Worksheet 4
Coarse-grained polymers and their properties

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Important remarks

- Due date: **Tuesday, June 3rd, 2014, 10:00**
- You can send a PDF file to Anand Narayanan Krishnamoorthy (anand@icp.uni-stuttgart.de) or submit a hand-written copy.
- If you have further questions, contact Jens Smiatek (smiatek@icp.uni-stuttgart.de) or Anand Narayanan Krishnamoorthy (anand@icp.uni-stuttgart.de).

Short Questions - Short Answers (6 points)

Please give precise and short answers to the questions.

1. Q1: What is the persistence length of a polymer and how it is defined?
2. Q2: Which real polymers can be described by the Worm-like-chain model?
3. Q3: What are the differences between the ideal chain, the worm-like-chain, the freely jointed chain and the self-avoiding chain?

You need to study literature in order to answer these questions. A good reference would be the one by Rubenstein "Polymer Physics".

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1 T1: Polymer properties and thermal blobs

Task : (6 points)

Consider an ideal linear chain with N Kuhn monomers of length b and fixed end to end vector R directed along the x axis. Demonstrate that the mean-square projection of the radius of gyration onto the direction of its end to end vector is

$$\frac{1}{N}\Sigma_{i=1}^{N} < ((\vec{R}_i - \vec{R_{cm}})_x)^2 >= \frac{1}{36}Nb^2 \tag{1}$$

Note that for $|\vec{R}| = 0$ the mean square radius of gyration of a ring polymer $< R_g^2 >= Nb^2/12$ is recovered, for $|\vec{R}| = bN^{0.5}$ the mean square radius of gyration of an ideal linear chain $< R_g^2 >= Nb^2/6$ is recovered and for $|\vec{R}| = bN$ the mean square radius of gyration $< R_g^2 >= (approx)Nb^2/12$ is recovered. It is interesting to point out that the asymmetry of the ideal linear chain,

$$(1 + \frac{3\vec{R}^2}{Nb^2})$$

is quite large and a typical shape is better represented by an elongated ellipsoid than by a sphere.

C1: Static properties of coarse-grained polymers (8 points)

The program package ESPResSo

The program package ESPResSo is developed and maintained at the Institute for Computational Physics and is mainly intended to perform coarse-grained simulations with Lattice-Boltzmann, Dissipative Particle Dynamics and Langevin Dynamics. It consists of a broad variety of electrostatic algorithms, analysis tools and various other features like the support of massively parallelized hardware architectures or GPU-platforms. In the following you will conduct coarse-grained simulations with the Lattice-Boltzmann and Dissipative Particle Dynamics method to learn how to work with ESPResSo. The package can be downloaded at

- ESPResSo-Homepage: http://espressomd.org/
- ESPResSo-Download: http://espressomd.org/wordpress/download/
- ESPResSo-Manual:
  http://espressomd.org/jenkins/job/ESPResSo/lastSuccessfulBuild/artifact/doc/ug/ug.pdf

Important Remark: It is good to have a look inside the manual to understand how it works. This tutorial is mainly intended to understand how the coarse-grained methods and the simulation package works.

Download and install ESPResSo

Download the ESPResSo package version 3.2.0 (espresso-3.2.0.tar.gz) and install it in your home directory. You can follow the commands as given in the manual on p. 14. Before compilation and after using "./configure", please uncomment the macros in "myconfig-sample.h" for

- LENNARD_JONES

and rename it to myconfig.h. Have a look at the test cases and the manual to understand how to set up a polymer with Langevin Dynamics. You need harmonic springs with the spring constant $k = 10$ to connect the monomers. The temperature equals $T = 1$ and the friction coefficient of the Langevin equation is given by $\gamma = 1$.

Ideal chain

Perform a simulation of an ideal coarse-grained polymer with Langevin Dynamics. Simulate different chain lengths $(N = 10, 20, 30, 40, 50, 100, 200)$ and calculate the radius of gyration R_g. Determine the parameter ν in the relation $R_g \sim N^{\nu}$.

Chain with excluded volume interactions

Now you simulate a coarse-grained polymer with the same interactions and parameters as given above. In addition, apply Lennard-Jones interactions to the monomers with $\epsilon = 1$ and $\sigma = 1$. Shift the Lennard-Jones function at the point $r_c = 2^{1/6}$ such that the force is zero. Repeat the simulations for the different values of N. Determine the ν by the relation given above.