Chapter 6

The numerical modeling of diffusion

The numerical modeling of a continuous phenomenon imposes the discretization of the implied continuous fields. The link between the continuous in time and space functions associated to the analytical problem and the discrete fields defined on the nodes of a grid is made by different interpolation methods, respectively, by different methods of approximation. The space-time coarse-grained averages defined in Chapter 4 allow an approach closer to the physical intuition. As shown in Section 4.1, the volume of the spatial averaging sphere and the length of the time averaging interval are related to the resolution of the measuring device, i.e., to the space-time scale at which the continuous description of a corpuscular system is defined. In this chapter we show how it is possible to evaluate the space-time scale of the averaging of the numerical results in order to obtain the continuous fields with a given error. To simplify the presentation in the following we confine ourselves to a one-dimensional diffusion case: a single type of particles which diffuse without being under the influence of any force field. Also, the particles do not participate to chemical reactions, so they cannot be created or annihilated. However, the number of particles can vary by introducing or extracting them from the domain where the diffusion takes place. The results from this chapter have been published in [68].

6.1 The random walk algorithm

The random walk is a discrete Markov process describing the motion on a grid of a particle which jumps with the same probability into all the neighboring nodes. Consider a one-dimensional grid with its nodes in $x_i = i\delta x$, $i \in \mathbb{Z}$,

where $\delta x > 0$ is the spatial step. At the moment $t_k = k\delta t$, $k \in \mathbb{N}$, where $\delta t > 0$ is the time step, the particle jumps to the right or to the left with equal probabilities. If we denote by $P(x_i, t_k)$ the probability distribution at the moment t_k and by $P(x_i, t_k|x_j, t_l)$ the corresponding transition probability, then the consistence property for discrete Markov processes is written

$$P(x_i, t_k) = \sum_j P(x_i, t_k|x_j, t_l)P(x_j, t_l), \tag{6.1}$$

where $t_k > t_l$. According to the random walk law the transition probability for successive time steps is equal with

$$P(x_i, t_{l+1}|x_j, t_l) = \begin{cases} \frac{1}{2} & \text{if } i = j \pm 1 \\ 0 & \text{if } i \neq j \pm 1 \end{cases}. \tag{6.2}$$

From the discrete Chapmann-Kolmogorov equation

$$P(x_i, t_k|x_h, t_m) = \sum_j P(x_i, t_k|x_j, t_l)P(x_j, t_l|x_h, t_m)$$

and (6.2) we have the evolution equation of the transition probability

$$P(x_i, t_{k+1}|0, 0) = \frac{1}{2}\left[P(x_{i-1}, t_k|0, 0) + P(x_{i+1}, t_k|0, 0)\right]. \tag{6.3}$$

It can be proved [18] that if the limit

$$\lim_{\delta x, \delta t \to 0} \frac{\delta x^2}{2\delta t} = D \tag{6.4}$$

is finite, then for $\delta x \to 0$ and $\delta t \to 0$ the limit solution of the equation (6.3) is the Gaussian transition probability

$$p(x, t|0, 0) = (4\pi D t)^{-1/2} \exp\left\{\frac{-x^2}{4Dt}\right\}. \tag{6.5}$$

For the same limit, the relation (6.1) becomes

$$p(x, t) = \int_{\mathbb{R}} p(x, t|x', 0)p(x', 0)dx' \tag{6.6}$$

which is the integral representation of the solution of the equation

$$\partial_t p = D\partial_x^2 p, \tag{6.7}$$

with the initial condition $p_0(x) = p(x, 0)$.

The relation between the equation (6.7) and the diffusion equation (1.5) is given by

$$c(x,t) = N\, p(x,t)\,, \tag{6.8}$$

where

$$N = \int_{-\infty}^{\infty} c(x,t)\, dx$$

is the number of diffusing particles. Replacing (6.8) in (6.7) we obtain the diffusion equation

$$\partial_t c = D\, \partial_x^2 c \tag{6.9}$$

corresponding to the equation (1.5) in which Fick's law (1.6) has been used. The relation between the random walk algorithm described by (6.1) and (6.3) and the solution (6.6) of the diffusion equation can be used to design a numerical method to solve the diffusion equation (6.9). Let us consider N fictitious particles moving on the grid previously described, their movement being governed by the random walk law. At the initial moment the distribution of the N particles approximates the initial concentration $c_0(x)$. At each time step, for each particle we generate a random number equal to-1 or $+1$ with the probability equal with $1/2$. If the random number is equal with -1, then the particle moves to the left and if it is equal with $+1$ the particle moves to the right. Thus the spatial distribution of the N particles at the moment t_k approximates the solution $c(x,t_k)$ of the diffusion equation (6.9). The approximation can be improved by increasing N and decreasing δx and δt.

This algorithm is not effective since for each jump of each particle a random number has to be generated, which requires many numerical operations. As shown in [69] the random walk algorithm can be substantially improved by a law of collective displacement of the particles from a grid node to the other, not one by one. As we are interested here only in the illustration of the space-time coarse-grained averages applications, we use the simple random walk algorithm.

We consider the stationary diffusion of the particles introduced at the origin of the coordinates axis and which are extracted at the ends of the interval $[-1,1]$. So the diffusion equation (6.9) is applied only within the intervals $(-1,0)$ and $(0,1)$. Because the diffusion is stationary, the particles flux density (1.6) has to be constant. Then the equilibrium concentration varies linearly with x

$$c_0(x) = \frac{J}{D}(1- \mid x \mid) \quad \text{for} \quad x \in (-1,0) \cup (0,1)\ , \tag{6.10}$$

where $J > 0$ is the absolute value of the particles flux and $c_0(\pm 1) = 0$. In order to maintain this flux constant it is necessary to introduce at the origin

$2J$ particles per time unit. At the ends of the interval $[-1, 1]$ at each time unit, J particles have to be extracted.

In order to obtain by means of the random walk, the solution (6.10) we consider the one-dimensional grid from the beginning of this section formed by $2L + 1$ nodes symmetrically arranged with respect to the origin $\{x_i = i\,\delta x \,|\, -L \leq i \leq L\}$. Due to the condition (6.4), between the space and time steps we have the relation

$$D = \frac{\delta x^2}{2\,\delta t}\,. \tag{6.11}$$

Initially in the node i of the grid there is a number of particles denoted by $n_0(i)$ whose value will be established later. At each time step we introduce $\Delta n = 2\,J\,\delta t$ particles in origin which afterwards are moved according to the random walk algorithm previously described. In order to satisfy the boundary condition $c_0(\pm 1) = 0$, all the particles that reach the ends of the grid $\pm L\,\delta x$ are eliminated from the grid. Therefore at a moment $t_k = k\,\delta t$ in the node $x_i = i\,\delta x$ there are $n(i, k)$ particles.

Repeating S times the simulation in the same conditions we obtain for each node and for each moment a set of values $n_s(i, k)$, $1 \leq s \leq S$. For a large enough S, the average $\overline{n(i,k)}$ after S realizations has negligible fluctuations and characterizes the ensemble average like in a Monte Carlo simulation. Assuming that the particles from the node x_i are assigned to an interval of length δx centered on the respective node, we attach to the mean distribution of the particles the concentration

$$c(x_i, t_k) = \frac{1}{\delta x}\overline{n(i,k)}. \tag{6.12}$$

By means of this relation we also can establish the initial distribution of the particles in the grid $n_0(i)$. Since all the S simulations have the same initial state it follows that the average after S simulations at the initial moment is also $n_0(i)$. Then, replacing (6.10) in (6.12) and taking into account that $x_i = i\,\delta x$ and $\delta x = 1/L$, we obtain

$$n_0(i) = \frac{J\,\delta x^2}{D}(L - |i|)\,.$$

If we use (6.11) and the notation introduced above $\Delta n = 2\,J\,\delta t$, it follows

$$n_0(i) = \Delta n\,(L - |i|)\,.$$

From this formula it follows that the total number of particles in the grid at a given moment is equal with $\Delta n\,L^2$ and then the probability that a particle should be in the node i is equal with

$$p(i) = \frac{n_0(i)}{\Delta n\,L^2} = \frac{1}{L^2}\,(L - |i|)\,. \tag{6.13}$$

6.2 The space-time scale evaluation

The relation (6.12), and the analogue one (4.1) as well, refers to the instantaneous values of the concentration and of the particle number. At small concentrations the numerical modeling of the diffusion may require a large number S of simulations to supply significant statistics. As discussed in section 4.1, the enhancement of the information needed to build the continuous fields can be obtained by increasing the averaging time interval. In this section we apply this method to the random walk modeling of the stationary diffusion described in the previous section. This method can also be applied to nonstationary diffusion processes [68].

In the time interval δt between two successive jumps we consider that the particles move with the constant velocity $\delta x/\delta t$ between two neighborhood nodes of the spatial grid. Each particle can be introduced into or extracted from the spatial grid, therefore we denote by t_i^+ the moment when it enters the grid and by t_i^- the moment it goes out. So the position of the particle i is given by the function $x_i : [t_i^+, t_i^-] \to [-1, 1] \subset \mathbf{R}$ which has discontinuities when the particle shifts its direction in one of the nodes of the spatial grid. The particle velocity $\xi_i = \dot{x}_i : [t_i^+, t_i^-] \to \{-\delta x/\delta t, \delta x/\delta t\}$ is a jump function.

In the one-dimensional case, the sphere $S(\mathbf{r}(t), a)$ from relation (4.5) becomes the interval $(x - a, x + a)$. Then the coarse-grained average of the number of particles of the discrete system at a point $(x, t) \in \mathbf{R} \times (\tau, T - \tau)$ is equal with

$$\langle 1 \rangle (x, t) = \frac{1}{4\tau a} \sum_{i=1}^{N} \int_{t-\tau}^{t+\tau} H^+(a - \mid x_i(t') - x \mid) dt' \tag{6.14}$$

and

$$\langle \xi \rangle (x, t) = \frac{1}{4\tau a} \sum_{i=1}^{N} \int_{t-\tau}^{t+\tau} \xi_i(t') H^+(a - \mid x_i(t') - x \mid) dt' \ . \tag{6.15}$$

These quantities can be computed at any point and any moment, not only for the discrete arguments defined by the grid.

Let us show that the formulas (6.14) and (6.15) are generalizations of the usual computing methods of the concentration and the particle flux. We compute $\langle 1 \rangle$ at a grid point x_i at a moment t_k multiple of δt. In analogy with (6.12), we consider that the particles in a node are assigned to an interval of length δx and we choose $2a = \delta x$. In order to obtain the "instantaneous" value of the concentration, we choose the averaging time interval much smaller than the time step $\tau \ll \delta t$. Then the particle j, which at the

moment t_k is at x_i, will be at the proximate vicinity of x_i within the interval $(t_k - \tau, t_k + \tau)$, i.e. the integrand from (6.14) is equal with unity in all the integration interval ant the integral is equal with 2τ. The particles which at the moment t_k are at the other nodes of the grid have a null contribution to $\langle 1 \rangle$. Therefore we obtain

$$\langle 1 \rangle (x_i, t_k) = \frac{n(i,k)}{2a} = \frac{n(i,k)}{\delta x}, \tag{6.16}$$

i.e. a formula identical with (6.12), but for the values of a single simulation.

In order to show that $\langle \xi \rangle$ represents the flux of the particles, we compute its value for $x = x_i + \delta x/2$ at the moment $t_k + \delta t/2$ such that it characterizes the particles flux between the nodes x_i and x_{i+1} in the interval $(t_k + \delta t/2 - \tau, t_k + \delta t/2 + \tau)$. In the same way as for $\langle 1 \rangle$ we consider that $2a = \delta x$ and $\tau \ll \delta t$ and then the particles with a nonvanishing contribution to the integral (6.15) are those jumping from x_i to x_{i+1} and inversely from x_{i+1} to x_i. Their velocity ξ_i is constant and equal to $\delta x \,/\, \delta t$, respectively $-\delta x \,/\, \delta t$, so that the integral in (6.15) is equal to $2\tau\, \delta x \,/\, \delta t$, respectively to $-2\tau\, \delta x \,/\, \delta t$. Taking into account that $2a = \delta x$, we obtain

$$\langle \xi \rangle (x_i + \delta x/2,\ t_k + \delta t/2) = \frac{1}{\delta t}[\delta n(i, i-1, k) - \delta n(i, i+1, k)]\,, \tag{6.17}$$

where $\delta n(i, j, k)$ is the number of the particles that at the moment t_k jump from x_i in x_j.

The formulas (6.16) and (6.17) in which the time averaging interval is very small in comparison with the time step of the numerical algorithm $\tau \ll \delta t$ coincide with the usual formulas for numerical estimation of the concentration and the particle flux. The difference consists in the fact that (6.16) and (6.17) refer to a single simulation, whereas in (6.12) we have the average over several simulations. Therefore the values obtained by means of (6.16) and (6.17) have all larger fluctuations when the number N of particles in the grid decreases. As discussed in section 4.1, a method to damp the fluctuations is to increase the time averaging interval, i.e., of the time scale. If the diffusion process is stationary as the one considered in the previous section, then we can consider $\tau \to \infty$.

We apply the coarse-grained averaging with $\tau \gg \delta t$ when the mean number of particles existing at a given moment in the grid is very small. The first particle is introduced into the origin at the initial moment and the next one is introduced only after the previous particle has been removed through one of the ends of the grid. This way the mean number of particles in the grid is equal with 1. From (6.13) it follows that the probability that a particle should be at the last but one node of the grid $i = \pm(L-1)$ is L^{-2}.

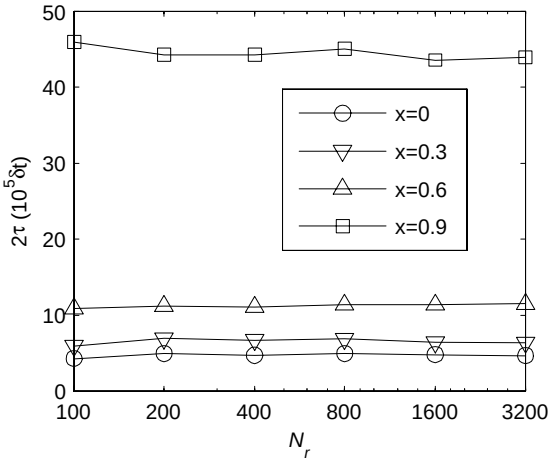

Figure 6.1: The time scale expressed in $10^5\delta t$ needed in order to obtain the concentration in the grid nodes with a relative error of 0,01 with respect to the particle number used for the computation of $\overline{\langle 1\rangle_i}$ and σ_i

The probability that the particle at the knot $i = \pm(L-1)$ leaves the grid is $1/2$. The grid has two ends, therefore the probability that at a time step the particle leaves the grid is L^{-2}, so the mean time in which a particle is in the grid is $L^2\delta t$. Then within the time averaging interval of length 2τ, since at a given moment a single particle is in the grid, the number of particles used in the simulation is equal with

$$N = \frac{2\tau}{L^2\delta t}\,. \tag{6.18}$$

The field $\langle 1\rangle$ can be obtained as a sum of the contributions $\langle 1\rangle_i$ of the $N = 2\tau/(L^2\delta t)$ particles contained by the grid within the time averaging interval

$$\langle 1\rangle(x,t) = \sum_{i=1}^{N}\langle 1\rangle_i(x,t)\ .$$

If the right-hand side term of this formula is divided by N, then it becomes the computation formula of the average of the quantities $\langle 1\rangle_i(x,t)$. Since the motions of the N particles are independent from each other, the average and standard deviation of these quantities as random variables are related through the relations $\overline{\langle 1\rangle} = N\,\overline{\langle 1\rangle_i}$ and $\sigma = \sqrt{N}\,\sigma_i$. The condition $3\sigma \le \varepsilon\overline{\langle 1\rangle}$ that the relative error of $\langle 1\rangle$ with respect to $\overline{\langle 1\rangle}$ should be ε with a confidence level of 0.997

$$3\sqrt{N}\sigma_i \le \varepsilon\, N\,\overline{\langle 1\rangle_i}$$

allows the determination of the particle number N needed to obtain this precision

$$N \geq \left(\frac{3\,\sigma_i}{\varepsilon\,\overline{\langle 1 \rangle_i}} \right)^2 . \tag{6.19}$$

According to the relation (6.18), this value corresponds to a time averaging interval, i.e., to a time scale

$$2\tau \geq \left(\frac{3\,\sigma_i\,L}{\varepsilon\,\overline{\langle 1 \rangle_i}} \right)^2 \delta t\ . \tag{6.20}$$

The values of N and τ for a given ε can be estimated if $\overline{\langle 1 \rangle_i}$ and σ_i are determined by means of a small number of particles N_r.

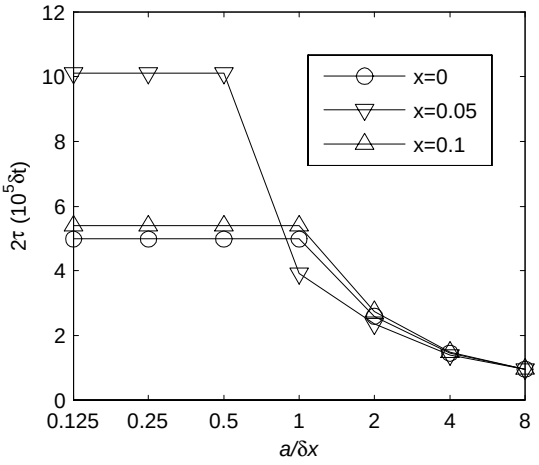

Figure 6.2: The time scale expressed in $10^5\delta t$ needed to obtain the concentration in the grid nodes with a relative error of 0,01with respect to the spatial averaging interval a.

As an exemplification we use the following values $\varepsilon = 0,01$, $L = 10$, $D = 0,5$, $\tau = 10^4\delta t$, $a = 0,125\,\delta x$. Estimations of $\overline{\langle 1 \rangle_i}$ and σ_i were performed using different numbers N_r.of particles The time scale 2τ computed according to (6.20) expressed in $10^5\delta t$ in the grid nodes is presented in figure 6.1. As one can see the magnitude order does not vary significantly with the particle number used to estimate $\overline{\langle 1 \rangle_i}$ and σ_i.

The time scale can be computed for any spatial scale a and at any point. In figure 6.2 we have computed the time scale expressed in $10^5\delta t$ for different

x and a, with $N_r = 200$. As one can see, the time scale decreases significantly while the space scale increases, but only for $a \geq \delta x$. For $a \leq \delta x$ one can see that between the spatial grid nodes the time scale is double, pointing to a larger variability of the coarse-grained averages.