Numerical Simulations of Ideal Chain Model of Polymer using the Freely Jointed Chain (FJC)

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1 Introduction

- General introduction about physics of polymer. Discrete models. Examples
- Theory of FJC model.
- Presentation of measure of extent (metrics). Relationship with experimental measurement.
- Goal of the practical work

Polymer physics deals with complex substances through a simple approach. Understanding the properties of polymers from a molecular point of view is key to unveil their complexity.

Given an ensamble of polymers, we can use tools from statistics to derive some properties that apply to the ensamble at any given instant. To do so we model each polymer as a (continuous or discrete) ideal chain of monomers along with some constraints. Some examples of these models include the Freely Jointed Chain, the Freely Rotating Chain, the wormlike chain, the hindered rotating chain, the rotational isometric state model, among others [5].

The first, most straightforward (yet illustrating) approach is the Freely Jointed Chain model. The FJC is a chain consisting of N links, each of length b and able to point in any direction independently of each other (thus the simplicity).

2 Methods

- Numerical simulations: Parameters + Brief description of the algorithm
- Examples of structures generated
- Time series + mean square and distributions statistical tools (theory) + Monte-Carlo
- Summary of data produced (ex: Table)

The first script analyzes the simulation data of a $3D$ FJC polymer for different chain lenghts N. The parameters are the bond length b, the N values we wish to test for, and the number of configurations T we wish to analyze. An XYZ file containing T polymer configurations is read, and for every configuration the end-to-end distance Q and the radius of gyration R_g is computed. Finally both quantities are squared and averaged over all configurations yielding $\langle Q^2 \rangle$ and $\langle R_g^2 \rangle$. This algorithm is looped over for every N.

The second script is built over the first one. The only extra parameter needed are the number of bins for the histogram. After computing the end-to-end distance Q, the algorithm builds a histogram out of these values, treating them as samples from a probability distribution. The histogram is then normalized so that it can be directly compared to the gaussian distribution.

The third simulation focuses on computing the structure factor for a polymer of `N = 100` and `b = 3`. An array k is introduced, spanning values from 0 to 1 (in our case, sampling every 0.01 steps). One of the files containing the simulated polymers is held in memory. Then, we use the formula

$$I(k) = \sum_{i=0}^{N} \sum_{j=0}^{N} \left\langle \frac{\sin\left(k\,|\mathbf{R}_i - \mathbf{R}_j|\right)}{k\,|\mathbf{R}_i - \mathbf{R}_j|} \right\rangle \tag{1}$$

where $\mathbf{R}_i$,$\mathbf{R}_i$ are coordinates of the monomers in 3D space obtained from the simulated polymer.

Then, the Guinier approximation is computed on the same k array to compare them side by side.

Fig. 1 Two polymer structures generated from FJC model simulations for $N = 100$ and $b = 3.0$.

3 Results and Discussion

- Description of the numerical results (Parts 1 to 4)
- Comparison with theoretical results (qualitatively and quantitatively)
- Discussion

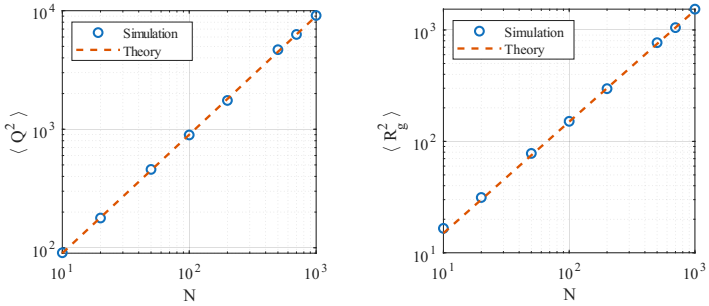

Fig. 2 $\langle Q^2 \rangle$ (left) and $\langle R_g^2 \rangle$ (right)

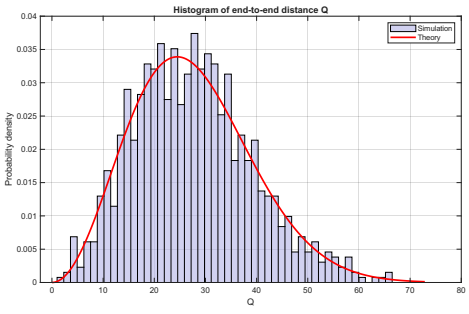

Fig. 3 Probability distribution

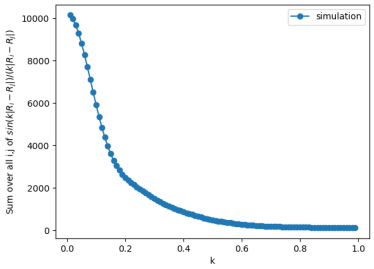

Fig. 4 Structure factor (simulated)

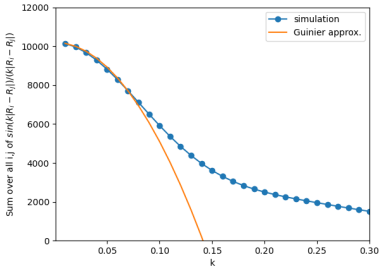

Fig. 5 Structure factor comparison (simulation and Guinier approximation)

4 Conclusion

- General conclusion about FJC model
- Summary of the main results
- Perspectives

5 References

1 Masao Doi and Samuel F. Edwards. *The Theory of Polymer Dynamics*. Oxford University Press, Oxford, 1986.

2 Nicholas J. Giordano. *Computational Physics*. Prentice Hall, Upper Saddle River, NJ, 2006.

3 Rubin H. Landau, Manuel J. Páez, and Cristian C. Bordeianu. *Computational Physics: Problem Solving with Python*. Wiley-VCH, Weinheim, 2015.

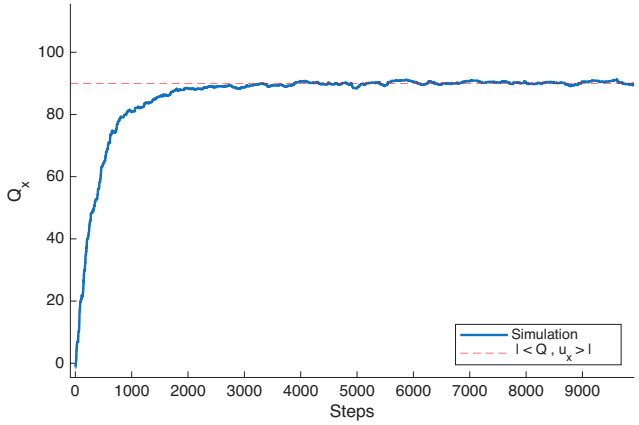

Fig. 6 Extension evolution of the polymer, sturating to the theoretical value

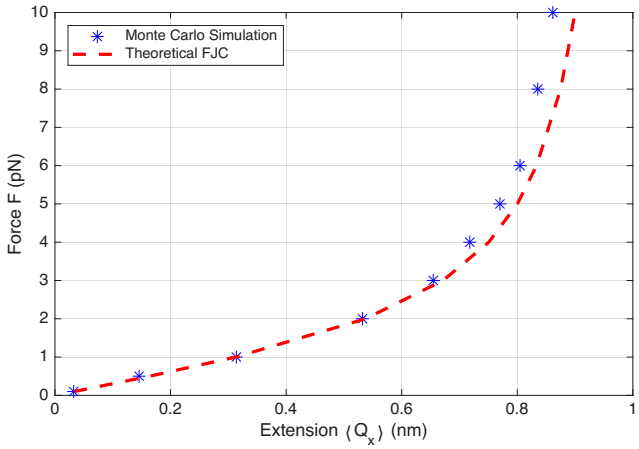

Fig. 7 Extension - Force curve

4 Fabio Manca, Stefano Giordano, P. L. Palla, Fabrizio Cleri, and Luciano Colombo. Monte carlo simulations of single polymer force-extension relations. In *Journal of Physics: Conference Series*, volume 383, page 012016. IOP Publishing, 2012.

5 Michael Rubinstein and Ralph H. Colby. *Polymer Physics*. Oxford University Press, Oxford, 2003.