Polymer Simulations
Report

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1 The random walk model:Gaussian Chain

Consider a linear polymer to be a freely-jointed chain with N beads, length of each bond is b , that occupy zero volume. The path of the chains is like a 'random walk 'in three dimensions, limited only by the constraint that each segment must be joined to its neighbors.

Consider the 'end to end' vector $\boldsymbol{R}$ joining one end of the polymer to the other,the average value $< \boldsymbol{R} >$ is zero,since the probability of R equals -R.Therefore we will calculate $< \boldsymbol{R^2} >$

$$< \boldsymbol{R^2} >= \sum_{n=1}^{N} \sum_{m=1}^{N} < r_n \cdot r_m > \tag{1}$$

We consider that there is no correlation between bead n and m,therefore we find :

$$< \boldsymbol{R^2} >= \sum_{n=1}^{N} < r_n^2 >= Nb^2 \tag{2}$$

The probability distribution of $\boldsymbol{R}$ is:

$$P(\boldsymbol{R}, N) = (\frac{3}{2\pi Nb^2})^{3/2} exp(-\frac{3\boldsymbol{R}^2}{2Nb^2}) \tag{3}$$

The probability distribution is Gaussian,so we also call it Gaussian Chain.

1.1 Random walk Simulation

```
%This program is used to simulate the brownian motion
classdef FirstTry<handle

properties
dimension%dimension=1,2 or 3
numParticles%number of particles in polymers;
dt%pas de temps
numSteps% number of motion
diffusionConst %constante diffusion
paths %the paths of polymer;
end

methods

%class constructor
function obj=FirstTry(dimension,numParticles,dt,diffusionConst,numSteps)
obj.dimension=dimension;
obj.numParticles=numParticles;
obj.dt=dt;
obj.numSteps=numSteps;
obj.diffusionConst=diffusionConst;
obj.paths = zeros(obj.numParticles,3,obj.numSteps);
```

```
end


function Calculate(obj)

for j=1
noise = [zeros(1,obj.dimension);...
sqrt(2*obj.diffusionConst*obj.dt)*randn(obj.numParticles-1,obj.dimension)];
obj.paths(:,1:obj.dimension,j)=cumsum(noise);

end

for j=2:obj.numSteps
noise = [sqrt(2*obj.diffusionConst*obj.dt)*randn(obj.numParticles,obj.dimension)];
obj.paths(:,1:obj.dimension,j)=obj.paths(:,1:obj.dimension,j-1)+noise;

end


end %'random walk 'simulation

function Plot(obj)
f=figure;
b =[-20 20];
a= axes('Parent',f,'NextPlot','replaceChildren','XLim',b,'YLim',b,'ZLim',b);
c=rand(1,3);

x = obj.paths(:,1,1);
y = obj.paths(:,2,1);
z = obj.paths(:,3,1);
%        end
l=line('XData',x,'YData',y,'ZData',z,'Color',c,'linestyle','-.','Marker','o','markersize',10,'Parent
for i=2:obj.numSteps

set(l,'XData',obj.paths(:,1,i),'YData',obj.paths(:,2,i),'ZData',obj.paths(:,3,i));

pause(1)

drawnow

end
end

end
end
```

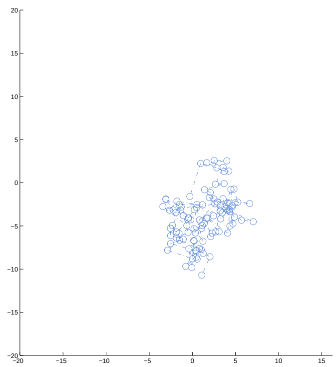

Figure 1: initial position

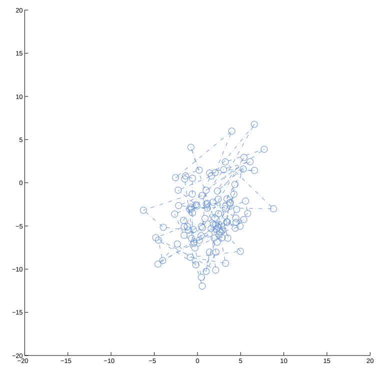

Figure 2: final position

1.2 Probability distribution function of $\boldsymbol{R}$

In order to verify that the PDF of $\boldsymbol{R}$ is Gaussian,we calculate the 'end to end distance' $\boldsymbol{R}$ for each simulation,then we plot it with histogram by coordinate (x, y, z) respectively.