Simulation of the Brownian movement using a new method based on cellular automata.

Eric Plaza\textsuperscript{1} and Rafael Martin\textsuperscript{2}

\textsuperscript{1}Universidad del Zulia, Laboratorio de Sistemas Desordenados, Facultad Experimental de Ciencias - Maracaibo, Venezuela.
\textsuperscript{2}Centro de Física Teórica y Computacional, Escuela de Física, Facultad de Ciencias, Universidad Central de Venezuela, Caracas, Venezuela

(Dated: April 16, 2009)

We propose a new model based on cellular automata technique to simulate the behavior of Brownian’s particles with restrictions. In our model each particle will moves randomly for each time-step in each of his possible directions for a two-dimensional network. The movement of each particle is the result of collisions with other particles and this interaction determines the movement in one direction; they can only occupy one cell at time. We take only a representative percentage of fluid particles. We calculate the square root of the arithmetic mean of particles displacements (SRAMPD) in order to make a comparison with the diffusion coefficient in an adiabatic fluid. We also observe the behavior of the (SRAMPD) when we change the network size of the simulation for a fixed concentration and when we change the particles concentration for a fixed network size.

PACS numbers: 87.55.kd, 05.40.Jc, 46.65.+g

1. INTRODUCTION

Brownian motion is the random movement for some nanoscopic particles in a fluid. It is named in honor of Robert Brown who described it in 1827. The random movement of these particles is the result of constant bombardment of his surface by fluid molecules under a thermal agitation. Atomic bombardment at this scale is not always completely uniform and have large statistical variations. The pressure on one side can vary, causing the movement observed \cite{4}.

The mathematical description of the phenomenon was developed by Albert Einstein \cite{1}. Einstein found a way to confirm the atomic nature of matter observing the relationships between the macroscopic diffusion coefficients $D$ and the atomic properties of matter. This relationship is:

$$D = \frac{(RT)}{(Na6\eta\pi)} \tag{1}$$

Since $R$ is the gas constant, $Na$ Avogadro number, $T$ is temperature in Kelvin, $\eta$ the viscosity, "a" the radius of the Brownian particles and $D$ is the diffusion coefficient of the material suspended in the liquid \cite{1,2}. The theory of Brownian motion was developed in order to describe the dynamic behavior of particles whose mass and size are much larger than the rest in the medium in which they are. Einstein was succeed in proving that the average movement of the brownians particles in one direction is an expression such as:

$$\lambda = \sqrt{(2Dt)} \tag{2}$$

In this work we present a new simple method to simulate the diffusive behavior of particles that interact in a fluid, we control the statistical characteristics of the particles movement by simples integers sums. We observed only the Brownians particles in the simulation. Each particle is localized in a two-dimensional network and they have for each time-step one movement direction. This direction will be chosen randomly by our algorithm.

The simulation represents a percentage of total particles immersed in fluid, showing the phenomenon of self-diffusion. We perform calculations for the (SRAMPD) in order to compare with the experimental values obtained for the diffusion coefficient in \cite{1}. We calculate the standard deviation (SD) of the values obtained for the (SRAMPD) in 50 simulations as a measure of the dispersion of the simulated data. Also we make simulations changing the concentration of particles fixing the network size, and changing the size of the network for a fixed concentration. In both cases we calculate the behavior of the (SRAMPD) and the (SD).

2. SIMULATION TECHNIQUE

Our model use two networks represented as two matrix (\textit{Mi} and \textit{Me}). Each number inside on the matrix cell's in "\textit{Mi}" represent the position in "\textit{Me}" matrix. This number may change for each time step and determine the particle position in the spatial matrix \textit{Me}. The supra-index of each cell in \textit{Mi} represents the name of each particle in \textit{Me}. (see Figure 1). This method will be called "Reticular Matrix Mapping" or MMR for his spanish acronym.

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 non-movement. To perform this movement, for each particle in \textit{Mi} one may
FIG. 1: Example: Particle 1 (position 1x1) displayed in the cell as the number "4" this number represent the position in Me (1x4). The particle 3 of Mi it is in the position 16 and so on for all other particles. The network size it’s represented by N3xN4 = 5x5 = 25, and the numbers of particles by N1xN2 = 3x3 = 9.

FIG. 2: Example of particle 6 displacement from position 13 to position 18.

sum a integer, for each time-step. This sum may possible the particles movement to other position. to move any particle to the right side we need to add (+1) at the corresponding Mi cell, this will move the particle to the right side in Me matrix. If we sum (-1) we will move the particles to the left side, (-N3) for up, (+N4) for down and (+0) for non-movement. N1 and N2 are the matrix components for Mi and N3, N4 the matrix components in Me.

As an example: We take the particle 6 in position 13, if we add (+5) to the particle 6 we will move the particle from position 13 to 18 in "Me" (see Figure 2).

Our particle systems have restrictions to moving up, down, right, left and no movement. We can assign a percentage of movement for each direction. Every time-step each particle will have the chance to move in a direction that will be chosen randomly. We assign a weight of probability for each of his possible directions. In this case for our propose, all direction must have the same probability weight to correspond a random movement in all directions like in a Brownian movement or a 2 dimensional random walk. (20% up, down, right and non moving).

This method allows us to stadistastically control the particles movement. In the Figure 4 we show snap-shots for particles which moves randomly with different weight percentage. In this case, the particles will move preferentially to the bottom part, like high density particles in a classic fluid, subject only to gravity forces, i.e. A more higher probability to move in a "down" direction. The simulation showed in the figure 4 correspond with weight percentage probabilities: down 30%, up 20%, right 20%, left 10% and non-movement of 10% in 1000 steps simulation. We can appreciate a clear trend for all particles to stay in the bottom part of the picture.

A mechanism in the code prevents particles with the same number in the Mi matrix, avoiding particles in the same position. For the boundary conditions are established rules on the border cells to determine the type of boundaries that we want. In our case, we choice as boundary conditions rigid-walls enclosing all particles.

3. SQUARE ROOT OF THE ARITHMETIC MEAN OF PARTICLES DISPLACEMENTS

In order to compute (SRAMPD) we take the initial and final position for all particles in the network. The number of particles is given by "n" sub-index. The initial position are represented by "i" sub-index and the final position by the "f" sub-index. Where n = N1xN2 is the number of particles in Mi. Using the familiar expression for the two-dimensional distance between two points; summing and dividing over all particles we obtain the (SRAMPD) in the simulation:
FIG. 5: Values of $\gamma$ obtained in 50 simulations with the same parameters $M_i \times 30 = 900$ particles, $M_e \times 100 = 10,000$ cells in 200 time-steps. The probability for each movement direction was 20% for each one: Up, down, right, left and not moving. The mean of $\gamma$ in the computational experiments carried was $\gamma = 10.3159$ cell units and the standard deviation was 0.0152 in the same units.

FIG. 6: $\gamma$ Values for different network sizes with the same particles concentration. The particles concentration was fixed at 20.25%. If $M_e = 6400 = 80 \times 80$ particles, and $M_i = 36 \times 36 = 1296$ particles the concentration will be 20.25%. Each data obtained for $\gamma$ was the average of 50 simulations. Each simulation was performed in 200 time-steps with the same characteristics. The probability for each motion direction was 20% up, down, left and right and non movement.

$$\gamma = \frac{1}{n} \sum_{n} \sqrt{(x_{n1} - x_{n2})^2 + (y_{n1} - y_{n2})^2} \tag{3}$$

To compate (SRAMPD) in the simulation $\gamma$, with the experimental (SRAMPD) $\lambda$ we need to establish a scale parameter $\sigma$ associating in this, the simulation scale with the real scale. This expression will be given by the product between the (SRAMPD) in the simulation $\gamma$ and the scale factor $\sigma$:

$$\lambda = \sigma \gamma \tag{4}$$

If $N$ is equal to $6 \times 10^3$ in accordance with the kinetic theory of gases, water at 17°C, $k = 1.35 \times 10^{-23} J/K$, the particles diameter 0.001mm we have that $\lambda$ in the x direction is $0.8\mu = 8 \times 10^{-5} cm$ and the displacement of a half minutes will be $0.6\mu$ [1]. This value is independent of the number of experiments made it and its a invariable value.

If we take the (SRAMPD) simulation value: $\gamma = 10.3159$ and divide between the experimental value of $\lambda = 6\mu$ in [1]. We can calculate the value of $\sigma$ using (4) $\sigma = 0.5816 \times 10^{-\gamma}\mu$.

Figures 6 and 7 show the behavior of $\gamma$ when we vary the network size maintaining the same particles concen-
FIG. 8: Graphic for $\gamma$ values varying the concentration of particles and fixing the size of the network $Me=100x100=10.000$ cells. Each measure is the average obtained from 50 simulations for $\gamma$, each simulation was performed under the same conditions 20% probability for each movement direction: up, down, left and right does not move in 200 time-steps.

FIG. 7: Standard deviation (SD) for the data obtained in the figure 6 for all of the 50 simulations in $\gamma$. These values represent a measure of data dispersion in the simulation.

Graphs 8 show the behavior of the (SRAMPD) when we varying the concentration of particles in the simulations and fix the network size. We obtained data for 18 different concentrations ranged from 1% to 90% of occupancy. Each point corresponded to the average value of $\gamma$ in 50 simulations; each simulation was performed in 200 time-steps with the same movement probability: up, down, left right and non movement 20%. The network size for all cases was 100x100 cells or 10,000 possible positions. We see as the value of (SRAMPD) decreases when we increasing the particle concentration. That is attributed to the fact that the movement of particles
depends of the numbers of available possibilities in his neighbors, if we have a more higher numbers of particles, the possibilities will be decrease changing the particles mobility. The values of (SD) remained in a relatively small variations if we compared with the size of the network and the simulation magnitud of (SRAMPD).

4. CONCLUSIONS

The properties on invariability obtained by Einstein in [1] for the compute of the (SRAMPD) and the respective comparison with the diffusion coefficient in a fluid, give us a prove of the randomness characteristic of the Brownian movement phenomenon. This is the same principle used in random walks in 2D. No matter how many times does the experiment we always get the same results. We represent this situation with our new method MMR and we obtained the same results for many experiment. The graphics 6 show us this result with a little dispersion proved by the smalls values of (SD). For 50 experiments we obtain a dispersion of 0.0152 cells units and the mean in 50 simulations was $\gamma = 10.3159$ cells units. In order to compare with real experiments showed in [1] we propose a scale parameter $\sigma$. We perform simulations changing the size of the network and fixing the concentration, and fixing the network size and changing the concentration. In the first case we observe an increase of $\gamma$ and a soft decline in the dispersion. In the second case we observe a decline of $\gamma$ caused by the increasing number of particles. For too many particles they lose possibilities to occupy positions and mobility in general decrease. The method allows us to implement a so higher complex situation, and this work represents only ones of the more simples experiment. We will go to perform simulations in: the particles movement having preferences to move in one special direction, simulations taking in a count the collisions between particles, 3D networks, fluid particles moving in a porous media, and so other situations.

[1] Albert Einstein, *Investigations on the theory of the Brownian movement* (Dover Publications, 1956).
[2] P. Langevin, R. Acad. Sci. 146, 530-533 (1908).
[3] Donald L., Ermaek J., and A. McCammon, Chem. Phys. 69, 1352 (1978).
[4] L. E. Reichl, *A Modern Course in Statistical Physics* (John Wiley Sons, 1998).
[5] Sauro Succi, *The Lattice Boltzmann Equation for fluid dynamics and beyond* (Clarendon Press, 2001).
[6] U. Frisch, B. Haslassher, Y. Pomeau. Phys. Rev. Lett 56, 14 (1986).
[7] J. Hardy, Y. Pomeau, Phys. Rev. A 16, 2 (1977).
[8] J. Hardy, O. de Pazzis, and Y. Pomeau, Phys. Rev. A 13, 5 (1976).