22.01.15

Tutorial from the book

- Rerun the simulation from the beginning, this time using different folders for each step of the simulation
- simulation started

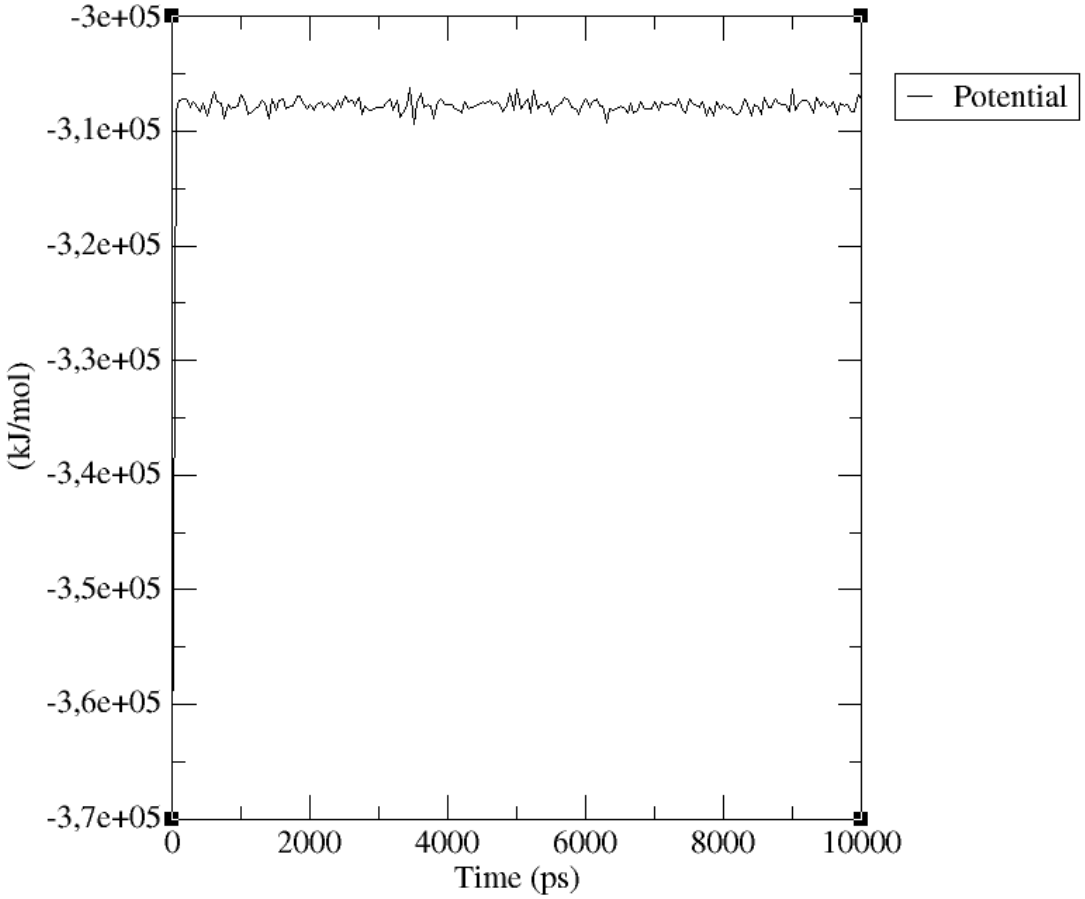
Trajectory Analysis of simulation from 20.01.15

- Simulation of the 2x Heptad
- Connect via ssh

```
ssh hvoehri@hvoehri.mpibpc.intern
```

- Potential energy

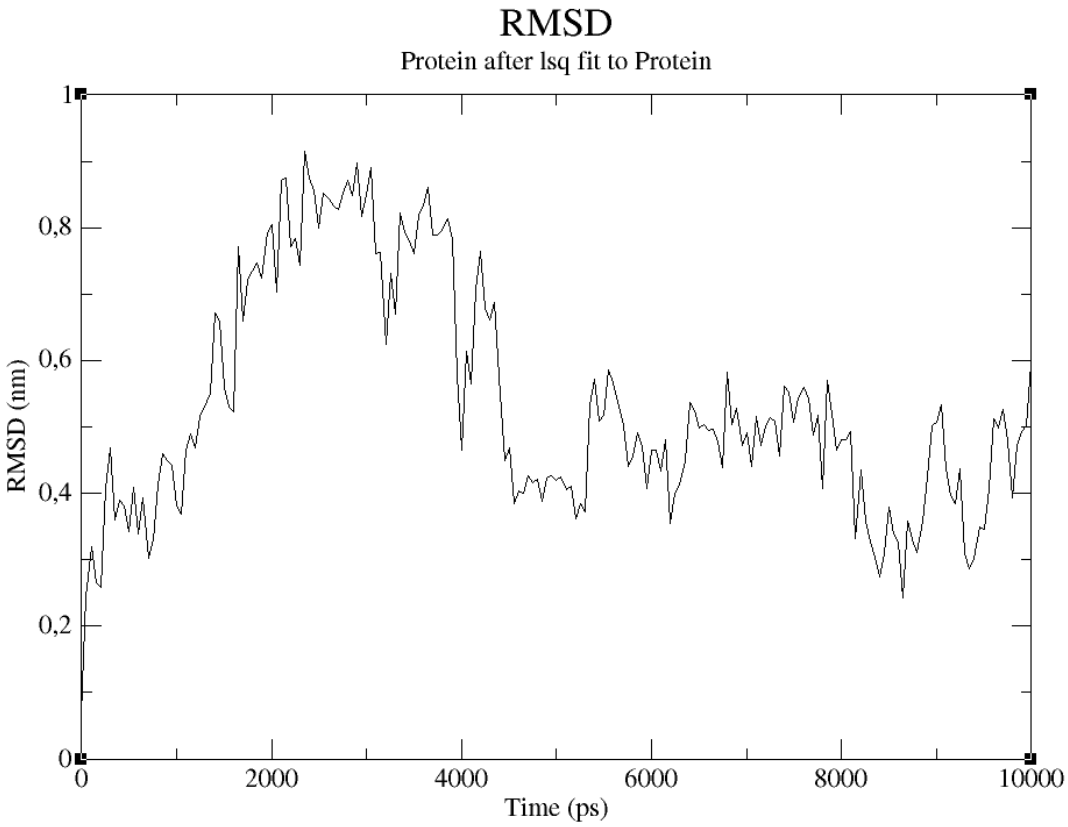
```
g_energy -f ener.part0001.edr
```



Potential Energy

- RMSD calculation performed as follows, selecting two times 1 for protein

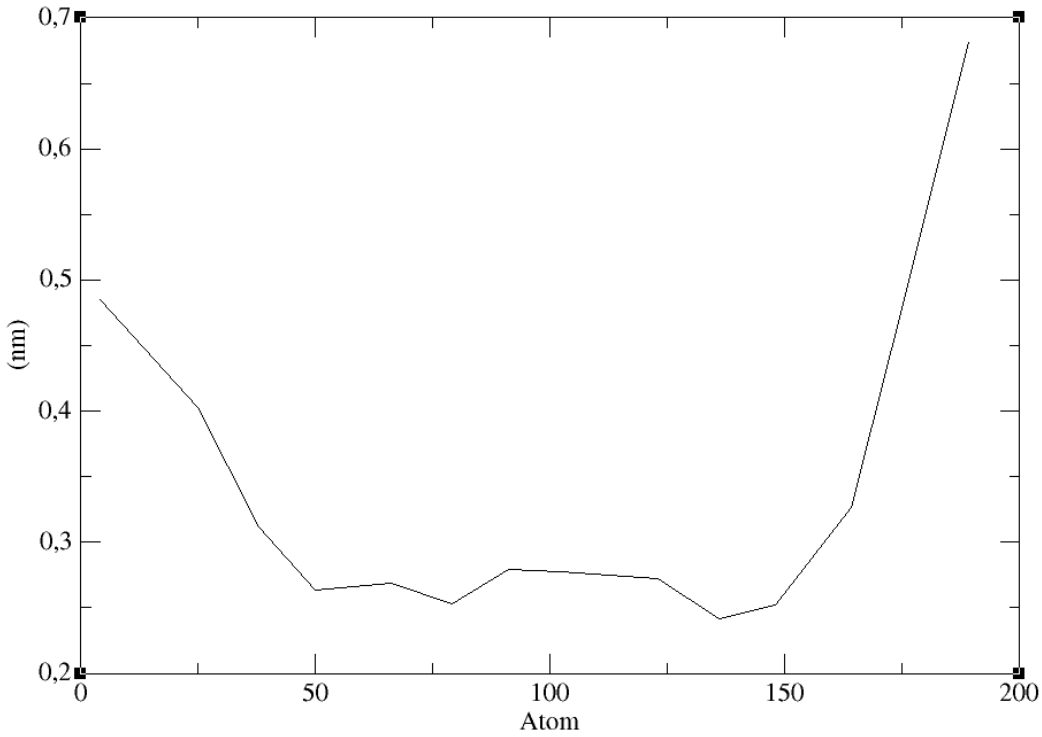
```
g_rms -s ../em.tpr -f traj.part0001.xtc
xmgrace rmsd.xvg
```



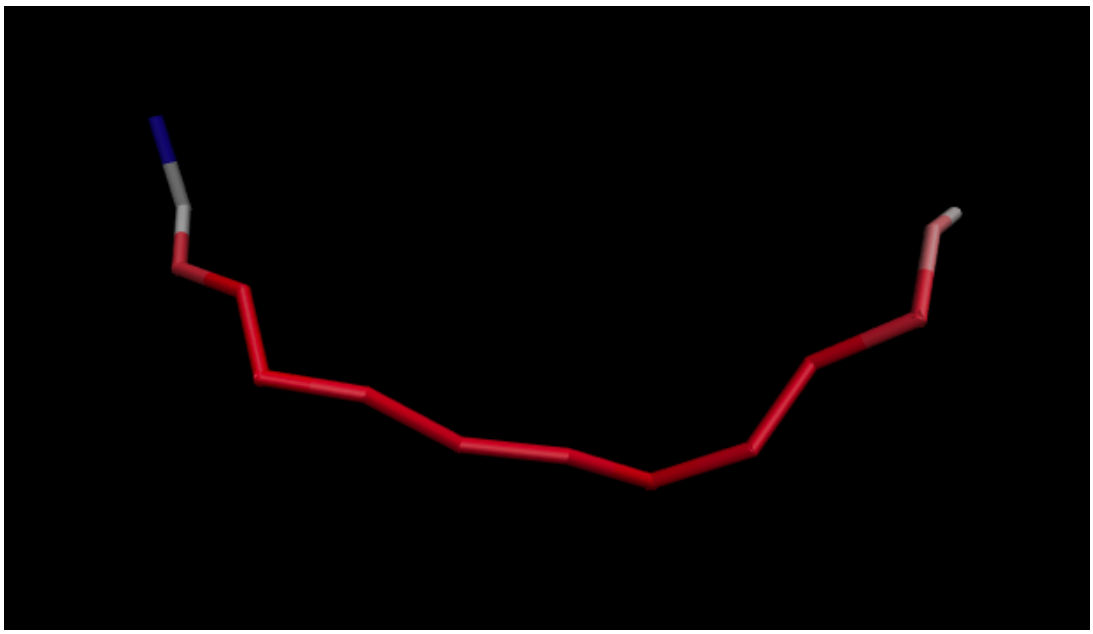
RMSD

- Comparing fluctuations of Cα-atoms with g_rmsf tool

```
g_rmsf -s md.tpr -f traj.part0001.xtc -o rmsf.xvg -oq bfaq.pdb
xmgrace rmsf.xvg
```



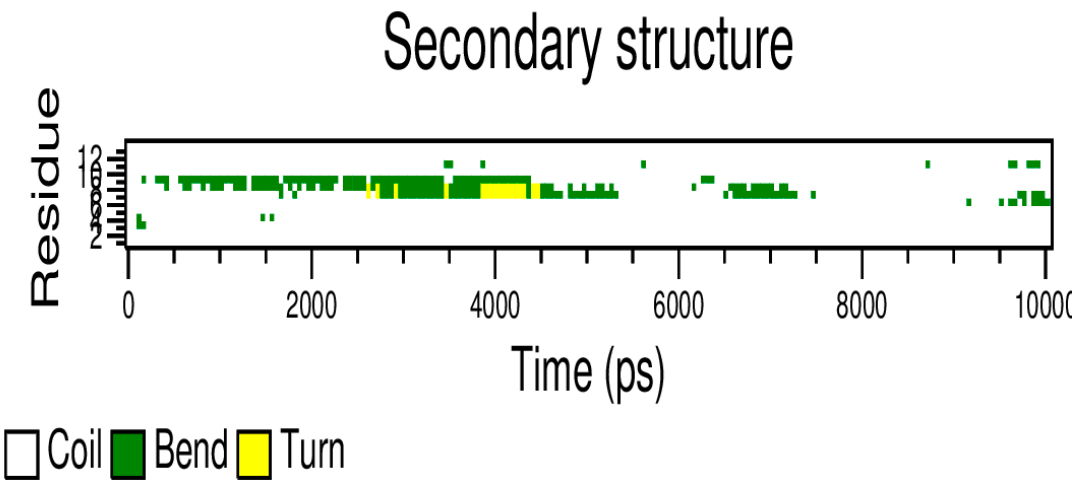
RMSF of Cα atoms



Trace

- Analysis of Secondary structures

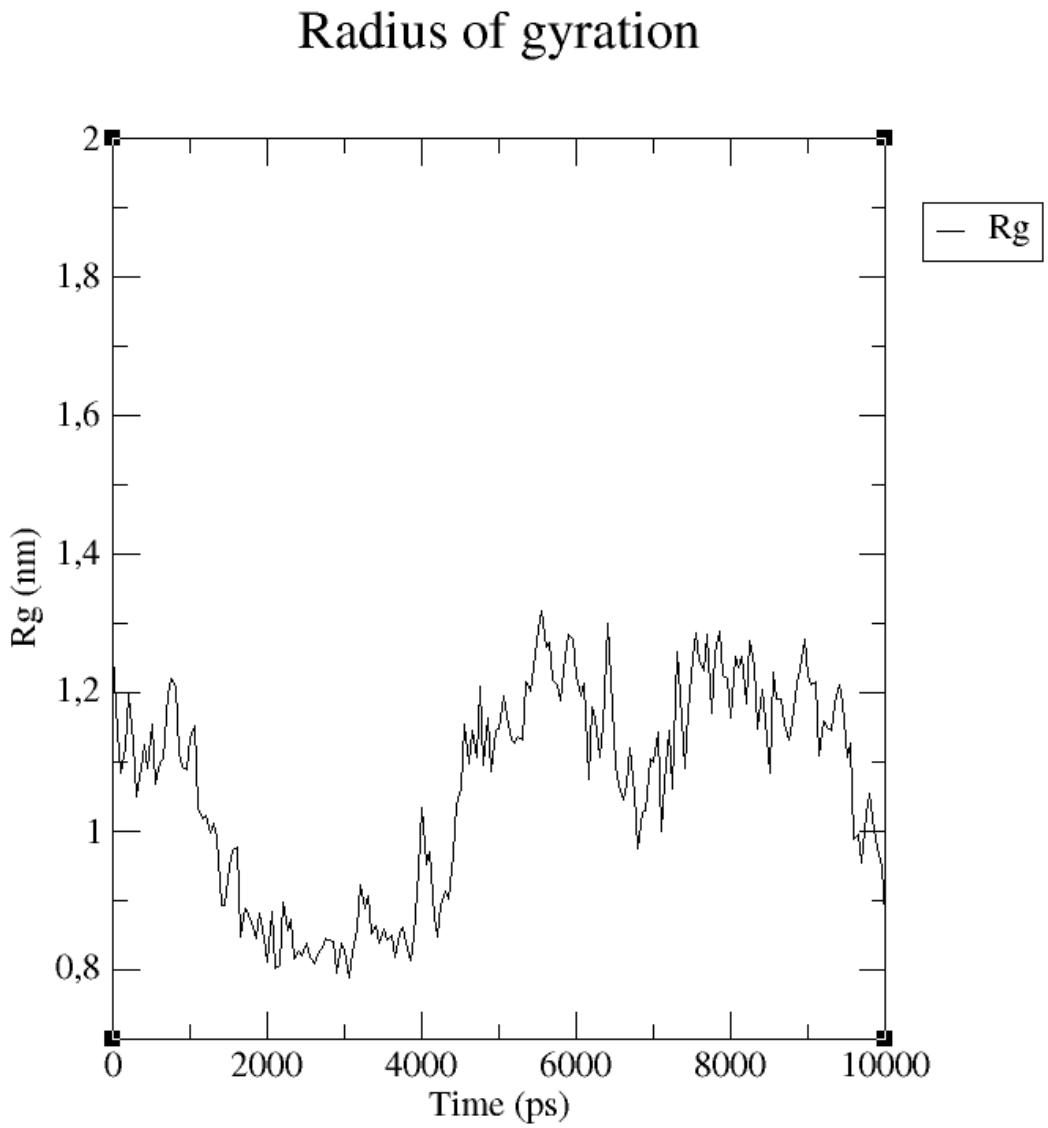
```
do_dssp -s md.tpr -f traj.part0001.xtc -ver 1
xmp2ps -f ss.xpm
gv plot.eps
```



Secondary Structures

- Radius of Gyration

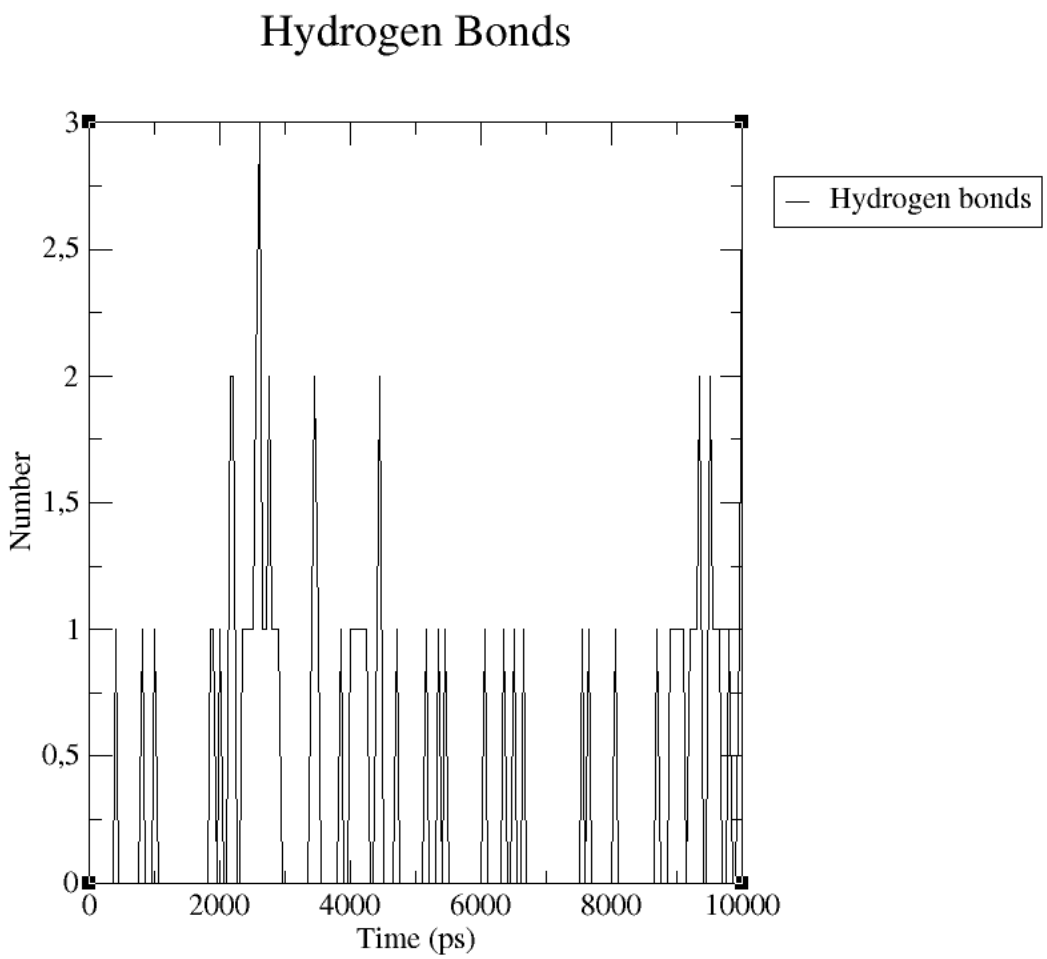
```
g_gyrate -s md.tpr -f traj.part0001.xtc
```



Radius of gyration

- Number of H-bonds between protein and protein itself

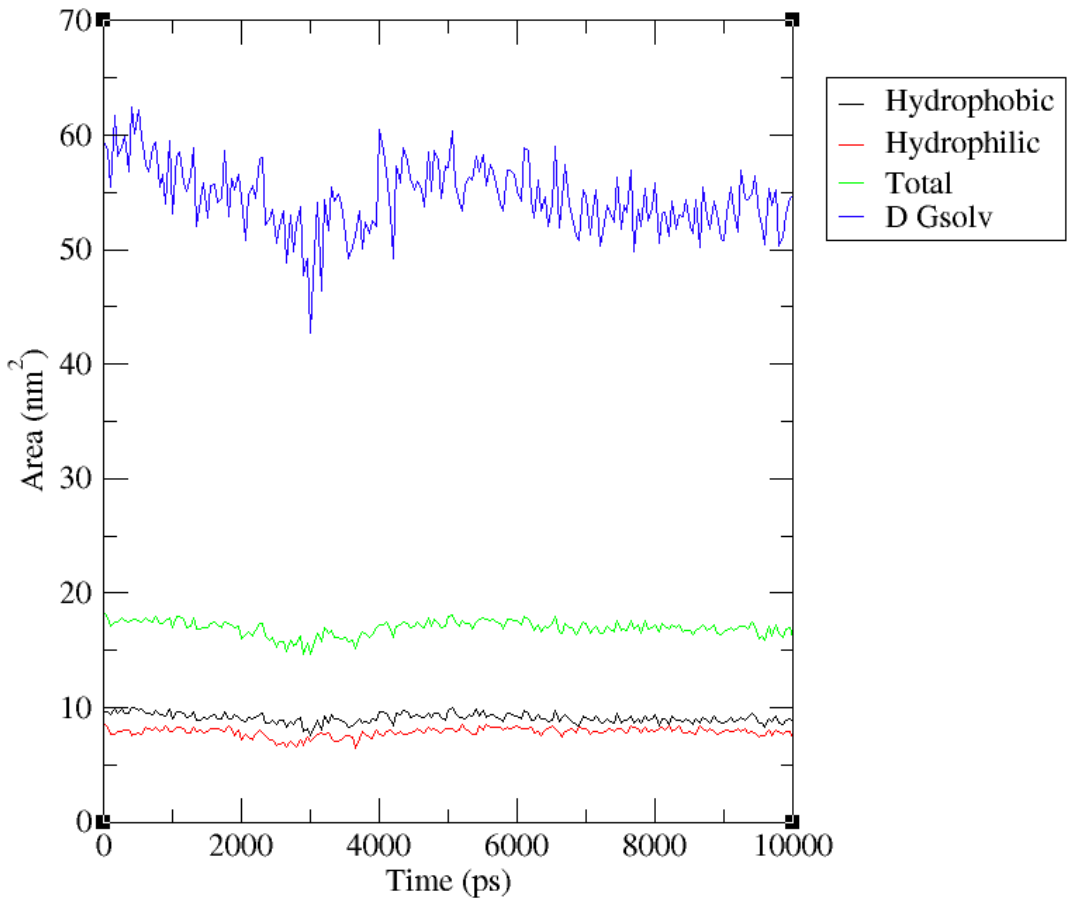
```
g_hbond -s md.tpr -f traj.part0001.xtc  -num hbnum.xvg
```



Number of H-bond formed by the protein itself

- Solvent accessible surface

```
g_sas -s md.tpr -f traj.part0001.xtc
xmgrace -nxy area.xvg
```



Soluble accessible area