Additional Materials: Energy minimization

About parameters in mdp file

- To comment a line out, use semicolon at the beginning
- Title is optional (but always recommended to keep track)
- integrator = steep ; Algorithm steepest descent minimization
- emtol = 500.0 : This step tells Gromacs to stop the energy minimization when the Fmax < 500.0 KJ/mol/nm (if lower tolerance is needed please change the value)
- nsteps = 10000 ; In case, Fmax does not go below 500 KJ, the process stops after 10000 steps (total energy minimization step)
- dt = 0.01 (time step)
- nstxout = 10 ; number of steps between writing coordinates
- cutoff-scheme = Verlet ; Neighbor searching methos and electrostatics is used
- nstlist = 20 ; Frequency to update the neighbor list
- pbc = xyz ; Periodic boundary conditions in xyz
- rvdw = 1.2 ; cut-off distance (Lennard-Jones)
- DispCorr = EnerPres ; apply long range dispersion corrections for Energy and Pressure
- constraints = none
- define = -DPOSRES , is the positional restriained if to be used, if any is desired.
    - It is specified in the grompp command with the flag -r file.gro. If there is no constraint on the residues in the system comment out the line.

Terminal commands used in the tutorial

Grace is already installed in my computer. **Windows** users may use **QtGrace**, which is a fork of **Grace**. Windows users can drag the **.xvg** file icon on the graph window to avoid error messages.

1. Type, **cd Documents/firstmd** and press **Enter**.
2. Type, **vmd ions-added.gro** .
    - Click on **Graphics, Representations**. In VMD Main window.
    - Select **Name** in **Coloring Method**.
    - Type **protein** for **Selected Atoms**. Press **Enter** and see only protein in the graphics window.
    - Click on **Create rep** and select the newly created display.
    - For **selected atoms** type **name CL** and press **Enter**.
    - For **Drawing method**, choose **Beads**.
    - Type, **pbc box** in the **vmd terminal prompt**.
    - Close **vmd**.
1. Type, **gmx grompp -f em.mdp -c ions-added.gro -p topol.top -o em.tpr** and press **Enter**.

2. Type, **gmx mdrun -v -deffnm em** and press **Enter**.
3. Press **Ctrl+C**. To abort the process if there is time constraint.
4. Type **ls** and press **Enter** to list the files.
5. Type, **gmx energy -f em.edr -o energy.xvg** and press **Enter**. Choose 11 (or number for temperature as appropriate for you) and press **Enter** to write the file.
6. Type, **xmgrace temperature.xvg** and press **Enter**.