Worksheet 4: Properties of Coarse-grained Polymers

David Sean, Jens Smiatek, Christian Holm, Johannes Zeman

Institute for Computational Physics, University of Stuttgart

Contents

General Remarks

- Deadline for the report is **Wednesday, 20th of June 2017, 12:00 noon**
- In this worksheet, you can achieve a maximum of 20 points.
- The report should be written as though it would be read by a fellow student who attends the lecture, but doesn't do the tutorials.
- To hand in your report, send it to your tutor via email.
  - David (`david.sean@icp.uni-stuttgart.de`)
- Please attach the report to the email. For the report itself, please use the PDF format (we will *not* accept MS Word doc/docx files!). Include graphs and images into the report.
- The report should be 5–10 pages long. We recommend using LaTeX. A good template for a report is available online.
- The worksheets are to be solved in **groups of two or three** people.

1 Introduction

In the first part of this worksheet, you will have to answer a few general questions about coarse-grained polymer models and solve a related mathematical task.
In the remainder of the worksheet, you will get to know our in-house software package ESPResSo (Extensible Simulation Package for Research on Soft matter). Using ESPResSo, you will perform several simulations involving coarse-grained polymers and analyze their properties.
All files required for this tutorial can be downloaded from the lecture's homepage.

2 Short Questions - Short Answers (6 points)

Task (6 points)
Answer the following questions:

- What is the persistence length of a polymer and how is it defined?
- Which real polymers can be described by the worm-like chain model?
- What are the differences between the ideal chain, the worm-like chain, the freely jointed chain and the self-avoiding chain?

Hint

- You might want to study literature to answer these questions. A good reference would be the book:
  Polymer Physics by Rubinstein and Colby, 2003,
  Oxford University Press, ISBN: 9781613449431

  From an ICP CIP-pool computer, you can find the second chapter under:
  `/group/sm/2018/tutorial_04/Rubinstein-Chapt2.pdf`

3 Polymer Properties (6 points)

The mean-square radius of gyration of a polymer with N Kuhn monomers of length b is defined as

$$\left\langle R_g^2 \right\rangle \equiv \frac{1}{N} \sum_{i=1}^{N} \left\langle \left(\vec{R}_i - \vec{R}_{\text{com}} \right)^2 \right\rangle , \tag{1}$$

where $\vec{R}_i$ denotes the position of the i-th monomer in the chain, and $\vec{R}_{\text{com}}$ the chain's center of mass.

Task (6 points)

- Starting from equation (1), show that the mean-square radius of gyration of a *worm-like chain* is

$$\left\langle R_g^2 \right\rangle = \frac{1}{3} R_{\max} l_p - l_p^2 + \frac{2 l_p^3}{R_{\max}} - \frac{2 l_p^4}{R_{\max}^2} \left(1 - e^{-\frac{R_{\max}}{l_p}} \right) . \tag{2}$$

  Here, $R_{\max}$ is the maximum end-to-end distance of the polymer and l_p is its persistence length.

Hints

- Read chapter 2 of *Polymer Physics* by Rubinstein. Sections 2.3.1, 2.3.2, 2.4, and 2.4.1 are the most important ones for this task.
- Rewrite equation (1) so that it loses its dependence on $\vec{R}_{\text{com}}$ and depends solely on the distances $\left(\vec{R}_j - \vec{R}_i \right)$.
- Sums may be transformed into integrals.
- Think about how equation (2.35) in section 2.3.2 is connected to this problem.

4 Static Properties of Coarse-grained Polymers with ESPResSo(8 points)

4.1 The Software Package ESPResSo

The software package ESPResSo is developed and maintained at the Institute for Computational Physics and is mainly intended to perform coarse-grained simulations with Lattice-Boltzmann (LB), Dissipative Particle Dynamics (DPD) and Langevin Dynamics (LD). It offers a broad variety of electrostatic algorithms, analysis tools and various other features such as the support of massively parallelized hardware architectures or GPU platforms.

- The package can be obtained free of charge under `http://espressomd.org/`.
- We shall be using Python to set up the ESPResSo simulations. To use this feature, the python branch needs to be taken from GitHub `https://github.com/espressomd/espresso`
- Be advised to also have a look at the ESPResSo manual to understand how it operates. Some Python documentation can be found in the older User's guide: `http://espressomd.org/jenkins/job/master-doc/lastSuccessfulBuild/artifact/doc/ug/ug.pdf`
  as we as the (often updated) online documentation `https://espressomd.github.io/doc`

In the following, you will conduct coarse-grained simulations of polymers with LD to learn how to work with ESPResSo. The simulations focus on the ideal chain model and the chain with excluded volume interactions. You can either use the computers in the ICP CIP pool or install ESPResSo on your own computer.

4.2 Installing ESPResSo

You may download and run the installation script `espresso_install_script_polymers.sh` from the lecture website, or follow the instructions below.
Download the latest ESPResSo version of the python branch.

```
git clone -b python https://github.com/espressomd/espresso.git
```

Enter the newly created ESPResSo directory, and create (and enter) a `build` directory inside

```
cd espresso
mkdir build
cd build
```

Run `cmake` inside the `build` directory

```
cmake ..
```

The computers in the CIP pool will have the needed dependencies and `cmake` should complete successfully. Once finished, a new file called `myconfig-sample.hpp` should have appeared. Create a copy called `myconfig.hpp`

```
cp myconfig-sample.hpp myconfig.hpp
```

and edit its contents. In order to enable the feature `LENNARD_JONES`, simply remove the comment symbol at the beginning of the line. You may now compile ESPResSo by running `make` after running `cmake` a second time

```
cmake ..
make -j8
```

Upon successful compilation, you can verify that the python-driven ESPResSo works by running

```
./pypresso
```

4.3 Setting up and Running the Simulations

Download the template Python script `template.py` from the lecture website.
Examine the template script and also have a look at the manual (and perhaps on the test cases, too) 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 should be set to $T = 1$ and the friction coefficient of the Langevin thermostat to $\gamma = 1$.
Once the Tcl script is prepared, you can run the simulation with

```
/<install_dir>/pypresso template.py
```

4.4 Ideal Chain

Task (4 points)

- Perform simulations of an ideal coarse-grained polymer with Langevin Dynamics for different chain lengths $N \in \{10, 20, 30, 40, 50, 100, 200\}$ and determine the average radii of gyration $R_g(N)$.
- Determine the size exponent ν in the relation $R_g(N) \propto N^{\nu}$.

4.5 Chain with Excluded Volume Interactions

Task (4 points)

- Simulate a coarse-grained polymer with the same interactions and parameters as given above. In addition, apply Lennard-Jones interactions to the monomers with $\epsilon = 1$, $\sigma = 1$, and cutoff radius $r_c = 2^{\frac{1}{6}}$. Shift the Lennard-Jones function such that the energy is zero for $r = r_c$.
- Repeat the simulations for the different values of N.
- Determine ν as in the previous task.