Monte Carlo Simulation of Probability Distribution of a Linear Homopolymer with *k*=2 Coincidences: the fBm Edwards Model

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I. Introduction

A polymer is a macromolecule composed of repeating structural units called monomers which can be classified into heteropolymer and homopolymer. A linear homopolymer consists of the same type of monomers in a linear architecture [1,2]. These polymers has a significant role in many modern technology nowadays which includes semiconductor devices, medical applications, among others.

In order to further understand the dynamics of a polymer, one can study its probability distribution *ρ (R)*, which describes the size of a polymer. In this study, we will consider a linear homopolymers and use the concept of fractional Brownian motion, B^H , where H is the Hurst parameter to obtain the probability distribution [2,3].

II. Methodology

The Metropolis algorithm of Monte Carlo simulation is integrated in this study in order to generate the conformation of the numbers of monomers, *N* and *k=2* self-intersection where monomers are allowed to intersect at least once.

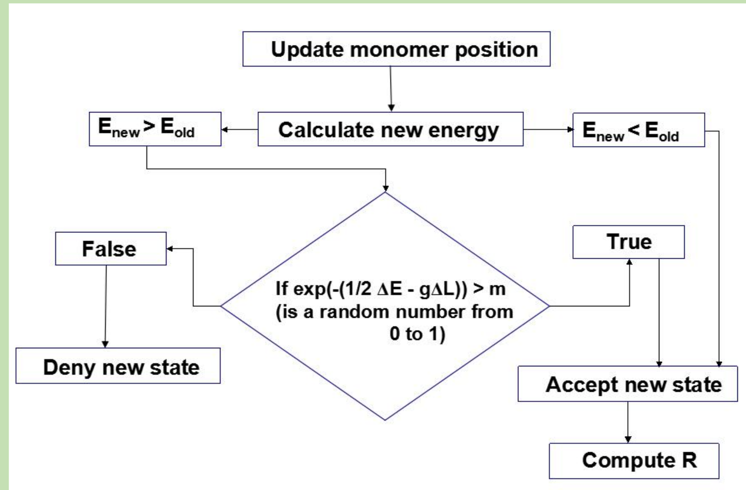

Fig. 1: Diagram of Metropolis Algorithm

Table 3.1: Notation and definition of parameters.

Notation	description
d	dimension
h	Hurst parameter
g	coupling constant
r	maximum range for the magnitude of update
*N*1 & *N*2	lower limit and upper limit range of values for *N* (number of monomer units)
step	interval for range of *N* values
Nr	lower limit for the range of the number of updates
s	upper limit for the range of the number of updates
dir	data location
f	filename

III. Results and Discussions

Previous studies conducted shows that there are suspected outliers that stem from the polymers that did not succeed to unwind to a relaxed conformation. Due to the presence of these outliers, a simulated annealing method is incorporated to reduce and eliminate them. In this study, the linear- exponential annealing method is incorporated with varying *H* and *N* in order to reduce the presence of the outliers.

Result shows that the linear-exponential annealing method (Fig.2a,2b and 2c) has better results compared to the exponential annealing (Fig.2d). It can be observe that the probability of the end-to-end distance of a are not entangled and less to no outliers were detected.

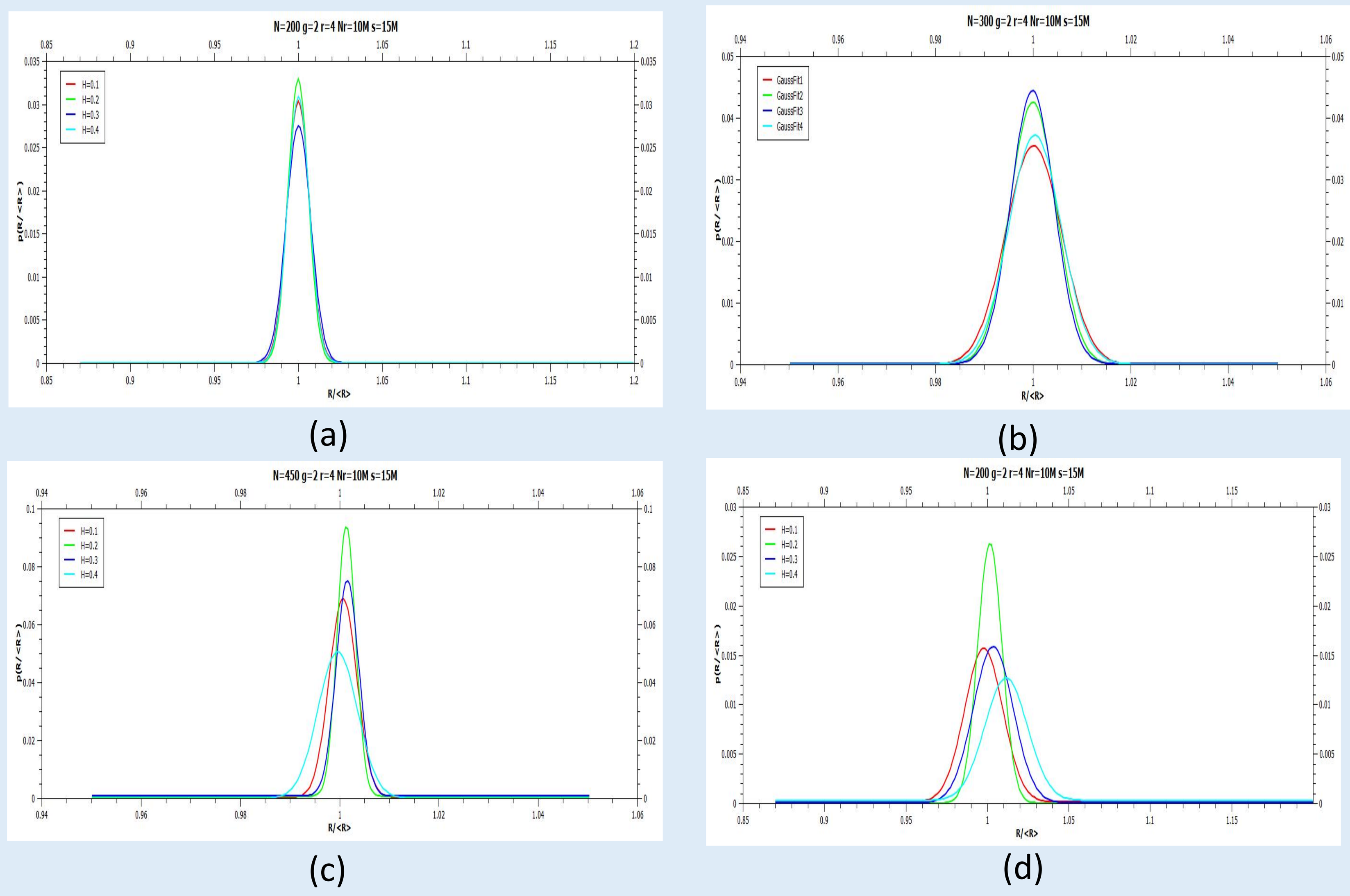

Fig. 2: Graphs results from a, b and c are from linear-exponential annealing method; (d) shows the exponential annealing.

IV. Conclusion

The probability distribution of *ρ (R)* with different *N* and each with varying *H*, shows a good result. It also shows that the linear-exponential annealing method is better than exponential annealing method.

With the k=2 and the liner-exponential annealing method, the polymer were able to unwind and achieve an equilibrium state which is important in cosidering if the polymer is shrinking or swelling.

V. References

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Acknowledgement