Worksheet 4
All-atom Molecular Dynamics simulations of the alanine dipeptide

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June 24, 2013
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Important remarks

- Due date: **Thursday, July 9^{th}, 2013, 8:00**
- You can either send a PDF file to Jens Smiatek (smiatek@icp.uni-stuttgart.de) or submit a hand-written copy.
- If you have further questions, contact Jens Smiatek (smiatek@icp.uni-stuttgart.de)

Computer simulations of the alanine dipeptide (20 points)

The alanine dipeptide is a small molecule which consists of two alanine amino acid units. The molecular structure is shown in Fig. 1. It consists of two dihedral angles ϕ and ψ and five backbone carbon atoms. In the following you will conduct a Molecular Dynamics GROMACS simulation in explicit water to calculate the distribution of the dihedral angles. The procedure is nearly identical for each simulation conducted bt GROMACS.
Important Remark 1: By adding the -h flag to each GROMACS command, the manual entry is shown.
Important Remark 2: An internet search may sometimes be helpful. The manual can be also found at www.gromacs.org. An example for setting up a GROMACS simulation can be found at [2].
Furthermore: Often the output files are the new input files for the next command.

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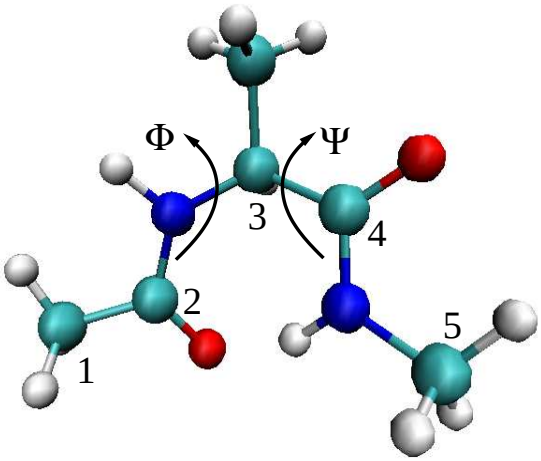

Figure 1: Molecular structure of the alanine dipeptide with the dihedral angles ϕ and ψ and the numbered carbon atoms. Taken from Ref. [1]

Task 1: Converting PDB files to GRO files

You can open the structure of the alanine dipeptide in VMD. Unfortunately, GROMACS cannot use PDB files. Therefore you have to convert the file format to a GRO-File.

- Use the command pdb2gmx
- We use the force field AMBER94 and the TIP3P water model

Always: Have a look after the command in the corresponding directory for the output files.

Task 2: Edit the simulation box

With the command editconf you can edit the simulation box (dimensions, shape...).

- Use the command editconf
- We simulate a cubic box
- The distance between the solute and the box is 1 nm

Task 3: Solvation with water

With the command genbox you can dissolve the alanine dipeptide with water.

- Use the command genbox and the flag -cs

Task 4: Preprocessor: Energy minimization

In the following you have to modify the file em.mdp. After modification, the preprocessor for the energy minimization can be created with the grompp command.

- Open the file em.mdp
- We use the steepest descend algorithm with a maximum tolerance of emtol=500 and emstep=0.01.
- Use the grompp command

Task 5: Perform the energy minimization

Perform the energy minimization by the mdrun command.

- Use the mdrun command and the -v option

What is displayed on the monitor and what is the result?

Task 6: Perform the warm up and the simulation

Perform the warm up and the simulation run with the grompp and mdrun command.

- Have a look at the full.mdp file. Some values are missing. We want to equilibrate the system for 200 ps with a time step of 2 fs. The Berendsen thermostat with a temperature of 300 K is used for all simulations. The simulation run should take 2 ns with a time step of 2 fs.
- Use grompp (output) $\rightarrow$ mdrun (input/output) $\rightarrow$ grompp (input) $\rightarrow$ mdrun (input)

What is the meaning of the entries in the mdp-files?

Task 8: Calculate the distribution of the dihedral angles

The distribution of the dihedral angles can be visualized by a Ramachandran Plot [3].

- Use the command g_rama

What is shown?

Task 9: Visualize the trajectory with VMD

Have a look at the simulation [4]. For this, we need a GRO-File and the TRR-trajectory-file.

- Open VMD
- Load the GRO-File
- Load the *.TRR file

References

[1] J. Smiatek, A. Heuer; *J. Comp. Chem.* **32**, 2084 (2011)

[2] http://manual.gromacs.org/online/speptide.html

[3] http://en.wikipedia.org/wiki/Ramachandran_plot

[4] http://www.csc.fi/english/csc/courses/archive/material/gmx-gpu-materials/vmd-gromacs-exercises.pdf