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# An Integral Algorithm for Numerical Integration of One-Dimensional Additive Colored Noise Problems

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We present an integral-closed algorithm for solving a Langevin equation driven by an additive colored noise. Both the mean first passage time in a bistable system and the diffusion current in a titled periodic potential are calculated and the comparison with existing algorithms is carried out. The dependence of the numerical results on the time steps is studied. Our algorithm is shown to have high accuracy and stability.

**KEY WORDS:** Algorithms; colored noise; Langevin equation; mean first passage time; current.

In the last fifteen years many researchers have developed different algorithms to simulate Langevin equations with a colored noise,(1) for instance, one-step collocation,(2) predictor-corrector scheme,(3) genuine second-order algorithm(4) and Runge–Kutta approach.(5) In these approaches an integral simulation for an Ornstein–Uhlenbeck noise source is firstly performed and then the deterministic portion of the equation is either expanded or iterated, thus one produces the numerical algorithms. One of the most debated problems within the community of stochastic physics has been the calculation of the activation rate in overdamped systems in the presence of the correlated fluctuations. It is the purpose of this paper to present and discuss an integral algorithm for numerical integration of one-dimensional Langevin equation driven by an additive colored noise. The algorithm is stable upon changing the time steps. The simulations of both the bistable

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potential and the titled ratchet-like periodic potential are tested to show the improved accuracy over the standard methods.

We consider a Brownian particle moving in a one-dimensional nonlinear potential $V(x)$, which is subject to an additive Ornstein-Uhlenbeck noise. The motion of the particle is described by the following Langevin equation:

$$\dot{x}(t) = f(x) + \varepsilon(t) \tag{1}$$

$$\langle \varepsilon(t) \rangle = 0, \qquad \{\langle \varepsilon(t)\, \varepsilon(t') \rangle\} = \frac{D}{\tau} \exp\left(-\frac{|t-t'|}{\tau}\right) \tag{2}$$

where $f(x) = -V'(x)$, $\varepsilon(t)$ indicates the noise source, $D$ and $\tau$ are the intensity and the correlation time of the noise. Here $\{\cdots\}$ refers to an average over the initial value of $\varepsilon$, i.e., the stationary distribution of $\varepsilon(0)$ is[6]: $P(\varepsilon(0)) = (2\pi D/\tau)^{-1/2} \exp(-\tau\varepsilon^2(0)/2D)$. This exponentially correlated colored noise can be produced by a white noise $\eta(t)$ as

$$\dot{\varepsilon}(t) = -\frac{1}{\tau}\varepsilon + \frac{\sqrt{2D}}{\tau}\eta(t) \tag{3}$$

with

$$\langle \eta(t) \rangle = 0, \qquad \langle \eta(t)\, \eta(t') \rangle = \delta(t-t') \tag{4}$$

An integral algorithm has been derived[7] for the simulation of Eq. (3). It reads

$$\varepsilon(t+\Delta t) = \exp(-\Delta t/\tau)\, \varepsilon(t) + \frac{\sqrt{2D}}{\tau}\omega_0 \tag{5}$$

where

$$\omega_0 = \int_t^{t+\Delta t} \exp\left(\frac{s-t-\Delta t}{\tau}\right) \eta(s)\, ds \tag{6}$$

We now develop an integral algorithm in a closed form in terms of the analytical solution of linearized Eq. (1). The first step is to expand the term $f(x(t))$ to the first order within the time interval $t \leqslant t' \leqslant t+\Delta t$,

$$f(x(t')) = f(x(t)) + f'(x(t))[x(t') - x(t)] \tag{7}$$

thus Eq. (1) becomes

$$\frac{dx(t')}{dt'} = f(x(t)) + f'(x(t))[x(t') - x(t)] + \varepsilon(t') \tag{8}$$

Integrate (8) with the initial condition $x(t')|_{t'=t} = x(t)$ and obtain

$$\begin{aligned} x(t+\Delta t) = x(t) - \frac{f(x(t))}{f'(x(t))} \{1 - \exp[f'(x(t))\,\Delta t]\} \\ + \int_t^{t+\Delta t} \exp[f'(x(t))(t+\Delta t - s)]\,\varepsilon(s)\,ds \end{aligned} \tag{9}$$

consequently,

$$\begin{aligned} x(t+\Delta t) = x(t) &- \frac{f(x(t))}{f'(x(t))} \{1 - \exp[f'(x(t))\,\Delta t]\} \\ &+ \frac{\tau \exp[f'(x(t))\,\Delta t]}{1 + \tau f'(x(t))} \{1 - \exp[-(f'(x(t)) + \tau^{-1})\,\Delta t]\}\,\varepsilon(t) \\ &+ \frac{\sqrt{2D}}{\tau}\,\omega_1 \end{aligned} \tag{10}$$

in which $\omega_1$ is defined by

$$\omega_1 = \int_t^{t+\Delta t} \exp[f'(x(t))(t+\Delta t - s)]\,ds \int_t^s \exp\left(\frac{s'-s}{\tau}\right) \eta(s')\,ds' \tag{11}$$

where $\omega_0$ and $\omega_1$ are two Gaussian variables with zero $-$ mean and their standard deviations and cross correlation are given by

$$\langle \omega_0^2 \rangle = \frac{\tau}{2}\,[1\text{-}\exp(-2\Delta t/\tau)] \tag{12}$$

$$\begin{aligned} \langle \omega_1^2 \rangle = &\frac{\tau^2}{1 - \tau f'(x(t))} \left\{ \frac{\exp[2f'(x(t))\,\Delta t] - 1}{2f'(x(t))} \right. \\ &\left. + \frac{\tau \exp[2f'(x(t))\,\Delta t]}{1 + \tau f'(x(t))}\,[\exp(-(f'(x(t)) + \tau^{-1})\,\Delta t) - 1] \right\} \\ &- \frac{\tau^3}{2} \exp[2f'(x(t))\,\Delta t] \left[ \frac{1 - \exp(-\Delta t f'(x(t)) - \Delta t/\tau)}{1 + \tau f'(x(t))} \right]^2 \end{aligned} \tag{13}$$

and

$$\langle \omega_0 \omega_1 \rangle = \frac{\tau^2}{2} \left\{ \frac{1 - \exp[(f'(x(t)) - \tau^{-1})\, \Delta t]}{1 - \tau f'(x(t))} + \frac{\exp(-2\Delta t/\tau) - \exp[(f'(x(t)) - \tau^{-1})\, \Delta t]}{1 + \tau f'(x(t))} \right\} \tag{14}$$

Define $R_0$ and $R_1$ as two uncorrelated Gaussian random numbers with mean zero and standard deviation one, thus we have for $\omega_0$ and $\omega_1$.[3,4]

$$\omega_0 = \sqrt{\langle \omega_0^2 \rangle}\, R_0 \tag{15}$$

$$\omega_1 = \frac{\langle \omega_0 \omega_1 \rangle}{\sqrt{\langle \omega_0^2 \rangle}}\, R_0 + \left[ \langle \omega_1^2 \rangle - \frac{\langle \omega_0 \omega_1 \rangle^2}{\langle \omega_0^2 \rangle} \right]^{1/2} R_1 \tag{16}$$

To demonstrate the superiority of the present method, let us now discuss the algorithm in the limit $|f'|\, \Delta t \ll \min(\Delta t/\tau, 1)$ and in the limit $\tau \to 0$. First, consider in the first limiting case.

Using (10) we have

$$-\frac{f(x(t))}{f'(x(t))} \{1 - \exp[f'(x(t))\, \Delta t]\} \approx f(x(t))\, \Delta t + \frac{1}{2} f(x(t))\, f'(x(t))\, \Delta t^2 \tag{17}$$

and

$$\begin{aligned} &\frac{\tau \exp[f'(x(t))\, \Delta t]}{1 + \tau f'(x(t))} \{1 - \exp[-(f'(x(t)) + \tau^{-1})\, \Delta t]\}\, \varepsilon(t) \\ &\quad \approx \tau[1 + f'(x(t))\, \Delta t][1 - \tau f'(x(t))] \\ &\qquad \times \{1 - \exp(-\Delta t/\tau)[1 - f'(x(t))\, \Delta t]\}\, \varepsilon(t) \\ &\quad \approx \tau(1 - \exp(-\Delta t/\tau))\, \varepsilon(t) + \tau^2 f'(x(t))[\Delta t/\tau + \exp(-\Delta t/\tau) - 1]\, \varepsilon(t) \end{aligned} \tag{18}$$

For $\langle \omega_1^2 \rangle$ and $\langle \omega_0 \omega_1 \rangle$ we have

$$\begin{aligned} \langle \omega_1^2 \rangle &\approx \tau^2\{\Delta t + \tau[\exp(-\Delta/\tau) - 1]\} - \frac{\tau^3}{2}[1 - \exp(-\Delta t/\tau)]^2 \\ &\approx \frac{\tau^3}{2}[2\Delta t/\tau - 3 - \exp(-2\Delta t/\tau) + 4\exp(-\Delta t/\tau)] \end{aligned} \tag{19}$$

and

$$\langle \omega_0 \omega_1 \rangle \approx \frac{\tau^2}{2} \frac{\Delta t}{\tau} \left\{ \frac{1-\exp(-\Delta t/\tau)}{\Delta t/\tau - f'\,\Delta t} + \frac{\exp(-2\Delta t/\tau) - \exp(-\Delta t/\tau)}{\Delta t/\tau + f'\,\Delta t} \right\}$$
$$\approx \frac{\tau^2}{2} [1 - 2\exp(-\Delta t/\tau) + \exp(-2\Delta t/\tau)] \tag{20}$$

We have exactly the second-order algorithm of Fox[4] and 3/2-order algorithm of Mannella–Palleshchi.[3]

In the other limit $\tau \to 0$, which corresponds to taking the limit of white noise, our algorithm becomes

$$x(t+\Delta t) = x(t) - \frac{f(x(t))}{f'(x(t))} [1 - \exp(f'(x(t))\,\Delta t)]$$
$$+ \left\{ \frac{D}{f'(x(t))} [\exp(2f'(x(t))\,\Delta t) - 1] \right\}^{1/2} R_1 \tag{21}$$

Thus the expression (21) agrees with Cecchi–Magnasco algorithm for the white noise.[8]

We have performed tests of the algorithm presented here on two types of problems concerned with improving existing algorithms. One of these is a mean first-passage-time (MFPT) problem that is not analytically solvable but for which the reliable results have been obtained by use of the one-step collocation algorithm, the stochastic Runge–Kutta algorithm and the genuine second-order algorithm as well as the theoretical predictions.[9, 10] The other one is the diffusion current of a particle in a tilted ratchet-like potential which has been studied by the matrix-continued fraction (MCF) method.[11] Both tests support the claim that the integral algorithm is efficient and stable on the changing the time steps.

Recent studies on MFPT behavior in a double well ($V(x) = -1/2x^2 + 1/4x^4$) with the parameters $D = 0.1$ and $\tau = 0.1$, 1.0 have been carried out by an improved algorithm[3] and a genuine second-order algorithm,[4] respectively. Up to $\Delta t = 0.1$ the above two methods reproduced the $\Delta t = 0.001$ value for MFPT quite well. In this paper, the numerical calculations for MFPT are done starting from $x = -1$ to reach the barrier at $x = 0$ with average over 2000 stochastic realizations. The results are shown in Fig. 1 and Table 1 by using the 3/2-order algorithm (ALGO 1), the stochastic Runge–Kutta approach (ALGO 2), the genuine second-order algorithm (ALGO 3) and our integral algorithm (ALGO 4) for the different values of $D$ and $\tau$. We choose $\tau = 0.1$ and $D = 0.3$ in Fig. 1. In Table 1 the white-noise limit $\tau = 10^{-4}$ is taken, the theoretical value of

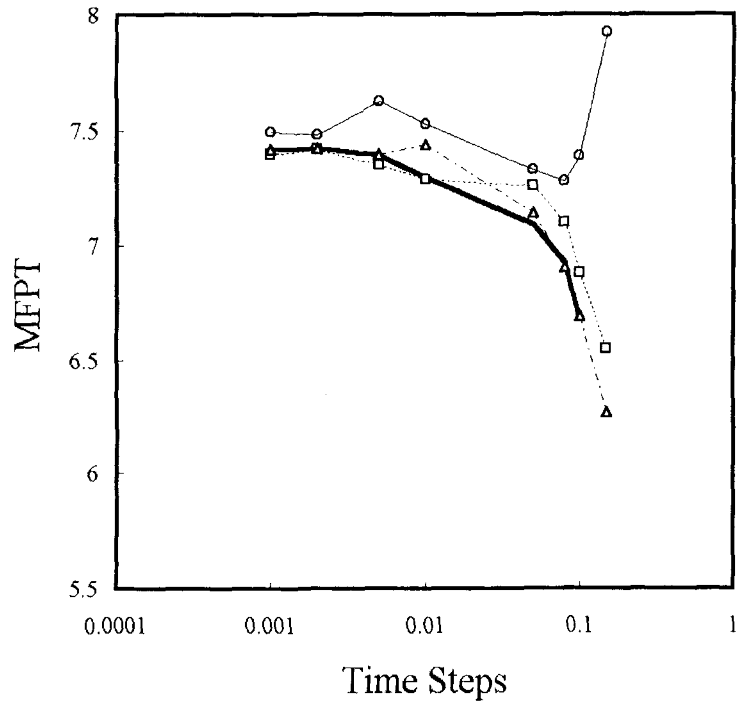


Fig. 1. Dependence of MFPT on time steps for $\tau = 0.1$ and $D = 0.3$. Triangles, ALGO 1; squares, ALGO 2; thin solid line with circles, ALGO 3; and thick solid line, ALGO 4.

MFPT is 30.86 for $D = 0.1$ as well as the one is 1.28 for $D = 1.0$. It is clear from Fig. 1 and Table 1 that both our algorithm (ALGO 4), the genuine second-order algorithm of Fox (ALGO 3) and the stochastic Runge–Kutta approach (ALGO 2) have an overall better convergence when $\Delta t$ is decreased, also the limit $\tau \to 0$, $\Delta t$ finite can be safely taken. On the other hand, however, as the noise intensity $D$ increases, numerical overflow will

**Table 1. MFPT vs. $\Delta t$ in the White-Noise Limit[a]**

| | $D = 0.1$ | | | | $D = 1.0$ | | | |
|---|---|---|---|---|---|---|---|---|
| | ALGO 1 | ALGO 2 | ALGO 3 | ALGO 4 | ALGO 1 | ALGO 2 | ALGO 3 | ALGO 4 |
| $\Delta t = 0.1$ | 37.4543 | 37.1914 | 42.6164 | 31.2229 | overflow | 1.7167 | 2.2113 | overflow |
| $\Delta t = 0.05$ | 35.6602 | 35.5612 | 37.8906 | 33.4442 | 1.6702 | 1.5945 | 1.7728 | 1.4189 |
| $\Delta t = 0.01$ | 33.3607 | 33.3607 | 33.9640 | 32.7790 | 1.4417 | 1.4401 | 1.4731 | 1.4204 |
| $\Delta t = 0.001$ | 31.4781 | 31.4781 | 31.5900 | 31.4306 | 1.3706 | 1.3706 | 1.3638 | 1.3690 |

develop when $\Delta t \geqslant 0.1$ with $D = 1.0$ for ALGO 1 and ALGO 4, these can be traced to the poor quality of the numerical integration for such large time steps. The Runge–Kutta algorithm and the second-order algorithm are also used to obtain a stable data, but the MFPT computed for $\Delta t = 0.1$ is about $20 \sim 30\%$ larger than the MFPT computed for $\Delta t = 0.001$. We solve this problem by interdicting a dimensionless restriction: $D\,\Delta t < 10^{-1}$.

The second example, we consider the diffusion current of a particle in a tilted ratchet-like potential[11] ($V(x) = -(1/2\pi)[\sin(2\pi x) + 0.25\sin(4\pi x)] - 0.5x$, cf. Fig. 2) driven by a colored noise. The simulation is done with $2 \times 10^4$ realizations to determine the average particle velocity $\langle \dot{x}(t) \rangle = \langle f(x(t)) \rangle$ at the stationary states (here, $t = 4.0$) when starting from a minimal state of the potential, the steady current is determined by $J = \langle \dot{x}(t) \rangle_{st}$. The dependence of the numerical results calculated by above four kinds of algorithms on the time steps with the parameters $D = 0.5$ and $\tau = 0.2$ is shown in Fig. 3. One can clearly see that the integral algorithm (ALGO 4) is more stable than other three algorithms, and it seems to show a platform for small-to-intermediate values of $\Delta t$. From Figs. 1 and 3 we have found

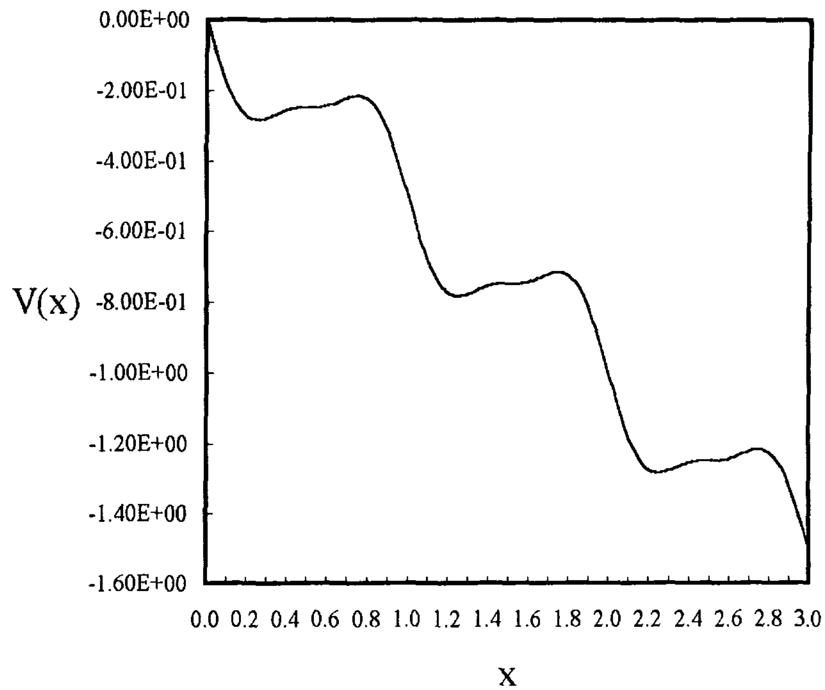


Fig. 2. The titled ratchet-like potential.

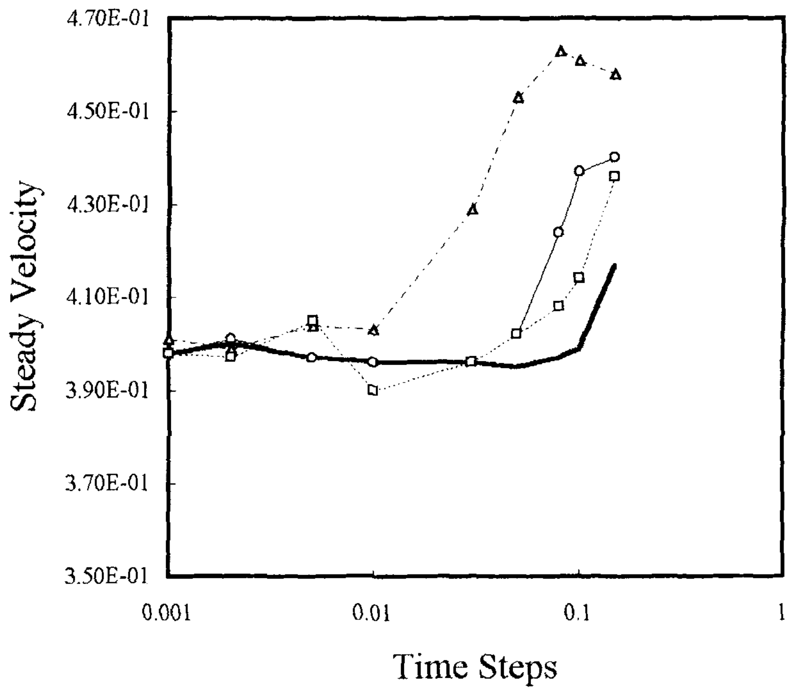


Fig. 3. Dependence of the steady velocity on time steps for $\tau=0.2$ and $D=0.5$. Triangles, ALGO 1; squares, ALGO 2; thin solid line with circles, ALGO 3; and thick solid line, ALGO 4.

that the second-order algorithm[4] (ALGO 3) is always slightly better than the 3/2-order algorithm (ALGO 1), and the results calculated by ALGO 3 and ALGO 4 are identical when the time steps become small, however the stochastic Runge–Kutta algorithm (ALGO 2) has a little oscillation.

In summary, we have derived an integral-closed algorithm for solving one-dimensional Langevin equation driven by an additive colored noise, only two Gaussian random numbers are required within each integration step as the same the genuine second-order algorithm.[4] The present algorithm has the nice properties that it can be reduced to the integral algorithm for the white noise and to the earlier colored noise algorithm for small enough time step. Two numerical tests are performed by using the various algorithms, and the dependence of numerical results on the time steps is also studied. For the integral algorithm presented here, any correlation time of colored noise and the more complex nonlinear potentials can be considered, however, one should not blindly use too large a time step when the noise intensity is increased.

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