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MDMovie: A molecular dynamics viewing tool

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The graphics program MDMovie (Molecular Dynamics Movie), written in C using IRIS GL graphics library calls, is designed to facilitate the visualization and interpretation of empirical force field data. MDMovie was created and initially adapted in accord with the needs of physical chemists and thereafter became an expandable analysis tool. Capabilities include the display of chemical structure, animation of molecular dynamics and Monte Carlo trajectories, and the visual representation of various vector and scalar dynamical properties. In addition to being a research tool, MDMovie has features for creating presentation videos and hardcopy output. A library is also available for linking to Fortran simulation codes running on a remote machine and connecting to MDMovie via a socket connection. MDMovie continues to be an ongoing research project and new features are actively being added in collaboration with various research groups. Future plans include porting to OpenGL and the design of an X11-based user interface.

Keywords: molecular dynamics, interactive computer graphics, SGI workstations

Introduction

Chemists today are presented with a wide choice of commercial and academic visualization software packages. Many of these codes have overlapping capabilities, and the choice of one over another may just be a matter of user preference. However, strong factors in the choice of a particular program may also involve compatibility with the format of a user's data set, output options, connections with particular simulation codes, and options for visual representation of data. MDMovie is the cumulative result of the need for research groups to have chemistry visualization software that is specific to their particular requirements. It was originally written to display the dynamics trajectories calculated by students and postdocs at the University of California San Diego (UCSD, San Diego, CA). These projects ranged from quantum dynamics simulations of small atomic clusters to classic calculations of van der Waals gases.

Subsequently, as a result of working with other research chemists, the general need for molecular graphics programs that perform specific functions became apparent. Thus, MDMovie has options and functions that satisfy particular niches within the research community. It allows the user to animate molecular trajectories either manually or automatically, view trajectories as they are calculated on a remote UNIX platform via socket connections, and depict data other then just Cartesian coordinates. The latter is one of its ultimate goals: to expand the scope of data that may be represented visually. Currently, this includes the display of scalar and vector properties. MDMovie can generate output for hardcopy devices such as color laser printers via the SDSC "vpr" program and the SDSC image tools library as well as produce animations for recording on laser disks and video tape. Images using MDMovie have been used in various publications[1–3] and have appeared in the SIGGRAPH Technical Slide Sets.[4]

Program Use and Features

When MDMovie is started, a banner appears, containing a display that indicates the kind of data being read and a count for each data type such as atoms, dynamics configurations, and bonds.

Input files

By default, MDMovie reads input files in the MOLPLOT[5] file format for the display of a single configuration. It also reads a modified version of MOLPLOT files in order to accommodate dynamics history files. Dynamics configurations follow one another, separated by a line that may contain characters (e.g., time step, energy) that can be displayed. Various other input file formats have also been added specifically to handle the output of custom dynamics codes.

Color Plates for this article are on pages 279.

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Received 5 June 1995; revised 6 November 1996; accepted 21 November 1996.

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0263–7855/97/$15.00
PII S0263–7855(96)00079-3

Command input

Color Plate 1 shows the main MDMovie display. The molecular structure is the minimum energy structure of a boron cluster.[6] Each option field contains items represented by boxes on the sides and the bottom of the screen. Selecting an item within the field, using the mouse, allows the user to change the value specified by that item interactively, enter specific values via the keyboard, or display a pop-up menu that gives more command options.

Transformation field

The items comprising the field at the bottom of the screen govern model transformations. When an item is chosen with the cursor, the structure may then be manipulated by moving the mouse. These items allow the user to rotate, translate, and scale the molecular system as well as to set the near and far clipping planes and the field of view for the perspective projection.

The yellow rectangles above each red transformation item label display the current value of each item (e.g., the amount that the structure has been translated along the z axis) on the top line and the value that it will be incremented by on each automatic update on the bottom line. If a value is entered from the keyboard, the transformation occurs with each automatic frame update. For example, if the number 5 is entered under the Z-ROT menu item, then the model will change 5 degrees about the z axis with each new frame. This is particularly useful when transforming each successive frame when making an animated video.

Property field

The property field appears on the left-hand side of the screen. It governs what features of a molecular system are displayed and how they are rendered. At the upper left-hand portion of the screen are items representing each atom type, followed by items for specifying the background color, bond rendering, vector, and color property options. At the lower left-hand portion of the screen are items that display values specific to various display objects. For example, selecting an atom-type item with the cursor displays a pop-up menu with options for atomic display. The options include lighted spheres, both solid and transparent, "beach ball" spheres (circles transformed about two axes), dots, circles, and color. After the "Color" option, a submenu appears that allows the user to select an atom color from among the eight basic colors. The current color of this atom type is also displayed in the COLOR item in the lower left-hand portion of the screen as an RGB value and it can also be changed by entering an RGB value in the COLOR item. Similarly, the current value of the atomic radius is displayed in the RADIUS item. When this item is chosen with the cursor along with a particular atom type, the radius may be changed interactively with the mouse or a specific value may be entered from the keyboard. Following the atom items is the BACKGROUND item, which allows the user to change the color of the screen background. Selecting the ALL item brings up the same pop-up menu as the ATOM item but the changes apply to all atom types.

Choosing the BOND item allows the user to select bond display characteristics such as lines, cylinders, bond lengths, and angles. Atom connectivity may be read from files or picked with the cursor. Moreover, MDMovie can evaluate all interatomic distances and draw bonds between all atoms whose distances fall below or equal to the value entered in the BOND LENGTH item. As a molecular dynamics trajectory evolves, interatomic distances change. The user has the option of having MDMovie update the bond list for each configuration or "freeze" the bond list for the entire simulation. When the BOND item is selected, the current value of the radius is shown in the RADIUS item and the color in the COLOR item. The user may change these values in the same manner as with atom types. The bond options are currently for display purposes only and do not constitute force field component assignments.

The V PROPERTY item controls the display of vectors. Typically these may represent properties such as a particular force component or velocity. The display options are similar to those for bonds: Vectors may be displayed as lines or cylinders, deleted or added by picking, and the colors chosen either via the pop-up menu or the COLOR item. The vector magnitudes can be displayed as well. Color Plate 2 illustrates the use of this option.

The VECTOR item is analogous to the RADIUS item for atoms and bonds. It controls the scaling of the lengths of the vectors. When this item is highlighted, the values of the vectors are scaled either by moving the mouse or by keyboard input.

The C PROPERTY item controls the display of scalar properties as a function of color. This is still in the experimental stage and has not yet been widely used. The user may specify in the input file ranges of data that are represented by a particular color. Colors then may either be scaled between the selected values, based on a linear interpolation between the chosen colors, or may be a single color for a given range of values. The intended use of this feature is to display a property such as the kinetic energy of individual atoms as a dynamic simulation proceeds. Color Plate 3 shows an atomic cluster whose atoms are colored according to the binding energy.[7]

The TRACE item allows the user to follow the movement of an atom in a dynamics simulation. The numbers of the atoms that are to be traced are entered from the keyboard. As the trajectory evolves, lines are drawn between successive configurations from the first up to the current one. The color of the line is the same as the corresponding atom.

All objects such as atoms, bonds, and surfaces that are represented by lines or wire frames are depth cued. The user may adjust the amount of depth cueing by changing the positions of the near and far clipping planes.

Animation and hardcopy fields

The items on the right-hand side of the screen control how a dynamics run is animated and the type of hardcopy device to which the output is sent. The upper value in the CONFIG item displays the current trajectory step, while the lower value is set by the user and specifies the number of steps to be incremented on each iteration. This number may be a negative number. The FRAMES item displays a value, set by the user, that determines how many steps of the anima-

tion are to be run. The FILE item displays the name of the file to which an SGI "rgb" file is written to if a hardcopy device has been specified. This feature has been modified for particular sites. For example, an SGI "rgb" file can be converted to a PostScript file via the SDSC Image Conversion Tools,[8] which can be called from within MDMovie. The user may enter the name of the queue in the QUEUE NAME item. Alternatively, the user may choose queue names from the pop-up menus when the VPR, LPR, or VIDEO item is picked with the cursor. These are specific to the devices at SDSC. However, they may easily be modified.

Selecting the GO item displays an animation and sends output to a device on the basis of transformation and configuration update parameters that have been selected. After each configuration update, a "checkpoint" file is overwritten so that the user may return to the last frame recorded and to the exact orientation and data display settings when the program is restarted. Dynamics may also be animated manually by using the arrow keys: the right arrow key advances the dynamics run by the number of frames specified in the CONFIG item. The left arrow key runs the simulation in reverse. The down arrow key displays the first configuration while the up key displays the last.

OTHER DISPLAY FEATURES

Surface and contour display

MDMovie is capable of displaying surfaces and contours. However, these features have been greatly enhanced in the QMView program[9] and it is recommended that the latter program be used for the display of surface data. The MDMovie manual explains how to read in surface data and display it.

Labeling

Users may label their figures by toggling a function key that brings up the "titles" display field. Fonts and type sizes that are available via the IRIS GL font manager can be selected as well as the color. Individual labels can be selected and moved about interactively with the mouse.

Stereo

Interactive stereo viewing is an option, if it is supported by the hardware, by selecting the STEREO field in the lower right-hand corner. Eye separation between the two views may be adjusted interactively. For publication and hardcopy output, a side-by-side stereo pair may be generated as in Color Plate 4.

Data plots

Two-dimensional data may be included in input files and plotted on a graph. The data for all iterations are represented by dots, and a solid line is drawn from the first up to the current configuration. The user may click with the mouse on either the line or the dots and the corresponding structure will be displayed. An example is shown in Color Plate 5.

VRML

MDMovie can produce VRML files for viewing structures interactively using a World Wide Web browser such as SDSC WebView.[10] Pressing a key creates a VRML file that will reproduce what is being displayed on the screen at the time.

Socket connections

MDMovie can connect to a dynamics program running on a remote platform via calls to the MDMovie distributed library. The molecular structure and values chosen by the user are displayed for each iteration as it is computed on the remote platform. The library is written in C and is designed to be linked to Fortran programs. Two subroutines must be inserted in the code. The first is an initialization routine whose arguments are the addresses of all the data that are to be passed to the graphics workstation. These include the names of the arrays where the coordinates are stored, the number and types of atoms, as well as the addresses of optional data such as energy components. The second routine, which contains no arguments, is placed in the code wherever a coordinate update is made. Each call to this routine sends the current data to the graphics workstation.

A user may start a job on the workstation and view the progress of the simulation. He or she may then stop the MDMovie program running on the workstation while the program on the remote machine continues to run. Later, they may reconnect to the running job in order to view its progress. This library has been tested on the Cray Research c90 and the Intel Paragon and results have been demonstrated at various conferences. For example, MDMovie has been used to display a dynamics run calculated by Euler-GROMOS, a parallel version of the GROMOS molecular mechanics program.[11]

CONCLUSION

MDMovie has proven to be a useful visualization tool and, in addition, accommodates chemists who require options that are not available in commercial programs and need interfaces to particular recording devices. MDMovie is under continual development and enhancement. The main emphasis in this development and future evolution is to display properties other then basic atomic Cartesian coordinates and bond connectivity, thus allowing chemists to interpret visually a wider variety of data. Developments in progress include (1) options for displaying multiple-phase simulations and (2) porting to OpenGL so that MDMovie will run on a wide variety of graphics workstations. A copy of the on-line manual, which gives a more detailed explanation of its use, is available either on the WWW[12] or in ASCII or PostScript versions via anonymous ftp.[13]

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