# LEARNING to WORK with GROMACS

August 20, 2013

## 1 Create a water box

1. Generate a water box:
   genbox -cs -box 3.2 -o water.gro
   *In the future you only need to change the size of the box in order to get more or less water molecules.*

2. Write the correct number of water molecules at the end of water.top (Everything else should not be changed).

3. Run the simulation *(For the future there is no reason to change anything in the *mdp files, since we will always do the same kind of simulation).*
   grompp -f Mini_ water.mdp -c water.gro -p water.top -o Mini_ water.tpr
   mdrun -deffnm Min_ water
   grompp -f NVT_ water.mdp -c Mini_ water.gro -p water.top -o NVT_ water.tpr
   mdrun -deffnm NVT_ water
   grompp -f NPT_ water.mdp -v NV_ water.gro -p water.top -o NPT_ water.tpr
   mdrun -deffnm NPT_ water

## 2 Put the waterbox onto the surface

### 2.1 Move water box

- Visualize NPT_water.gro file with VMD and determine position of last upper atom.

- Select Mouse\Pick. Then click on upper atom and look at the information on the vmd console (On the Labels Window appears the same information: Select Graphics\Labels)
- Write down position (VMD in Amstrongs, but GROMACS in nm!).
- Move water box up, leaving approx. 5 Amstrongs between the surface and the droplet.

### 2.2 Put droplet in the middle

- Open start.gro file with editor and look at the last lines → Size of surface in x-y-z-coordinates:

  80SAM H4059519 16.069 13.342 2.139 0.0000 0.0000 0.0000
  80SAM H4159520 16.009 13.423 2.267 0.0000 0.0000 0.0000
  15.00000 13.85640 12.00000

## 3 Let the water box equilibrate on the surface

## 4 Analyze the shape of the drop