Simulations of linear polymer chains in continuous space

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ABSTRACT HERE!

INTRODUCTION

The simulation of the dynamics of linear polymer chains in solution has attracted a lot of interest over the years. For this purpose, several computational methods based on Monte Carlo simulations have been successfully used [1]. In general, these methods are applied in on- and off-lattice models, either in two or three dimensions adnd, depending on the conditions being studied, the potential energy included in the sampling changes. In this work, we focus our attention in off-lattice models for dilute polymers in bad solvent. This allows us to use a mesoscopic model in which we simulate the monomers (taken of unit length) as beads interacting through a Lennard-Jones potential:

$$V(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} + C_{\text{bias}}\right] \qquad (1)$$

where we use $\sigma = 0.8$ following [2, 3]. The value of ϵ is defined through the non-dimensional variable ϵ/k_BT as in [2, 4]. Contrary to what is done in the previous cited references, we folloewd the idea in [1] and truncate the potential at twice the minimum of the potential, $r_{\text{cut}} = 2 \times 2^{1/6}\sigma$, including a small bias to make the potential zero at r_{cut}, $C_{\text{bias}} = 127/16384$.

!!!HERE I WRITE THE BLA BLA OF WHAT WE HAVE DONE IN THE PAPER!!!

SIMULATION DESCRIPTION

Agustin Part!

Rosenbluth Method

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PERM Method

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COMPARISON OF THE METHODS

Agustin Part! Talk here about end-to-end distance

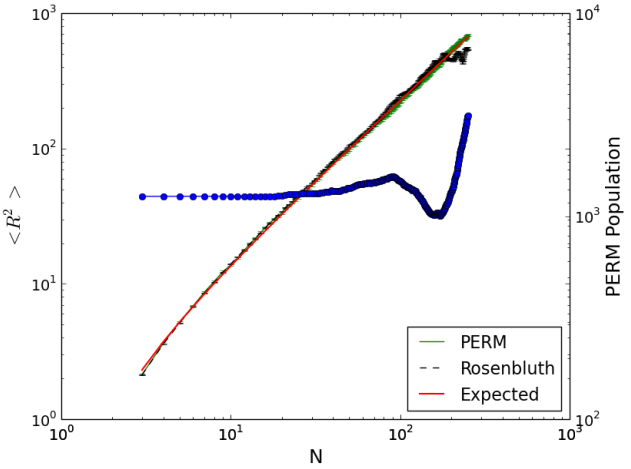

FIG. 1. Comparison of the squared end-to-end distance obtained using Rosenbluth and PERM methods for the three dimensional off-latice model. The results are compared with the predicted line, in which $< R^2 >= a(N-1)^{2\nu}$, with $\nu = 0.5876$ [5]. We used the data to obtain the parameter a. The blue circles show the population of polymers with different N using the PERM algorithm.

RESULTS

Follow PERM paper, I'll talk about the gyration radius here. Eduardo Part!

CONCLUSION

Agustin Part!

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* All files on https://github.com/bofo90/Monte_Carlo

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