

## NUMERICAL MODELLING OF THE ONE-DIMENSIONAL DIFFUSION BY RANDOM WALKERS

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### 1. THE MATHEMATICAL MODELLING OF THE DIFFUSION

The distribution of the particles in a domain  $\Omega \subset \mathbf{R}^3$  at a moment  $t \in \mathbf{R}$  is described by the continuous field of the concentration  $c : \Omega \times \mathbf{R} \rightarrow \mathbf{R}_+$ . The differentiability properties of  $c$  are different for different processes of diffusion, but  $c$  usually is a function of  $\mathbf{C}^2$  class in the definition domain. The number of particles in a subdomain  $A \subset \Omega$  at the moment  $t$  is given by

$$(1.1) \quad n(A, t) = \int_A c(\mathbf{r}, t) d\mathbf{r}.$$

The concentration verifies a local balance equation [11]

$$(1.2) \quad \partial_t c + \nabla \mathbf{j} = g,$$

where the vectorial field  $\mathbf{j} : \Omega \times \mathbf{R} \rightarrow \mathbf{R}^3$ , is the particles flux density and  $g : \Omega \times \mathbf{R} \rightarrow \mathbf{R}$  is the source term. The balance equation (1.2) should be completed by a constitutive law which should connect the flux  $\mathbf{j}$  and the concentration  $c$ . A simple constitutive law is Fick's law, valid for small gradients of concentration

$$(1.3) \quad \mathbf{j} = -\tilde{\mathbf{D}} \nabla c,$$

where  $\tilde{\mathbf{D}}$  is the tensor of the diffusion coefficients.

In the case of the homogeneous and one-dimensional diffusion the tensor  $\tilde{\mathbf{D}}$  is reduced to a real parameter  $D$  and if  $g = 0$ , (1.2) becomes the one-dimensional diffusion equation

$$(1.4) \quad \partial_t c - D \partial_x^2 c = 0.$$

Depending on the initial and boundary conditions, the equation (1.4) has different types of solutions [2, 3]. For the initial condition  $c(x, 0) = N\delta(x)$ ,

where  $\delta(x)$  is Dirac's function, and the conditions at infinity  $\lim_{|x| \rightarrow \infty} c(x, t) = 0$ ,  $\lim_{|x| \rightarrow \infty} \partial_x c(x, t) = 0$ , the solution of the equation (1.4) is the concentration of  $N$  independent particles in Brownian motion

$$(1.5) \quad c(x, t) = \frac{N}{\sqrt{4\pi Dt}} e^{-\frac{x^2}{4Dt}}, \quad x \in (-\infty, \infty), \quad t > 0.$$

The rigorous definition of the concentration field is a problem which has not a solution yet. The number of particles in a set  $A$  can not be modelled as a absolutely continuous set function. Therefore, the Radon-Nikodym theorem [8] does not guarantee the existence of a corresponding density, as in the case of other fields in the continuum mechanics [4]. The existence of the concentration field  $c$  is postulated and the corresponding global quantity  $n(A, t)$ , is defined by (1.1) [11].

In the statistical mechanics, the probability that a particle should exist in an element of infinitesimal volume  $d\mathbf{r}$  centered on  $\mathbf{r} \in \Omega$  at the moment  $t$  is given by  $p(\mathbf{r}, t)d\mathbf{r}$ , where  $p(\mathbf{r}, t)$  is the one-particle probability distribution [7]. The relation to the concentration is given by

$$(1.6) \quad c(\mathbf{r}, t) = Np(\mathbf{r}, t),$$

where  $N$  is the total number of particles. In this way, the concentration was substituted for another continuous field and its existence was postulated as well. The definition of the probability distribution in the statistical mechanics is so far an open problem [1]. For a diffusion process,  $p(\mathbf{r}, t)$  satisfies the Fokker-Planck equation which according to (1.6), is equivalent to the diffusion equation.

## 2. THE MICROSCOPIC DEFINITION OF THE CONCENTRATION

To discuss the problems occurring to the definition of the concentration, we present the method usually used in thermodynamics [10]. Consider  $N$  molecules in a volume  $V$ . The concentration at the point of the position vector  $\mathbf{r}$  at the moment  $t$  is defined as the number of particles per unit volume in a domain of volume  $\mathcal{V} < V$  centered at this point. The domain should be spherical, otherwise the concentration would depend not only on the position but also on the orientation of the domain. We denote by  $S(\mathbf{r}, a)$  the sphere of center  $\mathbf{r}$  and radius  $a$ . Then the concentration is defined as the function  $c: \mathbf{R}^3 \times \mathbf{R} \rightarrow \mathbf{R}_+$  given by

$$(2.1) \quad c(\mathbf{r}, t) = \frac{1}{\mathcal{V}} \sum_{i=1}^N H^+(a^2 - (\mathbf{r}_i(t) - \mathbf{r})^2),$$

where  $\mathbf{r}_i(t)$ ,  $t \in \mathbf{R}$ , is the position vector of the molecule  $i \leq N$  at the moment  $t$ . The left continuous Heaviside function  $H^+(a^2 - (\mathbf{r}_i(t) - \mathbf{r})^2)$  is equal to 1 if

the molecule  $i$  is inside the sphere  $S(\mathbf{r}, a)$  and vanishes otherwise. The function defined by (2.1) for given  $a$  and  $\mathbf{r}_i$ , is a finite linear combination of Heaviside functions having null derivatives except when their argument vanishes and the derivative does not exist. So (2.1) defines a step function which can not satisfy a partial derivative equation of the diffusion equation type.

In thermodynamics one considers that for a large enough  $N$  the function  $c(\mathbf{r}, t)$  given by (2.1) is well approximated by a continuous field. To obtain the condition that  $N$  should satisfy we analyze the simple case of the thermodynamical equilibrium state in absence of the exterior fields. Then the molecules are uniformly distributed in the  $V$  volume and, taken as a continuous field, the concentration has a constant value at any point in the volume and at any moment,  $c_o(\mathbf{r}, t) = N/V$ . If we want to verify this equilibrium distribution by definition (2.1), we count the number of molecules  $n$  at the moment  $t$  in the sphere  $S(\mathbf{r}, a)$ . It is obvious that the result is affected by fluctuations and the measured concentration  $c = n/\mathcal{V}$  differs from  $c_o$ . In [10], Section 114, one shows that  $n$  satisfies a Poisson repartition with dispersion  $\sigma = \sqrt{\bar{n}}$ , where  $\bar{n} = N\mathcal{V}/V$  is the mean number of molecules in  $\mathcal{V}$ . So, the dispersion of the concentration fluctuation is equal to  $\sigma_c = \sqrt{N/\mathcal{V}V}$ . If  $N$  is large enough,  $\Delta c = c - c_o$  has a normal repartition of zero average and dispersion  $\sigma_c$ . According to the "three sigma" rule of excluding rough errors [13], we impose that the relative error should be smaller than a value  $\varepsilon$  fixed with a confidence level of 0.997 and we obtain

$$(2.2) \quad 3\sigma_c \leq \varepsilon c_o \implies \frac{\mathcal{V}}{V} \geq \frac{9}{\varepsilon^2 N}.$$

For a large enough  $N$ , this formula gives the minimum volume  $\mathcal{V}$  (or the minimum radius  $a$ ) necessary to measure the concentration with the precision  $\varepsilon$ , i.e. the space scale for which the measured concentration behaves like a continuous field with approximation  $\varepsilon$ . If (2.2) is satisfied, we can write  $c(\mathbf{r}, t) \sim c_o(\mathbf{r}, t) + \mathcal{O}(\varepsilon)$ , for  $\varepsilon \rightarrow 0$ .

The classical definition of the concentration is not applicable when  $N$  or  $\mathcal{V}$  is too small. To exemplify, we consider the case when there is a single molecule in the volume  $V$ . Then  $c(\mathbf{r}, t) = \mathcal{V}^{-1}$  for  $\mathbf{r} \in S(\mathbf{r}_1(t), a)$ , and in the rest  $c$  vanishes. Therefore the concentration is completely different from the equilibrium concentration which is as well  $c_o(\mathbf{r}, t) = 1/V$  in the entire volume  $V$ . These difficulties occur because in definition (2.1) one implicitly supposes an instantaneous measurement of the molecules number in the volume  $\mathcal{V}$ . The actual measurement has a duration which defines the temporal scale as the volume  $\mathcal{V}$  (or the radius  $a$ ) defines space scale. If we denote by  $(t - \tau, t + \tau)$  the averaging interval, we define the concentration by

$$(2.3) \quad c(\mathbf{r}, t) = \frac{1}{2\tau\mathcal{V}} \sum_{i=1}^N \int_{t-\tau}^{t+\tau} H^+(a^2 - (\mathbf{r}_i(t') - \mathbf{r})^2) dt'.$$

In [14, 15] one proves that the function defined by (2.3) has a. e. continuous first order partial derivatives. That is, the temporal averaging transforms the step function (2.1) into a continuous field even if the discontinuities are conserved in the first order partial derivatives.

The new definition (2.3) is meaningful even when  $\mathcal{V}$  or  $N$  is very small and the classical definition (2.1) can not be applied. Consider again the thermodynamical equilibrium state with an uniform distribution of the molecules in the volume  $V$ . The number of molecules in  $\mathcal{V}$  is measured at each moment over the interval  $(t - \tau, t + \tau)$  and then it is averaged. We attach to this continuous temporal average a discrete one, to which we can apply the same Poisson distribution. We denote by  $\Delta t$  the mean time interval over which the molecule remains inside the volume  $\mathcal{V}$ . Consider the averaging interval  $(t - \tau, t + \tau)$  divided into  $2\tau/\Delta t$  subintervals of  $\Delta t$  length and suppose that the existence of the molecule in volume  $\mathcal{V}$  within an subinterval  $\Delta t$  is independent from its existence in the same volume within another subinterval  $\Delta t$ . Then the concentration fluctuations (2.3) for  $N$  molecules over a time interval of  $2\tau$  length, are equivalent to the fluctuations of  $2N\tau/\Delta t$  molecules in a  $\Delta t$  interval. Therefore instead of formula (2.2) we have

$$(2.4) \quad \mathcal{V}\tau \geq \frac{9\Delta t}{2\varepsilon^2 c_o}.$$

This formula expresses the relation between the space scale ( $\mathcal{V}$ ) and the temporal one ( $\tau$ ), necessary to obtain a continuous description of the concentration with a precision  $\varepsilon$ . Unlike (2.2), the relation (2.4) is valid for any  $N$ . The increase of the temporal scale can compensate the decrease of the space one.

### 3. THE NUMERICAL ALGORITHM

The random walk hypothesis is a simple form of microscopic evolution law of the form used in molecular dynamics [5, 9]. Consider a one-dimensional space lattice  $\{x_k = k\delta x \mid -m \leq k \leq m\}$ , where  $\delta x$  is the space step of the lattice. On the lattice there are  $N$  noninteracting particles which move according to the random walk law. If the  $i$ -th particle is at the site  $k$  at the moment  $t$ , then at the end of a time step  $\delta t$  the particle will be either at the site  $k - 1$ , or at  $k + 1$ , with probabilities equal to  $1/2$ . So in the time interval  $(t, t + \delta t)$  the  $k$  particle moves with  $-\delta x/\delta t$  velocity, respectively  $\delta x/\delta t$ , to neighboring site.

We denote by  $n_k$  the number of particles at the site  $k$  at the moment  $t$  and by  $n'_k$  (respectively  $n''_k$ ) the number of particles which move at the moment  $t + \delta t$  to the site  $k - 1$  (respectively  $k + 1$ ). Then the number of particles at the site  $k$  at the moment  $t + \delta t$  can be written

$$(3.1) \quad n_k(t + \delta t) = n'_{k+1} + n''_{k-1}.$$

It is well known that a diffusion process can always be approximated by a jump process [6, 16]. Consider a sufficiently smooth concentration field  $c(x, t)$

and  $n_k = c(x, t)\delta x$ . When the condition

$$(3.2) \quad D = \frac{\delta x^2}{2\delta t},$$

is satisfied then, for a lattice of infinite extent, in the limit  $\delta x \rightarrow 0$  and  $\delta t \rightarrow 0$  the number of particles given by (3.1) approaches the solution of the diffusion equation (1.4) multiplied by  $\delta x$ . This model is a one-dimensional multiple random walkers cellular automaton [12].

For the macroscopic description of this one-dimensional corpuscular system we use the method based on the time-space coarse grained averaging [14, 15]. We consider  $N$  particles moving on the real line during a temporal interval  $[0, T]$  according to the random walker rule given above. We also assume that each particle can be introduced or expelled from the lattice. We denote by  $t_i^+$  the moment when it appears and by  $t_i^-$  the moment when it disappears. So the position of the  $i$ -th particle is given by the function  $x_i : [t_i^+, t_i^-] \rightarrow [x_{-m}, x_m] \subset \mathbf{R}$ . We define the coarse grained average  $\langle 1 \rangle(x, t)$  of the particles number at the point  $(x, t) \in \mathbf{R} \times (\tau, T - \tau)$ , for the real parameters  $a$  and  $\tau < T/2$ , by the relation (2.3). Written for the one-dimensional case, it becomes

$$(3.3) \quad \langle 1 \rangle(x, t) = \frac{1}{4\tau a} \sum_{i=1}^{N^*} \int_{t-\tau}^{t+\tau} H^+(a - |x_i(t') - x|) dt'.$$

This function has first order a.e. continuous partial derivatives and it satisfies a balance equation of the form (1.2) [14, 15].

#### 4. THE NUMERICAL SIMULATION OF THE ONE-DIMENSIONAL NONSTATIONARY DIFFUSION

To simulate the diffusion process we apply the coarse grained averaging to the microscopic motion of the system described by the one-dimensional cellular automaton. The field  $\langle 1 \rangle$  can be obtained as a sum of the contributions  $\langle 1 \rangle_i$  of the  $N$  particles contained in the lattice over the temporal averaging interval

$$\langle 1 \rangle = \sum_{i=1}^N \langle 1 \rangle_i.$$

The average of the concentration field is obtained as the average of  $\langle 1 \rangle$  over all the possible evolutions of the particles from the origin to one of the extremities of the lattice. We obviously have  $\overline{\langle 1 \rangle} = N \overline{\langle 1 \rangle}_i$ . For the dispersion we have  $\sigma = \sqrt{N} \sigma_i$  and the condition  $3\sigma \leq \varepsilon \overline{\langle 1 \rangle}$  (the relative error of  $\langle 1 \rangle$  with respect to  $\overline{\langle 1 \rangle}$  be  $\varepsilon$  with a confidence level of 0.997) allows to determine the particles number needed to obtain this precision

$$(4.1) \quad 3\sqrt{N} \sigma_i \leq \varepsilon N \overline{\langle 1 \rangle}_i \implies N \geq \left( \frac{3\sigma_i}{\varepsilon \overline{\langle 1 \rangle}_i} \right)^2.$$

We consider that from the random walker algorithm a discrete description of a diffusion process is obtained, i.e. one knows the particles number  $n_k(t)$  at each of the lattice site and at the multiples of the time step. Since the numerical scheme assumes linear variations during the time and space steps and the averaging over smaller intervals can not bring further information, the minimum values for  $\tau$  and  $a$  are those given by the time and space discretization ( $\delta t/2$ ) and ( $\delta x/2$ ). Using  $N_0$  particles moving according to the initial and boundary conditions of the studied diffusion process, the one-particle averages  $\overline{\langle 1 \rangle}_i(x, t)$  and  $\sigma_i(x, t)$  are calculated. Then (4.1) provides the minimum number of particles  $N$  needed to obtain, by numerical modelling, a relative error of the concentration equal to  $\varepsilon$  at a confidence level of 0.997. We model the diffusion using  $N$  particles and we calculate  $\langle 1 \rangle(x, t)$ . The larger the values of  $\tau$  and  $a$  are, the smaller the number of particles  $N$ . But if  $\tau$  and  $a$  become too large it is possible that  $\langle 1 \rangle(x, t)$  should average to strongly the motion of particles and to lose useful information on the concentration evolution.

We consider that at the initial moment there are  $N$  particles located in origin, and in the rest all the sites of the lattice are empty. This diffusion process is nonstationary. Three distinctive periods in the concentration evolution can be identified. The first one lasts from the initial moment until the first particle reach the extremities of the lattice and it correspond to the Brownian motion (1.5). The second period is a transition one and it is characterized by the appearance of a particles flux at the ends of the lattice. In the third period the evacuation of particles continues but by a nonstationary diffusion, in which the leaving particles flux is proportional to the number of particles left in the lattice.

The initial distribution of the particles is singular. Besides, due to the random walker law, at the odd moments, the particles will be only at the odd sites of the lattice and at the even moments only at the even sites. So, the distribution of particles is very discontinuous both in space and time. In the following we show that those discontinuities are completely averaged if  $\tau \geq \delta t$  and not  $\tau \geq \delta t/2$ , i.e., if the temporal averaging is made over two time steps. For the space averaging, we shall use only the minimum value  $a = \delta x/2$  since the space resolution is small ( $m = 10$ ) and a further space averaging would mean a larger decrease of the space resolution.

First we analyze the particles distribution at the moment  $t = 9\delta t$ , i.e. before the first particles leave the lattice. We use 1000 particles to calculate  $\overline{\langle 1 \rangle}_i(x, t)$  and  $\sigma_i(x, t)$  at the sites of the lattice and at the half distance between two neighboring sites  $x = k\delta x/2$ ,  $0 \leq k \leq 18$ . Due to the symmetry of the problem we consider only the positive side of the lattice, including the origin. The last site  $x_{10} = 10\delta x$  is used only to formulate the boundary condition

$$(4.2) \quad n_m = n_{-m} = 0,$$

expressing the fact that the particles which reach the extremities are removed out.

Table 4 presents the results obtained by means of the relation (4.1) for two values of the averaging interval. For the minimum value  $\tau = \delta t$ , the particles number necessary to obtain the concentration relative error of 0.01 varies by two orders of magnitude between the origin and the extremity of the lattice. The particles number necessary at the points between the sites of the lattice is roughly twice than at the sites. One also notices an important decrease of  $N$  if the temporal interval of averaging increases. To calculate  $\langle 1 \rangle$  and to compare the probability density obtained by numerical simulation with the theoretical one we used 100000 particles. In this way, about the origin, a relative error of roughly 0.01 was provided, and at the extremities of the lattice it decreased according to relation (4.1) down to 0.10 for  $\tau = \delta t$ . In Table 1 we present the values calculated by space-time coarse-grained averaging for the probability distribution in comparison with the theoretical one of the Brownian motion (1.5). The relative error is in a good concordance with that estimated by relation (4.1). Thus, the concentration obtained by a time averaging over a larger interval,  $\tau = 4\delta t$ , is closer to the theoretical value than those obtained for a smaller  $\tau$ .

Table 1. The particles number  $N$  needed to obtain a relative error of the concentration of  $\varepsilon = 0.01$ , the probability density obtained by the simulation of diffusion using 100 000 particles and the theoretical probability density of the Brownian motion, at the moment  $t = 9\delta t$ .

$x$	$N(\times 10^5)$ ( $\tau = \delta t$ )	$N(\times 10^5)$ ( $\tau = 4\delta t$ )	$\langle 1 \rangle / N$ ( $\tau = \delta t$ )	$\langle 1 \rangle / N$ ( $\tau = 4\delta t$ )	$\frac{e^{-\frac{x^2}{4Dt}}}{\sqrt{4\pi Dt}}$
0.00	1.8	0.42	1.30	1.32	1.33
0.05	3.7	0.83	1.30	1.32	1.31
0.10	1.9	0.43	1.23	1.25	1.26
0.15	3.8	0.90	1.16	1.19	1.17
0.20	2.0	0.51	1.06	1.06	1.06
0.25	4.4	1.2	0.953	0.933	0.940
0.30	2.6	0.68	0.819	0.803	0.806
0.35	6.6	1.6	0.685	0.674	0.673
0.40	3.5	0.95	0.565	0.549	0.547
0.45	7.6	2.4	0.445	0.424	0.432
0.50	5.4	1.5	0.348	0.331	0.332
0.55	19	4.2	0.251	0.239	0.248
0.60	12	2.9	0.188	0.181	0.180
0.65	32	9.3	0.125	0.124	0.127
0.70	21	6.3	0.0921	0.0892	0.0874
0.75	64	19	0.0596	0.0539	0.0584
0.80	56	14	0.0379	0.0390	0.0380
0.85	450	47	0.0162	0.0241	0.0240
0.90	220	36	0.0106	0.0144	0.0148

In Table 4 we analyze the third period of evolution we considered the moment  $t = 100 \delta t$ , when  $2/3$  of the initial number of particles were eliminated from the lattice. The particles number needed for a relative error of 0.01 was calculated for the same values of the averaging interval, using 1000 particles too.

Table 2. The particles number  $N$  needed to obtain a relative error of the concentration of  $\varepsilon = 0.01$  and the probability density obtained by the simulation of diffusion using 100 000 particles, at the moment  $t = 100\delta t$ .

$x$	$N(\times 10^5)$ ( $\tau = \delta t$ )	$N(\times 10^5)$ ( $\tau = 4\delta t$ )	$\langle 1 \rangle / N$ ( $\tau = \delta t$ )	$\langle 1 \rangle / N$ ( $\tau = 4\delta t$ )
0.00	7.8	1.9	0.798	0.799
0.05	17	4.0	0.803	0.798
0.10	7.6	2.0	0.781	0.781
0.15	14	3.9	0.758	0.765
0.20	8.0	2.0	0.739	0.754
0.25	19	4.1	0.719	0.743
0.30	8.3	2.1	0.702	0.710
0.35	15	4.4	0.685	0.678
0.40	9.2	2.2	0.638	0.638
0.45	24	4.5	0.591	0.598
0.50	12	2.8	0.557	0.552
0.55	25	7.1	0.524	0.507
0.60	14	3.8	0.466	0.459
0.65	34	8.0	0.409	0.412
0.70	18	4.6	0.361	0.358
0.75	37	11	0.312	0.304
0.80	24	6.1	0.247	0.247
0.85	64	13	0.183	0.190
0.90	45	11	0.125	0.126

An interesting problem occurring for the third period of the concentration evolution is connected with the time needed for a certain fraction of the initial number of particles to leave the lattice. At the limit the magnitude order of the evacuation time of a volume by diffusion can be calculated. At a time step, the average number of particles leaving the lattice is equal to half the number of particles in the last but one sites  $x_{-m+1}$  and  $x_{m-1}$ . But on average in these sites we have the same number of particles, so on average at each time step  $\langle 1 \rangle(x_{m-1}, t) \cdot \delta x$  particles leave the lattice. To study the variation in time of the number of particles in the lattice we estimate  $\langle 1 \rangle$  for  $x_{m-1}$  and we act the same way as we did in the other two cases. As shown above, at the extremity of lattice a larger statistic is needed. Therefore we used 10 000 particles to establish the number of particles needed to obtain the concentration with a



relative error of 0.01 and a time averaging of  $\tau = 10 \delta t$ . The results are presented in the first column of the Table 3 for several moments. To obtain this precision we used 1 000 000 particles. The values obtained are given in Table 3 divided by the total number of particles from the lattice and are compared with the values established without any averaging. The probability distribution at the extremities of the lattice is constant in time and equal to  $p = 0.125$ . Thus, after  $n$  time steps, the number of particles left in the lattice is equal to a fraction  $(1 - p \cdot \delta x)^n$  of the initial number of particles. The larger the value of  $n$ , the more precise this formula is, because the influence of the initial concentration is smaller. If the initial number of particles is  $N_0$ , then to get a single particle in the lattice. we should have

$$(1 - p \cdot \delta x)^n = \frac{1}{N_0}$$

so there are needed

$$(4.3) \quad n = -\frac{\ln N_0}{\ln(1 - p \cdot \delta x)}$$

time steps. For  $N_0 = 10^6$  particles. we get  $n \sim 1000$ , in concordance with the numerical simulations.

Table 3. The particles number  $N$  needed to obtain a relative error of  $\varepsilon = 0.01$  and the probability density at the last but one site,  $k = m - 1$ , of the lattice obtained by the simulation of diffusion using 1 000 000 particles, by means of the coarse grained average and directly from the number of particles.

t	$N(\times 10^6)$ ( $\tau = 10\delta t$ )	$\langle 1 \rangle / N$ ( $\tau = 10\delta t$ )	$\frac{n_{m-1}}{N} / \delta x$
100	0.49	0.125	0.126
150	0.87	0.125	0.121
200	1.5	0.126	0.126
250	2.5	0.124	0.126
300	6.0	0.124	0.127
350	7.5	0.125	0.119
400	15	0.127	0.115
450	24	0.122	0.125
500	113	0.124	0.134

On the basis of (4.3) we can estimate the evacuation time by diffusion of a number of particles  $N_0$  from a layer of  $2L$  thickness. We emphasize that the discussion is valid only for the boundary condition (4.2), i.e., if the particles leaving the layer are instantaneously removed from the neighborhood of the layer surface. From (3.2) it follows that the magnitude of the time step for a

given diffusion coefficient is  $\delta t = \delta x^2/(2D)$ . The diffusion equation (1.4) for the layer of  $2L$  thickness can be reduced to the space interval  $(-1, 1)$  if the transformation  $x = Lx'$  is done and the diffusion coefficient becomes  $D/L^2$ . Then, from (4.3) it follows that the mean time needed to eliminate the  $N_0$  particles is

$$(4.4) \quad \Delta t = n\delta t = 0.4 \frac{L^2}{D} \ln N_0.$$

## 5. CONCLUSIONS

In this paper we have described a new numerical algorithm for diffusion simulation. It is based on the evolution of a set of fictitious particles shifting on a line according to the random walk law. This is a model of one-dimensional cellular automaton. The continuous macroscopical interpretation of the results is made in the molecular dynamics manner by means of the coarse grained space-time averages.

For a non-stationary diffusion we have established the space-time scale needed to obtain a continuous macroscopical description with a given precision. We have also shown that if the particles reaching the extremity of the space lattice are immediately eliminated from the neighborhood of the lattice, then the number of particles in the lattice exponentially decreases.

Recently [12] a model of cellular automaton has been proposed. Our results are comparable in the case of the small concentration when the effect of the interaction decreases. The main distinction between these two approaches is the coarse grained averaging. This has as a result the decrease of the needed number of particles and the computing time.

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