Molecular Dynamics Simulations
SS 2007

Alessandra Villa
Computer Lab

How to find me:

Alessandra Villa (Room NU140/229)
www.theochem.uni-frankfurt.de/~villa
villa@theochem.uni-frankfurt.de

Energy Minimization

Energy Minimization of butane using

All-atoms force field/
united atom force field

- Molecule in a box (geometry file *.gro)
- **Complete and correct** topology file (*.top)
- Parameter file (*.mdp)

To check
N. atoms in topology file = N atoms in geometry file

editconf: converts generic structure format and modifies box

Geometry file (*.gro/*.pdb)

To Create define a box around the molecule

editconf -f mol.gro -bt cubic -d 0.8 -o box.gro

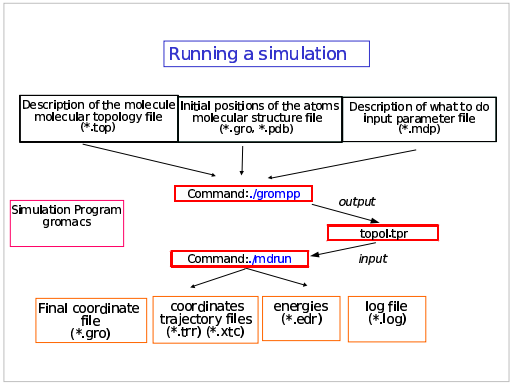
- Molecular coordinate file (*.gro) or (*.pdb)
- Box type
- Minimum distance solute-box wall
- Output name

Parameter file (*.mdp)

```
; LINES STARTING WITH ; ARE COMMENTS
title    =  Minimization of butane      ;Title of run
; Parameters describing what to do
integrator  = steep      ;Algorithm (steep = steepest decent minimization)
emtol       = 2.0        ;Stop minimization when the maximum force < 2.0 kJ/mol
; Parameters describing when to stop,
nsteps      = ???  ;Maximum number of (minimization) steps to perform
; Parameters describing what to save.
nstenergy   =   1          ;Write energies to disk every nstenergy steps (*.edr)
nstxout  =   1          ;Write coordinate to disk every nstxtcout steps (*.trr)

energygrps = XXX   ;which energy group(s) to write to disk
; Parameters describing how to find the neighbors of each atom and how to calculate
the interactions.
nstlist    = 0
ns_type  = simple
rlist = 0.0
coulombtype = cut-off
rcoulomb    = 0.0
rvdw     = 0.0

constraints = none       ;Bond types to replace by contraints
pbc  = no          ;Periodic Boundary Conditions (yes/no)
```



Mimimize a molecule:
Running simulation with GROMACS

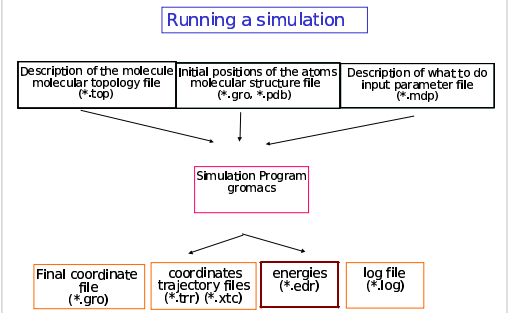
grompp makes a run input file

grompp -f *parameter_file* -c geometry_*file* -p topology_*file* -o TPR_*file*
*.mdp *.gro *.top

mdrun performs a simulation

topol.tpr

mdrun -v -s TPR_*file* (-deffnm *name*)



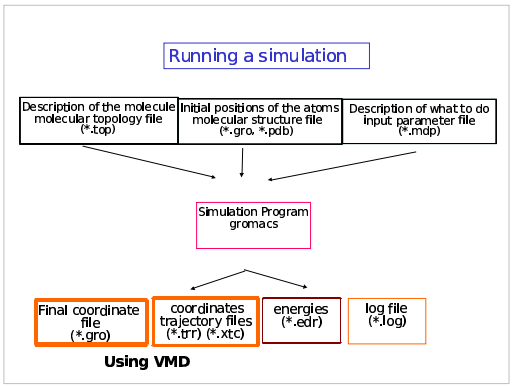
How to analyse the energy (*.edr) file:

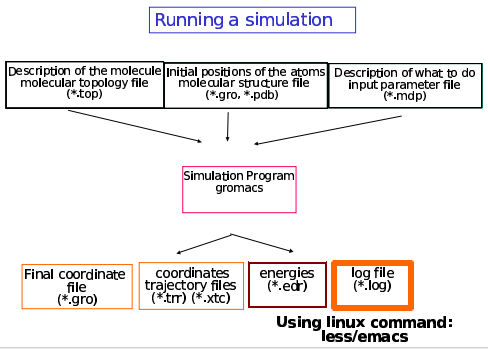
g_energy: extracts energy components and other data from the energy file.

input ***output***

g_energy -f ener.edr -s topol.tpr -o energy.xvg
•type the number correspond to your interest
•To finish put a 0 at the end of the number list

xmgrace -nxy energy.xvg: to display the file





Minimize the structure of the butene molecule :

•Create define a box using editconf.(geometry file *.gro)
•Choose the force field you want to use (all-atom/united-atom)
•Put the working directory: geometry file (*.gro); topology file (*.top)
•Check that the force field files are in the directory (*.itp)
•Complete the parameter file (em.mdp)
•Create the file topol.tpr using grompp
•Run the energy minimization using mdrun

The files, you need, are in our mdcourse directory under part3

For all-atom simulations
Geometry file: butane.pdb
Topology file: butane.top, ff.itp and ffnb.itp
Parameter file: em.mdp

For united-atom simulations
Geometry file: butane_uni.pdb
Topology file: butane_uni.top, ff_uni.itp and ff_uni_nb.itp
Parameter file: em.mdp

Questions:

- How many steps do you need to minimize the structures?
- How many energy contributions do you have? Which is the largest one (in absolute value)? See the last step in md.log file
- Plot the potential energies (using g_energy and xmgrace) .
- Look at the dihedral angles (C-C-C-C) in the confout.gro (using VMD) and in file traj.trr file using VMD

Energy Minimization of butane in water using

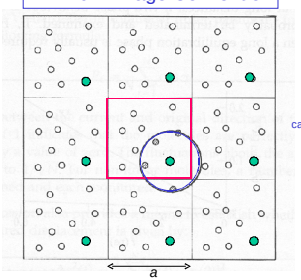
All-atoms force field

- Solvate minimized molecule (geometry file)
- Include water model in topology file: water.itp
- Parameter file

To check
N. atoms in topology file = N atoms in geometry file

Box Dimension should be at least two time bigger than the cut-off used in the non-bonded interaction

Minimum Image Convention



Use only nearest image when calculating interaction

cutoff < a/2

Parameter for non-bonded interactions in *.mdp file

```
; Parameters describing how to find the neighbors of each atom and how
to calculate the interactions.
nstlist     = 10        ;Frequency to update the neighbor list and long
range forces.
ns_type     = grid      ;Method to determine neighbor list (simple,
grid).
rlist   = 1.0       ;cutoff for making neighbor list (short range
forces).
coulombtype = cut-off  ;treatment of long range electrostatic
interactions
rcoulomb    = 1.0       ;long range electrostatic cutoff
rvdw    = 1.0       ;long range van der waals cutoff
```

Parameter for Periodic boundary conditions in *.mdp file

```
pbc  = xyz      ;Periodic Boundary Conditions (xyz/no)
```

Parameters for Energy Minimization in solution

```
;LINES STARTING WITH ; ARE COMMENTS
title    =  Minimization of meset      ;Title of run
; Parameters describing what to do.
integrator   = steep      ;Algorithm (steep = steepest decent minimization)
emtol        = 2000.0        ;Stop minimization when the maximum force < 2000
kJ/mol
; Parameters describing when to stop.
nsteps   = xxxx ;Maximum number of (minimization) steps to perform
; Parameters describing what to save.
nstenergy    = 1      ;Write energies to disk every nstenergy steps
nstxout    =  10        ;Write coordinate to disk every nstxtcout steps (*.trr)
energygrps  = MES SOL        ;which energy group(s) to write to disk
; Parameters describing how to find the neighbors of each atom and
how to calculate the interactions.
nstlist     = 10        ;Frequency to update the neighbor list and
long range forces.
ns_type     = grid      ;Method to determine neighbor list (simple,
grid).
rlist   = 1.0       ;cutoff for making neighbor list (short range
forces).
coulombtype = cut-off  ;treatment of long range electrostatic
interactions
rcoulomb    = 1.0       ;long range electrostatic cutoff
rvdw    = 1.0       ;long range van der waals cutoff


constraints  = all-bonds      ;Bond types to replace by contraints
pbc  = xyz      ;Periodic Boundary Conditions (xyz/no)
```

How to solvate a molecule box:

- Take a confout.gro of the minimization in vacuum.
- Check that the box dimensions or define a box
- Look at the help of genbox
- Use genbox to solvate the molecule using -cs water.gro
- Add to the topology file the number of water molecule and include the topology of the water (water.itp)

You find the file water.gro and tip3p.itp in the mdcourse directory

solute topology file

```
genbox -cp confout.gro -cs water.gro -p *.top -o  butane_w.gro
```

Solute coordinate file (*.gro) or (*.pdb)

Water box

Output

Minimization in solution

- Solvate the **minimized** molecule (using genbox)
- Create the parameter file
- Run a minimization for all atom force field

Analysis

- Use the tools g_energy to plot the potential energy and all the energy contributions.
- How many steps do you need to minimize the structures?
- What do you observed? Are there difference with the *in vacuo* results?
- Vizualise the minimized structures (confout.gro)
- Which value has the dihedral angle (C-C-C-C) in the minimized structures.