Reply to the "Comment on 'Numerical method for colored-noise generation and its application to a bistable system' "

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In the preceding Comment [Phys. Rev. A **46**, 8028 (1992)], Mannella and Palleschi critique the power spectral density method of colored-noise generation and its application to the bistable potential [Phys. Rev. A **42**, 7492 (1990)]. These writers make a critical analysis of the outlined advantages of the method and compare it to the stochastic differential equation approach. A reply to the Comment is given based on the work that was presented without adding any new results. It is emphasized that the primary intent of the original paper was to present *an option* for generating colored noise for use in many statistical physics problems.

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In Ref. [1] a method of colored-noise generation from power spectral density (PSD) was discussed, for which certain inherent advantages were claimed and outlined. The method, in essence, generates sample-time history of noise directly from a given power spectral density. This is in contrast to the commonly used method in statistical physics, namely, the stochastic differential equation method (SDE), in which white noise is first generated using the Box-Müller algorithm. In presenting the method, it is true that we did make some comparison with the SDE method [2] of noise generation, which might have led to the preceding Comment [3] from Mannella and Palleschi, who have used the latter in many well-known studies. It is pertinent to state at the outset that many attributes of our method were not presented in Ref. [1] due to the short format of the *Rapid Communication.* This reply does not discuss these attributes [4] but takes the opportunity to present our views about the preceding Comment.

The reply to the above Comment is presented in five sections.

1. *Value of N*

It is a fact, as Mannella and Palleschi [3] point out, that the PSD method has a period $2\pi/\Delta\omega$, but we fail to understand why the writers term this a "problem." We take exception to the writers comment that the N values for the O-U noise have to be in the range 10^5-10^6 based on this periodicity factor and the value of the upper cutoff frequency $\omega_{\max}$ (ω_u in Ref. [1]). We have explicitly stated in our paper that N values in the range of 1000 reproduced up to five standard deviations. For $\tau_c \leq 1$ the N values used in our calculation were all less than 1000 (see discussion below). However, it is true that for increasing τ_c larger N values are appropriate for producing noise with larger time periods. But this need is dictated by the physics of the mean first-passage time (MFPT) of an overdamped particle in a bistable potential. Even then, the N values used are much less than the suggested range.

It is patent that for the O-U noise, when τ_c is small $\omega_{\max}$ increases. This does not necessarily mean that the corresponding N values were increased proportionally. For small τ_c, the noise is "whitish," having a PSD that is largely constant over a substantial portion of the frequency; relatively large $\Delta\omega$ (i.e., smaller N) hardly has any effect on the O-U noise generation. We tested this last assertion in the original calculation. Recently, more calculations were carried out in which $\Delta\omega$ was decreased a thousand times (from a chosen value, for a small τ_c) and N was changed by a factor of 10 without resulting in any appreciable change of MFPT.

2. *Upper limit of frequency cutoff*

The assertion by Mannella and Palleschi that $\omega_{\max}\tau_c \gg 1$ must hold in our case is somewhat misconstrued. The value $\omega_{\max}\tau_c = 10$ (for the O-U noise) captures about 94% of the area under the PSD curve—an accuracy which is redundant for most physical problems. In our calculation, $\omega_{\max}\tau_c = 5$ (about 91% of the area) was used, which produced results that were hardly any different from those obtained using $\omega_{\max}\tau_c = 10$.

3. *CPU Time*

Subsequently in the comment, Mannella and Paleschi claim that the required CPU time of the PSD method (for a particular case study that they present) is 11 times greater than the SDE approach. They attribute this perceived difference largely to our use of the fast Fourier transform (FFT) ("very expensive"). In general, the FFT is considered to be an efficient algorithm since, for an $N \times N$ matrix, instead of N^2 operation, it requires $N \ln_2 N$ operations [5].

The calculated MFPT for a chosen case ($D = 0.1$, $\tau = 1$) is known to be about 250. For this study, Mannella and Palleschi suggest that the needed amount of random numbers for 100 averages must be about 2.5×10^5; this value does not depict our calculation, nor is it a generic one. The writers base their calculation on the number of random numbers needed by the SDE method. For our approach, such large random numbers were not essential. For an average MFPT of 250 units, N values as low as 200 were sufficient to produce the sample length; for 100 runs the number of random generators needed was 2.0×10^4.

The direct conversion of the required quantity of random numbers from the SDE approach to the PSD method is not appropriate. It is important to stress that the proportional need for random numbers for Δt (in the SDE method) is not present for the PSD method. If Δt is decreased to, say, 0.001, then, in the SDE method, the random-number generation must be increased by 100. But in our approach we did not need to increase N by this order. This is because, by using the FFT technique, the time step (as noted in Ref. [1]) is given by the relation $\Delta t = 2\pi/(M\Delta\omega)$, which clearly indicates that by increasing M 100 times, Δt can be reduced correspondingly, without changing N; and this N controls the random numbers needed as stated in Ref. [1].

Moreover, in the SDE method each random number is generated via the Box-Müller algorithm, which corresponds to involved multiplication and square-root operations [6]. This calculation, however, is included in the overhead category in the above comment.

Having differed on the reported CPU time, we want to present a point of view that we believe is pertinent at this juncture. This involves the advancement of computer speed. Notwithstanding all other advantages, in fairness, let us agree that the SDE approach will take less CPU time (but not such a difference as that claimed) for generating certain range O-U noise (not necessarily "higher-order" realistic noises). These CPU times under discussion are not very prohibitive. Now, computer speed up to 9000 megaflops are currently available (CM-200) and machines with teraflop capacity are expected by 1995. Even some workstations that a single individual uses are in the range of 4–10 megaflops. (Our original calculations were done on such a computer: SUN4.) At this point we question the purpose of such fast computers if we do not utilize and consume their efficiency for easier, faster, and importantly, accurate numerical solution. We question whether the fine counting of CPU time should take precedence when computer speeds are increasing exponentially and their availability is becoming commonplace. Of course, we are aware that the use of inefficient algorithms cannot be justified. But for the present case—where the method has many inherent advantages, involves efficient and modern algorithms, and the CPU time consumption is within bounds—we hold that the method is a viable option for colored-noise generation.

4. The physical problem: Particle in a bistable potential

When we compare T_{top} and T_{bot} we are aware that majority consensus holds that $1/2T_{bot}$ is not equivalent to T_{top}. In fact, this is also our belief—reinforced through the simulation study. The writers have the right to feel that the comparison of their calculation [7] with ours (Fig. 3, Ref. [1]) is unwarranted. But it is only when we discussed Fig. 4 (For the T_{top} case) did we state "that the present simulation . . . are at variance" with Ref. [7]. In fact, Fig. 4 clearly shows the scatter in the numerical values (of Ref. [7]) in the low-τ_c range with our calculation (not all values of Ref. [7] were plotted).

We agree with the writers that in our Fig. 3 (Ref. [1]) the good agreement of numerical calculation with the theory of Ref. [8] is fortuitous. But plotting variant theories with matching numerical results does not mean that we disregard the difference between T_{top} and T_{bot}. The figure was presented only to show the matching; no judgement as to "why and how" this occurred was made. In fact, we totally agree with the writer's concomitant comments on this aspect.

5. Miscellaneous

The authors present a convincing argument for slow convergence of the MFPT as being due to the nature of the probability distribution and not to "poor ergodicity" [2]. It must also be said that the PSD method generates (in accordance with the central limit theorem) a Gaussian distribution with a substantial portion of its "long tails," which are critical for many physical problems, e.g., first-passage-time calculations. For the SDE approach, Mannella and Palleschi note that this can be achieved "exerting the necessary care." This last qualitative statement may not translate to easy computational implementation and to date there has been no clear indication of how this can be accomplished as already noted in our paper.

In conclusion, we want to reiterate that the PSD method of colored-noise generation is efficient, has some attractive features, and is easy to implement for not only the O-H noise but higher-order noise [9,10] also. For colored-noise generation, we believe that the method should be considered as a viable option.

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