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

Andres Alvarez & Diego Guerrero

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

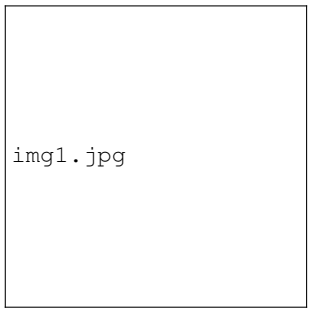
Polymer physics deals with complex substances through a simple approach. Understanding the properties of polymers from a molecular point of view is key to unveil their complexity.

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.

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)



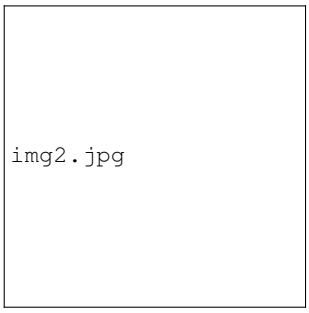


Fig. 1 Two polymer structures generated from FJC model simulations for $N = 100$ and $b = 3.0$.

3 Results and Discussion

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

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.

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.