Modeling and Simulation - Lab Assignment 6

Vaibhav Amit Patel (201401222)* and Tanmay Patel (201401409)*

E-mail: vaibhav290797@gmail.com; tanmaypatel273@gmail.com

Problem 1

(Radioactive decay)

Part A:

We have in the initial lectures modeled radioactive decay as a deterministic process. But radioactive decay is a nondeterministic process which can be simulated very naturally using the Monte carlo method. Suppose that the probability of any atom decaying over a time interval t is given by λ $(0 < \lambda < 1)$. Then the history of a single atom can be simulated by choosing a sequence of random numbers x_k , k = 1,2,...m uniformly distributed on [0,1]. The atom survives until the the first value of x_k for which $x_k < \lambda$. Use this approach to simulate an ensemble of atoms remaining after k intervals. Take λ = 0.1 and m = 50 and try values n = 10,100,1000 and 10000. How does the value of n (ensemble size) affect the smoothness of the resulting curve. Experiment with other values λ, n and m.

It is clear from the following plots that when the value of n is small the decrease in number of atoms is almost step wise. As the value of n increases, non-deterministic solution converges to analytical solution. Hence as the ensemble size of system increases, Monte-Carlo method converges to analytical method.

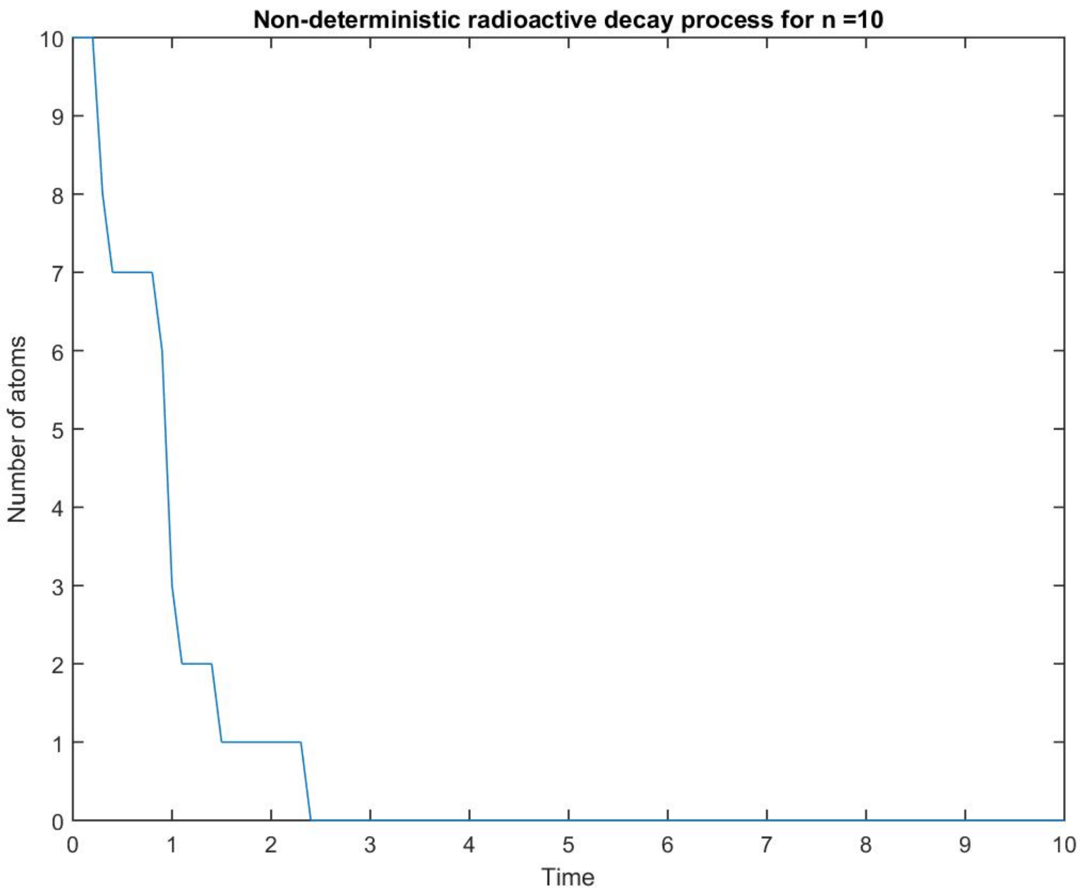


Figure 1

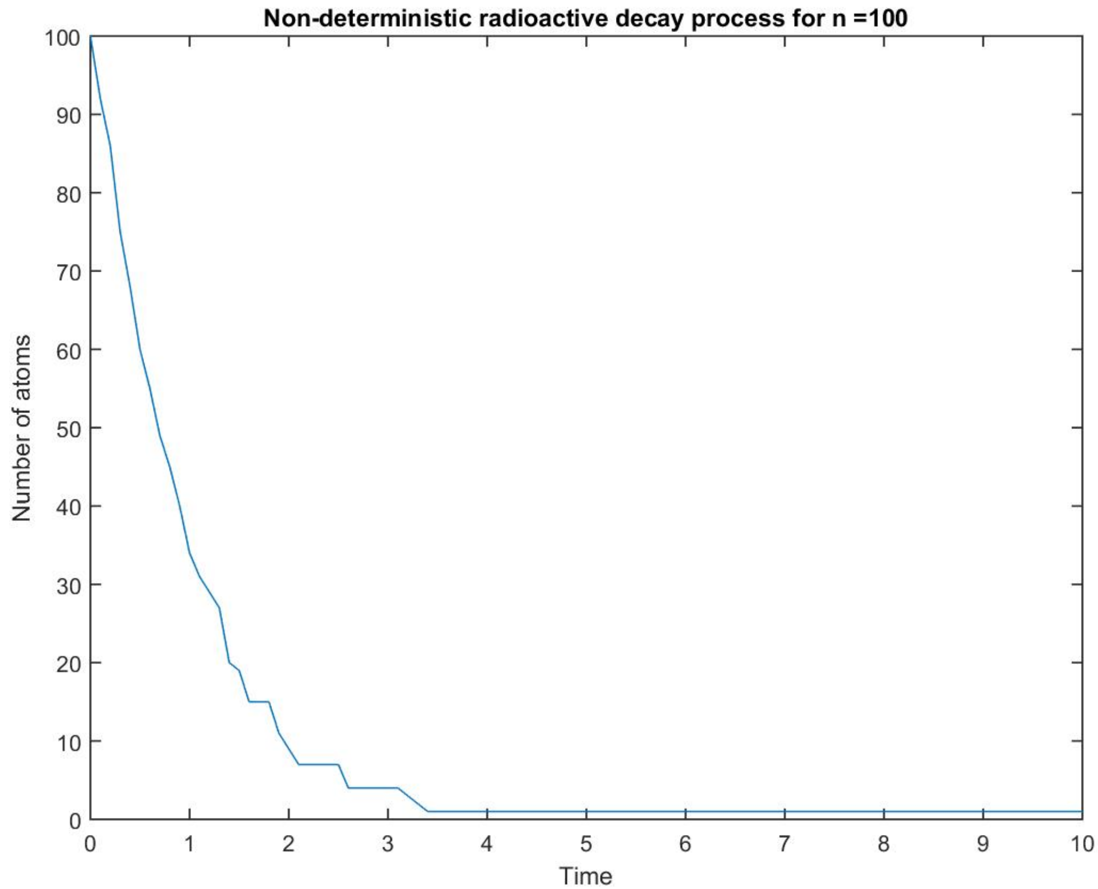

Non-deterministic radioactive decay process for n =100
Number of atoms
Time
100
90
80
70
60
50
40
30
20
10
0
0
1
2
3
4
5
6
7
8
9
10

Figure 2

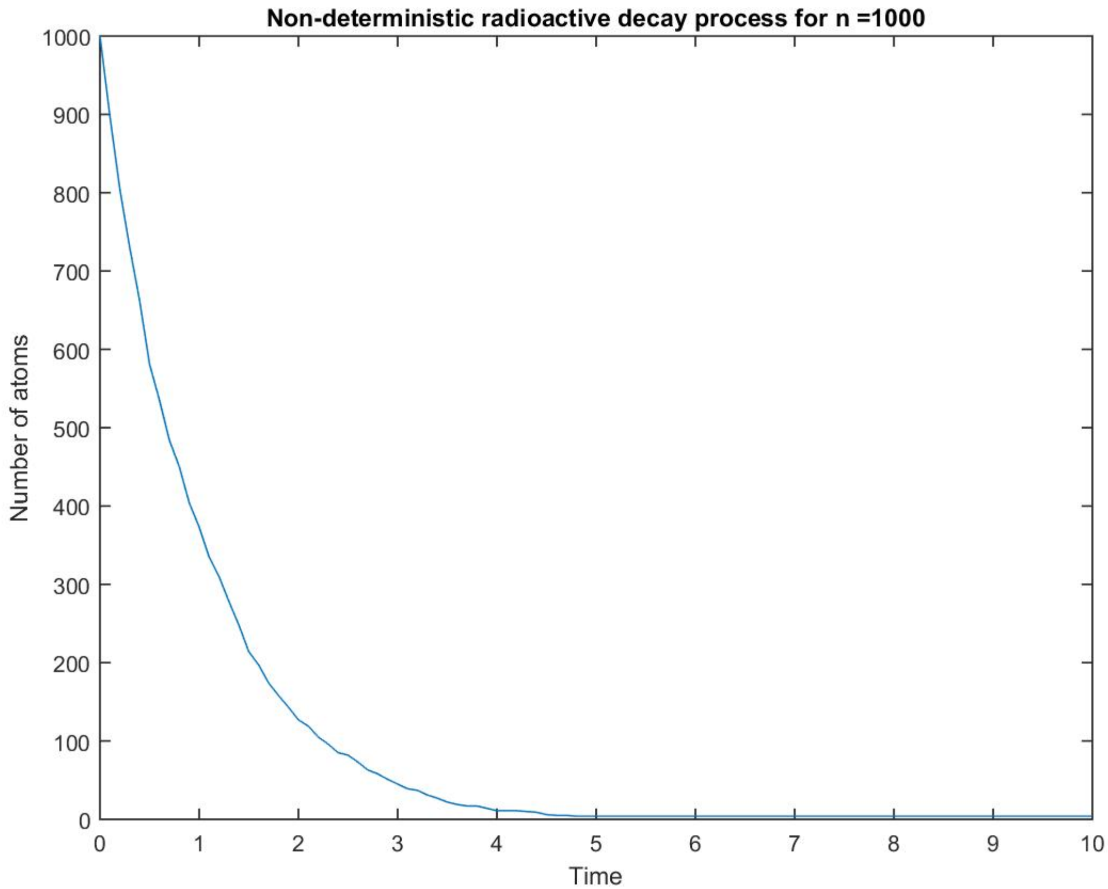

Non-deterministic radioactive decay process for n =1000
Number of atoms
Time
1000
900
800
700
600
500
400
300
200
100
0
0
1
2
3
4
5
6
7
8
9
10

Figure 3

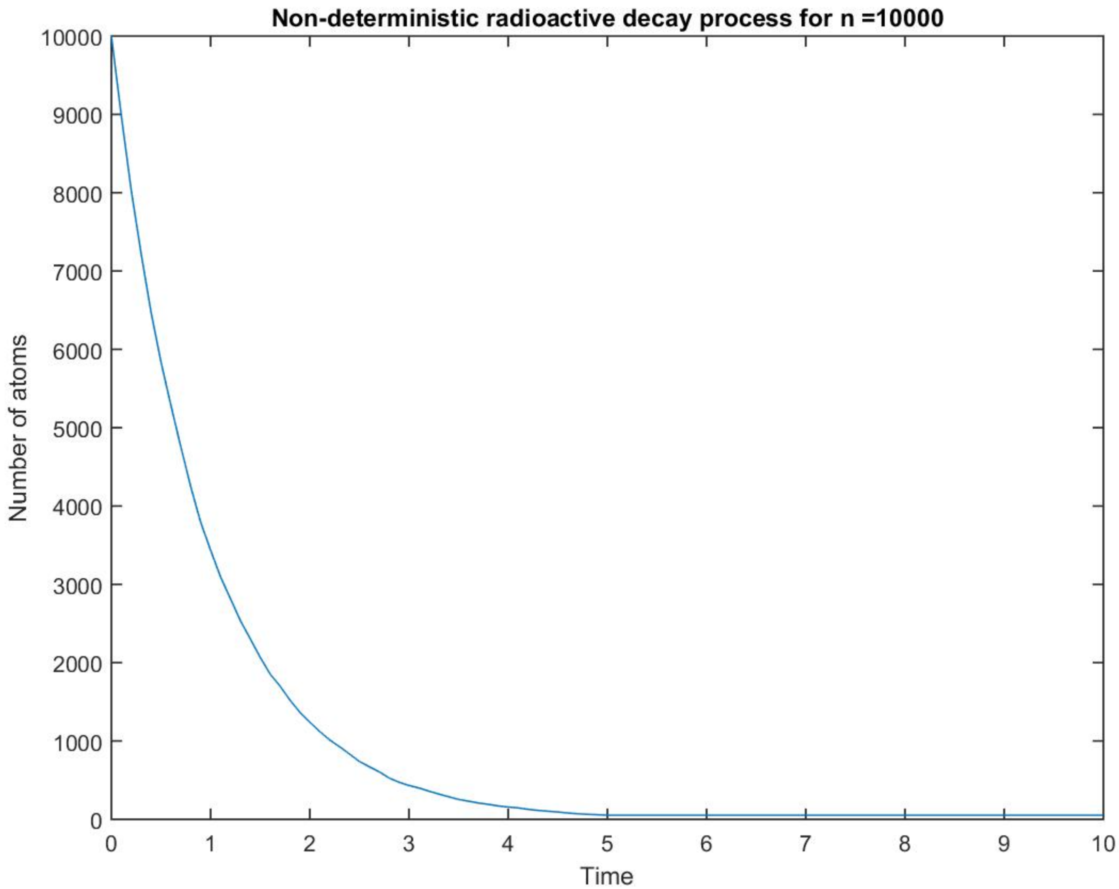


Figure 4

As we can see from following plot, as the value of λ increases, rate of decrease in atoms increases and hence number of atoms reaches to zero faster. Also by decreasing value of m, number of atoms will decay only till m steps and then system stops to change.

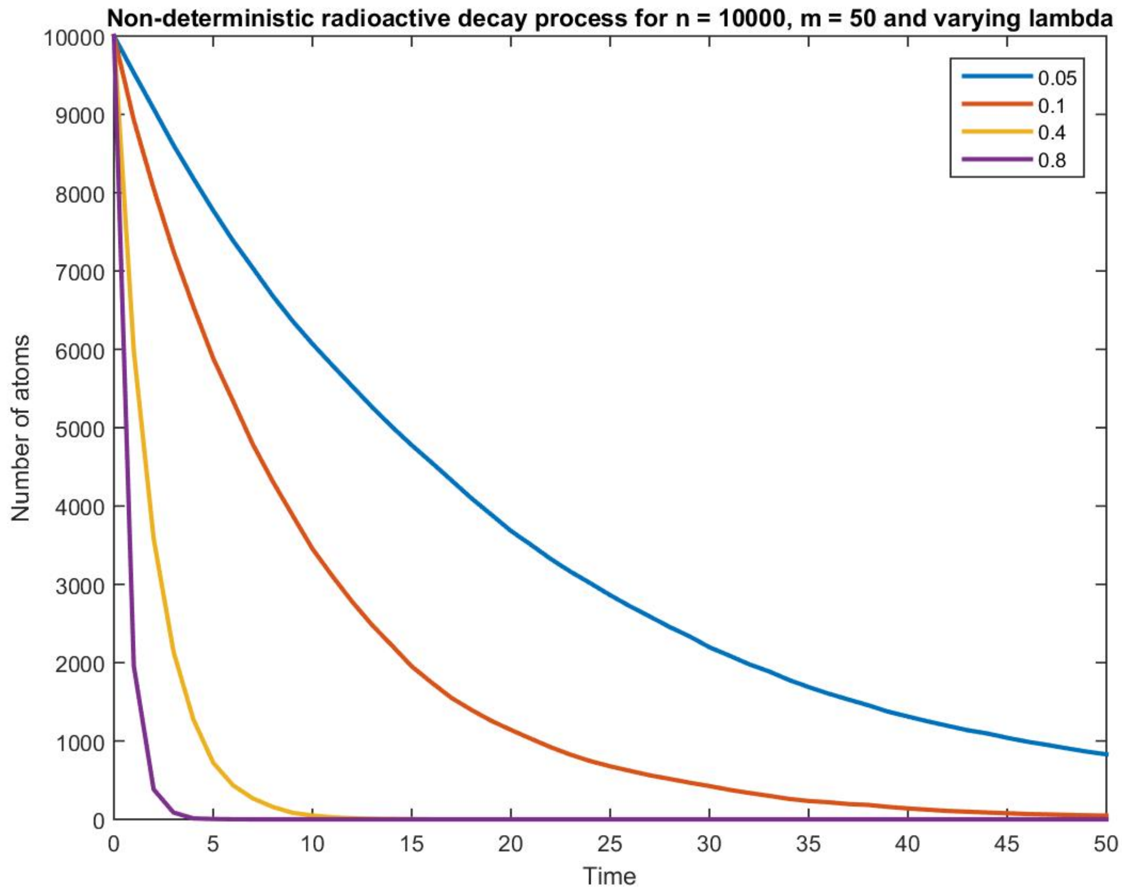
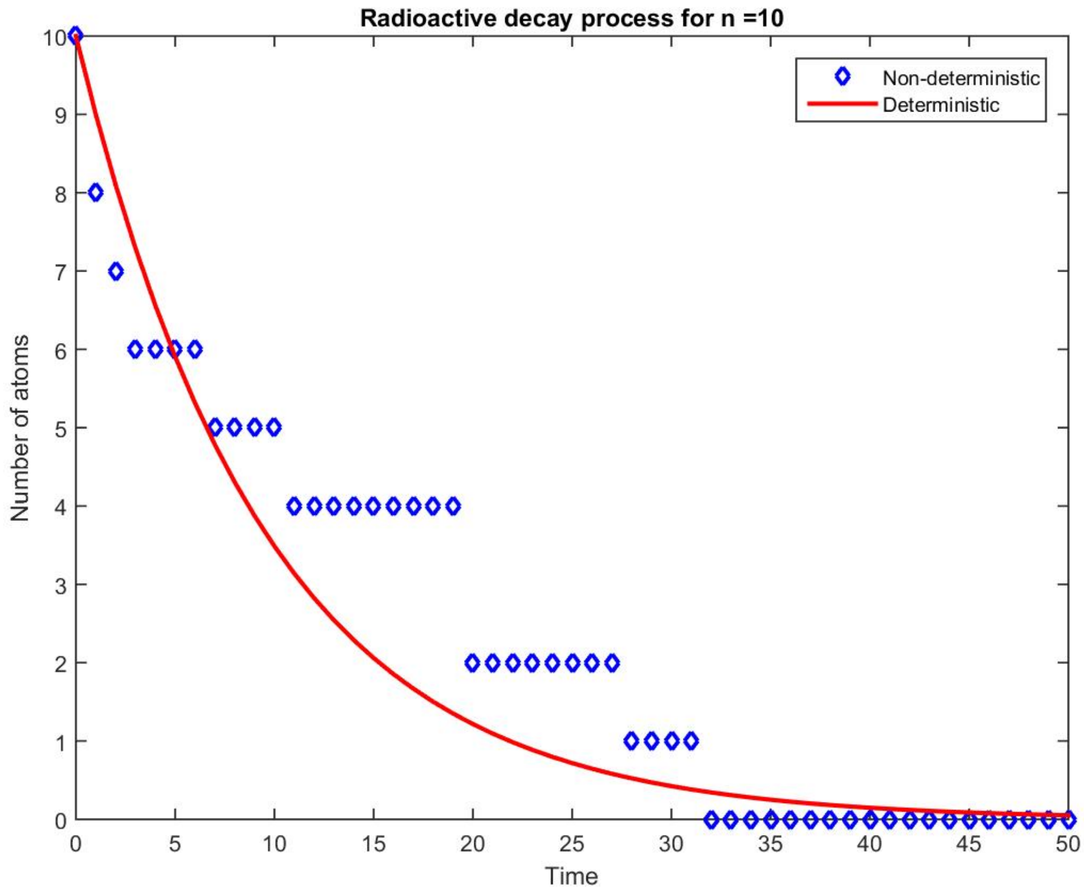


Figure 5

Part B:

Compare your results with the continuous, deterministic model of radioactive decay. Which model do you think is closer to the way nature actually behaves and why?

As the value of n increases, non-deterministic curve fits the deterministic curve. Non-deterministic model is better to the way nature actually behaves because the decay is not a completely deterministic process and deterministic model may fail for small value of n.



Radioactive decay process for n =10
Non-deterministic
Deterministic
Number of atoms
Time
0
1
2
3
4
5
6
7
8
9
10
0
5
10
15
20
25
30
35
40
45
50

Figure 6

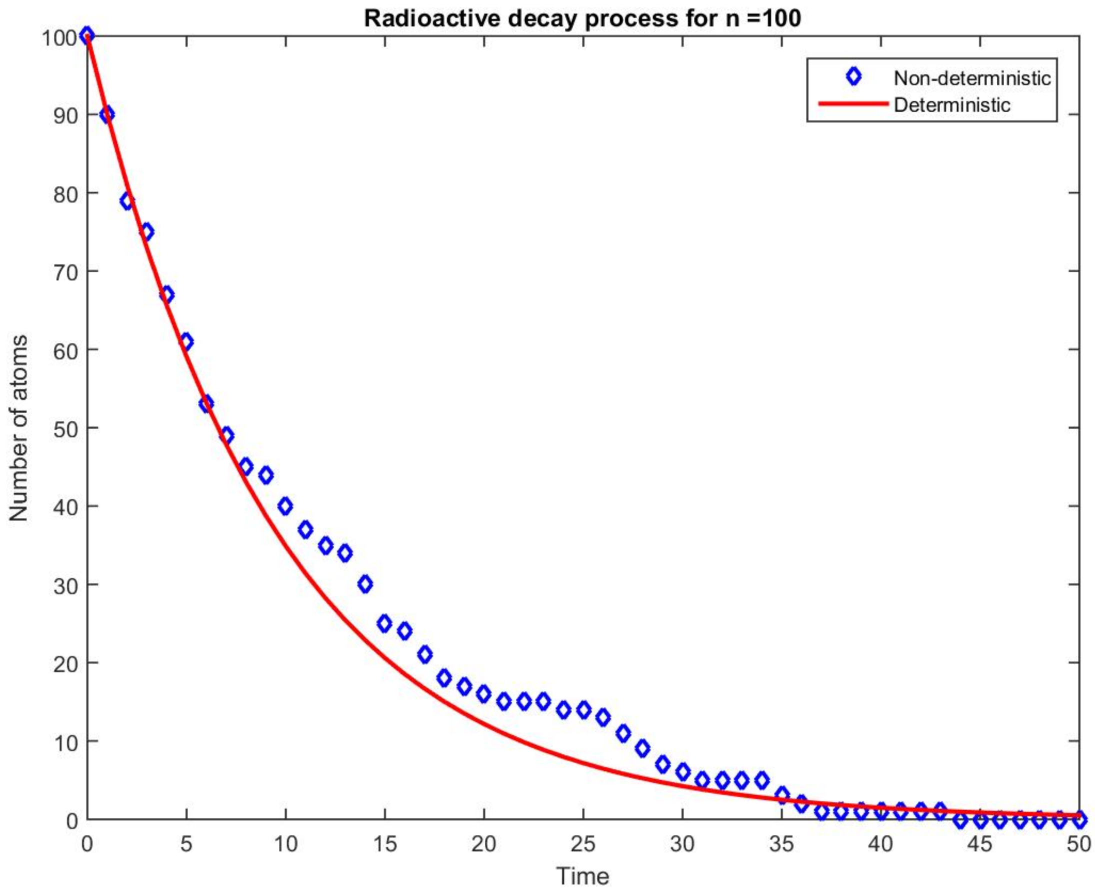
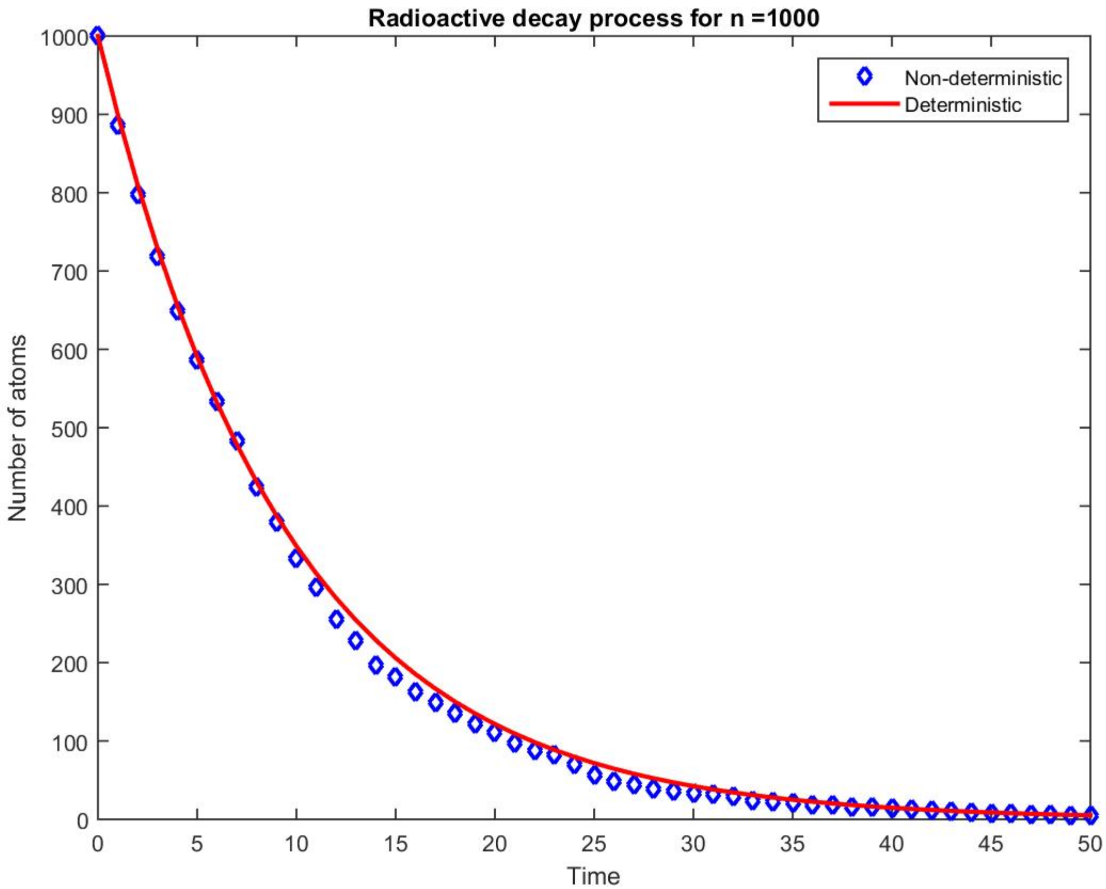

Radioactive decay process for n =100
Non-deterministic
Deterministic
Number of atoms
Time
100
90
80
70
60
50
40
30
20
10
0
0
5
10
15
20
25
30
35
40
45
50

Figure 7



Radioactive decay process for n =1000
Non-deterministic
Deterministic
Number of atoms
Time
1000
900
800
700
600
500
400
300
200
100
0
0
5
10
15
20
25
30
35
40
45
50

Figure 8

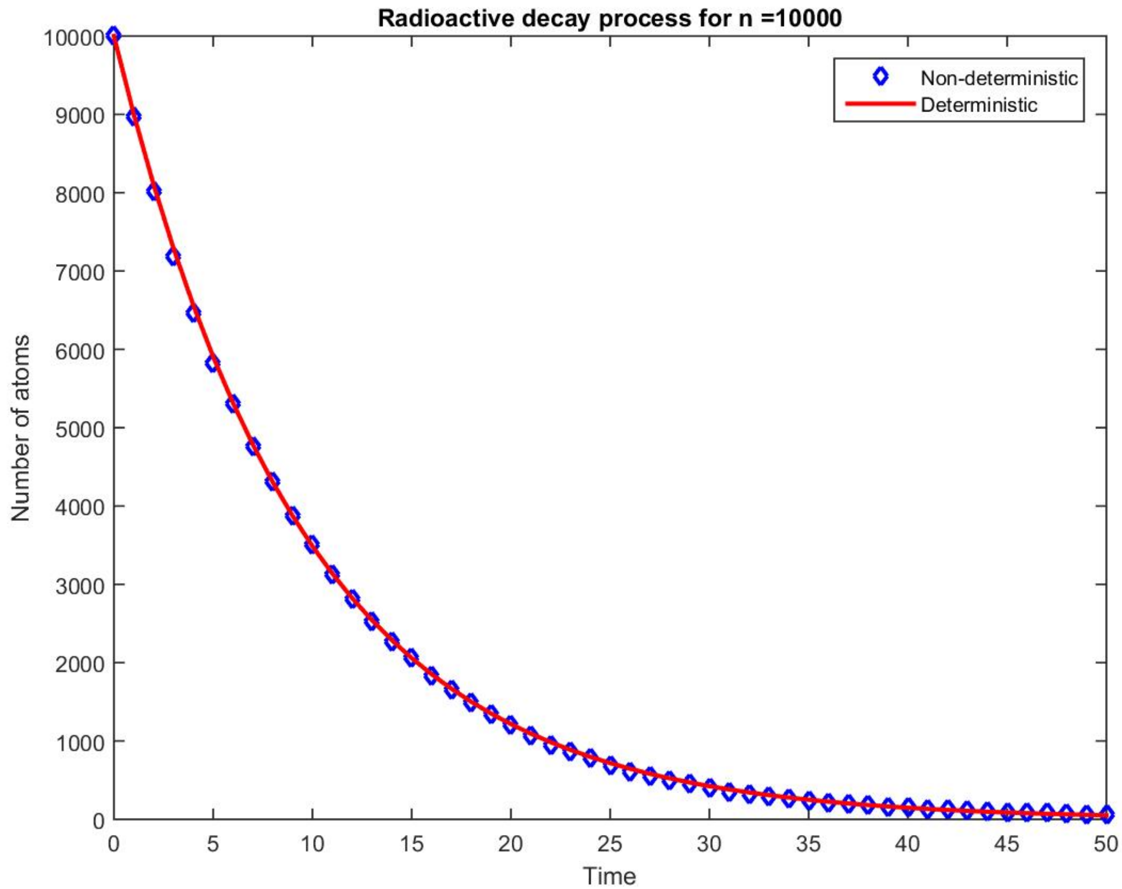


Figure 9

Problem 2

(1D Random walk)

Part A:

(Symmetric random walk) In this first part we will simulate the symmetric random walk. Let the probability of a random walker going left or right be the same p = q = 1/2. The walk starts from the site 0 and proceeds by successive steps of unit length. For direction we adopt

the convention that right is positive and left is negative. Write a program to implement the random walk of n steps, using a uniform random number generator to choose the direction of each step. Run your code to calculate the mean and mean square displacement(msd) . What is the size of the ensemble beyond which you observe Einstein's relationship (Show in a single figure by taking ensemble of different sizes). What is the value of Diffusion constant? Make a histogram of of the distribution 2 of p n (m) obtained from your data, where p n (m) is the probability of being at the mth site after n steps.

Here p = q = 0.5, so for higher number of time steps, the displacement is almost zero which can be seen from histogram plots of final position for different ensemble sizes (number of time steps n = 100 in all cases). As the ensemble size increases the plot becomes normal.

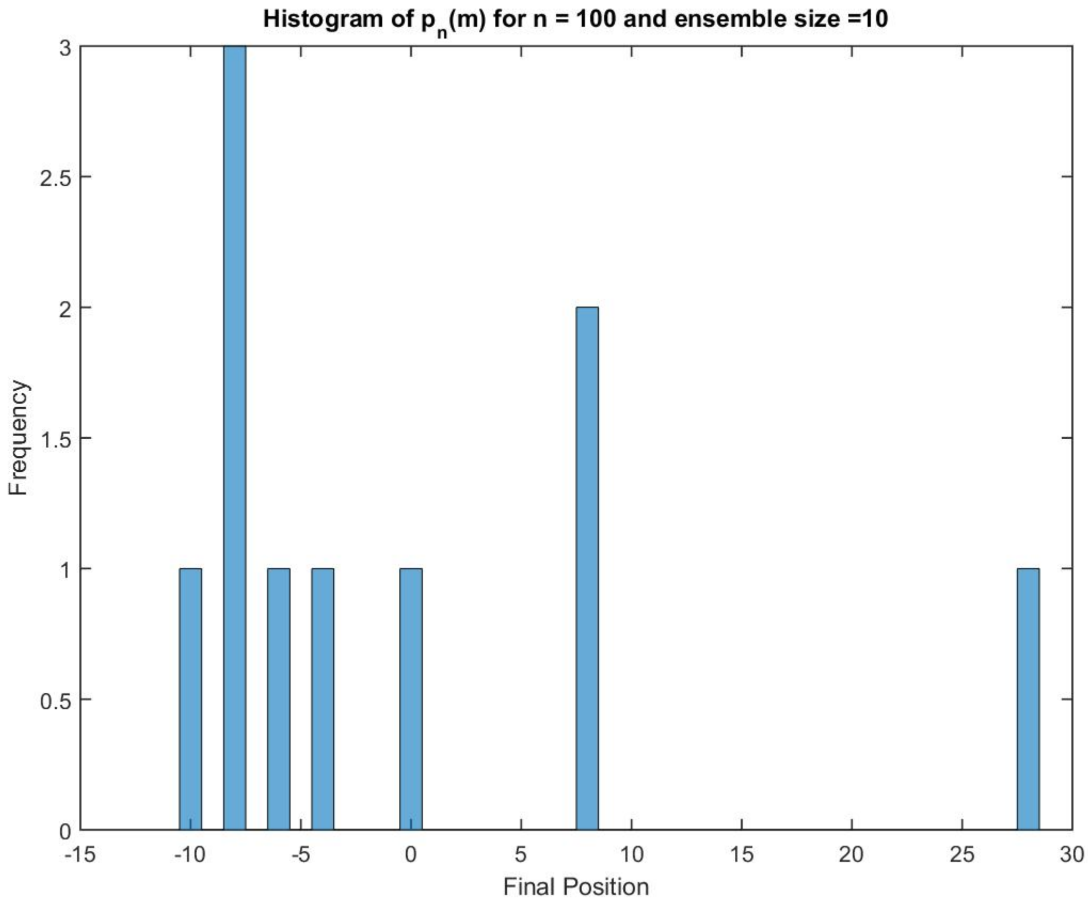

Histogram of $p_n(m)$ for n = 100 and ensemble size =10
Frequency
3
2.5
2
1.5
1
0.5
0
-15
-10
-5
0
5
10
15
20
25
30
Final Position

Figure 10

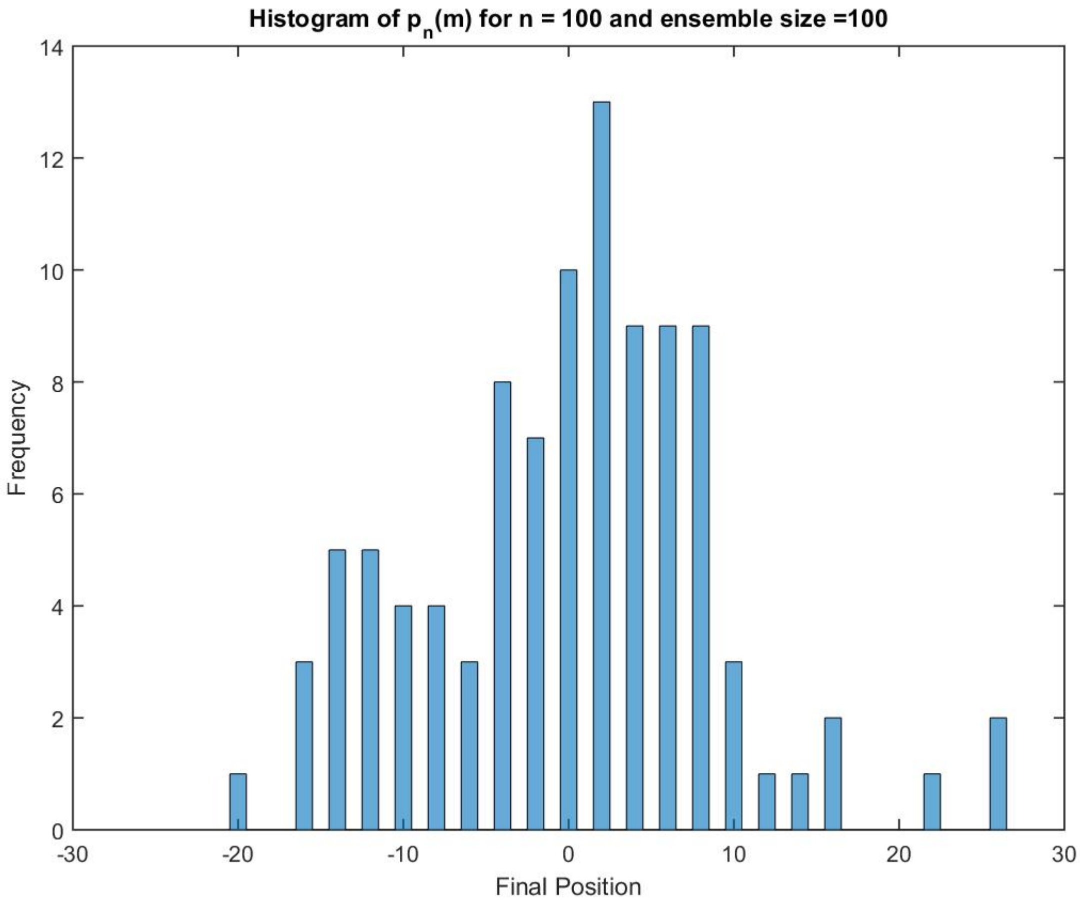

Histogram of $p_n(m)$ for n = 100 and ensemble size =100
Frequency
Final Position
14
12
10
8
6
4
2
0
-30
-20
-10
0
10
20
30

Figure 11

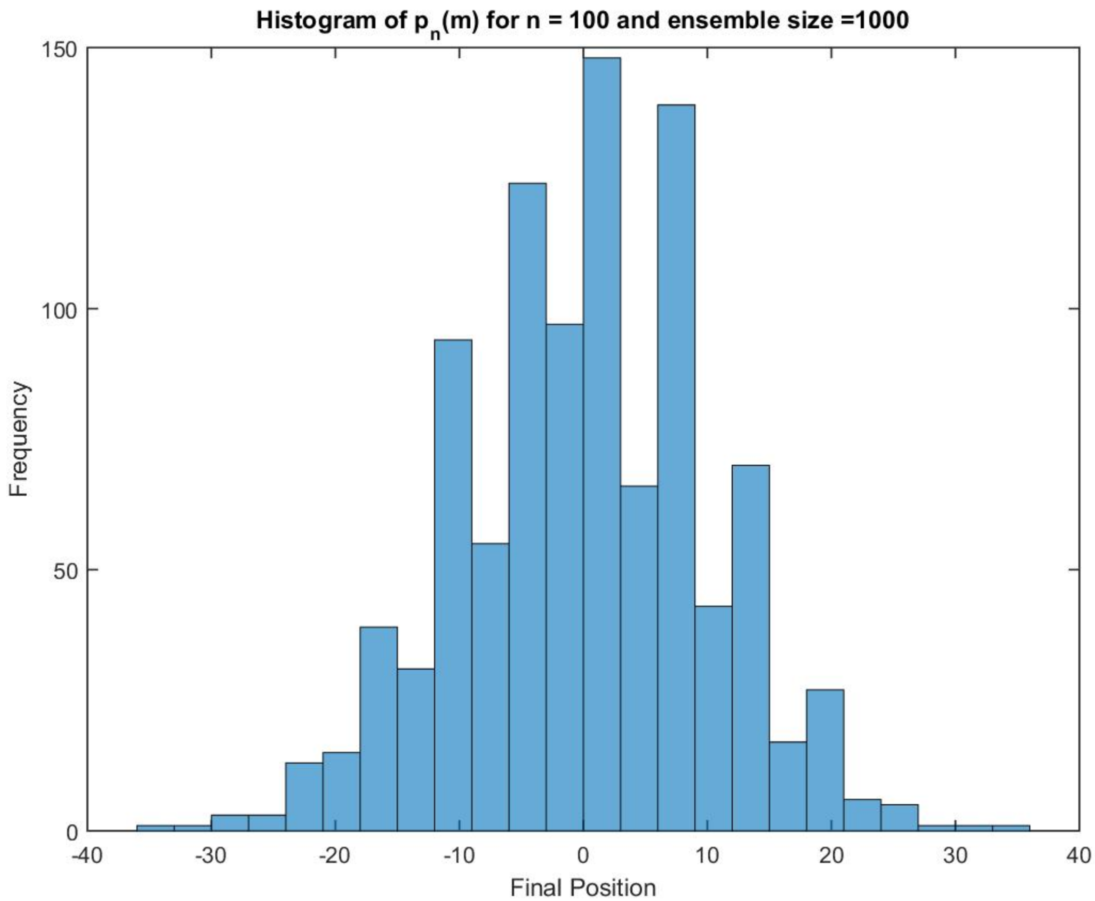

Histogram of $p_n(m)$ for n = 100 and ensemble size =1000
Frequency
Final Position
150
100
50
0
-40
-30
-20
-10
0
10
20
30
40

Figure 12

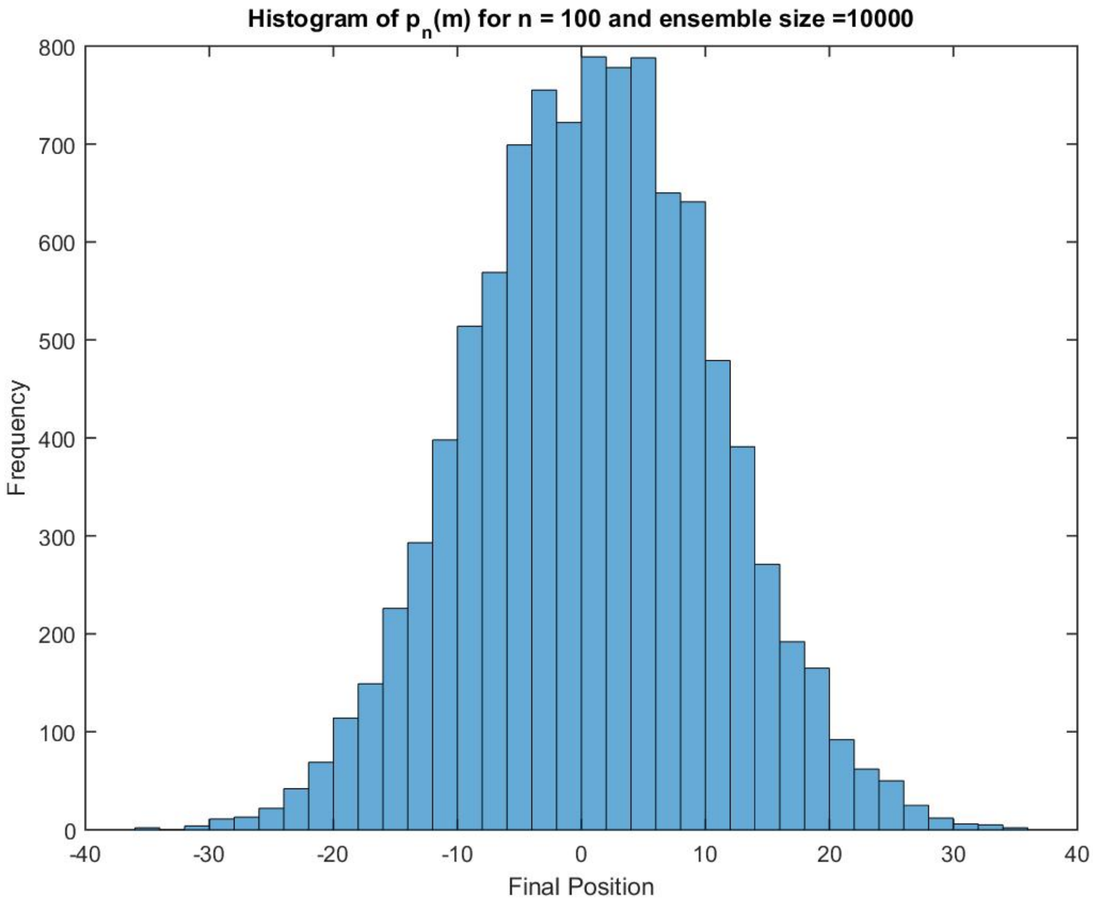
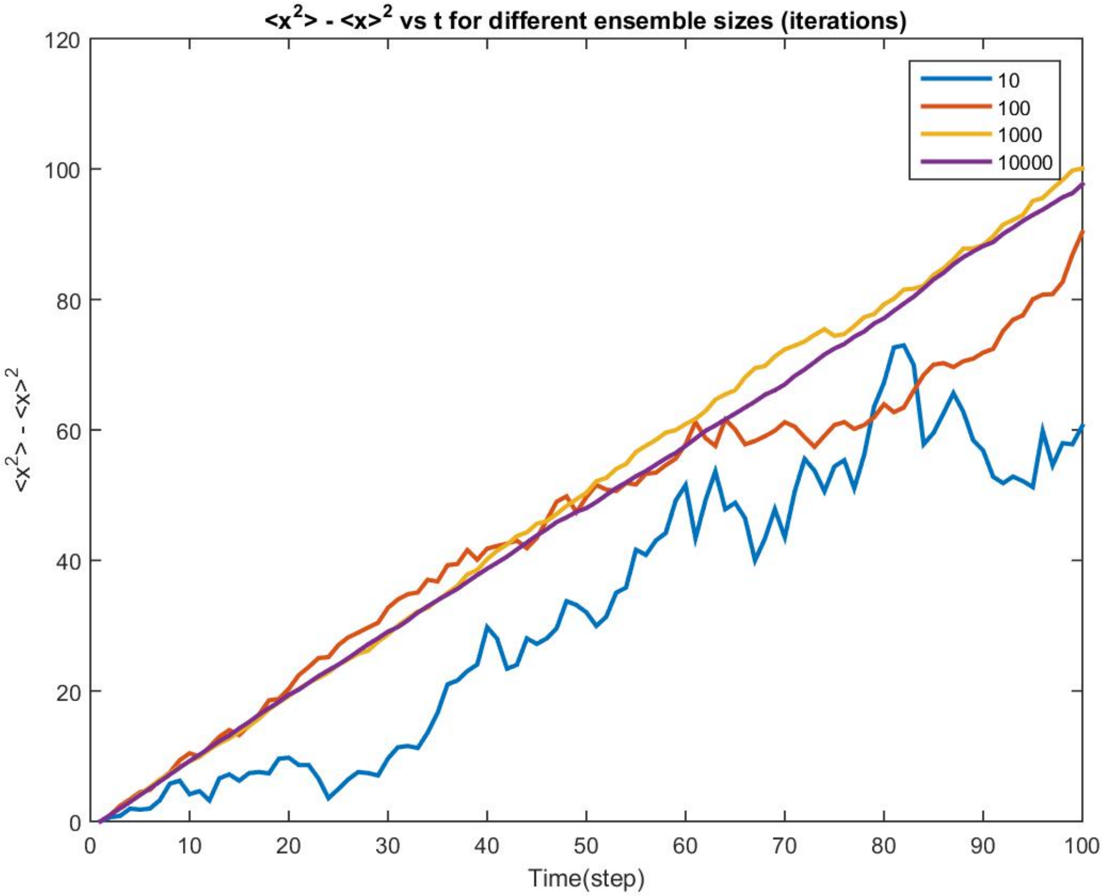

Histogram of p_n(m) for n = 100 and ensemble size =10000
Frequency
Final Position
800
700
600
500
400
300
200
100
0
-40
-30
-20
-10
0
10
20
30
40

Figure 13



<x^2> - <x>^2 vs t for different ensemble sizes (iterations)
10
100
1000
10000
120
100
80
60
40
20
0
0
10
20
30
40
50
60
70
80
90
100
Time(step)
<x^2> - <x>^2

Figure 14

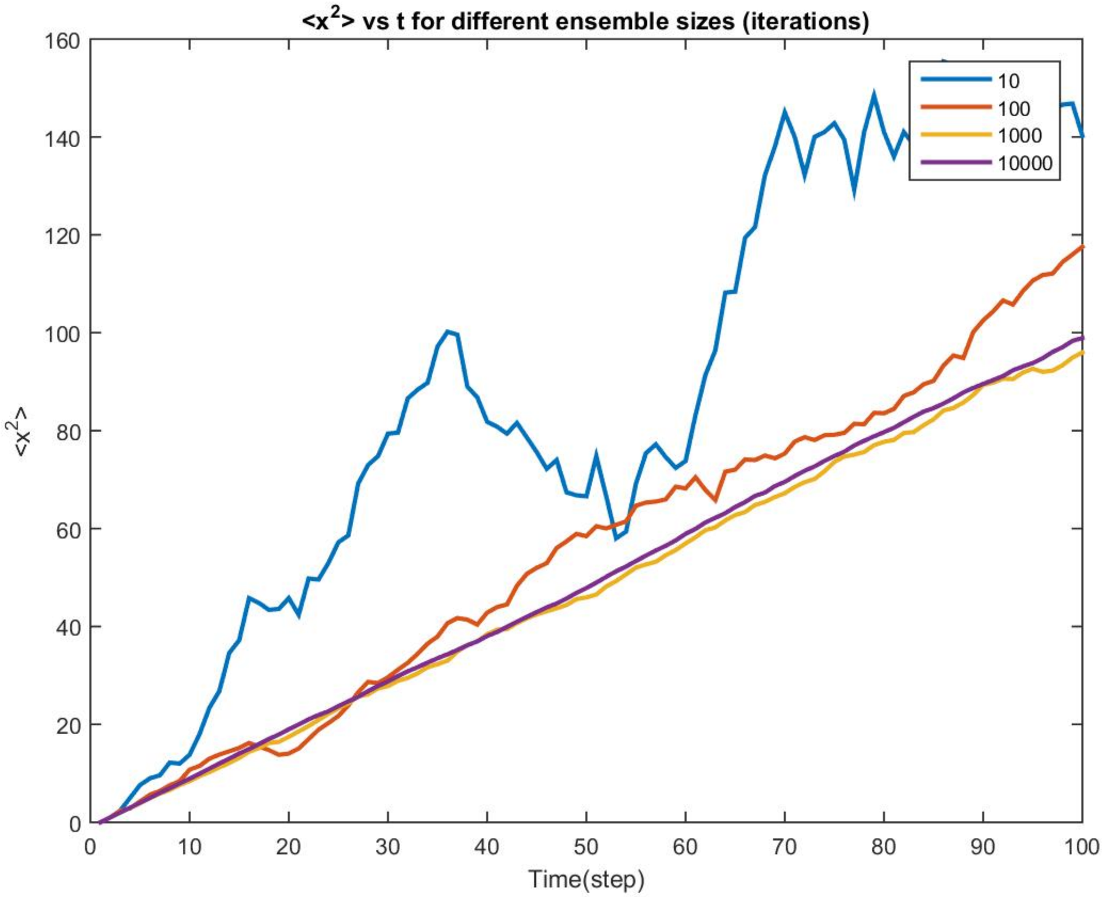

<x2> vs t for different ensemble sizes (iterations)
10
100
1000
10000
<x2>
Time(step)
0
20
40
60
80
100
120
140
160
0
10
20
30
40
50
60
70
80
90
100

Figure 15

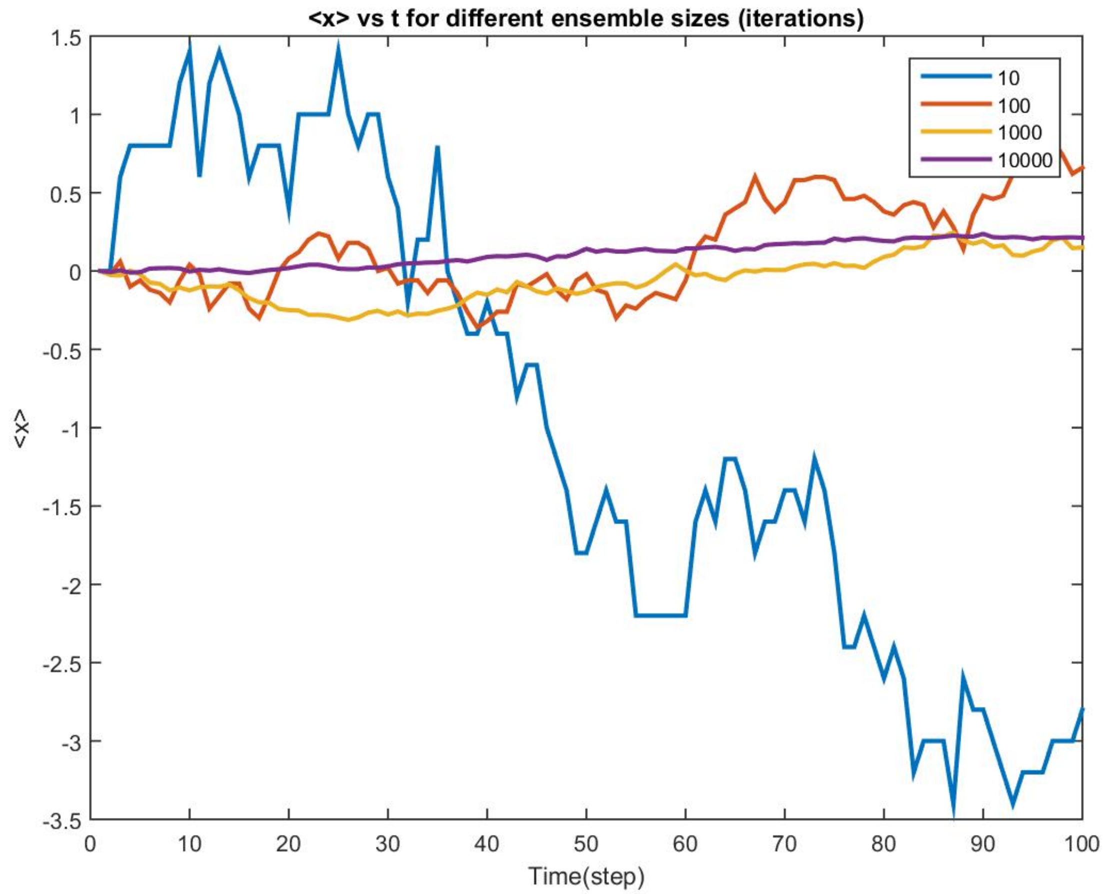


Figure 16

For ensemble size of 10000, the curve of $< x^2 > - < x >^2$ vs t is almost linear with non-zero slope. The curve of $< x >^2$ vs t is also linear with non-zero slope for large ensemble size and the curve of $< x >$ vs t is fitting x-axis i.e. $< x >$ = 0 for large ensemble size.

Diffusion constant D = Slope of $< x^2 > - < x >^2$ vs t.

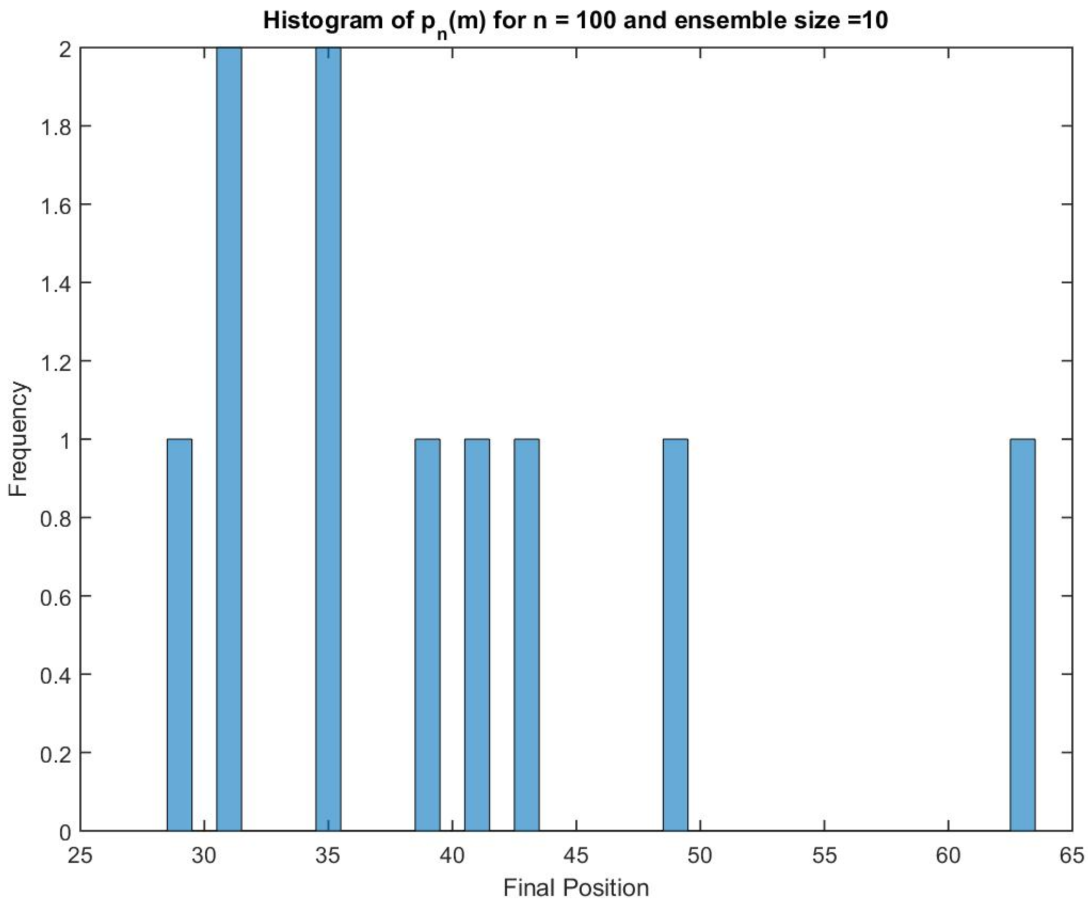
D = 97.72 / 100 = 0.977 $\approx$ 1.

It is clear that Einstein relationship is observed after ensemble size of 1000.

Part B:

(asymmetric random walk) Let us now consider the case of unequal probabilities of going left or right. Such a situation arises quite often when we force the random walker to prefer one of the directions. Think of the motion of an electron inside the metal in the presence of electric field. Let p be the probability of going right and q = 1 p be the probability of going left. Assuming that the random walker takes unit steps at each step what is the mean distance and mean squared displacement. Compare with the previous case.

Here $p = 0.7$ and $q = 0.3$. Hence after $n = 100$ steps there are almost 70 right steps and 30 left steps leading to final position of 40 which can be seen from following histogram plots. As the ensemble size increases the plot becomes normal.



Histogram of $p_n(m)$ for n = 100 and ensemble size =10
Frequency
Final Position
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
25
30
35
40
45
50
55
60
65

Figure 17

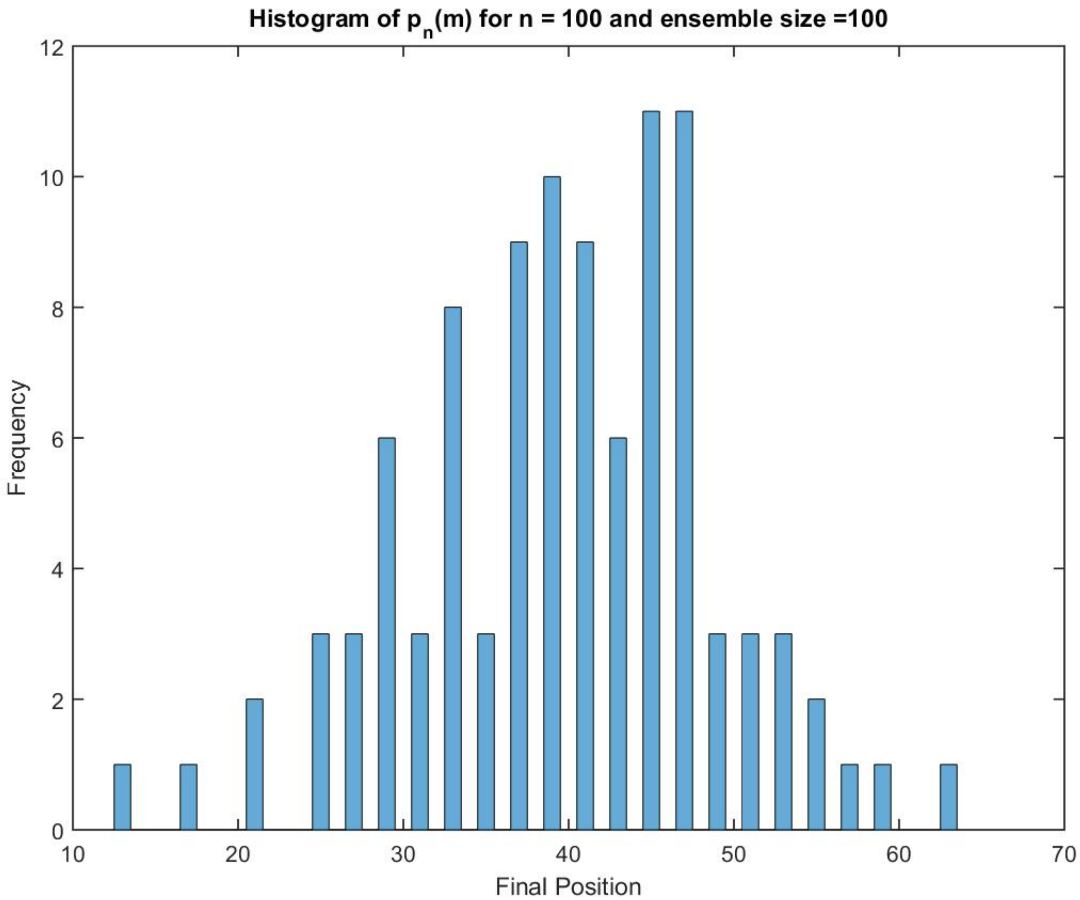
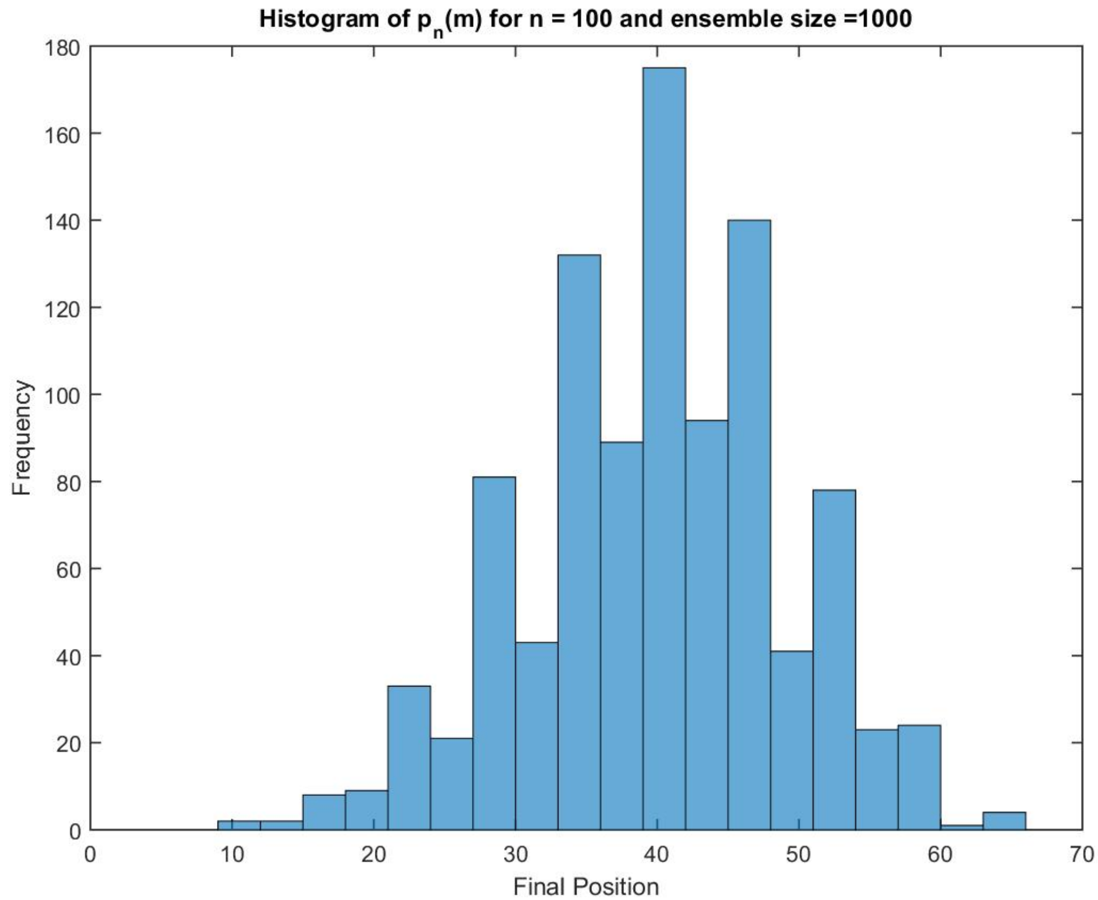

Histogram of $p_n(m)$ for n = 100 and ensemble size =100
Frequency
Final Position
0
2
4
6
8
10
12
10
20
30
40
50
60
70

Figure 18



Histogram of $p_n(m)$ for n = 100 and ensemble size =1000
Frequency
Final Position
0
20
40
60
80
100
120
140
160
180
0
10
20
30
40
50
60
70

Figure 19

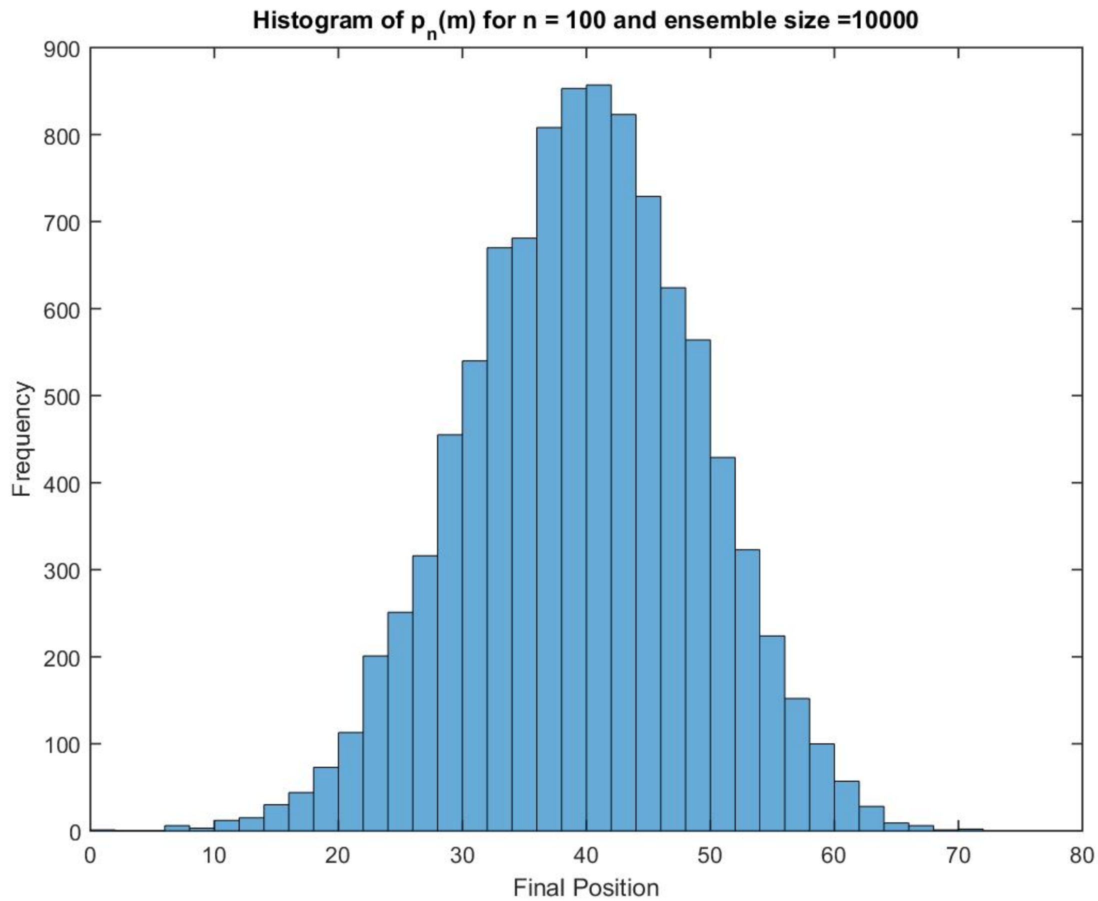
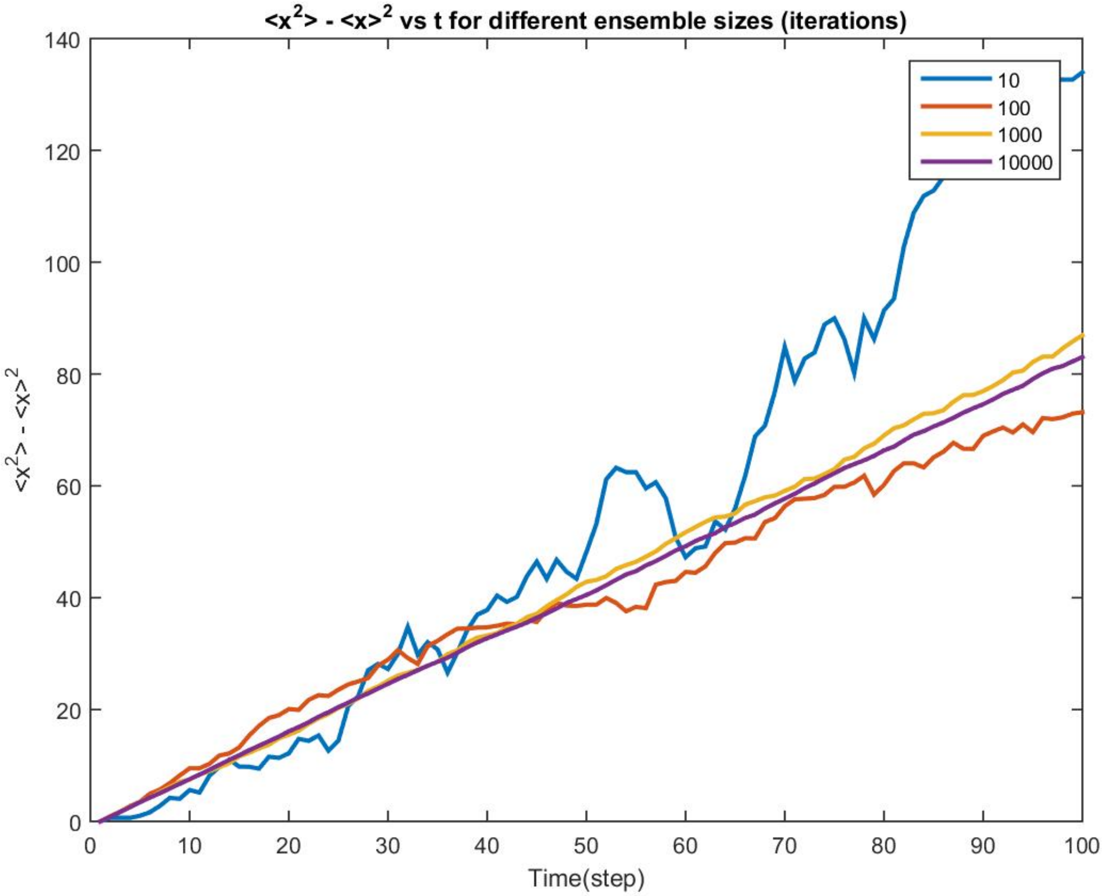
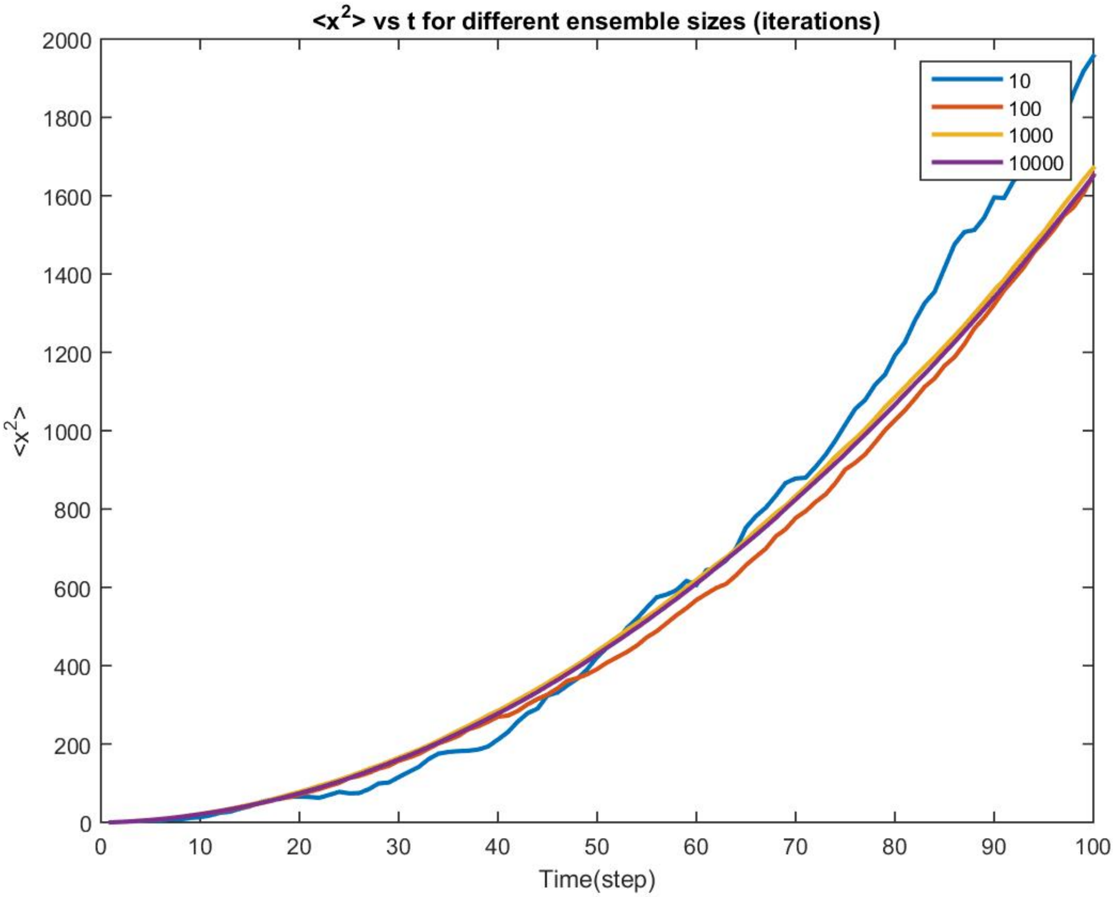

Histogram of $p_n(m)$ for n = 100 and ensemble size =10000
Frequency
Final Position
0
100
200
300
400
500
600
700
800
900
0
10
20
30
40
50
60
70
80

Figure 20



<x²> - <x>² vs t for different ensemble sizes (iterations)
10
100
1000
10000
<x²> - <x>²
Time(step)
0
20
40
60
80
100
120
140
0
10
20
30
40
50
60
70
80
90
100

Figure 21



<x^2> vs t for different ensemble sizes (iterations)
10
100
1000
10000
<x^2>
Time(step)

Figure 22

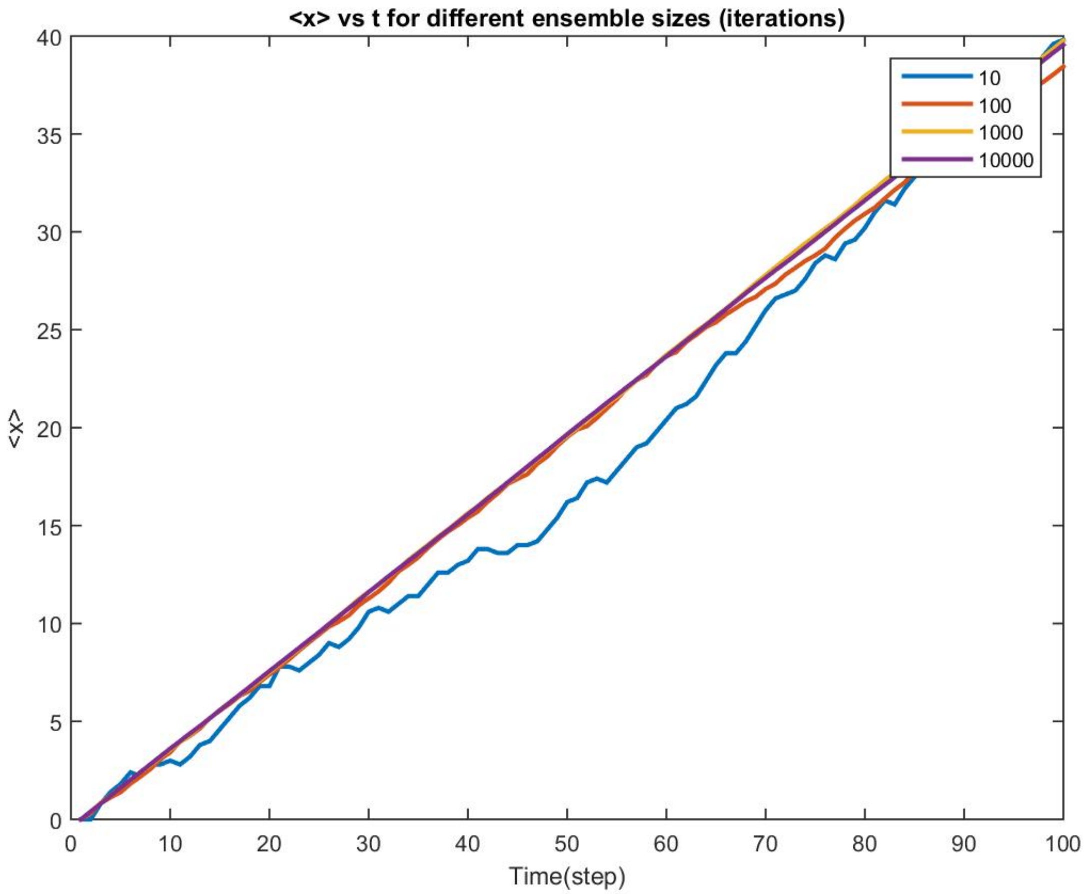


Figure 23

For ensemble size of 10000, the curve of $< x^2 > - < x >^2$ vs t is almost linear with non-zero slope. Also the curve of $< x >^2$ vs t is parabolic and the curve of $< x >$ vs t is not fitting x-axis.($< x >$ is non-zero)

Diffusion constant D = Slope of $< x^2 > - < x >^2$ vs t.

D = 84.12 / 100 = 0.84 < 1.

It is clear that Einstein relationship is observed after ensemble size of 1000.

Part C:

(Walk of varying lengths) Let us now allow the random walker to take steps of varying lengths. While we can in principle take any distribution for the step length let us assume that the length of the steps are normally distributed with with mean 0 and variance 1. From your simulations comment on the general behavior of the random walker in terms of the mean and msd, and calculate the diffusion constant. If the distribution was not standard normal but rather N(μ,) do you observe any difference in the behavior.

For N(0, 1):

Behaviour here is almost similar to that of Part (a). Highest frequency of final position is near position 0.

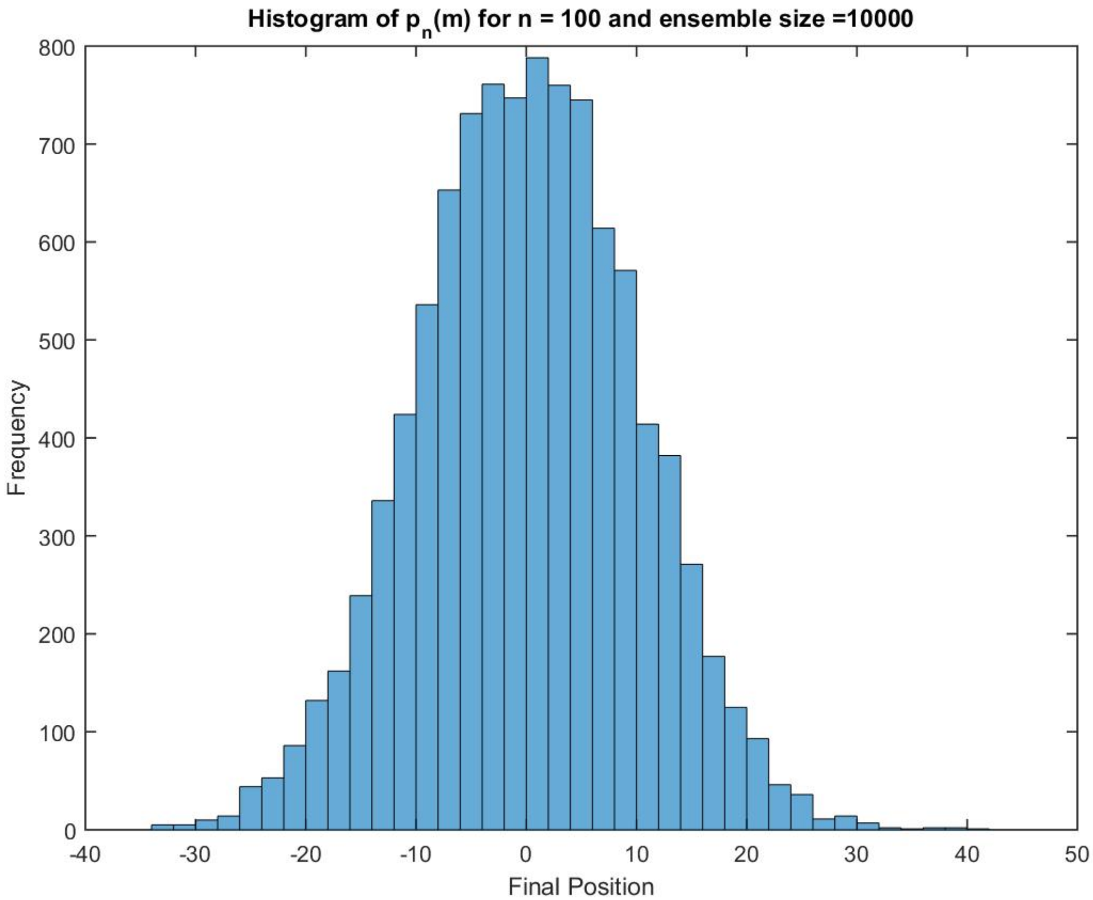
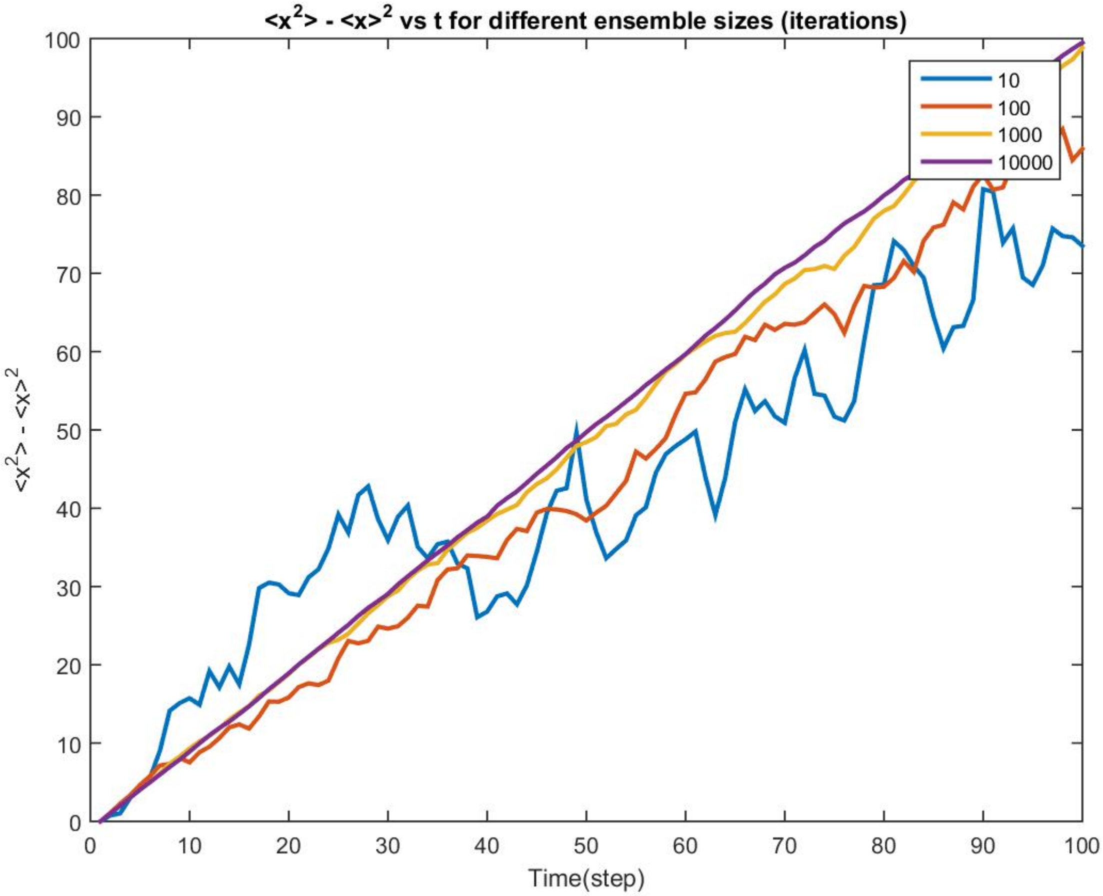

Histogram of $p_n(m)$ for n = 100 and ensemble size =10000
Frequency
Final Position
800
700
600
500
400
300
200
100
0
-40
-30
-20
-10
0
10
20
30
40
50

Figure 24



<x^2> - <x>^2 vs t for different ensemble sizes (iterations)
10
100
1000
10000
<x^2> - <x>^2
Time(step)
0
10
20
30
40
50
60
70
80
90
100

Figure 25

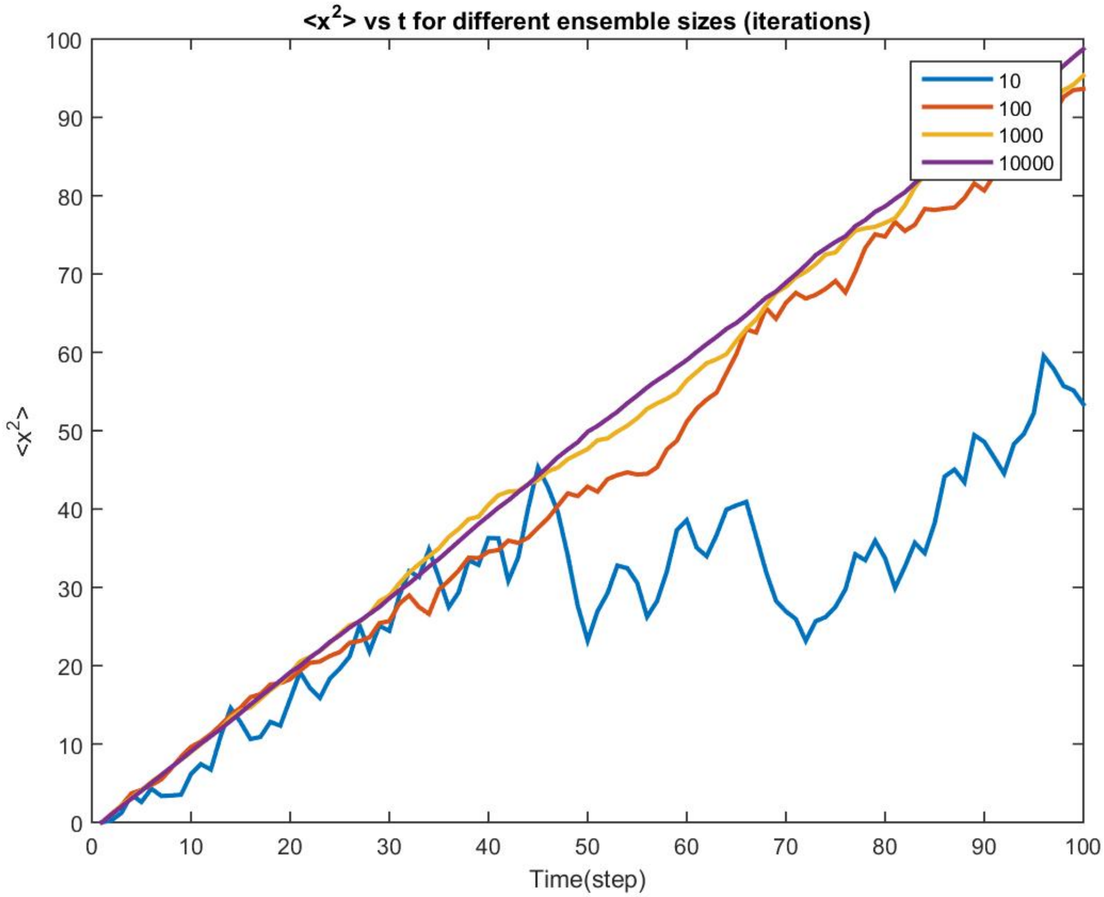

<x²> vs t for different ensemble sizes (iterations)
10
100
1000
10000
<x²>
Time(step)
0
10
20
30
40
50
60
70
80
90
100

Figure 26

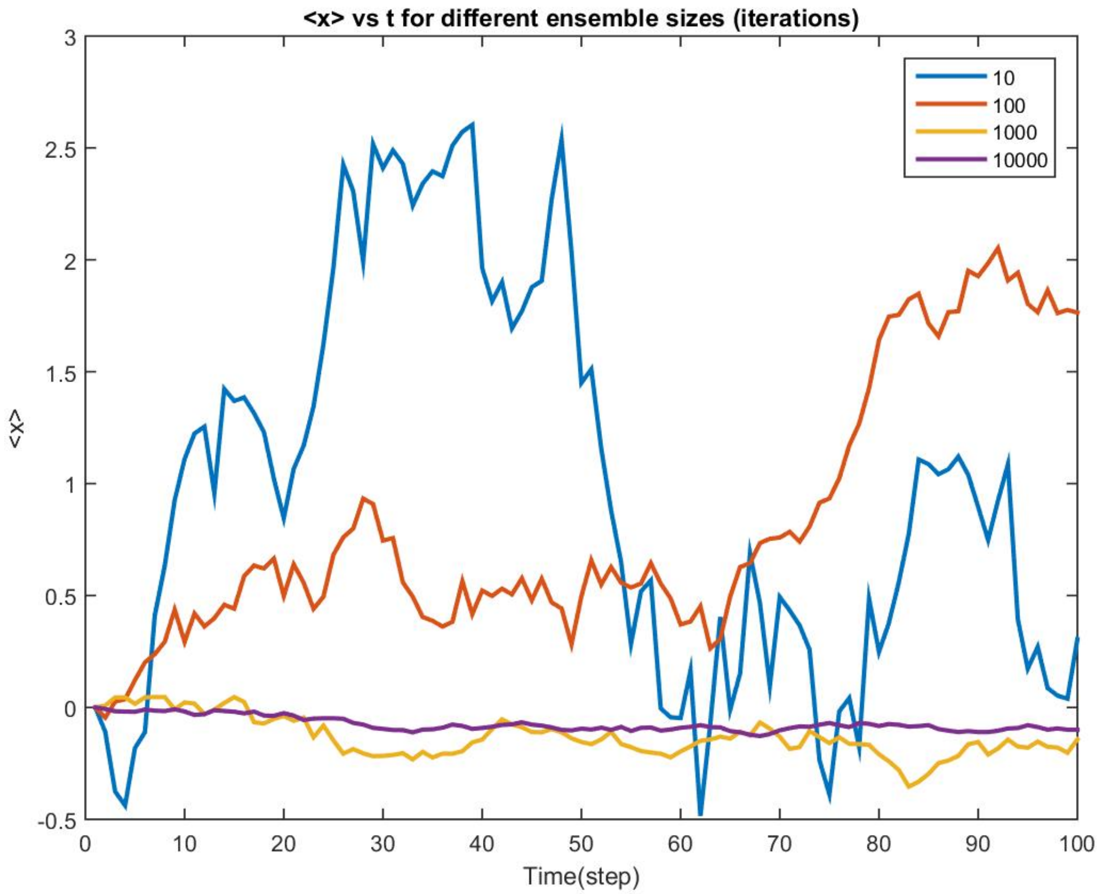


Figure 27

For ensemble size of 10000, the curve of $< x^2 > - < x >^2$ vs t is almost linear with non-zero slope. The curve of $< x >^2$ vs t is also linear with non-zero slope for large ensemble size and the curve of $< x >$ vs t is fitting x-axis i.e. $< x >$ = 0 for large ensemble size.

Diffusion constant D = Slope of $< x^2 > - < x >^2$ vs t.

D = 99.82 / 100 = 0.9982 $\approx$ 1.

It is clear that Einstein relationship is observed after ensemble size of 1000.

For N(5, 8):

Here also highest frequency of final position is near position 0.

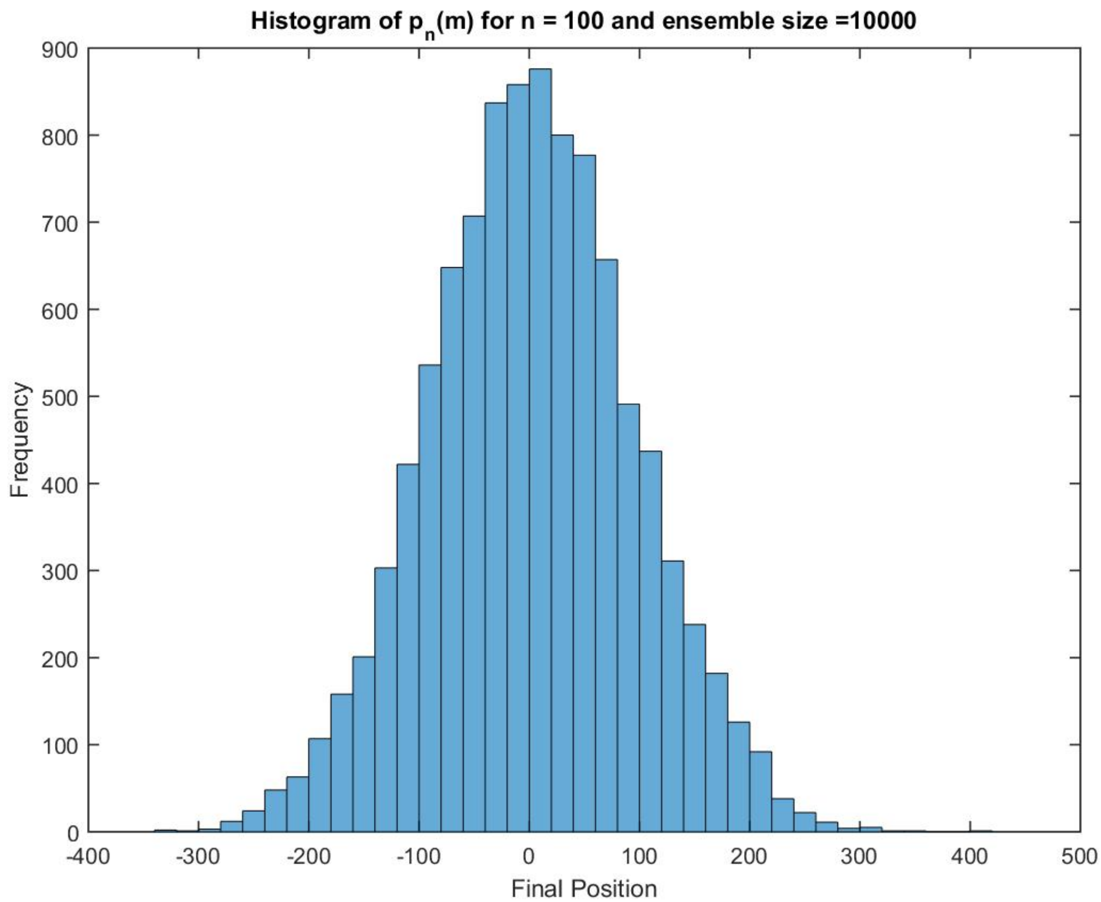


Figure 28

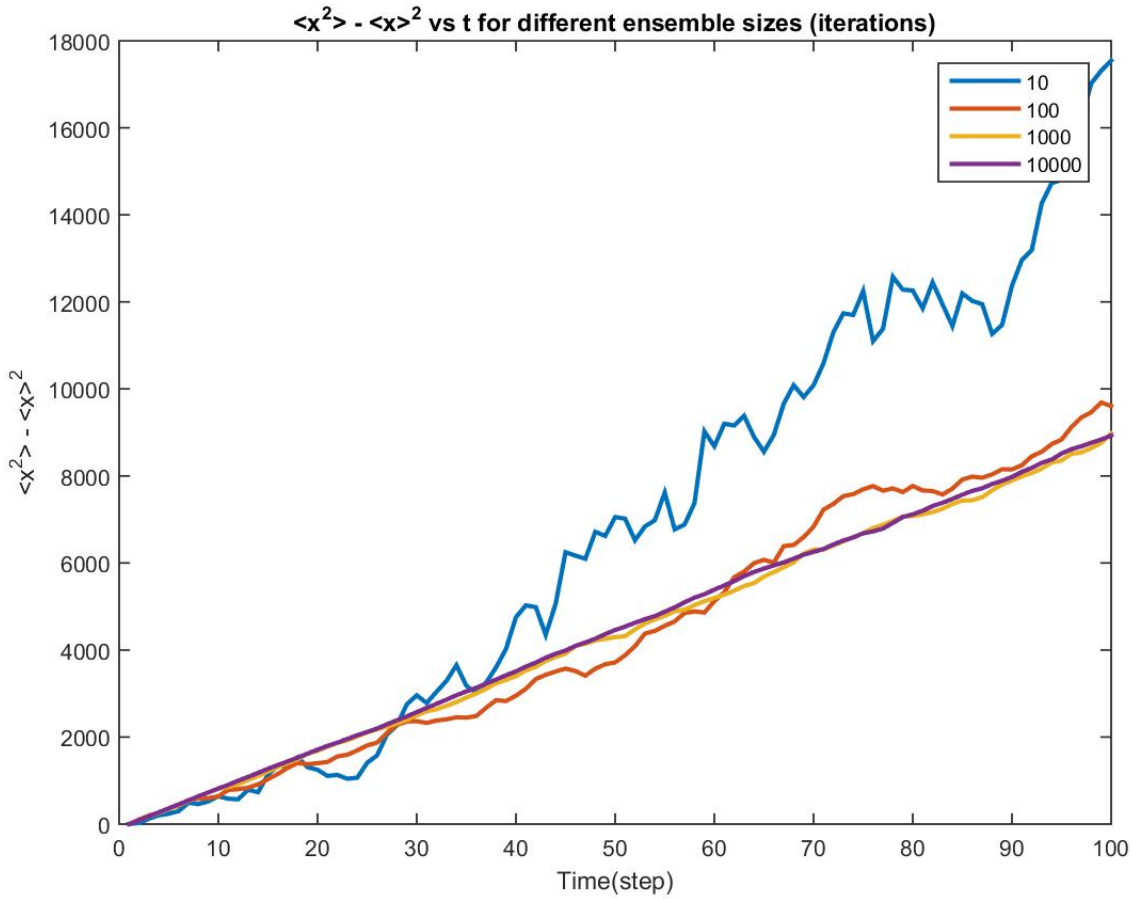
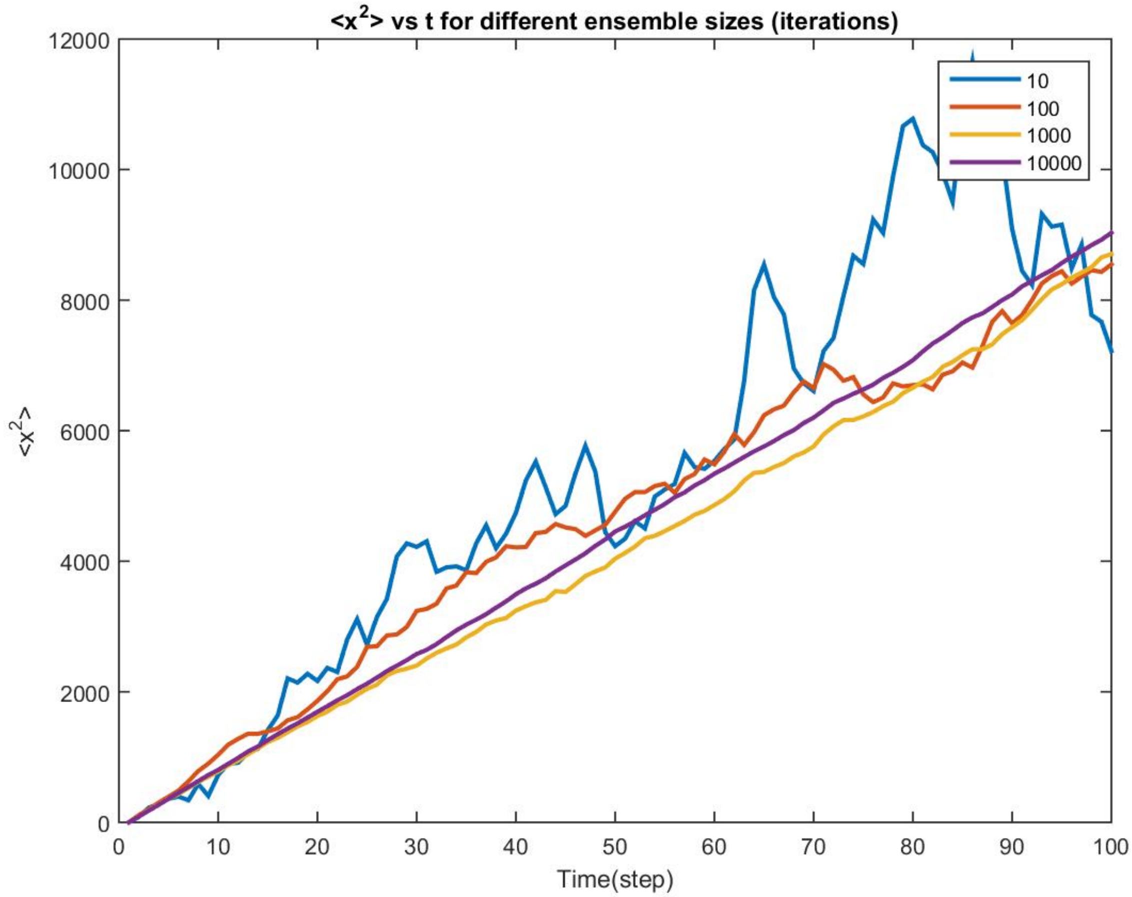

<x2> - <x>2 vs t for different ensemble sizes (iterations)
<x2> - <x>2
Time(step)
10
100
1000
10000

Figure 29



<x^2> vs t for different ensemble sizes (iterations)
10
100
1000
10000
<x^2>
Time(step)
0
2000
4000
6000
8000
10000
12000
0
10
20
30
40
50
60
70
80
90
100

Figure 30

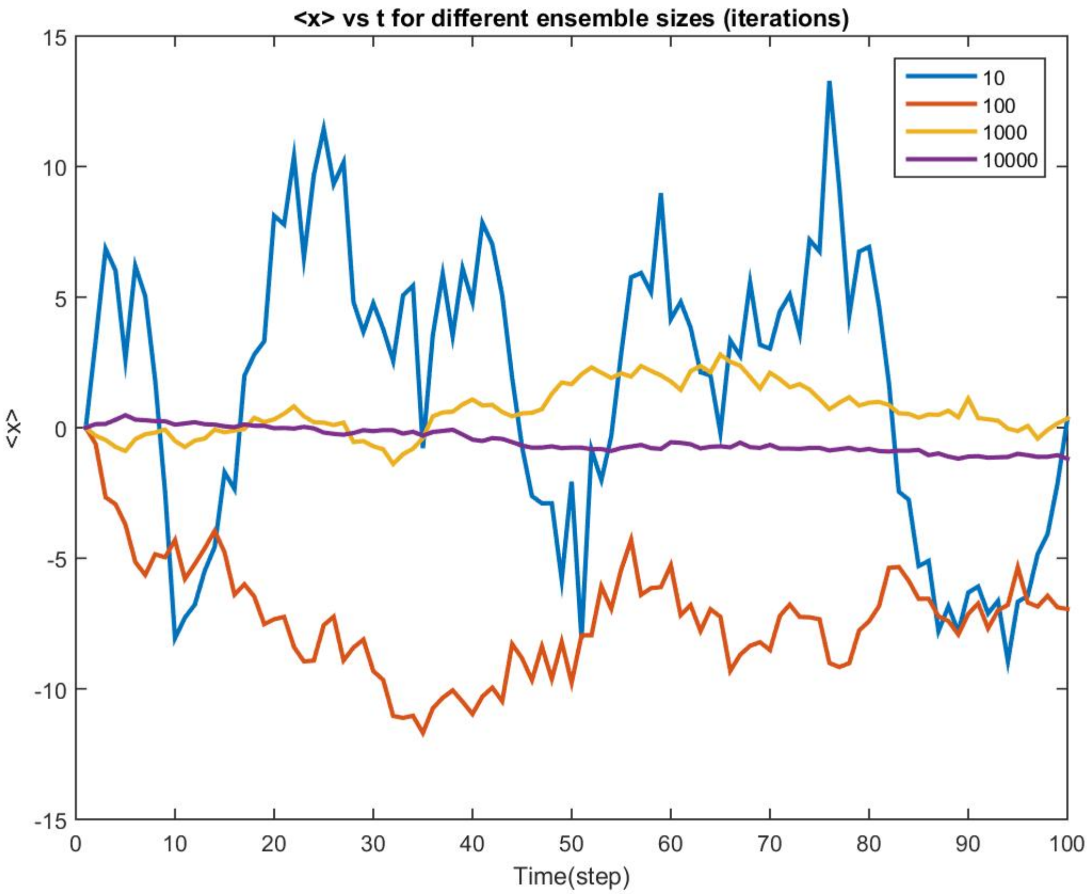


Figure 31

For ensemble size of 10000, the curve of $< x^2 > - < x >^2$ vs t is almost linear with large slope. The curve of $< x >^2$ vs t is also linear with large slope for large ensemble size and the curve of $< x >$ vs t is fitting x-axis i.e. $< x >$ = 0 for large ensemble size.

Diffusion constant D = Slope of $< x^2 > - < x >^2$ vs t.

D = 8872 / 100 = 88.72 $>$ 1.

It is clear that Einstein relationship is observed after ensemble size of 1000.

Thus here the value of Diffusion constant is much high than that in case of N(0, 1).

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