



LAMMPS Workshop

Converting PDB file to LAMMPS input

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Outline:

- About PDB
- Generating Protein Structure File
 - Visual Molecular Dynamics package (VMD)
- Converting PDB and PSF to LAMMPS input
- Run a simulation
- Check the results

PDB File

WWW.pdb.org : Just type a keyword or PDB ID

ATOM	2	CA	MET	A	1	12.980	51.045	106.100	1.00	8.94	C
ATOM	3	C	MET	A	1	11.624	50.763	106.674	1.00	6.28	C
ATOM	4	O	MET	A	1	10.883	49.764	106.349	1.00	7.00	O
ATOM	5	CB	MET	A	1	12.944	51.691	104.700	1.00	13.26	C
ATOM	6	CG	MET	A	1	12.598	53.174	104.844	1.00	19.60	C
ATOM	7	SD	MET	A	1	14.059	54.219	104.801	1.00	29.09	S
ATOM	8	CE	MET	A	1	15.164	53.592	106.046	1.00	30.27	C
ATOM	9	N	ASN	A	2	11.141	51.669	107.452	1.00	6.58	N
ATOM	10	CA	ASN	A	2	9.856	51.804	108.120	1.00	5.77	C
ATOM	11	C	ASN	A	2	9.569	53.324	108.060	1.00	3.63	C
ATOM	12	O	ASN	A	2	10.408	54.213	107.718	1.00	4.58	O
ATOM	13	CB	ASN	A	2	9.741	51.218	109.568	1.00	2.30	C
ATOM	14	CG	ASN	A	2	10.785	51.887	110.443	1.00	3.22	C
ATOM	15	OD1	ASN	A	2	10.684	53.100	110.631	1.00	3.59	O
ATOM	16	ND2	ASN	A	2	11.748	51.132	110.941	1.00	3.89	N
ATOM	17	N	ILE	A	3	8.361	53.636	108.454	1.00	3.23	N
ATOM	18	CA	ILE	A	3	7.784	54.980	108.480	1.00	2.23	C
ATOM	19	C	ILE	A	3	8.609	55.953	109.310	1.00	3.64	C
ATOM	20	O	ILE	A	3	8.765	57.123	108.903	1.00	2.87	O
ATOM	21	CB	ILE	A	3	6.273	54.912	108.919	1.00	5.35	C
ATOM	22	CG1	ILE	A	3	5.551	56.269	108.751	1.00	2.00	C
ATOM	23	CG2	ILE	A	3	6.121	54.330	110.401	1.00	3.13	C
ATOM	24	CD1	ILE	A	3	5.586	56.787	107.226	1.00	4.15	C
ATOM	25	N	PHE	A	4	9.128	55.434	110.438	1.00	2.26	N
ATOM	26	CA	PHE	A	4	9.966	56.300	111.293	1.00	5.69	C
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Generating Protein Structure File

- Using **psfgen** package directly
- ✓ The implemented **psfgen** in VMD

 - a. Making pgn file
 - b. Automatic psf builder



VMD

- ❖ Visualize your results using high graphical capabilities
- ❖ Measure bond, angle, etc. in the structure
- ❖ Modeling: Build protein, Nanotube and Membrane, Apply local changes to the structure like changing an angle or make a point mutation



Steps toward generating PSF

1. Make separate PDB files for individual chains of protein, solvent etc.
2. Match the residues and atoms of your PDB with the appropriate topology
3. Remove unwanted atoms
4. Generate new chain in the output PDB file
5. Read the PDB file
6. Guess coordinates of missing atoms
7. Writing output PSF and PDB

Preparation

- Delete all water molecules from the end of your pdb (ILYD.pdb) and rename it to ILYD-nw.pdb
- Find the force field files in a folder named toppar or Download **toppar_c35b2_c36a2.tgz** from:
http://mackerell.umaryland.edu/CHARMM_ff_params.html
- Copy top_all27_prot_lipid.rtp (topology) and par_all27_prot_lipid.prm (force field parameters)

Pgn file

Package require psfgen

Topology top_all27_prot_lipid.rtf

pdbalias residue HIS HSE

pdbalias atom ILE CDI CD

Segment U {pdb ILYD-nw.pdb}

coorpdb ILYD-nw.pdb

guesscoord

Write lys.pdb

Write lys.psf

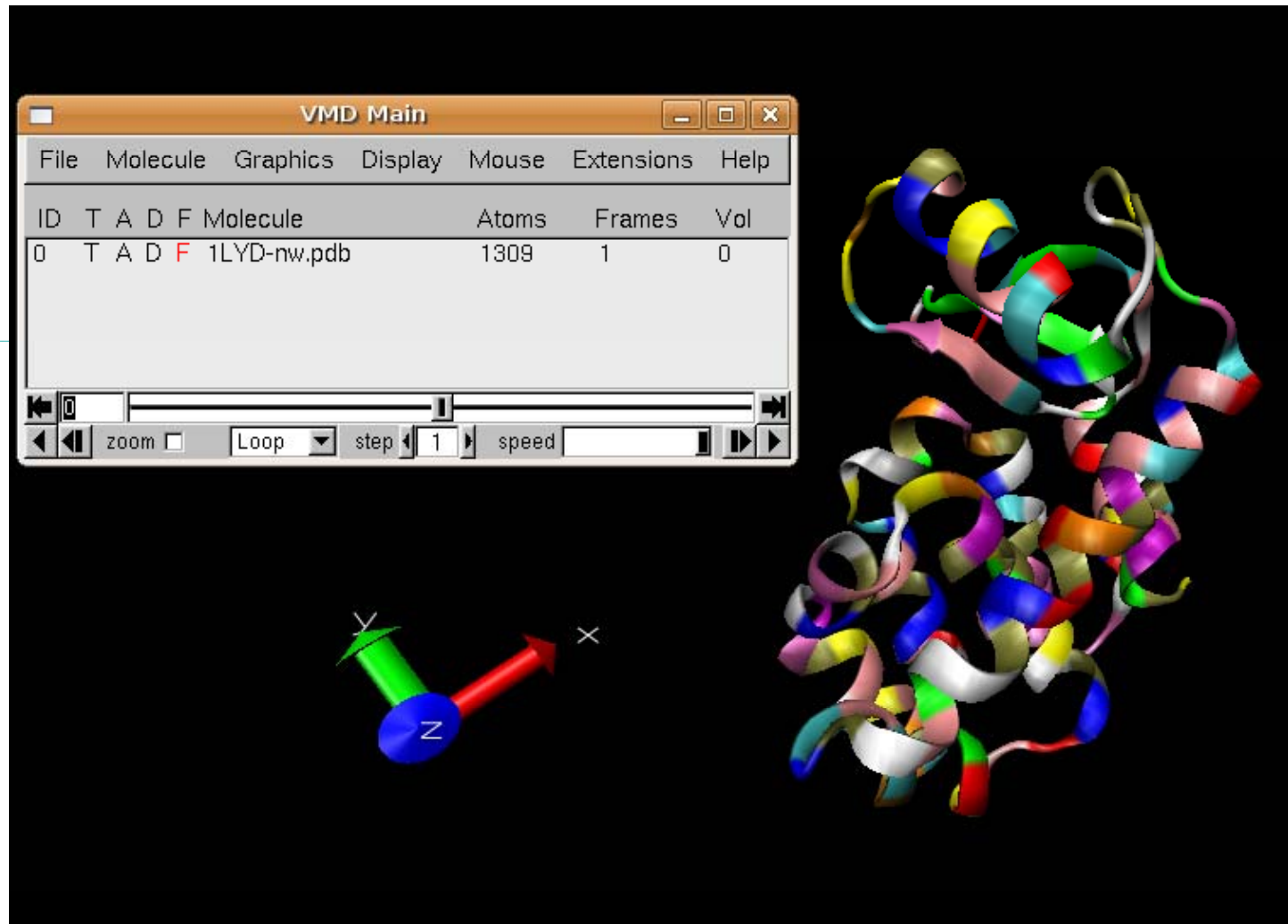


```
$ Vmd -dispdev text -e ILYD.pgn
```

-dispdev: specify display device

-e: Execute commands in <filename>

`$ vmd 1LYD-nw.pdb`



Automatic PSF builder

VMD main >
Extensions >
Modeling

The screenshot shows the AutoPSF dialog box with the following sections:

- Options** (with a Help button)
- Step 1: Input and Output Files**
 - Molecule: 0: 1LYD-nw.pdb
 - Output basename: 1LYD-nw_autopsf
 - Topology files: /home/hengameh/Desktop/LAMMPS-Workshop/top_all127_prot_1 (with Add and Delete buttons)
 - Load input files button
- Step 2: Selections to include in PSF/PDB**
 - Radio buttons: Everything (selected), Protein, Nucleic Acid
 - Other: protein or nucleic (with a text input field)
 - Guess and split chains using current selections button
- Step 3: Segments Identified**

Name	Length	Index	Range	Nter	Cter	Type

 - Add a new chain button
 - Edit chain button
 - Delete chain button
 - Create chains button
- Step 4: Patches**

Patch	Segid:Resid	Segid:Resid

 - Add patch button
 - Delete patch button
 - Apply patches and finish PSF/PDB button
- Reset Autopsf button
- I'm feeling lucky button



Compare the results of both method!

```
$ diff lys.psf /LYD-nw_autopsf.psf > out
```

As you can see there are some
differences!

Although the second method seems a lot easier, you have less control over the outputs so always check the outcome and don't get too comfortable with it!!



Converting PDB and PSF to LAMMPS input

- Copy charmm2lammmps.pl from lammps/tools to your working directory

```
$ Perl charmm2lammmps all27_prot_lipid lys -  
charmm -border=2 -water -ions
```

The in and data files are generated



➤ **Run a simulation**

- Copy `Imp_*` from `lammps/src` to the current directory

```
$ ./Imp_openmpi < lys.in
```

➤ **Convert the output to PDB**

- Copy `lammps2pdb.pl` from `lammps/tools/ch2Imp` to your directory

```
$ perl lammps2pdb.pl lys
```



References

- <http://www.ks.uiuc.edu/Training/Tutorials/namd/namd-tutorial-unix-html/node6.html>
 - <http://en.wikipedia.org/wiki/PSF>
 - <http://lammmps.sandia.gov/doc/Manual.html>
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- Thank you for your attention.
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