27.01.2015

Rerun simulation with berendsen equilibrated CTD

- Grompping with sim.mdp

```
grompp -f sim.mdp -c confout.part0001.gro -p topol.top -o sim.tpr
```

- Leads to the error observed before

```
Program grompp, VERSION 4.6.6-dev-20140325-693d2e6-unknown
Source code file: /tmp/git-gromacs-4-6-department/src/kernel/calc_verletbuf.c, line: 2

Fatal error:
In molecule type 'Protein_chain_A' Virtual site 3fad construction involves atom 5, whi
For more information and tips for troubleshooting, please check the GROMACS
website at http://www.gromacs.org/Documentation/Errors
```

Retry to run the simulation

- Create a new folder and copy CTD.pdb and charmm22star.ff folder over

```
mkdir 270115_CTD
cp 260115_CTD/CTD.pdb 270115_CTD/
cd 270115_CTD/
cp -r ../260115_CTD/charmm22star.ff/ ./
```

- Create topology, position restraint file, and a position restraint file
    - **Do not use virtual sites**
- Create box and ions

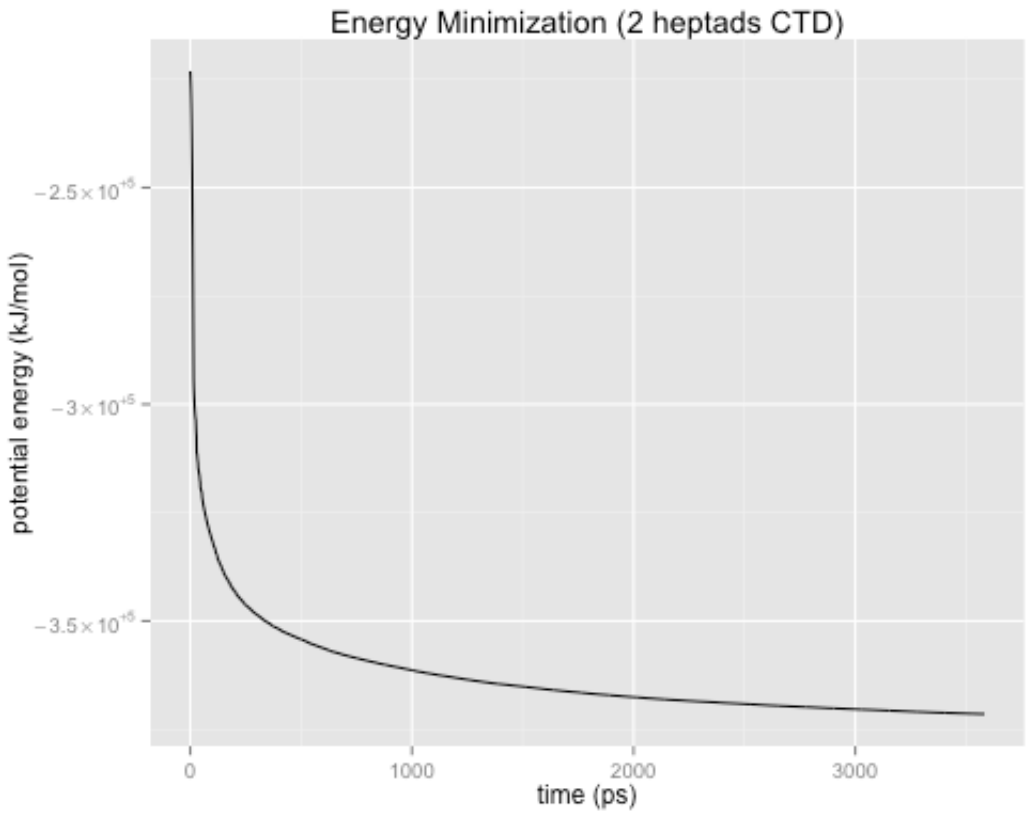
```
pdb2gmx -f CTD.pdb -ignh -ter
genbox -cp box.gro -cs spc216.gro -p topol.top -o solvated.gro
editconf -f conf.gro -o box.gro -bt dodecahedron -d 1.5 -center 0 0 0
genbox -cp box.gro -cs spc216.gro -p topol.top -o solvated.gro
touch ions.mdp
grompp -f ions.mdp -p topol.top -c solvated.gro -o ions.tpr
genion -s ions.tpr -neutral -conc 0.15 -p topol.top -o ions.gro
```

- Run energy minimization

```
grompp -f em.mdp -p topol.top -c ions.gro -o em.tpr
mdrun -v -deffnm em
```

- Check energy minimization

```
g_energy -f em.part0001.edr -o potential.xvg
```



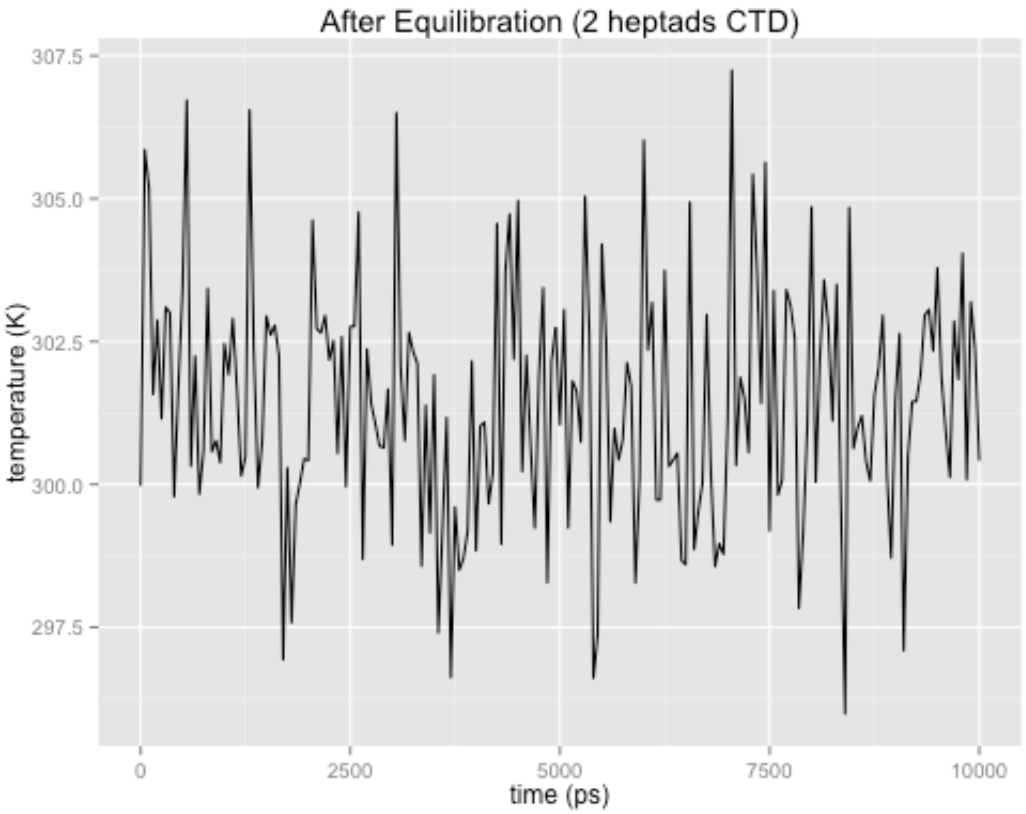
EM

- Run berendsen equilibration

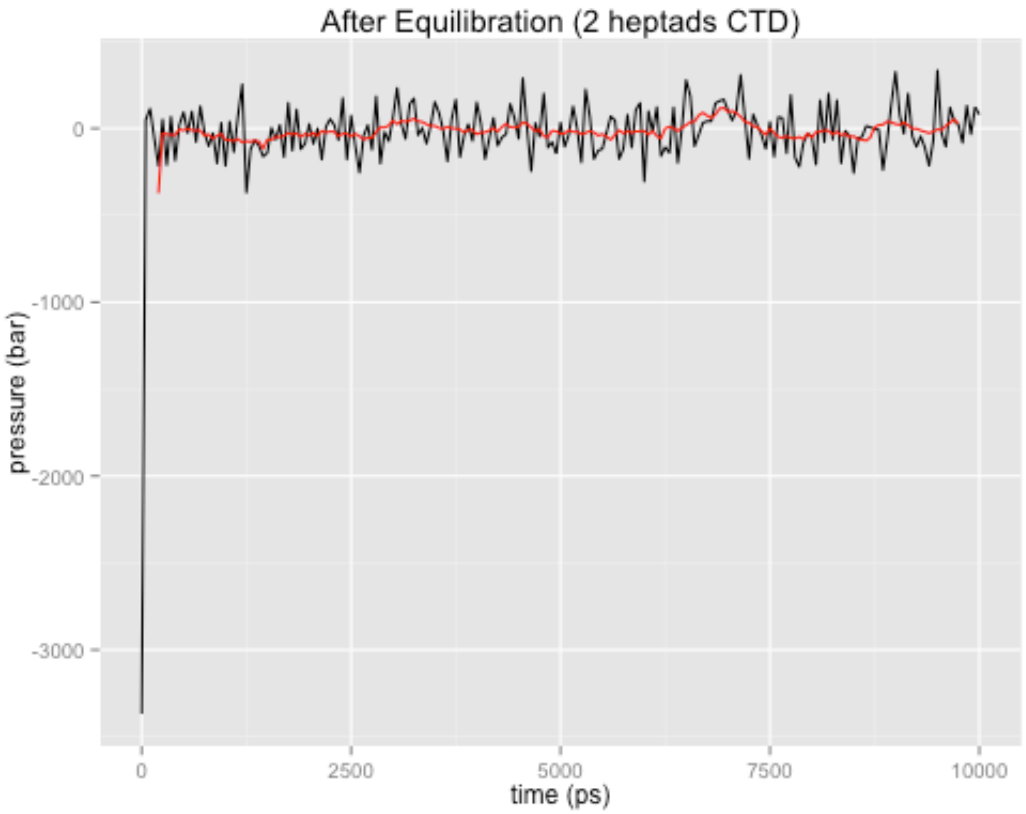
```
grompp -f berendsen.mdp -p topol.top -c em.part0001.gro -o berendsen.tpr
ssh owl3
g_submit -s berendsen.tpr
```

- Recover edr file (was overwritten by subsequent simulation)
- Check temperature, pressure and density

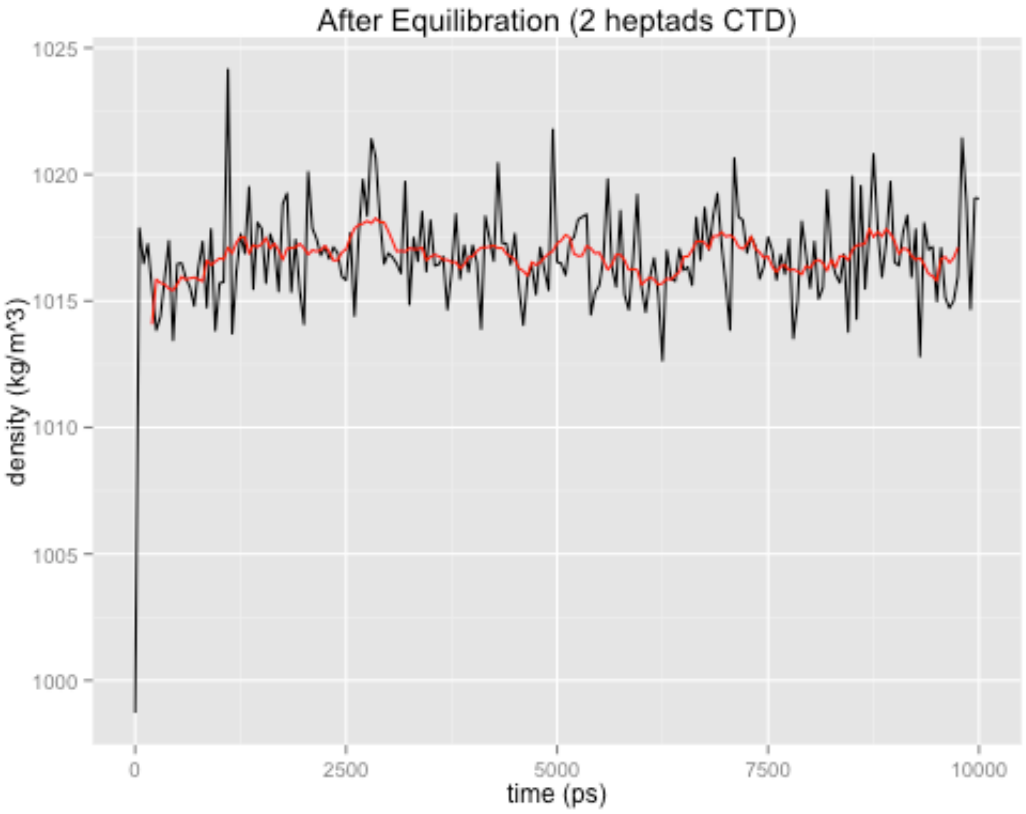
```
mv \#ener.part0001.edr.1# berendsen.edr
g_energy -f berendsen.edr -o temp.xvg
g_energy -f berendsen.edr -o press.xvg
g_energy -f berendsen.edr -o dens.xvg
```



Temperature



Pressure



Density

- Run Simulation

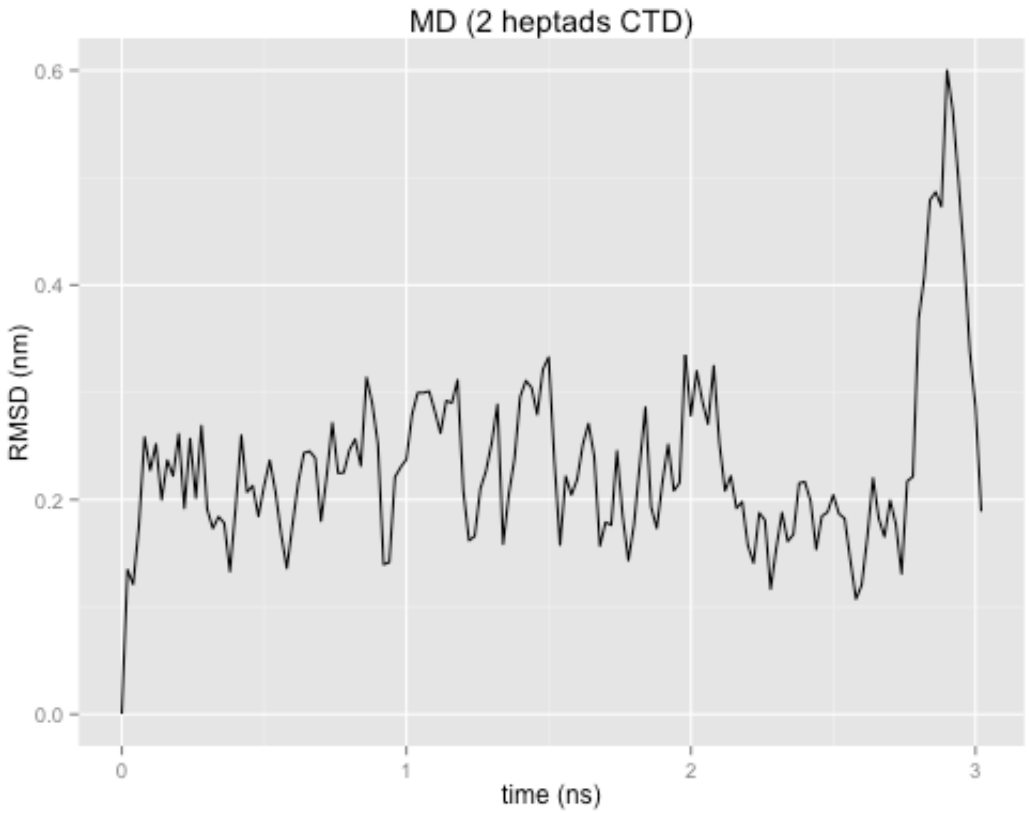
```
grompp -f sim.mdp -p topol.top -c confout.part0001.gro -o sim.tpr
ssh owl3
g_submit -s sim.tpr
```

- Correct trajectory

```
trjconv -s sim.tpr -f traj.part0001.xtc -o sim_noPBC.xtc -pbc mol -ur compact
```

- Check rmsd

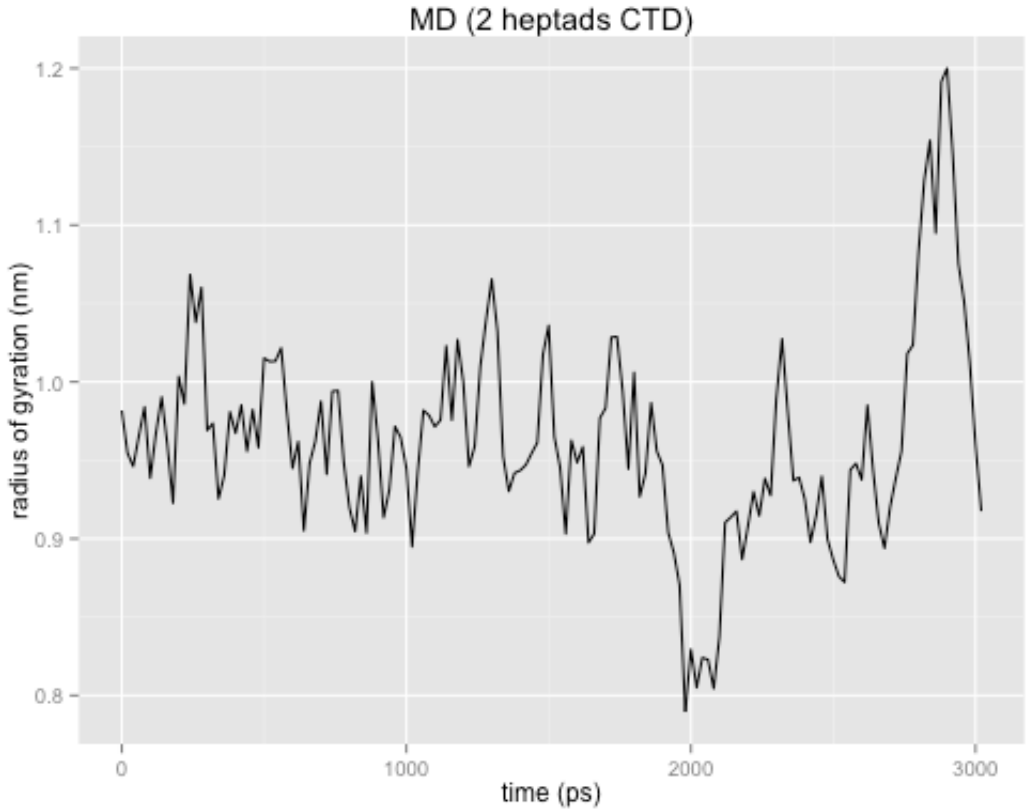
```
g_rms -s sim.tpr -f sim_noPBC.xtc -o rmsd.xvg -tu ns
```



RMSD

- Check Gyration

```
g_gyrate -s sim.tpr -f sim_noPBC.xtc
```



Radius of Gyration