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A Feedback Control of Fluctuations in Simple Molecular Dynamics

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Abstract: Suppression of diffusion processes generated by fluctuations in small-scale systems is crucial for its manipulation especially in nanotechnology. In this work, we focus on thermal fluctuations and their diffusion effect in a model of molecular dynamics. First, we propose time-delayed feedback control method instead of decreasing temperature which is a conventional way of controlling thermal fluctuations. We investigate numerically an effect of delayed-feedback on random walks in discrete time systems and find that diffusion processes of the controlled random walk is suppressed with increasing delay time. Second, we apply the proposed method to simple models of molecular dynamics which are composed of a single particle as well as two flocculated ones with the Lennard-Jones potential. Numerical simulations of the molecular dynamics show the effectiveness of the proposed method for suppressing diffusion processes observed in molecular dynamics.

Keywords: Delayed feedback control, stochastic process, molecular dynamics, diffusion

1. INTRODUCTION

According to recent developments of technology for very fine structure, i.e. nanotechnology, materials and devices in nanometer scale are of interest in many fields of engineering (1). For example, advancing nanotechnology is on demand from downsizing of computers, drag delivery systems and so on. However, several kinds of disturbances (or noise) such as thermal fluctuations and quantum effects are unignorable in those small scale devices, e.g. the nano disks (2), etc. In terms of conventional technology, those disturbances degrade the performance of systems assembled by nanoscale materials. Therefore, it is critically important to suppress noise in nano systems.

In order to take into account noise in small-scale systems, mathematical models are useful, because they are able to be readily simulated. Brownian motion is a typical example of such a system with noise, which can be modeled by a simple stochastic description like the Langevin equation (3). It would be helpful in practice for diffusion phenomena in Brownian motion to be suppressed (4). The most popular way for suppressing diffusion in Brownian motion would be decreasing temperature of the system which results in suppression of thermal fluctuations . However, decreasing temperature is not selective to a single target. So, we introduce alternative method which can control diffusion process of one particle in Brownian motion.

In nonlinear physics, controlling noisy dynamics, especially chaotic dynamics, has been extensively studied last few decades (5; 6). Among many control methods for chaotic dynamics, a time-delayed feedback control (DFC) method to stabilize periodic motion (7) is prevailed due to its simplicity and applicability to experimental systems such as laser, electronic circuits, etc (8).

In this paper, we focus on stochastic diffusion of random walks instead of chaotic dynamics, which corresponds to Brownian motion in discrete time, and apply a modified DFC method to control the degree of diffusion in random walks. First, we observe diffusion processes in a random walk model controlled by the DFC method. Then, we apply the method to a model of molecular dynamics regarding the case of single particle in one and two dimensional space as well as two flocculated particles with thermal fluctuations. We numerically confirm that both of the cases show suppression of diffusion by the proposed control method.

In Section II, brief explanation of basic idea of control of discrete time stochastic system by time-delayed feedback. In Section III, we introduce molecular dynamics with Lennard-Jones potential and demonstrate numerical simulations of single and two flocculated particles. Finally, summary is given in Section IV.

2. DELAYED FEEDBACK CONTROL OF RANDOM WALK

In this paper, a random walk model can be defined for discrete time n as

$$x_{n+1} = x_n + D\xi_n, \tag{1}$$

where x_n is a m-dimensional vector and ξ is a m-dimensional random variable following the normal distribution $N(0,\ 1)$ for each entry and D is an amplitude

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vector of noise. Without loss of generality, we consider one-dimensional case, i.e. $m = 1$.

In order to control the random walk x_n, we introduce an attractor dynamics described by

$$x_{n+1} = f(x_n, a), \tag{2}$$

where the map f has an stable fixed point. a is a parameter. We assume that the fixed point is denoted by $\tilde{x}$ and linearize f around $\tilde{x}$. Then, we have

$$x_{n+1} = f(\tilde{x}) + f'(\tilde{x})(x_n - \tilde{x}), \tag{3}$$

which can be described as

$$x_{n+1} = f'(\tilde{x})x_n + (1 - f'(\tilde{x}))\tilde{x}, \tag{4}$$

where we use the relation $\tilde{x} = f(\tilde{x})$. For this equation, if we denote $A = 1 - f'(\tilde{x})$, then $x_{n+1} = (1 - A)x_n + A\tilde{x}$. Moreover, we transform x_n as $X_n = x_n/A\tilde{x}$. Then, we can rewrite eq. (4) as

$$X_{n+1} = (1 - A)X_n + 1. \tag{5}$$

Let $\tilde{X} = 1/A$ be the fixed point of the dynamical system (5). Regarding this linear map, we add the noise term and rewrite as

$$X_{n+1} = X_n + D\xi_n + (1 - X_n/\tilde{X}). \tag{6}$$

Compared to eq. (1), the control input U_n is $U_n = 1 - X_n/\tilde{X}$. The dynamics of the system (6) is simple such that a trajectory wander around the fixed point $\tilde{X}$, if $\tilde{X}$ takes an appropriate value. It is possible to suppress diffusion of random walk by the form of (6). However, we have to set the value of $\tilde{X}$ in advance. On the other hand, if we replace the $\tilde{X}$ with $X_{n-\tau}$, then the system is

$$X_{n+1} = X_n + D\xi_n + (1 - X_n/X_{n-\tau}). \tag{7}$$

Note that $X_{n-\tau} \neq 0$. In this case, the control input is described as $U_n = -1/X_{n-\tau}(X_n - X_{n-\tau})$ and considered as a kind of DFC in which the gain is determined adaptively by the time delay $X_{n-\tau}$.

Figure. 1 shows the dynamics of (7). As can be seen, we observe that longer time delay suppresses the diffusion of a random walk. This result may be counterintuitive, since longer time delay make a system unstable in general. However, in the system (7), the opposite is observed. The detailed mechanism of the phenomenon and the analysis of the system (7) are discussed in (11).

It should be noted that similar discussion can be held for a continuous time system such as

$$\dot{y}_t = D\xi_t + (1 - y_t/y_{t-l}), \tag{8}$$

where y is a real variable and t and l is continuous time. For this system, let $\Delta = l/\tau$, $\tau \in \{2, 3, \ldots\}$. Then, we define t_n as $n\Delta$ that is $n\frac{l}{\tau}$, where $n \in \{-\tau, -\tau+1, \ldots, 0, 1, \ldots\}$. So, if we define $Y_n = y_{t_n}$ and $\xi_n = \xi_{t_n}$, eq. (8) can be rewritten as $Y_{n+1} = Y_n + D\Delta\xi_n + \Delta(1 - Y_n/Y_{n-\tau})$. This form is equivalent to eq. (7)

As can be seen from Figure 1, controlled random walk stay at almost stationary state. Therefore, we simplify the system (7) as follows.

$$X_{n+1} = X_n + D\xi_n + K(X_n - X_{n-\tau}), \tag{9}$$

where K is constant value satisfying $0 < K < 1$. This simplification can be held when the trajectories of suppressed fluctuations stay within a small region, which implies that the value of $1/x_{n-tau}$ can be approximated by a constant.

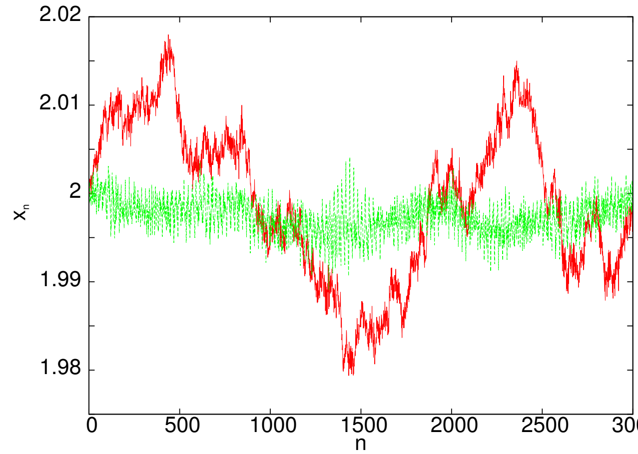

Fig. 1. Suppression of diffusion in random walks of the system (7). The red solid and green dashed lines are regarding $\tau = 2$ and $\tau = 20$, respectively. $D = 0.001$.

This form is the same as the original DFC with random walk. In order to analyze the stability of the simplified system (9), we consider $\tau + 1$ dimensional system without noise, namely $D = 0$:

$$\mathbf{x}_{n+1} = \mathbf{A}\mathbf{x}_n, \tag{10}$$

where $\mathbf{x}_n = (x_n^{(1)}\ x_n^{(2)}\ \ldots\ x_n^{(\tau)}\ x_n^{(\tau+1)})^T$ and

$$\mathbf{A} = \begin{bmatrix} 1-K & K & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 1 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 1 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 1 \\ 1 & 0 & 0 & 0 & \cdots & 0 & 0 \end{bmatrix}. \tag{11}$$

The characteristic equation of $\mathbf{A}$ is

$$\det(\mathbf{A} - \lambda I) = (1 - K - \lambda)\lambda^\tau + K = 0, \tag{12}$$

which has the largest eigenvalue $\hat{\lambda} = 1$ and the other eigenvalues λ_i's satisfy $|\lambda_i| < 1$. Therefore, the system (9) is damping with oscillations.

Fig. 2 (a) shows the eigenvalues for the matrix A. As can be seen, the number of the eigenvalues increases and those absolute values are approaching 1 with increasing the delay time τ. However, the dissipation rates, i.e. $\Pi\lambda_i$, are constant even if τ increases. Thus, the total stability of the fixed point is not changed. This result implies that it is not possible to explain the suppression of the diffusion in Figure 1 when there is no noise, i.e. $D = 0$. Then, we numerically calculate the largest Lyapunov exponent with respect to τ in the case of $D \neq 0$ shown in Figure 2 (b). We observe that the values of the largest Lyapunov exponent decrease with increase of τ. According to this, we guess that the increasing stability of the noisy system together with τ is due to the interaction between noise and time-delay.

3. APPLICATION TO MOLECULAR DYNAMICS

In this section, we apply the control scheme which is shown in §2 to molecular dynamics (9; 10).