Introduction to VMD

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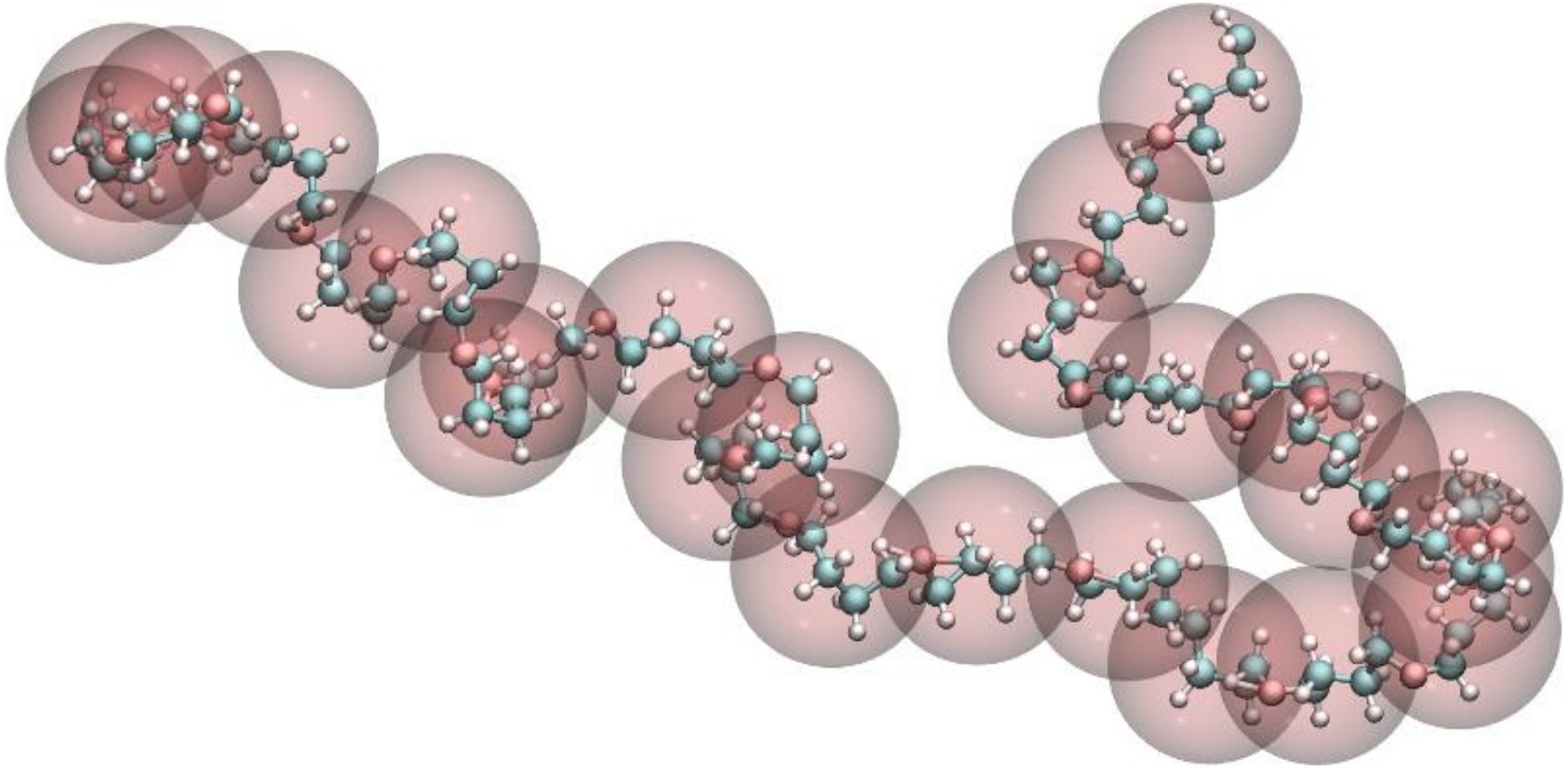
Last Week

- We talked discussed about the reference code



VMD

- VMD = Visual Molecular Dynamics
- VMD is a molecular visualization program for displaying, animating, and analyzing large biomolecular systems using 3-D graphics and built-in scripting

VMD Download and Registration

- To Download, go to
  - http://www.ks.uiuc.edu/Development/Download/download.cgi?PackageName=VMD
- To install (on Linux)
  - cd ~/Download/
  - tar –xzfvmd-1.9.2.bin.LINUXAMD64.opengl.tar.gz
  - cd vmd-1.9.2/
  - ./configure
  - cd src
  - sudo make install
  - vmd

Molecular file formats

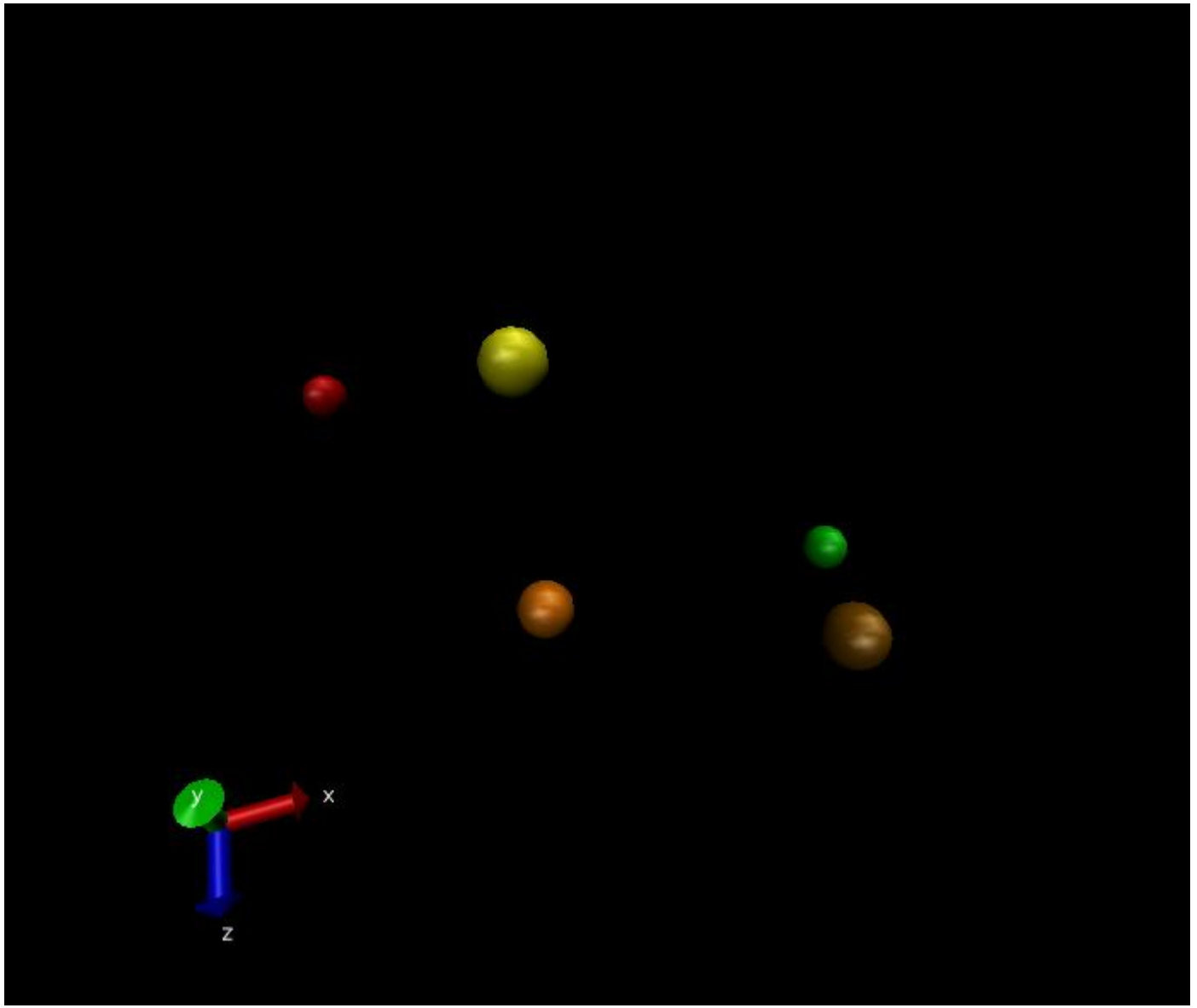
- **Molfile** plugin is responsible for translating the molecular file inputs
- VMD supports many common file types
- Molecular coordinate/structure file
  - AMBER structures
  - CHARMM coordinates/structures
  - NAMD structure
  - PDB files
  - XYZ coordinates
- Molecular dynamics trajectory files
  - AMBER, CHARMM, NAMD, Gromacs, Lammps trajectory, XYZ trajectory

XYZ Plugin

```
XYZ molecule file format:
  XYZ files are a simple molecule file format suitable for output
  by homegrown software since they are very minimalistic.  They don't
  even include bonding information.

[ # optional comment line ] comment line (can be blank)
                            ^^^ NOTE: comment lines aren't supported by
                                the current version of this plugin.
[ N                       ] # of atoms, required by this xyz reader plugin
[ molecule name           ] name of molecule (can be blank)
atom1 x y z [optional data] atom name followed by xyz coords
atom2 x y z [ ...         ] and and (optionally) other data.
...                         instead of atom name the atom number in
atomN x y z [ ...         ] the PTE can be given.

Note that this plugin currently ignores everything following the z
coordinate (the optional data fields).
```

Sample file

```
5

A 0 0 0
B 1 1 1
C 1 0 2
D 3 0 2
E 2 1 3
```



VMD Movie Maker

- VMD main >> Extensions >> Visualization >> Movie Maker
- Movie Settings >> Trajectory
- Format >> MPEG-1 (ffmpeg) or MPEG-2 (ffmpeg)
- Renderer >> Tachyon (Ray Tracer)
- http://www.ks.uiuc.edu/Training/Tutorials/vmd/tutorial-html/node3.html

- It may be necessary to install ffmpeg before generating movie for the first time. Turn off vmd, type "*sudo apt-get install ffmpeg*" in command line.

VMD Movie Maker

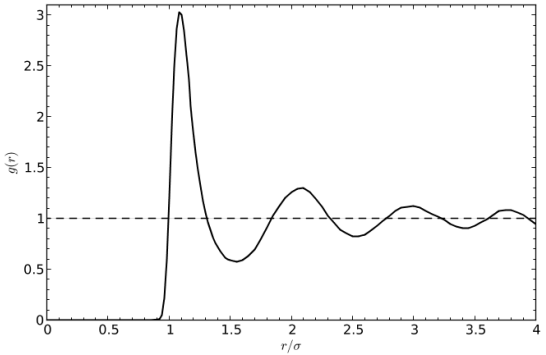
- Install mplayer after successfully generating a movie
  - sudo apt-get install mplayer

- Type “mplayer *{video name}.*mpg”, or
  type “mplayer –loop 0 *{video name}.*mpg” if want to replay video.

- In the future, you may want to convert video format into .wmv so that it can be inserted into PowerPoint. There is a convenient website:
- http://video.online-convert.com/convert-to-wmv

Some Simple Measurements Using VMD

- Calculate radial distribution function g(r)
  - VMD main >> Extensions >> Analysis >> g(r)
  - http://www.ks.uiuc.edu/Research/vmd/plugins/gofrgui/



g(r) of Lennard-Jones Fluid

- Calculate Root Mean Square Deviation/Displacement (RMSD)
  - VMD main >> Extensions >> Analysis >> RMSD Trajectory Tool
  - http://www.ks.uiuc.edu/Training/Tutorials/vmd/tutorial-html/node7.html

$$RMSD = \sqrt{\frac{\sum_{i=1}^{N}(\vec{r}_i(t_1) - \vec{r}_i(t_2))^2}{N}}$$

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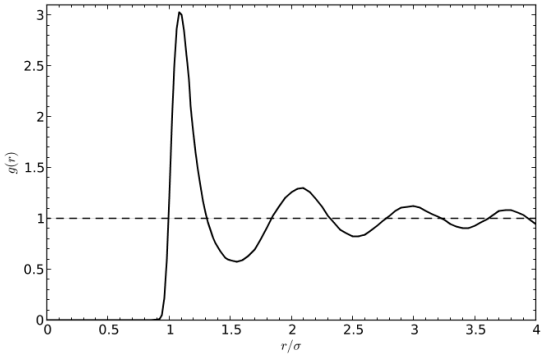

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Tk Console

- VMD has Tk Console extension
- Representations, colors and other attributes can be set through console environment

- It can also be automatically loaded with *.tcl scripts

Any Question?

Programming Exercise #3

- Programming Exercises can be found on the website of this course
- https://softphys.wordpress.com/

- Programming Exercise #3
- https://softphys.wordpress.com/2016/04/08/programming-exercise-3/