CREATE WATER BOX & PLANAR SYSTEM with GROMACS 5

June 29, 2016

Notes:

Changes in *genbox* Gromacs Version 5 or higher:

"This tool has been split to gmx solvate and gmx insert-molecules."

(Copied from:
http://www.gromacs.org/Documentation/How-tos/Tool_Changes_for_5.0)

Comments for "old" genbox:

"When using any 3-point model (e.g. SPC, SPC/E or TIP3P) you should specify -cs spc216.gro which will take this file from the gromacs/share/top directory (in our case the path is: "/usr/local/gromacs/share/gromacs/top"). After solvation, you should then be sure to equilibrate for at least 5-10ps at the desired temperature. You will need to select the right water model in your .top file, either with the -water flag to pdb2gmx, or by editing your .top file appropriately by hand."

(Copied from:
*http://www.gromacs.org/Documentation/How-tos/TIP3P_coordinate_file?highlight=genbo*x)

1 Create a water box

1. Generate a water box:
   gmx solvate -cs spc216.gro -box 6.000 5.196 1.522 -o waterbox_ptensor_v2
   We used the same size as the SAMs.

2. Write the correct number of water molecules at the end of waterbox_v2.top (old name was water.top)

3. Run the simulation
   gmx grompp -f Mini_water_v2.mdp -c waterbox_ptensor_v2.gro -p waterbox_v2.top -o Mini_water.tpr
   gmx mdrun -deffnm Mini_water
   gmx grompp -f NVT_water_v2.mdp -c Mini_water.gro -p waterbox_v2.top -o NVT_water.tpr
   gmx mdrun -deffnm NVT_water
   gmx grompp -f NPT_water_v2.mdp -c NVT_water.gro -p waterbox_v2.top -o NPT_water.tpr
   gmx mdrun -deffnm NPT_waterbox_ptensor_v2

(For parallel runs use a a batch script and add (before "gmx mdrun") "mpirun -np 8" with the number of nodes needed)

2 Put the water box on the surface (not reviewed yet)

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