

## Excercise 5

Thermalization from a bad  $\Gamma_0$  has to be made in steps, especially if pressure coupling is involved. In gromacs, every run saves the ending  $\Gamma$  as .gro file (where one has velocities too). Restarting run 2 from run1name.gro (and possibly using full precision trajectory **run1.trr**) of run 1 is simple

```
grompp -f run2.mdp -p ar.top -c run1.gro [-t run1.trr] -o run2
```

as the preprocessor can handle old configuration files. Needless to say, in restart one needs to remove any velocity generation in the input parameter (**.mpd**) file. More help is available in the end of this assignment pdf.

**Assignment 1. (1/3)** Starting from start.gro or your latest NVE.gro, run NVT for Ar at 80K. Use berendsen thermostat first and restart Nose-Hoover with -t option and 10 chain thermostats. For the NH run plot (and attach) conserved energy, and study thermalization by investigating temperature. Plot also the Ar RDF considering snapshots that belong to the thermalized part of the NH run ( using **-b** option)

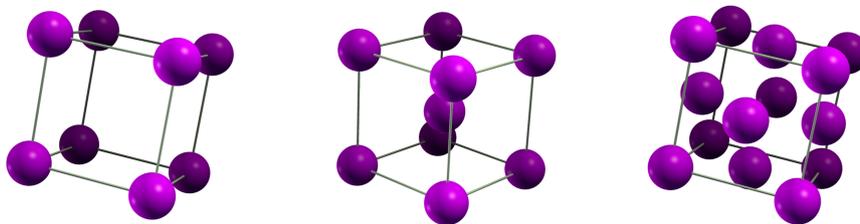
```
g_rdf -b [t_start in ps] ...
```

and if you made that for NVE, plot them both in same figure. Calculate also the pressure curve, attach a figure and comment. Can one use pressure curve to monitor thermalization?

**Assignment 2. (1/3)** Starting from your latest NVT.gro and NVT.trr, run NPT for Ar at 80K and 1 bar. Aim at doing MTTK run with 10 chain thermostats. For the MTTK run plot (and attach) conserved energy, and also discuss thermalization based on temperature and density. Plot also the Ar RDF and if you did it for NVE and NVT, plot them both in same figure and discuss them.

**Assignment 3. (1/3)** Starting from your latest NPT.gro and NPT.trr, run an NVT simulation for Ar at 3K Using Nose-Hoover chain thermostat. Visualize the trajectory, attach a the last snapshot and comment. Run then an NPT at 3K and 1 bar (Again aim using MTTK). Check thermalization, visualize and attach a snapshot. Please comment something.

The `-cn` option for `g_rdf` yields also the cumulative neighbor number curve as a function of  $r$ . Based on this and the standard RDF curve for thermalized Ar at 3K and 1 bar, which of the three cubic unit cells, simple, bulk centered or face centered would you say solid Ar at 3K and 1 bar probably has? What is the unit cell side length? Based on this, at which distances would you expect peaks in the RDF? Compare with the one you calculated.



Return your solutions to Ville [moleculardynamicssimulations@gmail.com](mailto:moleculardynamicssimulations@gmail.com), **latest by Friday exercise session 11.10.2013**. Please make the solution letter a single PDF.

**For some help, turn the page →**

## Thermostats and Barostats

To turn on a thermostats and barostats, you will need modify the `.mdp` file. If you need only thermostat, modify only that part... One may choose different relaxation times  $\tau$  and compressibility  $\kappa$  in certain cases. Here we will use  $\tau$  values of picoseconds and  $\kappa$  of water. Using Nose-Hoover chains requires velocity-Verlet integrator `integrator = md-vv` as the method needs velocities  $\mathbf{v}_i$ . Moreover if you want to use **NH chain and p-coupling**, use the MTTK run. yFor restart runs, you also need to remove the generate velocities section.

### Berendsen P&T

```
; Temperature coupling berendsen
tcoupl          = Berendsen
tc-grps         = system
tau_t          = XXX ;berendsen relaxation time in ps
ref_t          = XXX ;reference temperature, in Kelcin
;Pressure coupling 1
pcoupl         = Berendsen
pcoupltype     = isotropic
tau_p          = XXX ;berendsen coupling time in ps
ref_p          = XXX ;reference pressure, in bar
compressibility = 4.5e-5 ;water compressibility is 4.5e-5 [bar-1].
```

### Nose-Hoover and Parrinello-Rahman

```
;Temperature coupling nose-hoover
tcoupl          = Nose-Hoover
nh-chain-length = 1      ; IF SINGLE NH IS ENOUGH
tc-grps         = system
tau_t          = XXX    ; in ps (value should be at least 5 times
                        ;larger to berendsen tau)
ref_t          = XXX    ; reference temp, kelvin
;Pressure coupling isotropic parrinello-rahman = andersen
pcoupl         = Parrinello-Rahman ; IF SINGLE NH IS ENOUGH
pcoupltype     = isotropic
tau_p          = XXX    ; in ps (value should be at least 5 times
                        ;larger to berendsen tau)
ref_p          = XXX    ;reference pressure, in bar
compressibility = 4.5e-5
```

## MTTK

```
;Temperature coupling nose-hoover
tcoupl          = Nose-Hoover
nh-chain-length = XXX
tc-grps         = system
nsttcouple      = 1
tau_t           = XYZ ; in ps (value should be at least 5 times
                    ;larger to berendsen tau)
ref_t           = XXX ; reference temp, kelvin
;Pressure coupling isotropic parrinello-rahman = andersen
pcoupl         = mttk ; IF SINGLE NH IS NOT ENOUGH
pcoupltype     = isotropic
nstpcouple     = 1
tau_p          = XYZ ; in ps (value should be at least 5 times
                    ;larger to berendsen tau)
ref_p          = XXX ;reference pressure, in bar
compressibility = 4.5e-5
```