CELLULAR AUTOMATA TECHNIQUES: AN APPROACH TO MODEL AND SIMULATE BROWNIAN PARTICLES DIFFUSION

By

BIRHANU ABERA KIBRET

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ADDIS ABABA UNIVERSITY
DEPARTMENT OF
PHYSICS

Supervisor: ______________________
Dr.MULUGETA BEKELE

Examiners: ______________________
Dr.TATEK YERGOU

____

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Author: **BIRHANU ABERA KIBRET**

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For my family and all my friends who supported me in material and idea.

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Abstract

In this project, we investigate the diffusion coefficient of Brownian particles which are randomly generated on a two dimensional grid. By using the cellular automata techniques we investigate mean square displacement (MSD) and root mean square displacement (RMSD) of particles for fixed percent of concentration. We find the MSD and RMSD of particles at different values of concentration. In addition to these, we investigate MSD and RMSD of particles for fixed and different values of concentration at different time steps for a given number of cells.

Chapter 1

Introduction

Microscopically, nothing is ever still. Molecules of perfume from an open bottle will slowly diffuse across a room. Brownian particles diffusion is the random movement of microscopic particles in a gas or liquid. This motion was first observed by Robert Brown in 1827 for a suspension of pollen grains and particles of dust in a cup of water, which will show endless random movement. The mathematical description of the phenomenon was developed by Albert Einstein [1]. Still these days diffusion and Brownian motion are active research areas.

To come up with the result shown by Albert Einstein using computer simulation, many researchers used different approach but this project is done using the idea and work of Eric Plaza and Rafel Martin [2]. They have used a new technique called cellular automata. In their original work they have found the root mean square displacement (RMSD) of particles for fixed and different values of concentrations. In addition to this, they have investigated RMSD of particles for fixed and different values of concentration.

In this project, by applying the cellular automata model used by Plaza and Martin, we find the relation between RMSD and number of cells for 20 percent of concentration. We get the RMSD of particles for different values of concentration. Similarly, we investigate the value of root mean square displacement (RMSD) and mean square displacement (MSD) of particles for different number of cells and fixed concentration. In addition to this, we find the relation between MSD and time. By using similar steps, we investigate the relation between root mean square displacement and time.

The rest of this project is organized as follows:- In chapter two we describe the theory of the relation between mean square displacement and time steps. In chapter three we will discuss about the basic cellular automata simulation techniques and ways of implementations that help us to obtain MSD and RMSD as a function of time steps. Finally, in chapter five we will give conclusions about the results obtained in the data analysis part.

Chapter 2

Theory

In this chapter, we briefly describe the derivation of mean square displacement and its relation with time steps.

2.1 Mean displacement squared from the initial position after N steps

Einstein explained that the pollen grains are buffeted by collisions with molecules of water moving randomly in all directions. His theory showed that the mean distance traveled by a pollen grain (or other microscopic object) subject to random collisions increases as the square root of time. Brownian motion is the random movement of particles suspended in a fluid. It is caused by random bombardment by molecules of the fluid. Brownian motion is a kind of stochastic process. The particle does move and is certainly likely to cover large distance as time goes on. To find the mean displacement squared from the initial position after N steps, we can follow the following steps:

$$X(N) = X(N-1) \pm \delta \tag{2.1.1}$$

where, X is the displacement and δ is the change in displacement for each time step

$$X^2(N) = [\, X(N-1) \pm \delta.]^2 \tag{2.1.2}$$

$$X^2(N) = X^2(N-1) \pm 2\delta X(N-1) + \delta^2 \tag{2.1.3}$$

The average value is

$$\langle X^2(N)\rangle = \langle\ X^2(N-1)\rangle \pm 2\delta\langle X(N-1)\rangle + \delta^2 \tag{2.1.4}$$

The middle term is zero, because on average, the particle will get no where(X = 0) since it is equally likely to take left ward as right ward steps. so,

$$\langle X\rangle = 0 \tag{2.1.5}$$

$$\langle X^2(N)\rangle = \langle\ X^2(N-1)\rangle + \delta^2 \tag{2.1.6}$$

At each step, the mean squared displacement is increased by one step squared. Mathematically this can be shown as follows:

$$\langle X^2(0)\rangle = 0 \tag{2.1.7}$$

$$\langle X^2(1)\rangle = \delta^2 \tag{2.1.8}$$

$$\langle X^2(2)\rangle = 2\delta^2 \tag{2.1.9}$$

Then,we find that

$$\langle X^2(N)\rangle = N\delta^2 \tag{2.1.10}$$

Then characteristic distance traveled is

$$\langle X^2(N)\rangle^{\frac{1}{2}} = (N\delta^2)^{\frac{1}{2}} \tag{2.1.11}$$

$$\langle X^2(N)\rangle^{\frac{1}{2}} \propto N^{\frac{1}{2}} \tag{2.1.12}$$

Each step takes some amount of time τ. The total time is

$$t = N\tau \tag{2.1.13}$$

$$N = \frac{t}{\tau} \tag{2.1.14}$$

$$\langle X^2(t)\rangle = \frac{t}{\tau}\delta^2 = (\frac{\delta^2}{\tau})t \tag{2.1.15}$$

$$\langle X^2(t)\rangle^{\frac{1}{2}} \propto t^{\frac{1}{2}} \tag{2.1.16}$$

Rather than increasing linearly with time, the characteristic distance our of random walker increases as the square root of time. To go twice as far, the particle needs to take four times as many steps. This is the key characteristic of Brownian motion.

Using the defnition of diffusion coefficient, ($D = \frac{\delta}{2\tau}$)

$$\langle X^2(t)\rangle = (\frac{\delta^2}{\tau})t \tag{2.1.17}$$

but,

$$\delta = 2D\tau \tag{2.1.18}$$

$$\langle X^2(t)\rangle = 2Dt \tag{2.1.19}$$

this equation is the mean displacement squared from the initial position for one dimensional random walk. Similarly, in two dimension, this quantity can be easily shown as follows:

$$r^2 = X^2 + Y^2 \tag{2.1.20}$$

but the motion along X is equal to that along Y. Hence,

$$\langle r^2(t)\rangle = 4Dt \tag{2.1.21}$$

For three dimensions mean square displacement is

$$\langle r^2(t)\rangle = 6Dt \tag{2.1.22}$$

Chapter 3

Simulation technique

In this chapter, we briefly describe the simulation techniques that has been followed during the simulation. In the first section, we describe the basic steps that we followed during simulation. In the second section, we make a clear description of the implementations of cellular automata rules.

3.1 The rules of the cellular automaton

CA are regular arrangements of single cells of the same kind. Each cell holds a finite number of discrete states. The states are updated simultaneously at discrete time levels. The update rules are random and uniform in space and time. The rules for the evolution of a particle depend only on a local neighborhood of cells around it [3,4].

In a CA model, the time domain can be discretized into a series of finite time steps t_1, t_2,...,t_i, Some basic rules are outlined as follows:

(a) Each particle stays within one CA cell at time t_i.

(b) Each particle selects one exit as the movement direction.

(c) After the movement direction has been determined, each particle will only select one cell among all adjacent cells surrounding the current one for the new position at time $t_i + 1$.

(d) If one cell is selected by several particles at the same time step, it will be randomly assigned to one of them. The other occupants will have to wait within their current cells until the next time step.

(e) All particles update their positions at time t_i+1, and then based on the new situation, choose new exits and cells for themselves at time t_i+2.

(f) The motion can be toward the up, down, left, right or central cell, by mean of a random choice.

(g) If the destination cell is already occupied by a particle, the particle remains on its own row, with the same previous random choice as motion direction.

In a rectangular two dimensional box of 2s x 2s having identical grids, particles will be randomly generated, at the initial time $t_0 = 0$. The generated particles represent the Brownian particles. The particle jumps without friction on the grid at every temporal step $t_1 = 1$, $t_2 = 2$, ..., $t_N = N$. A particle moves on the next row or column on the basis of some predefined rules.

3.2 Implementation of the cellular automata rule

We denote with grid (xo(i),yo(i)) associated to the initial position coordinate (xo(i), yo(i)) of the i-th particle, of the computational grid at time t_k. If grid (xo(i),yo(i)) = 0, no particle are present in the position; if grid (xo(i),yo(i)) = 1 the position should be considered as occupied by one particle. We assume that the time variable is incremented by discrete unitary values. Fates of certain simple starting configurations in the distribution of particles will be considered before the diffusion of particles is started. CA work in a discrete manner. That is to say time goes step by step. In our case, after generation of particles on the grid is performed, each particle examines its environment and determines its future state. In each time step each particle will move randomly in one of the possible directions. Each particle will have 4 possible movement directions for the two dimensional case and 5 if we take the possibility of no movement.

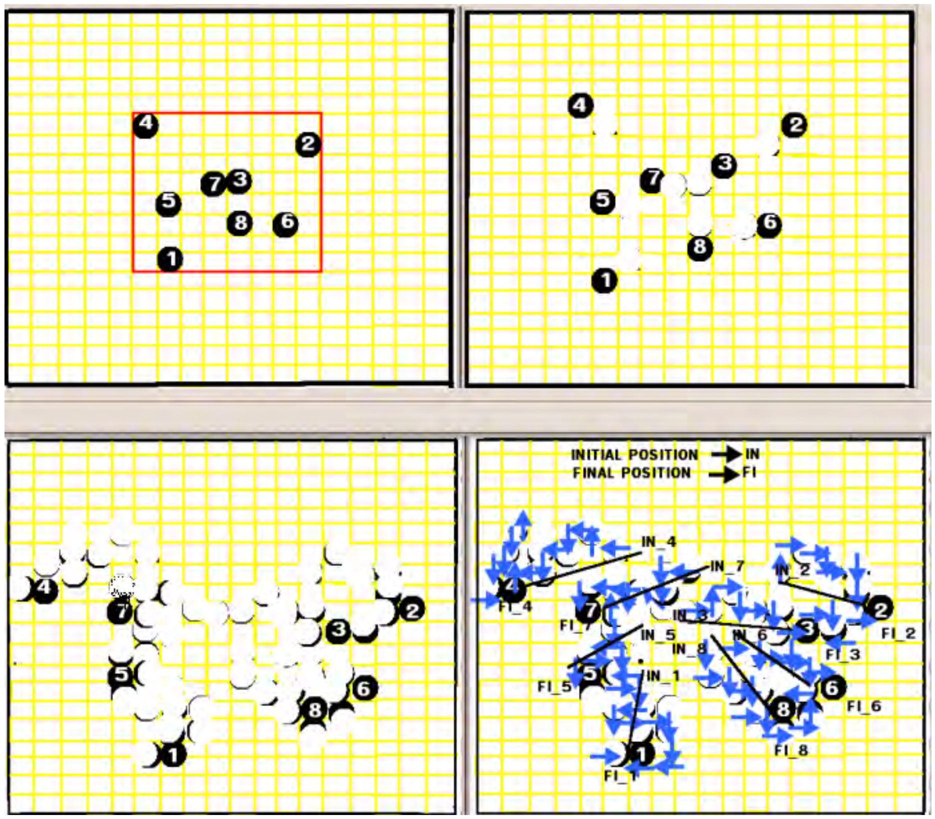

Figure 3.1: The left side graph of the upper plot is the initial configuration of 8 particles inside the 8 by 8 fictitious boundary, the right one tells that, the fictitious boundary is imaginary and the particles can pass it. The left side of one of the lower plots shows us particles movement after 13 time steps and the right one is particle displacement after 13 time steps.

In our simulation we gave an rank for each particles so as to identify initial and final position of all particles which are randomly generated on the grid. In addition to this, we have used an imaginary boundary in which we generate the initial positions of all particles. In our assumption we consider the following rules for the fictitious boundary:

(1) The fictitious boundary should not be an obstacle for the diffusion of particles, rather, it should pass the particles freely, for the motion of particles after they have been generated. Its main basic objective is only to keep the initial configuration bounded in the required boundary, so as to fix the time steps to use in the simulation in order to control the boundary effect.

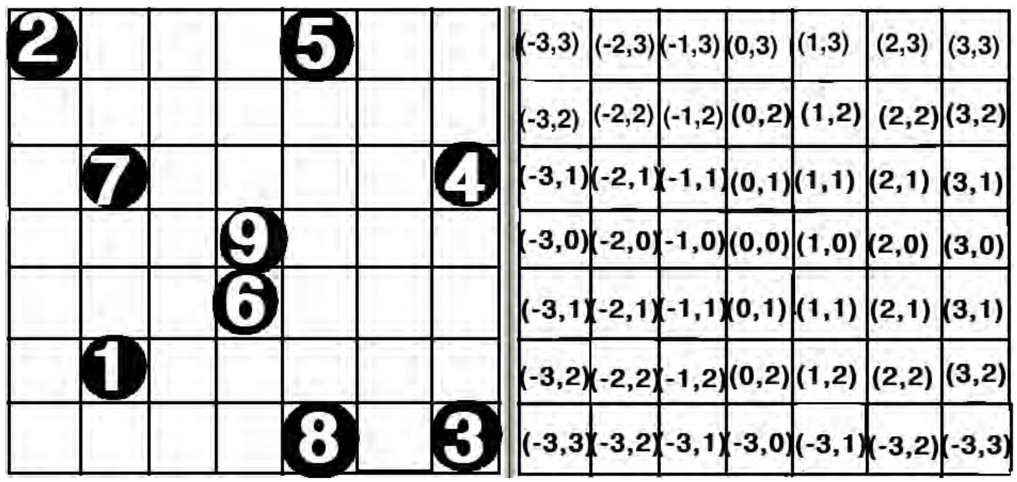

Figure 3.2: These plots are the initial configuration of 9 particles in side the 7 by 7 grids and the coordinates of each particle.

(2) It must give enough space for the diffusion of particles. In our simulation the number of cells in the fictitious boundary is at least 3 times greater than the number of particles generated inside it.

(3) No particle should be out side of this boundary during initialization of position.

(4) To perform movement, for each particle in the initial configuration one may sum ± 1, for each time step. This sum may possible the particles movement to the other position.

To move any particle to the right side we need to add (+1) at the x coordinate of the particle. If we sum (-1) to the x coordinate, we will move the particles to the left side, (-1) to the y coordinate for down, (+1) for up and (+0) for no movement.

In figure 3.2 we have the initial configuration of 7 particles in the 49 grids. In this configuration there is no particles overlap. After the initial time and position of each particles were assigned, each particles will be ready to move for the next position by checking their neighbors applying the cellular automata rule as shown in figure 3.3.

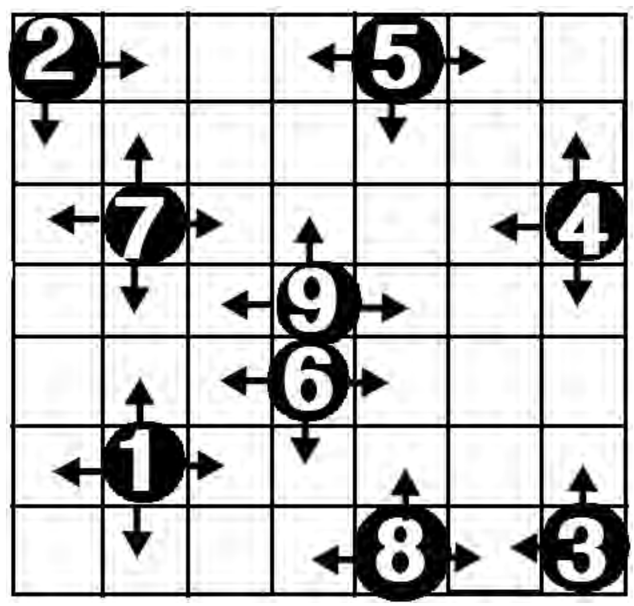

Figure 3.3: Each particles randomly select one of the four directions.

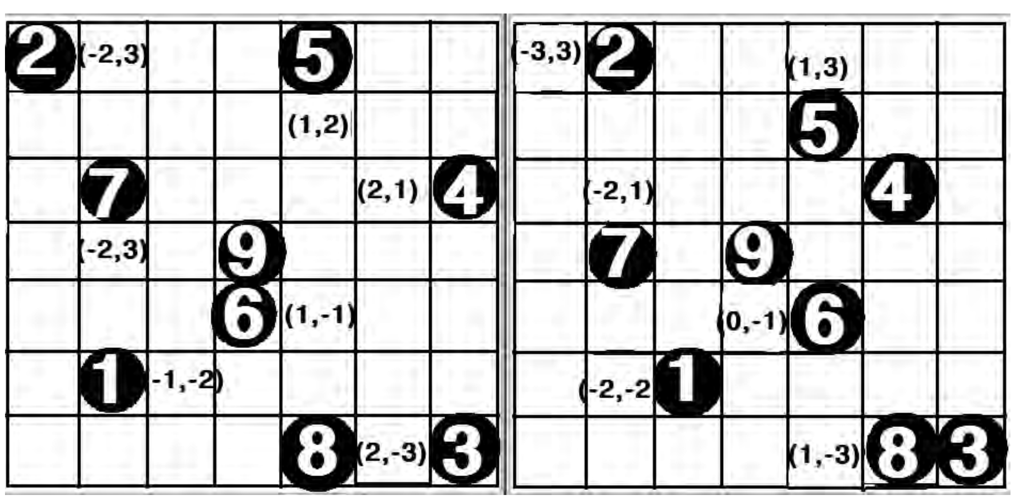

Figure 3.4: The figure in the left side shows us the randomly selected direction towards the selected grid, and figure at the right side shows us the old position coordinate.

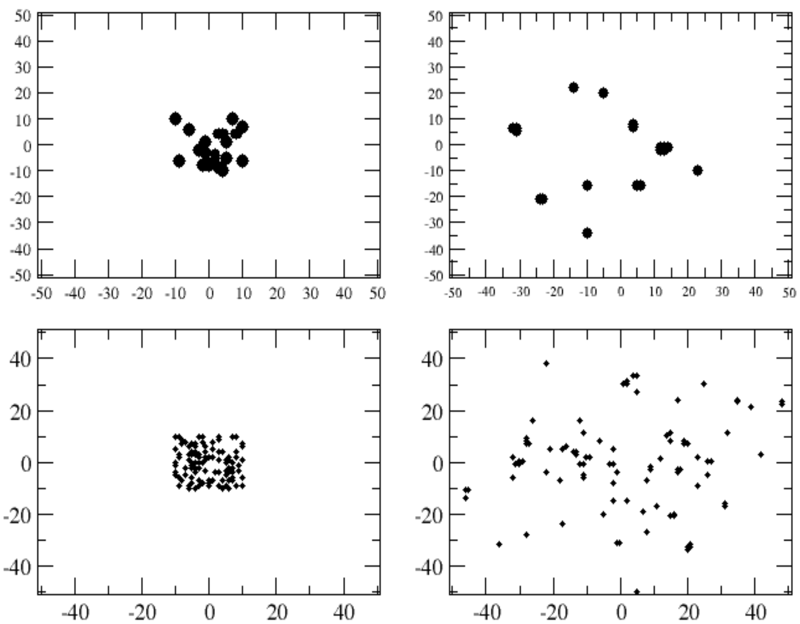

Figure 3.5: These graphs are the simulation result of initial position and position after 200 time steps starting diffusion from positions in an imaginary boundary box centered at the origin. The imaginary box size centered at the origin is 20 by 20 grids.

As an example: we take the particle 2 having coordinate (-3,3), if we add (+1) to the x coordinate we will move the particle from position coordinate (-3,3) to (-2,3) (see figure 3.4).

Chapter 4

Data analysis and discussion of the results

In the first section of this chapter, we describe how the initial position of each particle is assigned. In the second section, by assigning unequal percentage of preference on the selection of direction of motion. In the third section, we describe root mean square displacement for fixed percentage of concentration. In the fourth section, we investegate root mean square displacement for different percentage of concentrations. In the fifth section, we describe mean square displacement for different time steps. In the sixth section of this chapter, we describe root mean square displacement of Brownian particles for different time steps.

4.1 Random distribution of the particles on the two dimensional box

At the very beginning of the simulation the particles' position have to be assigned in a number of equal grid, which are parts of the two dimensional box. The number of all grid in the two dimensional box is equal to the area of the box, this means that each of the four sides of all grids in the box has one unit length. The initial positions of all particles should be assigned in the way that it consider the following initialization conditions:

1)Each grid should be occupied at most by one particle

2)A grid may or may not be occupied by a particle.

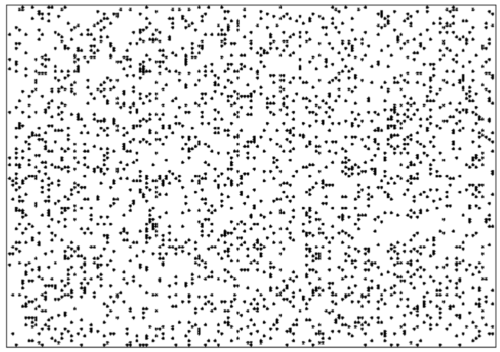

Figure 4.1: Initial configuration of 2500 particles in two dimensional grids in a box having 22500 grids.

3)The initial positions of each particle should be randomly given.

4)Before cellular automata rules are implemented every particle should have a rank to know which particle is changing its position after each time step.

4.2 Assigning unequal percentage of preference on the selection of direction of motion

Consider we change the percentage of direction preference of each particles rather than 20 percent for each directions, by making probability weights 20 percent left, 20 percent right, 20 percent zero movement, 10 percent up and 30 percent down. As the time step increases the final position of the particles will be to the direction of downwards, which is the most preferred direction by the particles as shown in the figure 4.2.

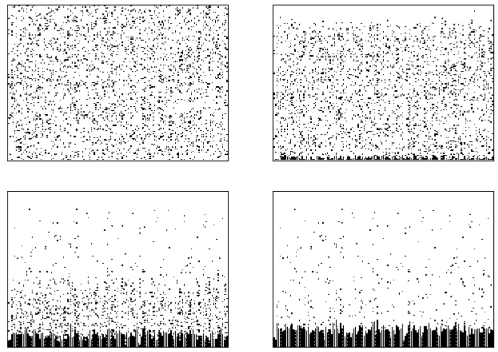

Figure 4.2: This graph is the simulation result of 2500 particles on 22500 grids after their random movement is performed for 50 time steps to one of the four direction or stay depending on probability. The probability weights are 30 percent down, 20 percent up, 20 percent right, 20 percent left and 10 percent zero movements. For many steps in time, the particles will move to the bottom of the simulation. The above figure correspond to the 0, 50, 500, 1000 time step.

4.3 Root mean square displacement for fixed percentage of concentration

Using cellular automata technique, after randomly generating a number of particles on the lattice, by changing the number of cells used in the simulation, and fixing the concentration of the particles, one can obtain diffusive behavior of Brownian particles in relation with the number of cells. From figure 4.3 it is clear to see that as the number of cells used in the simulation becomes large, by fixing the concentration of particles, the root mean square displacement increases.

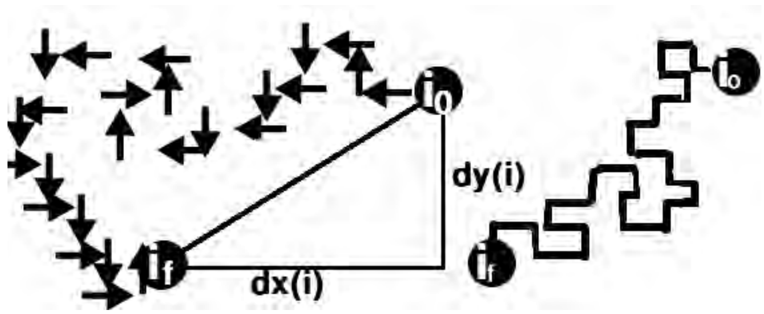

Figure 4.3: The plot is the initial and final position of a particle.

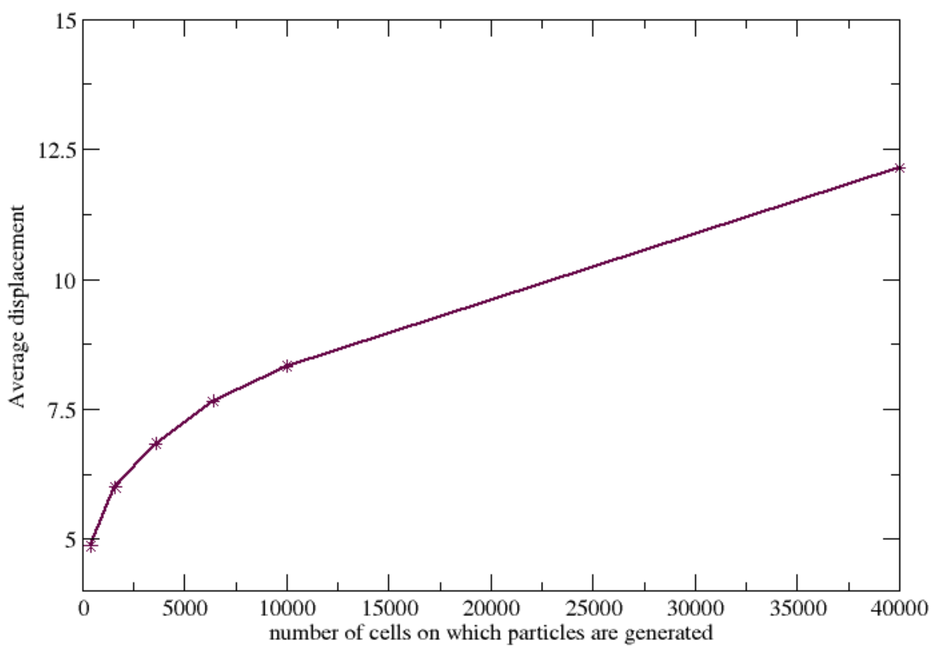

Figure 4.4: The graph is number of cells versus average displacement (root mean square displacement) of particles for 20 percent of concentration.

4.4 Root mean square displacement for different percentage of concentration

Similarly, using the automata rule, by fixing the number of cells and by varying the concentration (changing the number of particles) used in the simulation we get a result which is very different from figure 4.3. As the number of particles in the simulation is large for fixed number of cells, the obstacle for the movement of each particle increases and the root mean square displacement decreases as shown in figure 4.4. This graph is

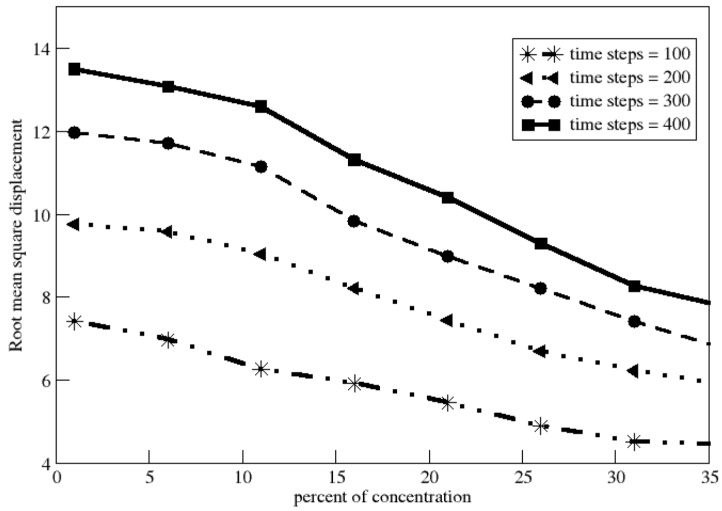

Figure 4.5: This graph is the simulation result of root mean square displacement vs percentage of concentration. It is the obtained by changing the concentration of particles inside 40,000 grids.

concentration versus displacement at 100, 200, 300 and 400 time steps. We can see the behavior of the graph of RMSD (root mean square displacement) at different concentration and in different time. From our simulation result we have proved that as the concentration of particles increases then the displacement of particles will also be increased.

4.5 Mean square displacement of Brownian particles for different time steps

We present a detailed derivation of the closed-form expression for the diffusion coefficient that was initially obtained by Einstein (look at equation 2.1.21).

Mean of displacement square is $\langle r^2(t) \rangle = 4Dt$, for the diffusion of particles in two dimensions. The mean square displacement of the Brownian particles diffusing in the 1,000,000 grids is plotted (see figure 4.5 and 4.6). It is the simulation result of 400 particles at 0, 5, 10, 15, 20 time steps. For very large time steps, the root mean square displacement will increase as a function of time.

Figure 4.5 is the simulation result of the mean square displacement of 400 particles for fixed number of cells and concentration of particles, but only the time steps are changed. In this graph we have seen the property of graphs which are plotted as a function of mean square displacement of particles (MSDP) versus time steps. In these graphs one can clearly observe that the increment of MSDP due to the increment of fictitious boundary. This is due to the fact that for equal number of particles as the number of cells in the fictitious boundary (FB) is large, most particles in it could not be able to move freely even from the beginning of the simulation. In contrast, the small number of cells in it will make the particle to be over crowded comparatively with the large one. This means at the beginning of the simulation, some particles will stay on their old position after they check the occupation of the randomly selected neighboring cells. The crowdedness of these particles will be reduced as time goes on, hence, those imaginary boundary system having greater number of cells inside, will have a better permission for the particles to diffuse inside them. In addition to this, fluctuation on the slope of the graph minimizes for those systems which are bounded by larger fictitious boundary (FB) representing the field of observation. The mean square displacement can be evaluated as follows:

$$MSDP = \frac{1}{NP}\Sigma_{i=1}^{NP}((xf(i) - xo(i))^2 + (yf(i) - yo(i))^2) \tag{4.5.1}$$

where, MSDP is mean square displacement of particles.

Let us take some points from figure 4.5, If we compare 1600 and 3600 cells inside the fictitious boundary, then the MSDP is large and the slope of the graph is better for particles inside 3600 cells. However, this condition is not observed at 6400 and 10,000 cells in this boundary. This shows us, after a certain greater number of cells inside FB, the value of RMS and the slope of the graph will not be changed. So to obtain a better result, we take 100 times simulated result and taking ensemble average.

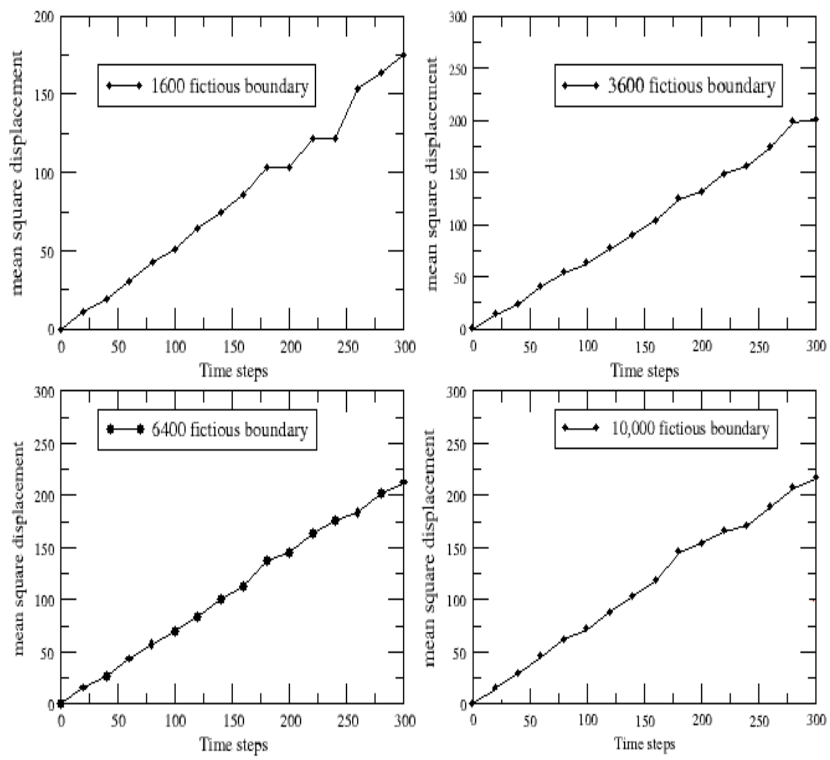

Figure 4.6: This graph is mean squared displacement of 400 particles vs time steps of four different fictitious boundary. These graph are the result of 10 simulations and taking sample average.

Figure 4.6 is the simulation result at 0, 50, 150, 200 time steps. As shown in this graph above as the concentration of particles increase, mean squared displacement will decrease for a given time step. The graph is the simulation result of the mean square displacement of 50, 500, 1000, 2000, 3000 particles for fixed number of cells. The simulation is done for 50 times to take ensemble average. When we change the number of particles generated in a given number of grids, we are changing the concentration of particles.

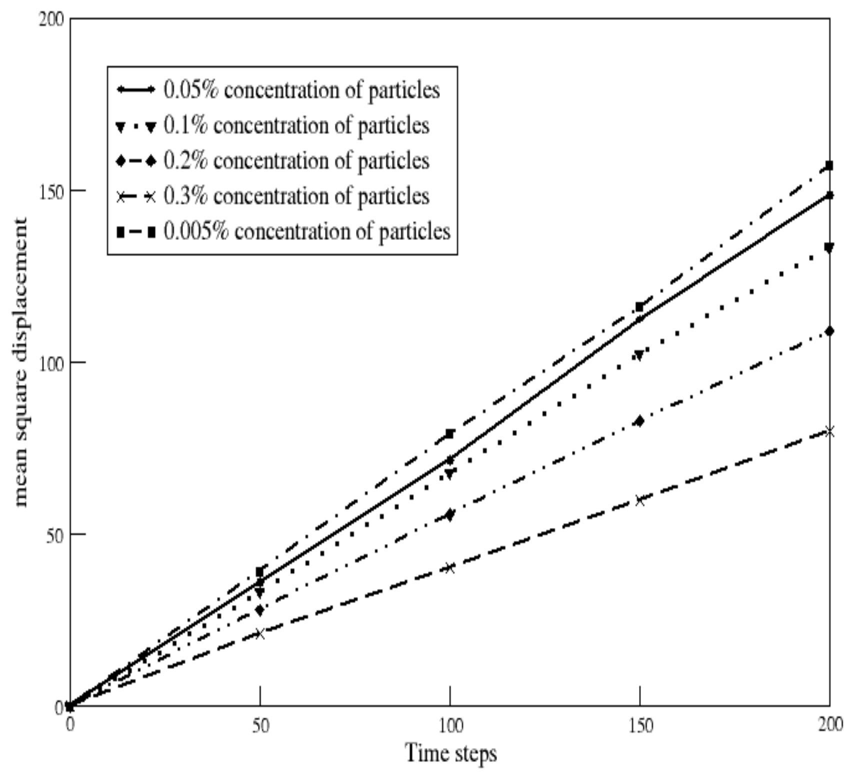

Figure 4.7: This graph is mean squared displacement of particles vs time steps of four different percent of concentration. We use 50, 500, 1000, 2000, 3000 particles by diffusing in 40,000 grids inside fictitious boundary. The fictitious boundary are included in 1,000,000 grids of the total grids in the real boundary.

concentration of Brownian particles	Diffusion coefficent of particles in $\left(\frac{\text{lattice size square}}{\text{montecarlo time step}}\right)$
0.3	0.4
0.2	0.6
0.1	0.7
0.05	0.75
0.005	0.8

Figure 4.8: This table is the concentration of Brownian particles used to plot figure 4.6 and the diffusion coefficient obtained during the diffusion of the particles.

4.6 Root mean square displacement for different time steps

The diffusion of Brownian particle is dependent on the time steps by which the particles are moving. By fixing the number of cells used to simulate and changing the time steps used in the simulation, we observed that the root mean squared displacement increases as the number of time steps in the simulation increases. In figure 4.8, similar to what we saw in the behavior of mean square displacement versus time graphs, we have generated different number of particles inside the fictitious boundary (FB) and let them to diffuse until they approach the real boundary, which is very far away from the FB. In the simulation part we know the initial and final positions of each particles. By using these two known values of a particle, we can find the displacement of each particles, the mean square displacement and the root mean square displacement. The root mean square displacement can be evaluated as follows:

$$RMSDP = \frac{1}{NP}\Sigma_{i=1}^{NP}\sqrt{(xf(i) - xo(i))^2 + (yf(i) - yo(i))^2} \tag{4.6.1}$$

where, RMSDP is square root of mean square displacement of particles. In the simulation part of this paper by using the above formula, we have plotted RMSDP versus time steps. Mean square displacement of particles is the square root of time, i.e

$$SRMSDP \propto \sqrt{t} \tag{4.6.2}$$

The graph of RMSDP versus time in our simulation, proves the theoretical and experimental results which have been done by many researchers. The main difference between these researchers work and ours is the method we followed to prove the relation between root mean square displacement and time. In this paper we followed the method of cellular automata.

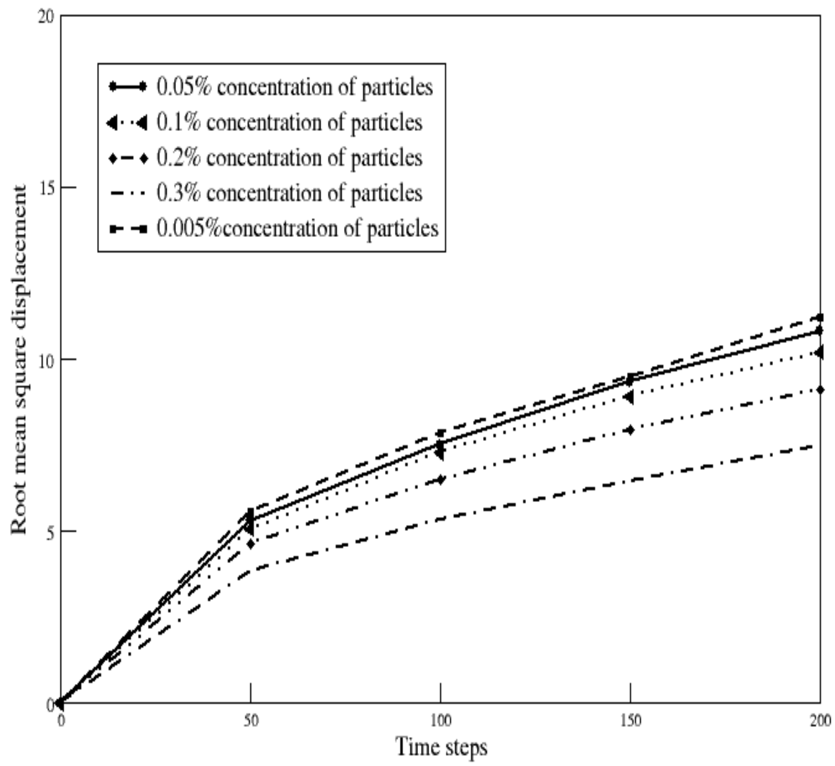

Figure 4.9: This graph is root mean square displacement of particles vs time steps. This graph is the simulation result of four different percent of concentrations of particles diffusion for 200 time steps. We use 50, 500, 1000, 2000, 3000 particles by diffusing in 40,000 grids inside fictitious boundary. The fictitious boundary are included in 1,000,000 grids of the total grids in the real boundary. Figure 4.8 is the result obtained after simulating 50 times for a fixed concentration and by taking ensemble average.

Chapter 5

conclusion

In this project, we have studied the diffusion coefficient of the Brownian particles. The particles were randomly generated on the grids. We made the particles to select one of the four directions and the stay. We observed that when the percentage of preference for the diffusion along one of the four directions and the stay is 20 percent, then the particles do not concentrate only at a fixed position. In contrast, we have seen that for different percentage of preference, the particles will concentrate around the most preferred direction. In our simulation, we have generated 2500 particles on 22500 grids. We have seen that the concentration of particles after 50, 500, 1000 time steps is around the most preferred direction depending on the time steps used for the diffusion of particles.

We have made a clear investigation on the mean square displacement (MSD) of particles and the root mean square displacement (RMSD) of particles. We have observed that the MSD and RMSD of the particles were increased as the number of grids got large. For 20 percent of concentration, we have obtained that, as the number of grids was changed from 400 to 40,000, the RMSD of particles were increased from 5 to 12.5. This means that large number of grids gave us a better possibility of changing positions for the diffusion of particles. In addition to this, RMSD of particles have been studied by changing the percentage of concentration from 10 to 40 percent. In this case, we have found that as the percent of concentrations of particles were increased from 10 to 40 percent, the RMSD of particles were decreased from 13.7 to 7.9. This result was very dependent on the time steps used in the simulation for the diffusion of particles.

MSD and RMSD of particles have been studied for different time steps by fixing and changing the value of concentration of particles in the grids. Firstly, we have obtained that the MSD of particles were increased as the time steps used in the simulation was getting large. During an investigation of this, we have used 50, 500, 1000, 2000, 3000 particles to diffuse in 40,000 grids inside the fictitious boundary. This boundary has been imagined inside the real boundary. In the real boundary there was 1,000,000 grids including grids in the fictitious boundary. We have obtained different value of mean square displacement and root mean square displacement for different values of concentration. For the case of mean square displacement we have obtained five values of diffusion for different values of concentration and time steps. From these results, we have concluded that, when the concentrations had been increased, then MSD were decreased. In addition to this we have investigated that MSD is directly proportional to the time steps.

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Declaration

All the sources of material used for the thesis have been fully acknowledged.

Name: birhanu abera

Signature:

Place and time of submission: Addis Ababa University, June 2009

This project has been submitted for examination with my approval as University advisor.

Name: Dr.Mulugeta Bekelle

Signature: