A New Random Walk Simulation Model for Study of Diffusion Behavior of Single Particle within Two-Dimensional Space

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Appendix A: Justification of Using Constant Speed

In our simulation model, a particle moves step by step whose speed is constant. In reality, the step speed of a diffusing particle cannot be constant but obeys a certain probability distribution. Although such probability distribution is usually unknown, according to the Central Limit Theorem, the unknown distribution can be represented by Gaussian (normal) distribution when the number of steps is very large. Then we need to justify that a particle's speed which obeys Gaussian distribution can be represented by its mean value, a constant speed.

We compare simulations using Gaussian distribution with $\mu = 1$, $\sigma = 0.1$ and constant value $\delta = 1$ (Fig. 11). The result shows that there is no significant difference between the two samples in the range from the beginning to around $t = 600$, and for $t > 600$ the D-t curves become noisy and are not reliable. It means that if the speed of a particle can be described by Gaussian distribution, it can be properly simulated using constant speed, with no significantly change in MSD behaviors. Hence all simulations in this article are carried out using constant speed.

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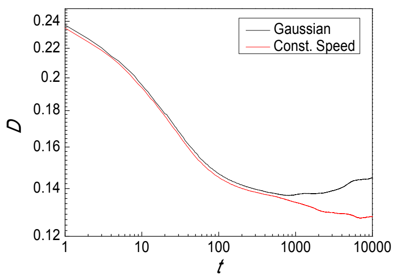
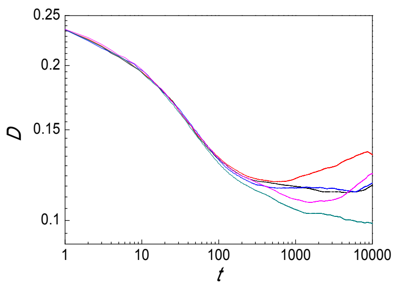


S1 D-t plot of simulations using Gaussian distribution for speed and constant speed.

Appendix B: Reproducibility of Simulated Data

The model used here is stochastic and the resulting data are got from statistical average, and the reproducibility of data is a basic requirement for reliability. The data have been tested and are proved reproducible. One of the tests is shown below.

The parameters are set as Series 3, half length of square = 2 (300,000 steps, 10 simulation runs for average). The results of 5 independent sets are shown in Fig 12. For small t, the results fit very well; for large t, the results are noisy and not reproducible, but they can be seen to be around a certain value. In fact, using more steps and more simulation runs, the noise can be weakened but calculation expense increases rapidly. As the results can be readily analyzed from the less noisy part, more steps and simulation runs are unnecessary.



S2 Reproducibility of D-t plots.

Appendix C: Relations of Free-diffusion MSD and Simulation Parameters

The free diffusion with no barrier or lateral drifting velocity is characterized by the straight MSD curve given by

$$MSD = 4Dt\,. \tag{1}$$

For two-dimensional free diffusion, D is constant and given by

$$D = \frac{1}{4} v^2 \tau \ , \tag{2}$$

in which v is speed and τ is step time. This expression can be proved mathematically following the similar procedure used by Berg[1] to derive D for one-dimensional random walk.

Define

$$\delta = v\tau \ , \tag{3}$$

where δ is the length of a step, v the speed and τ the step time. Now consider the x component of the distance of the particle from its original position after n steps:

$$x_n = x_{n-1} + \delta \cos\theta \ , \tag{4}$$

where θ is the angle from the x axis to the position vector counterclockwise, which is between 0 and 2π. And

$$x_n{}^2 = x_{n-1}{}^2 + \delta^2 \cos^2\theta + 2x_{n-1}\delta\cos\theta \ . \tag{5}$$

Then

$$\left\langle x_n{}^2 \right\rangle = \left\langle x_{n-1}{}^2 \right\rangle + \frac{1}{N}\sum_{i=1}^{N} \delta^2 \cos^2\theta_i + \frac{1}{N}\sum_{i=1}^{N} 2x_{n-1}\delta\cos\theta_i \ , \tag{6}$$

where N is the cases we take to get the average. Since θ is taken randomly from 0 to 2π, it is reasonable to take

$$\theta_i = 2\pi \frac{i}{N} \ , \tag{7}$$

and

$$\Delta\theta = \theta_{i+1} - \theta_i = \frac{2\pi}{N} \ . \tag{8}$$

Then

$$\left\langle x_n{}^2 \right\rangle = \left\langle x_{n-1}{}^2 \right\rangle + \frac{\delta^2}{2\pi}\sum_{i=1}^{N} \cos^2\theta_i \Delta\theta + \frac{\delta}{\pi}\sum_{i=1}^{N} x_{n-1}\cos\theta_i \Delta\theta \ . \tag{9}$$

When we take infinite number of cases, namely $N \rightarrow \infty$, x_{n-1} becomes constant and the summation becomes integrals, so we get

$$\left\langle x_n^{\ 2}\right\rangle = \left\langle x_{n-1}^{\ 2}\right\rangle + \frac{\delta^2}{2\pi}\int_0^{2\pi}\cos^2\theta\,\mathrm{d}\theta + \frac{\delta}{\pi}\left\langle x_{n-1}\right\rangle\int_0^{2\pi}\cos\theta\,\mathrm{d}\theta = \left\langle x_{n-1}^{\ 2}\right\rangle + \frac{\delta^2}{2}. \tag{10}$$

As $x_0^2 = 0$, we can iterate the calculation to get

$$\left\langle x_n^{\ 2}\right\rangle = \frac{\delta^2}{2}n. \tag{11}$$

In the same way we have

$$\left\langle y_n^{\ 2}\right\rangle = \frac{\delta^2}{2}n, \tag{12}$$

so

$$\left\langle r_n^{\ 2}\right\rangle = \left\langle x_n^{\ 2}\right\rangle + \left\langle y_n^{\ 2}\right\rangle = n\delta^2 = nv^2\tau^2. \tag{13}$$

The total time $t = n\tau$, so

$$MSD = \left\langle r_n^{\ 2}\right\rangle = nv^2\tau^2 = v^2\tau t. \tag{14}$$

Comparing the definition of D, the result can be derived.

Adding lateral drifting velocity to the free diffusion, the relations can also be derived by similar approach. First consider a one-dimensional random walk along x direction in which every step is randomly chosen to be δ or $-\delta$ with extra lateral velocity ε. We have

$$\begin{aligned} x_n &= x_{n-1} \pm \delta + \varepsilon \\ x_n^{\ 2} &= x_{n-1}^{\ 2} + \delta^2 + \varepsilon^2 + 2x_{n-1}\varepsilon \pm 2x_{n-1}\delta \pm 2\delta\varepsilon \end{aligned} \tag{15}$$

and

$$\begin{aligned} \left\langle x_n\right\rangle &= \left\langle x_{n-1}\right\rangle + \varepsilon \\ \left\langle x_n^{\ 2}\right\rangle &= \left\langle x_{n-1}^{\ 2}\right\rangle + \delta^2 + \varepsilon^2 + 2\left\langle x_{n-1}\right\rangle\varepsilon \end{aligned} \tag{16}$$

From $\langle x_0 \rangle = 0$, we have

$$\begin{aligned} \left\langle x_n\right\rangle &= n\varepsilon \\ \left\langle x_n^{\ 2}\right\rangle &= \left\langle x_{n-1}^{\ 2}\right\rangle + \delta^2 + \varepsilon^2 + 2n\varepsilon^2 \end{aligned} \tag{17}$$

From $\langle x_0^2 \rangle = 0$, we have

$$\begin{aligned} \left\langle x_n^{\ 2}\right\rangle &= n\delta^2 + n^2\varepsilon^2 \\ \frac{\mathrm{d}\left\langle x_n^{\ 2}\right\rangle}{\mathrm{d}\,n} &= \delta^2 + 2n\varepsilon^2 \end{aligned} \tag{18}$$

Then consider a two-dimensional random walk,

$$x_n = x_{n-1} + \delta\cos\theta + \varepsilon$$
$$x_n{}^2 = x_{n-1}{}^2 + \delta^2\cos^2\theta + \varepsilon^2 + 2x_{n-1}\varepsilon + 2x_{n-1}\delta\cos\theta + 2\varepsilon\delta\cos\theta \tag{19}$$

in which θ is randomly chosen from 0 to 2π. Similarly we can get

$$\left\langle x_n{}^2 \right\rangle = \frac{\delta^2}{2}n + \varepsilon^2 n^2$$
$$\frac{\mathrm{d}\left\langle x_n{}^2 \right\rangle}{\mathrm{d}n} = \frac{\delta^2}{2} + 2n\varepsilon^2 \tag{20}$$

MSD_y is unaffected by lateral velocity along x direction and given by

$$\left\langle y_n{}^2 \right\rangle = \frac{\delta^2}{2}n, \tag{21}$$

so total MSD is

$$\left\langle r_n{}^2 \right\rangle = \left\langle x_n{}^2 \right\rangle + \left\langle y_n{}^2 \right\rangle = \delta^2 n + \varepsilon^2 n^2$$
$$\frac{\mathrm{d}\left\langle r_n{}^2 \right\rangle}{\mathrm{d}n} = \delta^2 + 2n\varepsilon^2 \tag{22}$$

Reference

[1] Berg H C. Random walks in Biology [M]. Princeton: Princeton University Press, 1993.