How to Make a Molecular Dynamics Movie with Freeware

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This handout assumes that you already have read the first three hand-outs in the series:

- The Working Man's Guide to Molecular Dynamics Simulations
- The Working Man's Guide to Obtaining Self Diffusion Coefficients from Molecular Dynamics Simulations
- Molecular Dynamics for Multicomponent Systems

I. Introduction

One of the fine things about molecular dynamics simulations is that you can make movies of a system where you can visually observe phenomena occuring at the molecular level. This is cool.

In this handout, we describe in detail how to make a molecular dynamics movie with our FORTRAN code, using only freeware. This plug-in is called Chime.[1] It is a free molecular visualization tool.

II. Generating the Movie File

Chime can read various types of input. The simplest is an space-delimited text file. This we can easily create with our FORTRAN code. Since our code already saves positions for calculating a self-diffusion coefficient, all we are going to do here is convert the mean square displacement file, used for the self-diffusion coefficient into a format that Chime can read.

In appendix A, we provide the FORTRAN source code for a subroutine to generate movie from mean square displacement file. This subroutine can be placed at the end of the molecular dynamics code, after the self-diffusion coefficient calculation. The call to the routine would look something like this

```
      if (lmovie) then
            call makeamovie(maxstp, kmsd, N, ncomp, Nvec, cmsd, cname,
   & side)
      endif
```

where lmovie is a logical variable telling the code whether to create a movie or not.

This subroutine simply renders the position data into the correct format. The general format is as follows:

```
2

O    4.83786600   4.83786600   4.83786600
O    4.83786600   4.83786600   9.67573200
2

O    4.31892680   5.51409750   4.71572050
O    3.82347620   4.05128400  11.17209300
2

O    4.30679460   6.19066690   4.74016830
O    3.72448360   3.85222920  11.78613600
```

If this were the complete input file, we would create a movie of 2 oxygen atoms for three frames. The movie file must be in this format. Chime is picky. The movie file must end in .xyz. Thus if you generate a file md_msd.out, you have to manually rename it md_msd.xyz in order for Chime to read it. Furthermore, the numbers must be in fixed decimal notation. Chime doesn't read exponential notation.

The subroutine also removes periodically boundary conditions. You didn't want them form the diffusion calculation but you want them in the movie.

You can them copy this call this movie input file with a webpage, such as is given in Appendix B.

III. Chime

Chime is an interactive program. It can do a lot more than just show movies. However, we are just going to worry about showing movies here. In order to use Chime, the machine that you are on has to have Chime installed. Installation is trivial, but instructions are given at the Chime Website.[1] If you look at the HTML source code in Appendix B, all the Chime specific content of the webpage is in the following lines:

```
<embed src="./md_msd.xyz" display3d=spacefill animfps=5
startanim=true spiny=10 startspin=false width=90% height=90%>
```

This tells the browser to embed a Chime object with a source file of md_msd.xyz. You set the display to spacefill. You set the animate rate to 5 frames per second. You tell it to start the animation by default. I forget what spiny amd startspin control. Width and height define the size of the Chime box inside the webpage.

The explanation of all of these parameters and many more can be found in the Chime Tutorials online.

A variety of other molecular dynamics movies are located at my website under the interactive and animation menu tabs.[2]

References

1. Chime Website, http://www.mdli.com/cgi/dynamic/product.html?uid=$uid&key=$key&id=6
2. David Keffer Research Homepage, http://clausius.engr.utk.edu/

Appendix A. FORTRAN subroutine to generate movie from mean square displacement file

```
      subroutine makeamovie(maxstp, kmsd, N, ncomp, Nvec, cmsd, cname,
     & side)
c
c     This program will make a movie file readable by the web plug-in Chime
c
c     author  David Keffer
c     Department of Chemical Engineering
c     University of Tennessee, Knoxville
c     last updated  February 7, 2002
c
      integer, intent(in) :: maxstp, kmsd, N, ncomp
      integer, intent(in), dimension(0:ncomp) :: Nvec
      character*12, intent(in) :: cmsd
      character*2, dimension(1:ncomp), intent(in) :: cname
      double precision, allocatable :: md_msd(:,:)
      integer, dimension(1:ncomp) :: Nstart, Nend
c
      do i = 1, ncomp, 1
            if (i .eq. 1) then
                  Nstart(i) = 1
            else
                  Nstart(i) = Nend(i-1) + 1
            endif
            Nend(i) = Nstart(i) + Nvec(i) - 1
      enddo
c     number of times represented in data
      ntime = maxstp/kmsd + 1
c     number of rows of data
      ndata = N*ntime
      allocate (md_msd(1:ndata,1:3))
c     read data
      open(unit=2,file=cmsd,form='formatted',status='old')
      print *, ' ntime = ', ntime, ' ndata = ', ndata
      do i = 1, ndata, 1
            read(2,*) md_msd(i,1:3)
      enddo
      close (unit=2,status='keep')
c     apply pbc's on the data
      call pbc(ndata,md_msd,side)
c     write same data in format for movie
      open(unit=2,file=cmsd,form='formatted',status='old')
      k = 0
      do j = 1, ntime, 1
            write(2,*) N
            write (2,*) ' '
            do ic = 1, ncomp, 1
                  do i = Nstart(ic), Nend(ic), 1
                        k = k + 1
                        write(2,1009) cname(ic), md_msd(k,1:3)
                  enddo
            enddo
      enddo
```

```
      close (unit=2,status='keep')
1009 format(a2,1x,3(f12.8,1x))
      return
      end
```

Appendix B. Webpage for viewing movies

```
<HTML>
<TITLE> Molecular Dynamics - Animations</TITLE>
<BODY BGCOLOR="#000000" text="228B22" link="8b0000" vlink="B8860B">
<CENTER>
<BR>
<embed src="./md_msd.xyz" display3d=spacefill animfps=5
startanim=true spiny=10 startspin=false width=90% height=90%>
<!-- script="zoom 1000; rotate x 90; rotate z 90;"> -->
<BR><BR>
<table border=0 cellspacing=0 cellpadding=0 width=60%><tr><td valign=top align=left>
<FONT SIZE="+0" FACE="ARIAL">
<p>This  movie is a segment of a molecular dynamics simulation of a  bulk fluid.</p>
<ul>
        <li>System Parameters
                <ul>
                        <li>Temperature = 300 K
                        <li>density = 8.83x10<sup>-3</sup> molecules per Angstroms<sup>3</sup>
                        <li>pressure = 366 atm
                        <li>composition:
                                <ul>
                                        <li>80 mole percent methane (red)
                                        <li>20 mole percent ethane (gold)
                                </ul>
                        </li>
                </ul>
        </li><br><br>
        <li>Simulation Parameters
                <ul>
                        <li>number of atoms: N = 216
                        <li>number of equilibration steps:  0
                        <li>number of equilibration steps:  10,000
                        <li>size of steps:  2 fs
                        <li>Lennard-Jones potential
                        <li>collision diameter
                                <ul>
                                        <li>methane: 3.822 Angstroms
                                        <li>ethane: 4.418 Angstroms
                                </ul>
                        </li>
                        <li>energetic well depth
                                <ul>
                                        <li>methane: 137 K
                                        <li>ethane: 230 K
                                </ul>
                        </li>
                        <li>rcut = 15 Angstroms
                        <li>integrator:  Fifth Order Gear Predictor-Corrector
                        <li>time increment between movie frames:  200 fs
                </ul>
        </li><br><br>
        <li>Credits
```

```
                <ul>
                        <li>David Keffer
                        <li>Department of Chemical Engineering
                        <li>University of Tennessee, Knoxville
                        <li>February 7, 2001
                        <li>Contact:  <a href = "mailto:dkeffer@utk.edu">email</a>
                </ul>
        </li><br><br>
</ul>
</FONT>
</td></tr></table>
</CENTER>
</BODY>
</HTML
```