A lab tutorial to using Molecular Dynamics techniques

M. Smaoui & J. Waldispühl

March 26th, 2014 (Updated on November 2016)

McGill

School of Computer Science

Outline

- Download and install Gromacs
  - *www.gromacs.org/Downloads*
- Download your designated protein
  - *http://pdb.org*
- Run your MD simulation

Installation

Option 1: Local installation

- Download and install version 4.6
- The installation process can be tedious and take approx. 1h.

Option 2: Use CLUMEQ

- You must already have access to CLUMEQ
- Loading: "`module load gcc/4.7.2 ifort_icc FFTW/3.3-openmpi-intel openmpi FFTW/3.3-mvapich2-intel mvapich2/1.6-intel GROMACS/4.6.2-mvapich2-intel`"
- Commands: `pdb2gmx_mpi`, `editconf_mpi`, `grompp_mpi`, `mdrun_mpi`, etc..

Setup

- Unzip MD.zip to create a folder MD
- Open a shell and cd into the folder MD
- You should see 3 folders:
  - Proteins
  - workspace
  - mdp
  - tpr_trr
- Copy 1 of the 20 proteins into your workspace:
  - cp Proteins/molecule7.pdb ./workspace
- Move into your workspace folder
  - cd workspace

Commands

Prepare protein:

pdb2gmx -f molecule.pdb -o molecule.gro -ignh

editconf -f molecule.gro -o molecule-PBC.gro -bt triclinic -d 3.0

grompp -f ../mdp/em-vac-pme.mdp -c molecule-PBC.gro -p topol.top -o em-vac.tpr

mdrun -v -deffnm em-vac

Commands

Prepare solvent surroundings

genbox -cp em-vac.gro -cs spc216.gro -p topol.top -o molecule-b4ion.gro

grompp -f ../mdp/em-sol-pme.mdp -c molecule-b4ion.gro -p topol.top -o ion.tpr

genion -s ion.tpr -o molecule-b4em.gro -neutral -conc 0.15 -p topol.top -g ion.log

grompp -f ../mdp/em-sol-pme.mdp -c molecule-b4em.gro -p topol.top -o em-sol.tpr

mdrun -v -deffnm em-sol

Commands

Optimize for temperature and pressure

grompp -f ../mdp/nvt-pr-md.mdp -c em-sol.gro -p topol.top -o nvt-pr.tpr

mdrun -deffnm nvt-pr

grompp -f ../mdp/npt-pr-md.mdp -c em-sol.gro –p topol.top -o npt-pr.tpr

mdrun -deffnm npt-pr

Commands

Run Full simulation

grompp -f ../mdp/npt-nopr-md.mdp -c em-sol.gro -p topol.top -o npt-nopr.tpr

mdrun -deffnm npt-nopr

Commands

Analyze results

g_rms -s npt-nopr.tpr -f npt-nopr.trr -o molecule-bkbone-rmsd.xvg

trjconv -s npt-nopr.tpr -f npt-nopr.trr -o molecule-movie.pdb

(get the npt-nopr.tpr, npt-nopr.trr files from the tpr_trr directory)