GROMACS Beginners Guide

**Download software:** <https://manual.gromacs.org/>   
**Manual:** https://manual.gromacs.org/current/reference-manual/index.html

**Recommended tutorials:** <http://www.mdtutorials.com/gmx/index.html>

Type of files

In GROMACS we have MANY files, here are some explanations to start with -  
  
**File explanations and examples:**<https://www.compchems.com/gromacs-mdp-file-parameters/#mdp-file-for-npt-equilibrationsb>

**Input files**  
  
.top (topology file): you can think of the topology file as the molecular equivalent of a resume. The topology file is where you define the parameters for how the atoms in your molecule interact with each other. That includes [bonded interactions](https://www.compchems.com/molecular-dynamics-bonded-interactions/) and [non-bonded interactions](https://www.compchems.com/molecular-dynamics-non-bonded-interactions/), which ultimately dictate the motion of the system under study.

* .itp(included in the .top file): it is considered more practical to use the include mechanism in the .top file to add parameters/moleculetypes using .itp files. .itp file is simply another text file that contains molecular topology information, such as bond lengths, bond angles, dihedral angles, and force constants, for a specific molecule or group of molecules.

.gro: the gro file format is a plain text file storing spatial coordinates and velocities (if available) of atoms during a molecular dynamics simulation.   
1. Specifies the number of atoms in the system.   
2. Each line in the .gro file corresponds to an atom in the system and contains several columns with different information: residue number, residue name, atom name, atom number, position (x,y,z), and velocity (x,y,z).  
3. The last line of a .gro file contains information about the size of the simulation box. The line contains three numbers, which represent the size of the box in nanometers (nm) in the x, y, and z directions, respectively.

.mdp: includes the parameters to run the simulation.   
We need .mdp file for each simulation step:   
\*\*Energy minimization: we are simply interested in minimizing the potential energy of the system to avoid steric clashes.   
\*\*NVT equilibrations: this is required to bring the system to the desired temperature.

\*\*NPT equilibrations: this is required to bring the system to the desired pressure (thus density).  
\*\*MD run

.tpr (run input file): includes system topology, parameters, coordinates, and velocities.

**Output files**

.log: a .log file is a human-readble format. It is a computer-generated data file that contains information about usage patterns, activities, and operations within an operating system, application, server or another device. Log files show whether resources are performing properly and optimally.

.xtc: a compressed trajectory binary format.

.trr: the .trr file extension contains the trajectory of a simulation in binary format.

.edr: portable energy file. During a simulation, it is important to monitor a series of different thermodynamic properties to always make sure that everything is proceeding according to our plans. To this aim, we use the gmx energy command. This command simply takes an edr file as input and returns an output file in the xvg format which can be used to plot our data.

.cpt: the complete state of the simulation is stored in the checkpoint binary file, including extended thermostat/barostat variables, random number states and NMR time-averaged data.

General simulation steps

**Energy minimization**

Before we begin dynamics, we must ensure that the system has no steric clashes or inappropriate geometry. The structure is relaxed through a process called energy minimization (EM).  
  
Required files: em.mdp, .itp, .top, .gro

Commands:  
  
1. Assemble your files by creating a .tpr file  
gmx grompp -f em.mdp -c XXX.gro -p XXX.top -o em.tpr

2. Invoke mdrun to carry out the EM:  
gmx mdrun -v -deffnm em

Created files: em.log, em.edr, em.trr, em.gro

\* There are two very important factors to evaluate to determine if EM was successful. The first is the potential energy (printed at the end of the EM process). Epot should be negative, and (for a simple protein in water) on the order of 105-106, depending on the system size and number of water molecules. The second important feature is the maximum force, Fmax, the target for which was set in em.mdp - "emtol = 1000.0" - indicating a target Fmax of no greater than 1000 kJ mol-1 nm-1.

3. Analyze  
- Create a file with the potential energy information

gmx energy -f em.edr -o potential.xvg

**Equilibrium**

EM ensured that we have a reasonable starting structure, in terms of geometry and solvent orientation. To begin real dynamics, we must equilibrate the solvent.

Equilibration is often conducted in two phases: 1. NVT ensemble, and 2. NPT ensemble  
  
1. The first phase is conducted under an NVT ensemble (constant Number of particles, Volume, and Temperature). This ensemble is also referred to as "isothermal-isochoric" or "canonical."

Required files: nvt.mdp,.itp,.top, em.gro

Commands:

1. Assemble your .tpr file with the following:  
gmx grompp -f nvt.mdp -c em.gro -r em.gro -p XXX.top -o nvt.tpr

2. We are now ready to invoke mdrun to carry out the EM:  
gmx mdrun -deffnm nvt

Created files: nvt.xtc, nvt.log, nvt.gro, nvt.edr, nvt.cpt

3. Analyze: Produce the temperature progression:  
gmx energy -f nvt.edr -o temperature.xvg

B. The previous step, NVT equilibration, stabilized the temperature of the system. Prior to data collection, we must also stabilize the pressure (and thus also the density) of the system. Equilibration of pressure is conducted under an NPT ensemble, wherein the Number of particles, Pressure, and Temperature are all constant. The ensemble is also called the "isothermal-isobaric" ensemble, and most closely resembles experimental conditions.  
  
Required files: npt.mdp, nvt.cpt, topol.top, nvt.gro

1. Assemble your .tpr file with the following:  
gmx grompp -f npt.mdp -c nvt.gro -r nvt.gro -t nvt.cpt -p XXX.top -o npt.tpr  
  
2. We are now ready to invoke mdrun to carry out the EM:  
gmx mdrun -deffnm npt

Created files: npt.xtc, npt.log, npt.gro ,nvt.edr, nvt.cpt

3. Analyze

- Produce the pressure progression:  
gmx energy -f npt.edr -o pressure.xvg

- Let's take a look at density as well, this time using   
gmx energy -f npt.edr -o density.xvg

**MD**

Required files: md.mdp, npt.gro, npt.cpt, topol.top  
  
- Assemble your .tpr file with the following:  
gmx grompp -f md.mdp -c npt.gro -t npt.cpt -p XXX.top -o md.tpr

- Execute mdrun:  
gmx mdrun -deffnm md

Created files: md.xtc, md.trr, md.log, md.gro, md.edr, md.cpt, mdprev.cpt

Safe RUN and GOOD Luck ☺

Other useful sources

**VMD: molecular dynamic visualization**<https://www.ks.uiuc.edu/Research/vmd/>

**Protein Data Book (PDB)**

<https://www.rcsb.org/>

<https://www.wwpdb.org/documentation/file-format-content/format33/v3.3.html>

**CHARMM- Force field**  
<https://charmm-gui.org/>  
Polymer Builder: <https://charmm-gui.org/?doc=demo&id=polymer&lesson=2>