POLYMER TRANSLOCATION THROUGH NANOCHANNEL :- A Two Dimensional Monte Carlo Simulation Study

A Thesis Submitted in Partial Fulfillment of the
Requirements for the Degree of
Master of Science in Statistical and Computational Physics

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Abstract

In this paper we investigate Monte Carlo(**MC**) simulation of polymer translocation through a nanochannel. To this end we used the Bond Fluctuation Method (**BFM**) to study the translocation process of a polymer chain of length N in two dimensions, in the absence of external force on the polymer (i.e. unbiased translocation). To overcome the entropic barrier we consider a polymer, in which the center monomer is initially placed in the middle of the channel and study the escape time τ needed for the polymer to completely exit the channel on either side of the end. Numerically we find that the escape time τ scales with the chain length N as $\tau \sim N^{1+2\nu}$, where ν is the Flory exponent as far as the channel is small enough. And this scaling preferably agree with the translocation time of a polymer which passes through a nanopore in one direction only. In this work, we examine the interplay between the channel length L, width W and other parameters while simulating the translocation process.

Keywords: Nanochannel, Translocation time, Escape time, DNA sequencing

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Chapter 1

Introduction

Introduction to polymer physics

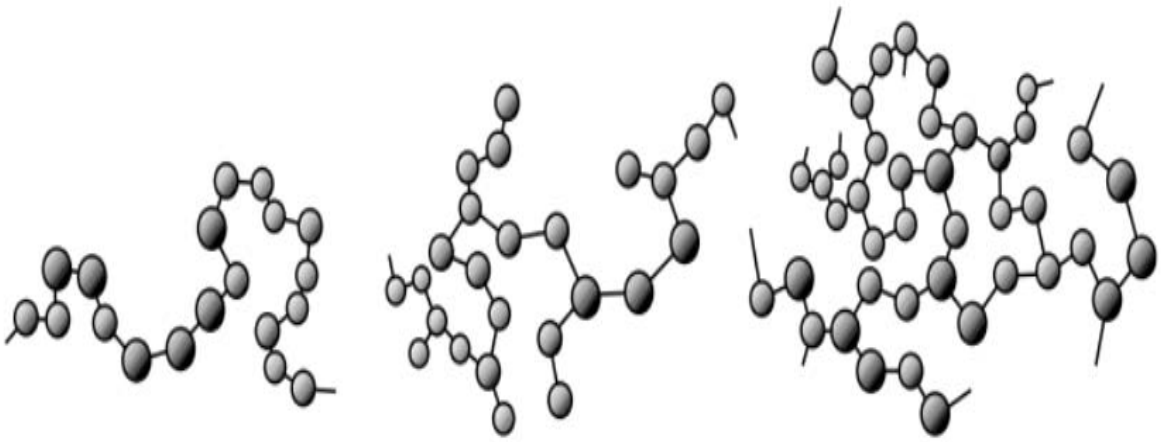
Yet scientific progresses in molecular biology have confirmed the idea that physical laws are indeed solely responsible for how life works. Another interesting aspect of biological systems is the dominant roles played by various kinds of polymer,which is inclusive in a huge field call polymer science.

Generally polymer science has many branches among which one is polymer physics. And it is the field of physics associated to the study of polymers, their fluctuation, mechanical properties, as well as the kinetic of reactions involving degradation and polymerization of polymers and monomers respectively. While it focuses on an aspect of the study of condensed matter physics, the field of polymer physics has developed as a branch of statistical physics. The statistical approach of polymer physics is based on an analogy between a polymer and a brownian motion, or some other type of random walk. Experimental approaches to polymer physics are also common to determine the chemical, physical, and material properties of polymers. These experimental approaches lead to more accuracy in theoretical model formulation and hence allow better understanding of polymer properties.

Polymers and biopolymers

The word polymer can have many definitions in respect to different aspects, but simply defining a ploymer is a long chain molecules, made of repeating monomer units. The

name polymer means many part. The degree of polymerization (DP), which ranges typically from 10^2 to 10^7, denotes the number of monomer units jointed together in a polymer. Natural polymeric materials consist of fossilic fuels, cellulose, amber, and rubber. Plastics contain a lot of different synthetic polymers, PVC for example. Other synthetic polymers also exist, for example, nylon and Kevlar. Polymers are also abundant in biological systems. This subclass of polymers is referred to as biopolymers, and consists, for example, of DNA, RNA, and proteins. Biopolymers are typically electrically charged, which is an important property related to many biological phenomena. Because of the wide applicability, it is not surprising that the study of polymers in different contexts has been, and still is, intense. A polymer can have various types of configurations, of which the three basic ones include linear, branched, and network (cross-linked chains) configurations as shown in figure 1.1 below. And if the available bonds for a monomer are two, then the process of polymerization leads to a linear polymer. A polymer with same type of monomers is called a homopolymer and that with different types of monomers is called a heteropolymer. In this report we shall deal with a linear polymer that may not be homopolymer.



a)linear chain b)branched chain c)Network chain

Figure 1.1: Architecture of polymer chain: a linear chain (a), a branched chain (b), and a cross-linked polymer (c).[1]

1.1 Properties of polymers

A natural way to characterize polymer in good solvent after equilibrium is the N-dependence of the mean-square end-to-end distance R and radius of gyration R_g averaged over the chain length. Let us see one by one.

1.1.1 Ideal chains

The simplest representation of a polymer chain, and surely the starting point of most polymer physics theories, is that of a chain with no interactions between non-adjacent monomers. In such a case, a polymer chain with N +1 monomers could be depicted as a finite length random-walk (RW) in which each step represents a link between two monomers. If no angular constraint is applied between two consecutive steps, this approach is called the freely-jointed chain (FJC) model. The two parameters of the RW, i.e. the number of steps, N , and the length of these steps, a , are respectively related to the degree of polymerization N + 1 of the chain and the distance between adjacent monomers. The total distance traversed during this RW, L = (N+1)a , is called the contour length [1], but this quantity does not give any information about the chain conformation.

The end-to-end vector

The first physical quantity we can compute for the ideal chain is the end-to-end vector R , which is the vector between the starting and the ending points of the RW (the end monomers), or net displacement. and it is defined as

$$\vec{R} = \sum_{i=1}^{N} \vec{r_i} = \vec{R}_N - \vec{R}_0 \tag{1.1.1}$$

Statistically, the average of the end-to-end distance is simply zero. This is true since the free chain does not have a preferential orientation, and this means that there is no orientation of any vector. This applies for every single bond vector and the end-to-end

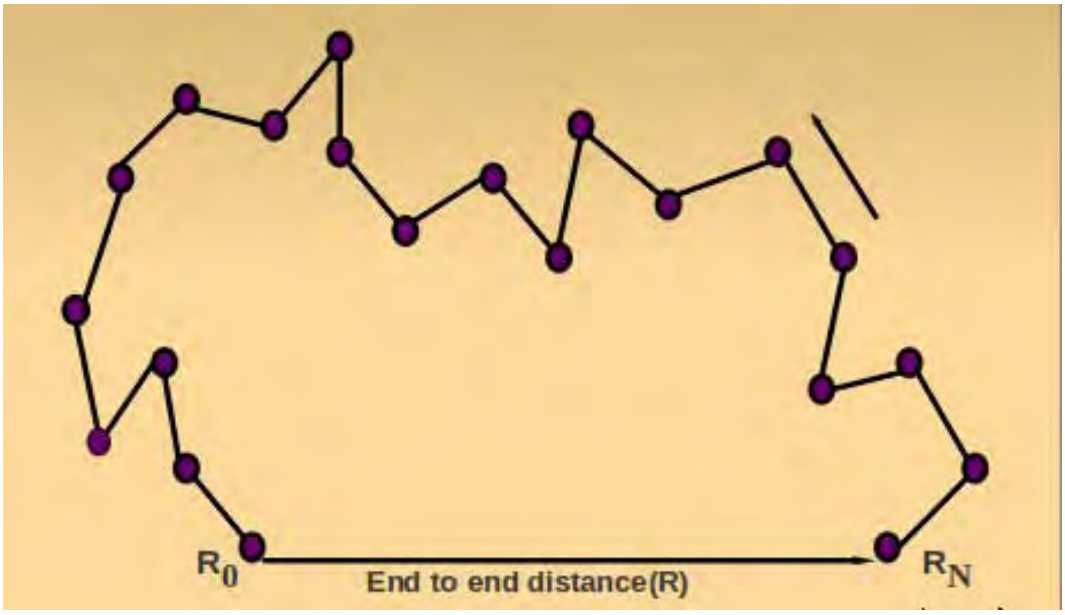


Figure 1.2: The freely jointed chain consists of N + 1 bonds at positions $\vec{R}_0$; . . . ; $\vec{R}_N$ and N links $\vec{R}_1$; . . . ; $\vec{R}_N$ of fixed length . The end-to-end vector R is defined by: $\vec{R}$ = $\vec{R}_N$ - $\vec{R}_0$.

vector vanishes:$\langle\vec{R}\rangle = 0$. But, the simplest non-zero average is the mean-square end-to-end vector,is given by[2]

$$\langle R^2\rangle = \langle\vec{R}.\vec{R}\rangle = \langle(\sum_{i=0}^{N}\vec{r}_i).\sum_{j=0}^{N}\vec{r}_j)\rangle = \sum_{i=0}^{N}\sum_{j=0}^{N}\langle\vec{r}_i.\vec{r}_j\rangle = (N+1)a^2 \qquad (1.1.2)$$

where the r vectors represent the N+1 uncorrelated bond vectors of the RW. The square root of Equation 1.1.2, $(N+1)^{1/2}$a , can be interpreted as a rough measure of the diameter of the spherical space occupied by the chain.

The radius of gyration

A second relevant measure of the size of the ideal chain is its radius of gyration Rg . For a chain in a given conformation, the mean square radius of gyration is the average square distance between each monomer and the polymers center of mass [1]:

$$R_g^2 = \langle\frac{1}{1+N}\sum_{i=0}^{N}(\vec{R}_i - \vec{R}_{cm})^2\rangle \qquad (1.1.3)$$

where $\vec{R}_{cm}$ is given in eq. 1.1.3

$$\vec{R}_{cm} = \frac{1}{1+N}\sum_{i=0}^{N}\vec{R}_i \tag{1.1.4}$$

where R_{cm} is the position of the center of mass while R_i is the position vector of each monomer. The square radius of gyration averaged over the ensemble of all possible conformations is given by [1]

$$R_g^2 = \frac{1}{2(1+N)^2}\sum_{i=0}^{N}\sum_{j=0}^{N}\langle(\vec{R}_i - \vec{R}_j)^2\rangle \tag{1.1.5}$$

For a very long FJC, the latter equation can be reduced to [1]

$$R_g^2 = \frac{Na^2}{6} = \frac{\langle R^2\rangle}{6} \tag{1.1.6}$$

However, one must be careful with the use of the word radius. The expressions given by Equations 1.1.2 and 1.1.5 are values averaged over the ensemble of allowed chain conformations, but they do not mean that the chain always adopt a spherical shape. In fact, the instantaneous shape of an ideal chain is almost always highly anisotropic [1].

1.1.2 Real chains

In real polymer chains, there are physical constraints such as the excluded volume effects that strongly affect the chain conformation. This means that real chains look more like self-avoiding walks (**SAW**) rather than random walk (**RW**), with the consequence of making them swell compared to ideal ones.

We now take into account interactions between monomers that are separated by many bond lengths along the polymer chain. In particular, we discuss alterations in the statistical properties if steric interactions are considered, i.e. the polymer consists of monomers with a finite lateral dimension. To keep things simple we restrict our analysis to spherical monomers.

Excluded volume interaction

In polymer physics, excluded volume(**EV**) interaction is referring to the idea that in any real polymer no two monomers occupy the same space at the same time. Hence, a real polymer chain can consequently be characterized as self-avoiding random walk, where it implies a random walk which does not allow to visit the same point more than once. The effect of excluded volume interaction plays a far more important role in polymer solution. A detailed analysis of real polymer chains was carried out by Flory [3]. Flory calculated configurations of real polymers based on the idea that their size is governed by two competing interactions. On one hand, steric repulsion is responsible for polymer swelling. On the other hand, chain connectivity creates an attraction counteracting monomer departure. Flory combined both interactions and derived a single parameter, ν , which summarizes the net interaction between monomers. An important result from Flory's theory for a polymer in good solvent is that it yields a universal power-law dependence of polymer size R on the number of monomers N , i.e

$$R^2 \sim N^{2\nu} \tag{1.1.7}$$

where

$$\nu = \frac{3}{2+d} \tag{1.1.8}$$

where d is the dimension in which the polymer resides. In contrast to ideal chains, the scaling behavior of the polymer size now exhibits a dependence on the dimension of space d in which the polymer resides. Compared to ideal linear polymers, where $\nu = 1/2$, Flory concluded the scaling exponent for real chains to be $\nu = 3/4$ and $\nu = 3/5$ in two and three dimensions respectively.

1.2 Polymer translocation through nanoscopic channel

Nanopore technology has opened a completely new window for probing the properties of polymers in general and biopolymers in particular [4, 5]. In a nanopore setup two macroscopic chambers filled with a buffer solution are separated from each other by a wall. Embedded into this wall is a single nanopore, i.e., a hole(pore) with a diameter in the few nanometer range, connecting the two chambers. Molecular transport through cell membranes is an essential mechanism in living organisms. Such events occur frequently in living cells. Often, the molecules are too long, and the pores in the membranes too narrow, to allow the large molecules to pass through as a single unit. In such circumstances, these molecules have to deform themselves to squeeze -i.e- translocate- themselves through the pores.

The translocation of biopolymers through nanometer-scale pores is one of the most crucial processes in biology, such as DNA and RNA translocation across nuclear pores, protein transport through membrane channels, and virus injection.[5, 6, 7] Moreover, translocation processes might eventually prove useful in various technological applications, such as rapid DNA sequencing,[8, 9, 10] gene therapy and controlled drug delivery, etc.[10] In addition to its biological relevance, the translocation dynamics is also a challenging topic in polymer physics. Accordingly, the polymer translocation has attracted a considerable number of experimental,[11]-[18] theoretical [19] - [32] and numerical studies.[33]-[39].

The translocation of a polymer through a nanopore faces a large entropic barrier due to the loss of a great number of available configurations. In order to overcome the barrier and to speed up the translocation, an external field or interaction is often introduced. The possible driving mechanisms include an external electric field, a chemical potential difference, or selective adsorption on one side of the membrane. For example, in 1996, Kasianowicz et al.[12] reported that an electric field can drive single-stranded DNA and RNA molecules through the α hemolysin channel of inside diameter 2 nm and that the

passage of each molecule is signaled by the blockade in the channel current. Inspired by the experiments [12], a number of recent theories [[21] - [34]] have been developed for the dynamics of polymer translocation. Even without an external driving force, polymer translocation remains a challenging problem. To this end, Park and Sung [21] and Muthukumar [24] considered equilibrium entropy of the polymer as a function of the position of the polymer through the nanopore. The geometric restriction leads to an entropic barrier. Standard Kramer analysis of diffusion through this entropic barrier yields a scaling prediction of the translocation time $\tau \sim N^2$ for long chains. However, as Chuang et al. [27] noted, this quadratic scaling behavior cannot be correct for a self-avoiding polymer. The reason is that the equilibration time; $\tau_{equil} \sim N^2$ for a phantom polymer and $\tau_{equil} \sim N^{1+2\nu}$ for a self-avoiding polymer, where ν is the Flory exponent ($\nu = 3/4$ and $3/5$ in 2D and 3D, respectively). Thus the exponent for τ_{equil} is larger than two for self-avoiding polymers, implying that the translocation time is shorter than the equilibration time of a long chain, thus rendering the concept of equilibrium entropy and the ensuing entropic barrier inappropriate for the study of translocation dynamics. Chuang et al.[27] performed numerical simulations with Rouse dynamics for a 2D lattice model to study the translocation for both phantom and self-avoiding polymers. They decoupled the translocation dynamics from the diffusion dynamics outside the pore by imposing the artificial restriction that the first monomer, which is initially placed in the pore, is never allowed to cross back out of the pore. We will refer to the translocation time obtained this way as τ_{tran} . Their results show that for large N, translocation time τ_{tran} scales approximately in the same manner as equilibration time, but with a larger prefactor.

Among the theoretical or computational simulations studied recently. The main three translocation process are

I. Unbiased translocation,where in the polymer translocates purely due to thermal fluctuations

II. Field-driven translocation, where in translocation is driven by a potential difference

across the pore or an electric field applied, and

III. Pulled translocation, where in translocation is facilitated by a pulling force at the head of polymer;

In this work we focus on the unbiased polymer translocation through a small channel. From the statistical physics perspectives, the translocation problem can be seen as a kind of tunneling process over an entropic barrier. This entropic barrier arises because the number of states available to the polymer is significantly decreased by the presence of the membrane or the nanochannel.

On a lattice of coordination number Z, the number of N - step random walks starting from the origin with it's all possibilities walks is given in equation (1.2.1) below

$$Z_N^{RW} = \mu^N. \tag{1.2.1}$$

But, If we constrain the random walks in to our basic work, for a polymer of length N which holds a SAW, the partition sum $Z_b(N)$ in the bulk scales as in equation (1.2.2) below.

$$Z_b^{SAW}(N) \approx B\mu^N N^{\gamma-1} \tag{1.2.2}$$

From the second factor μ is the connectivity constant and the last one is a power-law correction called the enhancement factor with universal exponent $\gamma = 49/\ 32$ and $\gamma \backsimeq 1.16$ in two and three dimensions respectively, While B and μ are not universal.

The corresponding number of states for the same polymer but whose end is tethered to the membrane is approximated as:

$$Z_U^{SAW}(N) \approx B_1\mu^N N^{\gamma_1-1} \tag{1.2.3}$$

in which μ is not affected by the introduction of the membrane, γ_1 is a different universal exponent $\gamma_1 = 61/64$ and $\gamma_1 \approx 0.68$ in two and three dimensions respectively, while B_1 is again not universal.

Considering a translocating polymer chain, These chains have lengths of s and (N-s), where N is the total length of these two parts, for which there are s monomers on one side from the middle of the channel and the rest (N-s) monomers on the other side of the channel. Since this situation can be seen as two strands of polymers with one end (of each strand) tethered on the membrane, the number of states for the polymer or the system entropy, is obtained from equation (1.2.2) is given below as equation (1.2.4):

$$Z_U^{SAW}(s,N) = \mu^N [s(N-s)]^{\gamma-1} \tag{1.2.4}$$

The number of states for the polymer attained it's minimum value when $s = \frac{N}{2}$.Thus the effective entropic barrier faced by the translocating polymer is $\triangle$S in which, $\triangle$S is the difference between the bulk entropy (S_b) and the entropy (S_U) after the introduction of the membrane .

And we know that: $S = k_B lnZ$, where k_B is the Boltzmann factor, and assuming $k_B = 1$, we get $\triangle$S as follows:

$$\triangle S = lnZ_b^{SAW} - lnZ_U^{SAW} \tag{1.2.5}$$

$$Z_U^{SAW}(s,N) = Z_U^{SAW}(s) Z_U^{SAW}(N-s) \tag{1.2.6}$$

at $s = \frac{N}{2}$

$$Z_U^{SAW}(s,N) = [Z_U^{SAW}(\frac{N}{2})]^2 \tag{1.2.7}$$

Thus, since we are studying unbiased polymer translocation, to overcome the entropic barrier we put the middle monomer tethered mid-way in the channel. We shall discuss this in detail later in chapter two. Generally, we investigate the unbiased translocation dynamics in a 2D lattice model by focusing on different parameters. In particular, we investigate the effect of varying the polymer chain lengths on the polymer translocation on a computed escape time, and the dependence of polymer translocation through varying channel lengths on a computed escape time and average escape time for a specific polymer chain N and width W.

Chapter 2

Computational techniques and methods

To study these properties of polymer in particular polymer translocation, we need a program to model using simulation methods and techniques . So, there are many methods and techniques to simulate any kind of simulation work. But, the two most widely used methods and preferably related to our work specially for atomic-level modeling are Monte Carlo (MC) and molecular dynamics (MD).[47]

In many cases, only static equilibrium properties are of interest, and then most dynamical models are equivalent. When looking at dynamical properties such as dynamical response functions, or at non-equilibrium situations, the choice of the dynamical model becomes relevant. In the following, I summarize about importance of the models that have been used to study polymer systems in relation to this thesis.

procedures of the above mentioned two widely used models are typically have the same system setup including representation of molecules as collections of atom-centered interaction sites, utilization of classical force fields for the potential energy terms, and implementation of periodic boundary conditions. The principal differences are in the modes of sampling the configuration space available to the system. For MC, a new configuration is generated by selecting a random molecule, translocating it, rotating it, and performing any internal structural variations. Acceptance of the new configuration is determined by the Metropolis

sampling algorithm; application over enough configurations yields properly Boltzmann-weighted averages for structure and thermodynamic properties. For MD, new configurations are generated by application of Newtons equations of motion to all atoms simultaneously over a small time step to determine the new atomic positions and velocities. In both cases, the force field controls the total energy (MC) and forces (MD), which determine the evolution of the systems.

A priori, the Monte Carlo (MC) method has been invented as a method to evaluate high dimensional integrals (i.e., thermal averages), and is designed for studying dynamics. Nevertheless, MC simulations are used for dynamical studies, based on the fact that like many static properties, dynamical phenomena are also often governed by universal principles. In dynamic MC simulations, one analyzes the artificial Monte Carlo evolution of a system in order to gain insight into real dynamical processes in the system. The main requirement is that the Monte Carlo moves are only local and reasonably realistic, i.e., chain crossings are not allowed. So, preferably 2D lattice Monte Carlo modeling methods have become a widely used simulation technique, to which we will also heavily refer in the following sections.

This modeling techniques are used for instance a subsequent configurations of the polymer chain is generated stochastically (randomly). The collective motion of a chain is modeled by the acceptance of an attempted new configuration. Under certain circumstances one can use such an approach not only for static properties but also for the investigation of the dynamics of the system. In order to use MC methods for the simulation of the dynamical properties of polymers, one needs a method which is based on local stochastic moves. For a non-reversal random walk (RW) or self-avoiding walk (SAW), that is a random walk with excluded volume for nearest and next-nearest neighbors along the chain only, it can be shown below. In such a case the local configurations and the

attempted moves are the same as in the case in which one includes the excluded volume interaction between all monomers. In order to fulfill this requirement, it is necessary to structure the algorithm which will be discussed later.

A realistic, microscopic model for the polymer would require too much computer time So, for the sake of computational efficiency, the chemical details of simulated polymer chains are not taken into account here, but Instead, for simulating our problem; polymer translocation, we use simple coarse grained models, which is a generic model and treats a group of chemical monomers as a bead (effective monomer) ignoring the microscopic degrees of freedom, which are invariably present; it retaining only features common to all polymers of the same chain topology. Thus,the simulations are performed with the standard bond-fluctuation model, which is described in detail below.

2.1 Lattice Model with Bond Fluctuation Method

2.1.1 Lattice model

About 50 years ago Orr and Montroll [48] proposed the self-avoiding walk (SAW) as a model for a linear polymer in a good solvent. The SAW is defined on a discrete lattice, often on a square or simple cubic lattice.

Lattice models have the oldest tradition among the coarse-grained particle models for polymer simulations, and are still very popular. A natural approach consists in placing the monomers on lattice sites and linking them by bonds that connect nearest-neighbor sites. For many applications, it has proven useful to apply less rigid constraints on the links and allow for bonds of variable length, which may also connect second-nearest neighbors[49] or stretch over even longer distances.[50] Moreover, the lattice is usually not entirely filled with monomers, but also contains a small fraction of voids. This is because most Monte

Carlo algorithms for polymers do not work at full filling, and special algorithms have to be devised for that case.[51] One particularly popular lattice model is the bond- fluctuation model, devised in 1988 by Carmesin and Kremer.[52] A different approach was used for the bond fluctuation method. The aim was to give an algorithm which allows for an analysis of dynamic properties in all spatial dimensions and which is ergodic.

2.1.2 Bond Fluctuation Method

The bond fluctuation method (BFM) is a lattice model for simulating polymer systems. It is useful for obtaining static and dynamic properties of polymers.

On a two dimensional square lattice, each monomer occupies four lattice sites of a unit cell .[52],[53] Each lattice site can at best be part of only one monomer by virtue of self avoidance condition. We implement it on a square lattice with lattice constant unity. Let l denotes length of a bond. Minimum bond length is $l \geq l_{Min} = 2$. A bond length (l) less than 2 violates self avoidance condition. We restrict to bond length less than 4. This condition ensures that no bond crossing takes place. The possible bond lengths (l) less than 4 are: $2; \sqrt{5}; \sqrt{8}; 3; \sqrt{10}$ and $\sqrt{13}$. In the present work, we restrict ourselves to four site model on a two dimension square lattice. Since we look for dynamic properties $l \leq l_{Max} = \sqrt{13}$ guarantees that bonds never cut through each other during the course of the simulation. We start with a configuration that is self avoiding and has no bond cuts. Generally, Figure (2.1) shows a bond fluctuating lattice polymer with all possible bond lengths and with the corresponding bond length restriction: $2 \leq l \leq \sqrt{13}$. For more detail of BFM algorithm ,there are steps written below briefly:

Step 1: Start with an initial state of a linear self avoiding conformation of a polymer chain consisting of N monomers.

Step 2 : Select a monomer randomly and select one of the four lattice directions randomly with equal probability.

Step 3 : Move the selected monomer in the selected direction by one lattice spacing.

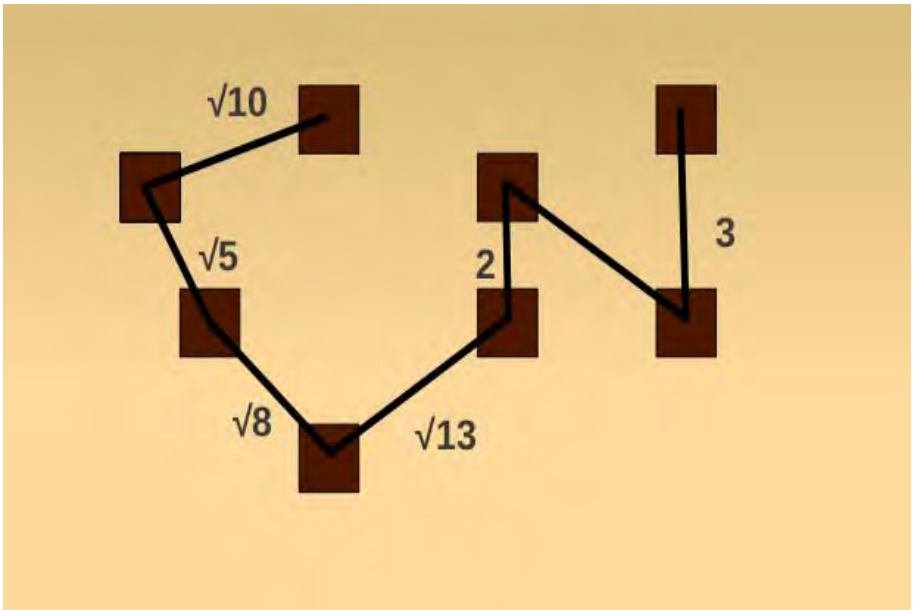


Figure 2.1: The above figure shows a two-dimensional system based on the BFM with the corresponding bond length restriction: $2 \leq l \leq \sqrt{13}$ and with all possibility moves in between these bond length restriction boundaries.

Call this a trial move.

Step 4 : Check if the trial move violates self avoidance condition(excluded volume and bond length restrictions). If it does, then reject the trial move by placing the monomer in its earlier lattice position and go to step 2.

Step 5 : Check if trial move increases the bond length beyond $\sqrt{13}$. If it does, then reject the trial move by placing the monomer in its earlier lattice position and go to step 2. **Step 6** : If both requirements self avoidance and bond length restrictions are met then take the trial conformation for further processing through Metropolis algorithm.

This will be Optional conditions, which proceed as follows

If the trial move leads to an energetic difference U for example due to an electric field or an adsorbing force to the walls. In this case the Metropolis algorithm is implemented which is defined as:

Step 7 : Calculate the energy change $\triangle U$ between the new and the old configurations of the system, and if $\triangle U < 0$ the move is accepted, otherwise

Step 8 : Generate a random number r such that $0 < r < 1$

Step 9 : If $r < e^{-U/K_BT}$,accept the move , After processing

Step 10 :Go to step 2. N elementary moves define one MC time step.

2.2 Simulation procedure

Since we use a lattice for our simulation purpose, the first thing that we do is preparing the lattice itself. Thus a 2000 X 2000 square lattice was formed. Then by putting the center of polymer at the center of the lattice, we tried to see how the chain diffuses through time by the bond fluctuation Monte Carlo method explained above.

To study the effect of self-avoidance on translocation in the coiled state, higher dimensional simulations ($d > 1$) are necessary. Two dimensional polymers are ideally suited to this purpose for dual reasons that excluded volume effects are more apparent, while computation times are shorter than three dimensional case.

In our simulation the membrane (wall) with the channel is constructed from a row of immobile monomers arranged in a straight line, with L lattice constant gap or length representing the channel. The length L and width W of the channel are free parameters which have influence on the translocation dynamics. For example a channel(pore) of L = 3 and W = 2 lattice units is small enough to allow only a single monomer to pass through. Since we are investigating a non-equilibrium process, the initial condition may play an important role. According to our setup, a polymer of size N is initially placed in a state in which the number of monomers, s ,on each side of the pore is equal.

Thus in the present work we consider a polymer which is initially placed symmetrically in the middle of the channel as shown in figure 2.2, to overcome the entropic barrier, i.e,

the initial configuration is constructed by fixing the middle monomer $\frac{N}{2}$ in the hole, and equilibrating the remaining monomers for more than the relaxation or equilibration time $\tau_{equil} \sim N^{2.50}$ in two dimension. After this equilibration is finished, at t = 0, the fixed middle monomer is allowed to move freely. Thus the simulation ends at a time $t = t' > 0$ when the entire polymer is on either side of the membrane. We call this t' the escape time. This procedure is repeated for a large number of times for each polymer length N , and take the escape time τ which happened most. Numerically, τ can be sampled much more efficiently than τ_{tran}, where τ_{tran} is defined as the time that the polymer needs to translocate through a pore by putting the first monomer at the gate of the pore under a restriction that it never gets back, and the whole translocation process ends when the last monomer is on the other side of the pore. We will show numerically that the escape time τ scales as $\tau^{1+2\nu}$ in agreement with our result [54]. Wolterrink et al. [55] have studied the translocation dynamics scaling for a 3D lattice model of a polymer. We have also found that τ scales as $\tau^{1+2\nu}$, in agreement with our work.

Now, we choose L = 20 and W = 3 just for simplicity as they both are free parameters. So, after we have placed the middle monomer of the polymer chain at the middle of the channel and the polymer chain is tethered mid way in the channel during the warm up as shown in figure (2.3) and then escapes on either side of the channel after relaxation figure (2.4).

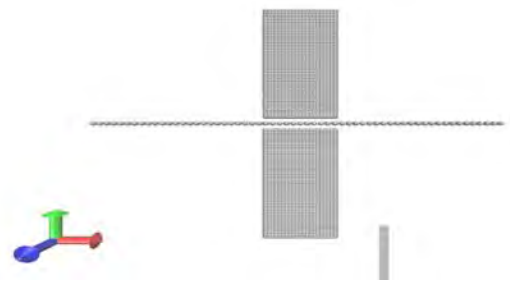


Figure 2.2: This figure shows that the initial stage of straight line of a linear conformation of a polymer chain consisting of 40 monomers.

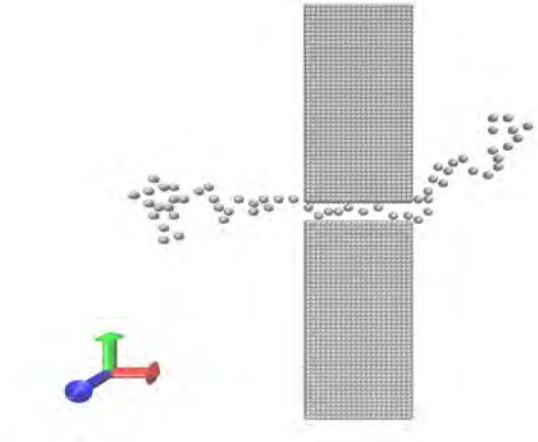


Figure 2.3: This is snapshot picture taken from the actual VMD(Visual Molecular Dynamics) graphics during the simulation work when the polymer chain (with chain length N = 60) starts to warm up after it has been initially placed at the center of the channel (with channel length L = 20)

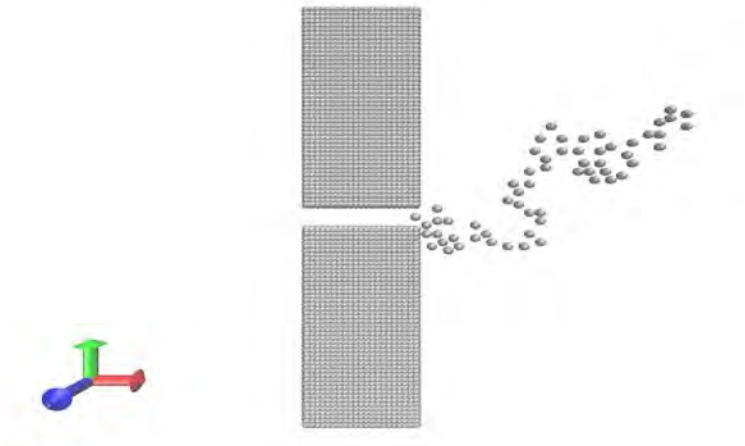


Figure 2.4: This visual shows snapshot taken from the actual VMD(Visual Molecular Dynamics) graphics during the simulation work when the polymer chain (with chain length N = 60) is already translocated from the channel(with channel length L = 20) on either side after some τ_{tran}

Chapter 3

Results and discussion

The organization of this chapter is as follows. we discuss the results from polymer translocation through a nanochannel with the bond fluctuating model combined with the single-segment Monte Carlo moves as we discussed previously. So this section shows the results and discussions about the polymer translocation of a computed results as written briefly below.

3.1 Results from translocation of a polymer

In this section we shall see the dependence of the translocation time or escape time(τ), average escape time(τ_{ave}) on different parameters such as polymer length N, channel length L and width W.

3.1.1 Escape time distribution for polymer translocation

We study the passage (translocation) of a self-avoiding polymer through a membrane channel in two dimensions. To do this we tried to see the distribution of the escape times of a polymer through a channel. We numerically measure the distribution $P_N(\tau)$ of the

escape time τ. Figure 3.1 shows the probability distribution function $P_N(\tau)$ of polymer translocation for different polymer chain N = 20,40,60 and 80. From the figure (3.1) we exhibit that the histogram of the escape time is a long tailed distribution in agreement with [56] as the probability distribution function decays for large values of escape times.

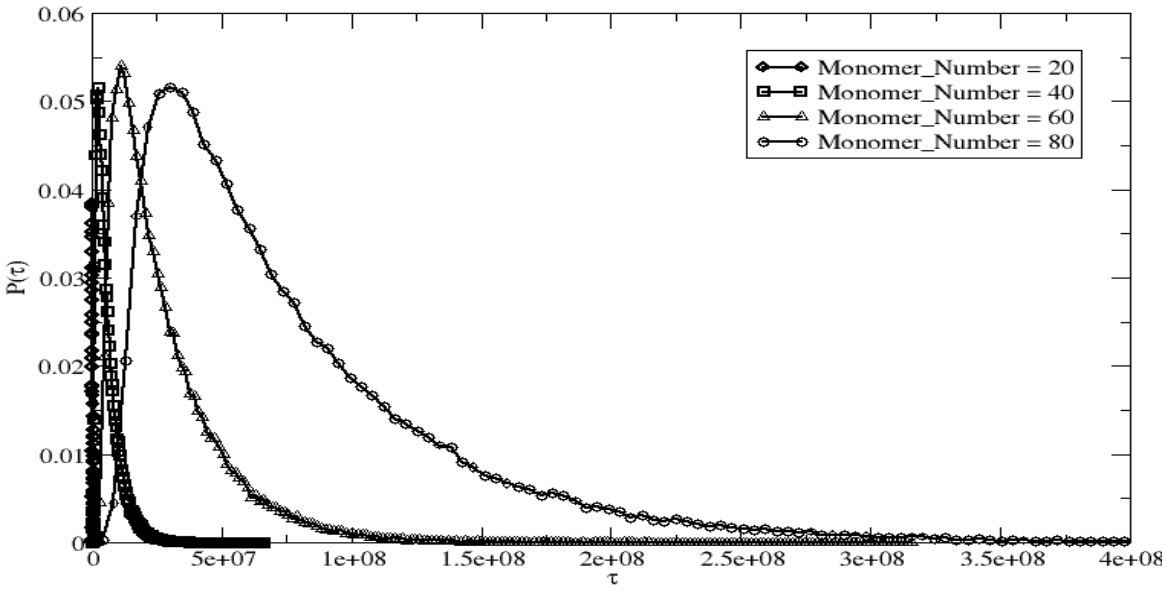


Figure 3.1: Escape time distribution of polymer translocation for N = 20,40,60 and N = 80 left to right, obtained from 10^5 runs each

3.1.2 Polymer translocation through nanochannel

As discussed in our simulation setup, the central monomer is placed at the middle of the channel; as a result the polymer can escape the channel from either side in a time defined as escape time τ. We computed the escape time for short polymer chains for the scale of τ and we considered the most probable values of the escape time in every simulation run. The log-log plot of the escape time τ versus N is shown in figure 3.2. That shows $\tau \sim N^{\alpha}$,

where we found α to be $\alpha = 2.04$ in agreement with the expected scaling power $\alpha = 1+2\nu$ but with a big difference with the agreement of $\tau \sim N^1$ with the numerically simulated for very long channel length(L = 800). So since our consideration is not pore but a channel with channel length (L = 20) we see a few difference with the above agreement $\tau \sim N^\alpha$, $\alpha = 1 + 2\nu$.

This a few difference could have different factors but mainly due to a bias when the channel length taken larger than the pore, which could bring increased entropic barrier as shown in the figure 3.3 .

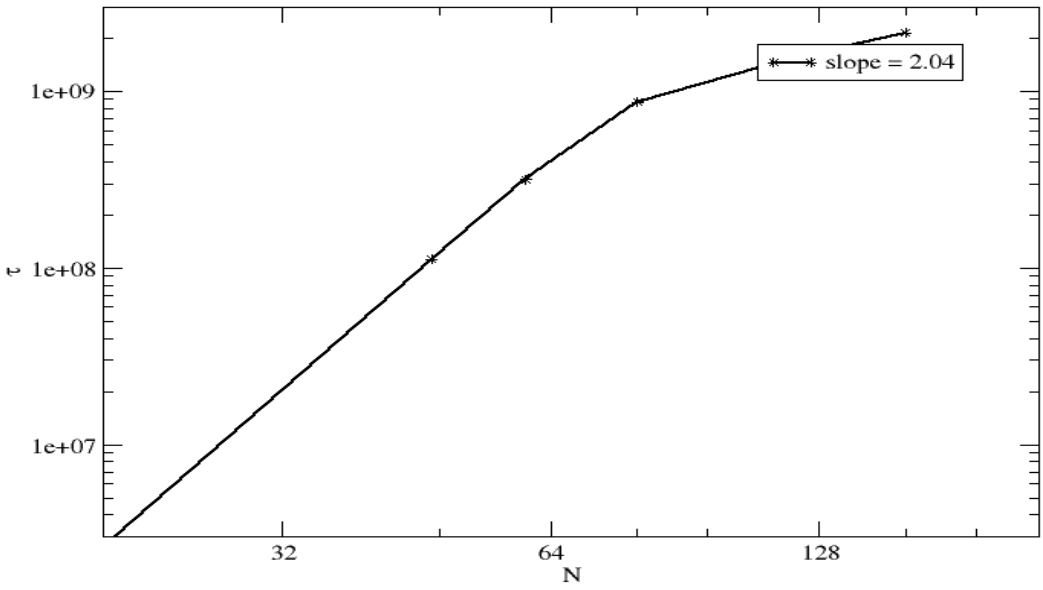


Figure 3.2: Log-log plot of most probable occurred escape time τ as a function of polymer chain length N

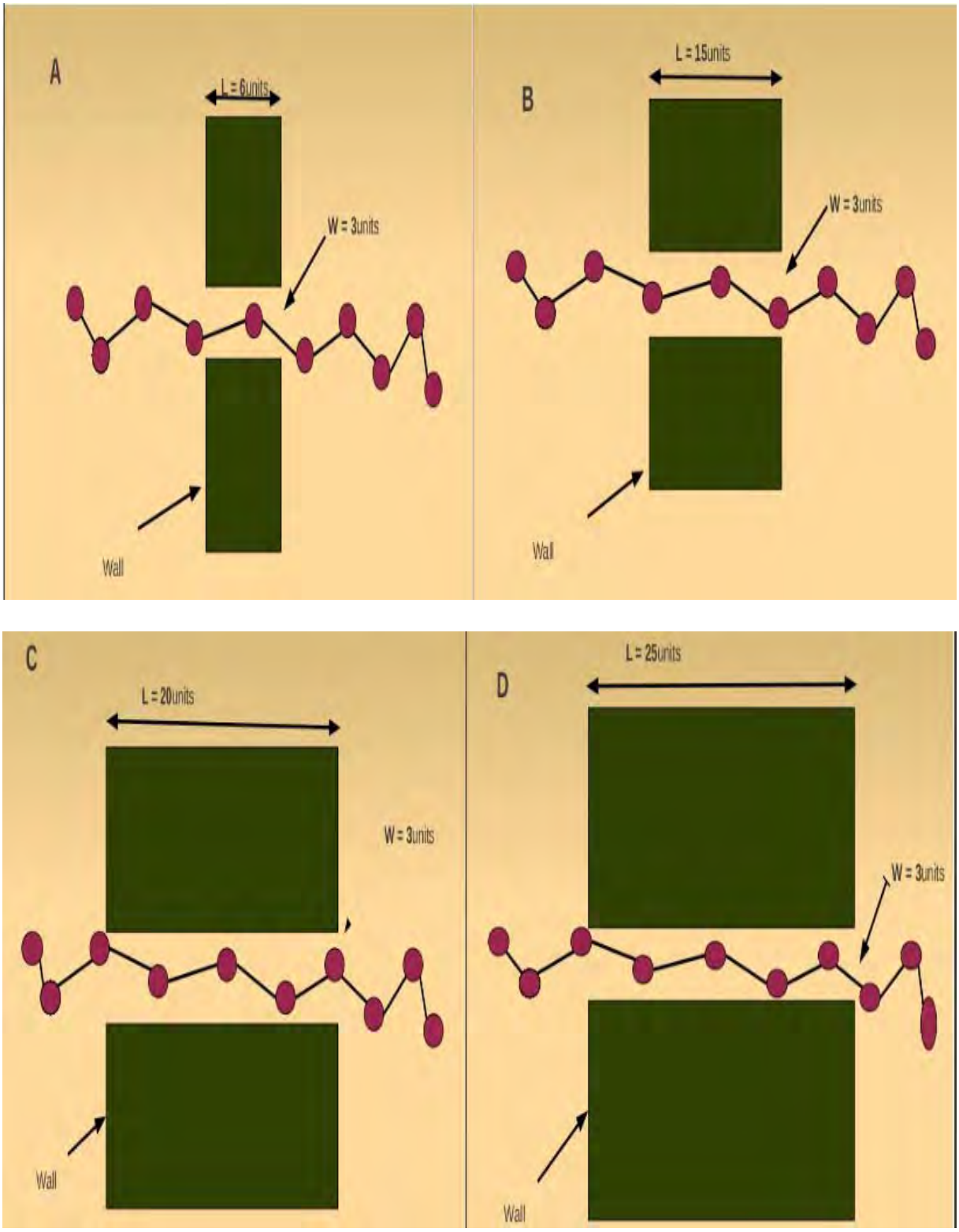


Figure 3.3: The above figure shows an increase entropic barrier as we go from A to D for a specific polymer chain N = 10 and channel width W = 3 but with different channel lengths L = 6,15,20 and 25.

3.1.3 The dependence of polymer translocation through varying channel lengths

Here we present and discuss the result from our simulation, for the dependence of polymer translocation with different parameters such as average escape time(τ), polymer chain(N), channel length(L) and channel width(W). Figure 3.4 below illustrates the translocation of a polymer chain through different channel lengths having values, L = 6, 20, 80,200. As it can be seen, when the channels length increase the escape time increases for the same size of a polymer chain (N = 20) and width of the channel (W = 3). Because it increases entropic barrier as it go through increased channel lengths as shown in the figure 3.3. Thus we can see a direct relation between the average escape time and the channel length.

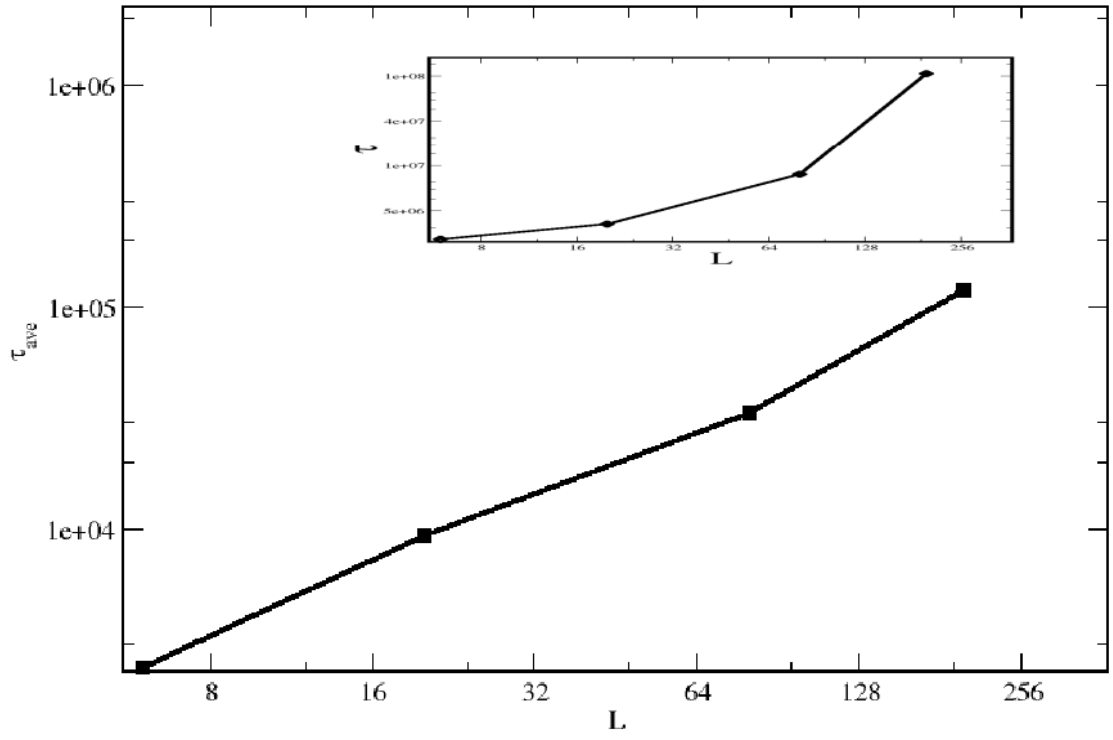


Figure 3.4: This is the computed log-log plot of average escape time τ versus the channel length for the simulation of polymer translocation through different channel lengths(L = 6 to L = 200) for a specific polymer chain N = 20 and channel width W = 3.

Figure 3.4 Clearly shows that the average escape time for a polymer chain of length N increases when the channel length increases. And similarly the most probable escape time increases as the channel length increases as shown in the figure 3.4 in small plot at the right top corner. So here both the average escape time and the most probable escape time increases as the channel length increases.

Chapter 4

Summary and conclusion

In this paper we presented and tested a Monte Carlo algorithm for simulations of translocating a polymer chain with similar or different beads through a very small channel can be used as a first step of modeling a DNA chain that passes through a nanopore. This translocation process offers a variety of possibilities in chemical and biological processes, for instance rapid DNA sequencing. In this thesis the chain is modeled as a polymer with similar or different types of monomers as beads. In the translocation process, we investigated the the relationship between the escape time with different parameters that influences the process. Some of these parameters are the polymer length N, the width of the channel through which the polymer translocates. As the presence of the wall produces an entropic barrier between the cis and trans side of the channel, we overcome this entropic barrier by initially placing the central monomer of the polymer at the center of the channel in a symmetric position. This symmetry means that a translocation of the polymer to the left or to the right is equally likely. Indeed, we observe for unbiased translocation that on average 50 percent of the polymers migrate to the left and the other half are finally found in the right side. Thus we studied the unbiased polymer translocation dynamics mainly by computing the escape time that the polymer chain leaves the channel either to the right or to the left of the channel instead of putting a restriction that the first monomer which is initially at the gate of the channel is never allowed to cross back out of the channel.

Though we have placed the central monomer in the middle of the channel to over come the entropic barrier there is still more entropic barrier since we consider a channel with channel length L = 20 instead of pore, so to this end our numerical results show that estimates for the scaling exponents of the escape time as a function of N are obtained, which is $\tau \sim N^{1+2\nu}$ with a few value difference as explaind in the previous section.

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Declaration

This thesis is my original work, has not been presented for a degree in any other University and that all the sources of material used for the thesis have been dully acknowledged.

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