COMP564: GROMACS 5 TUTORIAL

Example using molecule7.pdb as stated in presentation:

https://www.cs.mcgill.ca/~jeromew/teaching/564/W2019/MD_tutorial.pdf

The following are the GROMACS 5 version of the commands on slides 5 to 9 of this presentation.

Create gromacs topology for the protein from pdb structure
gmx pdb2gmx -f molecule7.pdb -o molecule.gro -ignh
choose force field : 14 (GROMOS, common polyvalent force field)
select water model : 1(default)

Place the protein into a triclinic box
gmx editconf -f molecule.gro -o molecule-PBC.gro -bt triclinic -d 3.0

preprocessing step to prepare energy minimization
gmx grompp -f ../mdp/em-vac-pme.mdp -c molecule-PBC.gro -p topol.top -o em-vac.tpr

energy minimization (find lowest energy coordinates)
gmx mdrun -v -deffnm em-vac

instead of genbox, use solvate to generate the solvent in the box (-cs identifies the solvent)
gmx solvate -cp em-vac.gro -cs spc216.gro -p topol.top -o molecule-b4ion.gro

preprocessing step to prepare the addition of ions
gmx grompp -f ../mdp/em-sol-pme.mdp -c molecule-b4ion.gro -p topol.top -o ion.tpr

randomly replace some of the solvent molecules by ions
gmx genion -s ion.tpr -o molecule-b4em.gro -neutral -conc 0.15 -p topol.top
choose solvent 13 (solution)

preprocessing step to prepare the energy minimization for the whole solution
gmx grompp -f ../mdp/em-sol-pme.mdp -c molecule-b4em.gro -p topol.top -o em-sol.tpr

run energy minimization for the whole solution
gmx mdrun -v -deffnm em-sol

the NVT stabilization step equilibrates temperature in the system
preprocessing
gmx grompp -f ../mdp/nvt-pr-md.mdp -c em-sol.gro -p topol.top -o nvt-pr.tpr
execution
gmx mdrun -deffnm nvt-pr

the NPT stabilization step equilibrates pressure in the system
preprocessing
gmx grompp -f ../mdp/npt-pr-md.mdp -c em-sol.gro -p topol.top -o npt-pr.tpr
execution
gmx mdrun -deffnm npt-pr

preprocessing step for the whole simulation
gmx grompp -f ../mdp/npt-nopr-md.mdp -c em-sol.gro -p topol.top -o npt-nopr.tpr

execution of the main run. This step is lengthy so the output is provided for you. Run it and stop it after a couple minutes once you see how it works.
gmx mdrun -deffnm npt-nopr

This program will output npt-nopr.tpr and npt-nopr.trr , the two files that you will use to do the next steps. The .tpr file contains the starting structure, the molecular topology and all the runs parameters. The .trr file contains the trajectory of each atom throughout the simulation.

generate RMSD graph of the backgone
gmx rms -s npt-nopr.tpr -f npt-nopr.trr -o molecule-bkbone-rmsd.xvg
choose options 4 and 4 (compare backbone to backbone)

generate a pdb movie file from the trajectory
gmx trjconv -s npt-nopr.tpr -f npt-nopr.trr -o molecule-movie.xvg
choose option 4(backbone)