Excercise 4

On the course web page you will find input files for NVE-simulation of Ar and a $\mathbf{r}(0)$ (start.gro). We are going to use GROMACS code (a real scientific MD code) for simulations. **See the end of this document for computer environment instructions and how to obtain the files.**

The gromacs package has plenty of useful routines and we will learn some of them today. Firstly, one needs parameters for the run to be made (**NVE.mdp** file), configuration to start with (**start.gro** file) and topology file describing bonds and forces (**ar.top** file). One can check all the files and compress them to one input file (**NVE.tpr**) with a preprocessor

Assignment (1/3) NVE for Ar. We have comments in **NVE.mdp** and **ar.top** files. Go through them both. Also check how your **start.gro** looks like using VMD. Then preprocess and run the calculation as it is. The run produces a number of output files and we will study some of them.

- The log file **NVE.log** is readable output of your simulation, printed in intervals given by the .mpd file.
- Energy file **NVE.edr** contains many different thermodynamical quantities written in intervals given by the .mpd file. One can study these easily by running

  g_energy -f NVE.edr

  and selecting quantity to be printed, like total energy for your system. The program outputs an **energy.xvg** figure file, which you can plot with **xmgrace** or simply open and copy the numbers from it and plot them with your favourite program.
- Trajectory file **NVE.trr** (written in intervals given by the .mpd file.) is a binary one, which can be converted to ASCII file by

  trjconv -f NVE.trr -s NVE.tpr -o NVE.ascii.gro

  One can open the **NVE.ascii.gro** directly in VMD and play the dynamics. Naturally restarting simulation can be done using the trajectory.

Is the run equilibrized in the end? Attach a plot to your answer. Also visualize your trajectory with VMD and attach a snapshot of your choice in the report.

Assignment 2. (1/3) Δt. Using different time steps study the energy conservation of your NVE run. How large time step can one use? Attach the plots you are studying to your report. You can assume that for 1 fs step, energy is conserved well. This is the case btw.
(One can define "conserved"as "to have drift less than 1.0×10^{-X} a.u./(atom*ps)". Energy of 1 a.u.=27.211eV and 1 eV is approx. 96 kJ/mol. X depends on person and studied system, typically X>6)

Assignment 3. (1/3) Other properties with largest possible Δt. Plot the temperature of your system for the largest Δt you find the simulation stable with. How does this temperature compare to the initiated one? Was the run started from potential energy minimum? And guess what kind of macig one can do with **g_rdf**!

g_rdf -f NVE.trr -s NVE.tpr

Prepare also a plot of Ar-Ar RDF (output will be **rdf.xvg**) for your system and attach that to the solution letter. The parameters we are using are approximately $\sigma = 3.405$ Å and $\epsilon = 1.00$ kJ mol^{-1}. Calculate the position of potential minimum for LJ with the parameters and compare it to the RDF.

Return your solutions to Ville *moleculardynamicssimulations@gmail.com*, **latest by Friday excercise session 4.10.2013**. Please make a solution letter a single PDF.

Turn the page for info →

A. LINUX on PC

If you have a LINUX machine home you can find gromacs and install it for free. (In Ubuntu it is as simple as **sudo apt-get install gromacs** and you are done.) Note that you can also install Ubuntu parallel to your windows and make the selection of operating system when booting.

grompp -f NVE.mdp -p ar.top -c start.gro -o NVE.tpr

running them on a desktop is then simple

mdrun -v -deffnm NVE

B. Alcyone cluster

You can do the excercise on a department cluster (alcyone.grid.helsinki.fi). You should have received an account and a password – if not, contact Johannes. On alcyone, you will need a batch job file **submitgromacs_scratch**, where you have the command for running the MD. The batch job file is then submitted to a queue and evaluated when resources are available. This is the supercomputer way of doing calculations. Small analysis programs can be run in the login node so the only part needing batch script is the **mdrun**. On alcyone, copy your files to a folder for example by

wget http://www.courses.physics.helsinki.fi/fys/moldyn/Exc4.files.tar.gz

Extract the tar by

tar -xvf Exc4.files.tar.gz

Now, you can load the gromacs environment on your login node by typing

module load gromacs

This loads the module and all the programs for your use. To run the preprocessor (for the given files) now type

g_grompp -f NVE.mdp -p ar.top -c start.gro -o NVE.tpr

Now you can edit **submitgromacs_scratch** so that you have the proper **NVE.tpr** in the call of **g_mdrun**. Submitting your MD to queue takes place when typing

sbatch submitgromacs_scratch

You can check your job status by

squeue -u [yourusernameonalcyone]

and after you have run the MD you can carry on with analysis. This you can do without batch jobs. You can naturally change the names of all the input and output files, as long as you do it consistently...