

Science-1 Tutorial

Topic: Basics of Visual molecular Dynamics
(VMD)

VMD Input – PDB files

Structure of a PDB file

index	name	resname	chain	resid	x	y	z	segname
ATOM	22	N	ALA B	3	-4.073	-7.587	-2.708	BH
ATOM	23	HN	ALA B	3	-3.813	-6.675	-3.125	BH
ATOM	24	CA	ALA B	3	-4.615	-7.557	-1.309	BH
ATOM	25	HA	ALA B	3	-4.323	-8.453	-0.704	BH
ATOM	26	CB	ALA B	3	-4.137	-6.277	-0.676	BH
ATOM	27	HB1	ALA B	3	-3.128	-5.950	-0.907	BH
ATOM	28	HB2	ALA B	3	-4.724	-5.439	-1.015	BH
ATOM	29	HB3	ALA B	3	-4.360	-6.338	0.393	BH
ATOM	30	C	ALA B	3	-6.187	-7.538	-1.357	BH
ATOM	31	O	ALA B	3	-6.854	-6.553	-1.264	BH
ATOM	32	N	ALA B	4	-6.697	-8.715	-1.643	BH
ATOM	33	HN	ALA B	4	-6.023	-9.463	-1.751	BH
ATOM	34	CA	ALA B	4	-8.105	-9.096	-1.934	BH
ATOM	35	HA	ALA B	4	-8.287	-8.878	-3.003	BH
ATOM	36	CB	ALA B	4	-8.214	-10.604	-1.704	BH
ATOM	37	HB1	ALA B	4	-7.493	-11.205	-2.379	BH
ATOM	38	HB2	ALA B	4	-8.016	-10.861	-0.665	BH
ATOM	39	HB3	ALA B	4	-9.245	-10.914	-1.986	BH
ATOM	40	C	ALA B	4	-9.226	-8.438	-1.091	BH
ATOM	41	O	ALA B	4	-10.207	-7.958	-1.667	BH

- Has 3-D structural data of the molecules
- Does not have connectivity information

Loading the pdb file and interaction modes

- Load pdb file
- Interaction mode: Rotate, translate, scale mouse modes

Drawing styles and coloring methods

- Atoms and molecules can be visualised in various drawing methods

Drawing Methods	Description
Lines	Default
HBonds	Draws Hydrogen Bonds
VDW	Space filling visualization
Ribbons/New Ribbons	Draws backbone of DNA/protein as a ribbon
Cartoon/New Cartoon	Draws secondary structure of proteins

Atom Selection

- Atom Selection in selections tab of the graphical representation window.
Example: all, protein, resname X, name X, resid X
- Multiple representation
- Loading a trajectory
- Saving an image with file -> render -> start rendering

Scripting in VMD

- Scripting in vmd is in the language called TCL
- TCL/TK console

- Write a tcl script to select the backbone atoms of the 1ubq.pdb protein and write it to a pdb file name backbone.pdb

[Hint : Use “\$selection writepdb output_name” to write the select atoms into a external pdb]

Trajectory file format

- Different file formats like .dcd,.xyz etc
- Format of .xyz file format:

```
<number of atoms>
comment line
atom_symbol11 x-coord11 y-coord11 z-coord11
atom_symbol12 x-coord12 y-coord11 z-coord12
...
atom_symbol1n x-coord1n y-coord1n z-coord1n
<number of atoms>
comment line
atom_symbol21 x-coord21 y-coord21 z-coord21
atom_symbol22 x-coord22 y-coord21 z-coord22
...
atom_symbol2n x-coord2n y-coord2n z-coord2n
.
.
.
<number of atoms>
comment line
atom_symbolm1 x-coordm1 y-coordm1 z-coordm1
atom_symbolm2 x-coordm2 y-coordm1 z-coordm2
...
atom_symbolmn x-coordmn y-coordmn z-coordmn
```


Submission

- Visualise your N random walkers for 10,000 steps and write the coordinates for each of the random walkers after each time step into a .xyz file and visualise it in vmd
- Submit your .xyz file on moodle
- Deadline : 12:00pm tonight (hard deadline)