An approach to generate deterministic Brownian motion

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ABSTRACT

We propose an approach for generation of deterministic Brownian motion. By adding an additional degree of freedom to the Langevin equation and transforming it into a system of three linear differential equations, we determine the position of switching surfaces, which act as a multi-well potential with a short fluctuation escape time. Although the model is based on the Langevin equation, the final system does not contain a stochastic term, and therefore the obtained motion is deterministic. Nevertheless, the system behavior exhibits important characteristic properties of Brownian motion, namely, a linear growth in time of the mean square displacement, a Gaussian distribution, and a -2 power law of the frequency spectrum. Furthermore, we use the detrended fluctuation analysis to prove the Brownian character of this motion.

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1. Introduction

Brownian motion has been extensively studied since the findings of the biologist Brown in 1828 [1] and first described by the mathematician Thiele [2] in his paper on the least squares method published in 1880. At that time, Brownian motion was defined as a continuous-time stochastic (or probabilistic) process characterized by normal distribution. The nature of the Brownian motion is uncertain and many questions still remain open of how it could depend on particle interactions with the environment, is this process stochastic or deterministic?

After the Thiele's paper, the study of Brownian motion has been followed independently by Bachelier [3] and Albert Einstein [4], who gave the first mathematical description of a free particle Brownian motion. Later, Smoluchowski [5] brought the solution of the problem to the attention of physicists. In 1908, Langevin [6] obtained the same result as Einstein, using a macroscopically description based on the Newton's second law. He referred his approach to as "infinitely simplest" because it was much simpler than the one proposed by Einstein. Since the pioneering work of Langevin, many papers have been devoted to the description of Brownian motion [7–16], where characteristic features of this behavior have been defined.

The dynamical model of Brownian motion provided by Langevin [6], who used a second-order differential equation with a stochastic term, seems apparently from the nature of randomness. On the other hand, it is widely believed that Brownian motion can be rigorously derived from totally deterministic Hamiltonian models of classical mechanics. One of the reasons for this conviction is related to the widely used Van Hove's method [17–19]. In one way or another, many attempts to establish a unified view of mechanics and thermodynamics [20] traced back to the Van Hove's approach. The result of their method depended on whether one adopted the Heisenberg perspective corresponding to the time evolution of observables,

or the Schrödinger perspective corresponding to the time evolution of the Liouville density. In [21] a Fokker–Planck equation has been derived with the aid of a set of variables of interest interacting with a booster, i.e., a dynamical system mimicking the action of an ideal thermostat with no need of ad hoc statistical assumptions; this approach is based on the assumption of a large number of degrees of freedom, the booster is an n-dimensional deterministic system. In the former case, the usual outcome was derived from the ordinary Langevin equation.

The idea of deterministic Brownian motion has been also moot in hydrodynamics and oscillatory chemical reactions, where in spite of an erratic or random character of time evolution, the observed motion is completely deterministic and sometimes it is referred to as *microscopic chaos* [22–26]. In 1998 Gaspard, et al. [27] have reported on the experimental evidence of microscopic chaos in fluids, obtained by direct observation of Brownian motion of a colloidal particle suspended in water. Deterministic random walk of a phase difference, similar to Brownian motion, has also been observed in coupled chaotic oscillators [28]. A deterministic Brownian motion generator has been previously proposed by Trefàn et al. [29], where the nonlinear generator has been presented by a discrete system which generates pseudo-random numbers [30]. The microscopic chaotic process drives a Brownian particle and has "statistical" properties that differ markedly from the standard assumption of Gaussian statistics.

In many paper devoted to Brownian motion, this behavior is characterized by specific properties, such as a linear in time growth of the mean square displacement, an exponential in time decay of the positional autocorrelation function, and the Lorentzian shape of the power spectrum with a -2 power law of a high-frequency slope [19,27,31]. Another important way to determine Brownian motion is the *detrended fluctuation analysis* (DFA) developed by Peng et al. [32]. The DFA allows one to measure a simple quantitative parameter, the scaling exponent β_v which characterizes correlation properties of a signal.

In this paper we introduce an approach to generate deterministic Brownian motion and determine its character by analyzing time series, power spectrum, and via DFA.

2. Model

A typical example of Brownian motion is particle mixing agitation in fluids. The perpetual motion of a particle occurs due to collisions with molecules of the surrounding fluid. Under normal conditions in a liquid, a Brownian particle suffers from about 10^{21} collisions per second, this is so frequent that we cannot really speak of separate collisions. Furthermore, since each collision can be thought of as producing a kink in the path of the particle, one cannot hope to follow the path in any detail, i.e., the details of the path are infinitely fine. Each of these collisions is always determined by the last event produced by physical interactions in the system.

The modern theory of Brownian motion of a free particle (in the absence of an external field of force) is generally governed by the Langevin equation [6]

$$\ddot{x} = -\gamma \dot{x} + A_f(t), \tag{1}$$

where $\dot{x} = dx/dt$ and $\ddot{x} = d^2x/dt^2$ denote the particle velocity and the acceleration, respectively. According to this equation, the influence of the surrounding medium on the particle motion can be split into two parts. The first term $-\gamma\dot{x}$ stands for the dynamical friction applied to the particle and the second term $A_f(t)$ is the fluctuation acceleration which provides a stochastic character of Brownian motion and depends on the fluctuation force F_f as $A_f(t) = F_f(t)/m$, where m is the particle mass.

It is assumed that the friction term $-\gamma\dot{x}$ is governed by the Stokes' law which states that the friction force $6\pi a\eta\dot{x}/m$ decelerates a spherical particle of radius a and mass m. Hence, the friction coefficient is

$$\gamma = 6\pi a\eta/m, \tag{2}$$

where η denotes the viscosity of the surrounding fluid.

Concerning the fluctuation term $A_f(t)$, we make two principal assumptions:

(i) $A_f(t)$ is independent of $\dot{x}$.
(ii) $A_f(t)$ varies extremely fast as compared with the variation of $\dot{x}$.

The latter assumption implies that there exists a time interval Δt during which the variations in $\dot{x}$ are very small. Alternatively, we may say that though $\dot{x}(t)$ and $\dot{x}(t + \Delta t)$ are expected to differ by a negligible amount, no correlation between $A_f(t)$ and $A_f(t + \Delta t)$ exists.

Because a particle is immersed in a liquid or gas at ordinary pressure, Einstein [4] used the Stokes formula to calculate the mean square $\overline{\Delta x^2}$ of displacement Δx of a spherical particle in a given direction x after a given time τ to be

$$\overline{\Delta x^2} = 2Dt = \frac{RT}{N}\frac{1}{3\pi\eta a}\tau, \tag{3}$$

where $\overline{\Delta x^2} = \overline{x^2} - \overline{x_0^2}$, D is the diffusion coefficient at temperature T, R is the gas constant, and N is the Avogadro number. Brownian motion occurs in systems where the mechanisms governing energy dissipation are distinct from those of energy storage [27,19,31]. In Brownian motion, the mean square displacement at short times grows linearly with time, i.e. $\overline{\Delta x^2} \propto t^\mu$.

By changing the variables in the Langevin equation (1) we get the system of two differential equations:

$$\dot{x} = y,$$
$$\dot{y} = -\gamma y + A_f(t). \tag{4}$$

The evolution of the flow Eq. (4) with the stochastic term A_f exhibits the characteristic properties of Brownian motion, such as a linear growth of the mean square displacement and an approximately -2 power law frequency spectrum. In order to generate deterministic Brownian motion we add an additional degree of freedom to the phenomenological system Eq. (4), where the fluctuating acceleration $A_f(t)$ is now replaced by variable z defined by a third differential equation. The proposed variable z, which acts as fluctuating acceleration, produces a deterministic dynamical motion with a chaotic behavior as in previous work [29]. However, in our model the fluctuation acceleration has a direct dependence on the position, velocity and acceleration due to the jerky equation involved [33]. When a particle is moving in a fluid, friction and collisions with other particles existing in the environment necessarily produces changes in the motion velocity and acceleration; all these changes are considered in the jerky equation. Without loss of generality, we define an unstable dissipative system in the same spirit that [34,35] as follows

$$\dot{x} = y,$$
$$\dot{y} = -\gamma y + z,$$
$$\dot{z} = -\alpha_1 x - \alpha_2 y - \alpha_3 z + \alpha_4, \tag{5}$$

where α_i, $i = 1, \ldots, 4$, are constants. The first two equations are derived from the Langevin equation 1 with a little change: the stochastic term is replaced by the deterministic term. The third derivative in Eq. (5), i.e. the rate of a change in acceleration, is technically known as jerk. This *jerky equation* is derived in the same spirit as those introduced by Campos-Cantón, et al. [34,35]. A great deal of qualitative information about the local behavior of this system near the equilibrium point x^* satisfying $f(x^*) = 0$ is determined by the Jacobian of the system Eq. (5) and specifically its eigenvalues $\Lambda = \{\lambda_1, \lambda_2, \lambda_3\}$.

For simplicity, the equilibrium can be given in terms of a single state by defining *switching surfaces* (SW). The SW are planes perpendicular to the x axis, which are considered as edges of each domain. In case of real systems, SW can be seen as multi-well potential with short fluctuation escape time, where x is bounded by SW as $-\frac{SW}{2} < x < \frac{SW}{2}$. For all SW, α_4 is defined as follows

$$\alpha_4 = C1 * Round(x/C2), \tag{6}$$

where $C1 = 0.9$ and $C2 = 0.6$ are constants which determine the system equilibrium and $Round(K)$ rounds K to a nearest integer less than or equal to K. Eq. (6) bounds the displacement of a Brownian particle when it is immersed in a short or a large container.

3. Numerical results

Numerical simulations are performed using the forth order Runge–Kutta algorithm by exploring different combinations of initial conditions. Fig. 1 shows the time series of the particle position where the memoryless behavior characterized Brownian motion can be clearly seen.

To study Brownian motion generated by Eq. (5), we fix $\gamma = 7 \times 10^{-5}$ and explore different values of α_1, α_2, and α_3. The trajectory of Brownian motion is determined by initial conditions and α's values. For initial conditions $x_0 = 1.0$, $y_0 = 1.0$, and $z_0 = 1.0$, deterministic Brownian motion is found for the following range of parameters α_{1-3}:
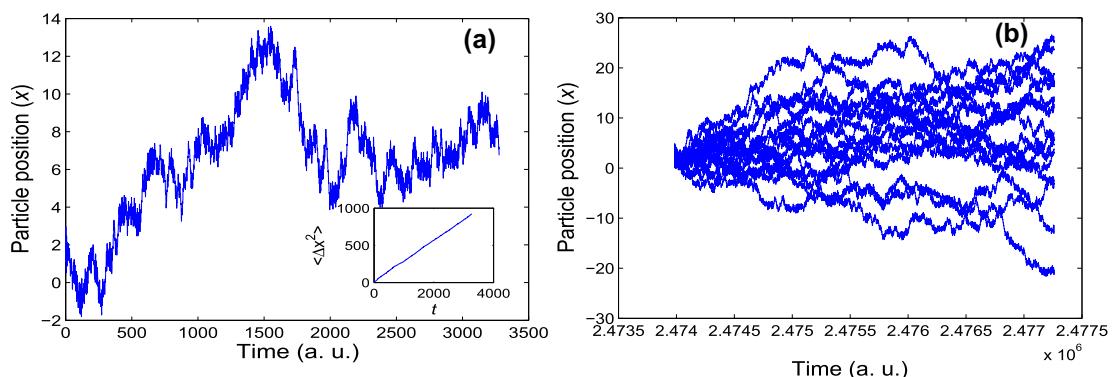

Fig. 1. (a) Trajectory of deterministic Brownian motion for one hundred *SW* generated by the proposed model. The inset shows a linear growth of the mean square displacement $\overline{\Delta x^2} \propto t^\mu$ ($\mu = 1$). (b) Trajectories of deterministic Brownian motion started from 16 different initial conditions. $\alpha_1 = 1.5$, $\alpha_2 = 1.2$, $\alpha_3 = 0.1$. Strong sensitivity to the initial conditions results in completely different trajectories.

$$1.49 \leqslant \alpha_1 \leqslant 1.52, \tag{7}$$

$$0.1 \leqslant \alpha_2 \leqslant 2.0, \tag{8}$$

$$0.1 \leqslant \alpha_3 \leqslant 1.5. \tag{9}$$

Since there are many steps with short time duration and few steps with long time duration, the predicted mean square displacement at short times is observed. Both the linear growth in time of the mean square displacement (inset in Fig. 1(a)) and the strong dependence on the initial conditions (Fig. 1(b)) indicate that the observed motion has a Brownian character.

It is known that traditional Brownian motion is characterized by zero-mean Gaussian probability distributions of system variables. Fig. 2 shows the probability distributions of a particle displacement (Fig. 2(a)), velocity (Fig. 2(b)), and acceleration (Fig. 2(c)) in our system. One can see that the distributions of the motion generated by our system are very close to Gaussian, similar to those obtained by the booster proposed in [21]. It is different from a U-shaped distribution obtained by Trefán et al. [29], typical for discrete chaotic systems [36–38] (see Fig. 3).

Another important feature of this motion is its specific power spectrum which obeys the scaling relation

$$I(\omega) \sim \omega^{\beta}, \tag{10}$$

where $I(\omega)$ is the spectral intensity at frequency ω. The experiments on the motion of a colloidal particle in a liquid [27] gave $\beta \sim -2$. By applying a Fourier transform to the time series of the displacement of our system Eq. (5), we obtain a $\beta \sim -2$ power law scaling in the frequency spectrum for different α_1, α_2, α_3, and different SW. Fig. 4 shows the power spectrum for the same parameters as those explored in Fig. 1, which yields $\beta \sim -2$.

Finally, to further ensure that the proposed system generates Brownian motion, we apply the DFA evaluation method for one hundred SW for the same values as those used in Fig. 1. The DFA is a scaling analysis which yields a simple quantitative parameter, the scaling exponent δ_v. The main advantages of the DFA over many other methods are that it allows the detection of long-range correlations of a signal embedded in seemingly nonstationary time series, and also avoids the spurious detection of apparent long-range correlations that are an artifact of nonstationarity. Fluctuation function $F(v;s)$ obeys the following power law scaling relation
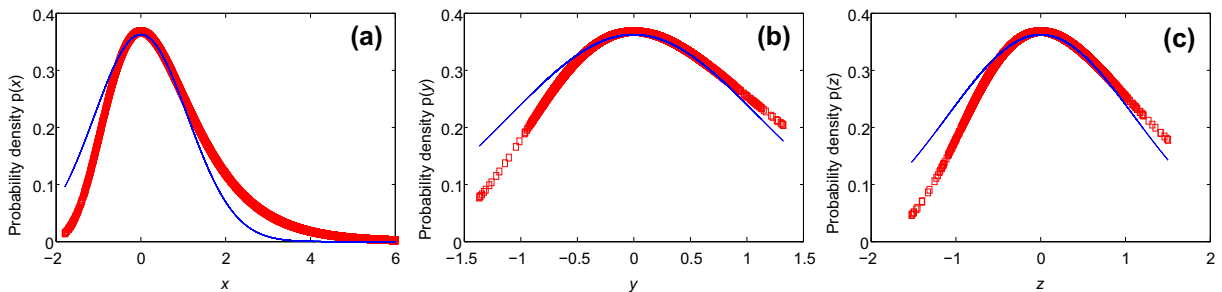

Fig. 2. Probability density, in red squares, obtained from the motion showed in Fig. 1(a), for (a) displacement, (b) velocity, (c) acceleration, compared with a fitted Gaussian distribution (straight blue line). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)
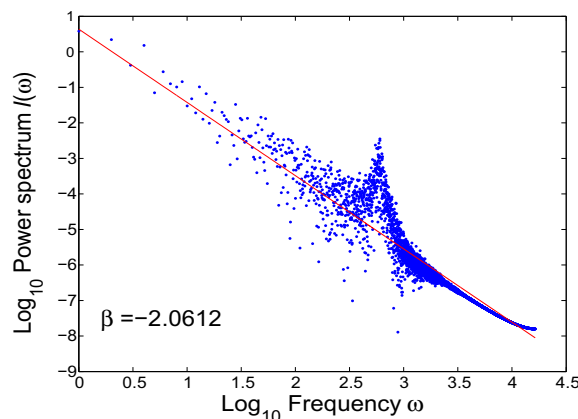

Fig. 3. Power spectrum of deterministic system Eq. (5) for one hundred SW represented a $\beta = -2.0612$ power law scaling, typical for Brownian motion.
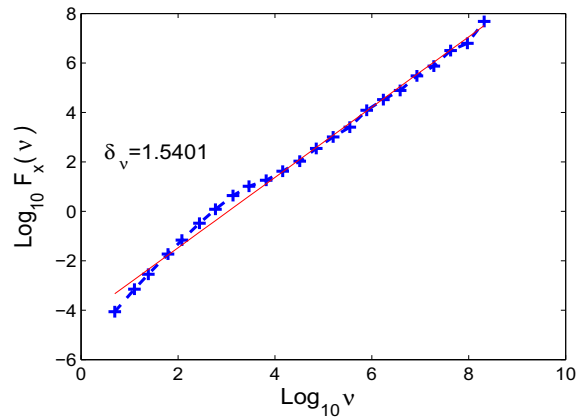
Fig. 4. Log–log plot of fluctuation function $F(v)$ versus segmented lengths (v) of time series of Eq. (5) for one hundred *SW*. $\delta_v \sim 1.5$ obtained by DFA indicates the Brownian character of the observed motion.
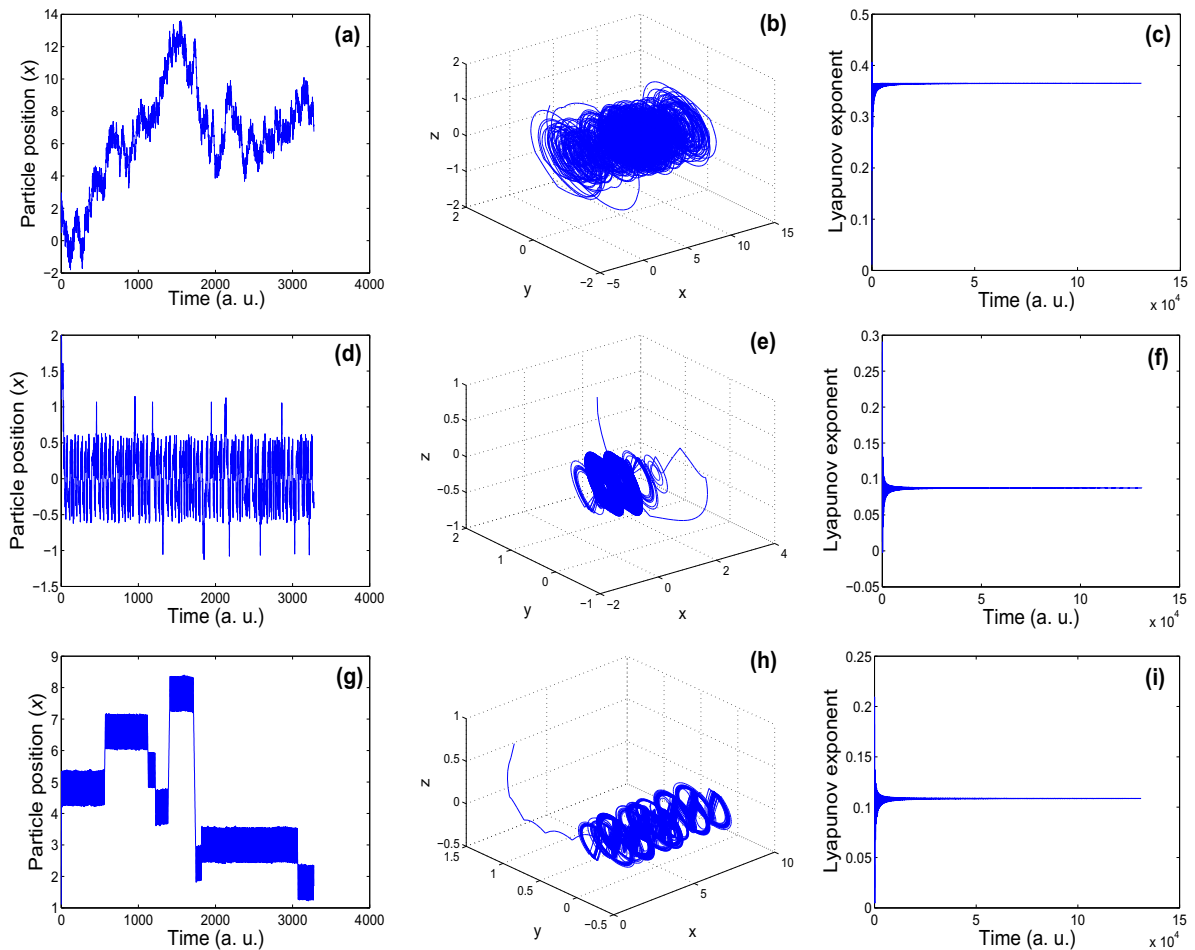

Fig. 5. Time series (left column), phase-space portraits (middle column), and leading the Lyapunov exponent (right column) of different dynamical regimes of system Eq. (5). (a)–(c) Brownian motion for $\alpha_1 = 1.5$, $\alpha_2 = 1.2$, and $\alpha_3 = 0.1$, (d)–(f) chaos for $\alpha_1 = 1.6$, $\alpha_2 = 1.3$, $\alpha_3 = 0.9$, and (g)–(i) intermittency (metastability) for $\alpha_1 = 1.5$, $\alpha_2 = 0.5$, $\alpha_3 = 1.5$.

$$F_q(v;s) \sim s^{\delta_v} \tag{11}$$

for which the time series is segmented in s pieces with length v. When the scaling exponent $\delta_v > 0.5$ three distinct regimes can be defined as follows.

1. If $\delta_v \sim 1$, DFA defines $1/f$ noise.
2. If $\delta_v > 1$, DFA defines a non stationary or unbounded behavior.
3. If $\delta_v \sim 1.5$, DFA defines Brownian motion or noise.

The scaling law with $\delta_v = 1.5401$ revealed by the DFA and shown in Fig. 4 confirms the Brownian character of the observed motion.

Finally, we should note that in addition to Brownian motion, the proposed system Eq. (5) displays other dynamical regimes for different sets of the parameters α, such as chaos, intermittency, limit cycles, and fixed points. Typical examples of different dynamical behaviors of our system are illustrated in Fig. 5 with the time series, phase-space diagrams, and the leading Lyapunov exponents.

During the Brownian motion shown in Fig. 5(a) and (b), the particle trajectory visits 16 SW, whereas in the chaotic (Fig. 5(d) and (e)) and intermittency (Fig. 5(g) and (h)) regimes the particle visits only 5 and 8 SW, respectively. Strong sensitivity to initial conditions inherent to Brownian motion is also an essential feature of chaos, because both are characterized by the positive leading Lyapunov exponent (Fig. 5(c) and (f)). However, there is a significant difference between Brownian and chaotic dynamics. While chaos is an attractor localized within a certain area of phase space, Brownian motion as noise is not an attractor and hence occupies infinite space.

4. Conclusions

In this paper we have introduced an approach to generate deterministic Brownian motion, by adding an additional degree of freedom to the Langevin equation. In our three-dimensional model, the fluctuation acceleration in the Langevin equation has been replaced by a new variable defined by a third differential equation with a Gaussian probability density distribution. Also, the numerical simulations of the resulted deterministic three-dimensional model displayed typical characteristics of Brownian motion, namely, a linear growth of the mean square displacement and an approximately -2 power law of the frequency spectrum, widely accepted in scientific literature. Furthermore, an approximately 1.5 power law scaling of the fluctuation function versus segmented lengths obtained by DFA, confirmed a Brownian character of the observed motion. Our results show that the main characteristics of the motion generated by our system do not represent a subtle difference from traditional Brownian motion.

Since the results of this paper have been obtained using a generic unstable dissipative system, we believe that the approach could help in the development of adequate realistic models with real parameters in order to obtain the Brownian motion in many natural systems. Based on the mathematical model proposed in this paper, an electronic device coupled can be developed to generate deterministic Brownian motion.

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