Hands-on in Molecular Dynamics in GROMACS

CD61004

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Bulk Salt Solution

Input files

- Coordinate file: *Conf.gro*
- Molecular topology file: *topol.top*
- Molecular dynamics parameter files:
  - Energy minimization: *min.mdp*
  - NVT run: *nvt.mdp*
  - NPT run: *npt.mdp*
  - Production run: *prod.mdp*

Topology file (topol.top)

```
#include "ff/forcefield.itp"
#include "ff/h2o.itp"
#include "ff/na.itp"
#include "ff/so4.itp"

[ System ]
Na2SO4 solution

[ Molecules ]
SO4 6
Na 12
SOL 701
```

Molecular dynamics parameter files (.mdp files)

- Used to set the parameters to run MD simulation in GROMACS
- The parameters are such as: *integrator, time step (dt), coordinate dumping frequency (nstxout-compressed), coulombtype, vdwtype, Temperature coupling (tcoupl), Pressure coupling (pcoupl)*

Running molecular dynamics simulations

- Create four directories and run the four steps of MD in the respective directories
- Energy minimization:
  - *gmx grompp -f inputs/min.mdp -c conf.gro -p topol.top -o min.tpr*
  - *gmx mdrun -ntomp 4 -v -deffnm min*

- NVT simulation:
  - *gmx grompp -f inputs/nvt.mdp -c min.gro -p topol.top -o nvt.tpr*
  - *gmx mdrun -v -deffnm nvt*

Running molecular dynamics simulations

- NPT Simulation:
  - *gmx grompp -f inputs/npt.mdp -c nvt.gro -p topol.top -o npt.tpr*
  - *gmx mdrun -v -deffnm npt*

- Production simulation:
  - *gmx grompp -f inputs/prod.mdp -c npt.gro -p topol.top -o prod.tpr*
  - *gmx mdrun -v -deffnm pro*

Plotting in GNUPLOT

Command:

>> gnuplot

>> plot ‘energy.xvg’ u 1:2 w l lw 2

Check these quantities

- Potential energy
- Temperature
- Simulation box length

Task

- Number of time steps to reach the desired temperature in NVT simulations
- Number of time steps to reach constant volume in NPT simulation
- Compute average simulation box length in production run
- Analyse the effect of temperature (300K, 320K, 340K, 360K, 400K) on the volume of the system (Start from output of NPT simulation)
- Compute constant-volume heat capacity from NVT simulation.
  - Heat capacity, $C_v = (kT^2)^{-1} \ <(\delta E)^2>$

Task: RDF

- Calculate the radial distribution function between water oxygen atoms using VMD

Command: VMD prod.xtc prod.gro

Note: water oxygen atom name **OW**

Task

- ❏ Run the MD simulation of methanol-water mixture
- ❏ Do the analysis discussed in previous slides

How would you go about estimating how long it would take to run an MD simulation? What information would you need to consider?

Solution: You would need to consider

- Number of time steps (depends on total time being simulated.)
- Total number of atoms in the system being simulated.
- The average number of non-bonded interactions to be computed for each atom at each time step (non-bonded interactions will dominate the overall computation). This will depend on the algorithm being used to compute the non-bonded interactions.
- Time to compute each non-bonded interaction.