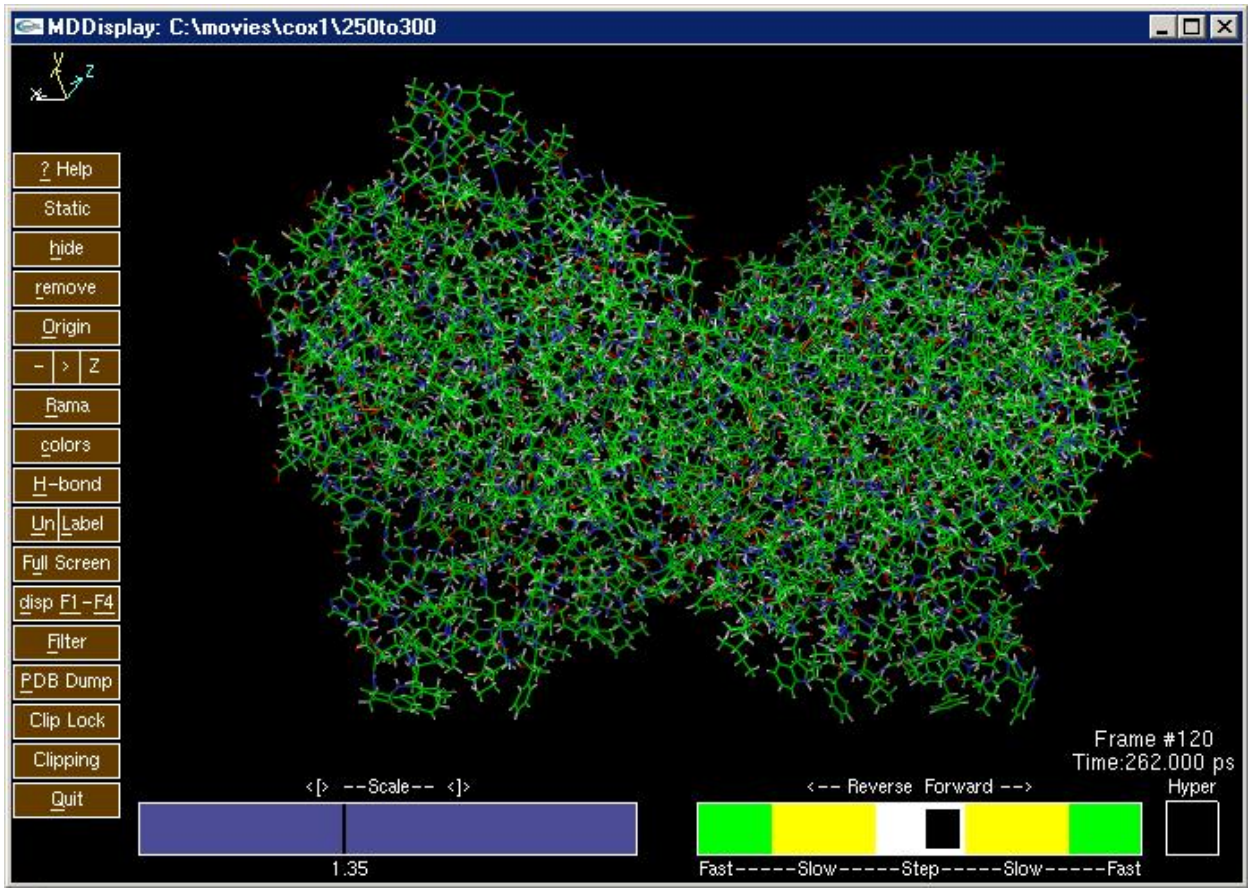
MD Display Version 3.0



Chris Moth, Tim Callahan, Eric Swanson, and Terry Lybrand

Vanderbilt University
Nashville, TN

http://www.structbio.vanderbilt.edu/~cmoth/mddisplay

TABLE OF CONTENTS

Introduction & Overview

Based on the design of MD Display version 2.0[1], MD Display version 3.0 turns molecular dynamics trajectory data into a colorful, animated, on-screen movie.

Key features of the package include:

- Mouse control of translation, rotation, scaling, and clipping
- Stereoscopic visualization through both legacy SGI split-buffer stereo and newer quad-buffered stereo hardware
- Half-bond coloring controls
- Animation speed and direction controls
- Dynamic monitoring of distances, bond angles, dihedrals, and hydrogen bonds
- Superimposition of static initial or average reference structures.
- Ramachandron plots
- Real-time filtering of higher frequency molecular motions
- PDB dump feature, for extracting movie frames on-the-fly
- Runs on SGI IRIX™, Microsoft Windows 95™ and higher, Linux, DEC UNIX, and other platforms with a complete implementation of the Ansi C Graphics Library Utility Toolkit[2]

MD Display consists primarily of two executable programs: *preproc* and *display*.

The **preproc**essor reads ASCII data from such sources as AMBER[3] prmtop and molecular dynamics coordinate files and outputs binary files optimized for movie viewing.

display reads preproc output, and provides the complete 3D movie user interface.

Additional utility programs in the package aid in the analysis of data, as well as the translation of alternate data sources.

Tutorial

This tutorial assumes that you have already created some AMBER trajectory data that you would like to visualize and analyze.

You will have:

1) Used AMBER's LEAP (or XLEAP) program and a command like:

```
saveAmberParm mymodel model.prmtop model.prmcrd
```

to create a prmtop file which lists all the residues, atoms, etc. in your simulation.

2) Used AMBER's SANDER tool with imin=0 in the min.in file and the

```
-x md.crd
```

command line option to create an ASCII file of movie frame-like atom coordinates.

With these output files from AMBER, you are ready to run preproc and then display.

First, preproc your movie coordinates with the command:

```
preproc –p model.prmtop –c md.crd –n movie
```

Preproc will display each frame number on the screen as it is read. (By default, preproc stops after reading 100 frames or reaching the end of the coordinate file, whichever comes first. To preproc more frames, add the `–f nnn` option to the command above).

Then binary, platform dependent output files are created:

movie.attr: the coloring of each atom, as well as labels for each atom and residue

movie.bnd: the list of bonded atoms

movie.cor: the md.crd coordinates scaled to two byte binary (short) integers.

To view the molecular dynamics data saved in these binary files, type:

```
mddisplay –n movie
```

Prior to displaying graphics, MD Display will show a splash screen and ask a few questions about your movie, starting with optional initial coloring:

```
_________ Initial coloring of residues & atoms _________

           0) invisible (remove)       1) white
           2) red                      3) blue
           4) aqua                     5) green
           6) magenta                  7) orange
           8) yellow                   9) gray
          98) each molecule a different color
          99) or <b>: automatic color by atom type

Enter optional initial coloring (0-99 or <b>) or press <ENTER> :
```

For now type <b><ENTER> to color oxygen red, hydrogen white, carbon green, etc. You will next be asked:

```
Enter #mol:res@atoms -->
```

Enter #*<ENTER> to color everything. Press <ENTER> one more time when the color menu appears for the second time. Initial coloring is now complete.

You will then be prompted:

```
Time interval per frame (picoseconds) :
```

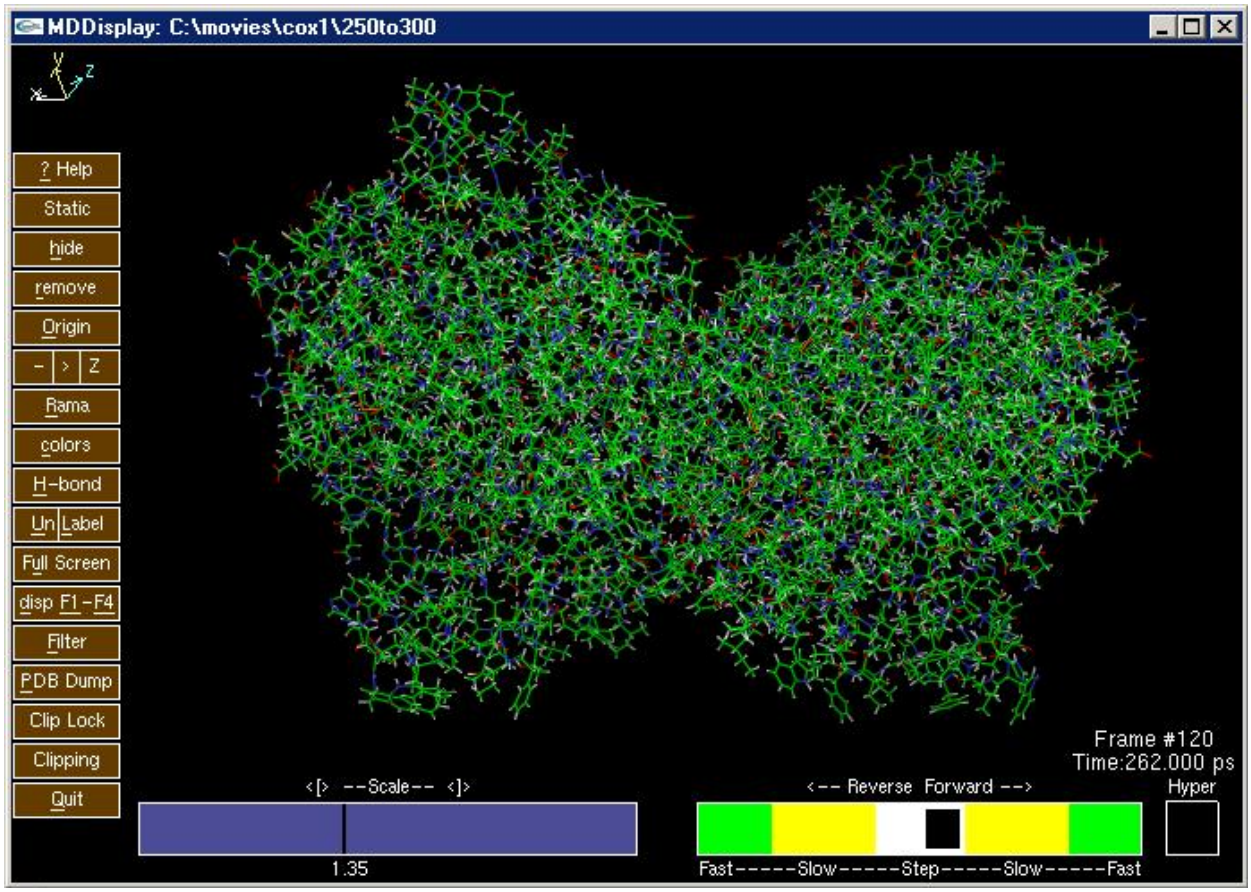
You are welcome to just press <ENTER>. Or, if you know that, for example, your AMBER (Sander) output consists of a frame every 100 ps, type 100<ENTER>.

You will finally be prompted for the

```
Initial offset (picoseconds) :
```

Again, you are welcome to just press <ENTER>. Or, you can enter the simulation time, in picoseconds, at which the current dataset starts.

After the binary files have been loaded into memory, the movie will begin:

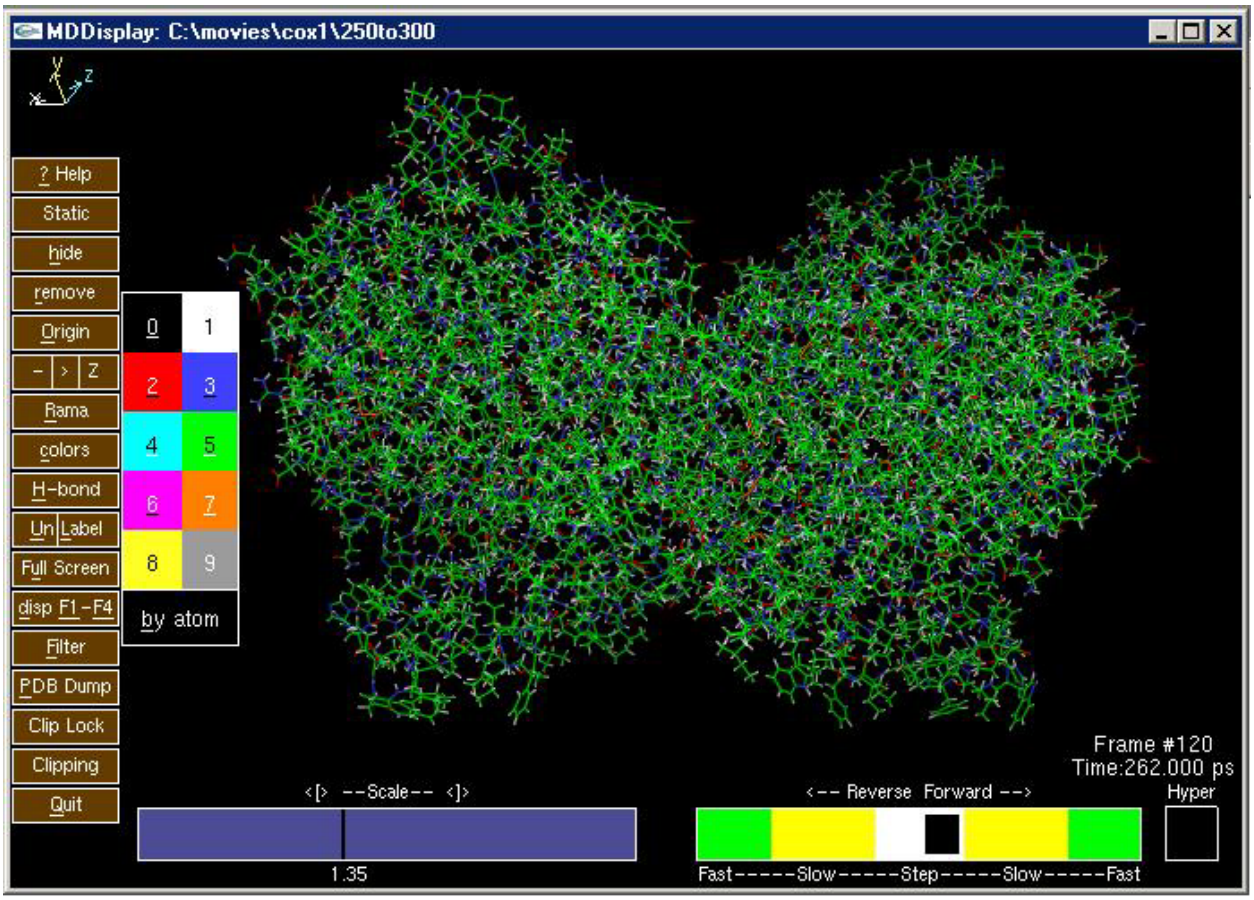


Notice that the left side of the display window contains a number of rectangular brown menu buttons. You can click on these to initiate actions. In cases where an underlined letter is shown, as in the menu button for "color", you can simply type the indicated letter instead of clicking. Note that MD Display is **case sensitive** with these menu button letter equivalents.

On the lower right side of the window, there is a green, yellow, and white bar for controlling the speed and direction of the movie. Click on the white "--Step--" area in this bar. The animation will pause.

To reduce the image to the protein backbone (thereby removing some visual clutter) press the lower case letter <c> or click on the 

menu box on the left side of the screen. You will see a color palette appear next to the brown menus:



Click on the black square of the color palette or type <0> (zero). You will be prompted for the areas of the molecule that you want to color black (invisible):

It takes a little practice to get used to the way that molecules, residues, and atoms are specified.

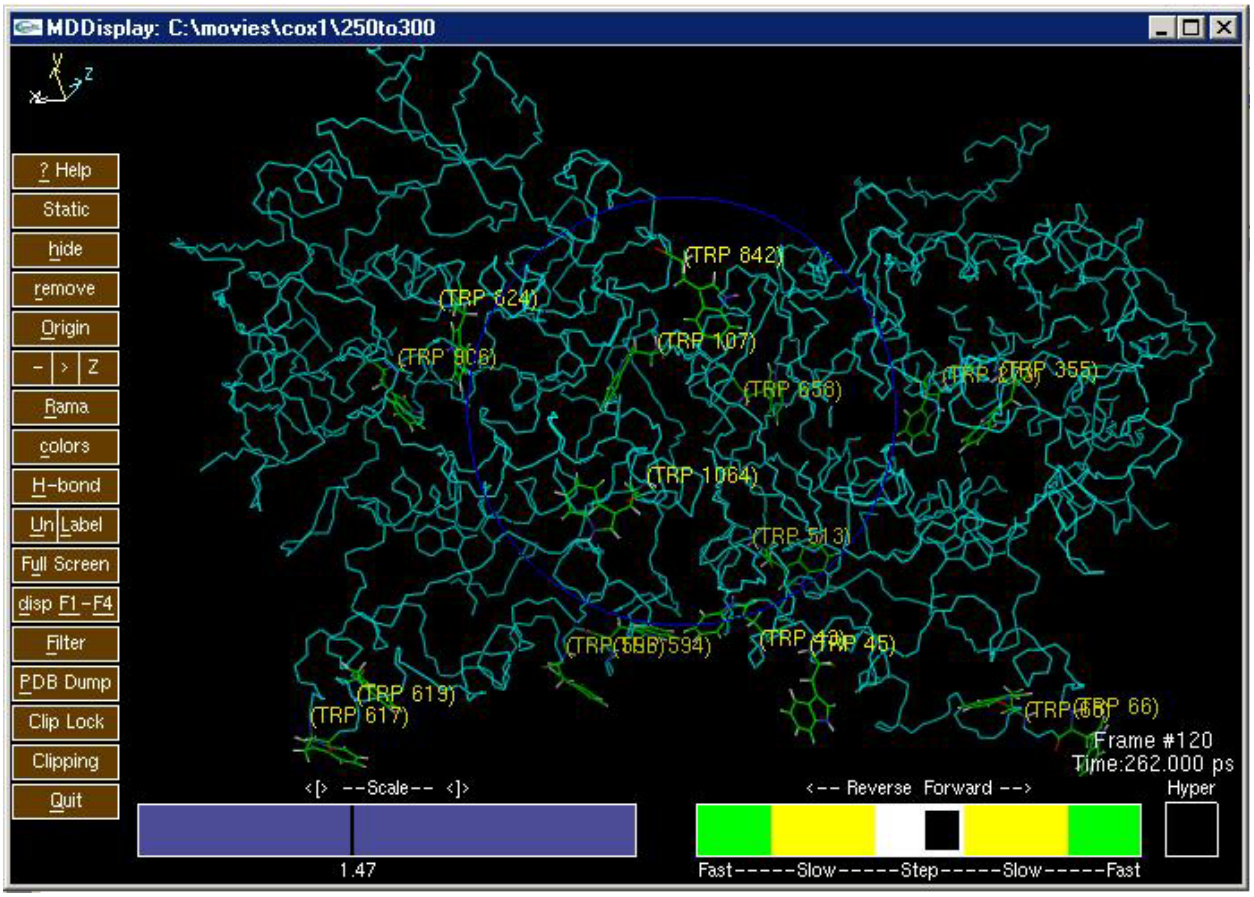
For now, type

@sc<ENTER>

This command will cause all side chains to be colored black (invisible). Now, press the number <4> to select aqua color. Let's color the backbone of the protein. Type

@bb<ENTER>.

Finally, let's color the Trp residues "by atom" and label them. Press <b> for "by atom" and then type **:TRP<ENTER>** when prompted. Press <L> or click on the Label menu box. Again, when prompted, type **:TRP<ENTER>.** Depending on the protein you are viewing, you might now see some labeled Tryptophan residues as in:



To quit your session, **do NOT** use your operating system's quit window option. Rather, for a graceful shutdown, press <Q> or click on the Quit menu button on the left side of the screen. This will give you the opportunity to exit gracefully, and save the current state of your visualization session.

MD Display has many other features for managing your perspective on the movie. Be sure to try out combinations of mouse buttons. With a little practice, you'll quickly be scaling, rotating, and translating your view. The reference manual sections that follow give more information and will help you get the most performance from MD Display.

Also, press <?> at any time to see the popup help window. Just be sure to close it down again with another press of <?> when you are done (**Do not** click or type ALT-F4 on many platforms. The GLUT library will exit and you will have to restart display, requiring the –r option to restore you interrupted session.)

Preprocessor Reference

The preprocessor reads one or two input files, creates three or four output files for handoff to *display*, and responds to three modifiers. All of these options are specified on the command line.

Preproc Input Options

-p The filename following this is the input parameter file (prmtop) in standard AMBER format. In the current release of MD Display, both AMBER 7 prmtop format, and the earlier (un-commented) formats are supported.

-c The filename following this is the input coordinate file (md.crd) in standard AMBER format (one title line, then 10f8.3).

-f The integer number following this specifies the maximum number of frames that will be preprocessed. By default, preproc will halt when 100 frames have been processed, or the end of the coordinate file is reached. To increase the limit beyond 100, use the –f nnn option. If nnn exceeds the number of frames in the coordinate file, then preproc will stop on reaching endof file.

-h The floating point number following this is the cutoff distance (in Angstroms) for generating a list of possible hydrogen bonds. See the section **Hydrogen Bond Display** on page 22 for important details.

-P The filename following this is a PDB file. If a (-c) file is also specified, then the PDB file will only be used for generating connectivity and labels. If no (-c) file is specified, then one frame of coordinates will be taken from the PDB file. This allows the user to display a stand-alone PDB file. If both (-P) and (-p) are specified, the results are unpredictable.

-s The file specified is an output file from MS, a program used to generate a Van der Waals surface. Use only in conjunction with the -P option.

-C Used only with the –P option, -C tells the preprocessor to use CONECT cards present in the PDB file to generate connectivity. Otherwise, connectivity is produced by measuring the distances between atoms.

Preproc Output Options

There are two ways of naming the output files. The first (and easiest) way is to use the –n option. For compatibility with earlier program versions, the -a -o -b options are still available.

-n As demonstrated in the Tutorial section, the filename following -n is appended with

".attr" to make the name of the attribute (colors and labels) file

".bnd" to make the name of the bond file

".cor" to make the name of the binary coordinate file.

Also, it is appended with ".srf" to make the name of the binary surface file if an input surface file was supplied with the -s option.

For legacy application compatibility, these file names can also be specified individually:

-a The filename following this is the name of the attribute file that will be created.

-o The filename following this is the name of the binary coordinate file that will be created.

-b The filename following this is the name of the output file which will contain the bonding information.

Preproc Examples

Example 1:

```
preproc -p model.prmtop -c md.crd -n movie -f 500
```

Here, the preprocessor will read in the parameter file model.prmtop and the coordinate file md.crd. Up to five hundred frames are read in and the output files named movie.attr (attribute file), movie.bnd (bond file), and movie.cor (binary coordinate file) are created in the current directory.

Example 2:

```
preproc -p model.prmtop -c md.crd -a attr -o bin -b bondfile -f 500
```

Same as example 1, except that the output files are explicitly named attr (attribute file), bin (binary coordinate file) and bondfile (bond file). These output files are also created in the current directory.

MD Display Reference

The movie viewer can be started most simply with a command like:

```
display –n movie
```

(This is the command line format used in the Tutorial section.) With this command, the preproc output files movie.attr (attribute file), movie.bnd (bond file), and movie.cor (binary coordinate file) are read in.

The files can also be specified explicitly as in:

```
display -a attr -o bin -b bondfile
```

Here, display will read “attr” for the attribute file, “bin” for binary coordinates, and “bondfile” for bonding information.

By default, display will read all the frames in the binary coordinate file created by preproc. However, the **–f nnn** option can be added to specify a maximum number of frames to read in. Or, in the form **–f first,last**, only a range of frames from the binary coordinate file will be loaded.

The –f options can be especially useful on hardware with little RAM memory. They also allow you to focus attention on a range of particularly interesting frames in an otherwise lengthy trajectory.

If your system has a quad-buffered stereo card, and does not crash on initialization of the GLUT_STEREO library option, you should add the –q option. This will allow the <F4> key to select this mode interactively.

Initial coloring can be accepted from the attribute file, which might have been saved during a previous display run. Or, you can specify some colorings prior to the opening of the graphics window, as shown in the Tutorial.

Next, if multiple frames have been read in, the program will prompt you for "time per frame" and "initial offset" so that this clock display is right. The program then enters graphics mode and displays the simulation’s atom coordinate frames.

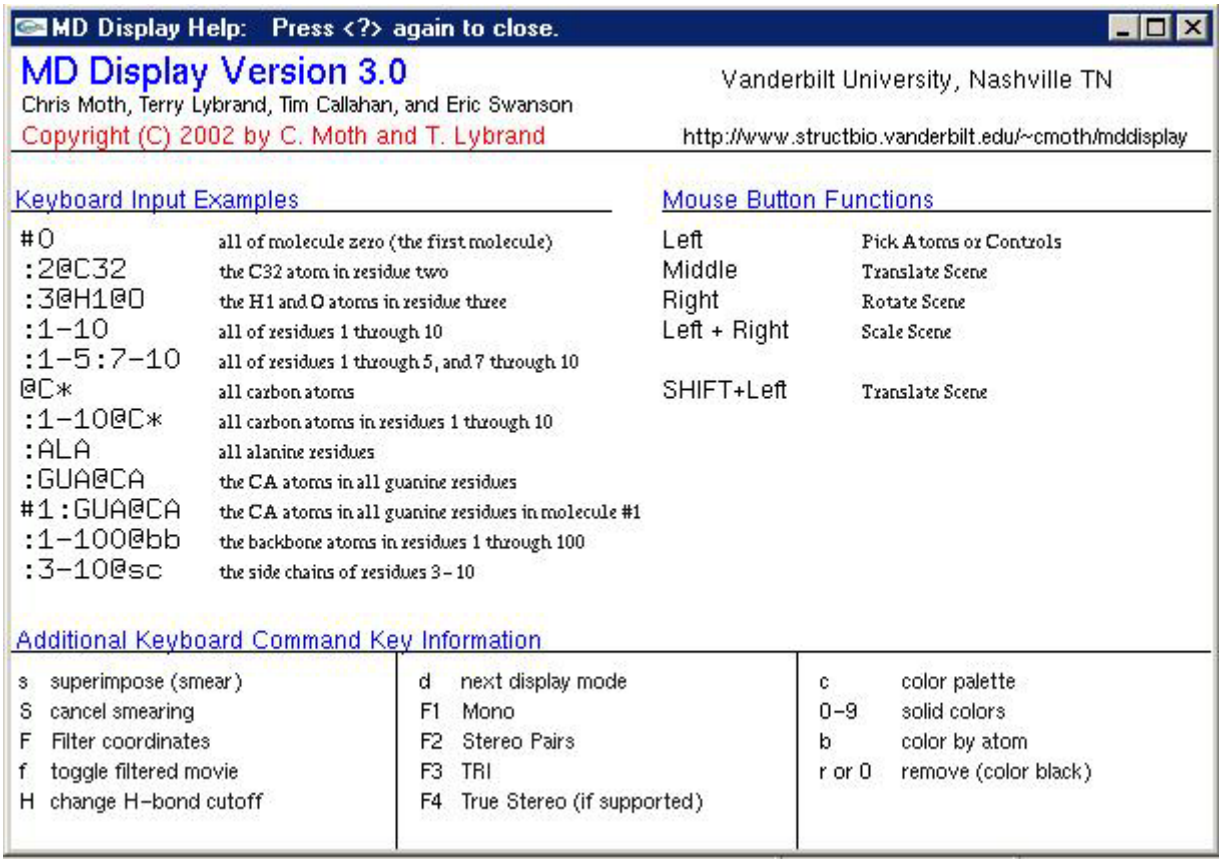
When you exit MD Display (by typing "Q" or by using the bottom left menu box), the program asks if you want to save the session. If you answer yes, then information about the display (coloring, labeling, distance measurements, etc.) will be saved in the attribute file and in the session file (saved as <dataset>.se3). This information will be reloaded the next time you use MD Display with that dataset

Note: **DO NOT Exit MD Display using the operating system window close command** (clicking  or ALT-F4 on many platforms). This will trigger the automatic shutdown system in GLUT, and you will not have the opportunity to properly save your data.

However, should you mistakenly do this, you can easily resume the session by adding the”-r” (resume) command line option when you restart display.

Getting Help

At any time, you can press the <?> key and the following popup box will appear. (As with the main movie window, **DO NOT EXIT** with a window close operation. Just press <?> again.)



Selecting molecules/residues/atoms (coloring)

You can easily change the color of residues and atoms. Click the left mouse button with the pointer over the colors menu button or type lower case <c>. A palette of colors will be displayed:

Click on a color square with the mouse or use the keyboard (<0>-<9> or <b> for 'by atom') to select a color.

If you click on an atom which is already the color you have selected, then all visible atoms of the residue are colored. So, in essence, double-clicking on an atom colors the entire residue, if it is visible.

Alternately, you may type in the molecules/ residues/ atoms, using the syntax described on the next page.

It does take a little practice with the keyboard input format to use MD Display efficiently. But, very soon, you'll be comfortable selecting regions of a system of interest for coloring, labeling, etc. The syntax for specifying the molecules/residues/atoms is best shown by example:

#0	(all of molecule zero)
:2@C32	(the C32 atom in residue two)
:3@H1@O	(the H1 and O atoms in residue three)
:1-10	(all of residues 1 through 10)
:1-5:7-10	(all of residues 1 through 5, and 7 through 10)
@C*	(all carbon atoms)
:1-10@C*	(all carbon atoms in residues 1 through 10)
:ALA	(all alanine residues)
:GUA@CA	(the CA atoms in all guanine residues)
#1:GUA@CA	(the CA atoms in all guanine residues in molecule #1)
:1-100@C@CA@N	(or **:1-100@bb**) (the backbone atoms in residues 1 through 100)
:3-10@sc	(the side chains of residues 3-10)

Note that molecule numbering starts with molecule #0.

Removing atoms is accomplished by coloring them black (color 0). This can be done either by clicking on "remove", pressing <r>, or selecting color <0>. Removed atoms can be restored by coloring them any non-black color.

Labeling

The label command is activated by clicking the right side of the 

menu button or typing <L>. You will then be prompted to specify which residues/atoms to label, and you may respond with the same input syntax described on the previous page in the Coloring section. (These examples are also shown when you press the <?> key).

If you specify just a residue or a range of residues (ex..**:10-40**), then only the residues, and not the atoms, will be labeled. If you specify atoms within a residue or range of residues, then the individual atoms will be labeled.

Examples:

:10:11@C2	will label residue 10 plus the C2 atom in residue 11.
:*	will label every residue.
@*	will label every atom.
#1	will label every residue in molecule #1.
:ALA@*	will label every atom in every alanine residue.

While the labeling option keyboard input prompt is active, (or in fact, if no blue text input box is shown) you can also change the labeling of atoms by picking them with the mouse. The labeling of an atom will cycle through the following states as you pick the atom:

nothing -> atom label -> residue label -> atom & residue labels -> nothing

The "Un-label" option removes labels from the display. It can be activated by clicking on the "Un" (label) rectangle or by typing <U>. To quickest way to clear all labels is to type:

#*:*@*<ENTER>

Translation and Rotation

To translate the movie left/right or up/down in the screen, click and hold the **middle** mouse button (SHIFT key together with the right button on a two button mouse) and the cursor will change shape. With the button held down, you can drag (translate) the movie image about the screen. Release the mouse button when you are satisfied with the new positioning.

To rotate the image, press the **right** mouse button alone. A blue disk will appear in most display modes.

Clicking and holding the right mouse button **outside** of this blue disk will allow you to rotate in the plane of the screen around the **Z axis** (which projects straight out of the screen towards you).

Clicking and holding the right mouse button **inside** the blue disk allows for rotations around the **X and Y axes**.

A small viewing aid at the top left corner of the screen: 

shows the current rotation of the movie relative to the start coordinates.

To change the center of rotation, click the 

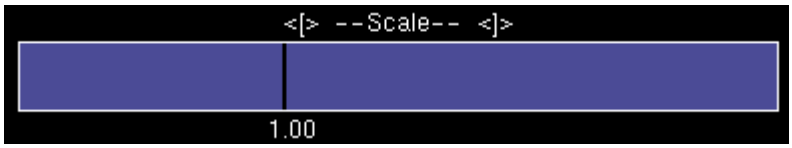
menu button or type capital letter <O>. Then, enter the residue number/atom label for the atom you want at the center of rotation (if you omit the atom label, the first atom in the residue will be used). Or, select an atom as the new center of rotation by clicking with the mouse.

If you just enter a carriage return, with no data, the center of rotation will return to its default value, usually the geometric center of the system.

Note: Centers of rotation are computed based on the 0th (first) frame in the system. This may make the new center of rotation at first feel incorrect, when picked from a frame far along into the movie.

Scaling

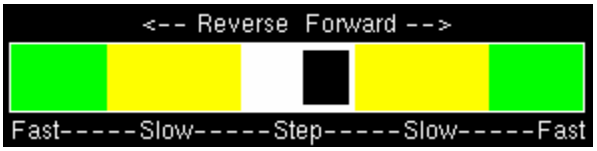
Scaling, or zooming, is controlled by a slide bar along the bottom left edge of the movie window:



You can click (and drag) the thin vertical line in the Scaling slide bar. Or, you can use the<[> and <]> keys to shrink or grow the image. Finally, dragging the mouse with both the left and right buttons down will also scale the image.

Speed Control

When MD Display first starts, movie frames are shown in the forward direction at maximum speed. Click on the speed control bar at the bottom right edge of the movie window:

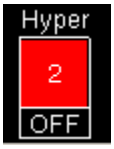


to slow down the animation, or reverse its course. To freeze the animation, click the left mouse button on the white block labeled "Step.". This will cause the current frame to be displayed indefinitely (all other operations, such as rotation and scaling, can still be performed).

With the frame progression frozen, you can manually step through the frames (either backwards or forwards) by positioning the mouse pointer on the correct side of the "Step" box and clicking the left mouse button. The movie will advance (or back up) one frame every time the button is clicked (unless the program is in hyperspeed mode -- see below).

You can also restart automatic frame progression by clicking in the yellow or green boxes. The closer the slide control is placed to the outer edge of the rectangle, the faster the frames will progress.

If you click on the red "Hyper" box at the bottom right corner of the screen, the program will go into hyperspeed mode. In this mode, only every Nth frame is displayed. (N-1 frames are skipped). The first time you click on "Hyper", N=2, and you will see:



Every other frame will be displayed as the movie progresses. Successive clicks on the red "Hyper" box will increase the number of frames skipped. To exit hyperspeed mode, click on the "OFF" rectangle. Hyperspeed also affects the increment while stepping through frames.

Smearing

A number of consecutive frames can be displayed simultaneously to produce a smear image. This is activated by pressing lower case <s> on the keyboard. As <s> is pressed repeatedly, more and more consecutive images are superimposed. To return to an unsmeared display, type upper case <S> (<SHIFT-S>). Note that this option works with hyperspeed so that every Nth frame can be superimposed.

Hiding Controls

To maximize the viewing area, click on the 

menu button or type <h>. The controls and menu buttons will vanish. To restore the controls, just click the left button anywhere (or type "h" again). All letter and number command keys will continue to function as normal with the control hidden.

Clipping

To activate the Z axis clipping control, click on the 

menu button. The clipping control will then be displayed in the extreme bottom left corner of the screen:

This control shows the positions of the front and rear clipping planes relative to the molecular system. I.e., atoms below and above the yellow bars are not displayed. The positions of the clipping planes can be adjusted by clicking the left mouse button in the bottom left. Depth-cueing is automatically controlled by the position of the clipping planes.

When the 

menu button is clicked, the distance between the front and rear clipping planes is held constant and the clipping plane indicator lines change from yellow to red. This allows fixed width sectioning of a large system.

Measurements (Distance, Angle, Dihedral)

To monitor a measurement, click on the menu 

box or type "-" for distance, ">" for bond angle, or upper case <Z> for dihedral.

When prompted, type two, three, or four atoms you are interested in (or pick them with the mouse) and the measurement will appear at the top right of the movie window. Note that order is important here.

For example, pressing <Z> and typing:

:27@O@CA@CB@N<ENTER>

displays the O-CA-CB-N dihedral in residue 27. A maximum of fifteen measurements can be displayed at one time. To remove a measurement, simply click on its text in the top right corner of the movie window.

Display Mode: Mono, Stereo Pairs, Tri, and True Stereo

By clicking on the "display" menu box, typing <d>, or specifically typing <F1>, <F2>, <F3>, or <F4>, you can select from these four different modes:

<F1> Mono One image of the molecule is displayed, taking up the entire window. This is what is shown in the tutorial screens.

<F2> Stereo Pairs A side-by-side stereo pair is displayed.

<F3> Tri Three (orthogonal) views of the molecule are displayed simultaneously: The lower right corner is the "front" view; the upper right is the "top" view; and the lower left is the "side" view.

<F4> True Stereo On SGI systems, the default behavior of the program is to engage legacy stereo support, splitting the 1280x1024 screen memory into two 620x1024 buffers in which the left and right eye images are rendered.

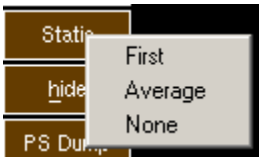
If you would like to engage the higher resolution quad-buffered stereo (GLUT_STEREO) available with newer hardware, you must start display with the –q option for “quad buffered stereo.”

On non-SGI systems, if you do not give the –q option, Stereo mode will not be available and the <F4> key will be simply ignored.

Static Display

To help you visualize the deviations in your trajectory, you can superimpose the movie on a grey static reference structure. Click on the 

menu button and select one of the three options in the popup menu:



- “First” simply shows the first (0th) frame of the trajectory in grey.
- “Average” takes a moment to compute the average of each (x,y,z) atom coordinate. This is then displayed in grey as the animation resumes
- “None” removes any static grey reference structure.

PDB Dump

This option is activated by selecting the 

menu box or by typing <P>. It allows the coordinates of the currently displayed frame to be dumped to a file in PDB format – which can then be read by more advanced presentation graphics software packages.

You will be prompted with a default .pdb file name, which includes both the base file name of your movie and the frame number.

Note that the view rotation and translation are not applied to the dumped coordinates, i.e., the PDB file will have the same coordinates as the preproc output file.

Note also that preproc stores coordinates as 16 bit short integers (**not floats**) in the .cor file. To accomplish this, coordinates are scaled to 1/200 of an angstrom. Therefore, only coordinates within the range +/- 160 angstroms are preprocessed correctly. **For systems with dimension larger than 320 $Å^3$, or applications which require precision beyond 2 x 10^{-2} Å, alternate routes to presentation graphics should be taken.**

Picking with the Mouse

When you click on an atom with the mouse, and a blue text input box is active, the selected atom will be treated as if its label were keyed into the input box. If no text input box is active, the atom will simply be labeled. In this case clicking again will cycle through the label option sequence:

nothing -> atom label -> residue label -> atom & residue labels -> nothing

If you then pick a menu option that requires atom selection, the currently selected atom will be processed. This is a subtle behavior – but it avoids the need to select the atom twice. Just be sure to click away from any atom before invoking a new program command if you do not want this behavior.

If you click on a point in a Ramachandron plot, then the current input box will be processed as if **:RES#** were entered at the keyboard.

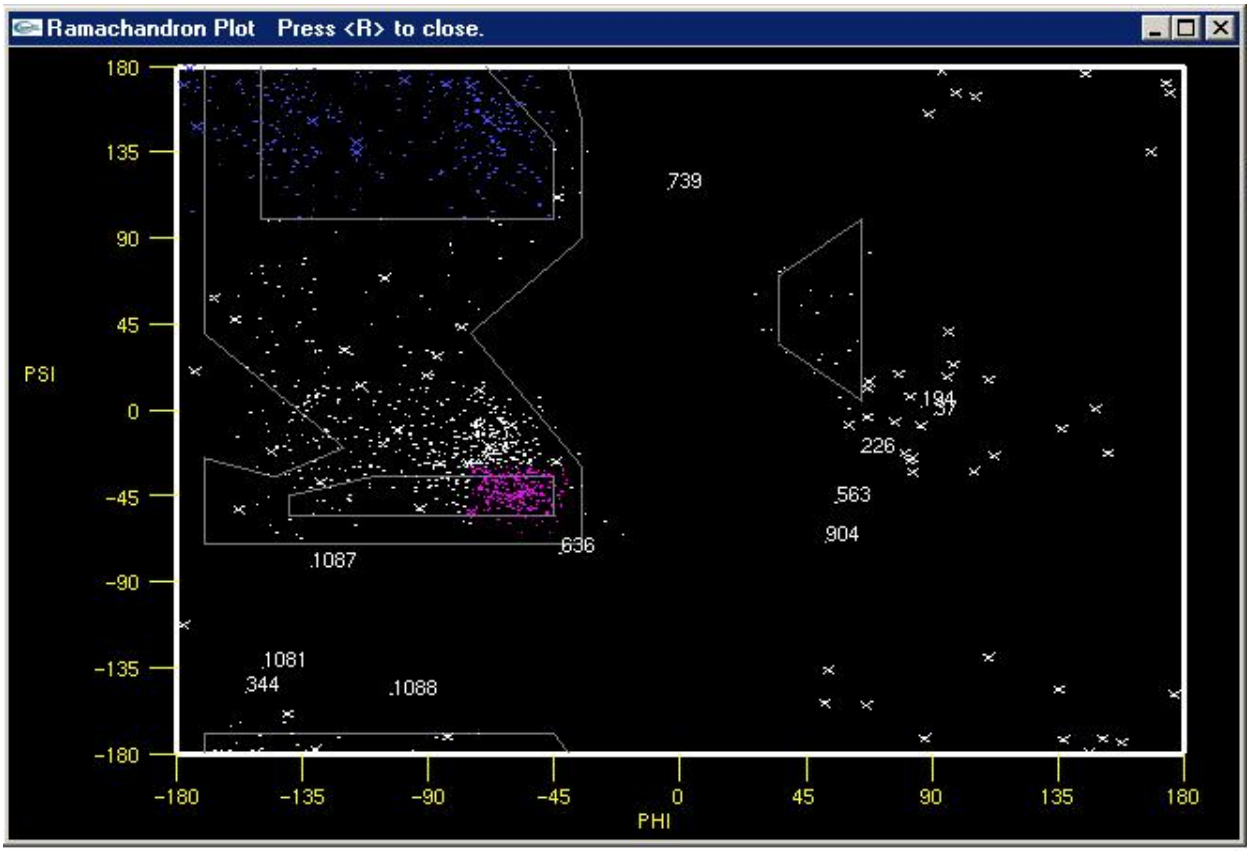
Mouse selection is particularly helpful with the measurement options ("-" for distance, ">" for bond angle, or <Z> for dihedral). To avoid frustration while learning the program, it is probably best to click away from any atoms first, then select a measurement option, and then pick the atoms in order.

In the coloring option, after the color is selected, you may start coloring atoms by picking them with the mouse. If a picked atom is already the color which you have selected, then the entire residue is colored. This allows the rapid coloring of an entire residue by double clicking on one of its atoms.

Ramachandron Plot Display

Select the 

menu button or type <R>. You will see a resizable window depicting a Ramachandran Φ-Ψ plot which is updated with each frame display.



Glycine residues are displayed as "X", while all other residues are displayed as dots. Residues which have been removed from the main display will not appear on the Ramachandran plot. When you select a data point on the plot with the left mouse button, the corresponding residue name and number will be displayed on the title bar of the Ramachandran window.

The data points which lie outside the acceptable range of Φ-Ψ angles are labeled automatically on the plot (by residue number).

DO NOT EXIT THE RAMA WINDOW with the close window command (clicking  or ALT-F4 on many platforms). Due to the way the GLUT multiplatform library is constructed, this will cause the entire application to exit. Instead, simply press <R> again to close the window.

You are welcome to minimize the RAMA window with the  button or whatever other means are provided by your operating system.

Low-pass filtering[4]

One challenge to trajectory interpretation can come from the many high frequency motions which are computed. While important, these motions can obscure slower frequency, larger scale, motions.

To filter out fast motions, click on 

or type <F>. If you initially entered a value for "picoseconds per frame" at program startup, then you will be prompted to enter a cutoff frequency for the low-pass filtering of atomic motion (in cm-1). Otherwise, you will be asked to enter a number of frames over which to average the motion of the atoms. After you have typed in the value, the program will take a while to calculate the filtered trajectory.

For initial experimenting, try values which encompass 5 frames or so. Computation times grow with the square of the number of frames.

The maximum number of frames which display can average over is 50.

If a "0" is typed in response to the text prompt, then the unfiltered trajectory will be restored.

Additionally, lower case <f> can be pressed to toggle between filtered and unfiltered coordinates after their calculation with the <F> option.

WARNING: If the cut-off frequency you choose is too low, i.e. you average over too many frames, physically unreasonable structures may result.

Hydrogen Bond Display

This option involves both the preproc and the display program. In preproc, a cutoff distance is specified with the -h option. Then, preproc makes a list of all possible donor/acceptor pairs which are separated by this distance or less in the **first** frame of the input coordinates. This list will be passed to the MD Display program.

When –h is specified, the hydrogen bond parameter text file “hb.parm” must be present in the current working directory. A sample “hb.parm” file is included in the software distribution. This parameter file contains information about which atoms are valid acceptors and which are valid donors in hydrogen bonds. An example of a line in the file is:

TYR OH D

which specifies that all atoms labeled OH (oxygen in hydroxyl group) found in tyrosine residues are valid donors. The following line is also valid:

* O A

which says that all atoms labeled O in any residue are valid acceptors. Any line beginning with '#' is considered to be a comment. It is permitted to have a specific atom type be both a donor and an acceptor.

In the display program, the user specifies a maximum length for a hydrogen bond by clicking on the 

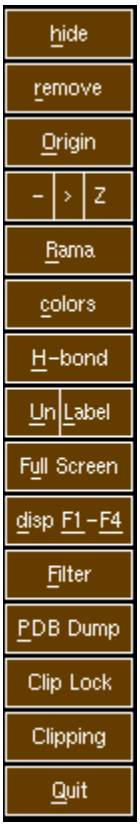
menu button or by typing <H>. For each frame, the display program will scan the list of possible H-bonds computed by preproc, and display those which fall within the acceptable bond length range. The hydrogen bonds are displayed with the color pink.

Note that if there is substantial motion in the system over the course of the trajectory, the cutoff hydrogen bond length specified in the preprocessor will have to be substantially longer than the hydrogen bond length used in the display program. This is because atoms which start far apart may come within hydrogen bonding distance of each other later in the trajectory, and therefore should be included in the list for the display program to check. However, if the cutoff H-bond length specified to the preprocessor is too long, then the list of possible H-bonds for the display program to check may get very large, and the performance of the display program will suffer.

The method used in checking for hydrogen bond formation is simply a distance measurement between the two heavy atoms involved. No check is made on the position of the hydrogen atom, i.e. hydrogen bonding angle, even if it is present.

Keyboard Quick Reference

Many keystroke commands are shown as underlined letters in the menu bar at the left of the screen:



Keystrokes for colors (<0> - <9> and <b>) are shown on the palette when <c> is pressed:

Here are the keystroke commands in text format:

<c>	color palette
<0> to <9>	solid colors
<b>	color by atom
<r>	remove (color black)
<d>	next display mode
<F1>-<F4>	select display mode
<h>	toggle hiding of controls
<l>	label
<u>	un-label (remove label)
<s>	superimpose (smear) two or more consecutive frames for smear display
<SHIFT-S>	cancel smearing (return to normal one-frame-at-a-time processing)
<F>	Filter coordinates
<f>	toggle filtered/unfiltered movie
<O>	new Origin
<H>	change Hbond cutoff
<P>	PDB Dump
<R>	Ramachandron plot
<[> and <]>	decrease/increase scale
<Q>	quit

Index

References

[1] Callahan, T. J., Swanson, E., Lybrand, T. P.: **MD Display: An interactive graphics program for visualization of molecular dynamics trajectories**, *Journal of Molecular Graphics*, 1996, **14:** 39-41

[2] Kilgard, Mark, and Robbins, Nate: **GLUT: Graphics Library Utility Toolkit**

http://freeware.sgi.com/Installable/glut-3.7.html

http://www.xmission.com/~nate/glut.html

[3] D.A. Pearlman, D.A. Case, J.W. Caldwell, W.S. Ross, T.E. Cheatham, III, S. DeBolt, D. Ferguson, G. Seibel & P. Kollman: **AMBER, a package of computer programs for applying molecular mechanics, normal mode analysis, molecular dynamics and free energy calculations to simulate the structural and energetic properties of molecules**. *Comp. Phys.Commun,.*1995 **91**: 1-41

[4] Oppenheim, A.V., and Schafer, R.W. **Discrete Time Signal Processing**. Prentice Hall, Englewood Cliffs, NJ, 1989 **Chap 7,** 444-452