Sup Galilée

Final year REPORT

Simulation and analysis of stochastic in polymer dynamics

Author:
chenyu ZHA

Supervisor:
Holcman DAVID
Ofir SHUKRON

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Acknowledgment

First I would like to thank David Holcman, the director of Director of Research Group of Applied Mathematics and Computational Biology , for giving me the opportunity to do an internship within the organization. For me it was a unique experience to be in IBENS and to study an interesting project. Furthermore I want to thank O.Shukron, without his assistance, comments, suggestion throughout this internship, this internship program could not be well.

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Chapter 1

Introduction

1.1 Presentation of IBENS

IBENS(Institut de Biologie de l'ENS)) is a institute of research mixed with ENS/CNRS/Inserm which focus on 4 themes:

- Biologie du développement
- Génomique environnementale et évolutive
- Génomique fonctionnelle
- Neurosciences

My internship is effected in the Group of Theoretical Modeling of Cellular Physiology under Neuroscience leaded by David Holcman.The main interest of group is to study the function of micro domains in cellular biology develop physical modeling, mathematical analysis, numerical simulations and data analysis.Our goal is to identify principles underlying cellular and network function. We develop mathematical multi scale models, statistical methods to treat data, analysis of the model equations and numerical simulations.[1]

[1] http://www.biologie.ens.fr/bcsmcbs/

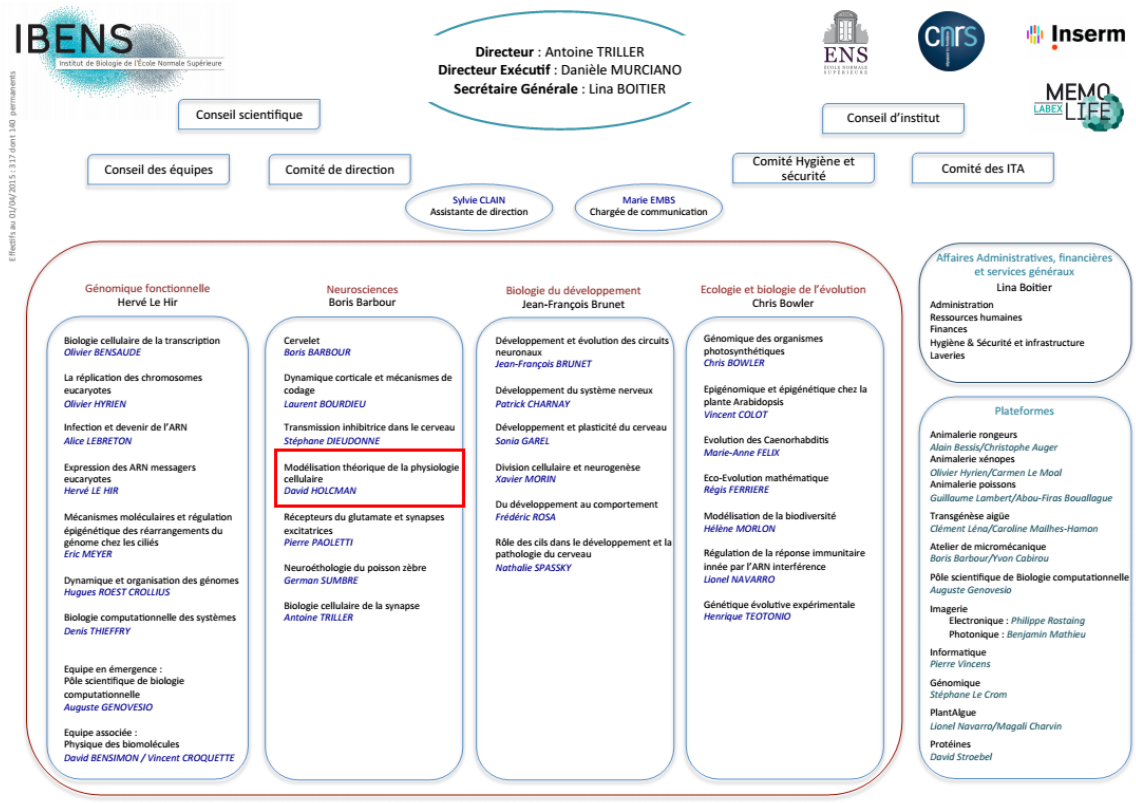


Figure 1.1: Organism of IBENS [a]

[a] http://www.biologie.ens.fr/depbio/spip.php?article22

1.2 Goal of internship

A polymer is a large molecule made of many small,simple chemical unit,joined together by chemical reaction .The purpose of internship is to simulate and analysis of stochastic in polymer dynamics,especially the simulation of chromosomes,which carry genetic information in the form of genes.In spite of recent progress in live cell microscopy, the chromosome dynamics is still unclear.Study this biology phenomena is indispensable for understanding the behavior of chromosomes.
This internship is effected with Ofir Shukron (phD of Group),my mainly works are the following:

- Simulate the motion of yeast chromosome and telomeres clustering.
- Simulate the mean first encounter time between 3 beads.
- Simulate the mean square displacement of beads in different contexts.
- Continue the development of framework by adding some functions and properties.

1.3 Structure of report

This report is structured with the following way:

The chapter 2 reviews some models of polymer chains and their basic properties.

The chapter 3 introduces the simulation of mean first encounter time in open domain,including the conception of algorithm, results obtained.

The chapter 4 introduces how to simulate the motion of yeast's chromosome in domain(sphere) and telomere clustering.

The chapter 5 introduces how to calculate the mean square displacement of beads in the Rouse Model for a single chain with different contexts.

The chapter 6 introduces other functions have been added in rouse framework and the related tests.

Chapter 2

Model of polymer chains

A polymer chain can have several architectures such as a linear chain, a branched chain , and a cross-linked polymer.For a linear chain polymer in a continuous space there exists various models : a bead-stick model, a bead-spring model, and a pearl-necklace model.
In the bead-spring model, the whole chain is represented by a series of beads connected by springs, and this model is a mechanical representation of the Gaussian chain.

2.1 Gaussian Chain

A Gaussian chain assumes that the vector $R_n - R_m$ between any two units n and m is Gaussian,being given by :

$$p(\boldsymbol{R_n - R_m}, \boldsymbol{n - m}) = [\frac{3}{2\pi b^2|n-m|}]^{\frac{3}{2}} exp[\frac{3(\boldsymbol{R_m - R_n})^2}{2|n-m|b^2}]$$

where b is the effective bond length.

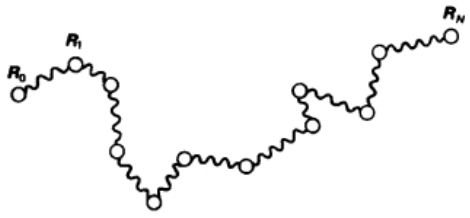


Figure 2.1: Gaussian Chain [a]

[a]The theory of polymer chains

Such a Gaussian chain is often represented by a mechanical model of beads

connected by harmonic spring,the potential energy is given by:

$$U = \frac{1}{2}k\sum_{n=1}^{N}(\boldsymbol{R_n} - \boldsymbol{R_{n-1}})^2$$

the spring constant k is chosen equal to :

$$k = \frac{3k_BT}{b^2}$$

where k_B is a Boltzmann constant,T is temperature. The Gaussian chain is used as a starting point for the Rouse Model,which is the simplest version of the bead-spring model that can treat the chain dynamics.

2.2 Dynamics simulations of Rouse model

In the Rouse Model,we assume that there exist only the nearest neighbor interactions between beads. The dynamics of the beads follow Brownian motion so that position of bead $R_n(t)$ can be described by Langevin Equation:

$$\frac{d\boldsymbol{R_n}}{dt} = \frac{-1}{\xi}\frac{\partial U}{\partial R_n} + g_n \tag{2.1}$$

By using the harmonic potential defined above,the governing equations of this model can be written as follows:

$$\frac{d\boldsymbol{R_n}}{dt} = \frac{k}{\xi}(\boldsymbol{R_{n+1}} + \boldsymbol{R_{n-1}} - 2\boldsymbol{R_n}) + \boldsymbol{g_n}, \forall n \in [1, 2...N-1] \tag{2.2}$$

For the bead 0 and N,we have :

$$\begin{cases} \frac{d\boldsymbol{R_0}}{dt} = \frac{k}{\xi}(\boldsymbol{R_1} - \boldsymbol{R_0}) + \boldsymbol{g_n}(t) \\ \frac{d\boldsymbol{R_n}}{dt} = \frac{k}{\xi}(\boldsymbol{R_{n-1}} - \boldsymbol{R_n}) + \boldsymbol{g_n}(t) \end{cases}$$

where $\boldsymbol{g_n}(t)$ is a random force following Gaussian distribution and the mean and variance is defined as:

$$< g_n(t) = 0 >$$

$$< g_{n\alpha}(t)g_{m\beta}(t') >= 2D\delta_{nm}\delta_{\alpha\beta}\delta(t-t')$$

where D is diffusion constant.
The random forces are needed to keep the chain in shape. Without the random forces, the beads would move until all of them collapse onto a single point and the spring forces disappear.

Chapter 3

Mean First Encounter Time Simulation

3.1 MFET in Rouse Model with 32 beads

The mean first encounter time between two ends of polymer is the mean time it takes for these 2 monomers to come to a proximity of ϵ at the first time,at which they interact to create a chemical bond between them. This time is key in the regulation of many reactions in the cell.As this case has already been simulated by Amitai A1, Kupka I, Holcman D [5],we want to simulate the mean first-encounter time(MFET) among 3 beads to study the probability distribution function of first encounter time(FET).

To calculate the FET of 3 beads,we set a rouse chain with 32 beads,we record the first time that two ends of a polymer(1 and 32)and bead 2 to 31 are located a distance of ϵ(encounter distance) from their center of mass(Figure 3.1).A priori , we can just simulate from 2 to 16 as it's symmetric,that means we have $[1, 2, 32], [1, 3, 32]...[1, 16, 32]$ cases.For each case,we calculate the first-encounter time(FET) then plot it by histogram.The MFET then is calculated by the average of FETs.

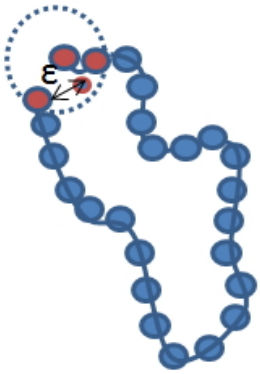


Figure 3.1: The encounter among 3 beads located at a distance ϵ from their center of mass

3.1.1 Simulation Results

From Figure 3.2 it's trivial to observe that the MFET for 3 beads are longer than the case of 2 beads. As the simulations of two ends of a polymer[5] show that the distribution of FETs of ends beads can be well approximated by a single exponential ,we would like also to study the FETs of 3 beads from [1 2 32] to [1 16 32]:

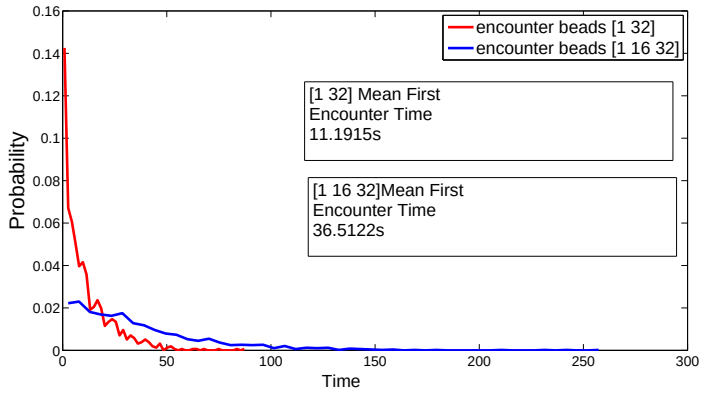


Figure 3.2: The first encounter time of [1,16,32] and [1,32] with d(dimension)=3,dt=0.01,b=1,D=10,ϵ=3b/5

According to Figure 3.3 and 3.4 , we fit the histograms of FETs by exponential distribution which is well captured.We can conclude that the distribution of FETs follows exponential distribution.Figure 3.5 describes the evolution of MFET.We observe that beads [1 16 32] took more time to encounter because

a priori, as a liner chain ,the length initial between two ends of beads and the center bead in the polymer are greater than other length.

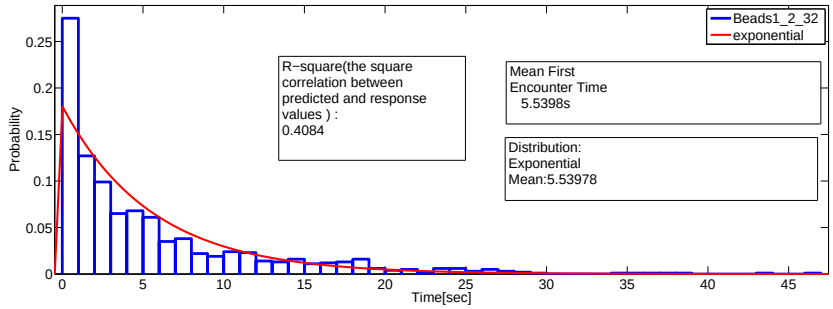


Figure 3.3: distribution of FETs of [1,2,32] fitted by exponential,d = 3,dt=0.01,b=1,D=10,ϵ=3b/5

.....

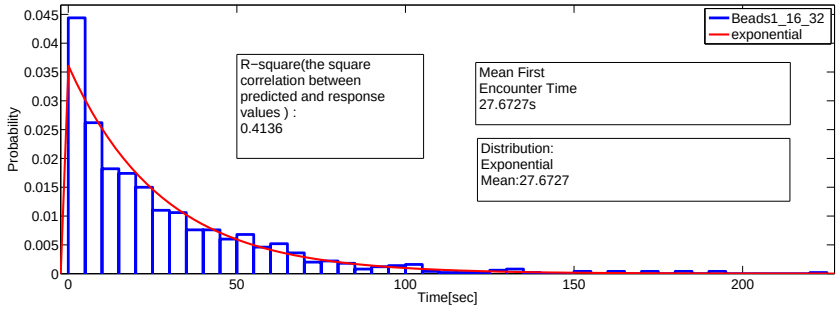


Figure 3.4: distribution of FETs of [1,16,32] fitted by exponential,d = 3,dt=0.01,b=1,D=10,ϵ=3b/5

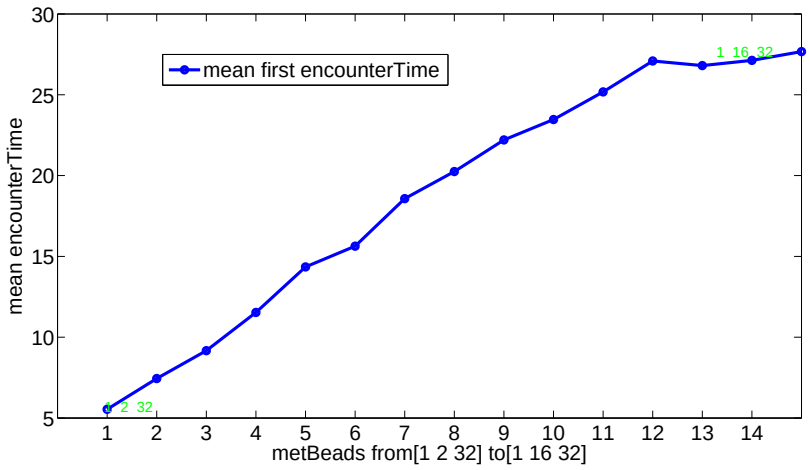


Figure 3.5: Evolution of MFET from [1,2,32] to [1,16,32]

To verify that it's symmetric,we calculate the MFET for all the beads with 10000 simulations for each pair then fit the graph by quadratic distribution.

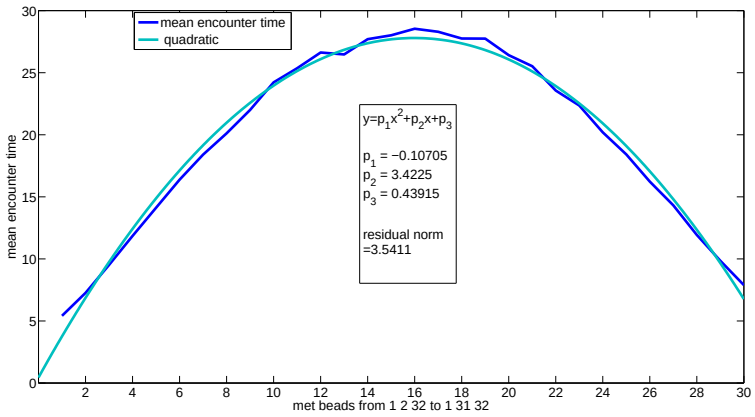


Figure 3.6: Evolution of MFET from [1,2,32] to [1,31,32] fitted by quadratic

3.2 MFET in Rouse Model with 64 beads

In order to see the result hold in general,we increase the number of beads to 64 and keep ϵ the same value to simulate the distribution of FETs and compute MFET.

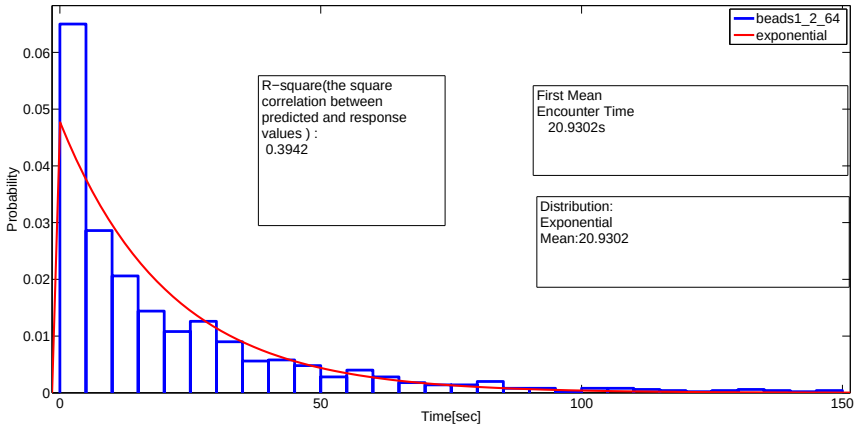


Figure 3.7: distribution of FETs of [1,2,64] fitted by exponential,d = 3,dt=0.01,b=1,D=10,ϵ=3b/5

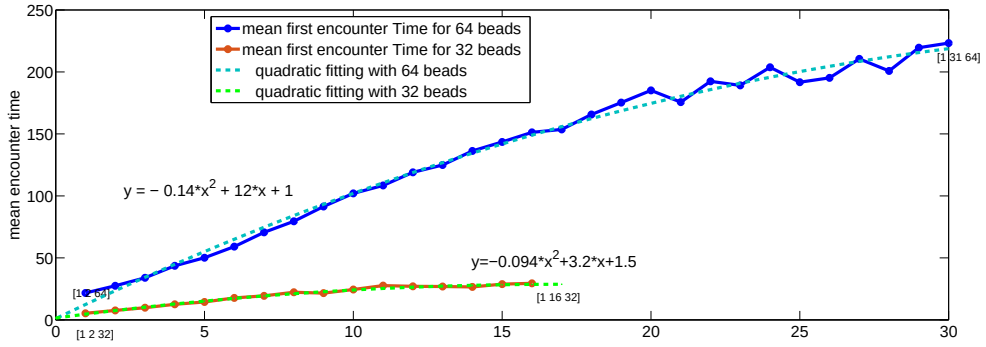


Figure 3.8: Evolution of MFET with N=32,64 and fitted by quadratic

By studying the MFET of 3 beads ,we can conclude that the FETs of 3 beads follows exponential distribution and the evolution of MFET follows quadratic distribution.For small N we find a great agreement with quadratic fit ,we need to explore this further .

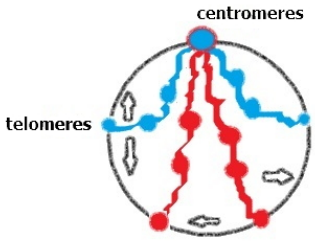
Chapter 4

Yeast chromosome motion simulation

4.1 Introduction

A chromosome is a long, stringy aggregate of genes that carries heredity information (DNA) and is formed from condensed chromatin. A non-duplicated chromosome is single-stranded and is comprised of a **centromere** region that connects two arm regions. The end region of a chromosome is called a **telomere**,which is a region of repetitive nucleotide sequences.[1] The centromeres (middle point) are anchored to the nucleus membrane, and the telomeres (end points) are either diffusion on the membrane or are detached and diffuse inside the nucleus.In yeast,the telomeres can associate in several clusters, leading to the unequal distribution of telomeres and telomere associated factors (Taddei et al., 2010). Understanding the principles of telomeres organization in yeast is a key step to elucidating the general mechanisms governing chromosome trans-interactions in eukaryotes.[6]

[1] http://biology.about.com/od/geneticsglossary/g/chromosome.htm



The motion of yeast chromosome in the nucleus can be characterized as a Brownian motion,which can be approached by rouse model.To simulate the yeast motion in the nucleus,the procedure will be broken down with mainly 5 steps :

1.Define domain(nucleus).

2.Define rouse chains(yeast chromosomes).

3.Imported middle points(centromeres) on surface;

4.Create Brownian bridge between middle point and ends points(for initialization);

5.Clustering telomeres in order to simulate the number of clusters in domain.

4.2 Brownian bridge

4.2.1 Introduction

At the initialization of the rouse chains,as the ends of beads can either move in domain or diffuse on the boundary,to create the path from middle points(centromeres) to ends points(telomeres) for the second case,one idea is to create a Brownian bridge .The Brownian bridge is a Brownian motion which is starting at x at time t_0 and passing through point y at T, $T \geq t$,it is defined as :

$$B(t) = w(t - t_0) - \frac{t - t_0}{T - t_0}[w(T - t_0) - y + x] + x \tag{4.1}$$

which $w(T)$ is a random walk process.

4.2.2 Implementation

Algorithm of Brownian bridge :

1.Initialization of beads on the domain's boundary;

2.List all constrain beads in ascending order $c = a_1, a_2, ...a_{N_c}$

3.Choose a random position for B_{a_1};

4.For $i = 2...N_c$,choose a position for B_{a_i} by diffusion on the boundary $a_i - a_{i-1}$ steps;

5.For all of points in c,if $a_i - a_{i-1} > 1$,construct a Brownian bridge between each 2 points by using the formula above;

6.If $a_1 \geq 1$ or $a_{N_c} \leq BeadsEnd$,sequentially build a path form the 1 to a_1 and a_{N_c} to $BeadsEnd$.

Diffusion On Sphere

To diffuse a path on the sphere, we do with the following steps :

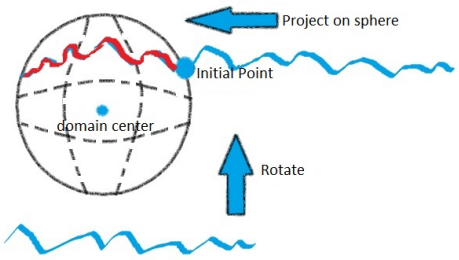
1.generate a path in 2D;

2.Set a initial point which is on the sphere ,find the polar angle θ and azimuthal angle ϕ

in the spherical coordinates;

3.By using the rotation matrix ,Rotate the path to the initial Point;

4.Project the path back on sphere;



To generate a path 2D, consider the Brownian motion of a free particle($U = 0$) for which the Langevin equation reads :

$$\frac{dX}{dt} = g(t) \tag{4.2}$$

Integrating from t to time $t+\Delta t$,and then discretizing with respect to time gives us:

$$X(t + \Delta t) = X(t) + \Delta G(t) \tag{4.3}$$

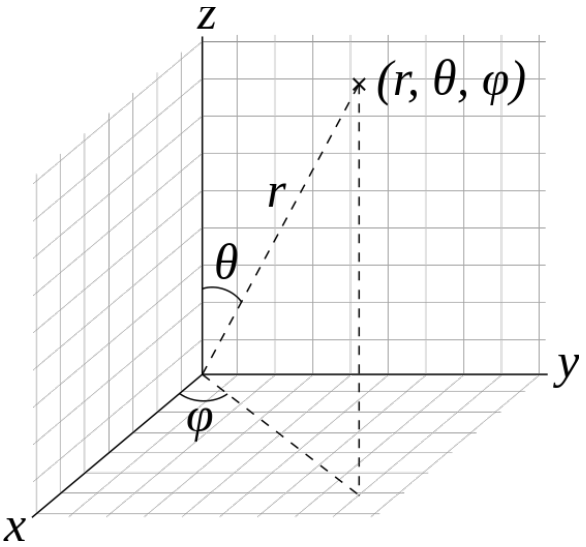
Here $\Delta G(t)$ is the PDF formed by integrating $g(t)$ from t to $t + \Delta t$.The mean and variance are calculated as follows :

$$< \Delta G(t) >= 0$$
$$< \Delta G(t)^2 >= 2D\Delta t$$

In order to carry out a simulation ,all we need is to generate a Gaussian distribution random function with mean and variance describing as above ,and use (8) to calculate the time evolution of $X(t)$.

We denote by $R_0 = (x, y, z)$ a initial point on sphere ,calculate the angles θ and ϕ :

$$\phi = \arctan \frac{y}{x}, \phi \in [0, 2\pi]$$
$$\theta = \arctan \frac{\sqrt{x^2 + y^2}}{z}, \theta \in [0, \pi]$$



Define the rotate matrix A:

$$A = Az * Ay; \tag{4.4}$$

$$Ay = \begin{pmatrix} cos(\theta) & 0 & -sin(\theta) \\ 0 & 1 & 0 \\ -sin(\theta) & 0 & cos(\theta) \end{pmatrix}, Az = \begin{pmatrix} cos(\phi) & -sin(\phi) & 0 \\ sin(\phi) & cos(\phi) & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

We move r units over the z-axis with 2D path X,then rotate the path such that the initial point becomes the first point on the path :

$$R_{rotate} = A * (r + X)$$

where r is the radius of sphere;

In order to project back on sphere ,calculate the distance between each point $P(i) = (P_x(i), P_y(i), P_z(i)), \forall i \in [1, N]$ on the path and the domain center $P_c = (P_{cx}, P_{cy}, P_{cz})$:

$$L(i) = \sqrt{(P_x(i) - P_{cx})^2 + (P_y(i) - P_{cy})^2 + (P_z(i) - P_{cz})^2}$$

Calculate the slope to find the intersection points $pI(i)$(points on sphere):

$$k(i) = L(i)/r;$$

$$\begin{cases} pI_x(i) = p_{cx} + (P_x(i) - p_{cx})k(i) \\ pI_y(i) = p_{cy} + (P_y(i) - p_{cy})k(i) \\ pI_z(i) = p_{cz} + (P_z(i) - p_{cz})k(i) \end{cases} \tag{4.5}$$

4.2.3 Simulation Graphs

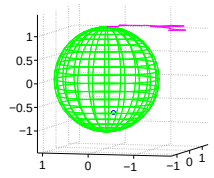


Figure 4.1: move r units over z-axis

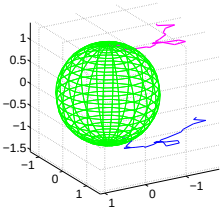


Figure 4.2: rotate to initial point

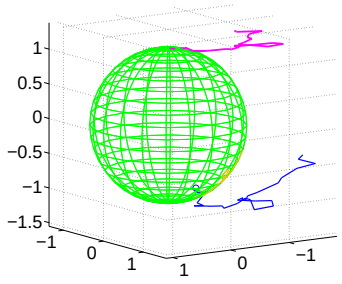


Figure 4.3: project back on sphere(yellow path)

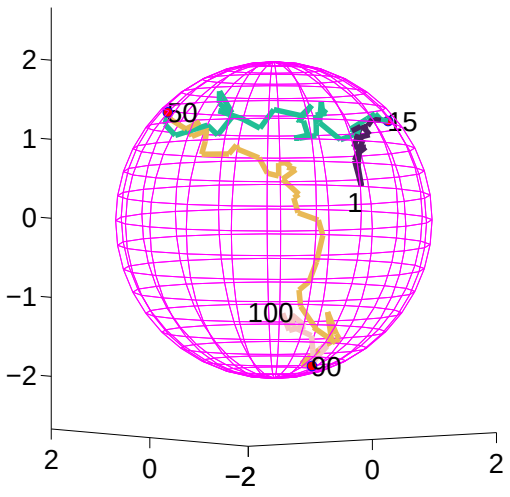


Figure 4.4: a example of a Brownian bridge in sphere,index of beads on the boundary=[15,50,90],$N = 100$,$d = 3$,$D = 1$,$dt = 0.01$

4.3 Telomeres clustering

4.3.1 Introduction

We are interested to study this phenomena by assuming that two telomeres at a distance $\leq \epsilon$ are considered to belong to the same cluster(see chapter 6.2 connect telomeres).We assume that the probability to form a cluster = 1,which follows a diffuse-associate model,and the stop condition(to pass to next simulation) is when telomeres are clustering in condition that the polymers are merging into one big polymer.

4.3.2 Dynamic simulations

We set 8 chains(16 telomeres) in sphere,which assume that all chromosomes are of same length, to simulate the telomeres clustering in addition to the following properties:

$$meanNumClustersSize = \frac{\sum_{j=1}^{L_i} c(j)/Nc(j)}{L_i}, \forall i = [1, N]$$

$$meanTotalTime = \frac{\sum_{i=1} T_i(end)}{N}, \forall i = [1, N]$$

$$meanTimeBetweenEvents = \frac{\sum_{j=0}^{L_i} T_i(j+1) - T_i(j)}{L_i}, \forall i = [1, N]$$

L_i :number of events(when number of clusters change) for each simulation
N :number of simulations
c :number of telomeres of each event
Nc :number of clusters of each event
T : the time related to each event

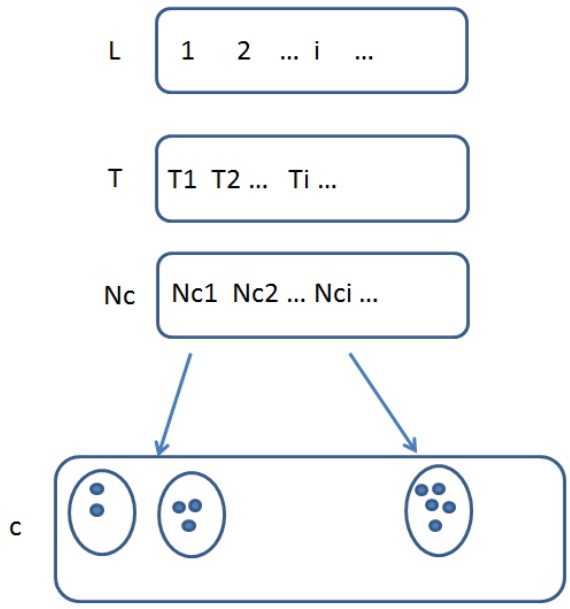


Figure 4.5: the architecture and component of each property.When a event happens(associate/dissociate a cluster),we count the number of events L, record the number of clusters Nc and the number of telomeres c in Nc,the time occurred T.

Simulation Results

Figure 4.6 represents the histograms of 3 properties when the telomeres are moving on the boundary while Figure 4.7 represents the case that the telomeres are moving in domain.We can suggest that the motion type of telomeres(in domain or on the boundary) do have some influence with $meanClusterSize$,$meanTotalTime$ and $meanEventTime$. Indeed,for the properties $meanTotalTime$ and $meanEventTime$ which also depends on the surface that polymer travels.As we set r(radius) $= 25$,the surface for the telomeres diffusing on the boundary $=4\pi r^2 = 7854$,while for the telomeres move inside the domain,the surface $= 4/3\pi r^3 = 65450$.

Telomeres are moving randomly on the boundary

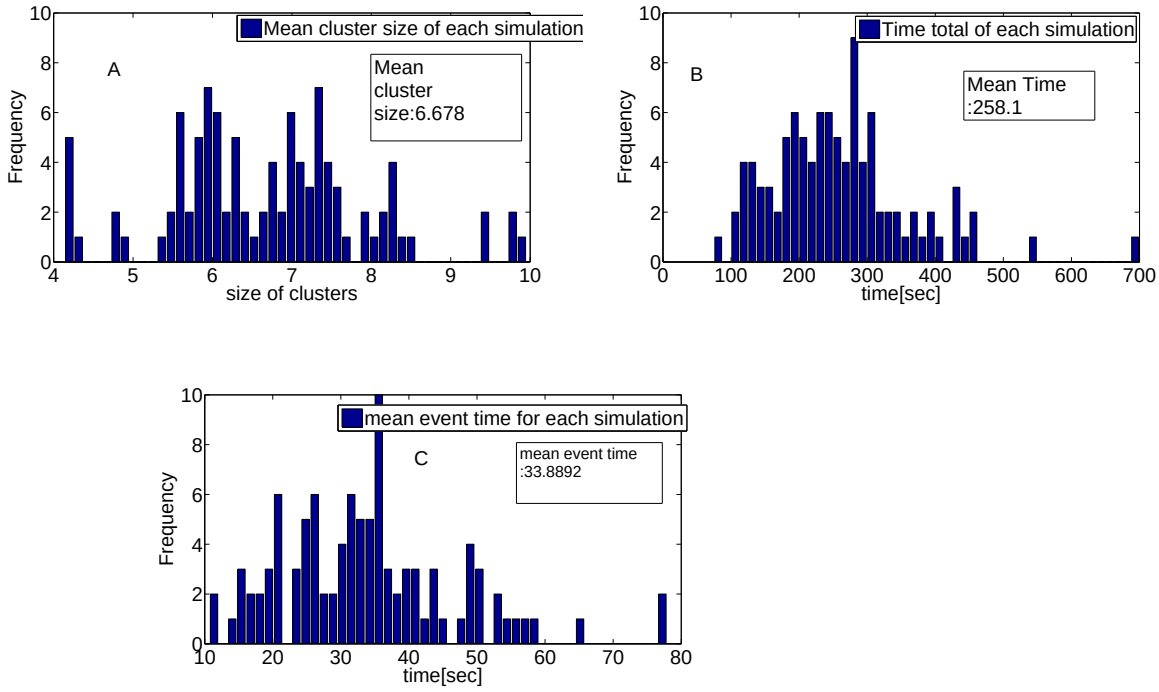
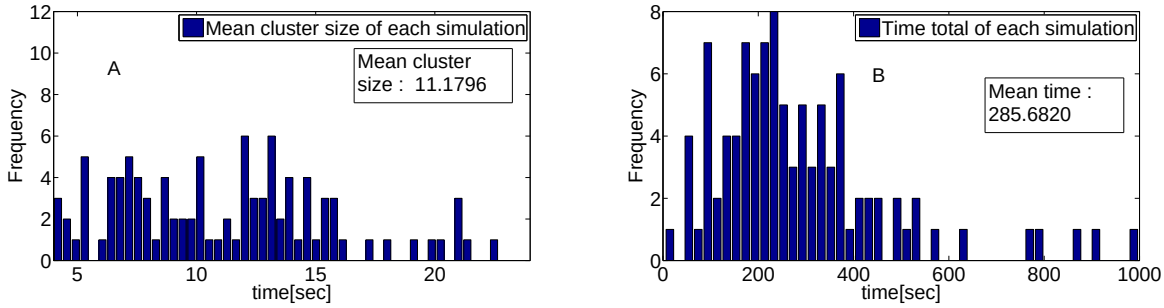


Figure 4.6: A:Mean cluster size ,B:Mean Total time ,C:mean event time,$D = 0.1$,$dt = 0.1$,number of telomeres=16,$\epsilon = b/5$,$b = \sqrt{3}$,$k = 1$,beads on boundary index:[1,64]

The telomeres are moving randomly in domain



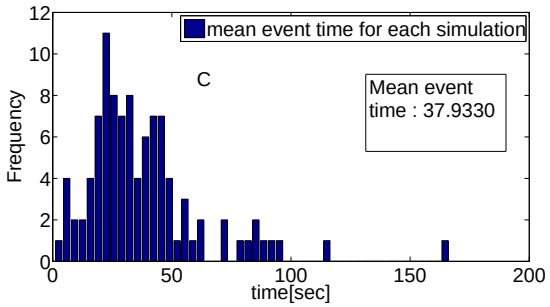


Figure 4.7: A:Mean cluster size ,B:Mean Total time ,C:mean event time,$D = 0.1$,$dt = 0.1$,number of telomeres=16,$\epsilon = b/5$,$b = \sqrt{3}$,$k = 1$

Chapter 5

Mean Square Displacement of monomers in Rouse Chains

5.1 Introduction

The examination of the various mean-square displacements gives insight in the dynamic behavior of polymer systems.When the MSD grows as a power law in time such that $< (R(t) - R(0))^2 > \propto D_\alpha t^\alpha$ with an exponent $\alpha \neq 1$, the underlying stochastic motion differs from normal diffusion,where D_α is anomalous diffusion constant .The origin of this behavior is not clear although a direct computation[7] of Rouse model shows that the exponent $\alpha = \frac{1}{2}$ .However,in order to compensate for the bias caused by cell rotation and motion,we would like to study the MSD of rouse chain with different motions of centromeres and fit the graphs to approach α.

5.2 Implementation

We distinguish 4 contexts of a rouse chain with 64 beads:

- Place first bead on the boundary and fixed ;
- Place first bead to move on the boundary;
- Place first bead to do oscillation motion on the boundary;
  (oscillatory in 2D : $x(t) = A_x cos(wt), y(t) = A_y cos(wt - \frac{\pi}{2})$)

- Unconstrained polymer freely diffuse;

The MSD is calculated as follows:

$$msd(t) =< (X_i(t) - X_i(0))^2 > \tag{5.1}$$

In this equation, $X_i(t) - X_i(0)$ is the (vector) distance traveled by particle i over some time interval of length t, and the squared magnitude of this vector is averaged (as indicated by the angle brackets) over many such time intervals.[1]

5.3 Simulations Results

Figure 5.1-5.4 represent the MSD of 64 beads for each case.We can see that for the case that first bead do oscillatory motion on the boundary,the mean square of all the other beads are greater than other 3 cases.

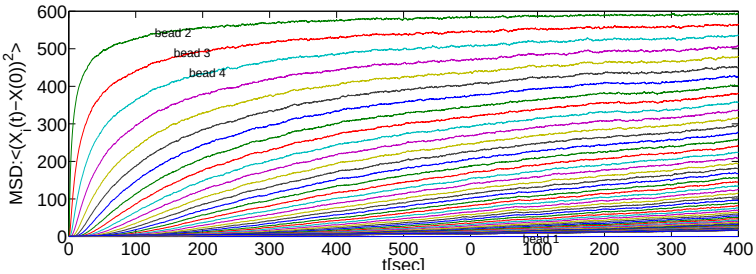


Figure 5.1: MSD of 64 beads with first bead fixed on the boundary,$N = 64$,$D = 0.1$,$k = 1$,$b = \sqrt{3}$,index of fixed beads=[1],$dt = 0.1$

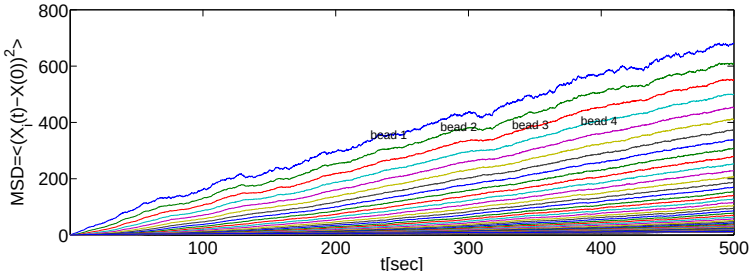


Figure 5.2: MSD of 64 beads with first bead move randomly on the boundary,$N = 64$,$D = 0.1$,$k = 1$,$b = \sqrt{3}$,index of beads on the boundary)=[1],$dt = 0.1$

[1] http://www.etomica.org/app/modules/sites/Ljmd/Background2.html

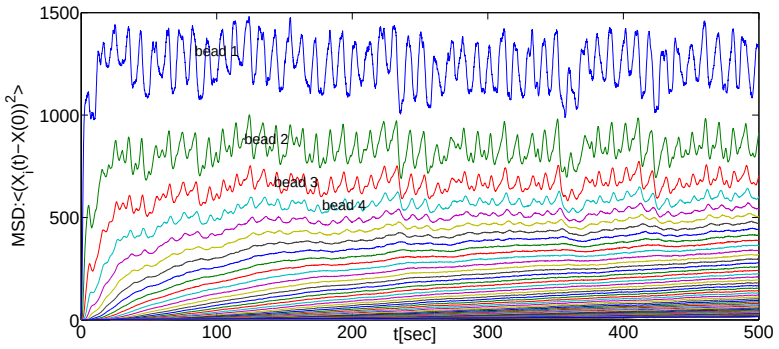


Figure 5.3: MSD of 64 beads with first bead do oscillatory motion on the boundary,$N = 64$,$D = 0.1$,$k = 1$,$b = \sqrt{3}$,index of beads on the boundary)=[1],$dt = 0.1$,$w = 1$,magnitude=1/2

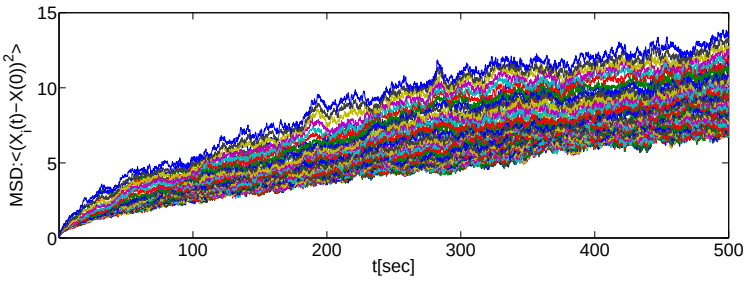


Figure 5.4: MSD of 64 beads freely diffuse in domain,$N = 64$,$D = 0.1$,$k = 1$,$b = \sqrt{3}$,$dt = 0.1$

To analysis and compare the MSD of beads according to different context,we pick up several beads to observe their MSD.
Through the Figure 5.5,we can suggest that the influence of motion of the first bead decays with the distance along the chain.To verify ,we'll then study the anomalous diffusion by fitting the graphs by power law to approach α.

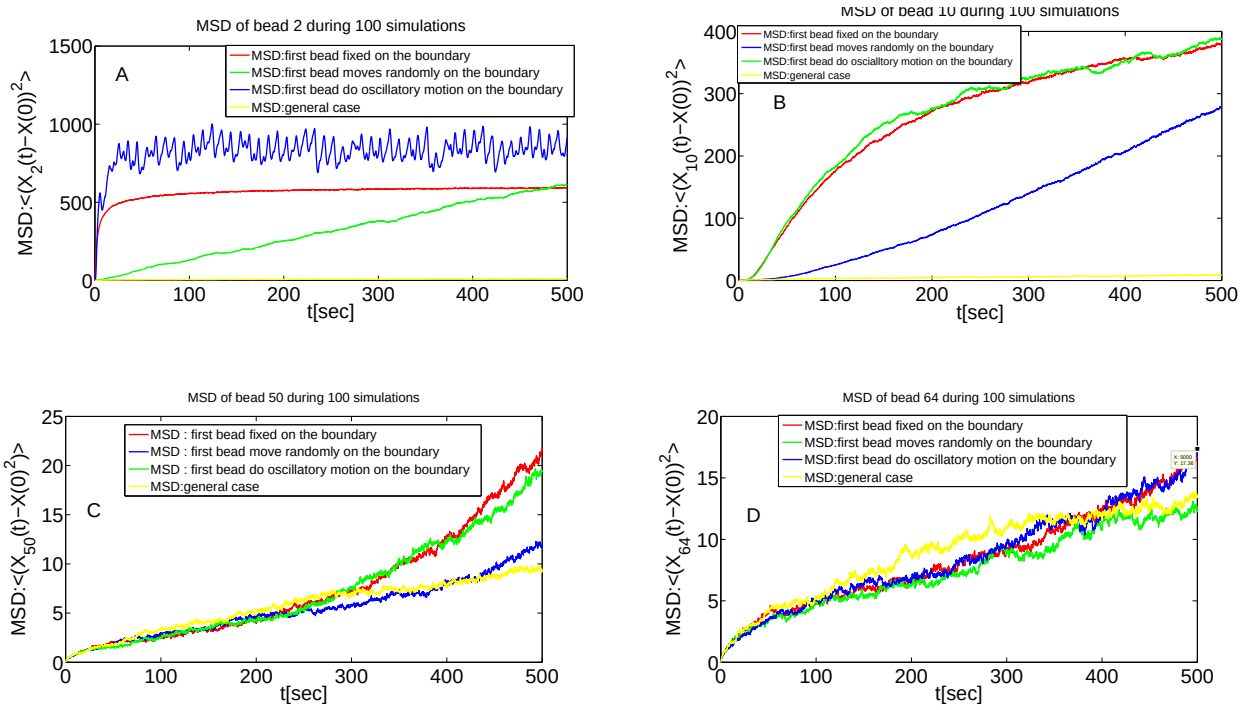


Figure 5.5: MSD of beads 2(A),10(B),50(C),64(D) with different contexts

5.4 Anomalous diffusion simulation

Using the analytical results[7] that during intermediate time $\tau_{N-1} \leq t \leq \tau_1$,the dynamics is described as anomalous diffusion,where τ describes a relaxation time:

$$\tau_p = \frac{1}{Dkp}$$

Figure 5.6-5.9 represent fitting the MSD by power law.As analytical result ensure that the anomalous exponent of rouse model equals $\frac{1}{2}$,which is being approached when all the beads unconstrained freely diffuse in sphere.For other contexts ,the first bead dynamic do affect the anomalous exponent and the influence decays along the distance of the chain.Figure 5.10 represents the evolution of α according to 4 contexts.We can assume that even change the behavior of one bead can lead to a very different interpretation of the dynamics of other beads.

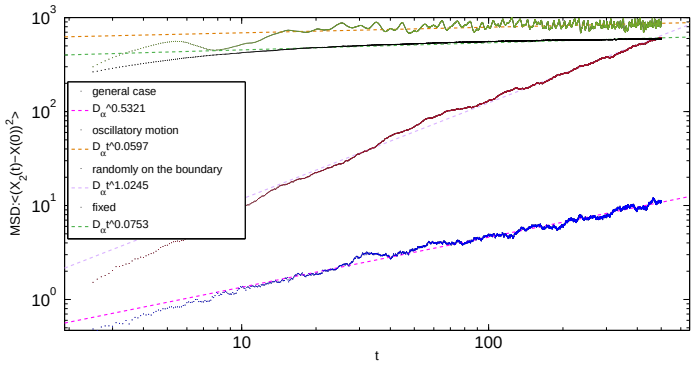


Figure 5.6: fitting with bead 2

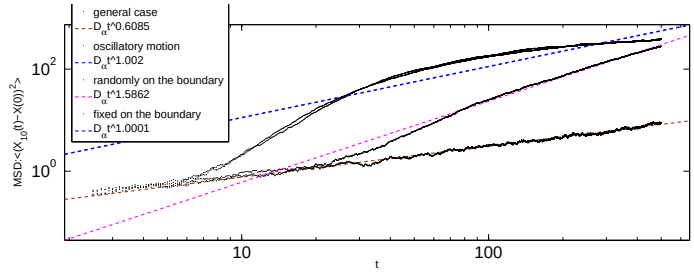


Figure 5.7: fitting with bead 10

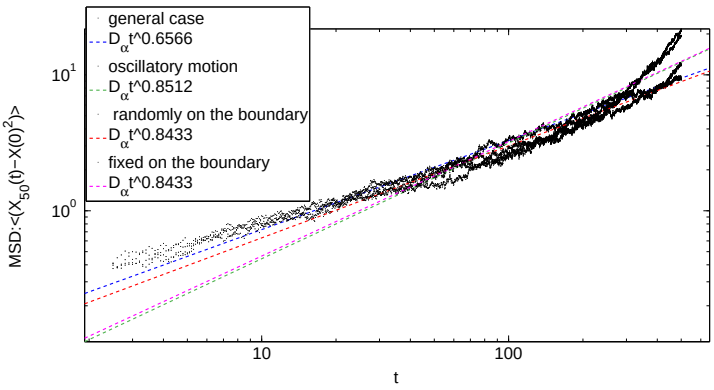


Figure 5.8: fitting with bead 50

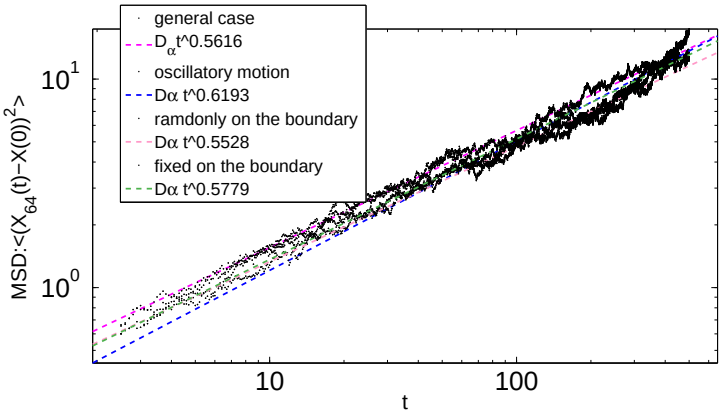


Figure 5.9: fitting with bead 64

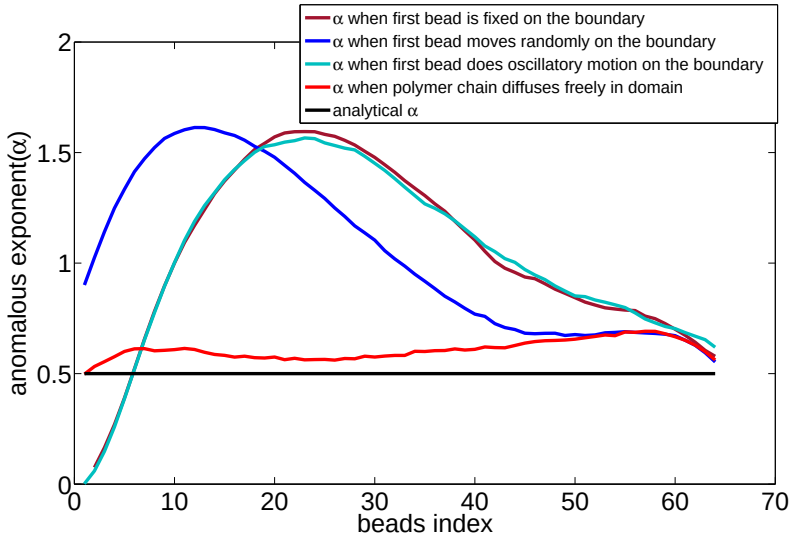


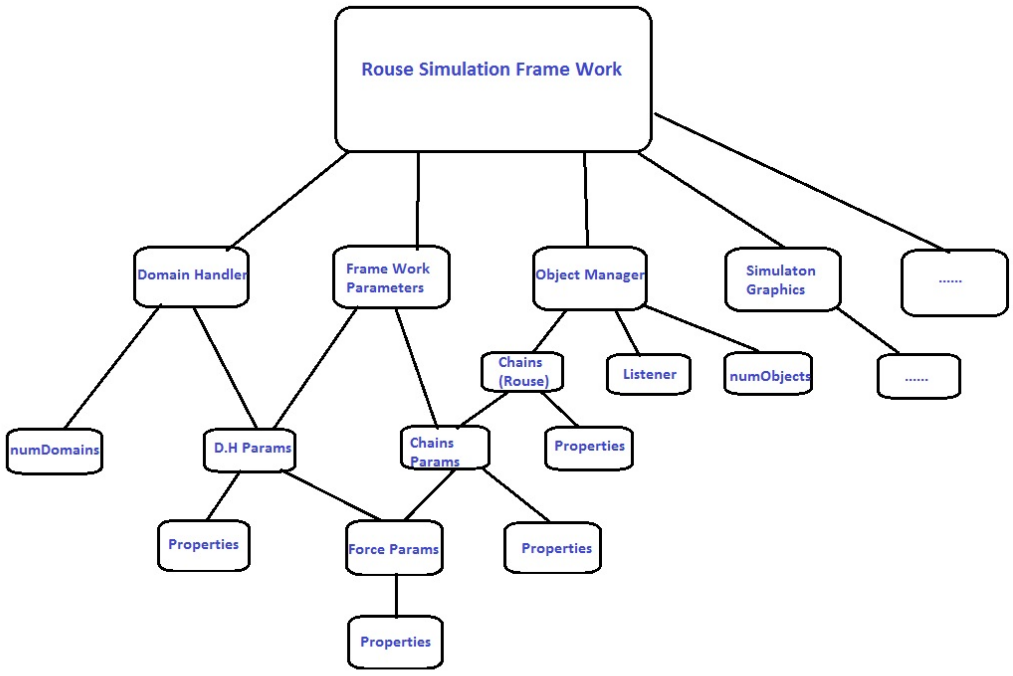
Figure 5.10: evolution of α

Chapter 6

Additions to framework

6.1 Structure of framework

The structure of framework(temporally) can be described as several classes in Matlab.



Using this Rouse Framework we are able to construct a model of rouse chains to simulate and analysis the chain dynamics.

6.2 Connect telomeres

This function is used to simulate the telomeres clustering,which predefine the index of telomeres. The algorithm is following:

Result: Connected or disconnceted of telomeres
for *each step* **do**
  for *each sticky bead(telomeres)* **do**
    Calculate distance D between each sticky bead;
    if $D \leq EncounterDistance$ **then**
      Set a random value p between 0 and 1;
      if $p \leq ConnectedProbability$ **then**
        Connect the telomeres;
      end
    end
  end
  for *conected beads(not include the connected beads in the same step)* **do**
    Set a random value p between 0 and 1;
    if $p \leq DisconnectedProbability$ **then**
      Disconnect the beads
    end
  end
end

6.2.1 Simulation graphs

Figure 6.1 represents at the initialization, there are 4 chains(with different colors).The Figure 6.2 and 6.3 show how they merge during the procedure(once they merge,the chain become the same color).The Figure 6.4 indicate that the chains are disconnected.

Telomeres clustering simulations $D = 0.1, k = 1, b = \sqrt{3}$,index of beads on boundary [1,64],$dt = 0.1$,probability to attach to sticky beads =0.5,$\epsilon = b/5$

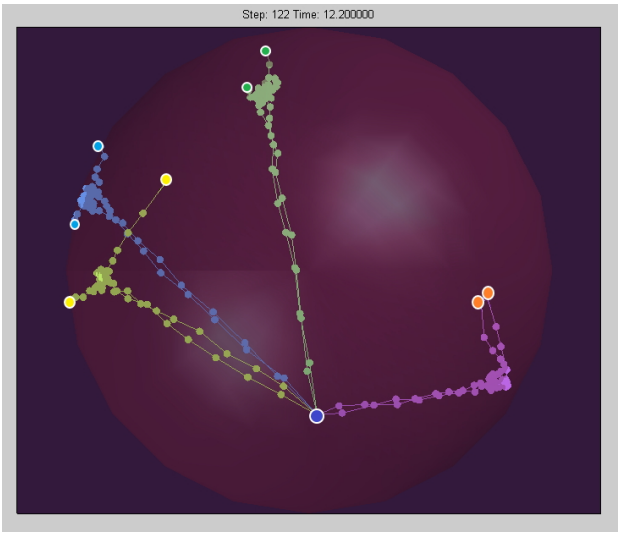


Figure 6.1: 4 chains

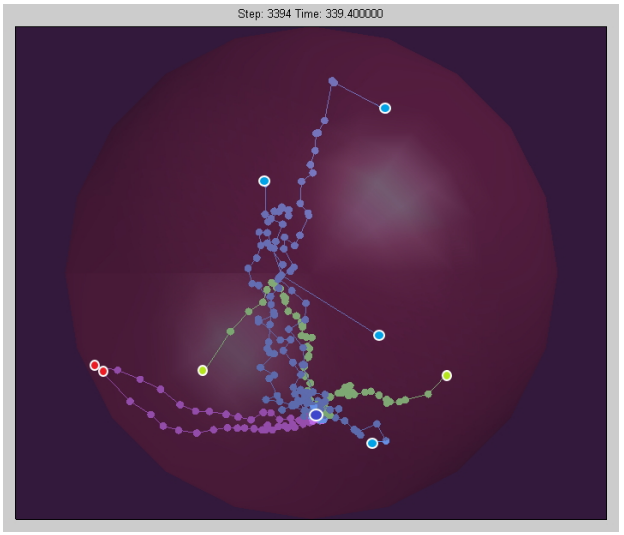


Figure 6.2: Merging :3 chains

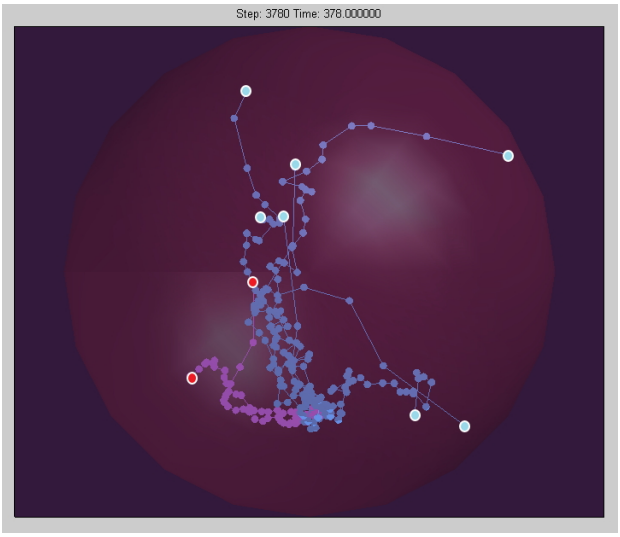


Figure 6.3: Merging :2 chains

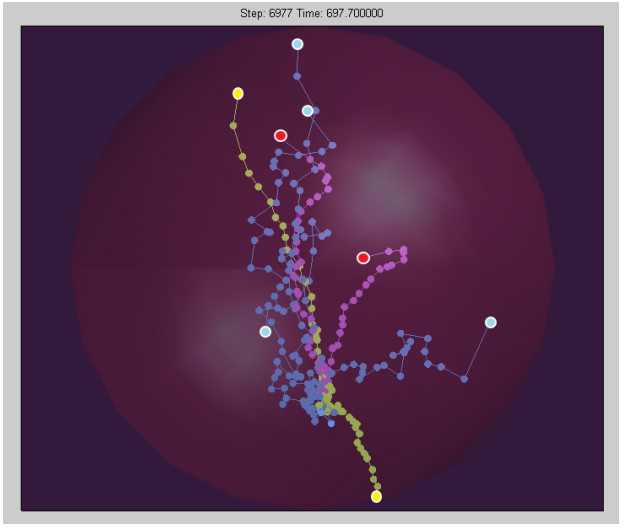


Figure 6.4: Disconnected:3 chains

6.3 Centromeres dynamic

The middle bead(centromeres) in the nucleus can be either fixed or moving on surface .The following figures represent the motion of 2 cases while telomeres are moving on the boundary.

Centromeres dynamics simulations $N = 64$,$D = 0.1, k = 1, b = \sqrt{3}$,index of beads on boundary [1,64],$dt = 0.1$,number of chains = 2,index of fixed bead =32

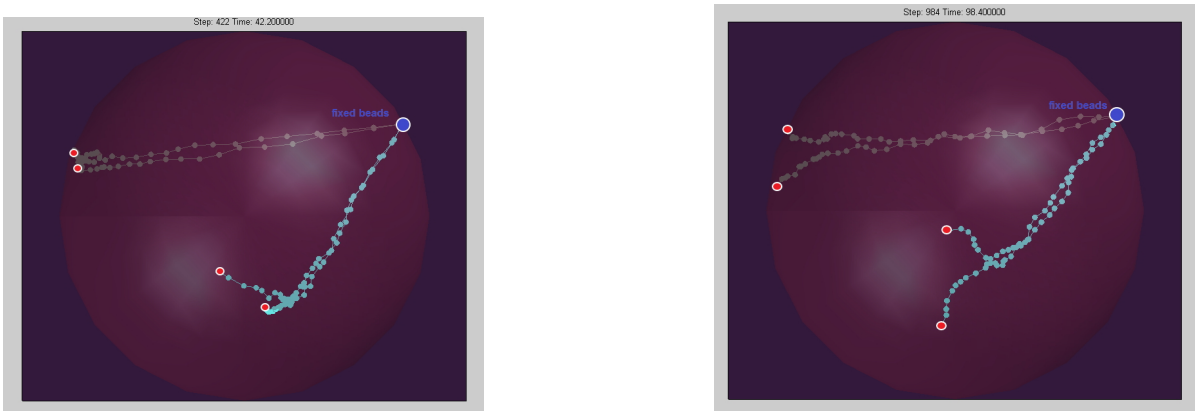


Figure 6.5: centromere is fixed during the simulation

Centromeres dynamics simulations $N = 64$,$D = 0.1, k = 1, b = \sqrt{3}$,index of beads on boundary [1,32,64],$dt = 0.1$,number of chains = 2

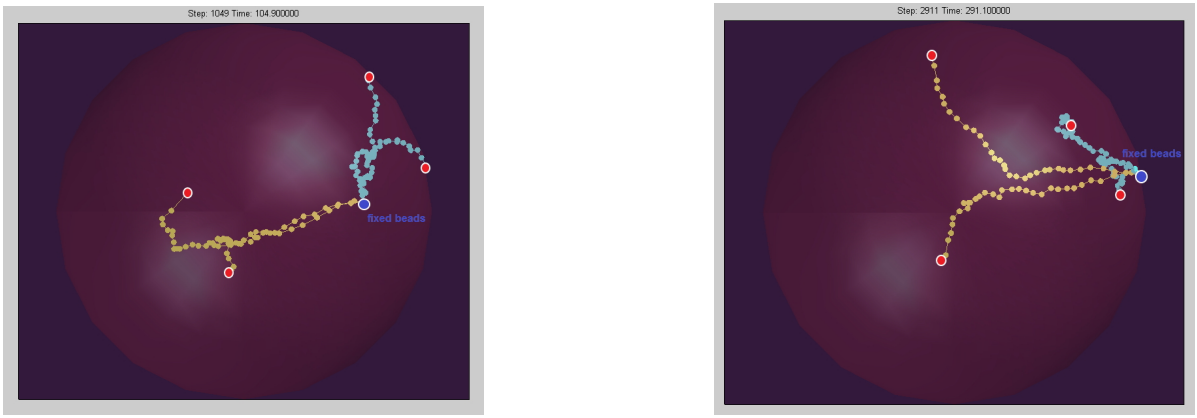


Figure 6.6: centromere moves randomly on domain

6.4 Attachment and Detachment from boundary

Attachment on boundary

In order to allow the beads in domain to attach on boundary , we calculate the distances between each bead and domain center L.Then $D = r - L$.If D $\leq \epsilon$ and satisfy a given attach probability , we allow them to move on the boundary. The algorithm is as follows :

Result: Attach the beads on the boundary
for *each step* **do**
  for *each chain and each bead* **do**
    if *AllowAttachOnBoundary* **then**
      Calculate $L = \parallel (x, y, z) - domainCenter \parallel$;
      Calculate $D = Radius - L$;
      if $D \leq EncounterDistance$ **then**
        Set a random value p between 0 and 1;
        if $p \leq AttanProbability$ **then**
          Update the list of $BeadsOnBoundary$;
          Update the current and previous position such that it's on the boundary;
        end
      end
    end
  end
end

Simulation of attachment on the boundary

Attachment on the boundary simulation,$N = 64$,$D = 0.1$, $k = 1$, $b = \sqrt{3}$,beads on boundary index [1,64],$dt = 0.1$,number of chains = 2,probability to attach= 0.007

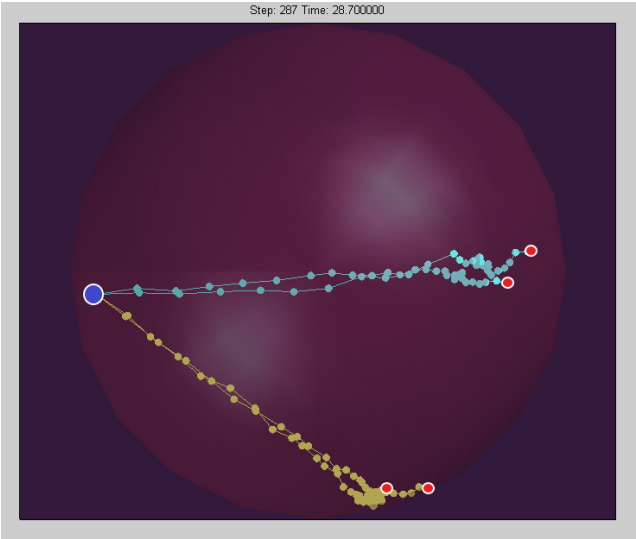


Figure 6.7: Time=28.7s

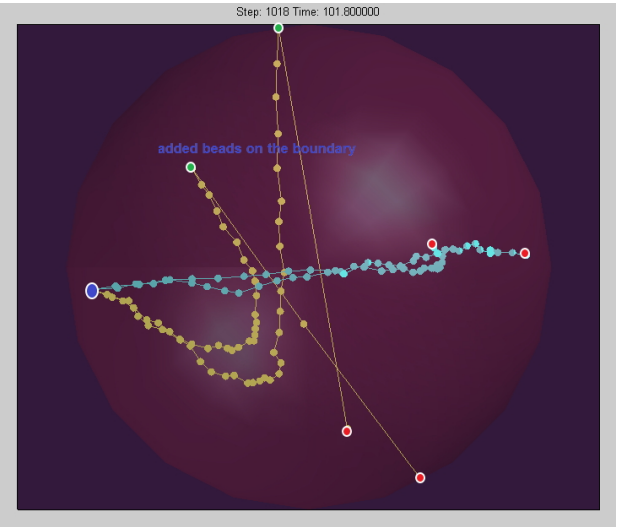


Figure 6.8: Time=101.8s

Detachment from boundary

This function is used to detach the last index of beads from boundary ,once the beads are detached , il move randomly in domain . The detachment is done with following steps :

- Calculate the vector between the domain center and the bead chosen to detach ;
- Set the number of steps when the chosen bead should be detached ;
- Reset the position by multiply the vector with a random number between [0,1];

Simulation of detachment from the boundary

Attachment on the boundary simulation,$N = 64$,$D = 0.1, k = 1, b = \sqrt{3}$,beads on boundary index [1,64],$dt = 0.1$,number of chains = 2,number of steps to detach=2000

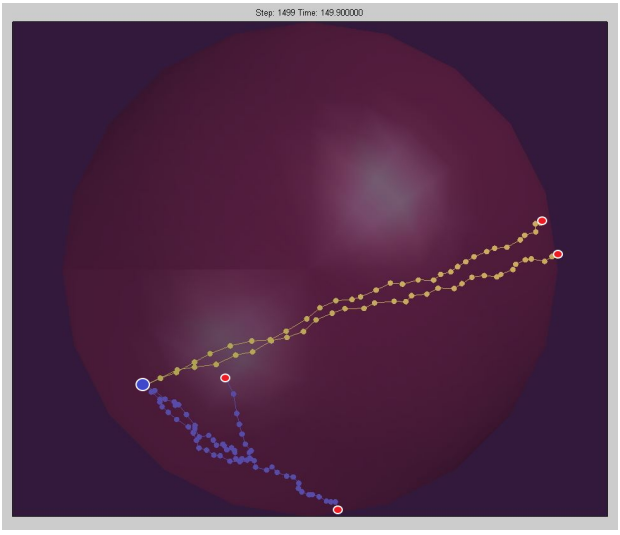


Figure 6.9: Attachment(Time=149.9s)

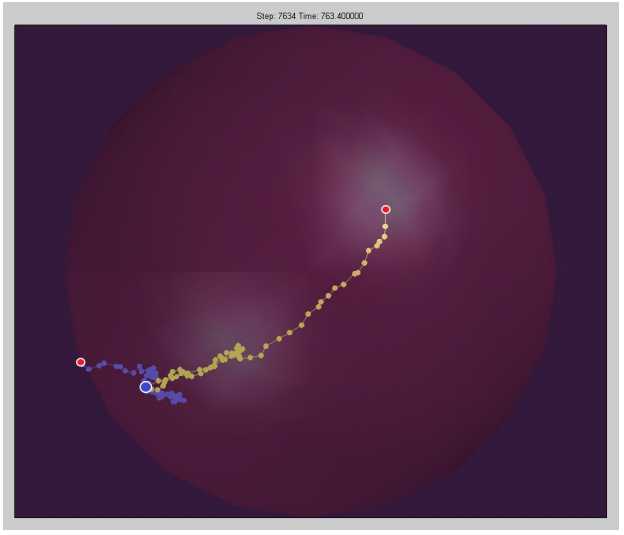


Figure 6.10: Detachment(Time=763.4s)

6.5 Multi Domain Simulation

In order to general the framework , we allow that the polymer can be generated in different domains doing different motions in the same time,with this propose we create the multi domain .

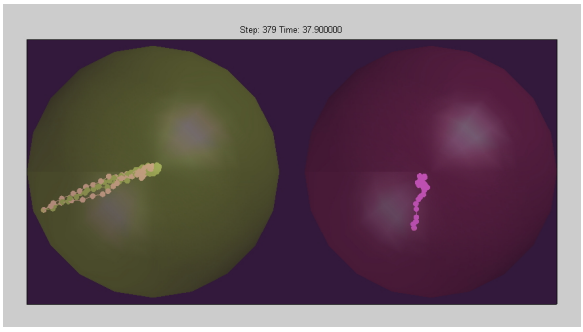


Figure 6.11: simulation with multi domain,domain 1 has 2 rouse chains of 64 beads each,domain 2 has 1 rouse chain of 32 beads

Conclusion

Through this internship,I learned at first the variety of polymer chains models,among which the properties of rouse model .Then pass static to dynamics to represent the motion of rouse chains by Langevin equation,which can be considered as a stochastic equation to approach Brownian motion.Later on start to simulate the polymer(chromosome) dynamic to compute MFET of 3 beads in open domain because this time has several implications in DNA looping and in cellular biology.After that ,build the functions and simulate the telomeres clustering in sphere to study and compare distribution of the size of clusters and the time while telomeres are moving on boundary or diffuse in domain. At last ,compute the MSD of beads in a polymer chain to track the anomalous diffusion.In the mean time,I learn to how to use Object-oriented programming in Matlab to manage a large data structure.

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