter. Instances of this class correspond to a set of atom indices in a particular molecule for a particular coordinate set. Once an atom selection is made, you can query the properties of the selected atoms, such as their names, residue ids, or coordinates. In a similar fashion, you can set the values of these properties. You can also perform logical operations on atom selections, including finding the intersection or union of two atom selections or finding the inverse of the set. Finally, you can perform tuple operations on the atom selection object to query the indices of the atoms in the selection.

Atom selection macros can be defined using the `macro` method of the AtomSel module. The syntax is just as in the corresponding `atomselect macro` and `atomselect delmacro` Tcl commands; see section 9.3.2 for details.

Below we summarize the methods available from the AtomSel class.

- `AtomSel(selection = 'all', molid = 0, frame = 0)`: Creates a new atom selection object.

  >>> sel = AtomSel('name CA', 1) # Selects the alpha carbons of molecule 1

- `select(selection)`: Change the selected atoms.

  >>> sel.select('resid 5')

- `list()`: Return a copy of the selected atom indices.

- `frame(value = -1)`: Set/get the coordinate frame for the selection. Nonpositive values will return the current value of the frame without changing it.

  >>> sel.frame(5)

  >>> sel.frame()

  5

- `get(attr1, attr2, ...)`: Takes any number of string arguments, which should correspond to a valid atom property such as "name", "x", or "water". Returns a list of the value of the property for each atom in the selection. For boolean properties such as "water", the returned value will be 1 if true and 0 if false.

  >>> x, y, z = sel.get('x', 'y', 'z')

- `set(attr, val)`: Set the atom property corresponding to *attr* using the values in *val*. The number of elements in *val* should be either 1 or the number in the atom selection.

  >>> len(sel)

  12

  >>> sel.set('beta',3)

  >>> sel.set('beta',(1,2,3,4,5,6,7,8,9,10,11,12))

- `write(filename, filetype=None)`: Write the atoms in the selection to filename. Filetype is guessed from the filename, or can be specified with filetype.

- `sel1 & sel2`: Create a new atom selection using the atoms found in both *sel1* and *sel2*.

- `sel1 | sel2`: Create a new atom selection using the atoms found in either *sel1* or *sel2*.

- `-sel`: Create a new atom selection using the atoms not found in *sel*.

- `len(sel)`: Returns the number of atoms in the selection.

- `sel[0], sel[0:3]`: Index and slice operations return the corresponding atoms in the selection.

- `center(weight=None)`: Return the center of the selected atoms, possibly weighted by `weight`, which must be a sequence.

- `sasa(srad, samples=-1, points=None, restrict=None)`: Returns the solvent-accessible surface area (SASA) of atoms in the selection using the assigned radius for each atom, extending each radius by `srad` to find the points on a sphere that are exposed to solvent. If a *restrict* selection is given, only solvent-accessible points near that selection bill be considered. The `points` parameter can be used to collect the points which are determined to be solvent-accessible; this must be a list variable.

- `getbonds()`: Returns a list of the atoms bonded to each atom in the selection.

- `setbonds(bonds)`: Set the bonds for the atoms in the selection. `bonds` must be a list of the same length as the selection; each element in the list must be a sequence containing the indices of the atoms to which the atom has a bond.

- `minmax()`: Returns the minimum and maximum coordinates of the atoms in the selection as a tuple of the form `(xmin, ymin, zmin), (xmax, ymax, zmax)`.
- `rmsd(sel, frame=None, weight=None)`: Returns the root-mean-square distance of the atoms in `sel` from the selection. If `frame` is given, the coordinates from the corresponding frame will be used (see the example). If `weight` is given, the computed RMSD will be weighted using the values in `weight`.
- `align(ref=None, move=None, frame=None, weight=None)`: Finds the transformation that aligns the atoms in the selection with the atoms in `ref`, with optional weights `weight`, and applies this transformation to the atoms in `move`. The following default values for all arguments are provided:
  - `ref`: Same molecule and atoms as selection, but always using the
  - `align(ref=None, move=None, frame=None, weight=None)`:
    Finds the transformation that aligns the atoms in the selection with the atoms in `ref`, with optional weights `weight`, and applies this transformation to the atoms in `move`. The following default values for all arguments are provided:
    * `ref`: Same molecule and atoms as selection, but always using the first timestep in the molecule.
    * `move`: All atoms in the selection molecule.
    * `frame`: overrides both the selection's frame and the `move` frame, but does not affect the `ref` frame.
    * `weight`: Defaults to uniform weights on all atoms in selection.

    first timestep in the molecule.
  - `move`: All atoms in the selection molecule.
  - `frame`: overrides both the selection's frame and the `move` frame, but does not affect the `ref` frame.
  - `weight`: Defaults to uniform weights on all atoms in selection.
- `contacts(cutoff, sel=None)`: Returns pairs of of atoms within `cutoff of each other`. If `sel` is `None`, atoms in the pairs must be in the selection; otherwise, the first atom in each pair will be from the selection, and the second will be from `sel`.

10.3.3 An atom selection example

In the first example, we load the molecule alanin.pdb, and create an atom selection consisting of the alpha carbons. Note that AtomSel is the name of the class which generates atom selection instances. We show the string representation of the object by entering its name and pressing return; this shows the text used in the selection.

Next we demenstrate how atom selections act like tuples: we can get their length using the built-in len() command,and return a copy of the selected atoms in a tuple by using the slice operator [:].

Finally, we demonstrate the get and set operations. The get() operation takes any number of string arguments; for each argument, it returns a Python list of values corresponding to that string. The set() operation allows only one property to be changed at a time. However, you can pass in

either a single value, which will be applied to all atoms in the selection, or a tuple or list of the same size as the atom selection, in which case values in the list will be assigned to the corresponding atom in the selection. We take advantage of this behavior in the following example by first saving the current value of beta for the selection, then setting the value of beta to 5 for all selected atoms, and finally resetting the original values using the results of the get().

```
>>> from molecule import *
>>> from AtomSel import AtomSel
>>> load('alanin.pdb')

>>> CA = AtomSel('name CA')
>>> CA
name CA
>>> len(CA)
12
>>> CA[:]
(0, 5, 11, 17, 23, 29, 35, 41, 47, 53, 59, 65)
>>> resname, resid = CA.get('resname', 'resid')
>>> resname
['ACE', 'ALA', 'ALA', 'ALA', 'ALA', 'ALA', 'ALA', 'ALA', 'ALA', 'ALA', 'ALA', 'C
BX']
>>> resid
[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12]
>>> x,y,z=CA.get('x','y','z')
>>> x
[-2.1840000152587891, 1.4500000476837158, 1.9809999465942383, 0.54100000858306885,
2.8090000152587891, 5.9079999923706055, 5.0440001487731934, 4.5659999847412109,
7.9340000152587891, 9.7329998016357422, 8.1689996719360352, 9.2229995727539062]
>>> y
[0.5910000205039978, 0.0, 3.6429998874664307, 4.8410000801086426, 2.5559999942779541,
3.7860000133514404, 7.4190001487731934, 6.7989997863769531, 5.0819997787475586,
7.9559998512268066, 10.515999794006348, 8.5710000991821289]
>>> z
[0.9100000262260437, 0.0, -0.9089999794960022, 2.3880000114440918, 4.3920001983642578,
2.5859999656677246, 3.244999885559082, 6.9559998512268066, 7.2639999389648438,
5.5669999122619629, 7.8870000839233398, 11.013999938964844]

>>> beta = CA.get('beta')
>>> CA.set('beta',5)
>>> CA.set('beta',beta)
>>>
```

10.3.4 Changing the selection and the frame

When molecule in VMD contains multiple coordinate sets (frames), atom selections must know which frame they are referring to, especially when you make distance-based atom selections or

request time-varying properties like the x, y, or z coordinates. By default, atom selections in Python use frame 0, i.e. the first coordinate set. You can specify the frame either when you create the atom selection, or by using the frame() method. Passing no arguments to frame() returns the current value of the frame.

```
>>> load('psf','alanin.psf','dcd','alanin.dcd')

>>> resid5 = AtomSel('resid 5', frame=50)
>>> resid5.frame()
50
>>> resid5.frame(22)
>>> resid5.frame()
22
```

In a similar way, you can change the selected atoms of an atom selection object using the select() operation. Continuing with the previous example:

```
>>> resid5
resid 5
>>> resid5.select('resid 7')
>>> resid5
resid 7
>>>
```

10.3.5 Combining atom selections

Once you've created one or more atom selections, you can combine them to create new ones.

```
>>> CA = AtomSel('name CA')
>>> resid5 = AtomSel('resid 5')
>>> CA
name CA
>>> resid5
resid 5
>>> ANDsel = CA & resid5
>>> ORsel = CA | resid5
>>> NOTsel = -CA
>>> ANDsel
(name CA) and (resid 5)
>>> ORsel
(name CA) or (resid 5)
>>> NOTsel
not (name CA)
>>>
```

When the combined atom selections are from different molecules or have different frame numbers, the molecule and frame from the first atom selection are used.

10.3.6 RMS example

Example: find the mass-weighted RMS distance from the initial frame. This assumes a molecule and its timesteps have already been loaded (see the description of the Molecule class).

```
from AtomSel import AtomSel
from Molecule import *

# Get a reference to the first molecule.
m=moleculeList()[0]

# Select all atoms.
sel=AtomSel()

# We are comparing to the first frame.
sel.frame(0)

# Get the mass weights.
mass = sel.get('mass')

Here's another RMSD example that uses the {\tt align} method:

\begin{verbatim}
from AtomSel import AtomSel
from Molecule import Molecule

mol1=Molecule()
mol1.load('proteins/alanin.psf')
mol1.load('proteins/alanin.dcd')
n = mol1.numFrames()

sel=AtomSel('backbone')

# align all frames with the first frame, using the backbone atoms
for i in range(1,n):
  sel.align(frame=i)

# align all frames with frame 10.
for i in range(1,n):
  sel.align(ref=sel.frame(10), frame=i)

# Align residues 1-3 from frame 10 with frame 20, but use all backbone atoms
# to perform the fit.
resid123=AtomSel('resid 1 to 3')
sel.align(ref=sel.frame(20), frame=10, move=resid123)
# GOTCHA ALERT: sel.frame(10).align(ref=sel.frame(20)) does not work!!
# That's because sel.frame(10) overrides frame 20 in this case since they
```

```
# are applied to the same AtomSel instance.  Either use the frame argument,
# as illustrated here, or create a new AtomSel instance for the reference.

# Perform a mass-weighted RMSD alignment and compute the mass-weighted
# RMS distance from the first frame.
w=sel.get('mass')
rms=[]
ref=AtomSel('backbone',frame=0)
for i in range(n):
  rms.append(sel.frame(i).align(ref=ref, weight=w).rmsd(ref, weight=w))

# Initialize result list.
rms=[]

# Go!
for i in range(m.numFrames()):
  rms.append(sel.rmsd(sel, frame=i, weight=mass))
```

Here's another RMSD example that uses the `align` method:

```
from AtomSel import AtomSel
from Molecule import Molecule

mol1=Molecule()
mol1.load('proteins/alanin.psf')
mol1.load('proteins/alanin.dcd')
n = mol1.numFrames()

sel=AtomSel('backbone')

# align all frames with the first frame, using the backbone atoms
for i in range(1,n):
  sel.align(frame=i)

# align all frames with frame 10.
for i in range(1,n):
  sel.align(ref=sel.frame(10), frame=i)

# Align residues 1-3 from frame 10 with frame 20, but use all backbone atoms
# to perform the fit.
resid123=AtomSel('resid 1 to 3')
sel.align(ref=sel.frame(20), frame=10, move=resid123)
# GOTCHA ALERT: sel.frame(10).align(ref=sel.frame(20)) does not work!!
# That's because sel.frame(10) overrides frame 20 in this case since they
# are applied to the same AtomSel instance.  Either use the frame argument,
# as illustrated here, or create a new AtomSel instance for the reference.
```

```
# Perform a mass-weighted RMSD alignment and compute the mass-weighted
# RMS distance from the first frame.
w=sel.get('mass')
rms=[]
ref=AtomSel('backbone',frame=0)
for i in range(n):
  rms.append(sel.frame(i).align(ref=ref, weight=w).rmsd(ref, weight=w))
```

10.4 Python callbacks

Some of your Python scripts may wish to be informed when various events in VMD occur. The mechanism for expressing this interest is to register a callback function with a special module supplied by VMD. When the event of interest occurs, all registered will functions will be called; VMD will pass the functions information specific to the event. The set of callbacks events is listed in Table 10.4.

Table 10.1: Description of callbacks available to Python scripts running in VMD.

Name	When called	Function arguments
display_update	Screen redraw	none
frame	Molecule changes coordinate frame	(molid, frame)
help	User pushes help button on Main window	(name of topic)
initialize_structure	Molecule created or deleted	(molid, 1 or 0)
pick_atom	Atom picked in graphics window	(molid, atomid, key_shift_state (1 if shift pressed, 0 otherwise)
pick_value	Bond, angle, or dihedral label created	(value)
timestep	New IMD coordinate frame received	(molid, frame)
trajectory	Completion of coordinate file read/write	(molid, filename)

All callback functions must take two arguments. The first argument will be an object given at the time the function is registered; VMD makes no use of this object, it simply saves it and passes it to the callback when the callback function is called. The second argument to the callback function will be a tuple containing 0 or more elements, depending on the type of callback. The type of information for each callback is listed in the third column of Table 10.4.

Callbacks are registered/deregistered using the add_callback/del_callback methods of the VMD.vmdcallbacks module. The syntax for these methods is:

```
def add_callback(name, func, userdata = None):

def del_callback(name, func, userdata = None):
```

`name` should be one of the callback names in Table 10.4. `func` is the function object. `userdata` is any object; if no object is supplied, None will be passed as the first argument to the callback function. To unregister a callback, use the same name, func, and userdata as were used when the callback was registered. The same function may be registered multiple times with different userdata objects.

10.4.1 Using Tkinter menus in VMD

The object-oriented interface to Tk known as Tkinter is included with the embedded Python interpreter. You can create Tkinter GUI's in the usual way, with one caveat: the Tkinter.mainloop() method should never be called, as it will interfere with VMD's own event loop. VMD will take care of updating your GUI windows for you.

10.5 Controlling VMD from Python

Commands for controlling VMD from Python are organized into modules which roughly correspond to Tcl commands. Importing all the commands in a module is not recommended as some of the functions (e.g., listall()) overlap. All commands are listed below, with the name of the module given by the section heading.

10.5.1 animate

Python operations available from the *animate* module, used to control which coordinate frames are displayed.

- `forward()`:
- `reverse()`: `forward()` and `reverse()` causes VMD to start animating frames automatically in order of increasing or decreasing frame number, respectively.
- `once()`:
- `rock()`:
- `loop()`: `once()`, `rock()`, and `loop()` control how frames are cycled when VMD is animating a series of frames. `once()` causes VMD to stop when it reaches the first or last frame. `rock()` causes VMD to reverse direction each time it gets to the beginning or end. `loop()` causes VMD to continue from the beginning when reaches the last frame, or from the last frame if it gets to the beginning.
- `style()`: Returns either `'Once'`, `'Rock'`, or `'Loop'`, corresponding to the animation mode VMD is currently in.
- `goto(frame)`: Set the animation to the given frame, and pause the animation.
- `prev()`: Step to the next-lowest frame, then pause.
- `next()`: Step to the next-highest frame, then pause.
- `pause()`: Stop animating frames.
- `speed(value)`: Get/set the relative rate at which VMD animates frames. `value` should lie between 0 and 1. If a value less than 0 is given, then the speed will not be changed. The new value of the speed is always returned.
- `skip(value)`: Get/set the number of frames to skip when animating. A value of 1 means every frame is shown; 2 means every other frame is shown; etc. If `value` is 0 or less, no change is made. The new value of the speed is always returned.

- `is_active(molid)`: Returns whether the molecule with the given id is active; that is; whether it responds to animation or not.
- `activate(molid, trueorfalse)`: Make the molecule with the given id active or not. Active molecules update their coordinate frames during animation; inactive molecules do not.

10.5.2 axes

Python operations available from the *axes* module, used to change where the axes are displayed in the graphics window.

- `OFF, ORIGIN, LOWERLEFT, LOWERRIGHT, UPPERLEFT, UPPERRIGHT`: String constants defined in the *axes* module for setting the location of the axes.
- `get_location()`: Returns a string object corresonding the current location of the axes.
- `set_location(location)`: Set the location of the axes, using one of constants defined in the module.

10.5.3 color

Python operations available from the *color* module, used to change the color definitions, color maps, or edit the color scale. All rgb and color scale values should be in the range 0 to 1.

- `categories()`: Returns a list of available color categories.
- `get_colormap(name)`: Returns a dictionary of name/color pairs for the given color category.
- `set_colormap(name, dict)`: Change the color definitions for the colors in the given color category. The keys in `dict` must come from the keys listed by `get_colormap` for that color category, though not all keys need be listed. The values must be legal color names.
- `get_colors()`: Returns a dictionary whose keys are all the legal color names and whose corresponding values are the RGB values of the color, represented as a 3-tuple.
- `set_colors(dict)`: Changes RGB values for colors in VMD. Keys must be chosen from the keys returned by `get_colors()`. Values must be 3-tuples of floats.
- `scale_method()`: Returns the current color scale method.
- `scale_methods()`: Returns a list of all available color scale methods.
- `scale_midpoint()`: Returns the current color scale midpoint.
- `scale_min()`: Returns the current color scale minimum.
- `scale_max()`: Returns the current color scale maximum.
- `set_scale(method, midpoint, min, max)`: Change the color scale method, midpoint, minimum, or maximum. All properties may be set using keyword arguments.

10.5.4 display

Python operations available from the *display* module, used to control the VMD camera as well as screen updates.

- `update()`: Force a display update, without checking the VMD FLTK menus
- `update_ui()`: Update the display as well as any other user interfaces.
- `update_on()`: Tell VMD to regularly update the display and the FLTK menus
- `update_off()`: Tell VMD not to regularly update the display. The display will be updated only when display.update() is called.
- `stereomodes()`: Returns a list of the available stereo modes.
- `PROJ_PERSP, PROJ_ORTHO`: String constants defined in the `display` module for setting the `projection` keyword in the `set` method.
- `set(**keywordlist)`:
- `get(key)`: set() and get() control various display properties. The following keywords accept/return floating-point values: `eyesep, focallength, height, distance, nearclip, farclip`. The following keywords accept boolean values for on or off, respectively: `antialias, depthcue, culling`. `stereo` should be one of the values returned by `stereomodes()`. `projection` should be one of the PROJ constants defined in this module. `size` should be a list of two integers corresponding to the width and height of the display in pixels.

10.5.5 evaltcl

The *evaltcl* method provides access to the main VMD Tcl interpreter from Python. It takes a string with Tcl commands as an argument and evaluates it. Its main purpose is to provide the Python interpreter with access to functionality that is only available from Tcl and for which no equivalent implementation yet exists in Python, for example the Tcl based plugins. Usage Examples:

```
from VMD import evaltcl

versionid=evaltcl('vmdinfo version')
evaltcl('play somescript.tcl')
```

10.5.6 graphics

Python operations available from the *graphics* module, used to create custom 3-D objects from graphics primitives. The first argument to all operations is the id of a Graphics molecule. Graphics molecules are created using the `load()` command in the *molecule* module: `load('graphics', 'test')` creates a Graphics molecule named 'test'. For vertices and normals, a tuple with three float items is required.

- `triangle(id, v1, v2, v3)`: Draw a triangle with the given vertices.
- `trinorm(id, v1, v2, v3, n1, n2, n3)`: Draw a triangle with the given vertices and vertex normals.

- `cylinder(id, v1, v2, radius=1.0, resolution=6, filled=0)`: Draw a cylinder with endpoints specified by the given points. Radius, resolution, and filled (whether the ends should be capped or not) may be optionally specified with keyword arguments.
- `point(id, v)`: Draw a point at the given coordinates.
- `line(id, v1, v2, style='solid', width=1)`: Draw a line between the given vertices. Optionally, the line style may be specified as either 'solid' or 'dashed', and width may be any positive integer.
- `materials(id, onoff)`: Turns materials on/off for subsequent graphics primitives. Primitives lying earlier in the stack are not affected. `onoff` should be either 0 (off) or 1 (on).
- `material(id, name)`: Sets the material for all graphics primitives in this molecule. `name` should be one of the material names returned by `material.listall()`.
- `color(id, color)`: Set the color for subsequent graphics primitives. `color` may be (1) a tuple containing three floats specifying the RGB value, (2) an integer corresponding to a color index, or (3) a string corresponding to a color name.
- `cone(id, v1, v2, radius=1.0, resolution=6)`: Draw a cone with base at `v1` and point at `v2`. radius and resolution may optionally be specified with keyword arguments.
- `sphere(id, center=(0.0, 0.0, 0.0), radius=1.0, resolution=6)`: Draw a sphere. The sphere center, radius, and resolution may optionally be specied with keyword arguments.
- `text(id, pos, text, size=1.0)`: Draw text at the given position (specified by a tuple of three floats, using the string `text`. Size may optionally be specified using keyword arguments.
- `delete(id, index)`: Deletes the graphics primitive with the given index. Alternatively, if the string 'all' is passed as the index, all graphics primitives will be deleted.
- `replace(id, index)`: Deletes the graphics primitive with the given index. The next graphics primitive added will go in the newly vacated position. Subsequent graphics primitives will resume at the end of the list.
- `info(ind, index)`: Returns a string describing the graphics primitive with the given index. If the index is invalid, an IndexError exception is raised.
- `listall(ind)`: Returns the indices of the valid graphics primitives in a list.

10.5.7 imd

Python operations available from the *imd* module, used to display and interact with a molecule in a molecular dynamics simulation.

- `connect(host, port)`: Connect to a simulation running on host `host` and listening for incoming connections on port `port`.
- `pause()`: If connected, cause the simulation to pause.

- `detach()`: If connected, detach from the simulation. The simulation will continue to run, but no more frames will be received until a connection is re-established.

- `kill()`: If connected, terminate the simulation. The connection will also be abolished.

- `transfer(rate)`: Set/get how often the remote simulation sends coordinate frames to VMD. If *rate* is omitted or is negative, no action is taken and the current value is returned. A value of 1 corresponds to every frame being sent; a value of 2 corresponds to every other frame, etc.

- `keep(rate)`: Set/get how often received coordinates frames are kept by VMD as part of an animation. If *rate* is omitted or is negative, no action is taken and the current value is returned. A value of 0 means no frames are saved. A value of 1 corresponds to every frame being saved; a value of 2 corresponds to every other frame, etc.

- `copyunitcell(True/False)`: Control how unitcell information is passed to the new frame that recieved via IMD. If set to `False` (the default) unit cell information would be taken from the IMD connection. Since the IMD protocol currently has no provisions for communicating the unit cell information, the unit cell dimensions are set to zero. If set to `True` the cell information is copied from the previous frame.
  WARNING: when using `imd.copyunitcell(True)` with simulations in the NPT ensemble, the resulting unitcell information will be incorrect.

10.5.8 label

Python operations available from the *label* module, used to create, show/hide, and delete labels for atoms, bonds, angles, or dihedrals.

- `ATOM, BOND, ANGLE, DIHEDRAL`: Label types defined by the label module, for use as the first argument to the add, listall, show, hide, and delete methods.

- `add(type, molids, atomids)`: Create a label of the given type. `molids` and `atomids` must be tuples containing 1, 2, 3, or 4 integers for ATOM, BOND, ANGLE, or DIHEDRAL labels, respectively. If the label already exists, no action is performed. Returns a dict corresponding to the referenced label that can be used in the show(), hide(), delete(), and getvalues() methods.

- `listall(type)`: Returns a list of labels of the given type. The elements of the list are python dictionary objects, with the following keys: `molid`, `atomid`, `value`, `on`. The values for `molid` and `atomid` are tuples containing the molecule id and atom id for the label. `value` is the numerical value of the geometry label, or zero for ATOM labels. `on` is 1 if the label is shown, and 0 if the label is hidden.

- `show(type, label)`: Turn the given label on. `label` must be a dictionary containing `molid` and `atomid` keys whose values are tuples. If the tuples match the molecule ids and atom ids of the atoms in an existing label, the label will be turned on. Raises ValueError if the label does not exist.

- `hide(type, label)`: Turn the given label off. `label` must be a dictionary containing `molid` and `atomid` keys whose values are tuples. If the tuples match the molecule ids and atom ids

of the atoms in an existing label, the label will be turned off. Raises ValueError if the label does not exist.

- `delete(type, label)`: Delete the given label. `label` must be a dictionary containing `molid` and `atomid` keys whose values are tuples. If the tuples match the molecule ids and atom ids of the atoms in an existing label, the label will be deleted. Raises ValueError if the label does not exist.

- `getvalues(type, label)`: Returns a list of values of the given label for each coordinate frame in the label. If the atoms in the label belong to different molecules, only the coordinates of the first molecule will be cycled. If the labels don't have values (like atom labels), None is returned.

10.5.9 material

Python operations available from the *material* module, used to create and modify material properties of molecular representations.

- `listall()`: Returns a Python list of the names of all available materials.

- `settings(name)`: Returns a Python dictionary of the material settings for material with the given `name`.

- `add(name=None, copy=None)`: Create a new material with the given name. Optionally, copy the properties from material `copy` into the new material. If no name is given, a new one will be provided.

- `delete(name)`: Delete the material with the given name.

- `rename(oldname, newname)`: Rename the material with the given name. The new name must not yet be used.

- `change(name, ambient, specular, diffuse, shininess, mirror, opacity)`: Change one or more of the material settings for the material with the given name. Keyword arguments may be used to specify each property.

10.5.10 molecule

Python operations available from the *molecule* module, used to load molecules and change their representations.

- `num()`: Returns the number of loaded molecules.

- `listall()`: Returns the molid's of the all the loaded molecules.

- `exists(molid)`: Returns true if the molid corresponds to an existing molecule.

- `new(name)`: Creates a new empty molecule with the given name and returns its id.

- `load(structure, sfname, coor, cfname)`: Load a molecule with structure type *structure* and filename *sfname*. Additionally, a separate coordinate file may be provided, of type *coor* and name *cfname*. **New in VMD 1.8:** All frames from *cfname* will be processed before the function returns. If successful, the function will return the id of the new molecule.

  >>> load('pdb','alanin.'pdb')

  >>> load('psf','alanin.psf','dcd','alanin.dcd')

- `cancel(molid)`: Cancel loading of coordinates file for the given molecule.

- `delete(molid)`: Delete the specified molecule.

- `read(molid, type, filename, beg = 0, end = -1, skip = 1, waitfor = 1, volsets = [1])`:

- `write(molid, type, filename, beg = 0, end = -1, skip = 1, waitfor = 1)`: Read or write a file to/from the specified molecule. For reading, if `molid` is -1, a new molecule will be created. Optional arguments `beg`, `end`, and `skip` may be specified with keywords; the default is to load/save all coordinate frames. **New in VMD 1.8:** The `waitfor` option will cause VMD to process the specified number of frames before returning. If `waitfor` is negative, all frames from the file will be processed before the function returns. For reading files containing volumetric datasets, set the volsets parameter to a list of set id's, starting from 0, to specify which datasets to load.

- `add_volumetric(molid, name, origin, xaxis, yaxis, zaxis, xsize, ysize, zsize, data)`: Add a volumetric data set to the given molecule. `origin`, `xaxis`, `yaxis`, and `zaxis` must be 3-tuples specifying the center and scale of the data. `xsize`, `ysize` and `zsize` give the number of elements along each dimension. `data` must be a Python list of the correct size as indicated by the three sizes.

- `get_filenames(molid)`: Returns a list of filenames that have been loaded into this molecule.

- `get_filetypes(molid)`: Returns a list of filetypes corresponding to `get_filenames`.

- `get_databases(molid)`: Returns a list of databases corresponding to `get_filenames`.

- `get_accessions(molid)`: Returns a list of accessiosn corresponding to `get_filenames`.

- `get_remarks(molid)`: Returns a list of remarks corresponding to `get_filenames`.

- `delframe(molid, beg=0, end=-1, skip=1)`: Delete frames from the specified molecule. Optional arguments `beg`, `end`, and `skip` may be specified with keywords; the default is to delete all coordinate frames.

- `dupframe(molid, frame)`: Copy the coordinates from the given frame and append them as a new frame.

- `numframes(molid)`: Return the number of coordinate frames in the specified molecule.

- `get_frame(molid)`: Return the current coordinate frame for the specified molecule.

- `set_frame(molid, frame)`: Set the current coordinate frames in the specified molecule.
- `numatoms(molid)`: Returns the number of atoms in the specified molecule.
- `ssrecalc(molid)`: Recalculate the secondary structure for the given molecule, using the current set of coordinates.
- `name(molid)`: Returns the name of the given molecule.
- `rename(molid,newname)`: Rename the given molecule.
- `get_top(molid)`:
- `set_top(molid)`: Get/set the molid of the top molecule.
- `get_periodic(molid, frame=-1)`:
- `set_periodic(molid, frame=-1, a, b, c, alpha, beta, gamma)`: Get/set periodic image settings for the given molecule and timestep (frame). `get_periodic` returns a dictionary whose keys are `a, b, c, alpha, beta, gamma`. `set_periodic` sets the corresponding values; negative values will be ignored.

10.5.11 molrep

Python operations available from the *molrep* module, used to add and modify representation of molecules.

- `num(molid)`: Returns the number of representations in the given molecule.
- `addrep(molid, style=None, color=None, selection=None, material=None)`: Add a representation to the specified molecule. If any of the optional keywords are specified as well, the new rep will have the specified properties. Note that these properties become the default for future calls to addrep, so that `addrep(0, style='VDW'); addrep(0, color='Name')` will create two reps, each with a style of 'VDW'.
- `delrep(molid, rep)`: Delete the specified rep from the given molecule.
- `modrep(molid, rep, style, sel, color, material)`: Modify the style, atom selection, color, and/or material for the specified molecule and representation. Any combination of the last four arguments may be specified, using positional or keyword arguments. Returns success.

  >>> modrep(0,0,color='name') # Color the first rep of molecule 0 by name.

  >>> modrep(0,2, selection='name CA', material='Transparent') # For the third representation of molecule 0, change the atom selection to "name CA" and the material to "Transparent"
- `get_style(molid, rep)`:
- `get_selection(molid, rep)`:
- `get_color(molid, rep)`:

- `get_material(molid, rep)`: Returns the representation style, selection, color, or material, respectively, for the given representation of the given molecule.
- `get_repname(molid, rep)`:
- `repindex(molid, name)`: These two commands let you assign names to reps and access them by that name. The name returned by `get_repname` is guaranteed to be unique for all reps in the molecule, and will stay with the rep it was assigned to even when the order of the reps changes. Use `repindex` to find the repid of the rep with the given name; -1 is returned if no rep with that name exists.
- `get_autoupdate(molid, rep)`:
- `set_autoupdate(molid, rep, onoff)`: These two commands let you turn on/off automatic updating of the atom selection for a given rep. Automatic updating means the atom selection for the rep will be recalculated every time the coordinate frame of the molecule changes.
- `get_colorupdate(molid, rep)`:
- `set_colorupdate(molid, rep, onoff)`: These two commands let you turn on/off automatic updating of the color for a given rep. Automatic updating means the color for the rep will be recalculated every time the coordinate frame of the molecule changes; this is useful for coloring by Position or User.
- `get_smoothing(molid, rep)`:
- `set_smoothing(molid, rep, n)`: These two commands let you get/set on-the-fly smoothing of molecular representations. Atom coordinates used to draw the given rep will be smoothed with a moving average window size of $2n - 1$.
- `get_scaleminmax(molid, rep)`:
- `set_scaleminmax(molid, rep, min, max)`:
- `reset_scaleminmax(molid, rep)`: Get/set the color scale range for this rep. Normally the color scale is automatically scaled to the minimum and maximum of the corresponding range of data. This command overrides the autoscaled values with the values you specify. Omit the *min* and *max* arguments to get the current values. Use `reset_scaleminax` to rescale the color scale to the maximum range again.
- `get_visible(molid, rep)`:
- `set_visible(molid, rep, onoff)`: These two commands let you show or hide a selected molecular representation, and retrieve the visibility status of a given rep.

10.5.12 render

Python operations available from the *render* module, used to export the scene to a file that can be read by external rendering programs.

- `listall()`: Return a Python list of the names of all supported rendering methods. One of these should be the first argument to the `render()` operation below.

- `render(method, filename)`: Using the the given rendering method, export the current scene to the file `filename`. `method` should be one of the values returned by `listall()`.

10.5.13 trans

Python operations available from the *trans* module, used to change the view of the rendered scene.

- `rotate(axis, angle)`: Rotate the scene about the specified axis by the given angle. `axis` should be 'x', 'y', or 'z'; `angle` is measured in degrees.
- `translate(x, y, z)`: Translate the scene by the given x, y, and z values.
- `scale(factor)`: Scale (zoom) the scene by the given factor.
- `resetview(molid)`: Sets the center, scale, rotation for all molecules so that the viewpoint is centered on the molecule with the given id.
- `get_center(molid)`:
- `set_center(molid, vector)`: Get/set the coordinates of the center of the given molecule as a Python list.
- `get_scale(molid)`:
- `set_scale(molid,scale)`: Get/set the scale factor used to display the given molecule.
- `get_rotation(molid)`:
- `set_rotation(molid, matrix)`: Get/set the rotation matrix for the given molecule as a 16-element Python list in row-major order.
- `get_trans(molid)`:
- `set_trans(molid, vector)`: Get/set the global translation applied to the given molecule as a Python list.
- `is_fixed(molid)`: Returns whether the molecule with the given id is fixed; that is, whether it is affected by translation, rotation, or scaling. Fixed molecules may still be animated (see `is_active` in the *animate* section).
- `fix(molid, trueorfalse)`: Make the molecule with the given id fixed or not.
- `is_shown(molid)`: Returns whether the molecule with the given id is shown or not.
- `show(molid, trueorfalse)`: Make the molecule with the given id shown or not.

10.5.14 vmdnumpy

This optional module is made available from within the toplevel VMD module if VMD detects a Numeric Python installation in the Python search path. When present, the following methods are provided:

- `timestep(molid, frame)`: Returns a single-precision Numeric array containing a **direct** reference to the given set of atom coordinates. Atom coordinates are arranged *xyzxyzxyz...* for each atom in the molecule. No copy of VMD's internal coordinates is made; therefore, modifications to this array will directly affect atom coordinates in VMD. Using the array after the timestep has been deleted will likely cause VMD to crash. The advantage is maximum efficiency and the ability to easily modify atom coordinates without going through the atom selection interface.

- `atomselect(molid, frame, selection)`: Returns an array of int's representing flags for on/off atoms in the given atom selection. The syntax for the selection is the same as for the AtomSel class. An array of this form can be used in conjunction with the Numeric `take` function to get selected coordinates from a timestep. Creating the array in this way can be 50-100 times faster than converting from an AtomSel object.

10.6 High-level Python Interface

VMD provides three modules for accessing and manipulating VMD state with objects that represent important entities. These objects can be thought of as references for the actual object within VMD: you can create as many references as you want and delete them, but modifying the reference changes the actual state of VMD. This is different from the AtomSel class, where each AtomSel instance is independent of the molecules and reps in VMD. These *proxy classes* are written in pure Python and use the lower level built-in interfaces to communicate with VMD.

10.6.1 Molecule

The Molecule class is a proxy for molecules loaded into VMD. Most operations raise ValueError if the proxy no longer refers to a valid molecule (i.e. if the molecule has been deleted).

Molecule instances provide the following methods:

- `__init__(id=None)`: Creating a new Molecule instance with no arguments will create a new empty molecule in VMD. Passing a valid molecule id will make the Molecule instance mirror the state of the corresponding molecule in VMD.

- `__int__()`: Casting a Molecule to an int returns the molecule ID.

- `rename(self, newname)`: Changes the name of the molecule.

- `name()`: Returns the name of the molecule.

- `delete()`: Deletes the molecule corresponding to this Molecule instance. The object can no longer be used.

- `load(filename, filetype=None, first=0, last=-1, step=1, waitfor=-1, volsets=[0])`: Load molecule data from the given file. The filetype will be guessed from the filename extension; this can be overrideen by setting the filetype option. `first`, `last`, and `step` control which coordinates frames to load, if any. `volsets` indicates which volumetric data sets to load from the file. Raises IOError if the file cannot be loaded.

- `save(filename, filetype=None, first=0, last=-1, step=1, waitfor=-1, sel=None)`: Save timesteps to the given file. The filetype will be guessed from the filename extension; this can be overridden by setting the filetype option. first, last, and step control which timesteps to save. Returns the number of frames written before the command completes. Pass an AtomSel instance as `sel` to write only a selection of atoms to the file. Note that this differs from the `AtomSel.write()` method in that `Molecule.save()` writes a range of timesteps, while `AtomSel.write()` writes only the coordinates corresponding to the selection's currently selected frame.
- `files()`:
- `types()`: Returns a list of filenames and file types, respectively, for the files that have been loaded into this molecule.
- `numAtoms()`: Returns the number of atoms in the molecule.
- `numFrames()`: Returns the number of coordinate frames in the molecule.
- `setFrame(frame)`: Set the coordinate frame to the given value. Must be in the range [0, numFrames())
- `curFrame()`: Returns the current coordinate frame for the molecule.
- `delFrame(first=0, last=-1, step=1)`: Deletes the given range of frames.
- `dupFrame(frame = None)`: Duplicate the given frame, apending it to the end. if `frame` is `None` then the current frame is used.
- `numReps()`: Returns the number of molecular representations (reps) in the given molecule.
- `reps()`: Returns a list of MoleculeRep objects, one for each rep in the molecule.
- `addRep(rep)`: Add the given MoleculeRep instance to the Molecule. Modifications to the rep will affect all Molecules to which the rep has been added. Raises ValueError if the rep has already been added to this molecule.
- `delRep(rep)`: Removes the given MoleculeRep from the Molecule. The rep is not affected and can be added to other molecules, but changes to it will no longer affect this Molecule.
- `clearReps()`: Removes all reps from this molecule.
- `autoUpdate(rep, onoff = None)`: If `onoff` is not `None`, sets the auto-update status for this rep and molecule (note that a rep's auto-update status may be different for different molecules). Returns the reps auto-update status.
- `ssRecalc()`: Recalculate the secondary structure for this molecule.

Examples:

```
>>> from VMD import *
>>> from Molecule import *
>>> bR=Molecule()
>>> bR.load('../proteins/brH.pdb')
```

```
    <snip>
<Molecule.Molecule instance at 0x406d878c>
>>> bR.name()
'molecule'
>>> bR.rename('bR')
<Molecule.Molecule instance at 0x406d878c>
>>> bR.name()
'bR'
>>> bR.numAtoms()
3762
>>> bR.dupFrame()
<Molecule.Molecule instance at 0x406d878c>
>>> bR.numFrames()
2
```

10.6.2 MoleculeRep

The MoleculeRep class, defined in the Molecule module, is designed to make it easy to keep track of the reps in a molecule and to update reps in many molecules simultaneously. The way it works is to create a MoleculeRep instance, then add it to as many molecules as you want using the Molecule.addRep() method. The only operations on MoleculeRep objects is to change their properties; when this occurs, all molecules to which the rep has been added will be updated. Deleting a MoleculeRep instance has no effect. A list of MoleculeRep instances for a given molecule can be gotten from the Molecule.reps() method.

The MoleculeRep class provides the following methods:

- `__init__(style=defStyle, color=defColor, selection=defSelection, material=defMaterial)`: Initialize the Rep object with optional style, color, selection and material properties. MoleculeRep objects also have attributes with the same names as the above keywords; these can be used to query the state of the rep. Don't set these attributes directly; use the `change*` methods below instead.
- `changeStyle(style)`:
- `changeColor(color)`:
- `changeSelection(selection)`:
- `changeMaterial(material)`: Set the draw style, color, atom selection and material for this rep. If the rep is assigned to any molecules, the molecule rep will be updated accordingly. `style` must be a valid draw style; see the `*Style` functions below.

In the following example, we load a molecule, add a new transparent VDW rep to the molecule, then change the atom selection for the rep to "name CA":

```
>>> from VMD import *
>>> from Molecule import *
>>> bR=Molecule()
>>> bR.load('../proteins/brH.pdb')
```

```
      <snip>
>>> reps=bR.reps()
>>> reps[0].style
'Lines'
>>> vdw=MoleculeRep(style='VDW', material='Transparent')
>>> bR.addRep(vdw)
>>> vdw.changeSelection('name CA')
```

10.6.3 Draw Style Methods

The syntax for changing the draw style in the MoleculeRep.changeStyle() method is fairly simple and easy to remember as long as the default values for each style are used; however, remembering that `rep.changeStyle("CPK 0.5 0.5 8")` is the way to set the bond radius, sphere scale, and sphere resolution for CPK is a little more difficult. The Molecule class defines a function for each draw style to make it easier to generate the required strings to pass to the changeStyle methods. Each function accepts keyword arguments for specifying the draw style parameters and returns a string suitable for `changeStyle()`.

10.6.4 Saving and Restoring Molecule State

Molecule and MoleculeRep instances can be saved used the `pickle` module from the Python standard library. Molecules will be saved with information about their name, files, and reps. The files themselves are not saved with the molecule; they will be reloaded when the molecule instance is recreated using `pickle.load()`. MoleculeRep instances can also be pickled; when restored they will be unassigned to any Molecules.

Chapter 11

Vectors and Matrices

Tcl does not handle mathematical expressions very well. It is slow at evaluating expressions, and provides no facility for handling vectors or matrices. Since the latter two are needed for structure analysis, we have added routines to manipulate them.

A vector in VMD is a list of numbers. All of the vector routines but one will work with vectors of any length; `veccross` will only use vectors of three numbers. A matrix is a 4x4 collection of numbers stored as a list of 4 vectors of 4 numbers, in row-major order.

Following are descriptions and examples of all the commands. For more examples of vectors, though without much documentation, the script used to test the vectors implementation is located at `$env(VMDDIR)/scripts/vmd/test-vectors.tcl`.

Since Tcl is slow at math, some of these commands have been reimplemented in C++. (The original definition is in the vmd script distribution, but it is redefined later on inside VMD). At times, the speedup is a factor of 40 or more. These commands are noted by (C++).

11.1 Vectors

- **veczero** – Returns the zero vector, {0 0 0}

  ```
  Example:
  vmd > veczero
  0 0 0
  ```

- (C++) **vecadd** *v1 v2* [*v3 ... vn*] – Returns the vector sum of all the terms.

  ```
  Examples:
  vmd > vecadd {1 2 3} {4 5 6} {7 8 9} {-11 -11 -11}
  1 4 7
  vmd > vecadd {0.1 0.2 0.4 0.8} {1 1 2 3} {3 1 4 1}
  4.1 2.2 6.4 4.8
  vmd > vecadd 4 5
  9
  ```

- **vecmul** *v1 v2* – Returns the vector of a term-by-term multiply.

```
Examples:
vmd > vecmul {1 2 3} {4 5 6}
4 10 18
vmd > vecmul {0.1 0.2 0.4 0.8} {1 1 2 3}
0.1 0.2 0.8 2.4
```

- (C++) **vecsub** *v1 v2* – Returns the vector subtraction of the second term from the first

```
Examples:
vmd > vecsub 6 3.2
2.8
vmd > vecsub {10 9.8 7} {0.1 0 -0.1}
9.9 9.8 7.1
vmd > vecsub {1 2 3 4 5} {6 7 8 9 10}
-5 -5 -5 -5 -5
```

- (C++) **vecsum** *v* – Returns the sum of the elements in v

```
Examples:
vmd > vecsum { 1 2 3 }
6.0
```

- (C++) **vecmean** *v* – Returns the mean of the elements in v

```
Examples:
vmd > vecmean { 1 2 3 }
2.0
```

- (C++) **vecstddev** *v* – Returns the standard deviation of the elements in v

```
Examples:
vmd > vecstddev { 1 2 3 4 5 6 7 8 9 10 }
2.87228131294
```

- (C++) **vecscale** *c v* –
- (C++) **vecscale** *v c* – Returns the vector of the scalar value c applied to each term of v

```
Examples:
vmd > vecscale .2 {1 2 3}
0.2 0.4 0.6
vmd > vecscale {-5 4 -3 2} -2
10 -8 6 -4
vmd > vecscale -2 3
-6
```

- **vecdot** *v1 v2* – Returns the scalar dot product of the two vectors

```
Examples:
vmd > vecdot {1 -2 3} {4 5 6}
12
vmd > vecdot {3 4} {3 4}
25
vmd > vecdot {1 2 3 4 5} {5 4 3 2 1}
35
vmd > vecdot 3 -2
-6
```

- **veccross** *v1 v2* – Returns the vector cross product of the two vectors.

```
Examples:
vmd > veccross {1 0 0} {0 1 0}
0 0 1
vmd > veccross {2 2 2} {-1 0 0}
0 -2 2
```

- **veclength** *v* – Returns the scalar length of v ($\|v\|$)

```
Examples:
vmd> veclength 5
5.0
vmd > veclength {5 12}
13.0
vmd > veclength {3 4 12}
13.0
vmd > veclength {1 -2 3 -4}
5.47723
```

- **veclength2** *v* – Returns the square of the scalar length of v ($\|v\|^2$)

```
Examples:
vmd > veclength2 5
25
vmd > veclength2 {5 12}
169
vmd > veclength2 {3 4 12}
169
vmd > veclength2 {1 -2 3 -4}
30
```

- **vecnorm** *v* – Returns the vector of length 1 directed along v

```
Examples:
vmd > vecnorm -10
-1.0
```

```
vmd > vecnorm {1 1 }
0.707109 0.707109
vmd > vecnorm {2 -3 1}
0.534522 -0.801783 0.267261
vmd > vecnorm {2 2 -2 2 -2 -2}
0.408248 0.408248 -0.408248 0.408248 -0.408248 -0.408248
```

- **vecdist** *v1 v2* – Returns the distance between the two vectors ($\|v_2 - v_1\|$)

```
Examples:
vmd > vecdist -1.5 5.5
7.0
vmd > vecdist {0 0 0} {3 4 0}
5.0
vmd > vecdist {0 1 2 3 4 5 6} {-6 -5 -4 -3 -2 -1 0}
15.8745
```

- **vecinvert** *v* – Returns the additive inverse of v ($-$v).

```
Examples:
vmd > vecinvert -11.1
11.1
vmd > vecinvert {3 -4 5}
-3 4 -5
vmd > vecinvert {0 -1 2 -3}
0 1 -2 3
```

11.2 Matrix routines

Because matrices are rather large when expressed in text form, the following definitions are used for the examples.

- **transidentity** – Returns the identity matrix.

```
Example:
vmd > transidentity
{1.0 0.0 0.0 0.0} {0.0 1.0 0.0 0.0} {0.0 0.0 1.0 0.0} {0.0 0.0 0.0 1.0}
```

- **transtranspose** *m* – Returns the matrix transpose of the given matrix

```
Example:
vmd > transtranspose {{0 1 2 3 4} {5 6 7 8} {9 10 11 12} {13 14 15 16}}
{0 5 9 13} {1 6 10 14} {2 7 11 15} {3 8 12 16}
```

- (C++) **transmult** *m1 m2* [*m3 ... mn*] – Returns the matrix multiplication of the given matrices

```
Examples:
vmd > set mat1 {{1 2 3 4} {-2 3 -4 5} {3 -4 5 -6} {4 5 -6 -7}}
vmd > set mat2 {{1 0 0 0} {0 0.7071 -0.7071 0} {0 0.7071 0.7071 0} {0 0 0 1}}
vmd > set mat3 {{0.866025 0 0 0} {0 1 0 0} {-0.5 0 0.866025 0} {0 0 0 1}}
vmd > transmult $mat1 [transidentity]
{1.0 2.0 3.0 4.0} {-2.0 3.0 -4.0 5.0} {3.0 -4.0 5.0 -6.0}
   {4.0 5.0 -6.0 -7.0}
vmd > transmult $mat1 $mat2 $mat3
{0.512475 3.5355 0.612366 4.0} {0.7428 -0.7071 -4.28656 5.0}
   {-0.58387 0.7071 5.5113 -6.0} {7.35315 -0.7071 -6.73603 -7.0}
```

- **transaxis** <**x**|**y**|**z**> *amount* [**deg**|**rad**|**pi**] – Returns the transformation matrix needed to rotate around the specified axis by a given amount. By default, the amount is specified in degrees, though it can also be given in radians or factors of pi.

```
Examples:
vmd > transaxis x 90
{1.0 0.0 0.0 0.0} {0.0 -3.67321e-06 -1.0 0.0} {0.0 1.0 -3.67321e-06 0.0}
         {0.0 0.0 0.0 1.0}
vmd > transaxis y 0.25 pi
{0.707107 0.0 0.707107 0.0} {0.0 1.0  0.0 0.0}
         {-0.707107 0.0 0.707107 0.0} {0.0 0.0  0.0 1.0}
vmd > transaxis z 3.1415927 rad
{-1.0 -2.65359e-06 0.0 0.0} {2.65359e-06 -1.0 0.0 0.0} {0.0 0.0 1.0 0.0}
         {0.0 0.0 0.0 1.0}
```

- **transvec** *v* – Returns the transformation matrix needed to bring the x axis along the v vector. This matrix is not unique, since a final rotation is allowed around the vector. The matrix is made from a rotation around y, then one about z.

```
Examples:
vmd > transvec {0 1 0}
{-3.67321e-06 -1.0 0.0 0.0} {1.0 -3.67321e-06 0.0 0.0} {0.0 0.0 1.0 0.0}
         {0.0 0.0 0.0 1.0}
vmd > vectrans [transvec {0 0 2}] {1 0 0}
0.0 0.0 1.0
```

- **transvecinv** *v* – Returns the transformation needed to bring the vector v to the x axis. This produces the inverse matrix to transvec, and is composed of a rotation about z then one about y.

```
Examples:
vmd > transvecinv {0 -1 0}
{-3.67321e-06 -1.0 0.0 0.0} {1.0 -3.67321e-06 0.0 0.0} {0.0 0.0 1.0 0.0}
    {0.0 0.0 0.0 1.0}
vmd > vectrans [transvecinv {-3 4 -12}] {-3 4 -12}
13.0 -1.8e-05 5.8e-05
```

```
vmd > transmult [transvec {6 -5 7}] [transvecinv {6 -5 7}]
{0.999999 2.29254e-07 -6.262e-09 0.0} {2.29254e-07 0.999999
    -4.52228e-07 0.0} {-6.262e-09 -4.52228e-07 1.0 0.0} {0.0 0.0 0.0 1.0}
```

- (C++) **transoffset** *v* – Returns the transformation matrix needed to translate by the given offset

  ```
  Examples:
  vmd > transoffset {1 0 0}
  {1.0 0.0 0.0 1} {0.0 1.0 0.0 0} {0.0 0.0 1.0 0} {0.0 0.0 0.0 1.0}
  vmd > transoffset {-6 5 -4.3}
  {1.0 0.0 0.0 -6} {0.0 1.0 0.0 5} {0.0 0.0 1.0 -4.3} {0.0 0.0 0.0 1.0}
  ```

- **transabout** *v amount* [**deg|rad|pi**] – Generates the transformation matrix needed to rotate by the given amount counter-clockwise around axis which goes through the origin and along the given vector. As with transvec, the units of the amount of rotation can be degrees, radians, or multiples of pi.

  ```
  Examples:
  # this is a rotation about x by 180 degrees
  vmd > transabout {1 0 0} 180
  {1.0 0.0 0.0 0.0} {0.0 -1.0 -2.65359e-06 0.0} {0.0 2.65359e-06
          -1.0 0.0} {0.0 0.0 0.0 1.0}
  # a rotation about z by 90 degrees
  # (compare this to "transaxis z 90"
  vmd > transabout {0 0 1} 1.5709 rad
  {0.999624 -0.027414 0.0 0.0} {0.027414 0.999624 0.0 0.0}
          {0.0 0.0 1.0 0.0} {0.0 0.0 0.0 1.0}
  vmd > transabout {1 1 1} 1 pi
  {-0.333335 0.666665 0.666669 0.0} {0.666668 -0.333334 0.666666
          0.0} {0.666666 0.66667 -0.333332 0.0} {0.0 0.0 0.0 1.0}
  ```

- **trans** [**center** {*x y z*}] [**origin** {*x y z*}] [**offset** {*x y z*}] [**axis x** *amount* [**rad|deg|pi**]] [**axis y** *amount* [**rad|deg|pi**]] [**axis z** *amount* [**rad|deg|pi**]] [**x** *amount* [**rad|deg|pi**]] [**y** *amount* [**rad|deg|pi**]] [**z** *amount* [**rad|deg|pi**]] [**axis** {*x y z*} *amount* [**rad|deg|pi**]] [**bond** {*x1 y1 z1*} {*x2 y2 z2*} *amount* [**rad|deg|pi**]] [**angle** {*x1 y1 z1*} {*x2 y2 z2*} {*x3 y3 z3*} *amount* [**rad|deg|pi**]] –

  This command can do almost everything the other ones can do, and then some. It is designed to be the main function used for generating transformation matrices.

Using it correctly calls for understanding how it works internally. There are three matrices: centering, rotation, and offset. The centering matrix determines where the center of rotation is located. By default, this is the origin, but it can be changed to pivot about any point. The rotation matrix defines the rotation about that centering point, and the offset matrix defines the final translation after the rotation.

For example, to rotate around a given point, the transformations would be 1) the centering matrix to bring that point to the origin, 2) the rotation about the center, and 3) the final offset to return the origin back to its original location.

The different options for the `trans` command modify the matrices in various ways.

- **center {***x y z***}** – Sets the centering matrix so that point x y z is brought to the origin
- **offset {***x y z***}** – Sets the offset matrix so that the origin is brought to x y z
- **origin {***x y z***}** – Sets both the centering and offset matrices to x y z
- **axis x** *amount* [**rad|deg|pi**] – Adds a rotation about the x axis by the given amount to the rotation matrix
- **axis y** *amount* [**rad|deg|pi**] – Adds a rotation about the y axis by the given amount to the rotation matrix
- **axis z** *amount* [**rad|deg|pi**] – Adds a rotation about the z axis by the given amount to the rotation matrix
- **axis {***x y z***}** *amount* [**rad|deg|pi**] – Adds a rotation of the given amount about the given vector to the rotation matrix
- **bond {***x1 y1 z1***} {***x2 y2 z2***}** *amount* [**rad|deg|pi**] – Sets the center and offset transformations to the first point, and defines a rotation about the bond axis by the given amount.
- **angle {***x1 y1 z1***} {***x2 y2 z2***} {***x3 y3 z3***}** *amount* [**rad|deg|pi**] – Sets the center and offset transformation to the second point, and defines a rotation about the axis perpendicular to the plane made by the three points (the vector is computed from the cross product of the vector connecting the first two points with that connected the last two).

11.3 Multiplying vectors and matrices

There are two commands to multiply a matrix and a vector, `vectrans` and `coordtrans`. They assume the vector is in column form and premultiply the matrix to the vector. If the vector contains four numbers, the two commands are identical. If the vector has three elements, a fourth is added; a 0 for `vectrans` and a 1 for `coordtrans`. The difference is that vectors are not affected by translations during transformations, while coordinates are.

- (C++) **vectrans** *m v* – Multiple the matrix m with the vector v (length 4); returns a vector
- **coordtrans** *m v* – Multiple the matrix m with the coordinate v (length 3); returns a vector

```
Examples:
vmd > vectrans [transaxis z 90] {1 0 0}
-3.67321e-06 1.0 0.0
vmd > vectrans [transvecinv {-3 4 -12}] {-3 4 -12}
13.0 -1.8e-05 5.8e-05
```

11.4 Misc. functions and values

Several other terms are added to the vectors package. The first is the variable M_PI, which contains the value of pi.

```
Examples:
vmd > set M_PI
3.14159265358979323846
vmd > expr 90 * ($M_PI / 180)
1.5708
```

The functions `trans_from_rot`, `trans_to_rot`, `trans_from_offset`, and `trans_to_offset` are used to get or set a transformation matrix from either a 3x3 rotation matrix or offset vector. As currently designed, these assume there is no scaling in the matrix. The `trans_from_offset` is identical to `transoffset` and is present for completeness.

The last is `find_rotation_value varname`, which takes a variable name and extracts from the beginning of it those terms which describe an amount of rotation. The rest of the data in the variable remains, and the amount of rotation, in radians, is returned. This is used by those functions which need a rotation. The valid values are: a number, followed by one of `rad`, `radian`, or `radians` for a value in radians, the word `pi` to give the rotation in factors of pi, or one of `deg`, `degree`, or `degrees` for a value in degrees. If no units are given, the value is assumed to be in degrees.

Examples:

```
vmd > set a "180 deg north"
180 deg north
vmd > find_rotation_value a
3.14159
vmd > set a
north
vmd > set a "1 pi to eat"
1 pi to eat
vmd > find_rotation_value a
3.14159
vmd > set a
to eat
vmd > set a 45
45
vmd > find_rotation_value a
0.785398
vmd > expr $M_PI * 3.0 / 2.0
4.71239
vmd > set a "4.71238 radians"
4.71238 radians
vmd > find_rotation_value a
4.71238
```

Chapter 12

Molecular Analysis

12.1 Using the `molinfo` command

This section covers how to extract information about molecules and atoms using the VMD text command `molinfo`.

Examples:

Two functions, one to save the current view position, the other to restore it. The position of the axis is not changed by these operations.

```
proc save_viewpoint {} {
   global viewpoints
   if [info exists viewpoints] {unset viewpoints}
   # get the current matricies
   foreach mol [molinfo list] {
      set viewpoints($mol) [molinfo $mol get {
center_matrix rotate_matrix scale_matrix global_matrix}]
   }
}
proc restore_viewpoint {} {
   global viewpoints
   foreach mol [molinfo list] {
      puts "Trying $mol"
      if [info exists viewpoints($mol)] {
         molinfo $mol set {center_matrix rotate_matrix scale_matrix
   global_matrix} $viewpoints($mol)
      }
   }
}
```

Cycle through the list of displayed molecules, turning each one on one at a time. At the end, return the display flags to their original state.

```
# save the current display state
foreach mol [molinfo list] {
  set disp($mol) [molinfo $mol get drawn]
```

```
}
# turn everything off
mol off all
# turn each molecule on then off again
foreach mol [molinfo list] {
  if $disp($mol) {
     mol on $mol
     sleep 1
     mol off $mol
  }
}
# turn the original ones back on
foreach mol [molinfo list] {
  if $disp($mol) {mol on $mol }
}
```

The last loop, which turns the originally drawn molecules back on, doesn't turn them on at the same time. That's because some commands (those which use the command queue) redraw the graphics when they are used. This can be disabled with the `display update` (see section 9.3.6 for more information). Using this, the final loop becomes

```
#turn the original ones back on
display update off
foreach mol [molinfo list] {
  if $disp($mol) {mol on $mol }
}
display update on
```

Alternatively, since the `drawn` option is settable, you could do:

```
foreach mol [molinfo list] {
  if $disp($mol) {molinfo $mol set drawn 1}
}
```

However, that won't set the flag to redraw the scene so you need to force a redraw with `display redraw`.

12.2 Using the `atomselect` command

Atom selection is the primary method to access information about the atoms in a molecule. It works in two steps. The first step is to create a selection given the selection text, molecule id, and optional frame number. This is done by a function called `atomselect`, which returns the name of the new atom selection. the second step is to use the created selection to access the information about the atoms in the selections.

Atom selection is implemented as a Tcl function. The data returned from `atomselect` is the name of the function to use. The name is of the form `atomselect%d` where '%d' is a non-negative number (such as 'atomselect0', atomselect26', ...).

The way to use the function created by the `atomselect` command is to store the name into a variable, then use the variable to get the name when needed.

```
vmd> set sel [atomselect top "water"]
atomselect3
vmd> $sel text
water
```

This is equivalent to saying

```
vmd> atomselect3 text
```

The easiest way of thinking about this is that the `atomselect` command creates an object. To get information from the object you have to send it a command. Thus, in the example above (`atomselect1 num`) the object "atomselect1" was sent the command "num", which asks the object to return the number of atoms in the selection. These derived object functions (the ones with names like atomselect3) take many options, as described in section 9.3.2,

For instance, given the selection

```
vmd> set sel [atomselect top "resid 4"]
atomselect4
```

you can get the atom names for each of the atoms in the selection with

```
vmd> $sel get name
N H CA CB C O
```

(which, remember, is the same as

```
vmd> atomselect4 get name
```

)

Multiple attributes can be requested by submitting a list, so if you want to see which atoms are on the backbone,

```
vmd> $sel get {name backbone}
{N 1} {H 0} {CA 1} {CB 0} {C 1} {O 1}
```

and the atom coordinates with

```
vmd>  $sel get {x y z}
{0.710000 4.211000 1.093000} {-0.026000 3.700000 0.697000} {0.541000
4.841000 2.388000} {-0.809000 4.462000 2.976000} {1.591000 4.371000
3.381000} {2.212000 5.167000 4.085000}
```

Note that the format of the data you get back from the `get` command depends on how many attributes you requested. If you request only one attribute, as in the `get name` example above, you will get back a simple list of elements. On the other hand, if you request two or more attributes, you will get back a list of sublists. Specifically, it is a list of size n where each element is itself a list of size i, where n is the number of atoms in the selection and i is the number of attributes requested.

Your scripts will run faster if you retrieve only one attribute at a time, because then VMD does not have to construct the sublists for each attribute. Remember that in Tcl you can loop over several lists at once using the `foreach` command:

```
foreach resid [$sel get resid] resname [$sel get resname] {
  # process each resid and resname here
}
```

One quick function you can build with the coordinates is a method to calculate the geometrical center (not quite the center of mass; that's a bit harder). This also uses some of the vector commands discussed in the section about vectors and matrices [§11], but you should be able to figure them out from context.

```
proc geom_center {selection} {
        # set the geometrical center to 0
        set gc [veczero]
        # [$selection get {x y z}] returns a list of {x y z}
        #    values (one per atoms) so get each term one by one
        foreach coord [$selection get {x y z}] {
           # sum up the coordinates
           set gc [vecadd $gc $coord]
        }
        # and scale by the inverse of the number of atoms
        return [vecscale [expr 1.0 /[$selection num]] $gc]
}
```

With that defined you can say (assuming $sel was created with the previous atomselection example)

```
vmd> geom_center $sel
0.703168 4.45868 2.43667
```

I'll go through the example line by line. The function is named `geom_center` and takes one parameter, the name of the selection. The first line sets the variable "gc" to the zero vector, which is 0 0 0. On the second line of code, two things occur. First, the command

```
$selection get {x y z}
```

is executed, and the string is replaced with the result, which is

```
{0.710000 4.211000 1.093000} {-0.026000 3.700000 0.697000} {0.541000
4.841000 2.388000} {-0.809000 4.462000 2.976000} {1.591000 4.371000
3.381000} {2.212000 5.167000 4.085000}
```

This is a list of 6 terms (one for each atom in the selection), and each term is a list of three elements, the x, y, and z coordinate, in that order.

The "foreach" command splits the list into its six terms and goes down the list term by term, setting the variable "coord" to each successive term. Inside the loop, the value of $coord is added to total sum.

The last line returns the geometrical center of the atoms in the selection. Since the geometrical center is defined as the sum of the coordinate vectors divided by the number of elements, and so far I have only calculated the sum of vectors, I need the inverse of the number of elements, which is done with the expression

```
expr 1.0 / [$selection num]
```

The decimal in "1.0" is important since otherwise Tcl does integer division. Finally, this value is used to scale the sum of the coordinate vectors (with vecscale), which returns the new value, which is itself returned as the result of the procedure.

The center of mass function is slightly harder because you have to get the mass as well as the x, y, z values, then break that up into to components. The formula for the center of mass is $\sum m_i x_i / \sum mass_i$

```
proc center_of_mass {selection} {
        # some error checking
        if {[$selection num] <= 0} {
                error "center_of_mass: needs a selection with atoms"
        }
        # set the center of mass to 0
        set com [veczero]
        # set the total mass to 0
        set mass 0
        # [$selection get {x y z}] returns the coordinates {x y z}
        # [$selection get {mass}] returns the masses
        # so the following says "for each pair of {coordinates} and masses,
#  do the computation ..."
        foreach coord [$selection get {x y z}] m [$selection get mass] {
           # sum of the masses
           set mass [expr $mass + $m]
           # sum up the product of mass and coordinate
           set com [vecadd $com [vecscale $m $coord]]
        }
        # and scale by the inverse of the number of atoms
        if {$mass == 0} {
                error "center_of_mass: total mass is zero"
        }
        # The "1.0" can't be "1", since otherwise integer division is done
        return [vecscale [expr 1.0/$mass] $com]
}

vmd> center_of_mass $sel
Info) 0.912778 4.61792 2.78021
```

The opposite of "get" is "set". Many keywords (most notably, "x", "y", and "z") can be set to new values. This allows, for instance, atom coordinates to be changed, the occupancy values to be updated, or user forces to be added. You can also change the resname, segid, and so forth, which may be easier to do within VMD than, for example, editing a PDB file by hand.

```
  set sel [atomselect top "index 5"]
  $sel get {x y z}
{1.450000 0.000000 0.000000}
  $set set {x y z} {{1.6 0 0}}
```

Note that just as the get option returned a list of lists, the set option needs a list of lists, which is why the extra set of curly braces were need. Again, this must be a list of size n containing elements which are a list of size i. The exeception is if n is 1, the list is duplicated enough times so there is one element for each atom.

```
  # get two atoms and set their coordinates
  set sel [atomselect top "index 6 7"]
  $sel set {x y z} { {5 0 0} {7.6 5.4 3.2} }
```

In this case, the atom with index 6 gets its (x, y, z) values set to 5 0 0 and the atom with index 7 has its coordinates changed to 7.6 5.4 3.2.

It is possible to move atoms this way by getting the coordinates, changing them (say by adding some offset) and replacing it. Following is a function which will do just that:

```
proc moveby {sel offset} {
  foreach coord [$sel get {x y z}] {
    lappend newcoords [vecadd $coord $offset]
  }
  $sel set {x y z} $newcoords
}
```

And to use this function (in this case, to apply an offset of (x y z) = (0.1 -2.8 9) to the selection "$movesel"):

```
moveby $movesel {0.1 -2.8 9}
```

However, to simplify matters some options have been added to the selection to deal with movements (these commands are also implemented in C++ and are much faster than the Tcl versions). These functions are `moveby`, `moveto`, and `move`. The first two take a position vector and the last takes a transformation matrix.

The first command, `moveby`, moves each of the atoms in the selection over by the given vector offset.

```
  $sel moveby {1 -1 3.4}
```

The second, `moveto`, moves all the atoms in a selection to a given coordinate (it would be strange to use this for a selection of more than one atom, but that's allowed). Example:

```
  $sel moveto {-1 1 4.3}
```

The last of those, `move`, applies the given transformation matrix to each of the atom coordinates. This is best used for rotating a set of atoms around a given axis, as in

```
  $sel move [trans x 90]
```

which rotates the selection 90 degrees about the x axis. Of course, any transformation matrix may be used.

A more useful example is the following, which rotates the side chain atoms around the CA-CB bond by 10 degrees.

```
# get the sidechain atoms (CB and onwards)
set sidechain [atomselect top "sidechain residue 22"]
# get the CA coordinates -- could do next two on one line ...
set CA [atomselect top "name CA and residue 22"]
set CAcoord [lindex [$CA get {x y z}] 0]
# and get the CB coordinates
set CB [atomselect top "name CB and residue 22"]
set CBcoord [lindex [$CB get {x y z}] 0]
# apply a transform of 10 degrees about the given bond axis
$sidechain move [trans bond $CAcoord $CBcoord 10 deg]
```

12.3 Analysis scripts

Following are some more examples of routines that could be used for analysing molecules. These are not the best routines to use since many of these can be implemented with the `measure` command, which calls a much faster built-in function.

Finding waters near a protein This example finds the waters near the protein for each frame of a trajectory and writes out a PDB file containing those waters:

```
set sel [atomselect top "water and same residue as (within 2 of protein)"]
set n [molinfo top get numframes]
for { set i 0 } { $i < $n } { incr i } {
  $sel frame $i
  $sel update
  $sel writepdb water_$i.pdb
}
```

The `frame` option sets the frame of the selection, `update` tells the atom selection to recompute which waters are near the protein, and `writepdb` writes the selected waters to a file.

Total mass of a selection

```
proc total_mass {selection} {
  set sum 0
  foreach mass [$selection get mass] {
    set sum [expr {$sum + $mass}]
  }
  return $sum
}
```

Note the curly braces after the `expr` command in the above example. Omitting those braces causes this script to run about three times slower! The moral of the story is: always put curly braces around the expression that you pass to `expr`.

Here's another (slightly slower) way to do the same thing. This works because the mass returned from the selection is a list of lists. Putting it inside the quotes of the eval makes it a sequence of vectors, so the vecadd command will work on it.

```
proc total_mass1 {selection} {
  set mass [$selection get mass]
  eval "vecadd $mass"
}
```

Coordinate min and max Find the min and max coordinate values of a given molecule in the x, y, and z directions (see also the `measure` command 'minmax'). The function takes the molecule id and returns two vectors; the first contains the min values and the second contains the max.

```
proc minmax {molid} {
  set sel [atomselect top all]
  set sx [$sel get x]
  set sy [$sel get y]
  set sz [$sel get z]
  set minx [lindex $sx 0]
  set miny [lindex $sy 0]
  set minz [lindex $sz 0]
  set maxx $minx
  set maxy $miny
  set maxz $minz
  foreach x $sx y $sy z $sz {
    if {$x < $minx} {set minx $x} else {if {$x > $maxx} {set maxx $x}}
    if {$y < $miny} {set miny $y} else {if {$y > $maxy} {set maxy $y}}
    if {$z < $minz} {set minz $z} else {if {$z > $maxz} {set maxz $z}}
  }
  return [list [list $minx $miny $minz] [list $maxx $maxy $maxz]]
}
```

Radius of gyration Compute the radius of gyration for a selection (see also `measure rgyr`). The square of the radius of gyration is defined as $\sum_i m_i(\vec{r}_i - \vec{r}_c)^2 / \sum_i m_i$. This uses the center_of_mass function defined earlier in this chapter; a faster version would replace that with `measure center`. Note that the `measure rgyr` command does the same thing as this script, only much much faster.

```
proc gyr_radius {sel} {
  # make sure this is a proper selection and has atoms
  if {[$sel num] <= 0} {
    error "gyr_radius: must have at least one atom in selection"
  }
  # gyration is sqrt( sum((r(i) - r(center_of_mass))^2) / N)
  set com [center_of_mass $sel]
  set sum 0
  foreach coord [$sel get {x y z}] {
    set sum [vecadd $sum [veclength2 [vecsub $coord $com]]]
  }
  return [expr sqrt($sum / ([$sel num] + 0.0))]
}
```

Applying this to the alanin.pdb coordinate file

```
vmd > mol new alanin.pdb
vmd > set sel [atomselect top all]
vmd > gyr_radius $sel
Info) 5.45443
```

Root mean square deviation Compute the rms difference of a selection between two frames of a trajectory. This takes a selection and the values of the two frames to compare.

```
proc frame_rmsd {selection frame1 frame2} {
  set mol [$selection molindex]
  # check the range
  set num [molinfo $mol get numframes]
  if {$frame1 < 0 || $frame1 >= $num || $frame2 < 0 || $frame2 >= $num} {
    error "frame_rmsd: frame number out of range"
  }
  # get the first coordinate set
  set sel1 [atomselect $mol [$selection text] frame $frame1]
  set coords1 [$sel1 get {x y z}]
  # get the second coordinate set
  set sel2 [atomselect $mol [$selection text] frame $frame2]
  set coords2 [$sel2 get {x y z}]
  # and compute the rmsd values
  set rmsd 0
  foreach coord1 $coords1 coord2 $coords2 {
    set rmsd [expr $rmsd + [veclength2 [vecsub $coord2 $coord1]]]
  }
  # divide by the number of atoms and return the result
  return [expr $rmsd / ([$selection num] + 0.0)]
}
```

The following uses the frame_rmsd function to list the rmsd of the molecule over the whole trajectory, as compared to the first frame.

```
vmd > mol new alanin.psf
vmd > mol addfile alanin.dcd
vmd > set sel [atomselect top all]
vmd > for {set i 0} {$i < [molinfo top get numframes]} {incr i} {
?   puts [list $i [frame_rmsd $sel $i 0]]
? }
0 0.0
1 0.100078
2 0.291405
3 0.523673
 ....
97 20.0095
98 21.0495
99 21.5747
```

The last example shows how to set the beta field. This is useful because one of the coloring methods is 'Beta', which uses the beta values to color the molecule according to the current color scale. (This can also be done with the occupancy field.) Thus redefining the beta values allows you to color the molecules based on your own definition. One useful example is to color the molecule based on the distance from a specific point (for this case, coloring a poliovirus protomer based on its distance to the center of the virus (0, 0, 0) helps bring out the surface features).

```
proc betacolor_distance {sel point} {
  # get the coordinates
  foreach coord [$sel get {x y z}] {
   # get the distance and put it in the "newbeta" list
    set dist [veclength2 [vecsub $coord $point]]
    lappend newbeta $dist
  }
  # set the beta term
  $sel set beta $newbeta
}
```

And here's one way to use it:

```
# load pdb2plv.ent using anonymous ftp to the PDB
vmd > mol new 2plv
vmd > set sel [atomselect top all]
vmd > betacolor_distance $sel {0 0 0}
```

Then go to the graphics menu and set the 'Coloring Method' to 'Beta'.

12.4 RMS Fit and Alignment

When one has two similar structures, one often wants to compare them. What's the difference between two X-ray structures? How much did the structure change during a simulation? To answer these questions, you must first figure out how to compare two structures, which usually means that you must find the root mean square deviation (RMSD).

Formally, given N atom positions from structure x and the corresponding N atoms from structure y with a weighting factor $w(i)$, the RMSD is defined as:

$$RMSD(N;x,y) = \left[\frac{\sum_{i=1}^{N} w_i \|x_i - y_i\|^2}{N \sum_{i=1}^{N} w_i}\right]^{\frac{1}{2}}$$

Using this equation by itself probably won't give you the answer you are looking for. Imagine two identical structures offset by some distance. The RMSD should be 0, but the offset prevents that from happening. What you really want is the minimum RMSD between two given structures; the best fit. There are many ways to do this, but for VMD we have implemented the method of Kabsch (Acta Cryst. (1978) A34, 827-828 or see file Measure.C in the VMD source code). This algorithm computes the transformation, needed to move one structure onto another in order to minimize the RMSD.

With the mathematical prerequisites behind us, we still need to be able to specify how to choose the atoms to compare. If you want to compare all the atoms in both structures, and they both

have the same number of atoms, then the problem is easy – N is everything. This occurs most often in MD simulations when the only thing different between two structures are the coordinates.

But what about homologous sequences? In this case, the number of atoms differ because while the number of residues is the same, the sidechains have different numbers of atoms. The usual solution is to determine the RMSD based solely on the backbone atoms or, in some X-ray structures where only the C_α atoms have been determined, based on the C_α atoms. VMD allows you to fit and align based on any valid atom selection, as long as the atom selection specifies the same number of atoms in each molecule being compared.

12.4.1 RMS Fit and Alignment Extension

To get started with RMS fitting and alignment, open the RMSD item from the **Extensions** menu. You should now have a new window titled RMSD Tool We'll describe the RMSD calculator function first.

RMSD calculation

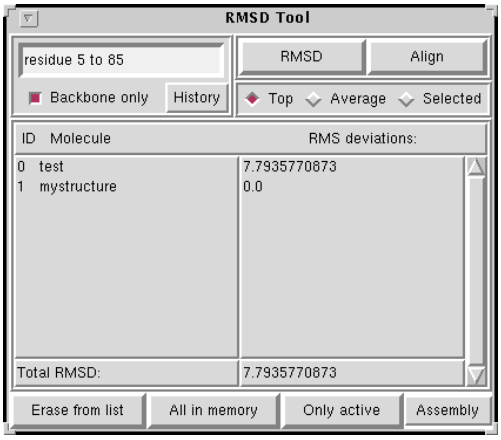


Figure 12.1: RMS calculation and alignment extension

The RMSD calculator button is used to calculate RMS distances between molecules. The upper left corner of the menu is where you specify which atoms are to be used in the calculation. In the input field, type the atom selection text just as you would in the Graphics window. The checkbox below the input field entitled *Backbone only* restricts whatever atom selection you typed to just the backbone atoms of the selection; in effect, it adds "and backbone" to the atom selection text.

The upper right corner of the menu has a button labeled **RMSD**. Its effect depends on which of the **Top**, **Average**, or **Selected** radio buttons are selected. If **Top** is selected, VMD calculates the RMS distance between the top molecule (which is usually the last molecule loaded) and every other molecule. If **Average** is selected, VMD first computes the average x, y, z coordinates of the selected atoms in each molecule, then computes the RMS distance of each molecule from that average structure.

Results of the RMS calculations for each molecule are shown in the browser in the bottom half of the menu. Note that this list is not updated until you presse the RMSD button, so the effects

of loading/deleting molecules will not be immediately reflected. The **Total RMSD** label at the bottom of the menu shows the average RMSD for all molecules listed.

RMS Alignment

The RMS Alignment button fits molecules based on selected groups of atoms. Whereas the RMSD calculator button finds the RMS distance between molecules without disturbing their coordinates, the RMS Alignment button actually moves molecules to new positions.

This button is quite simple: Enter an atom selection in the input field, and press Align to align the molecules based on the atoms in that selection. If you recompute the RMSD between molecules with the RMSD calculator button, you will probably find that the values are different; this is because the calculation is made based on the current positions of the atoms.

12.4.2 RMS and scripting

The same actions can be taken on the scripting level. The Text interface also gives you more flexibility through the atom selection mechanism allowing to choose the atoms to fit/compare.

RMSD Computation

There are two atom selections needed to do an RMSD computation, the list of atoms to compare in both molecules. The first atom of the first selection is compared to the first atom of the second selection, fifth to fifth, and so on. The actual order is identical to the order from the input PDB file.

Once the two selections are made, the RMSD calculation is a matter of calling the `measure rmsd` function. Here's an example:

```
      set sel1 [atomselect 0 "backbone"]
      set sel2 [atomselect 1 "backbone"]
      measure rmsd $sel1 $sel2
Info)  10.403014
```

This prints the RMSD between the backbone atoms of molecule 0 with those of molecule 1. You could also use a weighting factor in these calculations. The best way to understand how to do this is to see another example:

```
      set weighted_rmsd [measure rmsd $sel1 $sel2 weight mass]
Info)  10.403022
```

In this case, the weight is determined by the mass of each atom. Actually, the term is really one of the standard keywords available to an atom selection. Other ones include index and resid (which would both be rather strange to use) as well as charge, beta and occupancy. These last terms useful if you want to specify your own values for the weighting factors.

Computing the Alignment

The best-fit alignment is done in two steps. The first is to compute the 4×4 matrix transformation that takes one set of coordinates onto the other. This is done with the `measure fit` command. Assuming the same selections as before:

```
        set transformation_matrix [measure fit $sel1 $sel2]
Info) {0.971188 0.00716391 0.238206 -13.2877}
{0.0188176 0.994122 -0.106619 3.25415} {-0.23757 0.108029 0.965345 -2.97617}
{0.0 0.0 0.0 1.0}
```

As with the RMSD calculation, you could also add an optional `weight <keyword>` term on the end.

The next step is to apply the matrix to a set of atoms using the move command. So far you have two coordinate sets. You might think you could do something like `$sel1 move $transformation_matrix` to apply the matrix to all the atoms of that selection. You could, but that's not the right selection.

The thing to recall is that `$sel1` is the selection for the backbone atoms. You really want to move the whole fragment to which it is attached, or even the whole molecule. (This is where the discussion earlier comes into play.) So you need to make a third selection containing all the atoms which are to be moved, and apply the transformation to those atoms.

```
# molecule 0 is the same molecule used for $sel1
set move_sel [atomselect 0 "all"]
$move_sel move $transformation_matrix
```

As a more complicated example, say you want to align all of molecule 1 with molecule 9 using only the backbone atoms of residues 4 to 10 in both systems. Here's how:

```
# compute the transformation matrix
set reference_sel  [atomselect 9 "backbone and resid 4 to 10"]
set comparison_sel [atomselect 1 "backbone and resid 4 to 10"]
set transformation_mat [measure fit $comparison_sel $reference_sel]

# apply it to all of the molecule 1
set move_sel [atomselect 1 "all"]
$move_sel move $transformation_mat
```

A simulation example script

Here's a longer script which you might find useful. The problem is to compute the RMSD between each frame of the simulation and the first frame. Usually in a simulation there is no initial global velocity, so the center of mass doesn't move, but because of angular rotations and because of numerical imprecisions that slowly build up, the script aligns the molecule before computing its RMSD.

```
# Prints the RMSD of the protein atoms between each \timestep
# and the first \timestep for the given molecule id (default: top)
proc print_rmsd_through_time {{mol top}} {
        # use frame 0 for the reference
        set reference [atomselect $mol "protein" frame 0]
        # the frame being compared
        set compare [atomselect $mol "protein"]

        set num_steps [molinfo $mol get numframes]
        for {set frame 0} {$frame < $num_steps} {incr frame} {
```

```
                    # get the correct frame
                    $compare frame $frame

                    # compute the transformation
                    set trans_mat [measure fit $compare $reference]
                    # do the alignment
                    $compare move $trans_mat
                    # compute the RMSD
                    set rmsd [measure rmsd $compare $reference]
                    # print the RMSD
                    puts "RMSD of $frame is $rmsd"
            }
        }
```

To use this, load a molecule with an animation (for example, `$VMDDIR/proteins/alanin.DCD` from the VMD distribution). Then run `print_rmsd_through_time`. Example output is shown here:

```
vmd > print_rmsd_through_time
RMSD of 0 is 0.000000
RMSD of 1 is 1.060704
RMSD of 2 is 0.977208
RMSD of 3 is 0.881330
RMSD of 4 is 0.795466
RMSD of 5 is 0.676938
RMSD of 6 is 0.563725
RMSD of 7 is 0.423108
RMSD of 8 is 0.335384
RMSD of 9 is 0.488800
RMSD of 10 is 0.675662
RMSD of 11 is 0.749352
 [...]
```

12.5 VMD Script Commands for Colors

In order to fine tune color parameters, one typically needs more sophisticated controls than those offered in the GUI. For this reason, VMD provides a number of scripting level commands for color access. These commands will be discussed in detail in chapter 9, but to give you a flavor for their use, here are a couple of examples that you may find useful right away. Most things can be done with `color` [§9.3.4] and `colorinfo` [§9.3.5] commands.

12.5.1 Changing the color scale definitions

Suppose that of the 1024 colors, the first 511 should be red, then 2 whites, and finally 511 blues. You can use the 'color' command to modify the color scale values accordingly.

```
proc tricolor_scale {} {
  set color_start [colorinfo num]
```

```
  display update off
  for {set i 0} {$i < 1024} {incr i} {
    if {$i == 0} {
      set r 1;  set g 0;  set b 0
    }
    if {$i == 511} {
      set r 1;  set g 1;  set b 1
    }
    if {$i == 513} {
      set r 0;  set g 0;  set b 1
    }
    color change rgb [expr $i + $color_start     ] $r $g $b
  }
  display update on
}

tricolor_scale
```

12.5.2 Creating a set of black-and-white color definitions

To map grayscale on the color ids 0-16 (0=black; 16=white):

```
proc make_grayscale {} {
  display update off
  set coloridcount [colorinfo num]
  set colordiv [expr $coloridcount - 1.0]
  for {set i 0} {$i < $coloridcount} {incr i} {
    set val [expr $i / $colordiv]
    color change rgb $i $val $val $val
  }
  display update on
}
```

Note that the display updates are switched off for the time of redefinition, so that the screen would not be redrawn every time one color is changed. This way the procedure works faster. The only bad thing about this idea is that black becomes white, and white changes too, so the names of the colors (yellow, orange, etc.) become useless.

12.5.3 Revert all RGB values to defaults

After some of the color definitions have been changed and you want to restore the default definitions, the following procedure might be useful.

```
proc revert_colors {} {
  display update off
  foreach color [colorinfo colors] {
    color change rgb $color
  }
```

```
  display update on
}
```

12.5.4 Coloring Trick - Override a Coloring Category

There is currently no user-defined coloring method. This makes it hard to color residues by property "X" if X is not already defined in VMD. It is possible to get around this limitation somewhat by overriding one of the values in the PDB or PSF. For instance, suppose you wanted to color the atoms by the distance of the atom from a given point. One way is to compute the distance and put it in either the occupancy or beta field of the PDB file. Then when the molecule is colored by occupancy it is actually coloring by distance.

You could also override, say, the segment name field or even the residue name. Don't override the atom name unless you are really desperate as VMD uses it to determine which residues are proteins and nucleic acids, and hence which residues can be drawn as a tube or ribbon.

Chapter 13

Collective Variables Interface (Colvars)

In today's molecular dynamics simulations, it is often useful to reduce the large number of degrees of freedom of a physical system into few parameters whose statistical distributions can be analyzed individually, or used to define biasing potentials to alter the dynamics of the system in a controlled manner. These have been called 'order parameters', 'collective variables', '(surrogate) reaction coordinates', and many other terms.

Here we use primarily the term 'collective variable' (shortened to *colvar*), which indicates any differentiable function of atomic Cartesian coordinates, $\boldsymbol{x}_i$, with i between 1 and N, the total number of atoms:

$$\xi(t) = \xi\left(\boldsymbol{x}_i(t), \boldsymbol{x}_j(t), \boldsymbol{x}_k(t), \ldots\right) \ , \quad 1 \leq i, j, k \ldots \leq N \tag{13.1}$$

The Colvars module in VMD may be used to calculate these functions over a molecular structure, and to analyze the results of previous simulations. The module is designed to perform multiple tasks concurrently during or after a simulation, the most common of which are:

- apply restraints or biasing potentials to multiple colvars, tailored on the system by choosing from a wide set of basis functions, without limitations on their number or on the number of atoms involved;
- calculate potentials of mean force (PMFs) along any set of colvars, using different enhanced sampling methods, such as Adaptive Biasing Force (ABF), metadynamics, steered MD and umbrella sampling; variants of these methods that make use of an ensemble of replicas are supported as well;
- calculate statistical properties of the colvars, such as running averages and standard deviations, correlation functions of pairs of colvars, and multidimensional histograms: this can be done either at run-time without the need to save very large trajectory files, or after a simulation has been completed using VMD and the `cv` command.

Note: although restraints and PMF algorithms are primarily used during simulations, they are also available in VMD to test a new input for a simulation, or to evaluate the relative free energy of a new structure based on data from a previous calculation. *Options that only have an effect during a simulation are also included for compatibility purposes.*

To briefly illustrate the flexibility of the Colvars module, Figure 13.1 shows an example of a non-trivial configuration (the corresponding input can be found in 13.1.2).

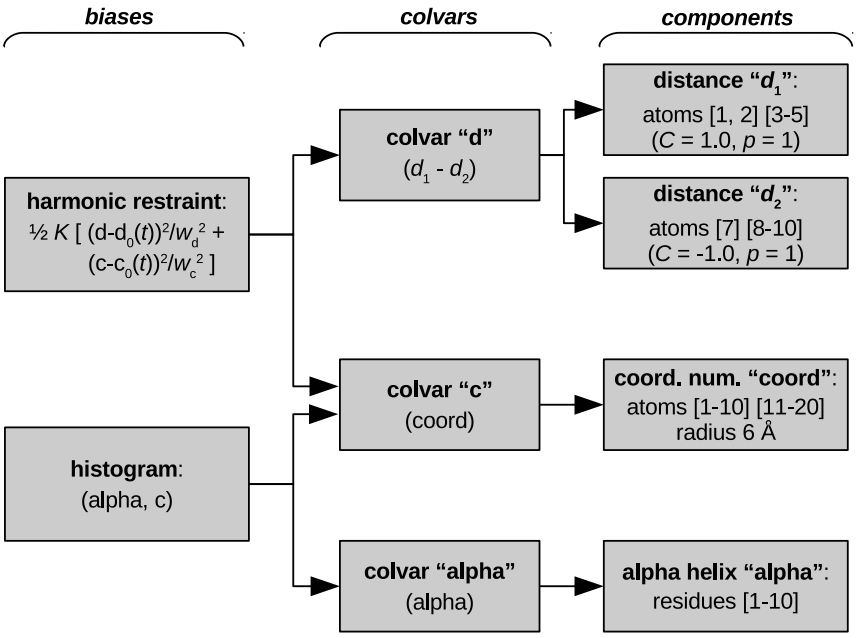


Figure 13.1: Graphical representation of a Colvars configuration. The colvar called "d" is defined as the difference between two distances: the first distance (d_1) is taken between the center of mass of atoms 1 and 2 and that of atoms 3 to 5, the second (d_2) between atom 7 and the center of mass of atoms 8 to 10. The difference $d = d_1 - d_2$ is obtained by multiplying the two by a coefficient $C = +1$ or $C = -1$, respectively. The colvar called "c" is the coordination number calculated between atoms 1 to 10 and atoms 11 to 20. A harmonic restraint is applied to both d and c: to allow using the same force constant K, both d and c are scaled by their respective fluctuation widths w_d and w_c. A third colvar "alpha" is defined as the α-helical content of residues 1 to 10. The values of "c" and "alpha" are also recorded throughout the simulation as a joint 2-dimensional histogram.

Detailed explanations of the design of the Colvars module are provided in reference [44]. Please cite this reference whenever publishing work that makes use of this module.

13.1 General parameters and input/output files

Here, we document the syntax of the commands and parameters used to set up and use the Colvars module in VMD. One of these parameters is the configuration file or the configuration text for the module itself, whose syntax is described in 13.1.2 and in the following sections.

13.1.1 Using the `cv` command

The Colvars module is accessed in VMD through the command `cv`. The command must be used the first time as `cv molid` <*molid*> to set up the Colvars module for a given molecule. In all following uses, the `cv` command will continue operating on the same molecule, regardless of its "top" status.

To use the `cv` command on a different molecule, use `cv delete` first and then `cv molid` <*molid*>. Invoking the `cv` command with no arguments prints a help screen.

Collective variables and biases can be added, queried and deleted through the scripting command `cv`, with the following syntax: `cv <subcommand> [args...]`. For example, to query the value of a collective variable named `myVar`, use the following syntax: `set value [cv colvar myVar value]`. All subcommands of `cv` are documented below.

Managing the colvars module

- `molid` <*molid*>: setup the colvars module for the given molecule; <*molid*> is the identifier of a valid VMD molecule, either an integer or `top` for the top molecule;
- `delete`: delete the colvars module; after this, the module can be setup again using `cv molid`;
- `configfile` <*file name*>: read configuration from a file;
- `config` <*string*>: read configuration from the given string; both `config` and `configfile` subcommands may be invoked multiple times; see 13.1.2 for the configuration syntax;
- `reset`: delete all internal configuration of the colvars module;
- `version`: return the version of the colvars code.

Input and output

- `list`: return a list of all currently defined variables; See 13.2, 13.4 and 13.3 for how to configure a collective variable;
- `list biases`: return a list of all currently defined biases (i.e. sampling and analysis algorithms);
- `load` <*file name*>: load a collective variables state file, typically produced during a previous simulation; this parameter requires that the corresponding configuration has already been loaded by `configfile` or `config`; see 13.1.4 for a brief description of this file; the contents of this file are not required for as long as the VMD molecule has valid coordinates and `cv update` is used;
- `load` <*prefix*>: same as above, but without the `.colvars.state` suffix;
- `save` <*prefix*>: save the current state in a file whose name begins with the given argument; if any of the biases have additional output files defined, those are saved as well using the same prefix;
- `update`: recalculate all colvars and biases based on the current atomic coordinates;
- `printframe`: return a summary of the current frame, in a format equivalent to a line of the collective variables trajectory file;
- `printframelabels`: return text labels for the columns of `printframe`'s output;
- `frame`: return the current frame number, from which colvar values are calculated;
- `frame` <*new frame*>: set the frame number; returns 0 if successful, nonzero if the requested frame does not exist.

Accessing collective variables

- `colvar` <*name*> `value`: return the current value of colvar <*name*>;
- `colvar` <*name*> `update`: recalculate colvar <*name*>;
- `colvar` <*name*> `type`: return the type of colvar <*name*>;
- `colvar` <*name*> `delete`: delete colvar <*name*>;
- `colvar` <*name*> `getconfig`: return config string of colvar <*name*>.
- `colvar` <*name*> `cvcflags` <*flags*>: for a colvar with several cvcs (numbered according to their name string order), set which cvcs are enabled or disabled in subsequent evaluations according to a list of 0/1 flags (one per cvc).

Accessing biases

- `bias` <*name*> `energy`: return the current energy of the bias <*name*>;
- `bias` <*name*> `update`: recalculate the bias <*name*>;
- `bias` <*name*> `delete`: delete the bias <*name*>;
- `bias` <*name*> `getconfig`: return config string of bias <*name*>.

13.1.2 Configuration syntax for the Colvars module

The Colvars configuration is usually read using the commands `cv configfile` or `cv config`. The syntax of the Colvars configuration is "`keyword value`", where the keyword and its value are separated by any white space. The following rules apply:

- keywords are case-insensitive (`upperBoundary` is the same as `upperboundary` and `UPPERBOUNDARY`): their string values are however case-sensitive (e.g. file names);
- a long value or a list of multiple values can be distributed across multiple lines by using curly braces, "{" and "}": the opening brace "{" must occur on the same line as the keyword, following a space character or other white space; the closing brace "}" can be at any position after that;
- many keywords are nested, and are only meaningful within a specific context: for every keyword documented in the following, the "parent" keyword that defines such context is also indicated;
- Tcl syntax is generally not available, but it is possible to use Tcl variables or bracket expansion of commands within a configuration string, when this is passed via the command `cv config ...`: for example, it is possible to convert the atom selection $*sel* into an atom group (see 13.3.1) using `cv config "atomNumbers { [$sel get serial] }"`;
- if a keyword requiring a boolean value (`yes|on|true` or `no|off|false`) is provided without an explicit value, it defaults to '`yes|on|true`'; for example, '`outputAppliedForce`' may be used as shorthand for '`outputAppliedForce on`';

- the hash character `#` indicates a comment: all text in the same line following this character will be ignored.

The following keywords are available in the global context of the colvars configuration, i.e. they are not nested inside other keywords:

- `colvarsTrajFrequency` ⟨ Colvar value trajectory frequency ⟩
  Context: global
  Acceptable values: positive integer
  Default value: `100`
  Description: The values of each colvar (and of other related quantities, if requested) are written to the file *outputName*`.colvars.traj` every these many steps throughout the simulation. If the value is `0`, such trajectory file is not written. For optimization the output is buffered, and synchronized with the disk only when the restart file is being written.

- `colvarsTrajAppend` ⟨ Append to trajectory file? ⟩
  Context: global
  Acceptable values: boolean
  Default value: `off`
  Description: If this flag is enabled, and a file with the same name as the trajectory file is already present, new data is appended to that file. Otherwise, a new file is created with the same name that overwrites the previous file.

- `colvarsRestartFrequency` ⟨ Colvar module restart frequency ⟩
  Context: global
  Acceptable values: positive integer
  Default value: `restartFreq`
  Description: Allows to choose a different restart frequency for the Colvars module. Redefining it may be useful to trace the time evolution of those few properties which are not written to the trajectory file for reasons of disk space.

- `indexFile` ⟨ Index file for atom selection (GROMACS "ndx" format) ⟩
  Context: global
  Acceptable values: UNIX filename
  Description: This option reads an index file (usually with a `.ndx` extension) as produced by the `make_ndx` tool of GROMACS. This keyword may be repeated to load multiple index files: the same group name cannot appear in multiple index files. The names of index groups contained in this file can then be used to define atom groups with the `indexGroup` keyword. Other supported methods to select atoms are described in 13.3.

- `smp` ⟨ Whether SMP parallelism should be used ⟩
  Context: global
  Acceptable values: boolean
  Default value: `on`
  Description: If this flag is enabled (default), SMP parallelism over threads will be used to compute variables and biases, provided that this is supported by VMD.

- `smp` ⟨ Whether SMP parallelism should be used ⟩
  Context: global

Acceptable values: boolean
Default value: `on`
Description: If this flag is enabled (default), SMP parallelism over threads will be used to compute variables and biases, provided that this is supported by VMD.

- `analysis` ⟨Turn on run-time statistical analysis⟩
  Context: global
  Acceptable values: boolean
  Default value: `off`
  Description: If this flag is enabled, each colvar is instructed to perform whatever run-time statistical analysis it is configured to, such as correlation functions, or running averages and standard deviations. See section 13.2.5 for details.

The example below defines the same configuration shown in Fig. 13.1. The options within the `colvar` blocks are described in 13.2 and 13.4, the ones within the `harmonic` and `histogram` blocks in 13.5. **Note:** *except* `colvar`*, none of the keywords shown is mandatory.*

```
colvar {
  # difference of two distances
  name d
  width 0.2 # 0.2 Å of estimated fluctuation width
  distance {
    componentCoeff 1.0
    group1 { atomNumbers 1 2 }
    group2 { atomNumbers 3 4 5 }
  }
  distance {
    componentCoeff -1.0
    group1 { atomNumbers 7 }
    group2 { atomNumbers 8 9 10 }
  }
}

colvar {
  name c
  coordNum {
    cutoff 6.0
    group1 { atomNumbersRange 1-10 }
    group2 { atomNumbersRange 11-20 }
  }
}

colvar {
  name alpha
  alpha {
    psfSegID PROT
    residueRange 1-10
  }
```

```
}

harmonic {
  colvars d c
  centers 3.0 4.0
  forceConstant 5.0
}

histogram {
  colvars c alpha
}
```

Section 13.2 explains how to define a colvar and its behavior, regardless of its specific functional form. To define colvars that are appropriate to a specific physical system, Section 13.3 documents how to select atoms, and section 13.4 lists all of the available functional forms, which we call "colvar components". Finally, section 13.5 lists the available methods and algorithms to perform biased simulations and multidimensional analysis of colvars.

13.1.3 Input state file (optional)

Aside from the colvars configuration, an optional input state file may be provided to load the relevant data from a previous simulation. The name of this file is provided through `cv load` <*file name* >.

13.1.4 Output files

During a simulation with collective variables defined, the following three output files are written:

- a *state file*, named *outputName*`.colvars.state`; this file is in ASCII format;
- if the parameter `colvarsRestartFrequency` is larger than zero, a *restart file* named *restartName*`.colvars.state` is written every that many steps: this file is equivalent to the final state file;
- if the parameter `colvarsTrajFrequency` is greater than 0 (default: 100), a *trajectory file* is written during the simulation: its name is *outputName*`.colvars.traj`; unlike the state file, it is not needed to restart a simulation, but can be used later for post-processing and analysis.

Other output files may be written by specific methods applied to the colvars (e.g. by the ABF method, see 13.5.1, or the metadynamics method, see 13.5.3). Like the colvar trajectory file, they are needed only for analyzing, not continuing a simulation. All such files' names also begin with the prefix *outputName*.

13.2 Defining collective variables and their properties

In the configuration file each colvar is defined by the keyword `colvar`, followed by its configuration options within curly braces: `colvar { ... }`. One of these options is the name of a colvar

component: for example, including `rmsd { ... }` defines the colvar as a RMSD function. *In most applications, only one component is used, and the component is equal to the colvar.*

The full list of colvar components can be found in Section 13.4, with the syntax to select atoms in Section 13.3. The following section lists several options to control the behavior of a single colvar, regardless of its type.

13.2.1 General options for a collective variable

The following options are not required by default; however, the first four are very frequently used:

- `name` ⟨ Name of this colvar ⟩
  Context: `colvar`
  Acceptable values: string
  Default value: "`colvar`" + numeric id
  Description: The name is an unique case-sensitive string which allows the Colvars module to identify this colvar unambiguously; it is also used in the trajectory file to label to the columns corresponding to this colvar.

- `width` ⟨ Colvar fluctuation scale, or resolution for grid-based methods ⟩
  Context: `colvar`
  Acceptable values: positive decimal
  Default value: 1.0
  Description: This number has the same physical unit as the colvar value and defines an effective colvar unit. Biasing algorithms use it for different purposes. Harmonic restraints (13.5.4) use it to set the physical unit of the force constant, which is useful for multidimensional restraints involving colvars with different units or scale which may then be defined by a single, scaled force constant. Histogram (13.5.7) and ABF biases (13.5.1) interpret it as the grid spacing in the direction of this variable. Metadynamics (13.5.3) uses it to set the width of newly added hills. In other cases, it is simplest to keep the default value of 1, so that harmonic force constants are provided in their usual physical unit. When a non-unity width is required by the application, the optimal value is application-dependent, but can often be thought of as a user-provided estimate of the fluctuation amplitude for the colvar. In those cases, it should generally be set smaller than or equal to the standard deviation of the colvar during a very short simulation run.

- `lowerBoundary` ⟨ Lower boundary of the colvar ⟩
  Context: `colvar`
  Acceptable values: decimal
  Description: Defines the lowest end of the interval of "relevant" values for the colvar. This number can be either a true physical boundary, or a user-defined number. Together with `upperBoundary` and `width`, it is used to define a grid of values along the colvar (not available for colvars based on `distanceDir`, `distanceVec`, and `orientation`). This option does not affect dynamics: to confine a colvar within a certain interval, the options `lowerWall` and `lowerWallConstant` should be used.

- `upperBoundary` ⟨ Upper boundary of the colvar ⟩
  Context: `colvar`
  Acceptable values: decimal
  Description: Similarly to `lowerBoundary`, defines the highest possible or allowed value.

- `hardLowerBoundary` ⟨Whether the lower boundary is the physical lower limit⟩
  Context: `colvar`
  Acceptable values: boolean
  Default value: `off`
  Description: This option does not affect simulation results, but enables some internal optimizations. Depending on its mathematical definition, a colvar may have "natural" boundaries: for example, a `distance` colvar has a "natural" lower boundary at 0. Setting this option instructs the Colvars module that the user-defined lower boundary is "natural". See Section 13.4 for the physical ranges of values of each component.

- `hardUpperBoundary` ⟨Whether the upper boundary is the physical upper limit of the colvar's values⟩
  Context: `colvar`
  Acceptable values: boolean
  Default value: `off`
  Description: Analogous to `hardLowerBoundary`.

- `expandBoundaries` ⟨Allow to expand the two boundaries if needed⟩
  Context: `colvar`
  Acceptable values: boolean
  Default value: `off`
  Description: If defined, biasing and analysis methods may keep their own copies of `lowerBoundary` and `upperBoundary`, and expand them to accommodate values that do not fit in the initial range. Currently, this option is used by the metadynamics bias (13.5.3) to keep all of its hills fully within the grid. This option cannot be used when the initial boundaries already span the full period of a periodic colvar.

- `subtractAppliedForce` ⟨Do not include biasing forces in the total force for this colvar⟩
  Context: `colvar`
  Acceptable values: boolean
  Default value: `off`
  Description: If the colvar supports total force calculation (see 13.4.3), all forces applied to this colvar by biases will be removed from the total force. This keyword allows to recover some of the "system force" calculation available in the Colvars module before version 2016-08-10. Please note that removal of *all* other external forces (including biasing forces applied to a different colvar) is *no longer supported*, due to changes in the underlying simulation engines (primarily NAMD). This option may be useful when continuing a previous simulation where the removal of external/applied forces is essential. *For all new simulations, the use of this option is not recommended.*

13.2.2 Artificial boundary potentials (walls)

The following options are useful to define restraints (confining potentials) for this colvar. To apply moving restraints, or restraints to more than one colvar simultaneously, a more convenient option is to use the `harmonic` bias (13.5.4).

- `lowerWallConstant` ⟨Lower wall force constant (kcal/mol/U^2)⟩
  Context: `colvar`

Acceptable values: positive decimal
Description: Defines the force constant for a confining restraint on the colvar, in the form of a "half-harmonic" potential. The potential starts at `lowerWall` if it is defined, or `lowerBoundary` otherwise. The energy unit of the constant is kcal/mol, while the spatial unit U is that of the colvar.

- `lowerWall` ⟨Position of the lower wall⟩
Context: `colvar`
Acceptable values: decimal
Default value: `lowerBoundary`
Description: Defines the value below which a confining restraint on the colvar is applied, in the form of a "half-harmonic" potential. Allows to use a different position of the wall than `lowerBoundary`.

- `upperWallConstant` ⟨Upper wall force constant (kcal/mol/U^2)⟩
Context: `colvar`
Acceptable values: positive decimal
Description: Analogous to `lowerWallConstant`.

- `upperWall` ⟨Position of the upper wall⟩
Context: `colvar`
Acceptable values: decimal
Default value: `upperBoundary`
Description: Analogous to `lowerWall`.

13.2.3 Trajectory output

- `outputValue` ⟨Output a trajectory for this colvar⟩
Context: `colvar`
Acceptable values: boolean
Default value: `on`
Description: If `colvarsTrajFrequency` is non-zero, the value of this colvar is written to the trajectory file every `colvarsTrajFrequency` steps in the column labeled "<name>".

- `outputVelocity` ⟨Output a velocity trajectory for this colvar⟩
Context: `colvar`
Acceptable values: boolean
Default value: `off`
Description: If `colvarsTrajFrequency` is defined, the finite-difference calculated velocity of this colvar are written to the trajectory file under the label "v_<name>".

- `outputEnergy` ⟨Output an energy trajectory for this colvar⟩
Context: `colvar`
Acceptable values: boolean
Default value: `off`
Description: This option applies only to extended Lagrangian colvars. If `colvarsTrajFrequency` is defined, the kinetic energy of the extended degree and freedom and the potential energy of the restraining spring are are written to the trajectory file under the labels "Ek_<name>" and "Ep_<name>".

- `outputTotalForce` ⟨ Output a total force trajectory for this colvar ⟩
  Context: `colvar`
  Acceptable values: boolean
  Default value: `off`
  Description: If `colvarsTrajFrequency` is defined, the total force on this colvar (i.e. the projection of all atomic total forces onto this colvar — see equation (13.19) in section 13.5.1) are written to the trajectory file under the label "`fs_<name>`". For extended Lagrangian colvars, the "total force" felt by the extended degree of freedom is simply the force from the harmonic spring. **Note:** not all components support this option. The physical unit for this force is kcal/mol, divided by the colvar unit U.

- `outputAppliedForce` ⟨ Output an applied force trajectory for this colvar ⟩
  Context: `colvar`
  Acceptable values: boolean
  Default value: `off`
  Description: If `colvarsTrajFrequency` is defined, the total force applied on this colvar by biases and confining potentials (walls) within the Colvars module are written to the trajectory under the label "`fa_<name>`". For extended Lagrangian colvars, this force is actually applied to the extended degree of freedom rather than the geometric colvar itself. The physical unit for this force is kcal/mol divided by the colvar unit.

13.2.4 Extended Lagrangian.

The following options enable extended-system dynamics, where a colvar is coupled to an additional degree of freedom (fictitious particle) by a harmonic spring. All biasing and confining forces are then applied to the extended degree of freedom. The "actual" geometric colvar (function of Cartesian coordinates) only feels the force from the harmonic spring. This is particularly useful when combined with an ABF bias (13.5.1) to perform eABF simulations (13.5.2).

- `extendedLagrangian` ⟨ Add extended degree of freedom ⟩
  Context: `colvar`
  Acceptable values: boolean
  Default value: `off`
  Description: Adds a fictitious particle to be coupled to the colvar by a harmonic spring. The fictitious mass and the force constant of the coupling potential are derived from the parameters `extendedTimeConstant` and `extendedFluctuation`, described below. Biasing forces on the colvar are applied to this fictitious particle, rather than to the atoms directly. This implements the extended Lagrangian formalism used in some metadynamics simulations [45].

- `extendedFluctuation` ⟨ Standard deviation between the colvar and the fictitious particle (colvar unit) ⟩
  Context: `colvar`
  Acceptable values: positive decimal
  Description: Defines the spring stiffness for the `extendedLagrangian` mode, by setting the typical deviation between the colvar and the extended degree of freedom due to thermal fluctuation. The spring force constant is calculated internally as $k_B T/\sigma^2$, where σ is the value of `extendedFluctuation`.

- `extendedTimeConstant` ⟨ Oscillation period of the fictitious particle (fs) ⟩
  Context: `colvar`
  Acceptable values: positive decimal
  Default value: `200`
  Description: Defines the inertial mass of the fictitious particle, by setting the oscillation period of the harmonic oscillator formed by the fictitious particle and the spring. The period should be much larger than the MD time step to ensure accurate integration of the extended particle's equation of motion. The fictitious mass is calculated internally as $k_B T(\tau/2\pi\sigma)^2$, where τ is the period and σ is the typical fluctuation (see above).

- `extendedTemp` ⟨ Temperature for the extended degree of freedom (K) ⟩
  Context: `colvar`
  Acceptable values: positive decimal
  Default value: thermostat temperature
  Description: Temperature used for calculating the coupling force constant of the extended variable (see `extendedFluctuation`) and, if needed, as a target temperature for extended Langevin dynamics (see `extendedLangevinDamping`). This should normally be left at its default value.

- `extendedLangevinDamping` ⟨ Damping factor for extended Langevin dynamics (ps^{-1}) ⟩
  Context: `colvar`
  Acceptable values: positive decimal
  Default value: `1.0`
  Description: If this is non-zero, the extended degree of freedom undergoes Langevin dynamics at temperature `extendedTemp`. The friction force is minus `extendedLangevinDamping` times the velocity. This is useful because the extended dynamics coordinate may heat up in the transient non-equilibrium regime of ABF. Use moderate damping values, to limit viscous friction (potentially slowing down diffusive sampling) and stochastic noise (increasing the variance of statistical measurements). In doubt, use the default value.

13.2.5 Statistical analysis of collective variables

When the global keyword `analysis` is defined in the configuration file, run-time calculations of statistical properties for individual colvars can be performed. At the moment, several types of time correlation functions, running averages and running standard deviations are available.

- `corrFunc` ⟨ Calculate a time correlation function? ⟩
  Context: `colvar`
  Acceptable values: boolean
  Default value: `off`
  Description: Whether or not a time correlaction function should be calculated for this colvar.

- `corrFuncWithColvar` ⟨ Colvar name for the correlation function ⟩
  Context: `colvar`
  Acceptable values: string
  Description: By default, the auto-correlation function (ACF) of this colvar, ξ_i, is calculated. When this option is specified, the correlation function is calculated instead with another colvar, ξ_j, which must be of the same type (scalar, vector, or quaternion) as ξ_i.

- `corrFuncType` ⟨ Type of the correlation function ⟩
  Context: `colvar`
  Acceptable values: `velocity`, `coordinate` or `coordinate_p2`
  Default value: `velocity`
  Description: With `coordinate` or `velocity`, the correlation function $C_{i,j}(t) = \langle \Pi\left(\xi_i(t_0), \xi_j(t_0+t)\right)\rangle$ is calculated between the variables ξ_i and ξ_j, or their velocities. $\Pi(\xi_i, \xi_j)$ is the scalar product when calculated between scalar or vector values, whereas for quaternions it is the cosine between the two corresponding rotation axes. With `coordinate_p2`, the second order Legendre polynomial, $(3\cos(\theta)^2 - 1)/2$, is used instead of the cosine.

- `corrFuncNormalize` ⟨ Normalize the time correlation function? ⟩
  Context: `colvar`
  Acceptable values: boolean
  Default value: `on`
  Description: If enabled, the value of the correlation function at $t = 0$ is normalized to 1; otherwise, it equals to $\langle O\left(\xi_i, \xi_j\right)\rangle$.

- `corrFuncLength` ⟨ Length of the time correlation function ⟩
  Context: `colvar`
  Acceptable values: positive integer
  Default value: `1000`
  Description: Length (in number of points) of the time correlation function.

- `corrFuncStride` ⟨ Stride of the time correlation function ⟩
  Context: `colvar`
  Acceptable values: positive integer
  Default value: `1`
  Description: Number of steps between two values of the time correlation function.

- `corrFuncOffset` ⟨ Offset of the time correlation function ⟩
  Context: `colvar`
  Acceptable values: positive integer
  Default value: `0`
  Description: The starting time (in number of steps) of the time correlation function (default: $t = 0$). **Note:** *the value at $t = 0$ is always used for the normalization.*

- `corrFuncOutputFile` ⟨ Output file for the time correlation function ⟩
  Context: `colvar`
  Acceptable values: UNIX filename
  Default value: `<name>.corrfunc.dat`
  Description: The time correlation function is saved in this file.

- `runAve` ⟨ Calculate the running average and standard deviation ⟩
  Context: `colvar`
  Acceptable values: boolean
  Default value: `off`
  Description: Whether or not the running average and standard deviation should be calculated for this colvar.

- `runAveLength` ⟨Length of the running average window⟩
  Context: `colvar`
  Acceptable values: positive integer
  Default value: `1000`
  Description: Length (in number of points) of the running average window.

- `runAveStride` ⟨Stride of the running average window values⟩
  Context: `colvar`
  Acceptable values: positive integer
  Default value: `1`
  Description: Number of steps between two values within the running average window.

- `runAveOutputFile` ⟨Output file for the running average and standard deviation⟩
  Context: `colvar`
  Acceptable values: UNIX filename
  Default value: `<name>.runave.dat`
  Description: The running average and standard deviation are saved in this file.

13.3 Selecting atoms for colvars: defining atom groups

13.3.1 Selection keywords

To define collective variables, atoms are usually selected by group. Each group is identified by a name that is unique in the context of the specific colvar component (e.g. for a distance component, the names of the two groups are `group1` and `group2`). The name is followed by a brace-delimited block of selection keywords: these may be used individually or in combination with each other, and each can be repeated any number of times. Selection is incremental: each keyword adds the corresponding atoms to the selection, so that different sets of atoms can be combined. However, atoms included by multiple keywords are only counted once. Below is an example configuration for an atom group named "`atoms`", which uses an unusually varied combination of selection keywords:

```
atoms {

  # add atoms 1 and 3 to this group (note:  the first atom in the system is 1)
  atomNumbers {
    1 3
  }

  # add atoms starting from 20 up to and including 50
  atomNumbersRange 20-50

  # add index group (requires a .ndx file to be provided globally)
  indexGroup Water

  # add all the atoms with occupancy 2 in the file atoms.pdb
  atomsFile atoms.pdb
  atomsCol O
```

```
  atomsColValue 2.0

  # add all the C-alphas within residues 11 to 20 of segments "PR1" and "PR2"
  psfSegID PR1 PR2
  atomNameResidueRange CA 11-20
  atomNameResidueRange CA 11-20
}
```

The resulting selection includes atoms 1 and 3, those between 20 and 50, and those in the index group called "Water"; the indices of this group are read from the file provided by `indexFile`, in the global section of the configuration file.

In the current version, the Colvars module does not manipulate VMD atom selections directly: however, these can be converted to atom groups within the colvars configuration string, using selection keywords such as `atomNumbers`. The complete list of selection keywords available in VMD is:

- `atomNumbers` ⟨ List of atom numbers ⟩
  Context: atom group
  Acceptable values: space-separated list of positive integers
  Description: This option adds to the group all the atoms whose numbers are in the list. *The number of the first atom in the system is 1: to convert from a VMD selection, use "atomselect get serial".*

- `indexGroup` ⟨ Name of index group to be used (GROMACS format) ⟩
  Context: atom group
  Acceptable values: string
  Description: If the name of an index file has been provided by `indexFile`, this option allows to select one index group from that file: the atoms from that index group will be used to define the current group.

- `atomNumbersRange` ⟨ Atoms within a number range ⟩
  Context: atom group
  Acceptable values: <Starting number>-<Ending number>
  Description: This option includes in the group all atoms whose numbers are within the range specified. *The number of the first atom in the system is 1.*

- `atomNameResidueRange` ⟨ Named atoms within a range of residue numbers ⟩
  Context: atom group
  Acceptable values: <Atom name> <Starting residue>-<Ending residue>
  Description: This option adds to the group all the atoms with the provided name, within residues in the given range.

- `psfSegID` ⟨ PSF segment identifier ⟩
  Context: atom group
  Acceptable values: space-separated list of strings (max 4 characters)
  Description: This option sets the PSF segment identifier for `atomNameResidueRange`. Multiple values may be provided, which correspond to multiple instances of `atomNameResidueRange`, in the order of their occurrence. This option is only necessary if a PSF topology file is used.

- `atomsFile` ⟨PDB file name for atom selection⟩
  Context: atom group
  Acceptable values: UNIX filename
  Description: This option selects atoms from the PDB file provided and adds them to the group according to numerical flags in the column `atomsCol`. **Note:** *the sequence of atoms in the PDB file provided must match that in the system's topology.*

- `atomsCol` ⟨PDB column to use for atom selection flags⟩
  Context: atom group
  Acceptable values: `O`, `B`, `X`, `Y`, or `Z`
  Description: This option specifies which PDB column in `atomsFile` is used to determine which atoms are to be included in the group.

- `atomsColValue` ⟨Atom selection flag in the PDB column⟩
  Context: atom group
  Acceptable values: positive decimal
  Description: If defined, this value in `atomsCol` identifies atoms in `atomsFile` that are included in the group. If undefined, all atoms with a non-zero value in `atomsCol` are included.

- `dummyAtom` ⟨Dummy atom position (Å)⟩
  Context: atom group
  Acceptable values: `(x, y, z)` triplet
  Description: Instead of selecting any atom, this option makes the group a virtual particle at a fixed position in space. This is useful e.g. to replace a group's center of geometry with a user-defined position.

13.3.2 Moving frame of reference.

The following options define an automatic calculation of an optimal translation (`centerReference`) or optimal rotation (`rotateReference`), that superimposes the positions of this group to a provided set of reference coordinates. This can allow, for example, to effectively remove from certain colvars the effects of molecular tumbling and of diffusion. Given the set of atomic positions $\mathbf{x}_i$, the colvar ξ can be defined on a set of roto-translated positions $\mathbf{x}'_i = R(\mathbf{x}_i - \mathbf{x}^{\mathrm{C}}) + \mathbf{x}^{\mathrm{ref}}$. $\mathbf{x}^{\mathrm{C}}$ is the geometric center of the $\mathbf{x}_i$, R is the optimal rotation matrix to the reference positions and $\mathbf{x}^{\mathrm{ref}}$ is the geometric center of the reference positions.

Components that are defined based on pairwise distances are naturally invariant under global roto-translations. Other components are instead affected by global rotations or translations: however, they can be made invariant if they are expressed in the frame of reference of a chosen group of atoms, using the `centerReference` and `rotateReference` options. Finally, a few components are defined by convention using a roto-translated frame (e.g. the minimal RMSD): for these components, `centerReference` and `rotateReference` are enabled by default. In typical applications, the default settings result in the expected behavior.

- `centerReference` ⟨Implicitly remove translations for this group⟩
  Context: atom group
  Acceptable values: boolean
  Default value: `off`
  Description: If this option is `on`, the center of geometry of the group will be aligned

with that of the reference positions provided by either `refPositions` or `refPositionsFile`. Colvar components will only have access to the aligned positions. **Note**: unless otherwise specified, `rmsd` and `eigenvector` set this option to `on` *by default*.

- `rotateReference` ⟨ Implicitly remove rotations for this group ⟩
  Context: atom group
  Acceptable values: boolean
  Default value: `off`
  Description: If this option is `on`, the coordinates of this group will be optimally superimposed to the reference positions provided by either `refPositions` or `refPositionsFile`. The rotation will be performed around the center of geometry if `centerReference` is `on`, around the origin otherwise. The algorithm used is the same employed by the `orientation` colvar component [46]. Forces applied to the atoms of this group will also be implicitly rotated back to the original frame. **Note**: unless otherwise specified, `rmsd` and `eigenvector` set this option to `on` *by default*.

- `refPositions` ⟨ Reference positions for fitting (Å) ⟩
  Context: atom group
  Acceptable values: space-separated list of `(x, y, z)` triplets
  Description: This option provides a list of reference coordinates for `centerReference` or `rotateReference`. If only `centerReference` is `on`, the list may contain a single (x, y, z) triplet; if also `rotateReference` is `on`, the list should be as long as the atom group.

- `refPositionsFile` ⟨ File containing the reference positions for fitting ⟩
  Context: atom group
  Acceptable values: UNIX filename
  Description: This keyword provides the reference coordinates for fitting from the given file, and is mutually exclusive with `refPositions`. The acceptable file format is XYZor PDB. Atomic positions are read differently depending on the three following scenarios: *i)* the file contains exactly as many records as the atoms in the group: all positions are read in sequence; *ii)* the file contains coordinates for the entire system: only the positions corresponding to the numeric indices of the atom group are read; *iii)* if the file is a PDB file and `refPositionsCol` is specified, positions are read according to the value of the column `refPositionsCol` (which may be the same as `atomsCol`).

- `refPositionsCol` ⟨ PDB column containing atom flags ⟩
  Context: atom group
  Acceptable values: `O`, `B`, `X`, `Y`, or `Z`
  Description: Like `atomsCol` for `atomsFile`, indicates which column to use to identify the atoms in `refPositionsFile` (if this is a PDB file).

- `refPositionsColValue` ⟨ Atom selection flag in the PDB column ⟩
  Context: atom group
  Acceptable values: positive decimal
  Description: Analogous to `atomsColValue`, but applied to `refPositionsCol`.

- `fittingGroup` ⟨ Use an alternate set of atoms to define the roto-translation ⟩
  Context: atom group
  Acceptable values: Block `fittingGroup { ... }`

Default value: This group itself
Description: If either `centerReference` or `rotateReference` is defined, this keyword defines an alternate atom group to calculate the optimal roto-translation. Use this option to define a continuous rotation if the structure of the group involved changes significantly (a typical symptom would be the message "Warning: discontinuous rotation!").

The following example illustrates the syntax of `fittingGroup`: a group called "`atoms`" is defined, including 8 C_α atoms of a protein of 100 residues. An optimal roto-translation is calculated automatically by fitting the C_α trace of the rest of the protein onto the coordinates provided by a PDB file.

```
# Example:  defining a group "atoms", with its coordinates expressed
# on a roto-translated frame of reference defined by a second group
atoms {

  psfSegID PROT
  atomNameResidueRange CA 41-48

  centerReference yes
  rotateReference yes
  fittingGroup {
    # define the frame by fitting the rest of the protein
    psfSegID PROT PROT
    atomNameResidueRange CA 1-40
    atomNameResidueRange CA 49-100
  }
  refPositionsFile all.pdb # can be the entire system
}
```

The following two options have default values appropriate for the vast majority of applications, and are only provided to support rare, special cases.

- `enableFitGradients` ⟨Include the roto-translational contribution to colvar gradients⟩
  Context: atom group
  Acceptable values: boolean
  Default value: `on`
  Description: When either `centerReference` or `rotateReference` is on, the gradients of some colvars include terms proportional to $\partial R/\partial \mathbf{x}_i$ (rotational gradients) and $\partial \mathbf{x}^{\mathrm{C}}/\partial \mathbf{x}_i$ (translational gradients). By default, these terms are calculated and included in the total gradients; if this option is set to `off`, they are neglected. In the case of a minimum RMSD component, this flag is automatically disabled because the contributions of those derivatives to the gradients cancel out.

- `enableForces` ⟨Apply forces from this colvar to this group⟩
  Context: atom group
  Acceptable values: boolean
  Default value: `on`
  Description: If this option is `off`, no forces are applied from this colvar to this group.

Other forces are not affected (i.e. those from the MD engine, from other colvars, and other external forces). For dummy atoms, this option is `off` by default.

13.3.3 Treatment of periodic boundary conditions.

When periodic boundary conditions are defined, the Colvars module requires that the coordinates of each molecular fragment are contiguous, without "jumps" when a fragment is partially wrapped near a periodic boundary. The Colvars module relies on this assumption when calculating a group's center of geometry, but the condition may fail if the group spans different molecules. In general, coordinate wrapping does not affect the calculation of colvars if each atom group satisfies one or more of the following:

i) it is composed by only one atom;

ii) it is used by a colvar component which does not make use of its center of geometry, but only of pairwise distances (`distanceInv`, `coordNum`, `hBond`, `alpha`, `dihedralPC`);

iii) it is used by a colvar component that ignores the ill-defined Cartesian components of its center of mass (such as the x and y components of a membrane's center of mass modeled with `distanceZ`).

If none of these conditions are met, wrapping may affect the calculation of collective variables: a possible solution is to use `pbc wrap` or `pbc unwrap` prior to processing a trajectory with the Colvars module.

13.3.4 Performance a Colvars calculation based on group size.

In simulations performed with message-passing programs (such as NAMD or LAMMPS), the calculation of energy and forces is distributed (i.e., parallelized) across multiple nodes, as well as over the processor cores of each node. Atomic coordinates are typically collected on one node, where the calculation of collective variables and of their biases is executed. This means that for simulations over large numbers of nodes, a Colvars calculation may produce a significant overhead, coming from the costs of transmitting atomic coordinates to one node and of processing them.

Performance can be improved in multiple ways:

- The calculation of variables, components and biases can be distributed over the processor cores of the node where the Colvars module is executed. Currently, an equal weight is assigned to each colvar, or to each component of those colvars that include more than one component. The performance of simulations that use many colvars or components is improved automatically. For simulations that use a single large colvar, it may be advisable to partition it in multiple components, which will be then distributed across the available cores. If printed, the message "SMP parallelism is available." indicates the availability of the option (will be supported in a future relase of VMD).

- As a general rule, the size of atom groups should be kept relatively small (up to a few thousands of atoms, depending on the size of the entire system in comparison). To gain an estimate of the computational cost of a large colvar, one can use a test calculation of the same colvar in VMD (hint: use the `time` Tcl command to measure the cost of running `cv update`).

13.4 Collective variable components (basis functions)

Each colvar is defined by one or more *components* (typically only one). Each component consists of a keyword identifying a functional form, and a definition block following that keyword, specifying the atoms involved and any additional parameters (cutoffs, "reference" values, ...).

The types of the components used in a colvar determine the properties of that colvar, and which biasing or analysis methods can be applied. In most cases, the colvar returns a real number, which is computed by one or more instances of the following components:

- `distance`: distance between two groups;
- `distanceZ`: projection of a distance vector on an axis;
- `distanceXY`: projection of a distance vector on a plane;
- `distanceInv`: mean distance between two groups of atoms (e.g. NOE-based distance);
- `angle`: angle between three groups;
- `dipoleAngle`: angle between two groups and dipole of a third group;
- `coordNum`: coordination number between two groups;
- `selfCoordNum`: coordination number of atoms within a group;
- `hBond`: hydrogen bond between two atoms;
- `rmsd`: root mean square deviation (RMSD) from a set of reference coordinates;
- `eigenvector`: projection of the atomic coordinates on a vector;
- `orientationAngle`: angle of the best-fit rotation from a set of reference coordinates;
- `orientationProj`: cosine of `orientationProj`;
- `spinAngle`: projection orthogonal to an axis of the best-fit rotation from a set of reference coordinates;
- `tilt`: projection on an axis of the best-fit rotation from a set of reference coordinates;
- `gyration`: radius of gyration of a group of atoms;
- `inertia`: moment of inertia of a group of atoms;
- `inertiaZ`: moment of inertia of a group of atoms around a chosen axis;
- `alpha`: α-helix content of a protein segment.
- `dihedralPC`: projection of protein backbone dihedrals onto a dihedral principal component.

Some components do not return scalar, but vector values. They can only be combined with vector values of the same type, except within a scripted collective variable.

- `distanceVec`: distance vector between two groups;

- `distanceDir`: unit vector parallel to distanceVec;
- `cartesian`: vector of atomic Cartesian coordinates;
- `orientation`: best-fit rotation, expressed as a unit quaternion.

In the following, all the available component types are listed, along with their physical units and the limiting values, if any. Such limiting values can be used to define `lowerBoundary` and `upperBoundary` in the parent colvar.

For each type of component, the available configurations keywords are listed: when two components share certain keywords, the second component simply references to the documentation of the first regarding that keyword. The keywords that are available for all types of components are listed at the end (see

13.4.1 List of available colvar components

`distance`: center-of-mass distance between two groups.

The `distance` {...} block defines a distance component between the two atom groups, `group1` and `group2`.

List of keywords (see also 13.4.4 for additional options):

- `group1` ⟨First group of atoms⟩
  Context: `distance`
  Acceptable values: Block `group1` {...}
  Description: First group of atoms.
- `group2`: analogous to `group1`
- `forceNoPBC` ⟨Calculate absolute rather than minimum-image distance?⟩
  Context: `distance`
  Acceptable values: boolean
  Default value: `no`
  Description: By default, in calculations with periodic boundary conditions, the `distance` component returns the distance according to the minimum-image convention. If this parameter is set to `yes`, PBC will be ignored and the distance between the coordinates as maintained internally will be used. This is only useful in a limited number of special cases, e.g. to describe the distance between remote points of a single macromolecule, which cannot be split across periodic cell boundaries, and for which the minimum-image distance might give the wrong result because of a relatively small periodic cell.
- `oneSiteTotalForce` ⟨Measure total force on group 1 only?⟩
  Context: `angle`, `dipoleAngle`, `dihedral`
  Acceptable values: boolean
  Default value: `no`
  Description: If this is set to `yes`, the total force is measured along a vector field (see equation (13.19) in section 13.5.1) that only involves atoms of `group1`. This option is only useful for ABF, or custom biases that compute total forces. See section 13.5.1 for details.

The value returned is a positive number (in Å), ranging from 0 to the largest possible interatomic distance within the chosen boundary conditions (with PBCs, the minimum image convention is used unless the `forceNoPBC` option is set).

`distanceZ`: projection of a distance vector on an axis.

The `distanceZ {...}` block defines a distance projection component, which can be seen as measuring the distance between two groups projected onto an axis, or the position of a group along such an axis. The axis can be defined using either one reference group and a constant vector, or dynamically based on two reference groups.
List of keywords (see also 13.4.4 for additional options):

- `main` ⟨ Main group of atoms ⟩
  Context: `distanceZ`
  Acceptable values: Block `main {...}`
  Description: Group of atoms whose position $\boldsymbol{r}$ is measured.

- `ref` ⟨ Reference group of atoms ⟩
  Context: `distanceZ`
  Acceptable values: Block `ref {...}`
  Description: Reference group of atoms. The position of its center of mass is noted $\boldsymbol{r}_1$ below.

- `ref2` ⟨ Secondary reference group ⟩
  Context: `distanceZ`
  Acceptable values: Block `ref2 {...}`
  Default value: none
  Description: Optional group of reference atoms, whose position $\boldsymbol{r}_2$ can be used to define a dynamic projection axis: $\boldsymbol{e} = (\|\boldsymbol{r}_2 - \boldsymbol{r}_1\|)^{-1} \times (\boldsymbol{r}_2 - \boldsymbol{r}_1)$. In this case, the origin is $\boldsymbol{r}_m = 1/2(\boldsymbol{r}_1 + \boldsymbol{r}_2)$, and the value of the component is $\boldsymbol{e} \cdot (\boldsymbol{r} - \boldsymbol{r}_m)$.

- `axis` ⟨ Projection axis (Å) ⟩
  Context: `distanceZ`
  Acceptable values: `(x, y, z)` triplet
  Default value: `(0.0, 0.0, 1.0)`
  Description: The three components of this vector define a projection axis $\boldsymbol{e}$ for the distance vector $\boldsymbol{r} - \boldsymbol{r}_1$ joining the centers of groups `ref` and `main`. The value of the component is then $\boldsymbol{e} \cdot (\boldsymbol{r} - \boldsymbol{r}_1)$. The vector should be written as three components separated by commas and enclosed in parentheses.

- `forceNoPBC`: see definition of `forceNoPBC` (`distance` component)

- `oneSiteTotalForce`: see definition of `oneSiteTotalForce` (`distance` component)

This component returns a number (in Å) whose range is determined by the chosen boundary conditions. For instance, if the z axis is used in a simulation with periodic boundaries, the returned value ranges between $-b_z/2$ and $b_z/2$, where b_z is the box length along z (this behavior is disabled if `forceNoPBC` is set).

`distanceXY`: modulus of the projection of a distance vector on a plane.

The `distanceXY {...}` block defines a distance projected on a plane, and accepts the same keywords as the component `distanceZ`, i.e. `main`, `ref`, either `ref2` or `axis`, and `oneSiteTotalForce`. It returns the norm of the projection of the distance vector between `main` and `ref` onto the plane

orthogonal to the axis. The axis is defined using the `axis` parameter or as the vector joining `ref` and `ref2` (see `distanceZ` above).
List of keywords (see also 13.4.4 for additional options):

- `main`: see definition of `main` (`distanceZ` component)
- `ref`: see definition of `ref` (`distanceZ` component)
- `ref2`: see definition of `ref2` (`distanceZ` component)
- `axis`: see definition of `axis` (`distanceZ` component)
- `forceNoPBC`: see definition of `forceNoPBC` (`distance` component)
- `oneSiteTotalForce`: see definition of `oneSiteTotalForce` (`distance` component)

`distanceVec`: distance vector between two groups.

The `distanceVec {...}` block defines a distance vector component, which accepts the same keywords as the component `distance`: `group1`, `group2`, and `forceNoPBC`. Its value is the 3-vector joining the centers of mass of `group1` and `group2`.
List of keywords (see also 13.4.4 for additional options):

- `group1`: see definition of `group1` (`distance` component)
- `group2`: analogous to `group1`
- `oneSiteTotalForce`: see definition of `oneSiteTotalForce` (`distance` component)

`distanceDir`: distance unit vector between two groups.

The `distanceDir {...}` block defines a distance unit vector component, which accepts the same keywords as the component `distance`: `group1`, `group2`, and `forceNoPBC`. It returns a 3-dimensional unit vector $\mathbf{d} = (d_x, d_y, d_z)$, with $|\mathbf{d}| = 1$.
List of keywords (see also 13.4.4 for additional options):

- `group1`: see definition of `group1` (`distance` component)
- `group2`: analogous to `group1`
- `oneSiteTotalForce`: see definition of `oneSiteTotalForce` (`distance` component)

`distanceInv`: mean distance between two groups of atoms.

The `distanceInv {...}` block defines a generalized mean distance between two groups of atoms 1 and 2, weighted with exponent $1/n$:

$$d_{1,2}^{[n]} \;=\; \left(\frac{1}{N_1 N_2} \sum_{i,j} \left(\frac{1}{\|\mathbf{d}^{ij}\|} \right)^n \right)^{-1/n} \tag{13.2}$$

where $\|\mathbf{d}^{ij}\|$ is the distance between atoms i and j in groups 1 and 2 respectively, and n is an even integer.
List of keywords (see also 13.4.4 for additional options):

- `group1`: see definition of `group1` (`distance` component)
- `group2`: analogous to `group1`
- `oneSiteTotalForce`: see definition of `oneSiteTotalForce` (`distance` component)
- `exponent` ⟨Exponent n in equation 13.2⟩
  Context: `distanceInv`
  Acceptable values: positive even integer
  Default value: 6
  Description: Defines the exponent to which the individual distances are elevated before averaging. The default value of 6 is useful for example to applying restraints based on NOE-measured distances.

This component returns a number in Å, ranging from 0 to the largest possible distance within the chosen boundary conditions.

`distancePairs`: set of pairwise distances between two groups.

The `distancePairs {...}` block defines a $N_1 \times N_2$-dimensional variable that includes all mutual distances between the atoms of two groups. This can be useful, for example, to develop a new variable defined over two groups, by using the `scriptedFunction` feature.
List of keywords (see also 13.4.4 for additional options):

- `group1`: see definition of `group1` (`distance` component)
- `group2`: analogous to `group1`
- `forceNoPBC`: see definition of `forceNoPBC` (`distance` component)

This component returns a $N_1 \times N_2$-dimensional vector of numbers, each ranging from 0 to the largest possible distance within the chosen boundary conditions.

`cartesian`: vector of atomic Cartesian coordinates.

The `cartesian {...}` block defines a component returning a flat vector containing the Cartesian coordinates of all participating atoms, in the order $(x_1, y_1, z_1, \cdots, x_n, y_n, z_n)$.
List of keywords (see also 13.4.4 for additional options):

- `atoms` ⟨Group of atoms⟩
  Context: `cartesian`
  Acceptable values: Block `atoms {...}`
  Description: Defines the atoms whose coordinates make up the value of the component. If `rotateReference` or `centerReference` are defined, coordinates are evaluated within the moving frame of reference.

`angle`: angle between three groups.

The `angle {...}` block defines an angle, and contains the three blocks `group1`, `group2` and `group3`, defining the three groups. It returns an angle (in degrees) within the interval $[0 : 180]$.
List of keywords (see also 13.4.4 for additional options):

- `group1`: see definition of `group1` (`distance` component)
- `group2`: analogous to `group1`
- `group3`: analogous to `group1`
- `oneSiteTotalForce`: see definition of `oneSiteTotalForce` (`distance` component)

`dipoleAngle`: angle between two groups and dipole of a third group.

The `dipoleAngle {...}` block defines an angle, and contains the three blocks `group1`, `group2` and `group3`, defining the three groups, being `group1` the group where dipole is calculated. It returns an angle (in degrees) within the interval $[0 : 180]$.
List of keywords (see also 13.4.4 for additional options):

- `group1`: see definition of `group1` (`distance` component)
- `group2`: analogous to `group1`
- `group3`: analogous to `group1`
- `oneSiteTotalForce`: see definition of `oneSiteTotalForce` (`distance` component)

`dihedral`: torsional angle between four groups.

The `dihedral {...}` block defines a torsional angle, and contains the blocks `group1`, `group2`, `group3` and `group4`, defining the four groups. It returns an angle (in degrees) within the interval $[-180 : 180]$. The Colvars module calculates all the distances between two angles taking into account periodicity. For instance, reference values for restraints or range boundaries can be defined by using any real number of choice.
List of keywords (see also 13.4.4 for additional options):

- `group1`: see definition of `group1` (`distance` component)
- `group2`: analogous to `group1`
- `group3`: analogous to `group1`
- `group4`: analogous to `group1`
- `oneSiteTotalForce`: see definition of `oneSiteTotalForce` (`distance` component)

`coordNum`: coordination number between two groups.

The `coordNum {...}` block defines a coordination number (or number of contacts), which calculates the function $(1 - (d/d_0)^n)/(1 - (d/d_0)^m)$, where d_0 is the "cutoff" distance, and n and m are exponents that can control its long range behavior and stiffness [45]. This function is summed over all pairs of atoms in `group1` and `group2`:

$$C(\texttt{group1}, \texttt{group2}) \;=\; \sum_{i \in \texttt{group1}} \sum_{j \in \texttt{group2}} \frac{1 - (|\mathbf{x}_i - \mathbf{x}_j|/d_0)^n}{1 - (|\mathbf{x}_i - \mathbf{x}_j|/d_0)^m} \tag{13.3}$$

List of keywords (see also 13.4.4 for additional options):

- `group1`: see definition of `group1` (`distance` component)
- `group2`: analogous to `group1`
- `cutoff` ⟨ "Interaction" distance (Å) ⟩
  Context: `coordNum`
  Acceptable values: positive decimal
  Default value: 4.0
  Description: This number defines the switching distance to define an interatomic contact: for $d \ll d_0$, the switching function $(1-(d/d_0)^n)/(1-(d/d_0)^m)$ is close to 1, at $d = d_0$ it has a value of n/m (1/2 with the default n and m), and at $d \gg d_0$ it goes to zero approximately like d^{m-n}. Hence, for a proper behavior, m must be larger than n.
- `cutoff3` ⟨ Reference distance vector (Å) ⟩
  Context: `coordNum`
  Acceptable values: "`(x, y, z)`" triplet of positive decimals
  Default value: `(4.0, 4.0, 4.0)`
  Description: The three components of this vector define three different cutoffs d_0 for each direction. This option is mutually exclusive with `cutoff`.
- `expNumer` ⟨ Numerator exponent ⟩
  Context: `coordNum`
  Acceptable values: positive even integer
  Default value: 6
  Description: This number defines the n exponent for the switching function.
- `expDenom` ⟨ Denominator exponent ⟩
  Context: `coordNum`
  Acceptable values: positive even integer
  Default value: 12
  Description: This number defines the m exponent for the switching function.
- `group2CenterOnly` ⟨ Use only `group2`'s center of mass ⟩
  Context: `coordNum`
  Acceptable values: boolean
  Default value: `off`
  Description: If this option is `on`, only contacts between each atoms in `group1` and the center of mass of `group2` are calculated (by default, the sum extends over all pairs of atoms in `group1` and `group2`). If `group2` is a `dummyAtom`, this option is set to `yes` by default.

This component returns a dimensionless number, which ranges from approximately 0 (all interatomic distances are much larger than the cutoff) to $N_{\texttt{group1}} \times N_{\texttt{group2}}$ (all distances are less than the cutoff), or $N_{\texttt{group1}}$ if `group2CenterOnly` is used. For performance reasons, at least one of `group1` and `group2` should be of limited size or `group2CenterOnly` should be used: the cost of the loop over all pairs grows as $N_{\texttt{group1}} \times N_{\texttt{group2}}$.

`selfCoordNum`: coordination number between atoms within a group.

The `selfCoordNum` {...} block defines a coordination number similarly to the component `coordNum`, but the function is summed over atom pairs within `group1`:

$$C(\texttt{group1}) = \sum_{i \in \texttt{group1}} \sum_{j>i} \frac{1-(|\mathbf{x}_i - \mathbf{x}_j|/d_0)^n}{1-(|\mathbf{x}_i - \mathbf{x}_j|/d_0)^m} \tag{13.4}$$

The keywords accepted by `selfCoordNum` are a subset of those accepted by `coordNum`, namely `group1` (here defining *all* of the atoms to be considered), `cutoff`, `expNumer`, and `expDenom`.
List of keywords (see also 13.4.4 for additional options):

- `group1`: see definition of `group1` (`coordNum` component)
- `group2`: analogous to `group1`
- `cutoff`: see definition of `cutoff` (`coordNum` component)
- `cutoff3`: see definition of `cutoff3` (`coordNum` component)
- `expNumer`: see definition of `expNumer` (`coordNum` component)
- `expDenom`: see definition of `expDenom` (`coordNum` component)

This component returns a dimensionless number, which ranges from approximately 0 (all interatomic distances much larger than the cutoff) to $N_{\texttt{group1}} \times (N_{\texttt{group1}} - 1)/2$ (all distances within the cutoff). For performance reasons, `group1` should be of limited size, because the cost of the loop over all pairs grows as $N^2_{\texttt{group1}}$.

`hBond`: hydrogen bond between two atoms.

The `hBond` {...} block defines a hydrogen bond, implemented as a coordination number (eq. 13.3) between the donor and the acceptor atoms. Therefore, it accepts the same options `cutoff` (with a different default value of 3.3 Å), `expNumer` (with a default value of 6) and `expDenom` (with a default value of 8). Unlike `coordNum`, it requires two atom numbers, `acceptor` and `donor`, to be defined. It returns an adimensional number, with values between 0 (acceptor and donor far outside the cutoff distance) and 1 (acceptor and donor much closer than the cutoff).
List of keywords (see also 13.4.4 for additional options):

- `acceptor` ⟨Number of the acceptor atom⟩
  Context: `hBond`
  Acceptable values: positive integer
  Description: Number that uses the same convention as `atomNumbers`.
- `donor`: analogous to `acceptor`
- `cutoff`: see definition of `cutoff` (`coordNum` component)
  Note: default value is 3.3 Å.
- `expNumer`: see definition of `expNumer` (`coordNum` component)
  Note: default value is 6.
- `expDenom`: see definition of `expDenom` (`coordNum` component)
  Note: default value is 8.

`rmsd`: root mean square displacement (RMSD) from reference positions.

The block `rmsd {...}` defines the root mean square replacement (RMSD) of a group of atoms with respect to a reference structure. For each set of coordinates $\{\mathbf{x}_1(t), \mathbf{x}_2(t), \ldots \mathbf{x}_N(t)\}$, the colvar component `rmsd` calculates the optimal rotation $U^{\{\mathbf{x}_i(t)\}\rightarrow\{\mathbf{x}_i^{(\mathrm{ref})}\}}$ that best superimposes the coordinates $\{\mathbf{x}_i(t)\}$ onto a set of reference coordinates $\{\mathbf{x}_i^{(\mathrm{ref})}\}$. Both the current and the reference coordinates are centered on their centers of geometry, $\mathbf{x}_{\mathrm{cog}}(t)$ and $\mathbf{x}_{\mathrm{cog}}^{(\mathrm{ref})}$. The root mean square displacement is then defined as:

$$\mathrm{RMSD}(\{\mathbf{x}_i(t)\}, \{\mathbf{x}_i^{(\mathrm{ref})}\}) \;=\; \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left|U\left(\mathbf{x}_i(t) - \mathbf{x}_{\mathrm{cog}}(t)\right) - \left(\mathbf{x}_i^{(\mathrm{ref})} - \mathbf{x}_{\mathrm{cog}}^{(\mathrm{ref})}\right)\right|^2} \tag{13.5}$$

The optimal rotation $U^{\{\mathbf{x}_i(t)\}\rightarrow\{\mathbf{x}_i^{(\mathrm{ref})}\}}$ is calculated within the formalism developed in reference [46], which guarantees a continuous dependence of $U^{\{\mathbf{x}_i(t)\}\rightarrow\{\mathbf{x}_i^{(\mathrm{ref})}\}}$ with respect to $\{\mathbf{x}_i(t)\}$.
List of keywords (see also 13.4.4 for additional options):

- `atoms` ⟨ Atom group ⟩
  Context: `rmsd`
  Acceptable values: `atoms {...}` block
  Description: Defines the group of atoms of which the RMSD should be calculated. Optimal fit options (such as `refPositions` and `rotateReference`) should typically NOT be set within this block. Exceptions to this rule are the special cases discussed in the *Advanced usage* paragraph below.

- `refPositions` ⟨ Reference coordinates ⟩
  Context: `rmsd`
  Acceptable values: space-separated list of `(x, y, z)` triplets
  Description: This option (mutually exclusive with `refPositionsFile`) sets the reference coordinates. If only `centerReference` is `on`, the list can be a single (x, y, z) triplet; if also `rotateReference` is `on`, the list should be as long as the atom group. This option is independent from that with the same keyword within the `atoms {...}` block (see 13.3.2). The latter (and related fitting options for the atom group) are normally not needed, and should be omitted altogether except for advanced usage cases.

- `refPositionsFile` ⟨ Reference coordinates file ⟩
  Context: `rmsd`
  Acceptable values: UNIX filename
  Description: This option (mutually exclusive with `refPositions`) sets the file name for the reference coordinates to be compared with. The format is the same as that provided by `refPositionsFile` within an atom group's definition (see 13.3.2).

- `refPositionsCol` ⟨ PDB column containing atom flags ⟩
  Context: `rmsd`
  Acceptable values: `O`, `B`, `X`, `Y`, or `Z`
  Description: If `refPositionsFile` is a PDB file that contains all the atoms in the topology, this option may be provided to set which PDB field is used to flag the reference coordinates for `atoms`.

- `refPositionsColValue` ⟨ Atom selection flag in the PDB column ⟩
  Context: `rmsd`
  Acceptable values: positive decimal
  Description: If defined, this value identifies in the PDB column `refPositionsCol` of the file `refPositionsFile` which atom positions are to be read. Otherwise, all positions with a non-zero value are read.

This component returns a positive real number (in Å).

Advanced usage of the `rmsd` component.

In the standard usage as described above, the `rmsd` component calculates a minimum RMSD, that is, current coordinates are optimally fitted onto the same reference coordinates that are used to compute the RMSD value. The fit itself is handled by the atom group object, whose parameters are automatically set by the `rmsd` component. For very specific applications, however, it may be useful to control the fitting process separately from the definition of the reference coordinates, to evaluate various types of non-minimal RMSD values. This can be achieved by setting the related options (`refPositions`, etc.) explicitly in the atom group block. This allows for the following non-standard cases:

1. applying the optimal translation, but no rotation (`rotateReference off`), to bias or restrain the shape and orientation, but not the position of the atom group;
2. applying the optimal rotation, but no translation (`translateReference off`), to bias or restrain the shape and position, but not the orientation of the atom group;
3. disabling the application of optimal roto-translations, which lets the RMSD component describe the deviation of atoms from fixed positions in the laboratory frame: this allows for custom positional restraints within the Colvars module;
4. fitting the atomic positions to different reference coordinates than those used in the RMSD calculation itself;
5. applying the optimal rotation and/or translation from a separate atom group, defined through `fittingGroup`: the RMSD then reflects the deviation from reference coordinates in a separate, moving reference frame.

`eigenvector`: projection of the atomic coordinates on a vector.

The block `eigenvector {...}` defines the projection of the coordinates of a group of atoms (or more precisely, their deviations from the reference coordinates) onto a vector in $\mathbb{R}^{3n}$, where n is the number of atoms in the group. The computed quantity is the total projection:

$$p(\{\mathbf{x}_i(t)\},\{\mathbf{x}_i^{(\mathrm{ref})}\}) \;=\; \sum_{i=1}^{n} \mathbf{v}_i \cdot \left(U(\mathbf{x}_i(t) - \mathbf{x}_{\mathrm{cog}}(t)) - (\mathbf{x}_i^{(\mathrm{ref})} - \mathbf{x}_{\mathrm{cog}}^{(\mathrm{ref})}) \right), \tag{13.6}$$

where, as in the `rmsd` component, U is the optimal rotation matrix, $\mathbf{x}_{\mathrm{cog}}(t)$ and $\mathbf{x}_{\mathrm{cog}}^{(\mathrm{ref})}$ are the centers of geometry of the current and reference positions respectively, and $\mathbf{v}_i$ are the components of the vector for each atom. Example choices for $(\mathbf{v}_i)$ are an eigenvector of the covariance matrix

(essential mode), or a normal mode of the system. It is assumed that $\sum_i \mathbf{v}_i = 0$: otherwise, the Colvars module centers the $\mathbf{v}_i$ automatically when reading them from the configuration.
List of keywords (see also 13.4.4 for additional options):

- `atoms`: see definition of `atoms` (`rmsd` component)
- `refPositions`: see definition of `refPositions` (`rmsd` component)
- `refPositionsFile`: see definition of `refPositionsFile` (`rmsd` component)
- `refPositionsCol`: see definition of `refPositionsCol` (`rmsd` component)
- `refPositionsColValue`: see definition of `refPositionsColValue` (`rmsd` component)
- `vector` ⟨ Vector components ⟩
  Context: `eigenvector`
  Acceptable values: space-separated list of `(x, y, z)` triplets
  Description: This option (mutually exclusive with `vectorFile`) sets the values of the vector components.
- `vectorFile` ⟨ PDB file containing vector components ⟩
  Context: `eigenvector`
  Acceptable values: UNIX filename
  Description: This option (mutually exclusive with `vector`) sets the name of a PDB file where the vector components will be read from the X, Y, and Z fields. **Note:** *The PDB file has limited precision and fixed point numbers: in some cases, the vector may not be accurately represented, and* `vector` *should be used instead.*
- `vectorCol` ⟨ PDB column used to flag participating atoms ⟩
  Context: `eigenvector`
  Acceptable values: `O` or `B`
  Description: Analogous to `atomsCol`.
- `vectorColValue` ⟨ Value used to flag participating atoms in the PDB file ⟩
  Context: `eigenvector`
  Acceptable values: positive decimal
  Description: Analogous to `atomsColValue`.
- `differenceVector` ⟨ The $3n$-dimensional vector is the difference between `vector` and `refPositions` ⟩
  Context: `eigenvector`
  Acceptable values: boolean
  Default value: `off`
  Description: If this option is `on`, the numbers provided by `vector` or `vectorFile` are interpreted as another set of positions, $\mathbf{x}'_i$: the vector $\mathbf{v}_i$ is then defined as $\mathbf{v}_i = \left(\mathbf{x}'_i - \mathbf{x}_i^{(\mathrm{ref})}\right)$. This allows to conveniently define a colvar ξ as a projection on the linear transformation between two sets of positions, "A" and "B". For convenience, the vector is also normalized so that $\xi = 0$ when the atoms are at the set of positions "A" and $\xi = 1$ at the set of positions "B".

This component returns a number (in Å), whose value ranges between the smallest and largest absolute positions in the unit cell during the simulations (see also `distanceZ`). Due to the normalization in eq. 13.6, this range does not depend on the number of atoms involved.

`gyration`: radius of gyration of a group of atoms.

The block `gyration {...}` defines the parameters for calculating the radius of gyration of a group of atomic positions $\{\mathbf{x}_1(t), \mathbf{x}_2(t), \dots \mathbf{x}_N(t)\}$ with respect to their center of geometry, $\mathbf{x}_{\mathrm{cog}}(t)$:

$$R_{\mathrm{gyr}} \;=\; \sqrt{\frac{1}{N}\sum_{i=1}^{N} |\mathbf{x}_i(t) - \mathbf{x}_{\mathrm{cog}}(t)|^2} \tag{13.7}$$

This component must contain one `atoms {...}` block to define the atom group, and returns a positive number, expressed in Å.
List of keywords (see also 13.4.4 for additional options):

- `atoms`: see definition of `atoms` (`rmsd` component)

`inertia`: total moment of inertia of a group of atoms.

The block `inertia {...}` defines the parameters for calculating the total moment of inertia of a group of atomic positions $\{\mathbf{x}_1(t), \mathbf{x}_2(t), \dots \mathbf{x}_N(t)\}$ with respect to their center of geometry, $\mathbf{x}_{\mathrm{cog}}(t)$:

$$I \;=\; \sum_{i=1}^{N} |\mathbf{x}_i(t) - \mathbf{x}_{\mathrm{cog}}(t)|^2 \tag{13.8}$$

Note that all atomic masses are set to 1 for simplicity. This component must contain one `atoms {...}` block to define the atom group, and returns a positive number, expressed in Å^2.
List of keywords (see also 13.4.4 for additional options):

- `atoms`: see definition of `atoms` (`rmsd` component)

`inertiaZ`: total moment of inertia of a group of atoms around a chosen axis.

The block `inertiaZ {...}` defines the parameters for calculating the component along the axis $\mathbf{e}$ of the moment of inertia of a group of atomic positions $\{\mathbf{x}_1(t), \mathbf{x}_2(t), \dots \mathbf{x}_N(t)\}$ with respect to their center of geometry, $\mathbf{x}_{\mathrm{cog}}(t)$:

$$I_{\mathbf{e}} \;=\; \sum_{i=1}^{N} \left((\mathbf{x}_i(t) - \mathbf{x}_{\mathrm{cog}}(t)) \cdot \mathbf{e}\right)^2 \tag{13.9}$$

Note that all atomic masses are set to 1 for simplicity. This component must contain one `atoms {...}` block to define the atom group, and returns a positive number, expressed in Å^2.
List of keywords (see also 13.4.4 for additional options):

- `atoms`: see definition of `atoms` (`rmsd` component)

- `axis` ⟨ Projection axis (Å) ⟩
  Context: `inertiaZ`
  Acceptable values: `(x, y, z)` triplet
  Default value: `(0.0, 0.0, 1.0)`
  Description: The three components of this vector define (when normalized) the projection axis **e**.

`orientation`**: orientation from reference coordinates.**

The block `orientation {...}` returns the same optimal rotation used in the `rmsd` component to superimpose the coordinates $\{\mathbf{x}_i(t)\}$ onto a set of reference coordinates $\{\mathbf{x}_i^{(\mathrm{ref})}\}$. Such component returns a four dimensional vector $\mathbf{q} = (q_0, q_1, q_2, q_3)$, with $\sum_i q_i^2 = 1$; this *quaternion* expresses the optimal rotation $\{\mathbf{x}_i(t)\} \rightarrow \{\mathbf{x}_i^{(\mathrm{ref})}\}$ according to the formalism in reference [46]. The quaternion (q_0, q_1, q_2, q_3) can also be written as $(\cos(\theta/2), \sin(\theta/2)\mathbf{u})$, where θ is the angle and $\mathbf{u}$ the normalized axis of rotation; for example, a rotation of 90° around the z axis is expressed as "`(0.707, 0.0, 0.0, 0.707)`". The script `quaternion2rmatrix.tcl` provides Tcl functions for converting to and from a 4×4 rotation matrix in a format suitable for usage in VMD.

As for the component `rmsd`, the available options are `atoms`, `refPositionsFile`, `refPositionsCol` and `refPositionsColValue`, and `refPositions`.

Note: `refPositions`and `refPositionsFile` define the set of positions *from which* the optimal rotation is calculated, but this rotation is not applied to the coordinates of the atoms involved: it is used instead to define the variable itself.

List of keywords (see also 13.4.4 for additional options):

- `atoms`: see definition of `atoms` (`rmsd` component)
- `refPositions`: see definition of `refPositions` (`rmsd` component)
- `refPositionsFile`: see definition of `refPositionsFile` (`rmsd` component)
- `refPositionsCol`: see definition of `refPositionsCol` (`rmsd` component)
- `refPositionsColValue`: see definition of `refPositionsColValue` (`rmsd` component)
- `closestToQuaternion` ⟨ Reference rotation ⟩
  Context: `orientation`
  Acceptable values: "`(q0, q1, q2, q3)`" quadruplet
  Default value: `(1.0, 0.0, 0.0, 0.0)` ("null" rotation)
  Description: Between the two equivalent quaternions (q_0, q_1, q_2, q_3) and $(-q_0, -q_1, -q_2, -q_3)$, the closer to `(1.0, 0.0, 0.0, 0.0)` is chosen. This simplifies the visualization of the colvar trajectory when samples values are a smaller subset of all possible rotations. **Note:** *this only affects the output, never the dynamics.*

Tip: stopping the rotation of a protein. To stop the rotation of an elongated macromolecule in solution (and use an anisotropic box to save water molecules), it is possible to define a colvar with an `orientation` component, and restrain it throuh the `harmonic` bias around the identity rotation, `(1.0, 0.0, 0.0, 0.0)`. Only the overall orientation of the macromolecule is affected, and *not* its internal degrees of freedom. The user should also take care that the macromolecule is composed by a single chain, or disable `wrapAll` otherwise.

`orientationAngle`**: angle of rotation from reference coordinates.**

The block `orientationAngle {...}` accepts the same base options as the component `orientation`: `atoms`, `refPositions`, `refPositionsFile`, `refPositionsCol` and `refPositionsColValue`. The returned value is the angle of rotation θ between the current and the reference positions. This angle is expressed in degrees within the range [0°:180°].
List of keywords (see also 13.4.4 for additional options):

- `atoms:` see definition of `atoms` (`rmsd` component)
- `refPositions:` see definition of `refPositions` (`rmsd` component)
- `refPositionsFile:` see definition of `refPositionsFile` (`rmsd` component)
- `refPositionsCol:` see definition of `refPositionsCol` (`rmsd` component)
- `refPositionsColValue:` see definition of `refPositionsColValue` (`rmsd` component)

`orientationProj`**: cosine of the angle of rotation from reference coordinates.**

The block `orientationProj {...}` accepts the same base options as the component `orientation`: `atoms`, `refPositions`, `refPositionsFile`, `refPositionsCol` and `refPositionsColValue`. The returned value is the cosine of the angle of rotation θ between the current and the reference positions. The range of values is [-1:1].
List of keywords (see also 13.4.4 for additional options):

- `atoms:` see definition of `atoms` (`rmsd` component)
- `refPositions:` see definition of `refPositions` (`rmsd` component)
- `refPositionsFile:` see definition of `refPositionsFile` (`rmsd` component)
- `refPositionsCol:` see definition of `refPositionsCol` (`rmsd` component)
- `refPositionsColValue:` see definition of `refPositionsColValue` (`rmsd` component)

`spinAngle`**: angle of rotation around a given axis.**

The complete rotation described by `orientation` can optionally be decomposed into two sub-rotations: one is a "*spin*" rotation around **e**, and the other a "*tilt*" rotation around an axis orthogonal to **e**. The component `spinAngle` measures the angle of the "spin" sub-rotation around **e**.
List of keywords (see also 13.4.4 for additional options):

- `atoms:` see definition of `atoms` (`rmsd` component)
- `refPositions:` see definition of `refPositions` (`rmsd` component)
- `refPositionsFile:` see definition of `refPositionsFile` (`rmsd` component)
- `refPositionsCol:` see definition of `refPositionsCol` (`rmsd` component)
- `refPositionsColValue:` see definition of `refPositionsColValue` (`rmsd` component)

- `axis` ⟨Special rotation axis (Å)⟩
  Context: `tilt`
  Acceptable values: `(x, y, z)` triplet
  Default value: `(0.0, 0.0, 1.0)`
  Description: The three components of this vector define (when normalized) the special rotation axis used to calculate the `tilt` and `spinAngle` components.

The component `spinAngle` returns an angle (in degrees) within the periodic interval $[-180 : 180]$.

Note: the value of `spinAngle` is a continuous function almost everywhere, with the exception of configurations with the corresponding "tilt" angle equal to 180° (i.e. the `tilt` component is equal to -1): in those cases, `spinAngle` is undefined. If such configurations are expected, consider defining a `tilt` colvar using the same axis **e**, and restraining it with a lower wall away from -1.

`tilt`: cosine of the rotation orthogonal to a given axis.

The component `tilt` measures the cosine of the angle of the "tilt" sub-rotation, which combined with the "spin" sub-rotation provides the complete rotation of a group of atoms. The cosine of the tilt angle rather than the tilt angle itself is implemented, because the latter is unevenly distributed even for an isotropic system: consider as an analogy the angle θ in the spherical coordinate system. The component `tilt` relies on the same options as `spinAngle`, including the definition of the axis **e**. The values of `tilt` are real numbers in the interval $[-1 : 1]$: the value 1 represents an orientation fully parallel to **e** (tilt angle = 0°), and the value -1 represents an anti-parallel orientation.
List of keywords (see also 13.4.4 for additional options):

- `atoms:` see definition of `atoms` (`rmsd` component)
- `refPositions:` see definition of `refPositions` (`rmsd` component)
- `refPositionsFile:` see definition of `refPositionsFile` (`rmsd` component)
- `refPositionsCol:` see definition of `refPositionsCol` (`rmsd` component)
- `refPositionsColValue:` see definition of `refPositionsColValue` (`rmsd` component)
- `axis:` see definition of `axis` (`spinAngle` component)

`alpha`: α-helix content of a protein segment.

The block `alpha {...}` defines the parameters to calculate the helical content of a segment of protein residues. The α-helical content across the $N+1$ residues N_0 to N_0+N is calculated by the formula:

$$\alpha\left(\mathrm{C}_\alpha^{(N_0)},\mathrm{O}^{(N_0)},\mathrm{C}_\alpha^{(N_0+1)},\mathrm{O}^{(N_0+1)},\dots\mathrm{N}^{(N_0+5)},\mathrm{C}_\alpha^{(N_0+5)},\mathrm{O}^{(N_0+5)},\dots\mathrm{N}^{(N_0+N)},\mathrm{C}_\alpha^{(N_0+N)}\right) = \tag{13.10}$$

$$\frac{1}{2(N-2)}\sum_{n=N_0}^{N_0+N-2}\mathrm{angf}\left(\mathrm{C}_\alpha^{(n)},\mathrm{C}_\alpha^{(n+1)},\mathrm{C}_\alpha^{(n+2)}\right) + \frac{1}{2(N-4)}\sum_{n=N_0}^{N_0+N-4}\mathrm{hbf}\left(\mathrm{O}^{(n)},\mathrm{N}^{(n+4)}\right), \tag{13.11}$$

where the score function for the $C_\alpha - C_\alpha - C_\alpha$ angle is defined as:

$$\mathrm{angf}\left(C_\alpha^{(n)}, C_\alpha^{(n+1)}, C_\alpha^{(n+2)}\right) = \frac{1 - \left(\theta(C_\alpha^{(n)}, C_\alpha^{(n+1)}, C_\alpha^{(n+2)}) - \theta_0\right)^2 / (\Delta\theta_{\mathrm{tol}})^2}{1 - \left(\theta(C_\alpha^{(n)}, C_\alpha^{(n+1)}, C_\alpha^{(n+2)}) - \theta_0\right)^4 / (\Delta\theta_{\mathrm{tol}})^4}, \tag{13.12}$$

and the score function for the $O^{(n)} \leftrightarrow N^{(n+4)}$ hydrogen bond is defined through a `hBond` colvar component on the same atoms.
List of keywords (see also 13.4.4 for additional options):

- `residueRange` ⟨ Potential α-helical residues ⟩
  Context: `alpha`
  Acceptable values: "<Initial residue number>-<Final residue number>"
  Description: This option specifies the range of residues on which this component should be defined. The Colvars module looks for the atoms within these residues named "`CA`", "`N`" and "`O`", and raises an error if any of those atoms is not found.

- `psfSegID` ⟨ PSF segment identifier ⟩
  Context: `alpha`
  Acceptable values: string (max 4 characters)
  Description: This option sets the PSF segment identifier for the residues specified in `residueRange`. This option is only required when PSF topologies are used.

- `hBondCoeff` ⟨ Coefficient for the hydrogen bond term ⟩
  Context: `alpha`
  Acceptable values: positive between 0 and 1
  Default value: 0.5
  Description: This number specifies the contribution to the total value from the hydrogen bond terms. 0 disables the hydrogen bond terms, 1 disables the angle terms.

- `angleRef` ⟨ Reference $C_\alpha - C_\alpha - C_\alpha$ angle ⟩
  Context: `alpha`
  Acceptable values: positive decimal
  Default value: 88°
  Description: This option sets the reference angle used in the score function (13.12).

- `angleTol` ⟨ Tolerance in the $C_\alpha - C_\alpha - C_\alpha$ angle ⟩
  Context: `alpha`
  Acceptable values: positive decimal
  Default value: 15°
  Description: This option sets the angle tolerance used in the score function (13.12).

- `hBondCutoff` ⟨ Hydrogen bond cutoff ⟩
  Context: `alpha`
  Acceptable values: positive decimal
  Default value: 3.3 Å
  Description: Equivalent to the `cutoff` option in the `hBond` component.

- `hBondExpNumer` ⟨ Hydrogen bond numerator exponent ⟩
  Context: `alpha`

Acceptable values: positive integer
Default value: 6
Description: Equivalent to the `expNumer` option in the `hBond` component.

- `hBondExpDenom` ⟨ Hydrogen bond denominator exponent ⟩
  Context: `alpha`
  Acceptable values: positive integer
  Default value: 8
  Description: Equivalent to the `expDenom` option in the `hBond` component.

This component returns positive values, always comprised between 0 (lowest α-helical score) and 1 (highest α-helical score).

`dihedralPC`: protein dihedral pricipal component

The block `dihedralPC {...}` defines the parameters to calculate the projection of backbone dihedral angles within a protein segment onto a *dihedral principal component*, following the formalism of dihedral principal component analysis (dPCA) proposed by Mu et al.[47] and documented in detail by Altis et al.[48]. Given a peptide or protein segment of N residues, each with Ramachandran angles ϕ_i and ψ_i, dPCA rests on a variance/covariance analysis of the $4(N-1)$ variables $\cos(\psi_1), \sin(\psi_1), \cos(\phi_2), \sin(\phi_2) \cdots \cos(\phi_N), \sin(\phi_N)$. Note that angles ϕ_1 and ψ_N have little impact on chain conformation, and are therefore discarded, following the implementation of dPCA in the analysis software Carma.[49]

For a given principal component (eigenvector) of coefficients $(k_i)_{1 \leq i \leq 4(N-1)}$, the projection of the current backbone conformation is:

$$\xi = \sum_{n=1}^{N-1} k_{4n-3} \cos(\psi_n) + k_{4n-2} \sin(\psi_n) + k_{4n-1} \cos(\phi_{n+1}) + k_{4n} \sin(\phi_{n+1}) \tag{13.13}$$

`dihedralPC` expects the same parameters as the `alpha` component for defining the relevant residues (`residueRange` and `psfSegID`) in addition to the following:
List of keywords (see also 13.4.4 for additional options):

- `residueRange`: see definition of `residueRange` (`alpha` component)
- `psfSegID`: see definition of `psfSegID` (`alpha` component)
- `hBondCoeff`: see definition of `hBondCoeff` (`alpha` component)
- `angleRef`: see definition of `angleRef` (`alpha` component)
- `angleTol`: see definition of `angleTol` (`alpha` component)
- `hBondCutoff`: see definition of `hBondCutoff` (`alpha` component)
- `hBondExpNumer`: see definition of `hBondExpNumer` (`alpha` component)
- `hBondExpDenom`: see definition of `hBondExpDenom` (`alpha` component)

- `vectorFile` ⟨ File containing dihedral PCA eigenvector(s) ⟩
  Context: `dihedralPC`
  Acceptable values: file name
  Description: A text file containing the coefficients of dihedral PCA eigenvectors on the cosine and sine coordinates. The vectors should be arranged in columns, as in the files output by Carma.[49]

- `vectorNumber` ⟨ File containing dihedralPCA eigenvector(s) ⟩
  Context: `dihedralPC`
  Acceptable values: positive integer
  Description: Number of the eigenvector to be used for this component.

13.4.2 Configuration keywords shared by all components

The following options can be used for any of the above colvar components in order to obtain a polynomial combination or any user-supplied function provided by `scriptedFunction`.

- `name` ⟨ Name of this component ⟩
  Context: any component
  Acceptable values: string
  Default value: type of component + numeric id
  Description: The name is an unique case-sensitive string which allows the Colvars module to identify this component. This is useful, for example, when combining multiple components via a `scriptedFunction`.

- `scalable` ⟨ Attempt to calculate this component in parallel? ⟩
  Context: any component
  Acceptable values: boolean
  Default value: `on`, if available
  Description: If set to `on` (default), the Colvars module will attempt to calculate this component in parallel to reduce overhead. Whether this option is available depends on the type of component: currently supported are `distance`, `distanceZ`, `distanceXY`, `distanceVec`, `distanceDir`, `angle` and `dihedral`. This flag influences computational cost, but does not affect numerical results: therefore, it should only be turned off for debugging or testing purposes.

13.4.3 Advanced usage and special considerations

Periodic components.

The following components returns real numbers that lie in a periodic interval:

- `dihedral`: torsional angle between four groups;

- `spinAngle`: angle of rotation around a predefined axis in the best-fit from a set of reference coordinates.

In certain conditions, `distanceZ` can also be periodic, namely when periodic boundary conditions (PBCs) are defined in the simulation and `distanceZ`'s axis is parallel to a unit cell vector.

The following keywords can be used within periodic components (and are illegal elsewhere):

- `period` ⟨Period of the component⟩
  Context: `distanceZ`
  Acceptable values: positive decimal
  Default value: 0.0
  Description: Setting this number enables the treatment of `distanceZ` as a periodic component: by default, `distanceZ` is not considered periodic. The keyword is supported, but irrelevant within `dihedral` or `spinAngle`, because their period is always 360 degrees.

- `wrapAround` ⟨Center of the wrapping interval for periodic variables⟩
  Context: `distanceZ`, `dihedral` or `spinAngle`
  Acceptable values: decimal
  Default value: 0.0
  Description: By default, values of the periodic components are centered around zero, ranging from $-P/2$ to $P/2$, where P is the period. Setting this number centers the interval around this value. This can be useful for convenience of output, or to set `lowerWall` and `upperWall` in an order that would not otherwise be allowed.

Internally, all differences between two values of a periodic colvar follow the minimum image convention: they are calculated based on the two periodic images that are closest to each other.

Note: linear or polynomial combinations of periodic components may become meaningless when components cross the periodic boundary. Use such combinations carefully: estimate the range of possible values of each component in a given simulation, and make use of `wrapAround` to limit this problem whenever possible.

Non-scalar components.

When one of the following components are used, the defined colvar returns a value that is not a scalar number:

- `distanceVec`: 3-dimensional vector of the distance between two groups;
- `distanceDir`: 3-dimensional unit vector of the distance between two groups;
- `orientation`: 4-dimensional unit quaternion representing the best-fit rotation from a set of reference coordinates.

The distance between two 3-dimensional unit vectors is computed as the angle between them. The distance between two quaternions is computed as the angle between the two 4-dimensional unit vectors: because the orientation represented by `q` is the same as the one represented by $-$`q`, distances between two quaternions are computed considering the closest of the two symmetric images.

Non-scalar components carry the following restrictions:

- Calculation of total forces (`outputTotalForce` option) is currently not implemented.
- Each colvar can only contain one non-scalar component.
- Binning on a grid (`abf`, `histogram` and `metadynamics` with `useGrids` enabled) is currently not implemented for colvars based on such components.

Note: while these restrictions apply to individual colvars based on non-scalar components, no limit is set to the number of scalar colvars. To compute multi-dimensional histograms and PMFs, use sets of scalar colvars of arbitrary size.

Calculating total forces.

In addition to the restrictions due to the type of value computed (scalar or non-scalar), a final restriction can arise when calculating total force (`outputTotalForce` option or application of a `abf` bias). total forces are available currently only for the following components: `distance`, `distanceZ`, `distanceXY`, `angle`, `dihedral`, `rmsd`, `eigenvector` and `gyration`.

13.4.4 Linear and polynomial combinations of components

To extend the set of possible definitions of colvars $\xi(\mathbf{r})$, multiple components $q_i(\mathbf{r})$ can be summed with the formula:

$$\xi(\mathbf{r}) = \sum_i c_i [q_i(\mathbf{r})]^{n_i} \tag{13.14}$$

where each component appears with a unique coefficient c_i (1.0 by default) the positive integer exponent n_i (1 by default).

Any set of components can be combined within a colvar, provided that they return the same type of values (scalar, unit vector, vector, or quaternion). By default, the colvar is the sum of its components. Linear or polynomial combinations (following equation (13.14)) can be obtained by setting the following parameters, which are common to all components:

- `componentCoeff` ⟨ Coefficient of this component in the colvar ⟩
  Context: any component
  Acceptable values: decimal
  Default value: `1.0`
  Description: Defines the coefficient by which this component is multiplied (after being raised to `componentExp`) before being added to the sum.

- `componentExp` ⟨ Exponent of this component in the colvar ⟩
  Context: any component
  Acceptable values: integer
  Default value: `1`
  Description: Defines the power at which the value of this component is raised before being added to the sum. When this exponent is different than 1 (non-linear sum), total forces and the Jacobian force are not available, making the colvar unsuitable for ABF calculations.

Example: To define the *average* of a colvar across different parts of the system, simply define within the same colvar block a series of components of the same type (applied to different atom groups), and assign to each component a `componentCoeff` of $1/N$.

13.4.5 Colvars as scripted functions of components

When scripting is supported (default in VMD), a colvar may be defined as a custom function of its components, rather than a linear or polynomial combination. When implementing generic functions of Cartesian coordinates rather than functions of existing components, the `cartesian` component may be particularly useful.

An example of elaborate scripted colvar is given in example 10, in the form of path-based collective variables as defined by Branduardi et al[50]. The required Tcl procedures are provided in the `colvartools` directory.

- `scriptedFunction` ⟨Compute colvar as a scripted function of its components⟩
  Context: `colvar`
  Acceptable values: string
  Description: If this option is specified, the colvar will be computed as a scripted function of the values of its components. To that effect, the user should define two Tcl procedures: `calc_<scriptedFunction>` and `calc_<scriptedFunction>_gradient`, both accepting as many parameters as the colvar has components. Values of the components will be passed to those procedures in the order defined by their sorted `name` strings. Note that if all components are of the same type, their default names are sorted in the order in which they are defined, so that names need only be specified for combinations of components of different types. `calc_<scriptedFunction>` should return one value of type <scriptedFunctionType>, corresponding to the colvar value. `calc_<scriptedFunction>_gradient` should return a Tcl list containing the derivatives of the function with respect to each component. If both the function and some of the components are vectors, the gradient is really a Jacobian matrix that should be passed as a linear vector in row-major order, i.e. for a function $f_i(x_j)$: $\nabla_x f_1 \nabla_x f_2 \cdots$.

- `scriptedFunctionType` ⟨Type of value returned by the scripted colvar⟩
  Context: `colvar`
  Acceptable values: string
  Default value: `scalar`
  Description: If a colvar is defined as a scripted function, its type is not constrained by the types of its components. With this flag, the user may specify whether the colvar is a scalar or one of the following vector types: `vector3` (a 3D vector), `unit_vector3` (a normalized 3D vector), or `unit_quaternion` (a normalized quaternion), or `vector` (a vector whose size is specified by `scriptedFunctionVectorSize`). Non-scalar values should be passed as space-separated lists, e.g. "1. 2. 3.".

- `scriptedFunctionVectorSize` ⟨Dimension of the vector value of a scripted colvar⟩
  Context: `colvar`
  Acceptable values: positive integer
  Description: This parameter is only valid when `scriptedFunctionType` is set to `vector`. It defines the vector length of the colvar value returned by the function.

13.5 Biasing and analysis methods

All of the biasing and analysis methods implemented (`abf`, `harmonic`, `histogram` and `metadynamics`) recognize the following options:

- `name` ⟨Identifier for the bias⟩
  Context: colvar bias
  Acceptable values: string
  Default value: `<type of bias><bias index>`
  Description: This string is used to identify the bias or analysis method in output messages and to name some output files.

- `colvars` ⟨Collective variables involved⟩
  Context: colvar bias

Acceptable values: space-separated list of colvar names
Description: This option selects by name all the colvars to which this bias or analysis will be applied.

- `outputEnergy` ⟨ Write the current bias energy to the trajectory file ⟩
  Context: colvar bias
  Acceptable values: boolean
  Default value: `off`
  Description: If this option is chosen and `colvarsTrajFrequency` is not zero, the current value of the biasing energy will be written to the trajectory file during the simulation.

13.5.1 Adaptive Biasing Force

For a full description of the Adaptive Biasing Force method, see reference [51]. For details about this implementation, see references [52] and [53]. **When publishing research that makes use of this functionality, please cite references [51] and [53].**

An alternate usage of this feature is the application of custom tabulated biasing potentials to one or more colvars. See `inputPrefix` and `updateBias` below.

Combining ABF with the extended Lagrangian feature (13.2.4) of the variables produces the extended-system ABF variant of the method (13.5.2).

ABF is based on the thermodynamic integration (TI) scheme for computing free energy profiles. The free energy as a function of a set of collective variables $\boldsymbol{\xi} = (\xi_i)_{i\in[1,n]}$ is defined from the canonical distribution of $\boldsymbol{\xi}$, $\mathcal{P}(\boldsymbol{\xi})$:

$$A(\boldsymbol{\xi}) = -\frac{1}{\beta}\ln\mathcal{P}(\boldsymbol{\xi}) + A_0 \tag{13.15}$$

In the TI formalism, the free energy is obtained from its gradient, which is generally calculated in the form of the average of a force $\boldsymbol{F}_\xi$ exerted on $\boldsymbol{\xi}$, taken over an iso-$\boldsymbol{\xi}$ surface:

$$\boldsymbol{\nabla}_\xi A(\boldsymbol{\xi}) = \langle -\boldsymbol{F}_\xi \rangle_{\boldsymbol{\xi}} \tag{13.16}$$

Several formulae that take the form of (13.16) have been proposed. This implementation relies partly on the classic formulation [54], and partly on a more versatile scheme originating in a work by Ruiz-Montero et al. [55], generalized by den Otter [56] and extended to multiple variables by Ciccotti et al. [57]. Consider a system subject to constraints of the form $\sigma_k(\boldsymbol{x}) = 0$. Let $(\boldsymbol{v}_i)_{i\in[1,n]}$ be arbitrarily chosen vector fields ($\mathbb{R}^{3N} \to \mathbb{R}^{3N}$) verifying, for all i, j, and k:

$$\boldsymbol{v}_i \cdot \boldsymbol{\nabla}_{\boldsymbol{x}}\, \xi_j = \delta_{ij} \tag{13.17}$$

$$\boldsymbol{v}_i \cdot \boldsymbol{\nabla}_{\boldsymbol{x}}\, \sigma_k = 0 \tag{13.18}$$

then the following holds [57]:

$$\frac{\partial A}{\partial \xi_i} = \langle \boldsymbol{v}_i \cdot \boldsymbol{\nabla}_{\boldsymbol{x}}\, V - k_B T \boldsymbol{\nabla}_{\boldsymbol{x}} \cdot \boldsymbol{v}_i \rangle_{\boldsymbol{\xi}} \tag{13.19}$$

where V is the potential energy function. $\boldsymbol{v}_i$ can be interpreted as the direction along which the force acting on variable ξ_i is measured, whereas the second term in the average corresponds to the geometric entropy contribution that appears as a Jacobian correction in the classic formalism [54].

Condition (13.17) states that the direction along which the total force on ξ_i is measured is orthogonal to the gradient of ξ_j, which means that the force measured on ξ_i does not act on ξ_j.

Equation (13.18) implies that constraint forces are orthogonal to the directions along which the free energy gradient is measured, so that the measurement is effectively performed on unconstrained degrees of freedom.

In the framework of ABF, $\mathbf{F}_\xi$ is accumulated in bins of finite size $\delta\xi$, thereby providing an estimate of the free energy gradient according to equation (13.16). The biasing force applied along the collective variables to overcome free energy barriers is calculated as:

$$\mathbf{F}^{\mathrm{ABF}} = \alpha(N_\xi) \times \boldsymbol{\nabla}_{\boldsymbol{x}} \widetilde{A}(\boldsymbol{\xi}) \tag{13.20}$$

where $\boldsymbol{\nabla}_{\boldsymbol{x}} \widetilde{A}$ denotes the current estimate of the free energy gradient at the current point $\boldsymbol{\xi}$ in the collective variable subspace, and $\alpha(N_\xi)$ is a scaling factor that is ramped from 0 to 1 as the local number of samples N_ξ increases to prevent nonequilibrium effects in the early phase of the simulation, when the gradient estimate has a large variance. See the `fullSamples` parameter below for details.

As sampling of the phase space proceeds, the estimate $\boldsymbol{\nabla}_{\boldsymbol{x}} \widetilde{A}$ is progressively refined. The biasing force introduced in the equations of motion guarantees that in the bin centered around $\boldsymbol{\xi}$, the forces acting along the selected collective variables average to zero over time. Eventually, as the undelying free energy surface is canceled by the adaptive bias, evolution of the system along $\boldsymbol{\xi}$ is governed mainly by diffusion. Although this implementation of ABF can in principle be used in arbitrary dimension, a higher-dimension collective variable space is likely to result in sampling difficulties. Most commonly, the number of variables is one or two.

ABF requirements on collective variables

The following conditions must be met for an ABF simulation to be possible and to produce an accurate estimate of the free energy profile. Note that these requirements do not apply when using the extended-system ABF method (13.5.2).

1. *Only linear combinations* of colvar components can be used in ABF calculations.

2. *Availability of total forces* is necessary. The following colvar components can be used in ABF calculations: `distance`, `distance_xy`, `distance_z`, `angle`, `dihedral`, `gyration`, `rmsd` and `eigenvector`. Atom groups may not be replaced by dummy atoms, unless they are excluded from the force measurement by specifying `oneSiteTotalForce`, if available.

3. *Mutual orthogonality of colvars.* In a multidimensional ABF calculation, equation (13.17) must be satisfied for any two colvars ξ_i and ξ_j. Various cases fulfill this orthogonality condition:

   - ξ_i and ξ_j are based on non-overlapping sets of atoms.
   - atoms involved in the force measurement on ξ_i do not participate in the definition of ξ_j. This can be obtained using the option `oneSiteTotalForce` of the `distance`, `angle`, and `dihedral` components (example: Ramachandran angles ϕ, ψ).
   - ξ_i and ξ_j are orthogonal by construction. Useful cases are the sum and difference of two components, or `distance_z` and `distance_xy` using the same axis.

4. *Mutual orthogonality of components*: when several components are combined into a colvar, it is assumed that their vectors $\boldsymbol{v}_i$ (equation (13.19)) are mutually orthogonal. The cases described for colvars in the previous paragraph apply.

5. *Orthogonality of colvars and constraints*: equation 13.18 can be satisfied in two simple ways, if either no constrained atoms are involved in the force measurement (see point 3 above) or pairs of atoms joined by a constrained bond are part of an *atom group* which only intervenes through its center (center of mass or geometric center) in the force measurement. In the latter case, the contributions of the two atoms to the left-hand side of equation 13.18 cancel out. For example, all atoms of a rigid TIP3P water molecule can safely be included in an atom group used in a `distance` component.

Parameters for ABF

ABF depends on parameters from collective variables to define the grid on which free energy gradients are computed. In the direction of each colvar, the grid ranges from `lowerBoundary` to `upperBoundary`, and the bin width (grid spacing) is set by the `width` parameter (see 13.2.1). The following specific parameters can be set in the ABF configuration block:

- `name`: see definition of `name` (biasing and analysis methods)
- `colvars`: see definition of `colvars` (biasing and analysis methods)
- `fullSamples` ⟨ Number of samples in a bin prior to application of the ABF ⟩
  Context: `abf`
  Acceptable values: positive integer
  Default value: 200
  Description: To avoid nonequilibrium effects due to large fluctuations of the force exerted along the colvars, it is recommended to apply a biasing force only after a the estimate has started converging. If `fullSamples` is non-zero, the applied biasing force is scaled by a factor $\alpha(N_\xi)$ between 0 and 1. If the number of samples N_ξ in the current bin is higher than `fullSamples`, the factor is one. If it is less than half of `fullSamples`, the factor is zero and no bias is applied. Between those two thresholds, the factor follows a linear ramp from 0 to 1: $\alpha(N_\xi) = (2N_\xi/\text{fullSamples}) - 1$.
- `maxForce` ⟨ Maximum magnitude of the ABF force ⟩
  Context: `abf`
  Acceptable values: positive decimals (one per colvar)
  Default value: disabled
  Description: This option enforces a cap on the magnitude of the biasing force effectively applied by this ABF bias on each colvar. This can be useful in the presence of singularities in the PMF such as hard walls, where the discretization of the average force becomes very inaccurate, causing the colvar's diffusion to get "stuck" at the singularity. To enable this cap, provide one non-negative value for each colvar. The unit of force is kcal/mol divided by the colvar unit.
- `hideJacobian` ⟨ Remove geometric entropy term from calculated free energy gradient? ⟩
  Context: `abf`
  Acceptable values: boolean

Default value: `no`
Description: In a few special cases, most notably distance-based variables, an alternate definition of the potential of mean force is traditionally used, which excludes the Jacobian term describing the effect of geometric entropy on the distribution of the variable. This results, for example, in particle-particle potentials of mean force being flat at large separations. Setting this parameter to `yes` causes the output data to follow that convention, by removing this contribution from the output gradients while applying internally the corresponding correction to ensure uniform sampling. It is not allowed for colvars with multiple components.

- `outputFreq` ⟨ Frequency (in timesteps) at which ABF data files are refreshed ⟩
Context: `abf`
Acceptable values: positive integer
Default value: Colvars module restart frequency
Description: The files containing the free energy gradient estimate and sampling histogram (and the PMF in one-dimensional calculations) are written on disk at the given time interval.

- `historyFreq` ⟨ Frequency (in timesteps) at which ABF history files are accumulated ⟩
Context: `abf`
Acceptable values: positive integer
Default value: 0
Description: If this number is non-zero, the free energy gradient estimate and sampling histogram (and the PMF in one-dimensional calculations) are appended to files on disk at the given time interval. History file names use the same prefix as output files, with "`.hist`" appended.

- `inputPrefix` ⟨ Filename prefix for reading ABF data ⟩
Context: `abf`
Acceptable values: list of strings
Description: If this parameter is set, for each item in the list, ABF tries to read a gradient and a sampling files named <`inputPrefix`>`.grad` and <`inputPrefix`>`.count`. This is done at startup and sets the initial state of the ABF algorithm. The data from all provided files is combined appropriately. Also, the grid definition (min and max values, width) need not be the same that for the current run. This command is useful to piece together data from simulations in different regions of collective variable space, or change the colvar boundary values and widths. Note that it is not recommended to use it to switch to a smaller width, as that will leave some bins empty in the finer data grid. This option is NOT compatible with reading the data from a restart file (`cv load` command).

- `applyBias` ⟨ Apply the ABF bias? ⟩
Context: `abf`
Acceptable values: boolean
Default value: `yes`
Description: If this is set to no, the calculation proceeds normally but the adaptive biasing force is not applied. Data is still collected to compute the free energy gradient. This is mostly intended for testing purposes, and should not be used in routine simulations.

- `updateBias` ⟨ Update the ABF bias? ⟩
Context: `abf`

Acceptable values: boolean
Default value: `yes`
Description: If this is set to no, the initial biasing force (e.g. read from a restart file or through `inputPrefix`) is not updated during the simulation. As a result, a constant bias is applied. This can be used to apply a custom, tabulated biasing potential to any combination of colvars. To that effect, one should prepare a gradient file containing the gradient of the potential to be applied (negative of the bias force), and a count file containing only values greater than `fullSamples`. These files must match the grid parameters of the colvars.

Output files

The ABF bias produces the following files, all in multicolumn text format:

- *outputName*`.grad`: current estimate of the free energy gradient (grid), in multicolumn;
- *outputName*`.count`: histogram of samples collected, on the same grid;
- *outputName*`.pmf`: only for one-dimensional calculations, integrated free energy profile or PMF.

If several ABF biases are defined concurrently, their name is inserted to produce unique filenames for output, as in *outputName*`.abf1.grad`. This should not be done routinely and could lead to meaningless results: only do it if you know what you are doing!

If the colvar space has been partitioned into sections (*windows*) in which independent ABF simulations have been run, the resulting data can be merged using the `inputPrefix` option described above (a run of 0 steps is enough).

Post-processing: reconstructing a multidimensional free energy surface

If a one-dimensional calculation is performed, the estimated free energy gradient is automatically integrated and a potential of mean force is written under the file name `<outputName>.pmf`, in a plain text format that can be read by most data plotting and analysis programs (e.g. gnuplot).

In dimension 2 or greater, integrating the discretized gradient becomes non-trivial. The standalone utility `abf_integrate` is provided to perform that task. `abf_integrate` reads the gradient data and uses it to perform a Monte-Carlo (M-C) simulation in discretized collective variable space (specifically, on the same grid used by ABF to discretize the free energy gradient). By default, a history-dependent bias (similar in spirit to metadynamics) is used: at each M-C step, the bias at the current position is incremented by a preset amount (the *hill height*). Upon convergence, this bias counteracts optimally the underlying gradient; it is negated to obtain the estimate of the free energy surface.

`abf_integrate` is invoked using the command-line:

```
abf_integrate <gradient_file> [-n <nsteps>] [-t <temp>] [-m (0|1)] [-h <hill_height>] [-f <factor>]
```

The gradient file name is provided first, followed by other parameters in any order. They are described below, with their default value in square brackets:

- `-n`: number of M-C steps to be performed; by default, a minimal number of steps is chosen based on the size of the grid, and the integration runs until a convergence criterion is satisfied (based on the RMSD between the target gradient and the real PMF gradient)

- `-t`: temperature for M-C sampling (unrelated to the simulation temperature) [500 K]
- `-m`: use metadynamics-like biased sampling? (0 = false) [1]
- `-h`: increment for the history-dependent bias ("hill height") [0.01 kcal/mol]
- `-f`: if non-zero, this factor is used to scale the increment stepwise in the second half of the M-C sampling to refine the free energy estimate [0.5]

Using the default values of all parameters should give reasonable results in most cases.

`abf_integrate` produces the following output files:

- `<gradient_file>.pmf`: computed free energy surface
- `<gradient_file>.histo`: histogram of M-C sampling (not usable in a straightforward way if the history-dependent bias has been applied)
- `<gradient_file>.est`: estimated gradient of the calculated free energy surface (from finite differences)
- `<gradient_file>.dev`: deviation between the user-provided numerical gradient and the actual gradient of the calculated free energy surface. The RMS norm of this vector field is used as a convergence criteria and displayed periodically during the integration.

Note: Typically, the "deviation" vector field does not vanish as the integration converges. This happens because the numerical estimate of the gradient does not exactly derive from a potential, due to numerical approximations used to obtain it (finite sampling and discretization on a grid).

13.5.2 Extended-system Adaptive Biasing Force (eABF)

Extended-system ABF (eABF) is a variant of ABF (13.5.1) where the bias is not applied directly to the collective variable, but to an extended coordinate ("fictitious variable") λ that evolves dynamically according to Newtonian or Langevin dynamics. Such an extended coordinate is enabled for a given colvar using the `extendedLagrangian` and associated keywords (13.2.4). The theory of eABF and the present implementation are documented in detail in reference [58].

Defining an ABF bias on a colvar wherein the `extendedLagrangian` option is active will perform eABF; there is no dedicated option.

The extended variable λ is coupled to the colvar $z = \xi(q)$ by the harmonic potential $(k/2)(z-\lambda)^2$. Under eABF dynamics, the adaptive bias on λ is the running estimate of the average spring force:

$$F^{\text{bias}}(\lambda^*) = \langle k(\lambda - z) \rangle_{\lambda^*} \tag{13.21}$$

where the angle brackets indicate a canonical average conditioned by $\lambda = \lambda^*$. At long simulation times, eABF produces a flat histogram of the extended variable λ, and a flattened histogram of ξ, whose exact shape depends on the strength of the coupling as defined by `extendedFluctuation` in the colvar. Coupling should be somewhat loose for faster exploration and convergence, but strong enough that the bias does help overcome barriers along the colvar ξ.[58] Distribution of the colvar may be assessed by plotting its histogram, which is written to the *outputName*`.zcount` file in every eABF simulation. Note that a `histogram` bias (13.5.7) applied to an extended-Lagrangian colvar will access the extended degree of freedom λ, not the original colvar ξ; however, the joint histogram may be explicitly requested by listing the name of the colvar twice in a row within the `colvars` parameter of the `histogram` block.

The eABF PMF is that of the coordinate λ, it is not exactly the free energy profile of ξ. That quantity can be calculated based on the CZAR estimator.

CZAR estimator of the free energy

The *corrected z-averaged restraint* (CZAR) estimator is described in detail in reference [58]. It is computed automatically in eABF simulations, regardless of the number of colvars involved. Note that ABF may also be applied on a combination of extended and non-extended colvars; in that case, CZAR still provides an unbiased estimate of the free energy gradient.

CZAR estimates the free energy gradient as:

$$A'(z) = -\frac{1}{\beta}\frac{d\ln\tilde{\rho}(z)}{dz} + k(\langle\lambda\rangle_z - z). \tag{13.22}$$

where $z = \xi(q)$ is the colvar, λ is the extended variable harmonically coupled to z with a force constant k, and $\tilde{\rho}(z)$ is the observed distribution (histogram) of z, affected by the eABF bias.

There is only one optional parameter to the CZAR estimator:

- `writeCZARwindowFile` ⟨ Write internal data from CZAR to a separate file? ⟩
  Context: `abf`
  Acceptable values: boolean
  Default value: `no`
  Description: When this option is enabled, eABF simulations will write a file containing the z-averaged restraint force under the name *outputName*`.zgrad`. The same information is always included in the colvars state file, which is sufficient for restarting an eABF simulation. These separate file is only useful when joining adjacent windows from a stratified eABF simulation, either to continue the simulation in a broader window or to compute a CZAR estimate of the PMF over the full range of the coordinate(s).

Similar to ABF, the CZAR estimator produces two output files in multicolumn text format:

- *outputName*`.czar.grad`: current estimate of the free energy gradient (grid), in multicolumn;
- *outputName*`.czar.pmf`: only for one-dimensional calculations, integrated free energy profile or PMF.

The sampling histogram associated with the CZAR estimator is the z-histogram, which is written in the file *outputName*`.zcount`.

13.5.3 Metadynamics

The metadynamics method uses a history-dependent potential [59] that generalizes to any type of colvars the conformational flooding [60] and local elevation [61] methods, originally formulated to use as colvars the principal components of a covariance matrix or a set of dihedral angles, respectively. The metadynamics potential on the colvars $\boldsymbol{\xi} = (\xi_1, \xi_2, \ldots, \xi_{N_{\mathrm{cv}}})$ is defined as:

$$V_{\mathrm{meta}}(\boldsymbol{\xi}(t)) \;=\; \sum_{t'=\delta t, 2\delta t, \ldots}^{t'<t} W \prod_{i=1}^{N_{\mathrm{cv}}} \exp\left(-\frac{(\xi_i(t) - \xi_i(t'))^2}{2\sigma_{\xi_i}^2}\right), \tag{13.23}$$

where V_{meta} is the history-dependent potential acting on the *current* values of the colvars $\boldsymbol{\xi}$, and depends only parametrically on the *previous* values of the colvars. V_{meta} is constructed as a sum of N_{cv}-dimensional repulsive Gaussian "hills", whose height is a chosen energy constant W, and whose centers are the previously explored configurations $(\boldsymbol{\xi}(\delta t), \boldsymbol{\xi}(2\delta t), \ldots)$.

During the simulation, the system evolves towards the nearest minimum of the "effective" potential of mean force $\tilde{A}(\boldsymbol{\xi})$, which is the sum of the "real" underlying potential of mean force $A(\boldsymbol{\xi})$ and the the metadynamics potential, $V_{\mathrm{meta}}(\boldsymbol{\xi})$. Therefore, at any given time the probability of observing the configuration $\boldsymbol{\xi}^*$ is proportional to $\exp\left(-\tilde{A}(\boldsymbol{\xi}^*)/\kappa_{\mathrm{B}}T\right)$: this is also the probability that a new Gaussian "hill" is added at that configuration. If the simulation is run for a sufficiently long time, each local minimum is canceled out by the sum of the Gaussian "hills". At that stage the "effective" potential of mean force $\tilde{A}(\boldsymbol{\xi})$ is constant, and $-V_{\mathrm{meta}}(\boldsymbol{\xi})$ is an accurate estimator of the "real" potential of mean force $A(\boldsymbol{\xi})$, save for an additive constant:

$$A(\boldsymbol{\xi}) \;\simeq\; -V_{\mathrm{meta}}(\boldsymbol{\xi}) + K \tag{13.24}$$

Assuming that the set of collective variables includes all relevant degrees of freedom, the predicted error of the estimate is a simple function of the correlation times of the colvars τ_{ξ_i}, and of the user-defined parameters W, σ_{ξ_i} and δt [62]. In typical applications, a good rule of thumb can be to choose the ratio $W/\delta t$ much smaller than $\kappa_{\mathrm{B}}T/\tau_{\boldsymbol{\xi}}$, where $\tau_{\boldsymbol{\xi}}$ is the longest among $\boldsymbol{\xi}$'s correlation times: σ_{ξ_i} then dictates the resolution of the calculated PMF.

To enable a metadynamics calculation, a `metadynamics` block must be defined in the colvars configuration file. Its mandatory keywords are `colvars`, which lists all the variables involved, and `hillWeight`, which specifies the weight parameter W. The parameters δt and σ_ξ specified by the optional keywords `newHillFrequency` and `hillWidth`:

- `name`: see definition of `name` (biasing and analysis methods)
- `colvars`: see definition of `colvars` (biasing and analysis methods)
- `outputEnergy`: see definition of `outputEnergy` (biasing and analysis methods)
- `hillWeight` ⟨ Height of each hill (kcal/mol) ⟩
  Context: `metadynamics`
  Acceptable values: positive decimal
  Description: This option sets the height W of the Gaussian hills that are added during this run. Lower values provide more accurate sampling of the system's degrees of freedom at the price of longer simulation times to complete a PMF calculation based on metadynamics.
- `newHillFrequency` ⟨ Frequency of hill creation ⟩
  Context: `metadynamics`
  Acceptable values: positive integer
  Default value: `1000`
  Description: This option sets the number of integration steps after which a new hill is added to the metadynamics potential. Its value determines the parameter δt in eq. 13.23. Higher values provide more accurate sampling at the price of longer simulation times to complete a PMF calculation.
- `hillWidth` ⟨ Relative width of a Gaussian hill with respect to the colvar's width ⟩
  Context: `metadynamics`
  Acceptable values: positive decimal
  Default value: $\sqrt{2\pi}/2$
  Description: The Gaussian width along each colvar, $2\sigma_{\xi_i}$, is set as the product between this number and the colvar's parameter w_i given by `width` (see 13.2.1); such product is

printed in the standard output of VMD. The default value of this number gives a Gaussian hill function whose volume is equal to the product of $\prod_i w_i$, the volume of one `histogram` bin (see 13.5.7), and W. **Tip:** *use this property to estimate the fraction of colvar space covered by the Gaussian bias within a given simulation time.* When `useGrids` is on, the default value also gives acceptable discretization errors [44]: for smoother visualization, this parameter may be increased and the `width` w_i decreased in the same proportion. **Note:** *values smaller than 1 are not recommended.*

Output files

When interpolating grids are enabled (default behavior), the PMF is written every `colvarsRestartFrequency` steps to the file *outputName*`.pmf`. The following two options allow to control this behavior and to visually track statistical convergence:

- `writeFreeEnergyFile` ⟨ Periodically write the PMF for visualization ⟩
  Context: `metadynamics`
  Acceptable values: boolean
  Default value: `on`
  Description: When `useGrids` and this option are `on`, the PMF is written every `colvarsRestartFrequency` steps.

- `keepFreeEnergyFiles` ⟨ Keep all the PMF files ⟩
  Context: `metadynamics`
  Acceptable values: boolean
  Default value: `off`
  Description: When `writeFreeEnergyFile` and this option are `on`, the step number is included in the file name, thus generating a series of PMF files. Activating this option can be useful to follow more closely the convergence of the simulation, by comparing PMFs separated by short times.

Note: when Gaussian hills are deposited near `lowerBoundary` or `upperBoundary` (see 13.2.1) and interpolating grids are used (default behavior), their truncation can give rise to accumulating errors. In these cases, as a measure of fault-tolerance all Gaussian hills near the boundaries are included in the output state file, and are recalculated analytically whenever the colvar falls outside the grid's boundaries. (Such measure protects the accuracy of the calculation, and can only be disabled by `hardLowerBoundary` or `hardUpperBoundary`.) To avoid gradual loss of performance and growth of the state file, either one of the following solutions is recommended:

- enabling the option `expandBoundaries`, so that the grid's boundaries are automatically recalculated whenever necessary; the resulting `.pmf` will have its abscissas expanded accordingly;
- setting `lowerWall` and `upperWall` well within the interval delimited by `lowerBoundary` and `upperBoundary`.

Performance tuning

The following options control the computational cost of metadynamics calculations, but do not affect results. Default values are chosen to minimize such cost with no loss of accuracy.

- `useGrids` ⟨Interpolate the hills with grids⟩
  Context: `metadynamics`
  Acceptable values: boolean
  Default value: `on`
  Description: This option discretizes all hills for improved performance, accumulating their energy and their gradients on two separate grids of equal spacing. Grids are defined by the values of `lowerBoundary`, `upperBoundary` and `width` for each colvar. Currently, this option is implemented for all types of variables except the non-scalar types (`distanceDir` or `orientation`). If `expandBoundaries` is defined in one of the colvars, grids are automatically expanded along the direction of that colvar.

- `rebinGrids` ⟨Recompute the grids when reading a state file⟩
  Context: `metadynamics`
  Acceptable values: boolean
  Default value: `off`
  Description: When restarting from a state file, the grid's parameters (boundaries and widths) saved in the state file override those in the configuration file. Enabling this option forces the grids to match those in the current configuration file.

Well-tempered metadynamics

The following options define the configuration for the "well-tempered" metadynamics approach [63]:

- `wellTempered` ⟨Perform well-tempered metadynamics⟩
  Context: `metadynamics`
  Acceptable values: boolean
  Default value: `off`
  Description: If enabled, this flag causes well-tempered metadynamics as described by Barducci et al.[63] to be performed, rather than standard metadynamics. The parameter `biasTemperature` is then required.

- `biasTemperature` ⟨Temperature bias for well-tempered metadynamics⟩
  Context: `metadynamics`
  Acceptable values: positive decimal
  Description: When running metadynamics in the long time limit, collective variable space is sampled to a modified temperature $T+\Delta T$. In conventional metadynamics, the temperature "boost" ΔT would constantly increases with time. Instead, in well-tempered metadynamics ΔT must be defined by the user via `biasTemperature`. The written PMF includes the scaling factor $(T + \Delta T)/\Delta T$ [63]. A careful choice of ΔT determines the sampling and convergence rate, and is hence crucial to the success of a well-tempered metadynamics simulation.

Multiple-replicas metadynamics

The following options define metadynamics calculations with more than one replica:

- `multipleReplicas` ⟨Multiple replicas metadynamics⟩
  Context: `metadynamics`

Acceptable values: boolean
Default value: `off`
Description: If this option is `on`, multiple (independent) replica of the same system can be run at the same time, and their hills will be combined to obtain a single PMF [64]. Replicas are identified by the value of `replicaID`. Communication is done by files: each replica must be able to read the files created by the others, whose paths are communicated through the file `replicasRegistry`. This file, and the files listed in it, are read every `replicaUpdateFrequency` steps. Every time the colvars state file is written (`colvarsRestartFrequency`), the file:
"*outputName*`.colvars.`*name*`.`*replicaID*`.state`" is also written, containing the state of the metadynamics bias for `replicaID`. In the time steps between `colvarsRestartFrequency`, new hills are temporarily written to the file:
"*outputName*`.colvars.`*name*`.`*replicaID*`.hills`", which serves as communication buffer. These files are only required for communication, and may be deleted after a new MD run is started with a different `outputName`.

- `replicaID` ⟨Set the identifier for this replica⟩
Context: `metadynamics`
Acceptable values: string
Description: If `multipleReplicas` is `on`, this option sets a unique identifier for this replica. All replicas should use identical collective variable configurations, except for the value of this option.

- `replicasRegistry` ⟨Multiple replicas database file⟩
Context: `metadynamics`
Acceptable values: UNIX filename
Default value: "*name*`.replica_files.txt`"
Description: If `multipleReplicas` is `on`, this option sets the path to the replicas' database file.

- `replicaUpdateFrequency` ⟨How often hills are communicated between replicas⟩
Context: `metadynamics`
Acceptable values: positive integer
Default value: `newHillFrequency`
Description: If `multipleReplicas` is `on`, this option sets the number of steps after which each replica (re)reads the other replicas' files. The lowest meaningful value of this number is `newHillFrequency`. If access to the file system is significantly affecting the simulation performance, this number can be increased, at the price of reduced synchronization between replicas. Values higher than `colvarsRestartFrequency` may not improve performance significantly.

- `dumpPartialFreeEnergyFile` ⟨Periodically write the contribution to the PMF from this replica⟩
Context: `metadynamics`
Acceptable values: boolean
Default value: `on`
Description: When `multipleReplicas` is `on`, the file *outputName*`.pmf` contains the combined PMF from all replicas, provided that `useGrids` is `on` (default). Enabling this option

produces an additional file *outputName*`.partial.pmf`, which can be useful to quickly monitor the contribution of each replica to the PMF.

Compatibility and post-processing

The following options may be useful only for applications that go beyond the calculation of a PMF by metadynamics:

- `name` ⟨Name of this metadynamics instance⟩
  Context: `metadynamics`
  Acceptable values: string
  Default value: "`meta`" + rank number
  Description: This option sets the name for this metadynamics instance. While it is not advisable to use more than one metadynamics instance within the same simulation, this allows to distinguish each instance from the others. If there is more than one metadynamics instance, the name of this bias is included in the metadynamics output file names, such as e.g. the `.pmf` file.

- `keepHills` ⟨Write each individual hill to the state file⟩
  Context: `metadynamics`
  Acceptable values: boolean
  Default value: `off`
  Description: When `useGrids` and this option are `on`, all hills are saved to the state file in their analytic form, alongside their grids. This makes it possible to later use exact analytic Gaussians for `rebinGrids`. To only keep track of the history of the added hills, `writeHillsTrajectory` is preferable.

- `writeHillsTrajectory` ⟨Write a log of new hills⟩
  Context: `metadynamics`
  Acceptable values: boolean
  Default value: `on`
  Description: If this option is `on`, a logfile is written by the `metadynamics` bias, with the name "*outputName*`.colvars.<name>.hills.traj`", which can be useful to follow the time series of the hills. When `multipleReplicas` is `on`, its name changes to "*outputName*`.colvars.<name>.<replicaID>.hills.traj`". This file can be used to quickly visualize the positions of all added hills, in case `newHillFrequency` does not coincide with `colvarsRestartFrequency`.

13.5.4 Harmonic restraints

The harmonic biasing method may be used to enforce fixed or moving restraints, including variants of Steered and Targeted MD. Within energy minimization runs, it allows for restrained minimization, e.g. to calculate relaxed potential energy surfaces. In the context of the Colvars module, harmonic potentials are meant according to their textbook definition:

$$V(\xi) = \frac{1}{2} k \left(\frac{\xi - \xi_0}{w_\xi} \right)^2 \tag{13.25}$$

Note that this differs from harmonic bond and angle potentials in common force fields, where the factor of one half is typically omitted, resulting in a non-standard definition of the force constant.

The formula above includes the characteristic length scale w_ξ of the colvar ξ (keyword `width`, see 13.2.1) to allow the definition of a multi-dimensional restraint with a unified force constant:

$$V(\xi_1, \ldots, \xi_M) = \frac{1}{2} k \sum_{i=1}^{M} \left(\frac{\xi_i - \xi_0}{w_\xi} \right)^2 \tag{13.26}$$

If one-dimensional or homogeneous multi-dimensional restraints are defined, and there are no other uses for the parameter w_ξ, *the parameter* `width` *can be left at its default value of* 1.

A harmonic restraint is set up by a `harmonic {...}` block, which may contain (in addition to the standard option `colvars`) the following keywords:

- `name`: see definition of `name` (biasing and analysis methods)
- `colvars`: see definition of `colvars` (biasing and analysis methods)
- `outputEnergy`: see definition of `outputEnergy` (biasing and analysis methods)
- `forceConstant` ⟨ Scaled force constant (kcal/mol) ⟩
  Context: `harmonic`
  Acceptable values: positive decimal
  Default value: `1.0`
  Description: This defines a scaled force constant k for the harmonic potential (eq. 13.26). To ensure consistency for multidimensional restraints, it is divided internally by the square of the specific `width` for each colvar involved (which is 1 by default), so that all colvars are effectively dimensionless and of commensurate size. For instance, setting a scaled force constant of 10 kcal/mol acting on two colvars, an angle with a `width` of 5 degrees and a distance with a width of 0.5 Å, will apply actual force constants of 0.4 kcal/mol×degree^{-2} for the angle and 40 kcal/mol/Å^2 for the distance.
- `centers` ⟨ Initial harmonic restraint centers ⟩
  Context: `harmonic`
  Acceptable values: space-separated list of colvar values
  Description: The centers (equilibrium values) of the restraint, ξ_0, are entered here. The number of values must be the number of requested colvars. Each value is a decimal number if the corresponding colvar returns a scalar, a "`(x, y, z)`" triplet if it returns a unit vector or a vector, and a "`(q0, q1, q2, q3)`" quadruplet if it returns a rotational quaternion. If a colvar has periodicities or symmetries, its closest image to the restraint center is considered when calculating the harmonic potential.

Tip: A complex set of restraints can be applied to a system, by defining several colvars, and applying one or more harmonic restraints to different groups of colvars. In some cases, dozens of colvars can be defined, but their value may not be relevant: to limit the size of the colvars trajectory file, it may be wise to disable `outputValue` for such "ancillary" variables, and leave it enabled only for "relevant" ones.

Moving restraints: steered molecular dynamics

The following options allow to change gradually the centers of the harmonic restraints during a simulations. When the centers are changed continuously, a steered MD in a collective variable space is carried out.

- `targetCenters` ⟨Steer the restraint centers towards these targets⟩
  Context: `harmonic`
  Acceptable values: space-separated list of colvar values
  Description: When defined, the current `centers` will be moved towards these values during the simulation. By default, the centers are moved over a total of `targetNumSteps` steps by a linear interpolation, in the spirit of Steered MD. If `targetNumStages` is set to a nonzero value, the change is performed in discrete stages, lasting `targetNumSteps` steps *each*. This second mode may be used to sample successive windows in the context of an Umbrella Sampling simulation. When continuing a simulation run, the `centers` specified in the configuration file <`colvarsConfig`> are overridden by those saved in the restart file <`colvarsInput`>. To perform Steered MD in an arbitrary space of colvars, it is sufficient to use this option and enable `outputAppliedForce` within each of the colvars involved.

- `targetNumSteps` ⟨Number of steps for steering⟩
  Context: `harmonic`
  Acceptable values: positive integer
  Description: In single-stage (continuous) transformations, defines the number of MD steps required to move the restraint centers (or force constant) towards the values specified with `targetCenters` or `targetForceConstant`. After the target values have been reached, the centers (resp. force constant) are kept fixed. In multi-stage transformations, this sets the number of MD steps *per stage*.

- `outputCenters` ⟨Write the current centers to the trajectory file⟩
  Context: `harmonic`
  Acceptable values: boolean
  Default value: `off`
  Description: If this option is chosen and `colvarsTrajFrequency` is not zero, the positions of the restraint centers will be written to the trajectory file during the simulation. This option allows to conveniently extract the PMF from the colvars trajectory files in a steered MD calculation.

- `outputAccumulatedWork` ⟨Write the accumulated work of the moving restraint to the trajectory file⟩
  Context: `harmonic`
  Acceptable values: boolean
  Default value: `off`
  Description: If this option is chosen, `targetCenters` is defined, and `colvarsTrajFrequency` is not zero, the accumulated work from the beginning of the simulation will be written to the trajectory file. If the simulation has been continued from a previous state file, the previously accumulated work is included in the integral. This option allows to conveniently extract the PMF from the colvars trajectory files in a steered MD calculation.

Note on restarting moving restraint simulations: Information about the current step and stage of a simulation with moving restraints is stored in the restart file (state file). Thus, such simulations can be run in several chunks, and restarted directly using the same colvars configuration file. In case of a restart, the values of parameters such as `targetCenters`, `targetNumSteps`, etc. should not be changed manually.

Moving restraints: umbrella sampling

The centers of the harmonic restraints can also be changed in discrete stages: in this cases a one-dimensional umbrella sampling simulation is performed. The sampling windows in simulation are calculated in sequence. The colvars trajectory file may then be used both to evaluate the correlation times between consecutive windows, and to calculate the frequency distribution of the colvar of interest in each window. Furthermore, frequency distributions on a predefined grid can be automatically obtained by using the `histogram` bias (see 13.5.7).

To activate an umbrella sampling simulation, the same keywords as in the previous section can be used, with the addition of the following:

- `targetNumStages` ⟨ Number of stages for steering ⟩
  Context: `harmonic`
  Acceptable values: non-negative integer
  Default value: `0`
  Description: If non-zero, sets the number of stages in which the restraint centers or force constant are changed to their target values. If zero, the change is continuous. Each stage lasts `targetNumSteps` MD steps. To sample both ends of the transformation, the simulation should be run for `targetNumSteps` × (`targetNumStages` + 1).

Changing force constant

The force constant of the harmonic restraint may also be changed to equilibrate [65].

- `targetForceConstant` ⟨ Change the force constant towards this value ⟩
  Context: `harmonic`
  Acceptable values: positive decimal
  Description: When defined, the current `forceConstant` will be moved towards this value during the simulation. Time evolution of the force constant is dictated by the `targetForceExponent` parameter (see below). By default, the force constant is changed smoothly over a total of `targetNumSteps` steps. This is useful to introduce or remove restraints in a progressive manner. If `targetNumStages` is set to a nonzero value, the change is performed in discrete stages, lasting `targetNumSteps` steps *each*. This second mode may be used to compute the conformational free energy change associated with the restraint, within the FEP or TI formalisms. For convenience, the code provides an estimate of the free energy derivative for use in TI. A more complete free energy calculation (particularly with regard to convergence analysis), while not handled by the Colvars module, can be performed by post-processing the colvars trajectory, if `colvarsTrajFrequency` is set to a suitably small value. It should be noted, however, that restraint free energy calculations may be handled more efficiently by an indirect route, through the determination of a PMF for the restrained coordinate.[65]

- `targetForceExponent` ⟨ Exponent in the time-dependence of the force constant ⟩
  Context: `harmonic`
  Acceptable values: decimal equal to or greater than 1.0
  Default value: `1.0`
  Description: Sets the exponent, α, in the function used to vary the force constant as a function of time. The force is varied according to a coupling parameter λ, raised to the power α: $k_\lambda = k_0 + \lambda^\alpha (k_1 - k_0)$, where k_0, k_λ, and k_1 are the initial, current, and final

values of the force constant. The parameter λ evolves linearly from 0 to 1, either smoothly, or in `targetNumStages` equally spaced discrete stages, or according to an arbitrary schedule set with `lambdaSchedule`. When the initial value of the force constant is zero, an exponent greater than 1.0 distributes the effects of introducing the restraint more smoothly over time than a linear dependence, and ensures that there is no singularity in the derivative of the restraint free energy with respect to lambda. A value of 4 has been found to give good results in some tests.

- `targetEquilSteps` ⟨Number of steps discarded from TI estimate⟩
  Context: `harmonic`
  Acceptable values: positive integer
  Description: Defines the number of steps within each stage that are considered equilibration and discarded from the restraint free energy derivative estimate reported reported in the output.

- `lambdaSchedule` ⟨Schedule of lambda-points for changing force constant⟩
  Context: `harmonic`
  Acceptable values: list of real numbers between 0 and 1
  Description: If specified together with targetForceConstant, sets the sequence of discrete λ values that will be used for different stages.

13.5.5 Linear restraints

The linear restraint biasing method is used to minimally bias a simulation. There is generally a unique strength of bias for each CV center, which means you must know the bias force constant specifically for the center of the CV. This force constant may be found by using experiment directed simulation described in section 13.5.6. Please cite Pitera and Chodera when using [66].

- `name`: see definition of `name` (biasing and analysis methods)

- `colvars`: see definition of `colvars` (biasing and analysis methods)

- `forceConstant` ⟨Scaled force constant (kcal/mol)⟩
  Context: `linear`
  Acceptable values: positive decimal
  Default value: `1.0`
  Description: This defines a scaled force constant for the linear bias. To ensure consistency for multidimensional restraints, it is divided internally by the specific `width` for each colvar involved (which is 1 by default), so that all colvars are effectively dimensionless and of commensurate size.

- `centers` ⟨Initial linear restraint centers⟩
  Context: `linear`
  Acceptable values: space-separated list of colvar values
  Description: The centers (equilibrium values) of the restraint are entered here. The number of values must be the number of requested colvars. Each value is a decimal number if the corresponding colvar returns a scalar, a "`(x, y, z)`" triplet if it returns a unit vector or a vector, and a "`q0, q1, q2, q3)`" quadruplet if it returns a rotational quaternion. If a colvar has periodicities or symmetries, its closest image to the restraint center is considered when calculating the linear potential.

13.5.6 Adaptive Linear Bias/Experiment Directed Simulation

Experiment directed simulation applies a linear bias with a changing force constant. Please cite White and Voth [67] when using this feature. As opposed to that reference, the force constant here is scaled by the `width` corresponding to the biased colvar. In White and Voth, each force constant is scaled by the colvars set center. The bias converges to a linear bias, after which it will be the minimal possible bias. You may also stop the simulation, take the median of the force constants (ForceConst) found in the colvars trajectory file, and then apply a linear bias with that constant. All the notes about units described in sections 13.5.5 and 13.5.4 apply here as well. **This is not a valid simulation of any particular statistical ensemble and is only an optimization algorithm until the bias has converged**.

- `name`: see definition of `name` (biasing and analysis methods)
- `colvars`: see definition of `colvars` (biasing and analysis methods)
- `centers` ⟨ Collective variable centers ⟩
  Context: `alb`
  Acceptable values: space-separated list of colvar values
  Description: The desired center (equilibrium values) which will be sought during the adaptive linear biasing. The number of values must be the number of requested colvars. Each value is a decimal number if the corresponding colvar returns a scalar, a "`(x, y, z)`" triplet if it returns a unit vector or a vector, and a "`q0, q1, q2, q3)`" quadruplet if it returns a rotational quaternion. If a colvar has periodicities or symmetries, its closest image to the restraint center is considered when calculating the linear potential.
- `updateFrequency` ⟨ The duration of updates ⟩
  Context: `alb`
  Acceptable values: An integer
  Description: This is, N, the number of simulation steps to use for each update to the bias. This determines how long the system requires to equilibrate after a change in force constant ($N/2$), how long statistics are collected for an iteration ($N/2$), and how quickly energy is added to the system (at most, $A/2N$, where A is the `forceRange`). Until the force constant has converged, the method as described is an optimization procedure and not an integration of a particular statistical ensemble. It is important that each step should be uncorrelated from the last so that iterations are independent. Therefore, N should be at least twice the autocorrelation time of the collective variable. The system should also be able to dissipate energy as fast as $N/2$, which can be done by adjusting thermostat parameters. Practically, N has been tested successfully at significantly shorter than the autocorrelation time of the collective variables being biased and still converge correctly.
- `forceRange` ⟨ The expected range of the force constant in units of energy ⟩
  Context: `alb`
  Acceptable values: A space-separated list of decimal numbers
  Default value: 3 k_bT
  Description: This is largest magnitude of the force constant which one expects. If this parameter is too low, the simulation will not converge. If it is too high the simulation will waste time exploring values that are too large. A value of 3 k_bT has worked well in the systems presented as a first choice. This parameter is dynamically adjusted over the course of

a simulation. The benefit is that a bad guess for the forceRange can be corrected. However, this can lead to large amounts of energy being added over time to the system. To prevent this dynamic update, add `hardForceRange yes` as a parameter

- `rateMax` ⟨ The maximum rate of change of force constant ⟩
  Context: `alb`
  Acceptable values: A list of space-separated real numbers
  Description: This optional parameter controls how much energy is added to the system from this bias. Tuning this separately from the `updateFrequency` and `forceRange` can allow for large bias changes but with a low `rateMax` prevents large energy changes that can lead to instability in the simulation.

13.5.7 Multidimensional histograms

The `histogram` feature is used to record the distribution of a set of collective variables in the form of a N-dimensional histogram. It functions as a "collective variable bias", and is invoked by adding a `histogram` block to the Colvars configuration file.

As with any other biasing and analysis method, when a histogram is applied to an extended-system colvar (13.2.4), it accesses the value of the fictitious coordinate rather than that of the "true" colvar. A joint histogram of the "true" colvar and the fictitious coordinate may be obtained by specifying the colvar name twice in a row in the `colvars` parameter: the first instance will be understood as the "true" colvar, and the second, as the fictitious coordinate.

In addition to the common parameters `name` and `colvars` described above, a `histogram` block may define the following parameter:

- `name`: see definition of `name` (biasing and analysis methods)
- `colvars`: see definition of `colvars` (biasing and analysis methods)
- `outputFreq` ⟨ Frequency (in timesteps) at which the histogram files are refreshed ⟩
  Context: `histogram`
  Acceptable values: positive integer
  Default value: `colvarsRestartFrequency`
  Description: The histogram data are written to files at the given time interval. A value of 0 disables the creation of these files (**note:** all data to continue a simulation are still included in the state file).
- `outputFile` ⟨ Write the histogram to a file ⟩
  Context: `histogram`
  Acceptable values: UNIX filename
  Default value: *outputName*`.<name>.dat`
  Description: Name of the file containing histogram data (multicolumn format), which is written every `outputFreq` steps. For the special case of 2 variables, Gnuplot may be used to visualize this file.
- `outputFileDX` ⟨ Write the histogram to a file ⟩
  Context: `histogram`
  Acceptable values: UNIX filename
  Default value: *outputName*`.<name>.dat`

Description: Name of the file containing histogram data (OpenDX format), which is written every `outputFreq` steps. For the special case of 3 variables, VMD may be used to visualize this file.

- `gatherVectorColvars` ⟨ Treat vector variables as multiple observations of a scalar variable? ⟩
  Context: `histogram`
  Acceptable values: UNIX filename
  Default value: `off`
  Description: When this is set to `on`, the components of a multi-dimensional colvar (e.g. one based on `cartesian`, `distancePairs`, or a vector of scalar numbers given by `scriptedFunction`) are treated as multiple observations of a scalar variable. This results in the histogram being accumulated multiple times for each simulation step or iteration of `cv update`). When multiple vector variables are included in `histogram`, these must have the same length because their components are accumulated together. For example, if ξ, λ and τ are three variables of dimensions 5, 5 and 1, respectively, for each iteration 5 triplets (ξ_i, λ_i, τ) $(i = 1, \ldots 5)$ are accumulated into a 3-dimensional histogram.

- `weights` ⟨ Treat vector variables as multiple observations of a scalar variable? ⟩
  Context: `histogram`
  Acceptable values: list of space-separated decimals
  Default value: all weights equal to 1
  Description: When `gatherVectorColvars` is `on`, the components of each multi-dimensional colvar are accumulated with a different weight. For example, if x and y are two distinct `cartesian` variables defined on the same group of atoms, the corresponding 2D histogram can be weighted on a per-atom basis: to compute an electron density map, it is possible to use `weights [$sel get atomicnumber]` in the definition of `histogram`.

Grid definition for multidimensional histograms

Like the ABF and metadynamics biases, `histogram` uses the parameters `lowerBoundary`, `upperBoundary`, and `width` to define its grid. These values can be overridden if a configuration block `histogramGrid { ...}` is provided inside the configuration of `histogram`. The options supported inside this configuration block are:

- `lowerBoundaries` ⟨ Lower boundaries of the grid ⟩
  Context: `histogramGrid`
  Acceptable values: list of space-separated decimals
  Description: This option defines the lower boundaries of the grid, overriding any values defined by the `lowerBoundary` keyword of each colvar. Note that when `gatherVectorColvars` is `on`, each vector variable is automatically treated as a scalar, and a single value should be provided for it.

- `upperBoundaries`: analogous to `lowerBoundaries`

- `widths`: analogous to `lowerBoundaries`

13.5.8 Probability distribution-restraints

The `histogramRestraint` bias implements a continuous potential of many variables (or of a single high-dimensional variable) aimed at reproducing a one-dimensional statistical distribution that is

provided by the user. The M variables $(\xi_1, \ldots, \xi_M)$ are interpreted as multiple observations of a random variable ξ with unknown probability distribution. The potential is minimized when the histogram $h(\xi)$, estimated as a sum of Gaussian functions centered at $(\xi_1, \ldots, \xi_M)$, is equal to the reference histogram $h_0(\xi)$:

$$V(\xi_1, \ldots, \xi_M) = \frac{1}{2} k \int \left(h(\xi) - h_0(\xi)\right)^2 \mathrm{d}\xi \tag{13.27}$$

$$h(\xi) = \frac{1}{M\sqrt{2\pi\sigma^2}} \sum_{i=1}^{M} \exp\left(-\frac{(\xi - \xi_i)^2}{2\sigma^2}\right) \tag{13.28}$$

When used in combination with a `distancePairs` multi-dimensional variable, this bias implements the refinement algorithm against ESR/DEER experiments published by Shen *et al* [68].

This bias behaves similarly to the `histogram` bias with the `gatherVectorColvars` option, with the important difference that *all* variables are gathered, resulting in a one-dimensional histogram. Future versions will include support for multi-dimensional histograms.

The list of options is as follows:

- `name`: see definition of `name` (biasing and analysis methods)
- `colvars`: see definition of `colvars` (biasing and analysis methods)
- `outputEnergy`: see definition of `outputEnergy` (biasing and analysis methods)
- `lowerBoundary` ⟨ Lower boundary of the colvar grid ⟩
  Context: `histogramRestraint`
  Acceptable values: decimal
  Description: Defines the lowest end of the interval where the reference distribution $h_0(\xi)$ is defined. Exactly one value must be provided, because only one-dimensional histograms are supported by the current version.
- `upperBoundary`: analogous to `lowerBoundary`
- `width` ⟨ Width of the colvar grid ⟩
  Context: `histogramRestraint`
  Acceptable values: positive decimal
  Description: Defines the spacing of the grid where the reference distribution $h_0(\xi)$ is defined.
- `gaussianSigma` ⟨ Standard deviation of the approximating Gaussian ⟩
  Context: `histogramRestraint`
  Acceptable values: positive decimal
  Default value: $2 \times$ `width`
  Description: Defines the parameter σ in eq. 13.28.
- `forceConstant` ⟨ Force constant (kcal/mol) ⟩
  Context: `histogramRestraint`
  Acceptable values: positive decimal
  Default value: `1.0`
  Description: Defines the parameter k in eq. 13.27.

- `refHistogram` ⟨ Reference histogram $h_0(\xi)$ ⟩
  Context: `histogramRestraint`
  Acceptable values: space-separated list of M positive decimals
  Description: Provides the values of $h_0(\xi)$ consecutively. The mid-point convention is used, i.e. the first point that should be included is for $\xi =$ `lowerBoundary`+`width`/2. If the integral of $h_0(\xi)$ is not normalized to 1, $h_0(\xi)$ is rescaled automatically before use.

- `refHistogramFile` ⟨ Reference histogram $h_0(\xi)$ ⟩
  Context: `histogramRestraint`
  Acceptable values: UNIX file name
  Description: Provides the values of $h_0(\xi)$ as contents of the corresponding file (mutually exclusive with `refHistogram`). The format is that of a text file, with each line containing the space-separated values of ξ and $h_0(\xi)$. The same numerical conventions as `refHistogram` are used.

- `writeHistogram` ⟨ Periodically write the instantaneous histogram $h(\xi)$ ⟩
  Context: `metadynamics`
  Acceptable values: boolean
  Default value: `off`
  Description: If `on`, the histogram $h(\xi)$ is written every `colvarsRestartFrequency` steps to a file with the name *outputName*`.<name>.hist.dat`This is useful to diagnose the convergence of $h(\xi)$ against $h_0(\xi)$.

13.5.9 Scripted biases

Rather than using the biasing methods described above, it is possible to apply biases provided at run time as a Tcl script. This option, also available in NAMD, can be useful to test a new algorithm to be used in a MD simulation.

- `scriptedColvarForces` ⟨ Enable custom, scripted forces on colvars ⟩
  Context: global
  Acceptable values: boolean
  Default value: `off`
  Description: If this flag is enabled, a Tcl procedure named `calc_colvar_forces` accepting one parameter should be defined by the user. It is executed at each timestep, with the current step number as parameter, between the calculation of colvars and the application of bias forces. This procedure may use the `cv` command to access the values of colvars and apply forces on them, effectively defining custom collective variable biases.

Chapter 14

Customizing VMD Sessions

There are a number of ways to change the behavior of VMD from the default settings, both in how the program starts up and in how the program behaves during a session. This Chapter describes the data files, command-line options, and environment variables which are used to customize a VMD session.

These files control the initial appearance and behavior of VMD at the start, and may be customized to suit each user's particular tastes. Default versions of these files are placed in the VMD installation directory (On Unix this is usually `/usr/local/lib/vmd`, on Windows this defaults to `C:\Program Files\University of Illinois\VMD`). Each user may specify their own versions of some of these files, but 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 giving each user the option to change the default behavior however they choose.

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

1. Command-line options.
2. Environment variable settings.
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. The Installation Guide describes how to change these default values when compiling VMD.

14.1 VMD Command-Line Options

When started, the following command-line options may be given to VMD. Note that if a command-line option does not start with a dash (-), and is not part of another option, it is assumed to be a filename, and its extension is matched to the extension registered by the proper plugin. Thus, the Unix command

```
vmd molecule.pdb
```

will start VMD and load a molecule from the file `molecule.pdb`, while the command

```
vmd molecule.psf molecule.dcd
```

will load the corresponding structure and coordinate files into the same molecule. On the Windows platform, one must preface the VMD invocation with the Windows `start` command

```
start vmd molecule.pdb
```

- `-h | --help` : Print a summary a command-line options to the console.
- `-e filename` : After initialization, execute the text commands in filename, and then resume normal operation.
- `-python` : After initialization, switch to the Python interpreter before executing commands in the file specified by `-e` (if any), and leave the text interpreter in Python mode.
- `filename` : Load the specified file at startup. The file type will be determined from the filename extension; if there is no filename extension, and the filename contains 4 letters, it is assumed to be a PDB accession code and will be loaded accordingly; otherwise the format is assumed to be PDB.
- `-<filetype> filename` : Load the specified file using the given filetype.
- `-f` : Load all subsequent files into the same molecule. This is the default. A new molecule is created for each invocation of `-f`; thus, `vmd -f 1.pdb 2.pdb -f 3.pdb` loads `1.pdb and 2.pdb` into the same molecule and `3.pdb` into a different molecule.
- `-m` : Load all subsequent files into separate molecules. The `-f` and `-m` options may be specified multiple times on the command line in order to load multiple molecule containing one or more files.
- `-dispdev < win | text | cave | caveforms | none >` : Specify the type of graphical display to use. The possible display devices include:
  - `win`: a standard graphics display window.
  - `text`: do not provide any graphics display window.
  - `cave`: use the CAVE virtual environment for display, windows are disabled.
  - `caveforms`: use the CAVE virtual environment for display and with windows enabled. This is useful with `-display machine:0` for remote display of the windows when the CAVE uses the local screen.
  - `none`: same as text.

  It is possible to use VMD as a filter to convert coordinate files into rendered images, by using the `-dispdev text` and `-e` options.
- `-dist z` : Specify the distance to the VMD image plane.
- `-height y` : Specify the height of the VMD image plane.
- `-pos x y` : Specify the position for the graphics display window. The position (x,y) is the number of pixels from the lower-left corner of the display to the lower-left corner of the graphics window.
- `-size x y` : Specify the size for the graphics display window, in pixels.

- `-nt` : Do not display the VMD title at startup.
- `-eofexit` : Make VMD exit when EOF on stdin is reached; for example, when a script is redirected to VMD. The combination `vmd -dispdev text -eofexit < input.tcl > output.log` is useful for batch mode scripting.
- `-startup filename` : Use filename as the VMD startup command script, instead of the default **.vmdrc** or **vmd.rc** file.
- `-args` : Pass subsequent command line arguments to the text interpreter. The Tcl interpreter will store these arguments in the list variable `argv`. By default, no arguments are stored in this variable.
- `-debug [level` : Turn on output of debugging messages, and optionally set the current debug level (1=few messages ... 5=many verbose messages). Note this is only useful if VMD has been compiled with debugging option included.

14.2 Environment Variables

Several environment variables are used by VMD to determine the location of certain files and directories. These variables are accessible to text interface through array `env`. These variables include:

- `DISPLAY` : **(Unix-only)** The X-Windows display that VMD should use for displaying the VMD windows and menus, as well as the graphics window. If this environment variable is not overridden by VMDGDISPLAY all VMD windows will be directed to this display.
- `VMDDIR` : The directory which contains the VMD data files (such as this help file) and architecture-specific executables. By default, this is /usr/local/lib/vmd on Unix systems, and `C:\Program Files\University of Illinois\VMD` on Windows sytems.
- `VMDTMPDIR` : The directory which VMD should use for temporary data files. By default, this is /tmp, or /usr/tmp on Unix systems, and `C:\` on Windows.
- `VMDCUSTOMIZESTARTUP` : **(Unix-only)** The name of a C-shell script to source prior to running the actual VMD process. This shell script can contain any commands necessary for performing machine-specific spaceball, graphics, and other customizations necessary to run VMD. This can be anything from a simple script that sets the right serial port for a Spaceball based on the hostname, or it can be a complex script for turning on a projection system, logging demos, configuring multi-display stereo-framelock features, etc.
- `VMDBABELBIN` : The complete path and filename for the program babel, which is used by VMD to convert molecular structure/coordinates files into PDB files which VMD can actually understand. If this is not set explicitly, the VMD startup script will attempt to find babel in the current path. If Babel cannot be found or is not installed, VMD will not be able to read molecular file formats other than PDB, PSF, and binary DCD files.
- `VMDFILECHOOSER` : Specifies which file chooser to use for loading and saving files from the GUI. At present, this should be either FLTK, which uses Fltk's platform- independent file chooser, or TK, which uses Tk's file chooser. The Tk file chooser is the default and uses a

native Windows interface on Windows platforms. The Fltk file chooser looks the same on all platforms, supports tab completion but not drive letters, and is probably most appropriate for Unix environments. The file chooser can be overridden at any time by changing the environment variable (e.g., in Tcl, `set env(VMDFILECHOOSER) FLTK`).

- `VMDFORCECPUCOUNT` : Specifies the maximum number of CPUs or CPU cores that VMD should use when running on a multiprocessor or multicore computer system. By default, VMD will use all of the processors on the host machine. This option can be used to prevent VMD from "hogging" CPUs or to make it abide by job submission policies required on large supercomputer systems, when running batch mode.

- `VMDCAVEMEM` : **(Unix-only)** This overrides the default size of the shared memory arena which is allocated by VMD when the CAVE starts up. The variable must be an integer number of megabytes. Since this is the only shared memory pool allocated, and it is done only once, you must choose a value sufficient to account for the largest scene you intend to render in VMD in that CAVE session. The default value unless otherwise specified is 80 Megabytes. Values of 200MB to 512MB are commonly needed for large molecular systems containing several hundred thousand atoms.

- `VMDFREEVRMEM` : **(Unix-only)** This overrides the default size of the shared memory arena which is allocated by VMD when the FreeVR starts up. The variable must be an integer number of megabytes. Since this is the only shared memory pool allocated, and it is done only once, you must choose a value sufficient to account for the largest scene you intend to render in VMD in that FreeVR session. The default value unless otherwise specified is 80 Megabytes. Values of 200MB to 512MB are commonly needed for large molecular systems containing several hundred thousand atoms.

- `VMDFORCECONSOLETTY` : **(Unix-only, intended only for clusters** This environment variable forces VMD to treat the text console as an interactive terminal, despite what the operating system says. This is only useful for running an interactive VMD session on a Clustermatic or Scyld Linux cluster node.

- `VMDGDISPLAY` : **(Unix-only)** The name of an X-Windows display that VMD will use to display the graphics window. This environment variable is only used on Unix systems. Through the use of the the DISPLAY and VMDGDISPLAY envrironment variables, the VMD graphics window can be placed on a separate screen from the windows and menus. This is particularly useful when giving 3-D demonstrations using a projector. The windows and menus can be kept on a different screen from the graphics so that they do not distract the audience.

- `VMDGLSLVERBOSE` : OpenGL Shading language compiler diagnostic errors only printed only when this environment variable is set.

- `VMDHTMLVIEWER` : The name of a command that will run a web browser in the background (Netscape, Mozilla, Firefox or whatever you prefer) that VMD should use to display HTML documents (such as this help file). By default, on UNIX, this is mozilla. (usage examples in Tcl: `set env(VMDHTMLVIEWER) ‘‘mozilla -remote openURL(%s)"`, `set env(VMDHTMLVIEWER) ‘‘mozilla %s &"`)

- `VMDIMAGEVIEWER` : The name of the external program to use for displaying VMD snapshots (or other images), in various formats.

- `VMDIMMERSADESKFLIP` : Enable a special reversed/reflected stereo projection mode for use with experimental displays based on LCD panels, phase plates, and beam splitters.
- `VMDMACENABLEEEXTENSIONS` : Enable performance-oriented OpenGL rendering extensions which are disabled by default. These extensions have been observed to trigger instability on some MacOS X systems.
- `VMDMAXAASAMPLES` : Override the maximum requested OpenGL multisample antialiasing sample depth with a user-specified value. The VMD default is normally 8 samples per pixel. Some video cards exhibit poor performance with large numbers of antialiasing samples and must be restricted to 5 or fewer samples per pixel.
- `VMDMSECDELAYHACK` : Add in a user-specified delay which causes VMD to sleep for specified number of milliseconds each time it renders the molecular scene on the display. This feature is meant as a workaround to poor performing display drivers which make the windowing system unresponsive if VMD is allowed to run unrestricted at maximum drawing rate.
- `VMDMSMSUSEFILE` : Force VMD to communicate with MSMS through the filesystem rather than with the socket-based network interface. This option can be used when the socket interface isn't working properly for some reason. This is the default behavior when using VMD on Windows.
- `VMDNOCUDA` : Force VMD not to use CUDA-based GPU acceleration, even if CUDA support was compiled in, and CUDA-capable devices are detected at startup. This can be used in cases where a GPU or GPU drivers prove to be unreliable for computation, for benchmarking vs. CPU-only implementations, and to prevent VMD from using a GPU that's already oversubscribed by other processes running on the same machine.
- `VMDCUDADEVICEMASK` This environment variable limits VMD to running GPU-accelerated algorithms on a specific subset of GPUs, based on a hexadecimal mask. For example, to allow rendering on only the first two GPUs, one would set the mask to 0x3; to use only the second GPU, the mask would be set to 0x2.
- `VMDDISABLESTEREO` : **(Unix)** Prevents VMD from enabling stereoscopic display features. This is normally only used as a workaround for buggy display drivers.
- `VMDPREFERSTEREO` : **(Unix, MacOS X)** On Unix systems using X11, this environment variable allows NVidia Quadro users to override the normal X11 visual search order, skipping multisample capable visuals in favor of stereo visuals. VMD still attempts to get the more complex visuals first, but if it comes down to a choice between stereo and multisample as mutually exclusive options, this variable provides the ability to force the use of stereo if available. On MacOS X, this environment variable tells VMD to create a a stereo-capable display window, even at the risk of terminating the program if the request is denied.
- `VMDSCRDIST` : Distance to the VMD image plane.
- `VMDSCRHEIGHT` : Height of the VMD image plane.
- `VMDSCRPOS` : Position of the VMD graphics window (x,y).
- `VMDSCRSIZE` : Size of the VMD graphics window (x,y).

- VMD_EXCL_GL_EXTENSIONS : Disable the use of named OpenGL extensions according to their official OpenGL extension names. This is intended to be used only when one encounters severe stability problems caused by buggy display drivers.
- VMDSHEARSTEREO : Enable the use of an alternative perspective projection mode which may result in improved stereoscopic display. Uses the shear-matrix stereo formulation rather than eye rotation.
- VMDSIMPLEGRAPHICS : Forces VMD to use absolutely minimalistic graphics features with no use of OpenGL extensions. Essentially, nothing but bread-and-butter vertex arrays and immediate mode rendering will be used. This mode is intended to be used only when one encounters severe stability problems caused by buggy display drivers.
- VMDWIREGL : This environment variable disables several graphics features which are unsupported (or poorly supported) by WireGL and Chromium. This variable will be superceded with a more general implementation in a future release.
- VMDOPTIXDEVICE This environment variable limits VMD to performing OptiX GPU-accelerated ray tracing on a specific GPU.
- VMDOPTIXDEVICEMASK This environment variable limits VMD to performing OptiX GPU-accelerated ray tracing on a specific subset of GPUs, based on a hexadecimal mask. For example, to allow rendering on only the first two GPUs, one would set the mask to 0x3; to use only the second GPU, the mask would be set to 0x2.
- VMDOPTIXNODISPLAYGPUS This environment variable limits VMD to performing OptiX GPU-accelerated ray tracing on GPUs that are not attached to a display, to prevent long-running batch mode OptiX renderings from interfering with interactive VMD sessions or other desktop applications.
- VMDOPTIX_CLUSTER This environment variable sets the remote access URL for VMD OptiX renderings on remote NVIDIA VCA clusters.
- VMDOPTIXVCACONFIG This environment variable selects the VCA cluster rendering configuration index for VMD OptiX renderings on remote NVIDIA VCA clusters, e.g., to favor increased image-space parallel decomposition, or conversely for increased stochastic sampling performance.
- VMDOPTIXVCANODES The number of VCA cluster nodes to request for the interactive VMD OptiX rendering session.
- VMDOPTIX_USER This environment variable sets the remote access user name for VMD OptiX renderings on remote NVIDIA VCA clusters.
- VMDOPTIX_PASSWD This environment variable sets the remote access password for VMD OptiX renderings on remote NVIDIA VCA clusters.
- VMDOPTIXBITRATE This environment variable controls the bitrate used for remote video streaming when VMD performs interactive ray tracing on a remote NVIDIA VCA cluster. A good typical value for high resolution, e.g., 4K images would be 15000000.

- `VMDOPTIXBUILDER` This environment variable allows the default fast-but-memory-intensive "Trbvh" acceleration structure to be overridden by "MedianBvh" or other algorithms that aren't as fast, but require much less GPU memory when rendering hundreds of millions of objects that could otherwise cause GPU out-of-memory errors.
- `VMDOPTIXIMAGESIZE` This environment variable allows the user to forcibly override the resolution of the images to be rendered, ignoring the incoming image height and width parameters VMD would normally use. This variable is particularly useful when combining interactive ray tracing with VR HMDs, where the ray traced image dimensions should generally be more than 3× higher horizontal resolution than the VR HMD display, and at least 2× higher vertical resolution.
- `VMDOPTIXAOMAXDIST` This environment variable specifies a maximum occlusion distance in eye coordinates, rather than the default of infinity, for use when computing the ambient occlusion factor for a hit point. By setting this to a small to moderate value, the interior region of closed structures such as virus capsids will be lit with soft shadows as they would with conventional AO, both on the interior and exterior. Without the reduced occlusion distance cutoff, closed surfaces would fall entirely into shadow.
- `VMDOPTIXHEADLIGHT` This environment variable enables a positional light that is always located at the center of projection, useful for interiors of virus capsids and the like.
- `VMDOPTIXDOMEMASTER` This environment variable allows the user to forcibly override the currently active VMD 3-D projection mode (only "Orthographic" or "Perspective" are currently implemented in the OpenGL-based renderer), allowing the OptiX ray tracer to generate hemispherical images for so-called "fulldome" projection systems such as those typically used in digital planetariums.
- `VMDOPTIXEQUIRECTANGULAR` This environment variable allows the user to forcibly override the currently active VMD 3-D projection mode (only "Orthographic" or "Perspective" are currently implemented in the OpenGL-based renderer), allowing the OptiX ray tracer to generate omnidirectional VR movies, e.g. for YouTube.
- `VMDOPTIXSTEREO` This environment variable allows the user to forcibly override the currently active VMD stereoscopic 3-D projection mode allowing the OptiX ray tracer to generate stereoscopic omnidirectional VR movies, e.g. for YouTube.
- `VMDOSPRAYAOMAXDIST` This environment variable specifies a maximum occlusion distance in eye coordinates, rather than the default of infinity, for use when computing the ambient occlusion factor for a hit point. By setting this to a small to moderate value, the interior region of closed structures such as virus capsids will be lit with soft shadows as they would with conventional AO, both on the interior and exterior. Without the reduced occlusion distance cutoff, closed surfaces would fall entirely into shadow.
- `VMDOSPRAYMPI` This environment variable enables the use of the MPI distributed memory rendering mode of OSPRay if it was compiled into the OSPRay library in use by VMD.
- `VMDOSPRAYIMAGESIZE` This environment variable allows the user to forcibly override the resolution of the images to be rendered, ignoring the incoming image height and width parameters VMD would normally use. This environment variable makes it easy to renderer very large images without changing the VMD display resolution.

14.3 Startup Files

14.3.1 Core Script Files

In the following, the value of `$VMDDIR` is the vmd installation directory. During the original installation this is the value of `INSTALLLIBDIR`. It can also be found by looking at the first few lines of the vmd startup script (`head ‘which vmd‘`) or by starting VMD and using the command `set env(VMDDIR)`.

As mentioned elsewhere, VMD uses the Tcl interpreter. VMD read Tcl scripts at initialization, which are contained in VMD distribution. The locations of the scripts is determined by the `TCL_LIBRARY` environment variable, which is set in the vmd startup script to `$VMDDIR/scripts/tcl`. In addition, VMD has its own directory of core Tcl routines.

The most important of these is `$VMDDIR/scripts/vmd/vmdinit.tcl`. This file sets up the basic Tcl initialization commands, defines some environment variables, and adds the vmd script directory to the Tcl autoindex path. Most of the other files are referenced through the `auto_path`.

There are a few non-Tcl scripts in this directory. Currently these are perl scripts used for the `urlload` command and `web client` startup (see section 9.3.20 and section 14.4).

14.3.2 User Script Files

A user-written run-time command file, `.vmdrc` on Unix, `vmd.rc` on Windows, can be used with a list of initial VMD text commands to process. This file may be changed to customize individual user's initial screen appearance and to set the proper display characteristics for displaying in stereo. If it does not exist, default values are used.

14.3.3 `.vmdrc` and `vmd.rc` Files

After everything is initialized, VMD reads the *startup* file using the equivalent of the command `play .vmdrc`. 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.

VMD searches for this file in three locations on Unix; `./.vmdrc`, `$HOME/.vmdrc` and `$VMDDIR/.vmdrc`. On Windows, VMD searches in `./vmd.rc`, `$HOME/vmd.rc` and `$VMDDIR/vmd.rc`. Only the first file found will be read in and processed.

See chapter 9 for a description of the VMD text commands which may be put in this file. Also, section 5.1.3 discusses how to put commands into the `.vmdrc` file to customize the behavior of the hot keys.

Here is an example of a startup file:

```
# add personalized keyboard shortcuts
user add key E echo on
user add key e echo off
user add key g display reset
user add key A stage location bottom
user add key m mol list

# position the stage and axes
```

```
axes location lowerleft
stage location off

# position and turn on menus
menu main move 5 196
menu display move 386 90
menu graphics move 5 455
menu files move 5 496

menu main on

# start the scene a-rockin'
rock y by 1
```

14.4 Using VMD as a WWW Client (for chemical/* documents)

Mosaic, Netscape, and possibly other browsers can be configured to use VMD as a helper application for viewing some `chemical/*` documents.

14.4.1 MIME types

When a web browser receives a document from a server it actually gets two pieces of information: the header and the body. The header contains information about the message and body. One of the most important pieces of data, called the *MIME type* specifies what the body of text describes. For instance, a GIF image is given the MIME type of `image/gif`, a JPEG image is `image/jpg`, and postscript is `application/postscript`. A class of types, `chemical/*`, has been created for chemical models so the MIME type for PDB files is `chemical/pdb`, for XYZ is `chemical/xyz`, etc.

Helper Applications

The web browser uses the MIME type to determine how to view the body of the message. Some of the documents are viewed by the browser itself, like `text/html` which describes HTML documents. In other cases, the browser has to start up another application. From here on, we'll describe how Mosaic and Netscape do this. First, it saves the incoming message body to a temporary file. It then scans the global and local *mailcap* files to determine which application is used to view the given MIME type. The application, which must take a file name on the command line, is then executed. When the application exits, the temporary file is deleted.

14.4.2 Setting up your `.mailcap`

The Unix versions of VMD have an extra `-webhelper` command line flag which causes VMD not to be spawned in the background, so that it has time to read temporary files downloaded by the web browser. This command line flag is just slightly simpler to use than the `chemical2vmd` script, as it does not depend on having Perl installed, so may be more appropriate for some cases.

In the VMD installation directory ($VMDDIR/scripts/vmd/) there is a perl script called `chemical2vmd` which will create a VMD command file and execute VMD. Since VMD does not block the calling process, Netscape and other web browsers cannot directly call VMD, as they do not

know when to delete the temporary file containing the molecule or other data. The `chemical2vmd` script starts VMD with the -e command line option which runs the saved VMD script or molecule file.

It is also possible to install the previous script in the global `.mailcap` file to make it accessible to everyone. You will have to consult the documentation for your web browser(s) to find out how.

14.4.3 Example sites

Some web sites that send `chemical/pdb` types are the Protein Data Bank at `http://www.rcsb.org/` and "Molecules R US" at `http://www.nih.gov/htbin/pdb`.

Bibliography

[1] William Humphrey, Andrew Dalke, and Klaus Schulten. VMD – Visual Molecular Dynamics. *J. Mol. Graphics*, 14:33–38, 1996.

[2] R. Sharma, T. S. Huang, V. I. Pavlovic, K. Schulten, A. Dalke, J. Phillips, M. Zeller, W. Humphrey, Y. Zhao, Z. Lo, and S. Chu. Speech/gesture interface to a visual computing environment for molecular biologists. In *Proceedings of 13th ICPR 96*, volume 3, pages 964–968, 1996.

[3] Rajeev Sharma, Michael Zeller, Vladimir I. Pavlovic, Thomas S. Huang, Zion Lo, Stephen Chu, Yunxin Zhao, James C. Phillips, and Klaus Schulten. Speech/gesture interface to a visual-computing environment. *IEEE Comp. Graph. App.*, 20:29–37, 2000.

[4] Simon Cross, Michelle M. Kuttell, John E. Stone, and James E. Gain. Visualization of cyclic and multi-branched molecules with VMD. *J. Mol. Graph. Model.*, 28:131–139, 2009.

[5] John E. Stone, Axel Kohlmeyer, Kirby L. Vandivort, and Klaus Schulten. Immersive molecular visualization and interactive modeling with commodity hardware. *Lect. Notes in Comp. Sci.*, 6454:382–393, 2010.

[6] John E. Stone, Kirby L. Vandivort, and Klaus Schulten. Immersive out-of-core visualization of large-size and long-timescale molecular dynamics trajectories. *Lect. Notes in Comp. Sci.*, 6939:1–12, 2011.

[7] John E. Stone, William R. Sherman, and Klaus Schulten. Immersive molecular visualization with omnidirectional stereoscopic ray tracing and remote rendering. *2016 IEEE International Parallel and Distributed Processing Symposium Workshop (IPDPSW)*, pages 1048–1057, 2016.

[8] Michael Zeller, James C. Phillips, Andrew Dalke, William Humphrey, Klaus Schulten, Rajeev Sharma, T. S. Huang, V. I. Pavlovic, Y. Zhao, Z. Lo, and S. Chu. A visual computing environment for very large scale biomolecular modeling. In *Proceedings of the 1997 IEEE International Conference on Application-specific Systems, Architectures and Processors (ASAP)*, pages 3–12. IEEE Computer Society Press, 1997.

[9] John E. Stone, Justin Gullingsrud, Paul Grayson, and Klaus Schulten. A system for interactive molecular dynamics simulation. In John F. Hughes and Carlo H. Séquin, editors, *2001 ACM Symposium on Interactive 3D Graphics*, pages 191–194, New York, 2001. ACM SIGGRAPH.

[10] Matthieu Chavent, Tyler Reddy, Joseph Goose, Anna Caroline E. Dahl, John E. Stone, Bruno Jobard, and Mark S.P. Sansom. Methodologies for the analysis of instantaneous lipid diffusion in MD simulations of large membrane systems. *Faraday Discuss.*, 169:455–475, 2014.

[11] Benjamin G. Levine, John E. Stone, and Axel Kohlmeyer. Fast analysis of molecular dynamics trajectories with graphics processing units–radial distribution function histogramming. *J. Comp. Phys.*, 230:3556–3569, 2011.

[12] John Stone and Mark Underwood. Rendering of numerical flow simulations using MPI. In *Second MPI Developer's Conference*, pages 138–141. IEEE Computer Society Technical Committee on Distributed Processing, IEEE Computer Society Press, 1996.

[13] John E. Stone. *An Efficient Library for Parallel Ray Tracing and Animation*. Master's thesis, Computer Science Department, University of Missouri-Rolla, April 1998.

[14] John E. Stone, Barry Isralewitz, and Klaus Schulten. Early experiences scaling VMD molecular visualization and analysis jobs on Blue Waters. In *Extreme Scaling Workshop (XSW), 2013*, pages 43–50, Aug. 2013.

[15] I. Wald, G. Johnson, J. Amstutz, C. Brownlee, A. Knoll, J. Jeffers, J. Gunther, and P. Navratil. OSPRay – a CPU ray tracing framework for scientific visualization. *IEEE Transactions on Visualization and Computer Graphics*, 23(1):1–1, 2017.

[16] John E. Stone, James C. Phillips, Peter L. Freddolino, David J. Hardy, Leonardo G. Trabuco, and Klaus Schulten. Accelerating molecular modeling applications with graphics processors. *J. Comp. Chem.*, 28:2618–2640, 2007.

[17] John D. Owens, Mike Houston, David Luebke, Simon Green, John E. Stone, and James C. Phillips. GPU computing. *Proc. IEEE*, 96:879–899, 2008.

[18] Christopher I. Rodrigues, David J. Hardy, John E. Stone, Klaus Schulten, and Wen-mei W. Hwu. GPU acceleration of cutoff pair potentials for molecular modeling applications. In *CF'08: Proceedings of the 2008 conference on Computing Frontiers*, pages 273–282, New York, NY, USA, 2008. ACM.

[19] David J. Hardy, John E. Stone, and Klaus Schulten. Multilevel summation of electrostatic potentials using graphics processing units. *J. Paral. Comp.*, 35:164–177, 2009.

[20] Volodymyr Kindratenko, Jeremy Enos, Guochun Shi, Michael Showerman, Galen Arnold, John E. Stone, James Phillips, and Wen-mei Hwu. GPU clusters for high performance computing. In *Cluster Computing and Workshops, 2009. CLUSTER '09. IEEE International Conference on*, pages 1–8, 2009.

[21] John E. Stone, David J. Hardy, Ivan S. Ufimtsev, and Klaus Schulten. GPU-accelerated molecular modeling coming of age. *J. Mol. Graph. Model.*, 29:116–125, 2010.

[22] John E. Stone, David Gohara, and Guochun Shi. OpenCL: A parallel programming standard for heterogeneous computing systems. *Comput. in Sci. and Eng.*, 12:66–73, 2010.

[23] Jeremy Enos, Craig Steffen, Joshi Fullop, Michael Showerman, Guochun Shi, Kenneth Esler, Volodymyr Kindratenko, John E. Stone, and James C. Phillips. Quantifying the impact of GPUs on performance and energy efficiency in HPC clusters. In *International Conference on Green Computing*, pages 317–324, 2010.

[24] John E. Stone, David J. Hardy, Barry Isralewitz, and Klaus Schulten. GPU algorithms for molecular modeling. In Jack Dongarra, David A. Bader, and Jakub Kurzak, editors, *Scientific Computing with Multicore and Accelerators*, chapter 16, pages 351–371. Chapman & Hall/CRC Press, 2011.

[25] David J. Hardy, Zhe Wu, James C. Phillips, John E. Stone, Robert D. Skeel, and Klaus Schulten. Multilevel summation method for electrostatic force evaluation. *J. Chem. Theor. Comp.*, 11:766–779, 2015.

[26] John E. Stone, Ryan McGreevy, Barry Isralewitz, and Klaus Schulten. GPU-accelerated analysis and visualization of large structures solved by molecular dynamics flexible fitting. *Faraday Discuss.*, 169:265–283, 2014.

[27] Abhishek Singharoy, Ivan Teo, Ryan McGreevy, John E. Stone, Jianhua Zhao, and Klaus Schulten. Molecular dynamics-based refinement and validation with Resolution Exchange MDFF for sub-5 Å cryo-electron microscopy maps. *eLife*, 10.7554/eLife.16105, 2016. (66 pages).

[28] John E. Stone, Juan R. Perilla, C. Keith Cassidy, and Klaus Schulten. GPU-accelerated molecular dynamics clustering analysis with OpenACC. In Robert Farber, editor, *Parallel Programming with OpenACC*, pages 215–240. Morgan Kaufmann, Cambridge, MA, 2016.

[29] John E. Stone, Jan Saam, David J. Hardy, Kirby L. Vandivort, Wen-mei W. Hwu, and Klaus Schulten. High performance computation and interactive display of molecular orbitals on GPUs and multi-core CPUs. In *Proceedings of the 2nd Workshop on General-Purpose Processing on Graphics Processing Units, ACM International Conference Proceeding Series*, volume 383, pages 9–18, New York, NY, USA, 2009. ACM.

[30] John E. Stone, David J. Hardy, Jan Saam, Kirby L. Vandivort, and Klaus Schulten. GPU-accelerated computation and interactive display of molecular orbitals. In Wen-mei Hwu, editor, *GPU Computing Gems*, chapter 1, pages 5–18. Morgan Kaufmann Publishers, 2011.

[31] John E. Stone, Michael J. Hallock, James C. Phillips, Joseph R. Peterson, Zaida Luthey-Schulten, and Klaus Schulten. Evaluation of emerging energy-efficient heterogeneous computing platforms for biomolecular and cellular simulation workloads. *2016 IEEE International Parallel and Distributed Processing Symposium Workshop (IPDPSW)*, pages 89–100, 2016.

[32] John E. Stone, Antti-Pekka Hynninen, James C. Phillips, and Klaus Schulten. Early experiences porting the NAMD and VMD molecular simulation and analysis software to GPU-accelerated OpenPOWER platforms. *Lect. Notes in Comp. Sci.*, 9945:188–206, 2016.

[33] Michael Krone, John E. Stone, Thomas Ertl, and Klaus Schulten. Fast visualization of Gaussian density surfaces for molecular dynamics and particle system trajectories. In *EuroVis - Short Papers 2012*, pages 67–71, 2012.

[34] Elijah Roberts, John E. Stone, and Zaida Luthey-Schulten. Lattice microbes: High-performance stochastic simulation method for the reaction-diffusion master equation. *J. Comp. Chem.*, 34:245–255, 2013.

[35] John E. Stone, Kirby L. Vandivort, and Klaus Schulten. GPU-accelerated molecular visualization on petascale supercomputing platforms. In *Proceedings of the 8th International Workshop on Ultrascale Visualization*, UltraVis '13, pages 6:1–6:8, New York, NY, USA, 2013. ACM.

[36] Melih Sener, John E. Stone, Angela Barragan, Abhishek Singharoy, Ivan Teo, Kirby L. Vandivort, Barry Isralewitz, Bo Liu, Boon Chong Goh, James C. Phillips, Lena F. Kourkoutis, C. Neil Hunter, and Klaus Schulten. Visualization of energy conversion processes in a light harvesting organelle at atomic detail. In *Proceedings of the International Conference on High Performance Computing, Networking, Storage and Analysis*, SC '14. IEEE Press, 2014.

[37] Juan R. Perilla, Boon Chong Goh, John Stone, and Klaus Schulten. Chemical visualization of human pathogens: the Retroviral Capsids. *Proceedings of the 2015 ACM/IEEE Conference on Supercomputing*, 2015. (4 pages).

[38] John E. Stone, Melih Sener, Kirby L. Vandivort, Angela Barragan, Abhishek Singharoy, Ivan Teo, Joao V. Ribeiro, Barry Isralewitz, Bo Liu, Boon Chong Goh, James C. Phillips, Craig MacGregor-Chatwin, Matthew P. Johnson, Lena F. Kourkoutis, C. Neil Hunter, and Klaus Schulten. Atomic detail visualization of photosynthetic membranes with GPU-accelerated ray tracing. *Parallel Computing*, 55:17–27, 2016.

[39] Steven G. Parker, James Bigler, Andreas Dietrich, Heiko Friedrich, Jared Hoberock, David Luebke, David McAllister, Morgan McGuire, Keith Morley, Austin Robison, and Martin Stich. OptiX: a general purpose ray tracing engine. In *ACM SIGGRAPH 2010 papers*, SIGGRAPH '10, pages 66:1–66:13, New York, NY, USA, 2010. ACM.

[40] James C. Phillips, John E. Stone, Kirby L. Vandivort, Timothy G. Armstrong, Justin M. Wozniak, Michael Wilde, and Klaus Schulten. Petascale Tcl with NAMD, VMD, and Swift/T. In *SC'14 workshop on High Performance Technical Computing in Dynamic Languages*, SC '14. IEEE Press, 2014.

[41] Mark D. Klein and John E. Stone. Unlocking the full potential of the Cray XK7 accelerator. In *Cray User Group Conf.* Cray, May 2014.

[42] John E. Stone, Peter Messmer, Robert Sisneros, and Klaus Schulten. High performance molecular visualization: In-situ and parallel rendering with EGL. *2016 IEEE International Parallel and Distributed Processing Symposium Workshop (IPDPSW)*, pages 1014–1023, 2016.

[43] En Cai, Pinghua Ge, Sang Hak Lee, Okunola Jeyifous, Yong Wang, Yanxin Liu, Katie Wilson, Sung Jun Lim, Michelle Baird, John Stone, Kwan Young Lee, Michael Davidson, Hee Jung Chung, Klaus Schulten, Andrew Smith, William Green, and Paul R. Selvin. Stable small quantum dots for synaptic receptor tracking on live neurons. *Angew. Chem. Int. Ed. Engl.*, 126:12692–12696, 2014.

[44] G. Fiorin, M. L. Klein, and J. Hénin. Using collective variables to drive molecular dynamics simulations. *Mol. Phys.*, 111(22-23):3345–3362, 2013.

[45] M. Iannuzzi, A. Laio, and M. Parrinello. Efficient exploration of reactive potential energy surfaces using car-parrinello molecular dynamics. *Phys. Rev. Lett.*, 90(23):238302, 2003.

[46] E A Coutsias, C Seok, and K A Dill. Using quaternions to calculate RMSD. *J. Comput. Chem.*, 25(15):1849–1857, 2004.

[47] Yuguang Mu, Phuong H. Nguyen, and Gerhard Stock. Energy landscape of a small peptide revealed by dihedral angle principal component analysis. *Proteins*, 58(1):45–52, 2005.

[48] Alexandros Altis, Phuong H. Nguyen, Rainer Hegger, and Gerhard Stock. Dihedral angle principal component analysis of molecular dynamics simulations. *J. Chem. Phys.*, 126(24):244111, 2007.

[49] Nicholas M Glykos. Carma: a molecular dynamics analysis program. *J. Comput. Chem.*, 27(14):1765–1768, 2006.

[50] Davide Branduardi, Francesco Luigi Gervasio, and Michele Parrinello. From a to b in free energy space. *J Chem Phys*, 126(5):054103, 2007.

[51] Eric Darve, David Rodríguez-Gómez, and Andrew Pohorille. Adaptive biasing force method for scalar and vector free energy calculations. *J. Chem. Phys.*, 128(14):144120, 2008.

[52] J. Hénin and C. Chipot. Overcoming free energy barriers using unconstrained molecular dynamics simulations. *J. Chem. Phys.*, 121:2904–2914, 2004.

[53] J. Hénin, G. Fiorin, C. Chipot, and M. L. Klein. Exploring multidimensional free energy landscapes using time-dependent biases on collective variables. *J. Chem. Theory Comput.*, 6(1):35–47, 2010.

[54] A. Carter, E, G. Ciccotti, J. T. Hynes, and R. Kapral. Constrained reaction coordinate dynamics for the simulation of rare events. *Chem. Phys. Lett.*, 156:472–477, 1989.

[55] M. J. Ruiz-Montero, D. Frenkel, and J. J. Brey. Efficient schemes to compute diffusive barrier crossing rates. *Mol. Phys.*, 90:925–941, 1997.

[56] W. K. den Otter. Thermodynamic integration of the free energy along a reaction coordinate in cartesian coordinates. *J. Chem. Phys.*, 112:7283–7292, 2000.

[57] Giovanni Ciccotti, Raymond Kapral, and Eric Vanden-Eijnden. Blue moon sampling, vectorial reaction coordinates, and unbiased constrained dynamics. *ChemPhysChem*, 6(9):1809–1814, 2005.

[58] A. Lesage, T. Lelièvre, G. Stoltz, and J. Hénin. Smoothed biasing forces yield unbiased free energies with the extended-system adaptive biasing force method. *J. Phys. Chem. B.* (submitted).

[59] A. Laio and M. Parrinello. Escaping free-energy minima. *Proc. Natl. Acad. Sci. USA*, 99(20):12562–12566, 2002.

[60] Helmut Grubmüller. Predicting slow structural transitions in macromolecular systems: Conformational flooding. *Phys. Rev. E*, 52(3):2893–2906, Sep 1995.

[61] T. Huber, A. E. Torda, and W.F. van Gunsteren. Local elevation - A method for improving the searching properties of molecular-dynamics simulation. *Journal of Computer-Aided Molecular Design*, 8(6):695–708, DEC 1994.

[62] G. Bussi, A. Laio, and M. Parrinello. Equilibrium free energies from nonequilibrium metadynamics. *Phys. Rev. Lett.*, 96(9):090601, 2006.

[63] Alessandro Barducci, Giovanni Bussi, and Michele Parrinello. Well-tempered metadynamics: A smoothly converging and tunable free-energy method. *Phys. Rev. Lett.*, 100:020603, 2008.

[64] P. Raiteri, A. Laio, F. L. Gervasio, C. Micheletti, and M. Parrinello. Efficient reconstruction of complex free energy landscapes by multiple walkers metadynamics. *J. Phys. Chem. B*, 110(8):3533–9, 2005.

[65] Yuqing Deng and Benoît Roux. Computations of standard binding free energies with molecular dynamics simulations. *J. Phys. Chem. B*, 113(8):2234–2246, 2009.

[66] Jed W. Pitera and John D. Chodera. On the use of experimental observations to bias simulated ensembles. *J. Chem. Theory Comput.*, 8:3445–3451, 2012.

[67] A. D. White and G. A. Voth. Efficient and minimal method to bias molecular simulations with experimental data. *J. Chem. Theory Comput.*, ASAP, 2014.

[68] Rong Shen, Wei Han, Giacomo Fiorin, Shahidul M Islam, Klaus Schulten, and Benoît Roux. Structural refinement of proteins by restrained molecular dynamics simulations with non-interacting molecular fragments. *PLoS Comput. Biol.*, 11(10):e1004368, 2015.