Running Gromacs

http://www.gromacs.org/

Input files: *.pdb, *.gro, *.itp, *.top, *.mdp, *.tpr

Output files: *.trr, *.xtc, *.edr, *.log

Input:

- pdb : Protein data bank format
- gro: Gromacs format (atom co-ordinates)
- itp: atom topologies (charges, mass, radii, etc)
- top: forcefields, number of molecules, water, etc
- mdp: molecular dynamics simulation parameters
- tpr: all of the above

Output:

- trr: trajectory file (co-ordinates and velocity)
- xtc: trajectory file (co-ordinates only)
- edr: trajectory file (energies)
- log: CPU time, MFLOP, etc.

Creating Input Files

Converting pdb to gro:

pdb2gmx –f input.pdb –o output.gro -o protein.top –inter

inter = interactive, (prompts you for different things

such as charge on polarizable residues,

protonoation state of histidine,

force-field

N-term, C-term patches (NH2, NH3, COO-, COOH)

Move protein.top to protein.itp

Solvation of the system:

editconf –f output.gro -box lx ly lz –o presol.gro

To check box size is OK

editconf –f presol.gro –o presol.pdb

Rasmol presol.pdb (graphics software)

Set unitcell on (check that protein is in the center of the box and the edge is about 3 nm away from the protein)

Solvation (continued)

Once you are satisfied with the box

•Genbox –cp presol.gro –cs spc216.gro –o sol.gro

Spc216: spc water molecules (you can take any other water type as well, tip3p, tip4p, tip5p)

Check once again that water and protein are inside the box and check the box size

- Editconf –f sol.gro –o sol.pdb
- Rasmol sol.pdb

Set unitcell on

Electroneutrality:

If you are happy with the system, check the total charge. If net charge is not zero, then add counter ions to get neutral system. (select random water molecules and replace with ion). Eg: H2O -> Cl- (remove H1, H2, and rename O as Cl-) or use genion (which does the same thing)

Once again check the system with rasmol or any other graphics software you like.

Creating tpr file

Grompp –f emin.mdp –p protein.top –c sol.gro -o emin.tpr

Protein.top: file which contains the following

protein.itp (created by pdb2gmx)

spc.itp

number of protein molecules

number of water molecules

number of counter ions

emin.mdp: molecular dynamics parameter file for energy minimzation of the system. Energy minimization is a must, before the production run.

To begin with, use the default parameters.

For all the gromacs commands, typing –h(help) will give the various options available for each command:

Eg:

pdb2gmx- -h

Editconf –h

Genbox –h, (etc)

Running Gromacs

On the liszt server:

Groit –q –np –n –r –s

- q : que type (tenday, fourweek)
- np: number of processors (1 for energy minimization)
- n: notify when job exits
- r : run (???)
- s: the tpr file (emin.tpr)

This will create the following outputs

emin.gro (energy minimized system in gro format)

emin.trr & emin.xtc : Co-ordinates and velocity (which are not meaningful here)

emin.log: The log file which gives the final energy of the system. Check to see that the energy is negative

Once you are satisfied with the energy minimzation,

Create the tpr file for the the MD simulation (production run)

Grompp -np 2 –f md.mdp –p protein.top –c emin.gro -o md.tpr

Here you have to specify the number of processors, since you can run it in parallel

np = 1 (two processors, 1 node on a dual node CPU)

2 (four processors, 2 nodes)

Run as: Groit –q –np –n –r –s

Do trajectory analysis using the gromacs software (check gromacs online)

http://www.gromacs.org/documentation/reference_3.2/online.html

This link also gives example mdp files and the meaning of each parameter.

Good Luck with your MD simulations!!