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Numerical method for colored-noise generation and its application to a bistable system

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A methodology for generating sample functions for colored noise which has some relative advantages over existing ones is outlined. This involves simulating a stochastic process in terms of harmonic functions, the amplitude of which is related to the power spectral density of the noise. The computational advantages of the fast Fourier transform are utilized and the numerical integration of the noise equation is avoided. In light of this methodology, existing algorithms for colored-noise simulation are critiqued and compared with the present one. Numerical results for a particular case study, namely that of an overdamped particle in a bistable potential, are presented and the results are compared with existing theories.

Numerical simulation in colored noise studies¹ is often used as a yardstick for theoretical approaches. For this purpose presently, some digital simulation techniques²⁻⁴ are used that are largely similar in that Gaussian white noise is generated first from uniform random variates using the well-known *Box-Mueller algorithm*.⁵

In the present work, a simulation technique highly suited for colored noise is presented which is different from existing ones in terms of its analytical formulation. The innovative attribute of the method is that it generates Gaussian colored noise directly from uniform random variates by expressing the sample functions in terms of harmonic functions and using the powerful fast Fourier transform (FFT) method to facilitate calculations. Although the concept of expanding a stochastic process in terms of harmonic function had been used as early as 1910 by Einstein⁶ and followed through by others,⁷ only in recent years has the method been developed to take the advantages of modern computational advancements.^{8,9} In this paper the methodology is applied to simulate the mean first passage time (MFPT) T_F of an overdamped particle in a bistable potential.¹⁰⁻²¹ Although some simulation studies exist (for review see Ref. 10) for this problem, the calculations presented here have two merits: details and sufficient control on accuracy and repeatability. However, the goal of the paper is not to produce an encompassing study of the chosen problem but in essence to introduce an effective simulation technique for colored noise (see conclusion).

The dynamic equation (in terms of dimensionless variables) is

$$\dot{x}(t) = -U'(x) + f(t) = -x + x^3 + f(t), \quad (1)$$

where $U(x) = x^4/2 - x^2/2$, with an unstable position at $x = 0$ and two stable ones at $x = -1, 1$; where $f(t)$ is zero-centered, stationary Gaussian noise with

$$\langle f(t)f(t') \rangle = (D/\tau) \exp(-|t-t'|/\tau),$$

D is the noise intensity, and τ the correlation time. This noise can be generated from a Gaussian white noise $\xi(t)$ [$\langle \xi(t)\xi(t') \rangle = 2D\delta(t-t')$], through the equation

$$\tau \dot{f}(t) = -f(t) + \xi(t) \quad (2)$$

with probability distribution of $f(0)$ being a Gaussian of half-width $(D/\tau)^{1/2}$.

To date, largely three different methods have been used, and all involve solving coupled equations [Eqs. (1) and (2)]. In the algorithm due to Sancho *et al.*² and Fox *et al.*³ (A1 and A2, respectively) Eq. (1) is approximated as

$$x(t+h) = x(t) + [x(t) - x^3(t) + f(t)]h,$$

where h is the discretized time step. In the algorithm of Mannella and Palleschi⁴ (A3) higher-order terms of h are taken into consideration. In A1, Eq. (2) is approximated as

$$f(t+h) = f(t) + [\xi(t) - f(t)]h/\tau,$$

whereas in A2 and A3 it is considered as

$$f(t+h) = f(t) \exp(-h/\tau) + b(t),$$

where $b(t)$ is a Gaussian number of zero mean and variance, $\{D[1 - \exp(-h/\tau)]/\tau\}$.

The putative advantage of A2 and A3 lies in the fact that it uses the exact solution of Eq. (2). From a simula-

tion point of view this means that the deterministic parts of A2 and A3 are more accurate than A1. However, all algorithms follow the same procedure (Box-Mueller algorithm) to generate the randomness and thus share the common properties of the method. It is not the authors' intent to present a detailed critique on this issue but a few critical points are delineated, necessitated for later comparison with the present algorithm.

One primary concern of any simulation method of a colored stochastic process is "how Gaussian is the end product?" Although the Box-Mueller algorithm is exact from a mathematical point of view the distribution of sample values may be "seriously different"²² when used with a *linear congruential random number generator* (used by the above algorithms). Surprising "short tails" even with generated 10⁶ standard normal deviates are obtained—values within three standard derivatives were difficult to obtain for the case study.²³ Special techniques²⁴ may have to be followed in order to generate the needed tail of the distribution. Even then "the effect is worrying, since the experimenter will often not know the value of the [random] multiplier."²²

The other difficulty surrounds the time step of integration. Since Eqs. (1) and (2) are solved as coupled equations, "forcing" Eq. (1) to be integrated over the time step of Eq. (2) which may in many cases produce totally inconsistent results. [In one version of A3 this is circumvented by integrating Eq. (1) by a predictor-corrector method.]

The other aspect has to do with ergodicity. This is not a necessary property of the noise but facilitates calculations as convergence values with respect to the number of realization is obtained faster. The generated samples of A1, A2, and A3 are not ergodic and in literature this shortcoming has been pointed out.²⁵ The absence of ergodicity results in each sample case with vastly different "energy flow," and hence numerous realizations have to be generated to obtain meaningful results. Averages taken over an arbitrary number such as 1000 or 5000 realizations do not signify any steady value. The MFPT should be obtained as the average converges and with the ergodic assumption the MFPT values are obtained faster.

For the present method a stochastic process $f(t)$ is simulated by the following series,^{8,9} as $N \rightarrow \infty$

$$f_s(t) = \sqrt{2} \sum_{n=1}^N [2S_f(\omega_n)\Delta\omega]^{1/2} \cos(\omega t + \Phi_n), \quad (3)$$

where $\omega_n = n\Delta\omega$, $n = 1, 2, 3, \dots, N$, and $\Delta\omega = \omega_u/N$; ω_u represents an upper cutoff frequency for the power spectral density (PSD) curve beyond which its value may be taken to be zero. The Φ_i 's in Eq. (3) are independent random-phase angles uniformly distributed over the interval $[0, 2\pi]$. Equation (3) provides a digitized simulated stochastic process $f_s(t)$ which is asymptotically Gaussian as $N \rightarrow \infty$ due to the central limit theorem. The authors' experience and approximate analysis²⁶ have shown that a reasonable (and computable) value of N can produce substantial portion of the tail of the Gaussian process as shown in what follows. Furthermore, it can be shown that each sample run is ergodic in the mean as well as in the correlation and that the simulated stochastic process repeats itself with a simulated period $T_s = 2\pi/\Delta\omega$. It is of

paramount importance to note that Eq. (3) *directly converts uniform random deviates to a stationary, Gaussian colored noise compared to the linear transformations and a numerical integration for existing algorithms.*

In order to take advantages of the FFT techniques²⁶ Eq. (3) is rewritten in the following form for a sample function $f^{(i)}$

$$f^{(i)}(p\Delta t) = \text{Re} \left[\sum_{n=0}^{M-1} b_n e^{in p 2\pi/M} \right]; \quad p = 0, 1, \dots, M-1, \quad (4)$$

where $b = \sqrt{2}[2S_f(n\Delta\omega)\Delta\omega]^{1/2} e^{i\phi_n^{(i)}}$, $n = 0, 1, \dots, M-1$, and $\phi_n^{(i)}$ is the i th realization of a sequence of random variable Φ_n . For simulation, three parameters of Eq. (4), namely N , M , and ω_u , are pivotal. Amongst other things, N controls the Gaussian character of the simulated process, M controls the digitized time step of the stochastic process; by varying M noise at desired timewidth can be generated.

Corresponding to the exponential correlation function the PSD, $S(\omega) = (D/\pi\tau^2)/[\omega^2 + (1/\tau)^2]$. For MFPT calculation, Eq. (1), along with noise characteristics given by $S(\omega)$, represents the physics of the phenomenon for the present method; the proposed method is effectively one-dimensional and not two like existing ones. (For higher-order noise, like the harmonic noise,²⁷ the method thus has a great advantage as the system is still one-dimensional.) This means that for the deterministic system equation [Eq. (1) with $F=0$] the question^{15,19,20} of the "separatrix" does not arise. The MFPT from $x = -1$ (starting point in all present studies) to say $x = 0$ or 1 (or any x location) for any arbitrary value of the colored noise. This in itself reflects the physics of the phenomenon; the question of separatrix arises due to the introduction of an artifice [enlarged space of Eq. (2)] for theoretical analyses. In the analysis by Doering, Hagan, and Levermore,¹⁷ the location of the end point is taken to be $x=0$ (f arbitrary) for which the simulation value $(T_F)_{x=0}$ will be used for comparison. On the other hand, it has been pointed out^{10,19} that for small τ , $(T_F)_{x=0}$ of the other theories should be interpreted as $\frac{1}{2}(T_F)_{x=1}$.

For a given τ , the ratio of area for say $\omega\tau (=p) = 10$ to

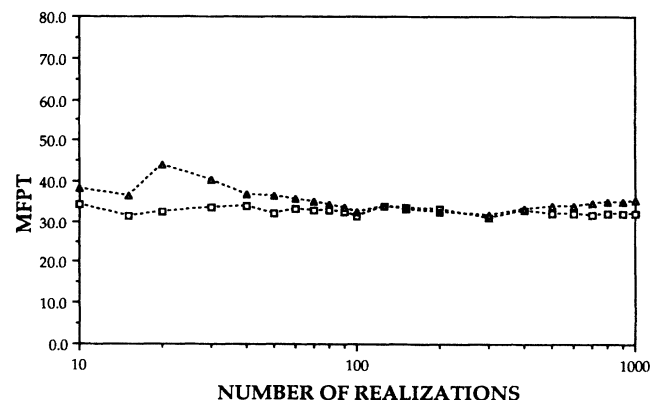


FIG. 1. $(T_F)_{x=0}$ vs number of runs for $D=0.1$. \square : $\tau=0.01$; \triangle : $\tau=0.05$.

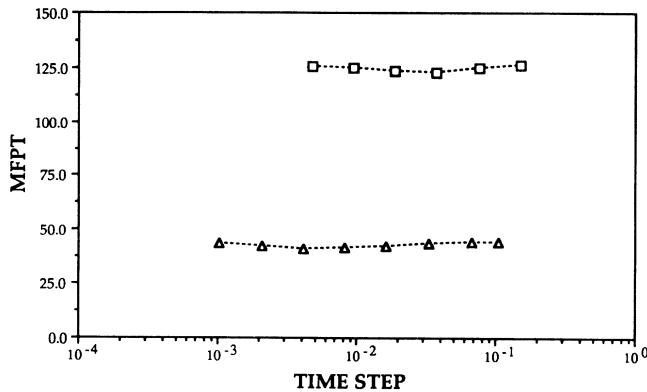


FIG. 2. MFPT vs integration time steps. \square : $(T_F)_{x=1}$ for $D=0.1$ and $\tau=0.5$; \triangle : $(T_F)_{x=0}$ for $D=0.1$ and $\tau=0.1$.

the total area under the PSD curve is 93.7% (for $p=40, 20, 7, 5,$ and 1 , the values are 98.4, 96.8, 90.96, 87.4, and 50, respectively). If p is taken to be 1 ($\omega = \tau$) or less results are inconsistent, as of course, only 50% (or less) of the area under the PSD curve is taken into account. Also high p values (≥ 40) include the asymptotically decreasing portion of the PSD curve without much "power" contribution. In the present tests p was varied from 7 to 20.

As noted before, in principle, "high" value of N is necessary for generating the tail of the Gaussian distribution. Thus, the following question is of importance: How fast is $f_s(t)$ converging to Gaussian character as a function of N ? Values of N were used such that in every run the MFPT was much smaller than the simulated time period T_s . For this, the values of N used were much larger typically (12000–26000) than those usually used in this type of simulation study. In general this improves the Gaussian character of the sample functions; even with N values of about 1000 the tail portion up to five standard deviations are obtained with practically less than 5% error.²⁶

Before comparing the numerical results with existing theories, some general characteristics of the simulation

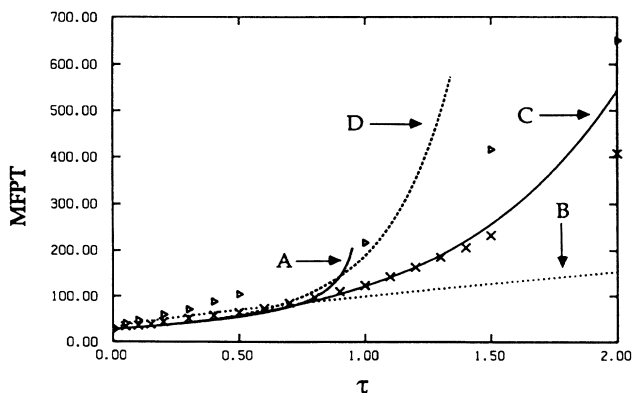


FIG. 3. $\frac{1}{2}(T_F)_{x=1}$ vs τ for $D=0.1$. Theories. A: Fox (Ref. 16); B: Doering, Hagan, and Levermore (Ref. 17); C: Masoliver, West, and Linderberg (Ref. 12); D: Luciani and Verga (Ref. 18); \triangle : Ref. 4; \times : present method.

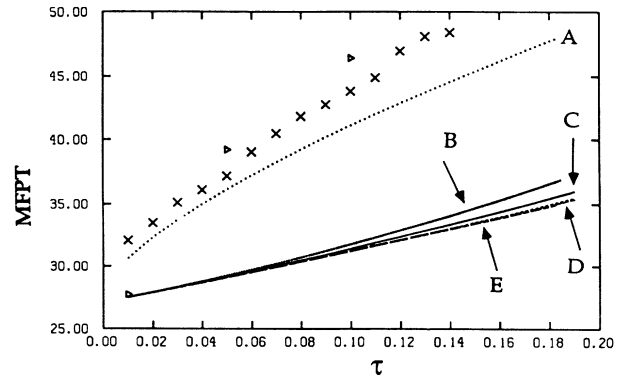


FIG. 4. $(T_F)_{x=0}$ for small τ for $D=0.1$. A: Doering, Hagan, and Levermore (Ref. 17); B: Klosek-Dygas, Matkowsky, and Schuss (Ref. 15); C: Masoliver, West, and Linderberg (Ref. 12); D: Luciani and Verga (Ref. 18); E: Fox (Ref. 16); \triangle : Ref. 4; \times : present method.

study are presented next. Figure 1 shows $(T_F)_{x=0}$ versus the number of realizations. The desired MFPT values (≈ 32 and 35) are obtained with few sample averages and with more averaging a "steady state" is obtained. For all MFPT values presented, the averages were not arbitrarily taken over any number of realizations (say 500 or 1000) but the process was carried through until such "steady state" was obtained. As mentioned earlier, due to the ergodicity of the sample runs, steadiness was obtained quite fast.

Figure 2 shows the advantage of the parameter M . By varying M , a sample run of the noise was discretized with different time steps but with practically no change in the value of MFPT. The values of this figure are to be compared with those obtained through existing methods where large fluctuations are known to occur (see Fig. 1 in Ref. 10 and Figs. 1 and 2 in Ref. 4).

Figure 3 compares the simulation results of $\frac{1}{2}(T_F)_{x=1}$ with the theories of Fox,¹⁶ Doering *et al.*,¹⁷ Masoliver, West, and Linderberg,¹² and that of Luciani and Verga.¹⁸

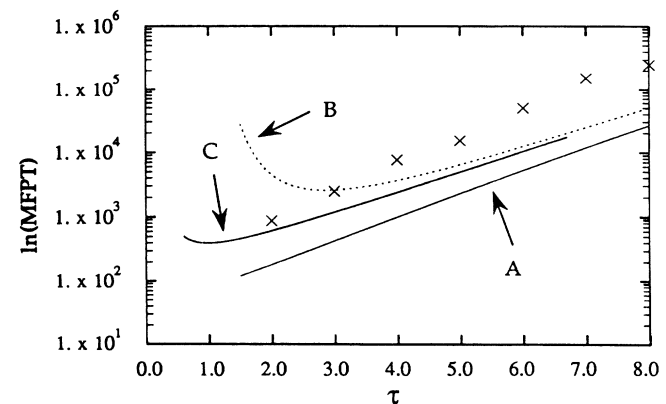


FIG. 5. $(T_F)_{x=1}$ for large τ for $D=0.1$. A: Tsironis and Grigolini (Ref. 14); B: de la Rubia *et al.* (Ref. 21); C: approximate Eq. (13) in de la Rubia *et al.* (Ref. 21); \times : present method.

Good matching between the theories and experiment for values of τ to 0.8 and in particular for the theory of Ref. 12 for up to 1.4. (References 10 and 19 hold that the theories should be good for values a little beyond $\tau=1$.) Figure 4 shows the values of $(T_F)_{x=0}$ for very small τ . In this case, the values obtained by Doering *et al.* (with its $\sqrt{\tau}$ correction) have a very good match with experimental results (to about $\tau=0.15$). It is to be noted that the present simulation results as given by Figs. 4 and 5 are at variance with those of Ref. 4.

Figure 5 represents the T_F values for large τ , i.e., for $\tau=2-8$ [$(\tau U_0)/D=5-20$, where U_0 is the height of the potential barrier]. For such τ values the physical process is quite complicated^{10,21} and the authors intend to address the additional features in much more detail in another paper.

In conclusion, the paper presented a method to generate colored, Gaussian stochastic processes with certain characteristics that offer some advantages over existing methods. It was applied to simulate the MFPT for a particle in an overdamped bistable potential. The simulation method, in essence, can be applied with relative ease for higher-order systems driven by exponential colored noise (e.g., including inertial effect²⁸ in the studied case) or for higher-order noise (e.g., harmonic noise²⁷) for which not much work has been done to date. Two important problems of the higher-order system are that of stability of underdamped particle in a potential well²⁹ and electrohydrodynamic instabilities.³⁰ Simulation studies carried out to date have problems.³¹ Using the present technique the authors have carried out preliminary work on these particular topics with promising success.

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