Numerical Studies of an Active Worm Like Chain

Bharti Yadav

A dissertation submitted for the partial fulfilment
of BS-MS dual degree in Science

Indian Institute of Science Education and Research Mohali
April 2017

Certificate of Examination

This is to certify that the dissertation titled **"Numerical Studies of an Active Worm Like Chain"** submitted by **Bharti Yadav** (Reg. No. MS12022) for the partial fulfillment of BS-MS dual degree programme of the Institute, has been examined by the thesis committee duly appointed by the Institute. The committee finds the work done by the candidate satisfactory and recommends that the report be accepted.

Dr. Sanjeev Kumar	Dr. Rajeev Kapri	Dr. Abhishek Chaudhuri (Supervisor)

Dated: April 21, 2017

Declaration

The work presented in this dissertation has been carried out by me under the guidance of Dr. Abhishek Chaudhuri at the Indian Institute of Science Education and Research Mohali.

This work has not been submitted in part or in full for a degree, a diploma, or a fellowship to any other university or institute. Whenever contributions of others are involved, every effort is made to indicate this clearly, with due acknowledgement of collaborative research and discussions. This thesis is a bonafide record of original work done by me and all sources listed within have been detailed in the bibliography.

Bharti Yadav
(Candidate)

Dated: April 21, 2017

In my capacity as the supervisor of the candidates project work, I certify that the above statements by the candidate are true to the best of my knowledge.

Dr. Abhishek Chaudhuri
(Supervisor)

Acknowledgment

Foremost, I would like to express my sincere gratitude to my thesis advisor Prof. Abhishek Chaudhuri for his continuous support, his patience, motivation, enthusiasm, and immense knowledge. His guidance helped me in all the time of research and writing of this thesis. I could not have imagined having a better advisor and mentor like him.

I would also like to thank Nisha Gupta who gave me various ideas to understand my topic clearly and helped me by allowing me to use her system for my work.

I am also thankful to my parents, family and friends.

List of Figures

Abstract

In this work, I have studied the statistical properties of polymer in passive and active scenarios. For an ideal chain, I have reviewed the results for a freely jointed chain. For such chain, I have also performed numerical simulations using Langevian Dynamics. There I have Incorporated bending energy and simulated a worm like chain. For such a chain, the introduction of an active propulsion force on each monomer unit, re-normalises the stiffness of the chain which i investigated by looking at distribution of end-to-end distance.

Contents

Chapter 1

Introduction

1.1 Active Matter

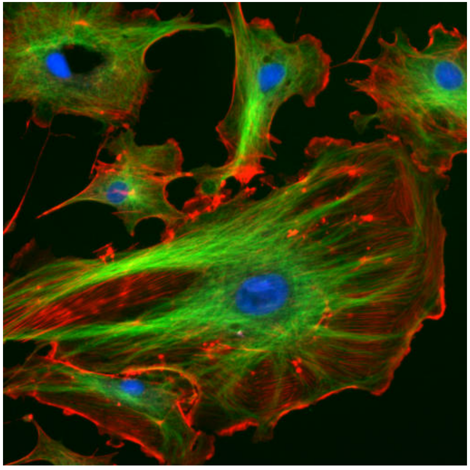
In active matter, the particles use internal energy or take up energy from the environment and perform directed movement. Examples of such systems include flocks of birds, molecular motors and the cellular cytoskeleton and bacterial suspensions to name a few. The individual and collective behavior of these systems show very interesting behavior unlike their passive counterparts. There have been several recent studies using experiments, simulations and analytics to understand the emergent properties of such systems. However there are several things that are as yet unexplored.

1.2 The Active Cytoskeleton

Inside the cell, there are a large number of filamentous structures which are semiflexible polymers with varying stiffness.

There are also molecular motors which are like the active particles we talked about which hydrolyse ATP to perform several functions like carrying cargo, etc. These filaments also undergo growth and shrinkage through the hydrolysis of GTP. There are also cross-linkers which connect different kinds of filaments forming a elastic network 1.1. There have been a large number of experiments performed by taking the filaments and motor proteins outside the cell. In these experiments, the molecular motors are irreversibly attached on a substrate such as a glass slide such that their heads stick to the substrate. Their tail ends stick out and the filaments are then put on this bed of motor proteins. It is seen that these filaments due to the motion of the motor proteins, slide in the opposite direction and their collective motion shows interesting features like vortices and swirls. Can we understand this behavior by modelling them using active particles ?

.5



.5

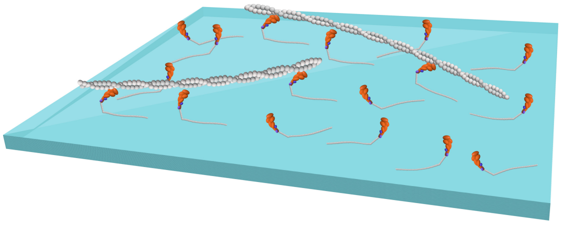


Figure 1.1: (a) A eukaryotic cell. Actin filaments shown in red, microtubules in green. Source : Wikipedia (b) An in-vitro motility assay showing motor proteins attached to the substrate and a cytoskeletal filament sliding on them.

1.3 Natural swimmers

Further, there are a large number of natural swimmers which propel themselves with the help of cilia and flegella. Cilia and flegella are attached with the outer body of the cell. They move liquid past the cell which makes the cells move. For single cells such as sperms, this enables them to swim. These filaments are semiflexible with bending rigidity, which are observed to be re-normalised by the effect of activity in the form of motor movements and ATP hydrolysis.

1.4 Plan of the thesis

In this thesis, I first review ideal polymers and discuss the various physical properties that characterize them. I then model a polymer with a finite bending rigidity and show that the simulation results match with the exact analytical expressions for special cases. Finally I study the case of a semiflexible polymer which is being self propelled by the action of active forces on each monomer. Here I look at the probability distribution of the end-to-end vector of the polymer to characterize its behavior due to changing stiffness and strength of activity.

Chapter 2

Ideal Chain polymer

2.1 Ideal Chain Polymer

Polymer is a large chain molecule which is made up of smaller units which are repeated. These units are called monomers and consecutive units are covalently bonded. Typically in a real polymer(synthetic or bio polymer), these monomer units interact via excluded volume interactions which prevent overlapping. In the case of ideal chain we relax these interactions.

2.1.1 Freely jointed Chain

The simplest model of an ideal chain is the freely jointed chain model. In such a chain, there are N beads joined together by (N-1) bonds of equal length b_0. Every successive bond can orient in any direction independent of the previous bond.

2.2 Conformations of FJC Polymer

Let $\{\vec{r_n}\} = (\vec{r_1}, \vec{r_2}, ...r_{\vec{N-1}})$ denote the set of bond vectors. Then, the distribution function of Fjc is :

$$\psi(\{\vec{r_n}\}) = \prod_{i=1}^{N-1} \psi(\vec{r_i}); \qquad \psi(\{\vec{r_n}\}) = \frac{1}{4\pi {b_0}^2} \delta(\mid \vec{r} \mid - b_0) \tag{2.1}$$

The size of the polymer is characterised by the end-to-end vector as follows:

$$\vec{R} = \sum_{i=1}^{N-1} \vec{r_i} \tag{2.2}$$

Since every bond direction is uncorrelated, the average end-to-end vector of an ideal chain of N monomers is zero.

$$\langle \vec{R} \rangle = 0 \tag{2.3}$$

Lets calculate the second moment $\langle R^2 \rangle$[CR03]:

$$\begin{aligned} \langle R^2 \rangle &= \langle \sum_{j=1}^{N-1} \vec{r}_j . \sum_{k=1}^{N-1} \vec{r}_k \rangle \\ &= \sum_{j=1}^{N-1} \sum_{k=1}^{N-1} \langle \vec{r_j} . \vec{r_k} \rangle \end{aligned} \tag{2.4}$$

Now, assuming all bond lengths are equal, $\mid \vec{r} \mid = b_0$, therefore;

$$\vec{r_j} . \vec{r_k} = b_0^2 \cos \theta_{jk} \tag{2.5}$$

Where, θ_{jk} is the angle between bond vectors.

$$\langle \vec{R^2} \rangle = b_0^2 \sum_{j=1}^{N-1} \sum_{k=1}^{N-1} \langle \cos \theta_{jk} \rangle \tag{2.6}$$

Since every successive bond in a FJC polymer are uncorrelated, ($\langle \cos \theta_{jk} \rangle = 0$ for $j \neq k$). Only N terms will contribute to the sum ($\langle \cos \theta_{jk} \rangle = 1$ for $j = k$). Therefor,for FJC model:

$$\langle R^2 \rangle = N b_0^2 \tag{2.7}$$

2.3 Radius of Gyration

Another quantity to characterise the size of a polymer is radius of gyration. It is the mean square distance between each monomer and center of mass of the polymer chain as[CR03],

$$R_g^2 = \frac{1}{N} \sum_{i=1}^{N} \left(\vec{R_i} - \vec{R_{cm}} \right)^2 \tag{2.8}$$

R_{cm} is the centre of mass of the polymer :

$$\vec{R_{cm}} = \frac{1}{N} \sum_{i=1}^{N} \vec{R_i} \tag{2.9}$$

Using this we can write;

$$
\begin{aligned}
R_g^2 &= \frac{1}{N}\sum_{i=1}^{N}\left(\vec{R_i}^{\,2} - 2\vec{R}_i\vec{R}_{cm} + \vec{R_{cm}}^{\,2}\right) \\
&= \frac{1}{N}\sum_{i=1}^{N}\left(\vec{r_i}^{\,2}\frac{1}{N}\sum_{j=1}^{N}1 - 2\vec{R}_i\frac{1}{N}\sum_{j=1}^{N}\vec{R}_{cm} + \frac{1}{N}\sum_{i=1}^{N}R_i\right)^2
\end{aligned}
\tag{2.10}
$$

The last term can be written as follows:

$$
\begin{aligned}
\frac{1}{N}\sum_{i=1}^{N}\left(\frac{1}{N}\sum_{i=1}^{N}\vec{R}_i\right)^2 = \left(\frac{1}{N}\sum_{i=1}^{N}\vec{R}_i\right)^2 &= \left(\frac{1}{N}\sum_{i=1}^{N}\vec{R}_i\right)\left(\frac{1}{N}\sum_{i=1}^{N}\vec{R}_i\right) \\
&= \frac{1}{N^2}\sum_{i=1}^{N}\sum_{j=1}^{N}\vec{R}_i.\vec{R}_i
\end{aligned}
\tag{2.11}
$$

Therefor the final expression for square of radius of gyration can be written as follows:

$$
\begin{aligned}
R_g^2 &= \frac{1}{N^2}\sum_{i=1}^{N}\sum_{j=1}^{N}\left(\vec{R}_i^2 - 2\vec{R}_i\vec{R}_j + \vec{R}_i\vec{R}_j\right) \\
&= \frac{1}{N^2}\sum_{i=1}^{N}\sum_{j=1}^{N}\left(\vec{R}_i^2 - \vec{R}_i\vec{R}_j\right) \\
&= \frac{1}{2}\left[\frac{1}{N^2}\sum_{i=1}^{N}\sum_{j=1}^{N}\left(\vec{R}_i^2 - \vec{R}_i\vec{R}_j\right) + \frac{1}{N^2}\sum_{i=1}^{N}\sum_{j=1}^{N}\left(\vec{R}_j^2 - \vec{R}_i\vec{R}_j\right)\right] \\
&= \frac{1}{2N^2}\sum_{i=1}^{N}\sum_{j=1}^{N}\left(\vec{R}_i^2 - 2\vec{R}_i\vec{R}_j + \vec{R}_j^2\right) \\
&= \frac{1}{2N^2}\sum_{i=1}^{N}\sum_{j=1}^{N}\left(\vec{R}_i - \vec{R}_j\right)^2
\end{aligned}
\tag{2.12}
$$

Now, $\frac{1}{2N^2}\sum_{i=1}^{N}\sum_{j=1}^{N} = \frac{1}{N^2}\sum_{i=1}^{N}\sum_{j=i+1}^{N}$,

$$
\left\langle R_g^2\right\rangle = \frac{1}{N^2}\sum_{i=1}^{N}\sum_{j=i+1}^{N}\left\langle\left(\vec{R}_i - \vec{R}_j\right)^2\right\rangle
\tag{2.13}
$$

Now, $\left\langle \left(\vec{R}_i - \vec{R}_j\right)^2 \right\rangle = b_o^2 \mid j - i \mid$

$$\begin{aligned} R_g^2 &= \frac{1}{N^2}\sum_{i=1}^{N}\sum_{j=1}^{N} \mid j-i \mid = \frac{1}{N^2}\sum_{i=1}^{N-1}\sum_{j=1}^{N-i} \mid j \mid = \frac{b_0^2}{N^2}\sum_{i=1}^{N-1}\frac{\big(N-i\big)\big(N-i+1\big)}{2} \\ &= \frac{b_0^2}{2N^2}\sum_{i=1}^{N-1}\Big[(N-i)^2 + (N-i)\Big] = \frac{b_0^2}{2N^2}\Big[\sum_{i=1}^{N-1}(N-i)^2 + \sum_{i=1}^{N-1}(N-i)\Big] \\ &= \frac{b_0^2}{2N^2}\Big[\sum_{i=1}^{N-1} i^2 + \sum_{i=1}^{N-1} i\Big] = \frac{b_0^2}{2N^2}\Big[\frac{\big(N-1\big)N\big(2N-1\big)}{6} + \frac{\big(N-1\big)N}{2}\Big] \\ &= \frac{b_0^2}{6N}\big(N^2-1\big) = \frac{b_0^2 N}{6}\big(1 - \frac{1}{N^2}\big) \end{aligned} \tag{2.14}$$

For $N >> 1$

$$\left\langle R_g^2 \right\rangle = \frac{N b_0^2}{6} \tag{2.15}$$

Finally;

$$\frac{\langle R^2 \rangle}{\langle R_g^2 \rangle} = 6 \tag{2.16}$$

Chapter 3

Worm Like Chain Polymer

Real polymers like DNA are stiff molecules. The FJC model Can not work. We need to account for the bending rigidity of the polymers. One way to do that is to restrict the angle that every successive bond is allowed to take. This discrete version is called the freely rotating model. We here add an energy for bending. The distribution function is modified as;

$$\psi(\vec{r_n}) = \prod_{i=1}^{N-1} \frac{1}{4\pi b_0^2} \delta(\mid \vec{r} \mid - b_0) \exp\left(k_b \sum_{i=1}^{N-1} \hat{r_i}.\hat{r_j} \right) \tag{3.1}$$

Where $\hat{r_i} = \frac{\vec{r_i}}{b_0}$ is the normalised bond vector, k_b is the bending rigidity. The continuum version of this model is called worm like chain model. We now give the details how to simulate such a chain.

3.1 Forces

The Hamiltonian of a semiflexible polymer chain has three components U_{bond},$U_{bend}$and U_{ex}.

$$U = U_{bond} + U_{bend} + U_{ex} \tag{3.2}$$

3.1.1 Excluded Volume Effect

The excluded volume effect makes the ideal chain nonideal. Excluded volume effect refers to the idea that one part of the long chain polymer can not occupy space that is already occupied by the other part of the same molecule. So to put this effect mathematically for our polymer we used the purely repulsive Lennard-Jones potential.

Purely repulsive Lennard-Jones potential describes the weak interactions between natural atoms and molecules. It is between any two monomers and given by the equation 3.3. And in our case we have used the shifted Lennard-Jones potential[GK86].

$$U_{ex} = \begin{cases} 4\epsilon\big[(\frac{\sigma}{r_{ij}})^{12} - (\frac{\sigma}{r_{ij}})^{6} + \frac{1}{4}\big], & \text{if } r_{ij} \leq \sigma 2^{1/6} \\ 0, & \text{otherwise} \end{cases} \tag{3.3}$$

ϵ and σ are the characteristic volume exclusion energy and bead size and r_{ij} is the vector between the position of beads i and j.

3.1.2 FENE Potential

FENE stands for finitely extensible nonlinear elastic model of a long chained polymer. FENE potential is like a spring potential, in case of spring it can be extended to infinite limit, but in case of the potential considered in the semiflexible polymer, if two monomers are stretched apart then they will try to come to their equilibrium bond length which is b_0. It is composed of the bond contribution of neighbouring beads. The Hamiltonian for this stretching is given by following FENE potential[GK86].

$$U_{bond} = \begin{cases} -0.5 k_s {r_{ij}}^2 \log_e(1 - (\frac{r_{ij}}{b_0})^2), & \text{if } r_{ij} \leq \mathrm{b}_0 \\ 0, & \text{otherwise} \end{cases}. \tag{3.4}$$

Where k_s is the bond stiffness .

3.1.3 Bending Rigidity

Conformations of the polymer chain costs bending energy and the bending energy for a conformation is give as: [HABB14]

$$U_{angle} = \frac{\kappa}{2} \int_0^L \left(\frac{\partial^2 r(s)}{\partial s} \right)^2 ds \tag{3.5}$$

κ is the bending rigidity.

3.2 The Integration Method

The motion of the i^{th} monomers in a viscous fluid is given by the langevian equation[AT89]:

$$\ddot{r}_i = -\nabla U_i - \tau \dot{r}_i + W_i(t) \tag{3.6}$$

Where τ is the coefficient of the viscous force, and $\tau \dot{r}_i$ is the viscous force. $W_i(t)$ describes the random force(due to random collisions of the fluid particles) acting on the each monomer, And also the random force is given by the Gaussian distribution with the following correlation function In $3d$:

$$\langle W_i\big(t\big).W_j\big(t_1\big)\rangle = \delta_{ij}\delta\big(t-t_1\big)6K_bT\tau \tag{3.7}$$

K_b is the Boltzmann's constant, T is the absolute temperature and $\delta(t-t_1)$ is Dirac delta function.
And by solving the above equation of motion we will get

$$r\big(t+\delta t\big) = r\big(t\big) + C_1\delta t v\big(t\big) + C_2\delta t^2 a\big(t\big) + \delta r^G \tag{3.8}$$

$$v\big(t+\delta t\big) = c_0 v\big(t\big) + \big(c_1-c_2\big)\delta t a\big(t\big) + c_2\delta t a\big(t+\delta t\big) + \delta v^G \tag{3.9}$$

$$C_0 = \exp\big(-\delta t\tau\big) \tag{3.10}$$

$$C_1 = \frac{1-C_0}{\tau\delta t} \tag{3.11}$$

$$C_2 = \frac{1-C_1}{\tau\delta t} \tag{3.12}$$

Where a is the force on the monomer by itself. δr^G and δv^G are the changes in r and v due to the Gaussian random numbers with the following variance :

$${\sigma_r}^2 = \frac{\Big(2-\big(\delta t\tau\big)^{-1}\big(3-4\exp\big(-\delta t\tau\big)+2\exp\big(-2\delta t\tau\big)\Big)}{\delta t\tau} \tag{3.13}$$

$${\sigma_v}^2 = \frac{KT}{m}\big[1-\exp\big(-2\delta t\tau\big)\big] \tag{3.14}$$

3.3 Initialisation

At first the first bead was positioned at the origin and the subsequent beads are placed at the distance of b_0 from its adjacent beads, with the small variations in the bond length due to the FENE potential. After assigning the position of the beads in the x,y,z direction we assigned the initial velocities of each and every monomer by using random no generator in between $[-0.5, 0.5]$.

3.4 Results of semiflexible polymer without excluded volume effect

3.4.1 End-To-End Distance

In case of non self avoiding polymer r^2 and r^4 were calculated, where r is the end-to-end distance of the polymer. To find the end-to-end vector the monomers are numbered starting from 1 to N, where r_1 and r_n are the initial and final positions vector of the polymer respectively.

$$\vec{R} = \vec{R_N} - \vec{R_1} = \sum_{i=1}^{N} \vec{r_i} \tag{3.15}$$

Because of no correlation in every $\vec{r_i}$,

$$\langle R \rangle = \sum_{i=1}^{N} \langle \vec{r_i} \rangle = 0 \tag{3.16}$$

It means polymer is behaving like a random walk.So there is no meaning of calculating mean of end to end distance. So instead of taking mean of end-to-end vector we took the mean square end-to-end distance vector. This gives the better way to analyse the polymer. As the each step of the simulation occurs at a fix time step then the averaging of the square of the end to end distance vector can be written as following.

$$\begin{aligned} \langle R^2 \rangle &= \sum_{n=1}^{N} \sum_{m=1}^{N} \langle r_n . r_m \rangle \\ &= \sum_{m=1}^{N} \langle {r_n}^2 \rangle \delta_{m,n} \\ &= \sum_{n=1}^{N} \langle {r_n}^2 \rangle \end{aligned} \tag{3.17}$$

The simulated data of even moments $\left(\langle r^2 \rangle\right)$ and $\langle r^4 \rangle)$ for different persistence length is compared for $N = 16, 32, 64, 80, 90$ for two and three dimensional case with the following analytical results[DC02].

$$\langle R^2 \rangle = \frac{4\kappa L}{d-1} - \frac{8\kappa^2 \left(1 - \exp\left(\frac{(1-dL)}{2\kappa}\right)\right)}{(1-d)^2} \tag{3.18}$$

$$\begin{aligned}\langle R^4\rangle = {} & \frac{64^4(d-1)\exp\frac{-dL}{\kappa}}{d^3(d+1)^2} - \frac{128^4(d+5)^2\exp\frac{-(d-1)L}{2\kappa}}{(d-1)^4(d+1)^2} \\ & + \frac{64^3L(d^2-8d+7)\exp\frac{-(d-1)L}{2\kappa}}{(d-1)^4(d+1)} + \frac{64^4(d^3+23d^2-7d+1)}{(d-1)^4(d)^3} \\ & + \frac{64^3(d^3+5d^2-7d+1)}{(d-1)^4(d)^2} + \frac{16^2(d^3-3d+2)}{(d-1)^4d}\end{aligned} \tag{3.19}$$

The analytical (equation 3.18 and equation 3.19) and simulated results are compared for the persistence length 4.27 and 6.4.

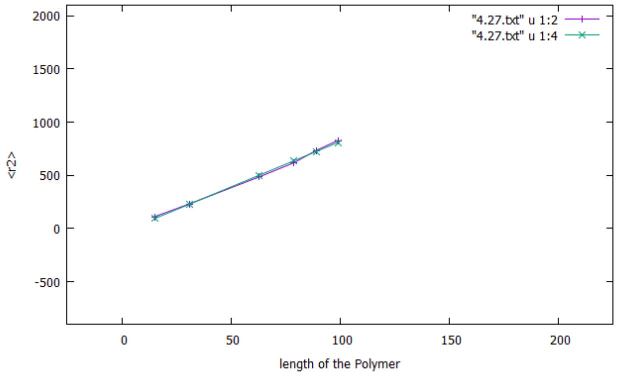


Figure 3.1: Plots showing a comparison in between simulated and analytical results shown in the equation 3.18 shows the comparison of simulated results for$\langle r^2\rangle$for persistence length 4.27.Green lines represents the analytical results and purple lines shows the simulated results.

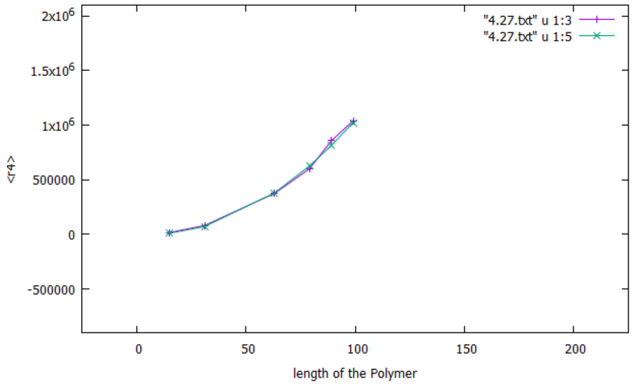


Figure 3.2: Plots showing a comparison in between simulated and analytical results shown in the equation 3.19 shows the comparison of simulated results for $\langle r^2\rangle$for persistence length 4.27.Green lines represents the analytical results and purple lines shows the simulated results.

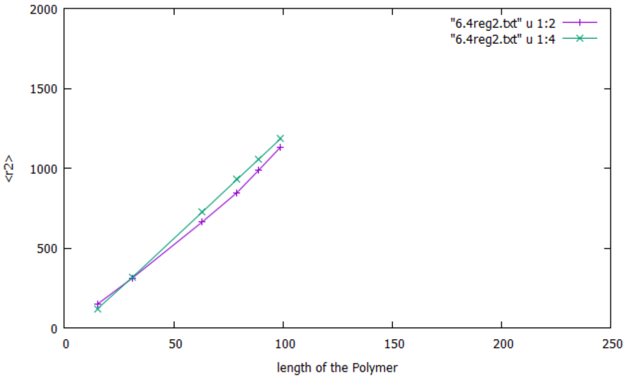


Figure 3.3: Plots showing a comparison in between simulated and analytical results shown in the equation 3.18 shows the comparison of simulated results for $\langle r^2 \rangle$for persistence length 6.4.Green lines represents the analytical results and purple lines shows the simulated results.

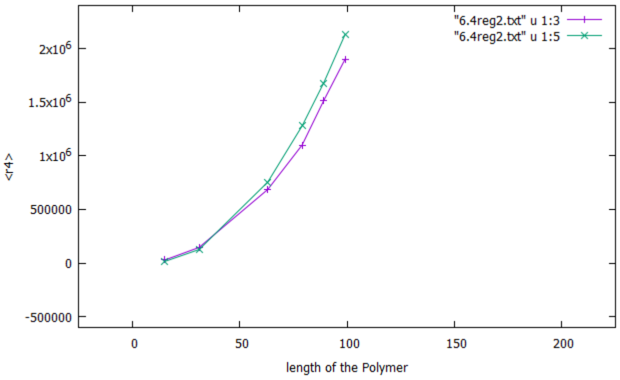


Figure 3.4: Plots showing a comparison in between simulated and analytical results shown in the equation 3.19 shows the comparison of simulated results for $\langle r^4 \rangle$for persistence length 6.4.Green lines represents the analytical results and purple lines shows the simulated results.

3.4.2 Probability Distribution

An important quantity to calculate is the probability distribution of end-to-end distance $p(v,t)$,where $v = r/L$ and $t = L/P_l$. In d-dimensional space the bending rigidity is related to the persistence length as follows.

$$\kappa = \frac{(d-1)P_l}{2} \tag{3.20}$$

In case of real polymers there can be wide range of the parameter t, based on the values of persistence length and length of the polymer. For example, $P_l = 18\mu m$ for Actin filaments and t can be varied by changing length of the polymer. Higher persistence length means higher rigidity. So actin filaments are stiffer then DNA, and DNA is stiffer then RNA based on their persistence lengths.

To calculate p(v,t), first we calculate ($P(r, L)$). As we have taken the spherically symmetric case, the spherical probability distribution is related to radial probability distribution ($S(r, L)$) as follows.[DC02]

$$S(r, L) = Cr^{d-1}P\big(r, L\big) \tag{3.21}$$

Where C is the area of a d-dimensional unit sphere. And the radial probability distribution ($P(r, L)$) is related to $p(v, t)$ as follows.

$$P(r, L) = \frac{1}{L^d}p(\frac{r}{L}, \frac{L}{p_l}) \tag{3.22}$$

So finally from equation 3.19 and equation 3.20 we can write :

$$S(r, L) = Cr^{d-1}\frac{1}{L^d}p(\frac{r}{L}, \frac{L}{p_l}) \tag{3.23}$$

For $v = r/L$ and $t = L/P_l$,

$$S(r, L) = Cr^{d-1}\frac{1}{L^d}p(v, t) \tag{3.24}$$

$$Cp(v, t) = \frac{L^d S(r, L)}{r^{d-1}} \tag{3.25}$$

Chapter 4

Self Propelled Worm Like Chain Polymer

4.1 Activity

As discussed in the introduction, in nature, there are several instances where the role of activity is extremely important to the dynamics of the polymer. The example of the bio-filaments such as actin and micro-tubules which forms the cytoskeletal, shows patterns in their collective behaviour when observed inside the cell or in motility average. Here, we consider a polymer chain where every monomer unit is propelled by a force acting tangentially to the bond between adjacent monomers. This model was introduced by Holder[IHEG15]

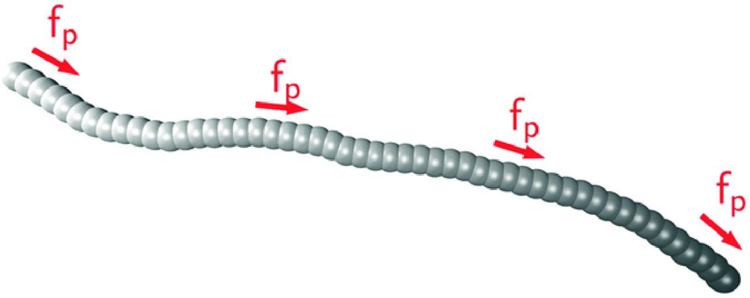


Figure 4.1: Beads are connected via stiff springs.the active force acts tangentially along all bonds. Colour gradient indicates the force direction.[IHEG15]

4.1.1 Force

The tangential force on every bond between two adjacent monomers is given by the following equation:[IHEG15]

$$F_p = \sum_{n=1}^{N} f_p r_{i,i+1} \tag{4.1}$$

f_p is the force per unit length acting on adjacent monomers in the direction tangent to the bond between them and is distributed equally onto both adjacent monomers. We consider system with parameters chosen such that k_s is sufficiently large that the bond length is approximately constant r_0.

$$\frac{P_l}{L} = \frac{\kappa}{k_B T L} \tag{4.2}$$

$$P_e = \frac{f_p L^2}{k_B T} \tag{4.3}$$

P_l and L are the persistence length and length of the polymer. P_l/L is the measure of bending rigidity of the polymer. P_e (peclet number) is the measure of degree of activity.

4.2 Probability Distribution Plots

We look at the probability distribution of end-to-end distance as introduced in section 3.4.2. For the two dimensional case,the area of sphere is $2\pi r$. In a unit sphere,$r = 1$,hence $C = 2\pi$.

$$2\pi p(v,t) = \frac{LS(r,L)}{v} \tag{4.4}$$

For the three dimensional case,the area of sphere is $4\pi r^2$. In a unit sphere, $r = 1$, hence $C = 4\pi$.

$$4\pi p(v,t) = \frac{LS(r,L)}{v^2} \tag{4.5}$$

4.2.1 Without Excluded Volume Effect and Without Activity.

In case of Worm Like Chain polymer without excluded volume effect (in both two and three dimensional case), we looked at the probability distribution plot of end-to-end distance at $t = 1, 2, 3.3, 5, 10$

- At $t = 1$(at persistence length ($P_l = 15$ for $N = 16$)), mean of the distribution plot lies at nearly ($v = 1$).That means at higher persistence length the polymer is rigid as we can see in figure 4.2 and figure 4.3.

- as we increase t(by decreasing persistence length up-to $P_l = 1.5$ for $N = 16$) the mean of the distribution plots shifts towards $v = 0$. At lower persistence length the polymer is flexible as we can see in figure 4.2 and figure 4.3.

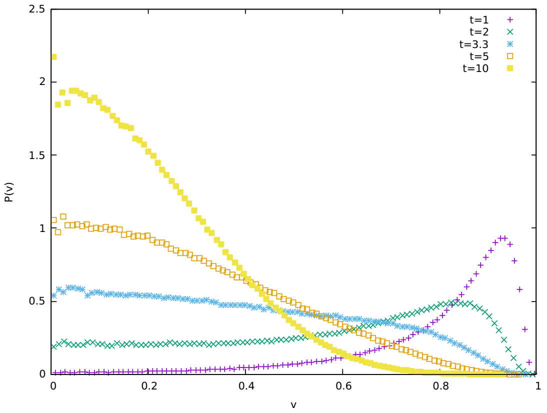


Figure 4.2: Probability distribution plot for two dimensional semiflexible polymer without excluded volume effect of $t = 1$, for $P_e = 0.1, 1, 10, 100, 1000, 10000$

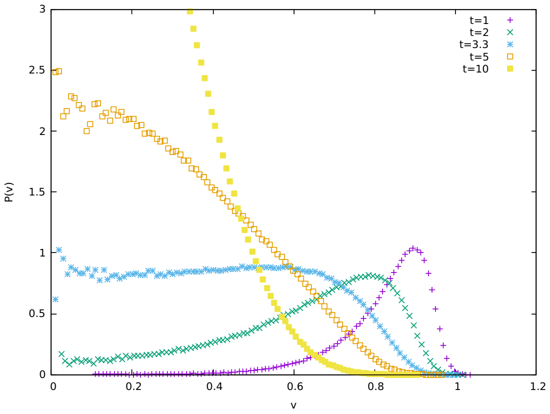


Figure 4.3: Probability distribution plot for three dimensional semiflexible polymer without excluded volume effect of $t = 1$, for $P_e = 0.1, 1, 10, 100, 1000, 10000$

4.2.2 Without Excluded Volume Effect and With Activity.

In case of Worm Like Chain polymer without excluded volume effect and with activity (for both two dimensional and three dimensional case), we looked at the behaviour of the probability distribution plot for peclet numbers $P_e = 0.1, 1, 10, 100, 1000, 10000$ at $t = 10$ and $t = 1$.

- For $t = 10$ the probability distribution plot shifts towards higher value of v as we increase peclet number from $P_e = 0.1$ to $P_e = 1000$, but as we further increase peclet number to $P_e = 10000$ it shifts towards lower number of v. That means the flexible polymer first becomes rigid and then for higher peclet number again it becomes flexible as we can see in figure 4.5.
- For $t = 1$ the probability distribution plot shifts towards lower value of v as we increase peclet number from $P_e = 0.1$ to $P_e = 10000$, That means the rigid polymer becomes

flexible as we increase activity as we can see in figure 4.4 and figure 4.6.

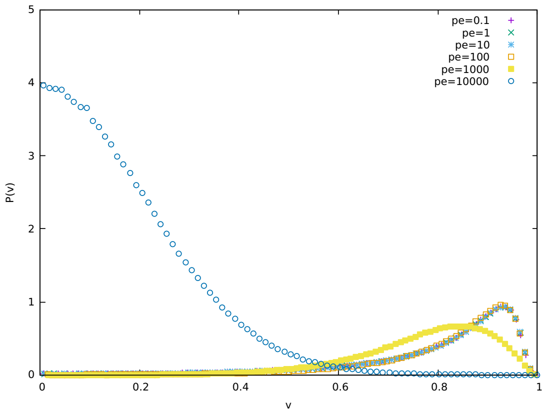


Figure 4.4: Probability distribution plot for two dimensional tangentially propelled semiflexible polymer without excluded volume effect of $t = 1$, for $P_e = 0.1, 1, 10, 100, 1000, 10000$

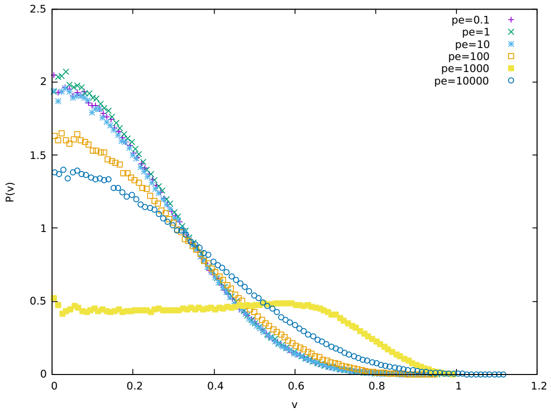


Figure 4.5: Probability distribution plot for two dimensional tangentially propelled semiflexible polymer without excluded volume effect of $t = 10$, for $P_e = 0.1, 1, 10, 100, 1000, 10000$

4.2.3 With Excluded Volume Effect and Without Activity.

In case of worm like chain with excluded volume effect(for both the two dimensional and three dimensional case) is little bit different from the results of the without excluded volume effect. Because of the presence of excluded volume effect the monomers can not coincide that means the distance between any two monomers cant be zero. So the mean of the probability distribution for flexible polymers(for $t = 10$ and $p_l = 1.5$ and $N = 15$) will shift towards higher value of v(as we compare with the without excluded volume effect) as we can see in figure 4.8 and figure 4.9.

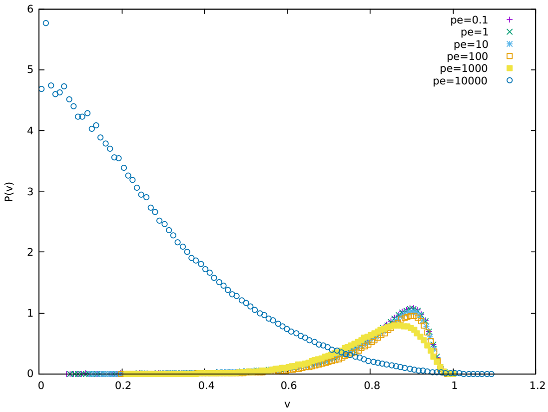


Figure 4.6: Probability distribution plot for three dimensional tangentially propelled semi-flexible polymer without excluded volume effect of $t = 1$, for $P_e = 0.1, 1, 10, 100, 1000, 10000$

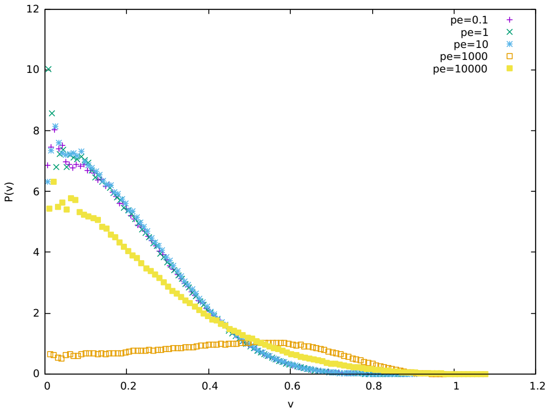


Figure 4.7: Probability distribution plot for three dimensional tangentially propelled semi-flexible polymer without excluded volume effect of $t = 10$, for $P_e = 0.1, 1, 10, 100, 1000, 10000$

4.2.4 With Excluded Volume Effect and With Activity.

In case of Worm Like Chain polymer with excluded volume effect and with activity(for both two dimensional and three dimensional case), we looked at the behaviour of the probability distribution plot for peclet numbers $P_e = 0.1, 1, 10, 100, 1000, 10000$ at $t = 10$ and $t = 1$.

- For $t = 10$ the probability distribution plot shifts towards higher value of v as we increase peclet number from $P_e = 0.1$ to $P_e = 1000$, but as we further increase peclet number to $P_e = 10000$ it shifts towards lower number of v. That means the flexible polymer first becomes rigid and then for higher peclet number again it becomes flexible as we can see in figure 4.11 and figure 4.13.

- For $t = 1$ the probability distribution plot shifts towards lower value of v as we increase peclet number from $P_e = 0.1$ to $P_e = 10000$, That means the rigid polymer becomes flexible as we increase activity as we can see in figure 4.10 and figure 4.12.

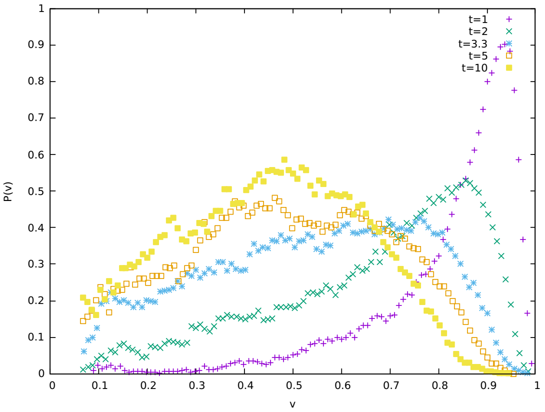


Figure 4.8: Probability distribution plot for two dimensional semiflexible polymer with excluded volume effect of for $t = 1, 2, 3.3, 5, 10$

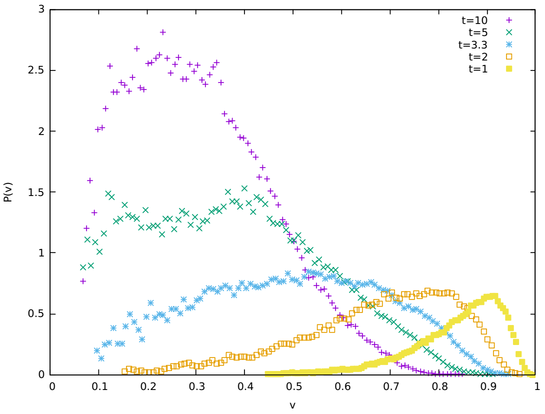


Figure 4.9: Probability distribution plot for three dimensional semiflexible polymer with excluded volume effect of for $t = 1, 2, 3.3, 5, 10$

4.3 Conclusion and Future Direction

In this thesis, I have obtained the statistical propulsion of an active worm like chain where the monomer units are propelled with a tangential force. The probability distribution of end-to-end vector revealed clearly the renormalisation of stiffness of the worm like chain due to activity. I would like to extend the study to the monomer dynamics of such chain with good solvent conditions.

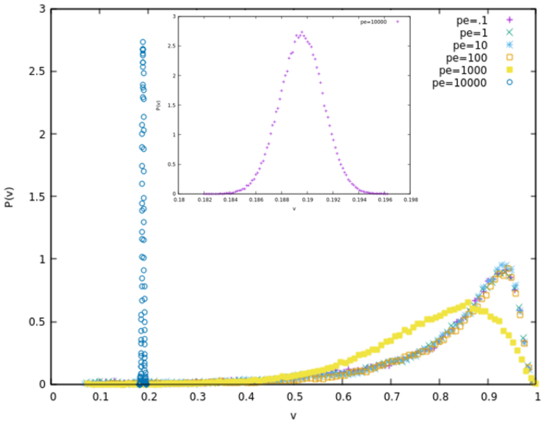


Figure 4.10: Probability distribution plot for two dimensional tangentially propelled semi-flexible polymer with excluded volume effect of $t = 1$, for $P_e = 0.1, 1, 10, 100, 1000, 10000$ the inset graph is for the $P_e = 10000$

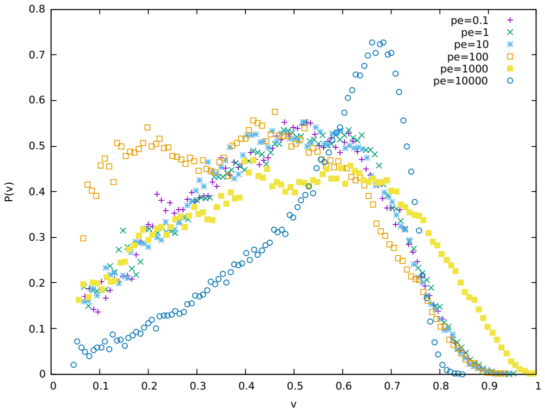


Figure 4.11: Probability distribution plot for two dimensional tangentially propelled semi-flexible polymer with excluded volume effect of $t = 10$, for $P_e = 0.1, 1, 10, 100, 1000, 10000$

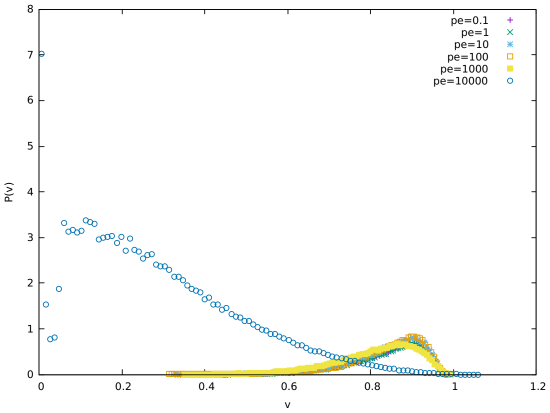


Figure 4.12: Probability distribution plot for three dimensional tangentially propelled semi-flexible polymer with excluded volume effect of $t = 1$, for $P_e = 0.1, 1, 10, 100, 1000, 10000$

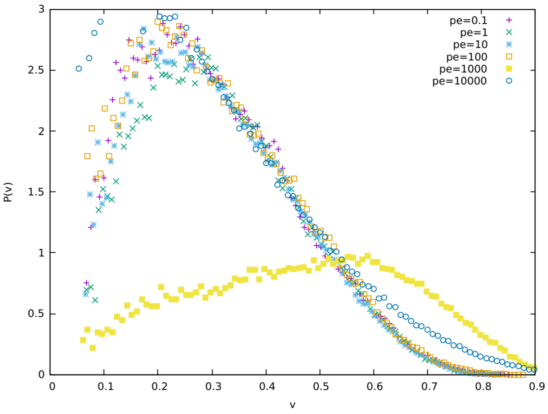


Figure 4.13: Probability distribution plot for three dimensional tangentially propelled semi-flexible polymer with excluded volume effect of $t = 10$, for $P_e = 0.1, 1, 10, 100, 1000, 10000$

Bibliography

[AT89] Mike P Allen and Dominic J Tildesley, *Computer simulation of liquids*, Oxford university press, 1989.

[CR03] RH Colby and M Rubinstein, *Polymer physics*, New-York: Oxford University (2003), 274–281.

[DC02] Abhishek Dhar and Debasish Chaudhuri, *Triple minima in the free energy of semiflexible polymers*, Physical review letters **89** (2002), no. 6, 065502.

[GK86] Gary S Grest and Kurt Kremer, *Molecular dynamics simulation for polymers in the presence of a heat bath*, Physical Review A **33** (1986), no. 5, 3628.

[HABB14] Aiqun Huang, Ramesh Adhikari, Aniket Bhattacharya, and Kurt Binder, *Universal monomer dynamics of a two-dimensional semi-flexible chain*, EPL (Europhysics Letters) **105** (2014), no. 1, 18002.

[IHEG15] Rolf E Isele-Holder, Jens Elgeti, and Gerhard Gompper, *Self-propelled worm-like filaments: spontaneous spiral formation, structure, and dynamics*, Soft matter **11** (2015), no. 36, 7181–7190.