

CHEM 579, Lab

Molecular dynamics of Lysozyme in Water

Goal: Simulation of a protein (lysozyme) in a box of water with ions using the GROMACS program package.

Lab Procedure:

Please follow the instructions in GROMACS Tutorial “Lysozyme in Water” by Justin Lemkul:

<http://www.bevanlab.biochem.vt.edu/Pages/Personal/justin/gmx-tutorials/lysozyme/index.html>

You can also consult with GROMACS manual (<http://www.gromacs.org/@api/deki/files/152/=manual-4.5.4.pdf>) if necessary.

Important Notices:

Since parameters of GROMACS programs depend on version of the package (GROMACS version 4.0.5 is installed on the Steele cluster), there are several differences from the tutorial by Justin Lemkul. These differences are listed below:

1. Before running any GROMACS command, set up the program environment by issuing the following command:

```
module load gromacs
```

2. To generate topology for lysozyme protein using *pdb2gmx*:

```
pdb2gmx -f 1AKI.pdb -o 1AKI_processed.gro -water spce
```

Select the Force Field:

```
5: OPLS-AA/L all-atom force field (2001 aminoacid dihedrals)
```

3. To add ions using *genion* type the following command:

```
genion -s ions.tpr -o 1AKI_solv_ions.gro -p topol.top -pname NA+ -nname CL- -nn 8
```

Pay attention to capital letters and ‘+’ and ‘-’ signs in names of sodium and chloride ions: “**NA+**” and “**CL-**”

4. To run the most time consuming energy minimization and molecular dynamics simulations jobs (e.g. *mdrun -v -deffnm em*, *mdrun -deffnm nvt*, *mdrun -deffnm npt*, and *mdrun -deffnm md_0_1*) you have to use the PBS submission scripts provided instead of direct call of *mdrun* tool.

For example, to run energy minimization take the following steps:

a. Download **em.csh** and **emsub.csh** scripts from <http://teach.kosenkov.org/>

b. Make the scripts executable:

```
chmod +x em.csh
```

```
chmod +x emsub.csh
```

c. Submit energy minimization job to PBS:

```
./emsub.csh
```

Similarly use `nvt.csh` and `nvtsub.csh` for NVT equilibration; `npt.csh` and `nptsub.csh` for NPT equilibration; `md_0_1.csh` and `md_0_1sub.csh` for MD run.

5. Obtained from *g_energy* tool *.xvg* files can be visualized using MS Excel program on Windows. In *.xvg* file delete all lines starting from symbols '#' and '@' then open *.xvg* file with MS Excel using 'delimiters space' mode.

Lab Report:

1. Summarize the results obtained for lysozyme in water:

- a. Visualize protein geometry using VMD program
- b. Plot potential energy vs. energy minimization (EM) step
- c. Plot temperature vs. time for NVT equilibration
- d. Plot pressure vs. time for NPT equilibration

2. Analyze the resulting MD trajectory:

- a. Plot Backbone RMSD vs. time
- b. Plot the radius of gyration for lysozyme vs. time

3. What conclusions can you draw about compactness of protein lysozyme in water based on analysis of obtained MD trajectory?