Exact numerical simulation of the Ornstein-Uhlenbeck process and its integral

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A numerical simulation algorithm that is exact for any time step $\Delta t>0$ is derived for the Ornstein-Uhlenbeck process $X(t)$ and its time integral $Y(t)$. The algorithm allows one to make efficient, unapproximated simulations of, for instance, the velocity and position components of a particle undergoing Brownian motion, and the electric current and transported charge in a simple R-L circuit, provided appropriate values are assigned to the Ornstein-Uhlenbeck relaxation time τ and diffusion constant c. A simple Taylor expansion in Δt of the exact simulation formulas shows how the first-order simulation formulas, which are implicit in the Langevin equation for $X(t)$ and the defining equation for $Y(t)$, are modified in second order. The exact simulation algorithm is used here to illustrate the zero-τ limit theorem. [S1063-651X(96)10908-9]

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I. INTRODUCTION

The Ornstein-Uhlenbeck (OU) process has a long history in physics. Introduced in essence by Langevin [1] in his famous 1908 paper on Brownian motion, the process received a more thorough mathematical examination several decades later by Uhlenbeck and Ornstein [2], Chandrasekhar [3], and Wang and Uhlenbeck [4], and it is nowadays offered as a fairly standard textbook topic [5–9]. Using the notation and nomenclature of Ref. [9], the OU process is understood here to be the univariate continuous Markov process X that evolves with time t (a real variable) according to any one of the following equivalent versions of the OU Langevin equation:

$$X(t+dt)=X(t)-\frac{1}{\tau}X(t)dt+c^{1/2}N(t)(dt)^{1/2}, \quad (1.1)$$

$$X(t+dt)=X(t)-\frac{1}{\tau}X(t)dt+c^{1/2}dW(t), \quad (1.2)$$

$$\frac{dX(t)}{dt}=-\frac{1}{\tau}X(t)+c^{1/2}\Gamma(t). \quad (1.3)$$

In these equations, τ and c are positive constants called, respectively, the *relaxation time* and the *diffusion constant*; dt is a ''positive infinitesimal,'' i.e., a real variable that is restricted to the interval $[0,\epsilon]$ where ϵ is arbitrarily close to zero; $N(t)$ is a temporally uncorrelated normal random variable with mean 0 and variance 1; $dW(t)$ is a temporally uncorrelated normal random variable with mean 0 and variance dt; and $\Gamma(t)$ is ''Gaussian white noise,'' which may be defined as the $dt\to 0$ limit of the temporally uncorrelated normal random variable with mean 0 and variance $1/dt$. The equivalence of Eqs. (1.1)–(1.3) is a straightforward consequence of the fact that $\mathcal{N}(m,\sigma^2)$, the normal random variable with mean m and variance σ^2, satisfies

$$\alpha+\beta\mathcal{N}(m,\sigma^2)=\mathcal{N}(\alpha+\beta m,\beta^2\sigma^2). \quad (1.4)$$

The density function P of the OU process X obeys the partial differential equation

$$\frac{\partial P(x,t)}{\partial t}=\frac{1}{\tau}\frac{\partial[xP(x,t)]}{\partial x}+\frac{c}{2}\frac{\partial^2 P(x,t)}{\partial x^2}, \quad (1.5)$$

which is the forward Fokker-Planck equation for the OU process. The four equations (1.1), (1.2), (1.3), and (1.5) are logically equivalent to each other; each provides a statistically complete description of the time evolution of the OU process.

The importance of the OU process in physics is owed to several facts. First, it plays a central role in the mathematical descriptions of Brownian motion and Johnson noise: Reference [9] gives a tutorial review of the arguments that lead one to conclude that any rectilinear velocity component of a Brownian particle of mass m and diffusion coefficient D at absolute temperature T can be regarded as an OU process with relaxation time and diffusion constant

$$\tau=\frac{Dm}{kT}, \quad c=\frac{2}{D}\left(\frac{kT}{m}\right)^2, \quad (1.6)$$

k being Boltzmann's constant, and also that the electrical current in a simple wire loop of resistance R and self-inductance L at absolute temperature T can be regarded as an OU process with relaxation time and diffusion constant

$$\tau=\frac{L}{R}, \quad c=\frac{2kTR}{L^2}. \quad (1.7)$$

Secondly, the OU process has lately been used by many investigators as a model of ''colored noise'' [10]; its stationary autocovariance function, in contrast to that of the δ-correlated Gaussian white noise process $\Gamma(t)$, decays exponentially with characteristic time constant τ. Finally, the fluctuations in many continuous Markov processes about a ''stable state,'' at least those fluctuations sufficiently small that a locally linear approximation to the drift function will be justified, can approximately be described as an OU process centered on the stable state.

The time integral of the OU process X (or indeed of any process X) is defined to be the process Y that satisfies

$$Y(t+dt)=Y(t)+X(t)dt. \quad (1.8)$$

Y is not itself a Markov process; however, X and Y together comprise a bivariate continuous Markov process [11]. In the Brownian motion problem of Eqs. (1.6) $Y(t)$ would be the corresponding position component of the Brownian particle at time t, and in the Johnson noise problem of Eqs. (1.7) $Y(t)$ would be the net charge transported past some fixed point on the wire loop by time t.

Construction of an algorithm for numerically simulating the OU process X and its integral Y ultimately comes down to finding valid ''updating'' formulas that allow one to calculate, from any given values of X and Y at any time t, the X and Y values at some later time $t+\Delta t$. *Approximate* updating formulas can be constructed simply by replacing the positive infinitesimal dt in Eqs. (1.1) and (1.8) with a positive *finite* variable Δt:

$$X(t+\Delta t)\approx X(t)-\frac{1}{\tau}X(t)\Delta t+c^{1/2}n(\Delta t)^{1/2}, \quad (1.9a)$$

$$Y(t+\Delta t)\approx Y(t)+X(t)\Delta t. \quad (1.9b)$$

In Eq. (1.9a), n represents a sample value of the unit normal random variable $N(t)=\mathcal{N}(0,1)$; such ''unit normal random numbers'' can easily be generated on a computer [12,13].

The shortcoming of the updating formulas (1.9) for X and Y is that they will be accurate *only* if Δt is ''suitably small.'' However, the fact that the coupled time-evolution equations (1.1) and (1.8) for X and Y are analytically solvable makes it possible to derive updating formulas that are *exact* for *any* positive value of Δt. Although it might be argued that such exact updating formulas are implicit in the analytical solution of the OU process, to the best of this writer's knowledge those formulas have never been published. In view of the prominent role that the OU process plays in physics applications of stochastic process theory, as recounted above, this omission deserves redressing. Not only should the exact updating formulas for X and Y afford interesting and useful insights into the OU process and its integral, but they may also suggest clues as to how we might improve simulation algorithms for stochastic processes that are not analytically solvable.

Actually, an exact updating formula for X by itself has been published; it reads [14]

$$X(t+\Delta t)=X(t)e^{-(1/\tau)\Delta t}+\left[\frac{c\tau}{2}(1-e^{-(2/\tau)\Delta t})\right]^{1/2}n. \quad (1.10)$$

It is easy to show that this formula reduces to the approximate formula (1.9a) whenever $\Delta t \ll \tau$, and that Eq. (1.9a) is in fact a first-order-in-Δt approximation to Eq. (1.10). In Secs. II and III we shall derive the companion exact updating formula for Y, which replaces the approximate updating formula (1.9b). In Sec. IV we shall expand the exact X and Y updating formulas in powers of Δt, and thereby infer the second-order-in-Δt updating formulas, the ''next step beyond'' Eqs. (1.9). We shall conclude in Sec. V by presenting the results of some numerical simulations that not only test the accuracies of the first- and second-order updating formulas as a function of Δt, but also verify that X and Y behave, in the problematic limit $\tau\to 0$ and $c\to\infty$ with $\tau c^{1/2}=1$, in the manner predicted by the zero-τ limit theorem [15].

II. SOLVING FOR $X(t)$ AND $Y(t)$

We wish to find the solutions $X(t)$ and $Y(t)$ to the coupled time-evolution equations (1.1) and (1.8) for the sure initial conditions

$$X(t_0)=x_0, \quad Y(t_0)=y_0. \quad (2.1)$$

For the sake of brevity, we first take note of the well-known result, which can be derived from either the Langevin equation (1.1) or the Fokker-Planck equation (1.5) [4,6–9], that for any $t>t_0$ the OU process $X(t)$ will be the *normal* random variable with mean and variance

$$\langle X(t)\rangle = x_0 e^{-(t-t_0)/\tau}, \quad (2.2)$$

$$\mathrm{var}\{X(t)\}=\frac{c\tau}{2}(1-e^{-2(t-t_0)/\tau}). \quad (2.3)$$

Next we recall the well known result in random variable theory that, if the two normal random variables $\mathcal{N}(m_1,\sigma_1^2)$ and $\mathcal{N}(m_2,\sigma_2^2)$ are *statistically independent*, then

$$\mathcal{N}(m_1,\sigma_1^2)+\mathcal{N}(m_2,\sigma_2^2)=\mathcal{N}(m_1+m_2,\sigma_1^2+\sigma_2^2); \quad (2.4)$$

indeed, the *normality* of the OU process $X(t)$ is most easily established by repeatedly applying rules (2.4) and (1.4) to the Langevin equation (1.1) at the successive times t, $t+dt$, $t+2dt$, etc. A result somewhat less well known than (2.4) is that the sum of any two statistically *dependent* normal random variables is normal, although the means and variances then do not combine so simply as in the statistically independent case of Eq. (2.4) [16]. Using this more general rule in conjunction with Eq. (1.4), we can prove from Eq. (1.8) that $Y(t)$ too is normal for all $t>t_0$. The argument goes as follows: Using Eqs. (1.8) and (2.1), we see that $Y(t_0+dt)$ is the sure number $y_0+x_0dt=\mathcal{N}(y_0+x_0dt,0)$. Then Eq. (1.8) gives

$$Y(t_0+2dt)=(y_0+x_0dt)+X(t_0+dt)dt.$$

Since $X(t_0+dt)$ is normal, it follows from Eq. (1.4) that $Y(t_0+2dt)$ also must be normal. Then we have from Eq. (1.8),

$$Y(t_0+3dt)=Y(t_0+2dt)+X(t_0+2dt)dt.$$

The two terms on the right are both normal random variables, although we *cannot* claim that they are statistically independent; nevertheless, by the general result just mentioned, we can infer that their sum $Y(t_0+3dt)$ must be normal. Repeating this last argument for t in Eq. (1.8) replaced successively by t_0+3dt, t_0+4dt, etc., and remembering that dt can be arbitrarily close to zero, we conclude that $Y(t)$ must be normal for *any* $t>t_0$.

Two *normal* random variables are completely specified by their means, variances, and covariance. For the normal random variables $X(t)$ and $Y(t)$ being considered here, we already know the mean and variance of $X(t)$ from Eqs. (2.2) and (2.3); so, it remains only to find the mean and variance of $Y(t)$, and the covariance of $X(t)$ with $Y(t)$. We can calculate those three averages directly from Eqs. (1.1) and (1.8) by proceeding as follows.

To compute the mean of $Y(t)$, we first take the average of Eq. (1.8). Then, subtracting $\langle Y(t)\rangle$ from both sides, dividing through by dt, and letting $dt\to 0$, we get

$$\frac{d\langle Y(t)\rangle}{dt}=\langle X(t)\rangle=x_0 e^{-(t-t_0)/\tau},$$

where the second equality has invoked Eq. (2.2). As can easily be verified, the solution to this simple differential equation for the required initial condition $\langle Y(t_0)\rangle=y_0$ is

$$\langle Y(t)\rangle=y_0+x_0\tau(1-e^{-(t-t_0)/\tau}). \tag{2.5}$$

To compute the covariance of $X(t)$ and $Y(t)$, we begin by multiplying Eqs. (1.1) and (1.8) together. That gives

$$\begin{aligned}X(t+dt)Y(t+dt)=X(t)Y(t)-\frac{1}{\tau}X(t)Y(t)dt\\ +c^{1/2}N(t)Y(t)(dt)^{1/2}+X^2(t)dt\\ +o(dt),\end{aligned}$$

where $o(dt)$ denotes terms of order >1 in dt. We next average this equation, taking note of the fact that since the zero-mean random variable $N(t)$ is statistically independent of $Y(t)$ then $\langle N(t)Y(t)\rangle=\langle N(t)\rangle\langle Y(t)\rangle=0$. Then, transposing the first term on the right side, dividing through by dt, and taking the limit $dt\to 0$, we get

$$\frac{d\langle X(t)Y(t)\rangle}{dt}=-\frac{1}{\tau}\langle X(t)Y(t)\rangle+\langle X^2(t)\rangle.$$

Since $\langle X^2(t)\rangle=\mathrm{var}\{X(t)\}+\langle X(t)\rangle^2$ is known explicitly from Eqs. (2.2) and (2.3), then this simple differential equation can be straightforwardly solved for $\langle X(t)Y(t)\rangle$ subject to the required initial condition $\langle X(t_0)Y(t_0)\rangle=x_0y_0$. The result is found to be

$$\begin{aligned}\langle X(t)Y(t)\rangle=\frac{c\tau^2}{2}+(x_0y_0+x_0^2\tau-c\tau^2)e^{-(t-t_0)/\tau}\\ +\left(\frac{c\tau^2}{2}-x_0^2\tau\right)e^{-2(t-t_0)/\tau}.\end{aligned} \tag{2.6}$$

From this result and Eqs. (2.2) and (2.5), we readily compute $\mathrm{cov}\{X(t),Y(t)\}\equiv\langle X(t)Y(t)\rangle-\langle X(t)\rangle\langle Y(t)\rangle$ to be

$$\mathrm{cov}\{X(t),Y(t)\}=\frac{c\tau^2}{2}(1-2e^{-(t-t_0)/\tau}+e^{-2(t-t_0)/\tau}). \tag{2.7}$$

Finally, to compute the variance of $Y(t)$, we first square Eq. (1.8) and then average:

$$\langle Y^2(t+dt)\rangle=\langle Y^2(t)\rangle+2\langle X(t)Y(t)\rangle dt+o(dt).$$

This implies that $d\langle Y^2(t)\rangle/dt=2\langle X(t)Y(t)\rangle$, and hence that

$$\langle Y^2(t)\rangle=y_0^2+2\int_{t_0}^{t}\langle X(t')Y(t')\rangle dt'.$$

So, $\langle Y^2(t)\rangle$ can be computed simply by substituting into the above integral the expression in Eq. (2.6) and then carrying out the integration. Upon doing that and then using Eq. (2.5), we find $\mathrm{var}\{Y^2(t)\}=\langle Y^2(t)\rangle-\langle Y(t)\rangle^2$ to be

$$\begin{aligned}\mathrm{var}\{Y(t)\}=c\tau^3\left[\frac{t-t_0}{\tau}-2(1-e^{-(t-t_0)/\tau})\right.\\ \left.+\frac{1}{2}(1-e^{-2(t-t_0)/\tau})\right].\end{aligned} \tag{2.8}$$

Having shown that the OU process $X(t)$ and its time integral $Y(t)$ are *normal* random variables with means given by Eqs. (2.2) and (2.5), variances given by Eqs. (2.3) and (2.8), and covariance given by Eq. (2.7), we now have a complete and exact solution to the problem of the time evolution of $X(t)$ and $Y(t)$. In the next section we shall use this information to construct a practicable set of exact Δt updating formulas for $X(t)$ and $Y(t)$.

III. EXACT UPDATING FORMULAS

For the updating formulas for X and Y, we regard $X(t)$ and $Y(t)$ as *given values*, and we seek the consequent values of the random variables $X(t+\Delta t)$ and $Y(t+\Delta t)$ for any $\Delta t>0$. By simply *replacing* in the arguments and formulas of the preceding section,

$$(t_0,t)\to(t,t+\Delta t),$$

we may infer that that the ''updates'' $X(t+\Delta t)$ and $Y(t+\Delta t)$ to the values $X(t)$ and $Y(t)$ will be *normal* random variables whose means, variances, and covariance are given by

$$\mathrm{mean}\{X(t+\Delta t)\}=X(t)e^{-\Delta t/\tau}, \tag{3.1a}$$

$$\mathrm{mean}\{Y(t+\Delta t)\}=Y(t)+X(t)\tau(1-e^{-\Delta t/\tau}), \tag{3.1b}$$

$$\mathrm{var}\{X(t+\Delta t)\}\equiv\sigma_X^2=(c\tau/2)(1-e^{-2\Delta t/\tau}), \tag{3.1c}$$

$$\begin{aligned}\mathrm{var}\{Y(t+\Delta t)\}\equiv\sigma_Y^2=c\tau^3\left[\frac{\Delta t}{\tau}-2(1-e^{-\Delta t/\tau})\right.\\ \left.+\frac{1}{2}(1-e^{-2\Delta t/\tau})\right],\end{aligned} \tag{3.1d}$$

$$\begin{aligned}\mathrm{cov}\{X(t+\Delta t),Y(t+\Delta t)\}\equiv\kappa_{XY}\\ =(c\tau^2/2)(1-2e^{-\Delta t/\tau}+e^{-2\Delta t/\tau}).\end{aligned} \tag{3.1e}$$

Next we turn to the following result in random variable theory: If N_1 and N_2 are statistically independent unit normal random variables, then the two random variables X_1 and X_2 defined by

$$X_1=m_1+\sigma_1N_1, \tag{3.2a}$$

$$X_2=m_2+\left(\sigma_2^2-\frac{\kappa_{12}^2}{\sigma_1^2}\right)^{1/2}N_2+\frac{\kappa_{12}}{\sigma_1}N_1, \tag{3.2b}$$

will be *normal* with respective means m_1 and m_2, respective variances σ_1^2 and σ_2^2, and covariance κ_{12}. (This incidently

implies, as mentioned earlier, that any two *normal* random variables are completely defined by their means, variances, and covariance.)

Since this result is not so widely known, we prove it here: We first use the definition (3.2a) and Eq. (1.4) to write

$$X_1 = m_1 + \sigma_1 \mathcal{N}(0,1) = \mathcal{N}(m_1, \sigma_1^2);$$

this proves that X_1 is indeed normal with the claimed mean and variance. Next, we use the definition (3.2b) and Eqs. (1.4) and (2.4) to write

$$\begin{aligned} X_2 &= m_2 + \left(\sigma_2^2 - \frac{\kappa_{12}^2}{\sigma_1^2}\right)^{1/2} \mathcal{N}(0,1) + \frac{\kappa_{12}}{\sigma_1}\mathcal{N}(0,1) \\ &= \mathcal{N}\left(m_2, \left(\sigma_2^2 - \frac{\kappa_{12}^2}{\sigma_1^2}\right)\right) + \mathcal{N}\left(0, \frac{\kappa_{12}^2}{\sigma_1^2}\right) \\ &= \mathcal{N}\left(m_2 + 0, \sigma_2^2 - \frac{\kappa_{12}^2}{\sigma_1^2} + \frac{\kappa_{12}^2}{\sigma_1^2}\right) = \mathcal{N}(m_2, \sigma_2^2); \end{aligned}$$

this proves that X_2 is also normal with the claimed mean and variance. Finally, for the covariance of X_1 and X_2, we have

$$\begin{aligned} \mathrm{cov}\{X_1, X_2\} &\equiv \langle (X_1 - \langle X_1\rangle)(X_2 - \langle X_2\rangle)\rangle \\ &= \langle (X_1 - m_1)(X_2 - m_2)\rangle \\ &= \left\langle [\sigma_1 N_1]\left[\left(\sigma_2^2 - \frac{\kappa_{12}^2}{\sigma_1^2}\right)^{1/2} N_2 + \frac{\kappa_{12}}{\sigma_1} N_1\right]\right\rangle \\ &= \sigma_1\left(\sigma_2^2 - \frac{\kappa_{12}^2}{\sigma_1^2}\right)^{1/2} \langle N_1 N_2\rangle + \kappa_{12}\langle N_1^2\rangle. \end{aligned}$$

Since N_1 and N_2 are statistically independent, zero-mean random variables, then $\langle N_1 N_2\rangle = \langle N_1\rangle\langle N_2\rangle = 0$. And since N_1 is a unit normal, then $\langle N_1^2\rangle = 1$. The last line therefore reduces to simply κ_{12}, and the covariance relation is established.

The result (3.2) allows us to express the two statistically *dependent* normals $X(t+\Delta t)$ and $Y(t+\Delta t)$ as linear combinations of two statistically *independent* unit normals. Taking account of the moment formulas (3.1), and defining

$$\mu \equiv e^{-\Delta t/\tau}, \tag{3.3}$$

so that the last three of those moment formulas can be written as

$$\sigma_X^2 = (c\tau/2)(1-\mu^2), \tag{3.4a}$$

$$\sigma_Y^2 = c\tau^3[\Delta t/\tau - 2(1-\mu) + (1/2)(1-\mu^2)], \tag{3.4b}$$

$$\kappa_{XY} = (c\tau^2/2)(1-\mu)^2, \tag{3.4c}$$

the foregoing theorem evidently allows us to write $X(t+\Delta t)$ and $Y(t+\Delta t)$ as follows:

$$X(t+\Delta t) = X(t)\mu + \sigma_X n_1, \tag{3.5a}$$

$$Y(t+\Delta t) = Y(t) + X(t)\tau(1-\mu) + \left(\sigma_Y^2 - \frac{\kappa_{XY}^2}{\sigma_X^2}\right)^{1/2} n_2 + \frac{\kappa_{XY}}{\sigma_X} n_1. \tag{3.5b}$$

Equations (3.5) are the *exact updating formulas* for the OU process X and its time integral Y. In these formulas, n_1 and n_2 are statistically independent unit normal random numbers [12], and μ, σ_X, σ_Y, and κ_{XY} are defined in terms of the time step Δt and the OU relaxation time τ and diffusion constant c according to Eqs. (3.3) and (3.4). Notice that Eq. (3.5a) is identical to the earlier mentioned formula (1.10), as expected.

For a succession of updates with a *fixed* time step Δt, as would occur in a typical simulation run, the values of μ, σ_X, σ_Y, and κ_{XY} on the right-hand sides of formulas (3.5) will all remain *constant*; the only variables there whose values will change at each time step are $X(t)$, $Y(t)$, n_1, and n_2. As a consequence, a numerical simulation of X and Y performed on a computer using the exact updating formulas (3.5) should proceed quite rapidly, and only slightly slower than a simulation performed using the approximate updating formulas (1.9) with the same time step size Δt.

IV. SECOND-ORDER UPDATING FORMULAS

We expect formulas (3.5) to reduce to the approximate formulas (1.9) when Δt is ''suitably small.'' To show that this indeed happens, and to see what a second-order-in-Δt improvement on formulas (1.9) would look like, we let

$$\Delta t/\tau \equiv \alpha. \tag{4.1}$$

Then if Δt is small compared to τ, we will have $\alpha \ll 1$, and we can approximate

$$\mu \equiv e^{-\alpha} \approx 1 - \alpha + \frac{\alpha^2}{2} - \frac{\alpha^3}{6} \quad (\Delta t \ll \tau). \tag{4.2}$$

It is then a simple matter of algebra to show from Eqs. (3.4) that, to *third* order in α,

$$\sigma_X^2 \approx c\tau\alpha(1 - \alpha + 2\alpha^2/3),$$

$$\sigma_Y^2 \approx c\tau^3\alpha^3/3,$$

$$\kappa_{XY} \approx c\tau^2\alpha^2(1-\alpha)/2.$$

Upon substituting these approximations into the exact updating formulas (3.5), we find that those formulas become, to *second* order in Δt,

$$X(t+\Delta t) \approx X(t) + \left[-\frac{1}{\tau}X(t)\Delta t + c^{1/2} n_1 (\Delta t)^{1/2}\right]\left(1 - \frac{\Delta t}{2\tau}\right), \tag{4.3a}$$

$$Y(t+\Delta t) \approx Y(t) + X(t)\Delta t\left(1 - \frac{\Delta t}{2\tau}\right) + c^{1/2}\frac{1}{2}(n_1 + 3^{-1/2} n_2)(\Delta t)^{3/2}. \tag{4.3b}$$

Equations (4.3) are the second-order-in-Δt updating formulas for the Ornstein-Uhlenbeck process X and its integral Y. If all terms of order >1 in Δt are dropped, Eqs. (4.3) become identical to the first-order formulas (1.9). Formulas (4.3) evidently provide *deterministic* corrections to formulas (1.9) of order $(\Delta t)^2$, and *stochastic* corrections of order $(\Delta t)^{3/2}$.

The stochastic correction term in the second-order Y-updating formula (4.3b) is particularly intriguing, involving as it does an admixture of the *same* unit normal random number n_1 that appears in the X-updating formula (4.3a) and a *statistically independent* unit normal random number n_2. Notice that, by appealing to rules (1.4) and (2.4), we could have written the linear combination of n_1 and n_2 in Eq. (4.3b) as

$$\frac{1}{2}\,(n_1+3^{-1/2}n_2)=\frac{1}{3^{1/2}}\left(\frac{3^{1/2}}{2}\,n_1+\frac{1}{2}\,n_2\right)=\frac{1}{3^{1/2}}\,n',\tag{4.4}$$

where n' is also a unit normal random number. But of course, n' as thus defined *cannot* be considered to be statistically independent of the unit normal random number n_1 in Eq. (4.3a).

V. ILLUSTRATIVE SIMULATIONS AND CONCLUSIONS

Whether one uses the first-order updating formulas (1.9), the second-order updating formulas (4.3), or the exact updating formulas (3.5), the procedure for numerically simulating the OU process X and its integral Y is basically the same. One first specifies values for the OU relaxation time τ and diffusion constant c, the initial process values $X(0)=x_0$ and $Y(0)=y_0$, the time step Δt, a stopping time $t_{\rm stop}$, and a starting seed for the unit-interval uniform random number generator. One next sets $X=x_0$, $Y=y_0$, and $t=0$, and for the sake of efficiency precomputes the values of those combinations of τ, c, and Δt appearing in the updating formulas that will not change throughout the simulation. One then repeatedly applies the chosen set of updating formulas to compute, from the values of X and Y at time t, their values at time $t+\Delta t$, updating all variables and recording their values for later use, and finally stopping when the variable t reaches $t_{\rm stop}$. Each application of the updating procedure requires two unit *normal* random numbers (or just one in the case of the first-order formulas), and these are computed as needed from a set of unit *uniform* random numbers in a straightforward way [12].

Figure 1 shows the results of a simulation run using the *exact* updating formulas (3.5) with $\tau=c=1$, $x_0=y_0=0$, and $\Delta t=0.01$. The dotted lines in each plot show the appropriate one-standard-deviation envelope, namely, $\langle X(t)\rangle \pm \mathrm{sdev}\{X(t)\}$ in the upper plot as computed from Eqs. (2.2) and (2.3), and $\langle Y(t)\rangle \pm \mathrm{sdev}\{Y(t)\}$ in the lower plot as computed from Eqs. (2.5) and (2.8). The jagged curves are composed of unconnected dots that give the values of the processes at each time step; each trajectory here is thus composed of 6000 dots. Since $X(t)$ and $Y(t)$ are both normal, then we expect that, in the limit $t\to\infty$, their trajectories should be inside the one-standard-deviation envelopes about 68% of the time.

Since for this simulation $\Delta t/\tau=0.01$, which is ''small'' compared to one, then both the first-and second-order updating formulas ought to work reasonably well here. To test that expectation, the foregoing exact simulation was run *in parallel* with a first-order simulation and a second-order simulation, with the second-order updating formulas (4.3) using the *same* n_1 and n_2 values as used by the exact updating formulas, and the first-order updating formulas (1.9) using $n=n_1$. The resultant first-order and second-order trajectories were found to track the exact trajectories very closely; indeed, on the scale of the plots in Fig. 1, the first-order and second-order X and Y trajectories were virtually indistinguishable from the exact trajectories. Figure 2(a) shows the *difference* between the first-order and the exact X value at each time step, and Fig. 2(b) shows the difference between the second-order and the exact X value at each time step. The *average absolute discrepancy* was found to be 2.1×10^{-3} in the first-order X data, and 8.7×10^{-6} in the second-order X data. Figures 2(c) and 2(d) show the analogous discrepancies in the first-order and second-order Y trajectories, for which the respective average absolute discrepancies were computed to be 8.4×10^{-3} and 1.1×10^{-5}. So, even though both approximate trajectories are quite accurate in this case, the errors in the first-order trajectories are over 2 orders of magnitude larger than the errors in the second-order trajectories.

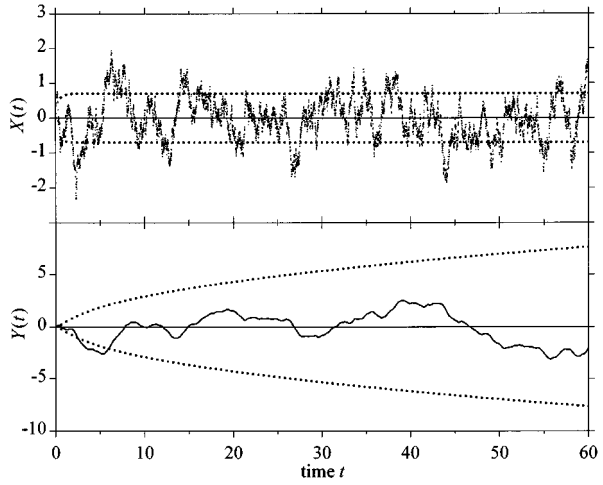

FIG. 1. Results of a numerical simulation of the Ornstein-Uhlenbeck process X and its time integral Y made with the exact updating formulas (3.5), with $\tau=c=1$, $x_0=y_0=0$, and $\Delta t=0.01$. The dotted lines show the theoretically predicted one-standard-deviation envelopes.

A simulation run with $\Delta t/\tau=0.001$ showed, as expected, even smaller errors: the average absolute first- and second-order X discrepancies for 6000 time steps were found to be 1.6×10^{-4} and 6.7×10^{-8}, respectively, and the average absolute first- and second-order Y discrepancies were found to be 3.4×10^{-4} and 8.2×10^{-8}. But of course, things get worse for larger values of $\Delta t/\tau$. As $\Delta t/\tau$ is increased from 0.1 to 1, the average absolute first-order X discrepancy rises from 0.022 to 0.35, while the average absolute second-order X discrepancy rises from 0.000 93 to 0.13; and the average absolute first-order Y discrepancy rises from 0.26 to 7.9, while the average absolute second-order Y discrepancy rises from 0.002 to 0.67. As $\Delta t/\tau$ is increased above 1, both of the approximate updating formulas rapidly become very inaccurate; e.g., for $\Delta t/\tau=2$, the average absolute first-order Y dis-

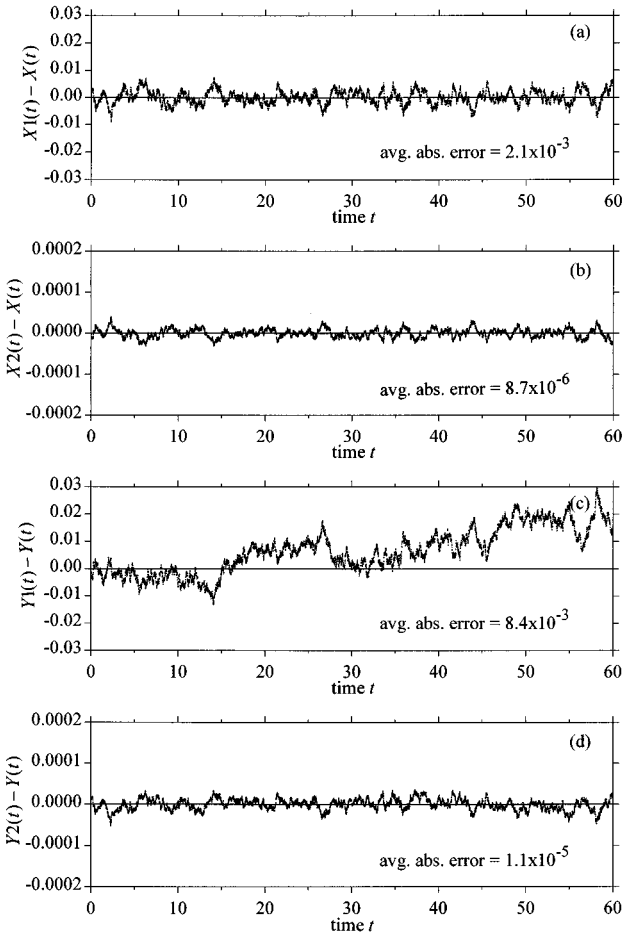

FIG. 2. Errors that would have occurred in the trajectories of Fig. 1 if the first-order updating formulas (1.9) or the second-order updating formulas (4.3) had been used instead of the exact updating formulas (3.5). (a) The error in the first-order X simulation; (b) the error in the second-order X simulation; (c) the error in the first-order Y simulation; and (d) the error in the second-order Y simulation. In each case, a simple average of the absolute values of the errors is indicated.

crepancy over 6000 time steps was found to be 91.

Although the second-order updating formula is clearly more accurate than the first-order updating formula, there is little reason to use it instead of the *exact* updating formula, because the second-order updating formula requires essentially the same number of computations to be done at each time step as the exact updating formula. The reason the second-order OU updating formula is of interest is that it shows us, by comparison, where the major shortcomings of the simple first-order OU updating formula are. The second-order OU updating formula thus serves as an instructive example to keep in mind when faced with the task of simulating a continuous Markov process for which an exact updating formula cannot be devised, but an improvement on the first-order updating formula is nonetheless desired.

One circumstance in which the restriction $\Delta t \ll \tau$ required by any finite-order approximate updating formula would pose a problem arises in connection with the so-called zero-τ limit theorem [15]. That theorem asserts that if $\tau \to 0$ and

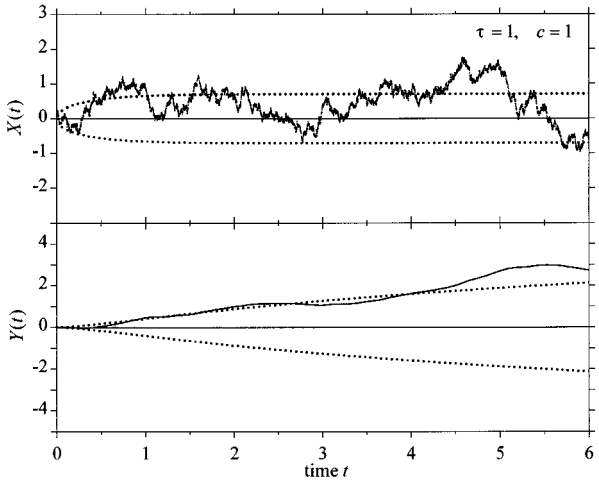

FIG. 3. Results of a numerical simulation of the OU process X and its time integral Y made with the exact updating formulas (3.5), with $\tau = c = 1$, $x_0 = y_0 = 0$, and $\Delta t = 0.001$. The dotted lines show the theoretically predicted one-standard-deviation envelopes.

$c \to \infty$ in such a way that $\tau c^{1/2} \equiv \epsilon$ stays constant, then X will approach $\epsilon \times$(Gaussian white noise), and Y will approach the driftless Wiener process with diffusion constant ϵ^2. The latter process is denoted by W_ϵ, and it can be defined by the Langevin equation

$$W_\epsilon(t+dt) = W_\epsilon(t) + \epsilon (dt)^{1/2} N(t), \tag{5.1}$$

where $N(t)$ is as usual a temporally uncorrelated, statistically independent, unit normal random variable. The first-order updating formula for this process, namely,

$$W_\epsilon(t+\Delta t) = W_\epsilon(t) + \epsilon (\Delta t)^{1/2} n, \tag{5.2}$$

is *exact* for *any* $\Delta t > 0$ [17].

Figures 3–6 show the results of four simulations of the OU process X and its integral Y, which were made using the

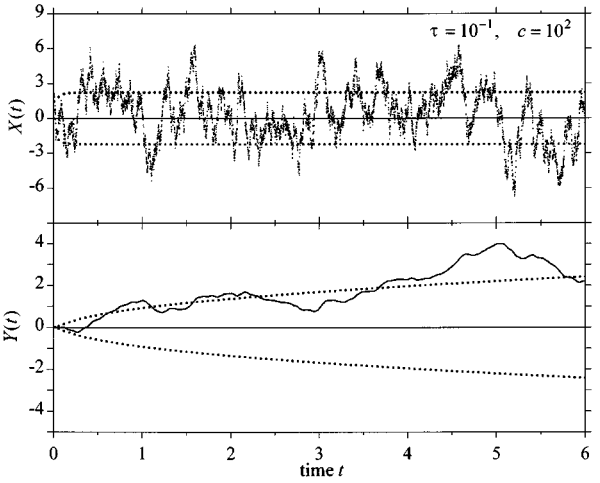

FIG. 4. As in Fig. 3, and constructed using the same random number sequence, except that $\tau = 0.1$ and $c = 100$. Note that $\tau c^{1/2} = 1$, as in Fig. 3.

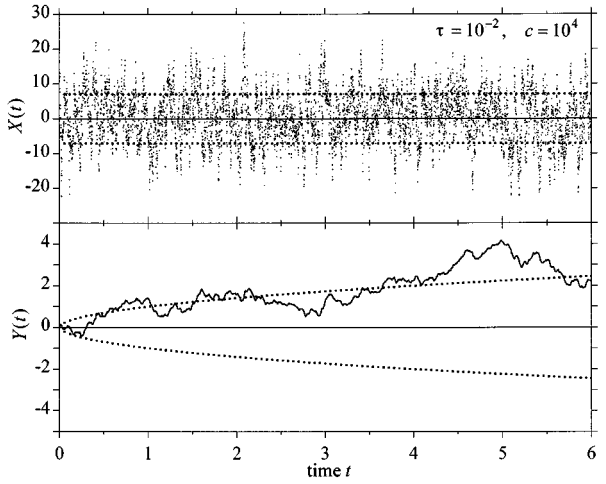

FIG. 5. As in Fig. 4, except that $\tau=10^{-2}$ and $c=10^4$.

exact updating formulas (3.5), and which differ only in the values assigned to the relaxation time τ and the diffusion constant c. As shown in the figures, each successive simulation has a smaller value of τ and a larger value of c, but in such a way that $\tau c^{1/2}$ is always equal to 1. Each simulation has the same initial conditions $x_0=y_0=0$ and the same time step $\Delta t=0.001$; furthermore, each simulation uses the same set of unit normal random numbers n_i for the 6000 time steps from $t=0$ to $t=6$. The dotted curves show, as before, the theoretically predicted one-standard-deviation envelopes.

The X plots in Figs. 3–6 show how, in accordance with the predictions of the zero-τ limit theorem, the OU process gradually evolves, as $\tau\to 0$, into the Gaussian white noise process $\Gamma(t)$, the temporally uncorrelated normal random variable with mean 0 and variance ∞. And the companion Y plots show how, again in accordance with the predictions of the zero-τ limit theorem, the integral of the OU process gradually evolves, as $\tau\to 0$, into the driftless Wiener process

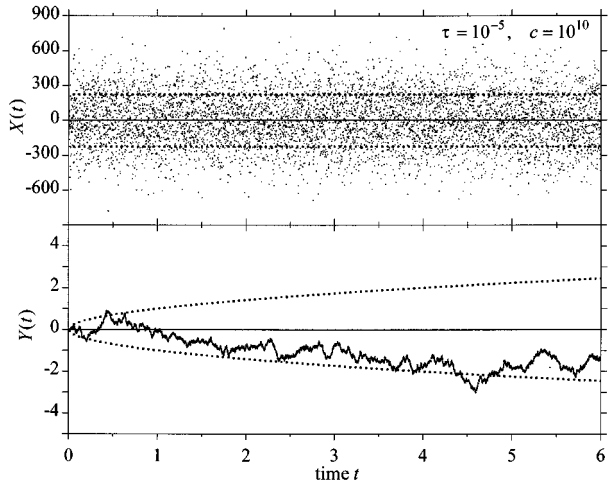

FIG. 6. As in Fig. 5, except that $\tau=10^{-5}$ and $c=10^{10}$. The X trajectory has now begun to resemble Gaussian white noise, in accordance with the predictions of the zero-τ limit theorem.

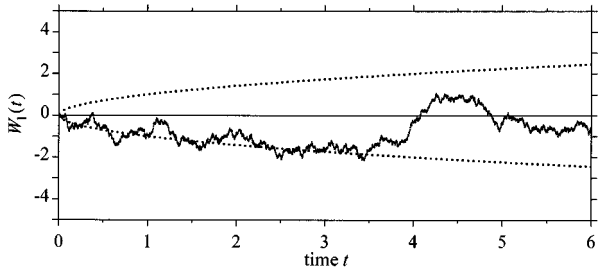

FIG. 7. Results of an exact numerical simulation of the driftless Wiener process W_1, which is defined by the Langevin equation (5.1) with $\epsilon=1$, along with its theoretically predicted one-standard-deviation envelope. The trajectory here is statistically indistinguishable from the Y trajectory in Fig. 6, in accordance with the predictions of the zero-τ limit theorem.

with the diffusion constant 1. A simulation of the latter process, made using the exact updating formula (5.2) with $\epsilon=1$, is shown in Fig. 7, along with its theoretically predicted one-standard-deviation envelope. The point to be noticed here is that the Y trajectory in Fig. 6 and the W_1 trajectory in Fig. 7 are, for all practical purposes, *statistically indistinguishable*. Also noteworthy of course is the fact that Δt in Fig. 6 is 100 times larger than τ, a circumstance that poses no problems for the exact updating formulas used in these simulations.

Our main goal in this paper has been to derive and illustrate the exact numerical simulation formulas (3.5) for the OU process X and its integral Y, and that goal has now been accomplished. But the last sequence of figures has an interesting historical connection, and we would be derelict if we did not pay some brief attention to that connection.

In Einstein's pioneering papers of 1905 and 1906 on Brownian motion [18], he used a ''coarse-grained time'' argument to infer that the position of a Brownian particle should be, to a good approximation, a random variable whose density function satisfies the elementary diffusion equation. But the elementary diffusion equation is precisely the forward Fokker-Planck equation for the driftless Wiener process W_ϵ, which can also be defined through the Langevin equation (5.1). So what Einstein proved was that, in some ''temporally coarse-grained'' sense, the position of a Brownian particle is a driftless Wiener process. A few years after Einstein's work, Langevin [1] presented another analysis of Brownian motion, which was based somewhat more cleanly on Newton's second law. In modern terminology [9], Langevin's analysis showed that the *velocity* of a Brownian particle should be an OU process, and hence that the *position* of a Brownian particle should be the time integral of an OU process. The relationship between the two different approaches to Brownian motion of Einstein and Langevin can therefore be appreciated *graphically* by comparing Figs. 6 and 7: Taking Einstein's ''coarse graining in time'' to mean simply the condition that observations of the Brownian particle are to be separated in time by an interval Δt that is *large* compared to the relaxation time τ of Langevin's analysis, we can see from the Y trajectory in Fig. 6 and the W_1 trajectory in Fig. 7 that such course graining causes the position of the Brownian particle in Langevin's

analysis to look just like the position of the Brownian particle in Einstein's analysis. It would certainly appear, though, that the *most general* mathematical representation of the position of a Brownian particle is provided by the time integral of an OU process, rather than by a driftless Wiener process.

ACKNOWLEDGMENTS

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[10] A few of the many recent papers to employ the OU process as a ''colored noise'' source are as follows: J. Müller and J. Schnakenberg, Ann. Phys. (Leipzig) **2**, 92 (1993); J. Luczka, P. Hänggi, and A. Gadomski, Phys. Rev. E **51**, 2933 (1995); M. Wu, K. Billah, and M. Shinozuka, *ibid*. **52**, 3377 (1995); P. Reimann, *ibid*. **52**, 1579 (1995); and F. Castro, A. Sánchez, and H. Wio, Phys. Rev. Lett. **75**, 1691 (1995).

[11] A pedagogical discussion of the non-Markovian nature of Y, and the bivariate Markovian nature of (X,Y), may be found in D. T. Gillespie, Am. J. Phys. (to be published).

[12] An exact method for generating unit normal random numbers is to first take two random numbers r_1 and r_2 *uniform* on [0,1] and compute $s=[2\ln(1/r_1)]^{1/2}$ and $\theta=2\pi r_2$; then $n_1=s\cos\theta$ and $n_2=s\sin\theta$ will be two statistically independent sample values of $\mathcal{N}(0,1)$. This is the Box-Muller algorithm, a rigorous derivation of which may be found in Ref. [8], Sec. 1.8.

[13] The tactic of some earlier modelers, of replacing in Eq. (1.9a) the *normal* random number n with some *uniform* random number u, should be avoided because this introduces inaccuracies in Eq. (1.9a) beyond those that are already present due to the finiteness of Δt. The updating formula (1.9a) as it stands has the virtue of ''compounding self-consistently,'' in that its successive application to the two intervals $[t,t+\frac{1}{2}\Delta t]$ and $[t+\frac{1}{2}\Delta t,t+\Delta t]$ gives a statistically identical result, at least to first order in Δt, as its single application to the interval $[t, t+\Delta t]$ (for a proof see Ref. [8], pp. 116–118); indeed, it is just such a self-consistency requirement that forces $N(t)$ in the Langevin equation (1.1) to be normal in the first place (see Ref. [9]). But self-consistent compounding will *not* occur if the normal random number n in Eq. (1.9a) is replaced by a uniform random number u. The underlying reason is that the class of *normal* random variables is *closed* under statistically independent addition, whereas the class of *uniform* random variables is *not*. With modern computers and the simple normal generating algorithm described in Ref. [12], there would seem to be no good excuse for such a corruption of Eq. (1.9a).

[14] To the best of this author's knowledge, the earliest published appearance of the exact OU updating formula (1.10) occurs in Ref. [8] at Eq. (E-12b). Later appearances occur in N. J. Kasdin, Proc. IEEE **83**, 802 (1995) at Eqs. (56) and (57), and also in Ref. [9] at Eq. (2.47).

[15] See, e.g., Ref. [9], Sec. II D.

[16] See M. D. Springer, *The Algebra of Random Variables* (Wiley, New York, 1979), pp. 67–75. But note that a much easier proof can be had by using the result at Eqs. (3.2) in conjunction with the results (1.4) and (2.4): They show quite handily that if X_1 and X_2 are normal random variables with respective means m_1 and m_2, respective variances σ_1^2 and σ_2^2, and covariance κ_{12}, then X_1+X_2 will be normal with mean m_1+m_2 and variance $\sigma_1^2+\sigma_2^2+2\kappa_{12}$.

[17] See, for example, Ref. [8], Sec. 3.9 A.

[18] A. Einstein, Ann. Phys. (Leipzig) **17**, 549 (1905); **19**, 371 (1906). See also Ref. [7], pp.2–6.