Two Simulation Methods of Brownian Motion

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Abstract. Einstein-Smoluchowski's theory and Langevin's theory are two main theories to describe Brownian motion. The Einstein-Smoluchowski theory regards Brownian motion as random walking of Brownian particles, while the Langevin theory establishes a random differential equation describing the motion of Brownian particles. Both theories involve random numbers, i.e., only the statistical results can be discussed. Based on the above theories, this paper presents the corresponding simulations, which verifies the statistical conclusions as well as compares their similarities, differences, and applicable conditions. These results offer a guideline for further studies on Brownian motion.

1. Introduction
Brownian motion is an important form of fluctuation. It refers to the random movement of tiny particles in a liquid discovered in 1827 by the English botanist R. Brown. At the beginning of the 20th century, A. Einstein¹, M. Von Smoluchowski², and P. Langevin³ published their theories on Brownian motion, respectively.

Einstein considered the Brownian motion as the random walking of particles, while Von Smoluchowski used continuous variables to describe Brownian particles' displacement and occurrence probability. Since the latter processing was not fundamentally different from Einstein's, i.e., it is known as the Einstein-Smoluchowski theory⁴. Differently, Langevin describes the motion of Brownian particles by establishing a motion differential equation.

Based on the theories, two simulation methods have been established in this paper accordingly. Using comparable simulations, we analysed the similarities and differences of the two methods and the applicable conditions. Besides, some additional problems were studied, including the case with different boundaries and force fields. This paper is organized as follow: section 2 introduces the theory of random walking and its simulation; section 3 discussed Langevin equation and its numerical solution method; a comparison between the two methods is given in section 4; a brief summary is presented in section 5 eventually.

2. Random walking
2.1. Description
According to the random walking model, every time a liquid molecule collides with a Brownian particle, the Brownian particle will move a small, fixed distance in any possible direction with the same probability. Based on the random walking model's basic ideas, the motion of a single particle can be formularized. We define the \( r_0 \) as initial position vector of the particle, \( r_n \) for the position vector after \( n \) times collisions, and \( s \) for the distance the particle moves after each collision. To consider the
random probability, a unitary random vector $k$ is used. Thus, one derives the relationship between the position of a Brownian particle before and after a collision:

$$ r_n = r_{n-1} + ks \quad (1) $$

It can be proved that after $n$ collisions, the probability density distribution of particles in coordinate space is approximately a Gaussian distribution\[5\]:

$$ P(r; n) = A \exp \left( -\frac{r^2}{ns^2} \right) \quad (2) $$

The value of the normalization constant $A$ is different when considering one-, two-, and three-dimensional motions of Brownian particles.

Subsequently, let’s consider the motion of a large number of Brownian particles. Considering $\langle k \rangle = 0$ (for random) and $\langle k^2 \rangle = 1$ (for unitary), two important statistical conclusions can be obtained by averaging and square averaging of equation (1):

$$ \langle r_n \rangle = \langle r_0 \rangle \quad (3) $$

$$ \langle r_n^2 \rangle = \langle r_0^2 \rangle + ns^2 \quad (4) $$

2.2. Simulation method

According to equation (1), the simulation of their motion can be completed by iterating step by step after defining the initial position of Brownian particles. The simulation’s key point is to obtain the unitary random vector $k$, which is different in one-, two- and three-dimensional cases.

Taking MATLAB as an example, we can generate the random numbers from its random generators. In the 1D case, particles can only walk in the positive or negative direction of the $x$-axis. As a consequence, we only need to generate a random number $k$ with 1 and $-1$ appearing randomly for each step. Then, the unitary random vector $k$ in 1D case should be:

$$ k_{1D} = k \hat{x} \quad (5) $$

In the 2D case, the particle can move at any angle, so for each step, we can simply generate a random number $\theta$ (as its role in the polar coordinates), which is between 0 and $2\pi$, as the direction of the particle to walk. Then, we get the unitary random vector $k$ in 2D case:

$$ k_{2D} = \cos(\theta) \hat{x} + \sin(\theta) \hat{y} \quad (6) $$

The three-dimensional case is relatively complex. The common idea is to define two random numbers $\theta$ and $\phi$ (as their role in the spherical coordinates) in a similar way for the 2D case. However, this causes a problem that the unitary random probability vector $k$ is not uniformly distributed on the unit sphere (see appendix A). A feasible approach is to generate three random numbers between 1 and $-1$ in each step, which is separately defined as $a$, $b$, and $c$, and normalize them as:

$$ \begin{align*}
\alpha &= \frac{a}{\sqrt{a^2 + b^2 + c^2}} \\
\beta &= \frac{b}{\sqrt{a^2 + b^2 + c^2}} \\
\gamma &= \frac{c}{\sqrt{a^2 + b^2 + c^2}}
\end{align*} \quad (7) $$

Then, the unitary random vector $k$ in 3D case is:

$$ k_{3D} = \alpha \hat{x} + \beta \hat{y} + \gamma \hat{z} \quad (8) $$

In light of this approach, we can redesign the acquiring method of the unitary random vector $k$ in two-dimension. There we generate two random numbers $a$ and $b$ between 1 and $-1$ in each step, and get them normalized similarly by:
\[
\begin{cases}
\alpha = \frac{a}{\sqrt{a^2 + b^2}} \\
\beta = \frac{b}{\sqrt{a^2 + b^2}}
\end{cases}
\]  

(9)

In this case, the redesigned \( k_{2D} \) would be:

\[
k_{2D} = \alpha \hat{x} + \beta \hat{y}
\]

(10)

Besides, it should be noted that both \( k_{2D} \) and \( \overrightarrow{k}_{2D} \) are uniformly distributed on the unit ring, which is different from the 3D case.

2.3. Results

For the convenience of observation, the Brownian particle's trajectory is plotted by considering the 2D case, as shown in figure 1. Subsequently, we simulate the Brownian motion of a large number of particles to get the statistical results. MATLAB matrix operation can greatly simplify the workload. Figure 2 shows the simulation process of multiple Brownian particles in 2D (figure 2(a)) and 3D (figure 2(b)) cases, where the particles seem distributed evenly in the space. Figure 3 presents the comparison of particle number distribution's statistical results with the theoretical standard distribution in both 1D and 2D cases. Obviously, the simulation results tally well with the analytical results. Figure 4 illustrates the changing trend of \( \langle x \rangle \) and \( \langle x^2 \rangle \) for multiple Brownian particles, which is in agreement with the statistic descriptions in equations (3) and (4).

Figure 1. The trajectory of a 2D Brownian particle simulated by random walking model.

Figure 2. The simulation process of multiple 2D (A) and 3D (B) Brownian particles for 10,000 Brownian particles.
Figure 3. Comparison of simulated distribution (as the bar showed) and theoretical distribution (as the contour line or surface showed) of 1D (A) and 2D (B) cases.

Figure 4. The evolution of 1D Brownian particles’ \( \langle x \rangle \) (A) and \( \langle x^2 \rangle \) (B).

2.4. With different boundaries
The problem of particle diffusion in the container can also be dealt with by the random walking model. As for such processing, the particle will reflect when it collides with the boundary in the simulation process, i.e., it limits all particles in the container. The simulation results of a rectangular container (2D case, of course) and the corresponding \( \langle r^2 \rangle \) trend are depicted in figure 5. Differently, the distribution becomes uneven, and the evolution of \( \langle r^2 \rangle \) is convergence.

Figure 5. Brownian particles’ diffusion in a rectangular container for 10,000 particles. (A) The simulation process. (B) The evolution of \( \langle r^2 \rangle \).
3. The Langevin theory

3.1. Description
The random differential equation of the motion of Brownian particles established by Langevin was:

\[
m \frac{d^2 \mathbf{r}}{dt^2} = -\alpha \frac{d \mathbf{r}}{dt} + \mathbf{R}(t) + \mathbf{F}(t)
\]

(11)

Wherein, the first term on the right side of the equal sign is the damping force, and the second term is the random fluctuating force, while the third term is other external forces. Due to the existence of random fluctuating force \( \mathbf{R}(t) \), one can only solve the Langevin equation numerically. Besides, one notices that the above equation describes the classical Brownian motion without external forces. At this point, the statistical conclusion of multiple Brownian particles should be similar to that described in the random walking model, which will be verified in the following simulation solution.

3.2. Simulation method
The key point of the solution is the handling of \( \mathbf{R}(t) \). Like the random walking model, where the direction of particles remains unchanged in a very short time, we can treat the value of \( \mathbf{R}(t) \) as a constant similarly. Accordingly, the solution interval can be divided into multiple cells, and a random number can be generated in each region to determine the \( \mathbf{R}(t) \) on the region. Subsequently, the solution can be carried out for each cell respectively. The termination value of the previous intercell serves as the initial condition for the next intercell.

3.3. Results
In the 2D case, the simulated motion of a Brownian particle is shown in figure 6. Compared with figure 1 given by the random walking model, the motion track is smoother this time. The changing trend of \( \langle x \rangle \) and \( \langle x^2 \rangle \) of multiple Brownian particles is shown in figure 7, which is consistent with the random walking model's simulated results.

![Figure 6. The trajectory of a 2D Brownian particle simulated by the Langevin theory.](image)
3.4. With forces
In order to give a comprehensive analysis for external terms in equation (11), a magnetic tweezers simulation case is carried out. In this case, the corresponding external force is an approximately linear restoring force, which can be described as:

$$ F = -k(r - r_0) $$

This is the case of the Brownian Harmonic Oscillator (BHO). The following will analyze the case of 1D BHO as an example. Considering BHO particles obey the Boltzmann distribution, it can be proved that the probability density distribution of a single BHO particle is also approximately Gaussian distributed[6]. Besides, it is proved that the stiffness coefficient $k$ of the restoring force is inversely proportional to the variance of the position fluctuation $\sigma_x^2$ of a single BHO particle (see appendix B), as:

$$ k = \frac{k_B T}{\sigma_x^2} $$

These two conclusions are commonly used in biophysics, where they treat the magnetic balls in the magnetic tweezers as BHO particles[7].

For the sake of verifying these conclusions, the simulation results are presented. Figure 8 shows the position distribution of Brownian particles with different stiffness coefficients, which is approximately Gaussian type in line with the conclusions. Figure 9 exhibits the fitting line for the reciprocal of the stiffness coefficient and position variance. The fitting results indicate that the stiffness coefficient is inversely proportional to the position variance, i.e., verifying the correctness of equation (13).
Figure 9. The fitting line of the inverse of position variance - stiffness coefficient. The goodness of fit: SSE: $7.424 \times 10^6$; R-square: 0.9925; Adjusted R-square: 0.9921; RMSE: 642.2

4. Comparison
From the above discussion, it can be seen that the random walking model and Langevin theory can both be used to simulate Brownian motion well. Nevertheless, the Langevin theory is more suitable for the simulation of a single Brownian particle on account of the smooth motion trajectories. At the same time, the random walking model is more suitable for the simulation of multiple Brownian particles due to the fast calculation speed. The diffusion problem in a container can be well treated by using the random walking model. In contrast, the Brownian motion problem with other external forces can be well treated by Langevin theory. In practical application, the simulation method can be selected according to the needs.

5. Conclusion
In summary, we established two simulating Brownian motion methods based on the random walking model and the Langevin theory. According to the analysis, the two methods can do simulation well, but they each show different strengths in their respective fields. In addition to the classical Brownian motion, the diffusion process of Brownian particles in the container and the BHO model are also discussed for the established simulation methods. Nevertheless, many other available scenarios have not been presented in this paper, which we hope to be investigated in the future. These results may pave a path for the further study of complex Brownian motion systems.

Appendix A
Here we would like to discuss why we cannot create the three-dimensional unitary random vector $k_{3D}$ using two random numbers $\theta$ and $\phi$ which correspond to the spherical coordinates. Firstly, we use evenly spaced $(\theta, \phi)$ data to plot a grid on the unit sphere. The result is shown in figure A1. The probability that $k_{3D}$ occurs somewhere on the unit sphere is proportional to the density of points on the grid. As seen in figure A1, the density of points is not a constant on the sphere but is denser near the poles and less dense near the equator. This means that the probability of $k_{3D}$ appearing near the pole is greater, thus destroying the requirement of its equal probability distribution in full space.
Figure A1. Evenly spaced \((\theta, \phi)\) points on the unit sphere.

In addition, this can also be seen from the coordinate transformation expression:

\[
\begin{align*}
    x &= \sin(\theta) \cos(\phi) \\
    y &= \sin(\theta) \sin(\phi) \\
    z &= \cos(\theta)
\end{align*}
\]  

(A. 1)

By calculating the variance \(\langle x^2 \rangle\), \(\langle y^2 \rangle\) and \(\langle z^2 \rangle\) for separate random numbers \((\theta, \phi)\), one obtains:

\[
\begin{align*}
    \langle x^2 \rangle &= \langle \sin^2(\theta) \rangle \langle \cos^2(\phi) \rangle = \frac{1}{2} \times \frac{1}{2} = \frac{1}{4} \\
    \langle y^2 \rangle &= \langle \sin^2(\theta) \rangle \langle \sin^2(\phi) \rangle = \frac{1}{2} \times \frac{1}{2} = \frac{1}{4} \\
    \langle z^2 \rangle &= \langle \cos^2(\theta) \rangle = \frac{1}{2}
\end{align*}
\]  

(A. 2)

We could see that the variances are not equal, which also implies that the \(k_{3D}\) created by this way is not well randomly distributed on the unit sphere.

**Appendix B**

Here we would like to introduce a simple derivation of equation (13). Considering 1D Brownian motion, suppose that the linear restoring force on a BHO particle is:

\[ F = -k(x - x_0) \]  

(B. 1)

This corresponds to potential energy:

\[ V_k = \frac{1}{2} k (x - x_0)^2 \]  

(B. 2)

According to the equipartition theorem, there should be:

\[ \langle V_k \rangle = \frac{1}{2} k_B T \]  

(B. 3)

Substitute equation (B.2) into equation (B.3), one derives:

\[ k = \frac{k_B T}{\langle (x - x_0)^2 \rangle} = \frac{k_B T}{\sigma_x^2} \]  

(B. 4)

Apparently, the stiffness coefficient of the restoring force is inversely proportional to the variance of the position fluctuation.
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