

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

Task : (6 points)

Consider an ideal linear chain with N Kuhn monomers of length b and fixed end to end vector \vec{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

$$\frac{1}{N} \sum_{i=1}^N \langle ((\vec{R}_i - \vec{R}_{cm})_x)^2 \rangle = \frac{1}{36} N b^2 \left(1 + 3 \frac{R^2}{N b^2}\right) \quad (1)$$

While the mean square projection of the radius of gyration onto the perpendicular direction is independent of the magnitude of the end to end vector.

$$\frac{1}{N} \sum_{i=1}^N \langle ((\vec{R}_i - \vec{R}_{cm})_y)^2 \rangle = \frac{1}{N} \sum_{i=1}^N \langle ((\vec{R}_i - \vec{R}_{cm})_z)^2 \rangle = \frac{1}{36} N b^2 \quad (2)$$

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

$$\left(1 + \frac{3\vec{R}^2}{N b^2}\right)$$

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.