Second-order algorithm for the numerical integration of colored-noise problems

Ronald F. Fox
School of Physics, Georgia Institute of Technology, Atlanta, Georgia 30332
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A second-order algorithm for the numerical integration of colored-noise stochastic processes is presented. It goes beyond recent efforts in this direction that are really only $\frac{3}{2}$ order. Generation of the noise for this algorithm requires the generation of two uniformly distributed random numbers at each integration step. Some of the earlier algorithms require four, or if they also only use two, they do so without requiring all cross correlations to hold up to second order as in the algorithm presented here. Several numerical results are presented that demonstrate the improvement over the well-known first-order algorithm.

I. INTRODUCTION

During the last ten years, several advances have been made in the numerical simulation of stochastic differential equations.[1-5] Physical applications have increasingly involved colored noise in place of white noise. This has led to the necessity of the Stratonovich point of view[3,6] that is invoked in this paper.

The algorithm presented here differs from previous results[1,5] in three ways. It is genuinely second order for both the deterministic and the stochastic portions. Some earlier work[5] is only order $\frac{3}{2}$ in the stochastic portion. In other work,[1] while putatively second order in the stochastic portion, the cross correlations of certain noise terms are not properly determined to second order. While we are in complete agreement with some earlier second-order work[2] for white noise, the present paper deals with colored noise and treats white noise as the short correlation time limit[3] of colored noise.

The generation of the various noise terms in the algorithm requires the generation of uniform random numbers that are inserted into the Box-Muller algorithm[7] to make Gaussian random numbers. In our algorithm, only two such numbers are required for each integration step. This is the same number needed for the first-order algorithm and it is two less than the number needed in one of the earlier algorithms.[5] This fact results in a substantial savings in computation time.

The paper is organized as follows. In Sec. II the algorithm is derived. The remarks of the previous paragraph are enlarged upon and explained. In Sec. III generalizations of the algorithm to greater numbers of variables are presented. In Sec. IV, numerical tests of the improved algorithm are described.

II. DERIVATION OF THE ALGORITHM

We begin by considering the one variable stochastic differential equation

$$\frac{d}{dt}x = f(x) + g(x)\epsilon(t) \tag{1}$$

in which $f(x)$ is generally a nonlinear function, $g(x)$ may be constant or a possibly nonlinear function, and $\epsilon(t)$ is Gaussian, colored noise satisfying the equation

$$\frac{d}{dt}\epsilon = -\lambda\epsilon + \lambda g_w(t)\ , \tag{2}$$

in which λ is the reciprocal of the colored-noise correlation time, and $g_w(t)$ is Gaussian white noise with the stochastic properties

$$\langle g_w(t)\rangle = 0 \quad \text{and} \quad \langle g_w(t)g_w(t')\rangle = 2D\delta(t-t') \tag{3}$$

in which D is the white-noise variance. If $g(x)$ is a constant, the process is additive, otherwise it is multiplicative.

We begin the derivation by formally integrating Eq. (1)

$$x(t+\Delta t) = x(t) + \int_t^{t+\Delta t} dt' f(x(t')) + \int_t^{t+\Delta t} dt' g(x(t'))\epsilon(t')\ . \tag{4}$$

Now we expand $f(x(t'))$ and $g(x(t'))$ as follows:

$$f(x(t')) = f_t^{(0)} + f_t^{(1)}(x(t')-x(t)) + \tfrac{1}{2}f_t^{(2)}(x(t')-x(t))^2 + \cdots\ , \tag{5}$$

$$g(x(t')) = g_t^{(0)} + g_t^{(1)}(x(t')-x(t)) + \tfrac{1}{2}g_t^{(2)}(x(t')-x(t))^2 + \cdots \tag{6}$$

in which the superscripts i denote the ith derivative of the function and the subscript t refers to the time at which the derivatives are to be evaluated. When these expansions are inserted into (4) we obtain

$$x(t+\Delta t) = x(t) + \Delta t f_t^{(0)} + f_t^{(1)}\int_t^{t+\Delta t} dt'[x(t')-x(t)] + \tfrac{1}{2}f_t^{(2)}\int_t^{t+\Delta t} dt'[x(t')-x(t)]^2 + \cdots + g_0^{(t)}[\Gamma_0(t+\Delta t)-\Gamma_0(t)] + g_t^{(1)}\int_t^{t+\Delta t} dt'[x(t')-x(t)]\epsilon(t') + \tfrac{1}{2}g_t^{(2)}\int_t^{t+\Delta t} dt'[x(t')-x(t)]^2\epsilon(t') + \cdots\ , \tag{7}$$

in which

$$\Gamma_0(t+\Delta t)-\Gamma_0(t)=\int_t^{t+\Delta t}dt'\epsilon(t') \ . \tag{8}$$

For the integrands in (7) we need an expansion of $x(t')-x(t)$ good to first order only. This can be obtained from (7) which implies

$$x(t')-x(t)=(t'-t)f_t^{(0)}+f_t^{(1)}\int_t^{t'}dt''[x(t'')-x(t)]+g_t^{(0)}[\Gamma_0(t')-\Gamma_0(t)]+g_t^{(1)}\int_t^{t'}dt''[x(t'')-x(t)]\epsilon(t'') \ . \tag{9}$$

Inserted into (7), an expression good to second-order results

$$\begin{aligned}x(t+\Delta t)=x(t)+\Delta t f_t^{(0)}+\tfrac{1}{2}(\Delta t)^2 f_t^{(1)}f_t^{(0)}+g_t^{(0)}[\Gamma_0(t+\Delta t)-\Gamma_0(t)]+f_t^{(1)}g_t^{(0)}[\Gamma_1(t+\Delta t)-\Gamma_1(t)-\Delta t\Gamma_0(t)]\\ +g_t^{(1)}f_t^{(0)}\int_t^{t+\Delta t}dt'(t'-t)\epsilon(t')+g_t^{(1)}g_t^{(0)}\int_t^{t+\Delta t}dt'[\Gamma_0(t')-\Gamma_0(t)]\epsilon(t')+O(\Delta t^3) \ ,\end{aligned} \tag{10}$$

in which

$$\Gamma_1(t+\Delta t)-\Gamma_1(t)=\int_t^{t+\Delta t}dt'\Gamma_0(t') \ . \tag{11}$$

The sixth and seventh terms on the right-hand side of (10) may be simplified using integration by parts

$$\begin{aligned}\int_t^{t+\Delta t}dt'(t'-t)\epsilon(t')&=\Delta t\Gamma_0(t+\Delta t)\\ &\quad-[\Gamma_1(t+\Delta t)-\Gamma_1(t)] \ ,\end{aligned} \tag{12}$$

$$\int_t^{t+\Delta t}dt'[\Gamma_0(t')-\Gamma_0(t)]\epsilon(t')=\tfrac{1}{2}[\Gamma_0(t+\Delta t)-\Gamma_0(t)]^2 \ . \tag{13}$$

Equation (10) does not contain a term proportion to $f_t^{(2)}g_t^{(0)}g_t^{(0)}$ and to an integral of the square of $\Gamma_0(t')-\Gamma_0(t)$ as might be expected from the fourth term on the right-hand side of (7). This is because this term has an average of order Δt^3. This is the Z_3 term of Ref. 5 that caused so much consternation in that paper and unnecessarily led to the restriction of the order of the stochastic terms to $\frac{3}{2}$. Such a term, however, is required for the second-order white-noise algorithm,[2] and indeed creates precisely the difficulty alluded to in Ref. 5. Although this difficulty can be overcome in the Stratonovich version of the white-noise algorithm, the resulting algorithm becomes overly unwieldy and inefficient. Indeed, the colored-noise algorithm for a short correlation time is the effective way to approach the white-noise simulation to second order.[3,5]

An integral algorithm has been derived[4] for the solution to Eq. (2). It reads

$$\epsilon(t+\Delta t)=\exp(-\lambda\Delta t)\epsilon(t)+G_0(t,\Delta t) \tag{14}$$

in which $G_0(t,\Delta t)$ is defined by

$$G_0(t,\Delta t)=\lambda\int_t^{t+\Delta t}ds\,\exp[-\lambda(t+\Delta t-s)]g_w(s) \tag{15}$$

and is Gaussian. This result and its derivation are easily extended to include $\Gamma_0(t)$ and $\Gamma_1(t)$. The extensions are

$$\Gamma_0(t+\Delta t)=\Gamma_0(t)+\frac{1}{\lambda}[1-\exp(-\lambda\Delta t)]\epsilon(t)+G_1(t,\Delta t) \ , \tag{16}$$

in which $G_1(t,\Delta t)$ is defined by

$$G_1(t,\Delta)=\int_t^{t+\Delta t}ds\{1-\exp[-\lambda(t+\Delta t-s)]\}g_w(s) \tag{17}$$

and

$$\begin{aligned}\Gamma_1(t+\Delta t)&=\Gamma_1(t)+\Delta t\Gamma_0(t)\\ &\quad+\frac{1}{\lambda^2}[\lambda\Delta t+\exp(-\lambda\Delta t)-1]\epsilon(t)\\ &\quad+G_2(t,\Delta t) \ ,\end{aligned} \tag{18}$$

in which $G_2(t,\Delta t)$ is defined by

$$\begin{aligned}G_2(t,\Delta t)=\frac{1}{\lambda}\int_t^{t+\Delta t}ds\{&\lambda(t+\Delta t-s)\\ &+\exp[-\lambda(t+\Delta t-s)]-1\}\\ &\times g_w(s) \ .\end{aligned} \tag{19}$$

Both $G_1(t,\Delta t)$ and $G_2(t,\Delta t)$ are Gaussian too.

In summary, Eq. (10) is the second-order algorithm in which the noise terms are determined by Eqs. (12)–(14), (16), and (18). These noise terms require the generation of three Gaussian random numbers, $G_0(t,\Delta t)$, $G_1(t,\Delta t)$, and $G_2(t,\Delta t)$. It is desired that their statistical properties are correct up to and including order Δt^2. This is where our work goes beyond earlier efforts.[1,3,5] Moreover, we are able to achieve our goal using only two uniformly distributed random numbers (on the unit interval), which is the optimum procedure.

The variance and the cross correlations of the $G_i(t,\Delta t)$'s, each of which has zero mean, are readily determined from their definitions

$$\langle G_0^2\rangle=D\lambda[1-\exp(-2\lambda\Delta t)]\approx O(\Delta t) \ , \tag{20}$$

$$\langle G_1^2\rangle=2D\left[\Delta t-\frac{3}{2\lambda}+\frac{2}{\lambda}\exp(-\lambda\Delta t)-\frac{1}{2\lambda}\exp(-2\lambda\Delta t)\right]\approx O(\Delta t^3) \ , \tag{21}$$

$$\langle G_2^2\rangle=\frac{2D}{\lambda^2}\left[\frac{\lambda^2}{3}\Delta t^3-\lambda\Delta t^2+\Delta t+\frac{2}{\lambda}[1-\exp(-2\lambda\Delta t)]-2\Delta t\exp(-\lambda\Delta t)\right]\approx O(\Delta t^5) \ , \tag{22}$$

$$\langle G_0G_1\rangle=D[1-\exp(-\lambda\Delta t)]^2\approx O(\Delta t^2) \ , \tag{23}$$

$$\langle G_0G_2\rangle=2D\left[\frac{1}{2\lambda}[1-\exp(-2\lambda\Delta t)]-\Delta t\exp(-\lambda\Delta t)\right]\approx O(\Delta t^3)\ , \tag{24}$$

$$\langle G_1G_2\rangle=\frac{D}{\lambda^2}[\lambda\Delta t+\exp(-\lambda\Delta t)-1]^2\approx O(\Delta t^4)\ . \tag{25}$$

These results are identical to those quoted in Ref. 5. To maintain an algorithm to order Δt^2, it is necessary to satisfy Eqs. (20)–(25) through order Δt^4. If we had to satisfy all six conditions, then we would need three[5] independent Gaussian random numbers to do it. However, since we do not need to require (22) because it is order Δt^5, we can satisfy the other five equations with just two Gaussian random numbers as is shown below.

Let Ψ_1 and Ψ_2 be two independent Gaussian random numbers with zero means and unit variances. This means that

$$\langle\Psi_1\rangle=0,\quad\langle\Psi_2\rangle=0,\quad\langle\Psi_1^2\rangle=\langle\Psi_2^2\rangle=1,\quad\langle\Psi_1\Psi_2\rangle=0\ . \tag{26}$$

Now we write

$$G_0=a(\langle G_0^2\rangle)^{1/2}\Psi_1+b(\langle G_0^2\rangle)^{1/2}\Psi_2\ , \tag{27}$$

$$G_1=c(\langle G_1^2\rangle)^{1/2}\Psi_1+d(\langle G_1^2\rangle)^{1/2}\Psi_2\ , \tag{28}$$

$$G_2=e(\langle G_2^2\rangle)^{1/2}\Psi_1+f(\langle G_2^2\rangle)^{1/2}\Psi_2\ . \tag{29}$$

Equations (20)–(25) require the identities

$$a^2+b^2=1\ , \tag{30}$$

$$c^2+d^2=1\ , \tag{31}$$

$$ac+bd=\frac{\langle G_0G_1\rangle}{(\langle G_0^2\rangle\langle G_1^2\rangle)^{1/2}}\ , \tag{32}$$

$$ae+bf=\frac{\langle G_0G_2\rangle}{(\langle G_0^2\rangle\langle G_2^2\rangle)^{1/2}}\ , \tag{33}$$

$$ce+df=\frac{\langle G_1G_2\rangle}{(\langle G_1^2\rangle\langle G_2^2\rangle)^{1/2}}\ . \tag{34}$$

We have not required $e^2+f^2=1$ as was explained above. Equations (30–(34) are easily solved yielding

$$a=1\ , \tag{35}$$

$$b=0\ , \tag{36}$$

$$c=\frac{\langle G_0G_1\rangle}{(\langle G_0^2\rangle\langle G_1^2\rangle)^{1/2}}\ , \tag{37}$$

$$e=\frac{\langle G_0G_2\rangle}{(\langle G_0^2\rangle\langle G_2^2\rangle)^{1/2}}\ , \tag{38}$$

$$d=\left[1-\frac{\langle G_0G_2\rangle^2}{\langle G_0^2\rangle\langle G_1^2\rangle}\right]^{1/2}\ , \tag{39}$$

$$f=\frac{\dfrac{\langle G_1G_2\rangle}{(\langle G_1^2\rangle\langle G_2^2\rangle)^{1/2}}-\dfrac{\langle G_0G_1\rangle\langle G_0G_2\rangle}{\langle G_0^2\rangle(\langle G_1^2\rangle\langle G_2^2\rangle)^{1/2}}}{\left[1-\dfrac{\langle G_0G_1\rangle^2}{\langle G_0^2\rangle\langle G_1^2\rangle}\right]^{1/2}}\ . \tag{40}$$

The Gaussian random variables Ψ_1 and Ψ_2 are generated by the Box-Muller algorithm[7] from two uniformly distributed random numbers (on the unit interval), r_1 and r_2, by the identities

$$\Psi_1=[-2\ln(r_1)]^{1/2}\cos(2\pi r_2)\ , \tag{41}$$

$$\Psi_2=[-2\ln(r_1)]^{1/2}\sin(2\pi r_2)\ . \tag{42}$$

As is seen from these expressions, two uniform random numbers are needed to make one Gaussian random number, but a second, statistically independent Gaussian random number is created by the change from cosine to sine. Thus, the second-order algorithm apparently requires no more random number generation per integration step than does the first-order algorithm. (In the first-order algorithm, one usually generates both uniform random numbers on one step, creates both possible Gaussian random numbers, uses one of them and saves the other for the next integration step, waiting another step before generating two more uniform random numbers). If one demands satisfaction of Eq. (22) as well, then three Gaussian random numbers must be created for each step and this requires four uniform random numbers. This in essence doubles the random number generation. (Again, as with the first-order algorithm, one could create a fourth Gaussian random number and save it for later.) Fortunately, this doubling is unnecessary in a second-order algorithm.

In Ref. 1, the putatively second-order algorithm does not treat the random integrals of Eq. (10) in the exact way presented above. Instead, they replace Eqs. (8) and (11), respectively, with

$$\int_t^{t+\Delta t}dt'\epsilon(t')=\Delta t\epsilon(t)\ , \tag{43}$$

$$\int_t^{t+\Delta t}dt'\Gamma_0(t')=\tfrac{1}{2}\Delta t^2\epsilon(t)\ . \tag{44}$$

The right-hand sides of these expressions do not reproduce the correlations of the left-hand sides up to order Δt^4, as they should, but only up to order Δt^3. Even this agreement depends upon use of the identity

$$\langle\epsilon(t)\epsilon(t')\rangle=D\lambda\exp(-\lambda|t-t'|)\ , \tag{45}$$

which implicitly assumes that the average is over both the white noise $g_w(t)$ and the distribution of initial values of $\epsilon(0)$ (see next paragraph).

The final difference between our algorithm and the work of others[1,5] is that the initial values for $\epsilon(0)$ must be given by a Gaussian distribution and an additional average over this distribution is generally required, as has been emphasized elsewhere.[3,5] In the present algorithm, the dependence on $\epsilon(0)$ is implicitly respected throughout [it is an intrinsic part of the extended integral algorithm of Eqs. (14), (16), and (18)] and the $\epsilon(0)$ average must be performed to guarantee stationarity.[3] In fact, if one correctly interprets the averaging expressed on the left-hand side of (45) as with respect to $g_w(t)$ only, then the identity should read

$$\langle\epsilon(t)\epsilon(t')\rangle=[\epsilon(0)]^2\exp[-\lambda(t+t')]+D\lambda\{\exp(-\lambda|t-t'|)-\exp[-\lambda(t+t')]\}\ . \tag{46}$$

Asymptotically in time, this consideration is not important, but for times of order λ^{-1} it is critical, and this is especially true for many first-passage time problems.[3]

Note that in executing this algorithm Eqs. (20)–(25) and (30)–(40) are implemented once and for all at the outset before the DO-LOOP commences, and only Eqs. (27)–(29), (41) and (42) are required for each integration step.

III. GENERALIZATIONS

It is straightforward to generalize the algorithm presented above to more than one dependent variable. Consider the system of stochastic differential equations

$$\frac{d}{dt}x^{\alpha}=f^{\alpha}(x)+g^{\alpha}{}_{\beta}(x)\epsilon^{\beta}(t) \tag{47}$$

in which α and β range from 1 to n, and pairs of repeated upper and lower Green indices are to be summed. There are now n colored noises satisfying

$$\frac{d}{dt}\epsilon^{\beta}=-\lambda^{\beta}\epsilon^{\beta}+\lambda^{\beta}g^{\beta}{}_{w}(t) \tag{48}$$

with n independent Gaussian white noises satisfying

$$\begin{aligned}&\langle g^{\beta}{}_{w}(t)\rangle=0\ ,\\ &\langle g^{\alpha}{}_{w}(t)g^{\beta}{}_{w}(t')\rangle=2\delta^{\alpha\beta}D^{\beta}\delta(t-t')\ .\end{aligned} \tag{49}$$

We proceed as in the one variable case and generate the analogs to Eqs. (4)–(10). The analog to Eq. (4) is obvious. Equations (5) and (6) become

$$\begin{aligned}f^{\alpha}(\mathbf{x}(t'))=f^{\alpha}&+f^{\alpha}{}_{,\beta}(x(t')-x(t))^{\beta}\\ &+\tfrac{1}{2}f^{\alpha}{}_{,\beta\eta}[x(t')-x(t)]^{\beta}[x(t')-x(t)]^{\eta}\\ &+\cdots\ ,\end{aligned} \tag{50}$$

$$\begin{aligned}g^{\alpha}{}_{\beta}(\mathbf{x}(t'))=g^{\alpha}{}_{\beta}&+g^{\alpha}{}_{\beta,\rho}[x(t')-x(t)]^{\rho}\\ &+\tfrac{1}{2}g^{\alpha}{}_{\beta,\rho\eta}[x(t')-x(t)]^{\rho}[x(t')-x(t)]^{\eta}+\cdots\end{aligned} \tag{51}$$

in which the following shorthand notation has been used:

$$\begin{aligned}&f^{\alpha}=f^{\alpha}(\mathbf{x}(t)),\quad f^{\alpha}{}_{,\beta}=\frac{\partial f^{\alpha}}{\partial[x(t)]^{\beta}}\ ,\\ &f^{\alpha}{}_{,\beta\eta}=\frac{\partial f^{\alpha}}{\partial[x(t)]^{\beta}\partial[x(t)]^{\eta}}\ ,\end{aligned} \tag{52}$$

$$\begin{aligned}&g^{\alpha}{}_{\beta}=g^{\alpha}{}_{\beta}(\mathbf{x}(t)),\quad g^{\alpha}{}_{\beta,\rho}=\frac{\partial g^{\alpha}{}_{\beta}}{\partial[x(t)]^{\rho}}\ ,\\ &g^{\alpha}{}_{\beta,\rho\eta}=\frac{\partial g^{\alpha}{}_{\beta}}{\partial[x(t)]^{\rho}\partial[x(t)]^{\eta}}\ .\end{aligned} \tag{53}$$

Note that each partial derivative is evaluated at time t. Equation (7) becomes

$$\begin{aligned}x^{\alpha}(t+\Delta t)=x^{\alpha}(t)&+\Delta t f^{\alpha}+f^{\alpha}{}_{,\beta}\int_{t}^{t+\Delta t}dt'[x(t')-x(t)]^{\beta}+\tfrac{1}{2}f^{\alpha}{}_{,\beta\eta}\int_{t}^{t+\Delta t}dt'[x(t')-x(t)]^{\beta}[x(t')-x(t)]^{\eta}+\cdots\\ &+g^{\alpha}{}_{\beta}[\Gamma^{\beta}{}_{0}(t+\Delta t)-\Gamma^{\beta}{}_{0}(t)]+g^{\alpha}{}_{\beta,\rho}\int_{t}^{t+\Delta t}dt'[x(t')-x(t)]^{\rho}\epsilon^{\beta}(t')\\ &+\tfrac{1}{2}g^{\alpha}{}_{\beta,\rho\eta}\int_{t}^{t+\Delta t}dt'[x(t')-x(t)]^{\rho}[x(t')-x(t)]^{\eta}\epsilon^{\beta}(t')+\cdots\ ,\end{aligned} \tag{54}$$

in which the analog to (8) is used

$$\Gamma^{\beta}{}_{0}(t+\Delta t)-\Gamma^{\beta}{}_{0}(t)=\int_{t}^{t+\Delta t}dt'\epsilon^{\beta}(t')\ . \tag{55}$$

For the analog of (9) we get

$$\begin{aligned}[x(t')-x(t)]^{\beta}=(t'-t)f^{\beta}&+f^{\beta}{}_{,\eta}\int_{t}^{t'}dt''[x(t'')-x(t)]^{\eta}+g^{\beta}{}_{\eta}[\Gamma^{\eta}{}_{0}(t')-\Gamma^{\eta}{}_{0}(t)]\\ &+g^{\beta}{}_{\eta,\rho}\int_{t}^{t'}dt''[x(t'')-x(t)]^{\rho}\epsilon^{\eta}(t'')+\cdots\ .\end{aligned} \tag{56}$$

Inserting (56) into (54) produces the analog to (10)

$$\begin{aligned}x^{\alpha}(t+\Delta t)=x^{\alpha}(t)&+\Delta t f^{\alpha}+\tfrac{1}{2}(\Delta t)^{2}f^{\alpha}{}_{,\beta}f^{\beta}+g^{\alpha}{}_{\beta}[\Gamma^{\beta}{}_{0}(t+\Delta t)-\Gamma^{\beta}{}_{0}(t)]\\ &+f^{\alpha}{}_{,\beta}g^{\beta}{}_{\eta}[\Gamma^{\eta}{}_{1}(t+\Delta t)-\Gamma^{\eta}{}_{1}(t)-\Delta t\Gamma^{\eta}{}_{0}(t)]+g^{\alpha}{}_{\beta,\rho}f^{\rho}\int_{t}^{t+\Delta t}dt'(t'-t)\epsilon^{\beta}(t')\\ &+g^{\alpha}{}_{\beta,\rho}g^{\rho}{}_{\eta}\int_{t}^{t+\Delta t}dt'[\Gamma^{\eta}{}_{0}(t')-\Gamma^{\eta}{}_{0}(t)]\epsilon^{\beta}(t')+O(\Delta t^{3})\ .\end{aligned} \tag{57}$$

The stochastic integrals in the sixth and seventh terms on the right-hand side of (57), in analogy with (12) and (13), are given by

$$\begin{aligned}\int_{t}^{t+\Delta t}dt'(t'-t)\epsilon^{\beta}(t')&=\Delta t\Gamma^{\beta}{}_{0}(t+\Delta t)\\ &\quad-[\Gamma^{\beta}{}_{1}(t+\Delta t)-\Gamma^{\beta}{}_{1}(t)]\ ,\end{aligned} \tag{58}$$

$$\begin{aligned}\int_{t}^{t+\Delta t}dt'[\Gamma^{\eta}{}_{0}(t')-\Gamma^{\eta}{}_{0}(t)]\epsilon^{\beta}(t')&\\ =(1-\tfrac{1}{2}\delta^{\eta\beta})[\Gamma^{\eta}{}_{0}(t+\Delta t)-\Gamma^{\eta}{}_{0}(t)]&\\ \times[\Gamma^{\beta}{}_{0}(t+\Delta t)-\Gamma^{\beta}{}_{0}(t)]\ .&\end{aligned} \tag{59}$$

Equations (14)–(42) may be applied to each of the n independent noise processes since the $g^{\beta}{}_{w}(t)$'s are statisti-

cally independent. All that needs to be done is to add the appropriate superscript. This, of course, means that at each integration step $2n$ uniform random numbers must be generated.

IV. NUMERICAL EXAMPLES

We have performed tests of the algorithm presented here on two types of problems used in earlier papers concerned with improving existing algorithms. One of these is the Kubo oscillator[2,8,9] which may be solved analytically, so that one compares the simulations with explicit formulas. The other is a first-passage-time problem[3,5] that is not solvable analytically but for which a reliable result can be obtained using a first-order algorithm and a very short step size; the results of the higher-order algorithms for larger step sizes are then compared to the reliable result. Both tests support the claim that the algorithm presented here is correct, efficient, and an improvement on earlier algorithms.

Recent study[8] of extant algorithms identified the earlier use[9] of the Kubo oscillator as an excellent choice for testing the quality of algorithms. In our earlier tests of this system, we used an algorithm of first order in Δt and a step size of order 10^{-4}. Excellent agreement with analytic expressions was achived[9] from averages over 5000 iterations. In the present study, the step size has been increased to 10^{-1}, and for the second-order algorithm the results are still very good, whereas for the first-order algorithm, the increased step size creates substantial deviations from the analytic expressions.

For a detailed description of the Kubo oscillator problem, the reader is referred to the earlier literature.[2,9] Application of the new algorithm presented in this paper produces the second-order algorithm

$$\begin{aligned} x(t+\Delta t)=x(t)-\Delta t\omega_0 y(t)-\tfrac{1}{2}\Delta t^2\omega_0^2 x(t) \\ -[\Gamma_0(t+\Delta t)-\Gamma_0(t)]y(t) \\ -\tfrac{1}{2}[\Gamma_0(t+\Delta t)-\Gamma_0(t)]^2 x(t)\ , \end{aligned} \tag{60}$$

$$\begin{aligned} y(t+\Delta t)=y(t)+\Delta t\omega_0 x(t)-\tfrac{1}{2}\Delta t^2\omega_0^2 y(t) \\ +[\Gamma_0(t+\Delta t)-\Gamma_0(t)]x(t) \\ -\tfrac{1}{2}[\Gamma_0(t+\Delta t)-\Gamma_0(t)]^2 y(t) \end{aligned} \tag{61}$$

for the real and imaginary parts, respectively, of the complex Kubo oscillator amplitude. These equations may be though of as a complex realization of Eqs. (10)–(12), or as a two-component realization of Eqs. (57)–(59) with the special added feature that the two noises, $\epsilon^{\beta}(t)$ for $\beta=1,2$, in corresponding Eq. (47), are the same. The third and fifth terms on the right-hand sides of these equations are the second order in Δt terms. According to both sets of equations (10)–(12) and (57)–(59), each should contain two types of Γ_1 terms as well. For the Kubo oscillator, however, these additional terms cancel exactly. This means that the Kubo oscillator tests are not testing all possible contributions to second order. However, these terms do play a role in our other tests, as will be discussed below.

Numerical tests for the Kubo oscillator were done for $\Delta t=0.1$, $D=0.05$, and $\lambda=1.0$, with averages over 5000 stochastic realizations. In our earlier tests,[9] $\Delta t=1.5915\times10^{-4}$ was used to obtain better than 1% agreement with analytic expressions. Using the second-order algorithm for 100 time steps produced averaged values for the Kubo oscillator phase and radius of 243.883 and 1.003 21, respectively. The correct values are 247.072 and 1.000 00. When the second-order terms in Eqs. (60) and (61) are dropped, leaving the first-order algorithm, the results are 243.34 and 1.683 06 instead. This demonstrates the improvement produced by the second-order algorithm over the first-order version, and shows that the major difference is in the radius, not the phase. The big difference in performance for the radius can be explained using Eqs. (60) and (61). Computation of x^2+y^2 using the first-order version produces an error of order Δt^2, whereas the second-order version produces an error of order Δt^4 on account of several cancellations. Thus, 100 time steps of size 0.1 will yield an error of roughly 1.0 in the first case, but of roughly 0.01 in the second, as is seen. When these tests are done again for 200 time steps, the second-order algorithm yields 136.814 and 1.009 90 for the correct values of 139.461 and 1.000 00, while the first-order version produces 134.547 and 2.840 99. As the number of time steps is increased, the superiority of the second-order algorithm over the first-order algorithm grows more dramatic. Moreover, a major portion of the time taken by the two algorithms is devoted to the generation of random numbers and is virtually the same for both first and second order, as has been discussed in Sec. II.

Recent studies of first-passage-time behavior[5] compared an improved algorithm[5] with our earlier[4] first-order method. Our first-order method[4] was used[5] for the small step size of $\Delta t=0.001$ to obtain an accurate value for a particular first-passage-time calculation. This value was then used to ascertain the quality of our first-order algorithm and an improved algorithm[5] of order $\Delta t^{3/2}$ for step sizes ranging from 0.001 up to 1.0. Up to $\Delta t=0.1$ the improved algorithm reproduced the $\Delta t=0.001$ value for the first-passage time quite well, although the scatter in the published data is rather large on account of the use of only 1000 stochastic realizations per average. In addition, the first-order algorithm showed a systematic decrease in value, beginning around $\Delta t=0.01$ and becoming about 10–20% by $\Delta t=0.1$, depending on various choices of the parameters. These results[5] clearly indicated that a higher-order algorithm produces marked improvement. We have tested our second-order algorithm for $\Delta t=0.1$ for 5000 stochastic realizations per average and find no significant deviation from the first-order result obtained for $\Delta t=0.001$. These tests do include the Γ_1 terms absent in the Kubo oscillator tests. For Δt larger than 0.1, however, large deviations develop, these can be traced to the poor quality of the second-order algorithm with regard to the nonstochastic part of the numerical integration for such large step sizes. Consideration of this possibility is always called for so that one does not blindly use too large a step size.

While these two types of tests complement each other,

it is desirable to identify an analytically tractable multiplicative stochastic process for which the Γ_1 terms of the second-order algorithm are not accidentally absent, and for which analytic expressions may be obtained, preferably for a more than one component system. This would enable us to thoroughly benchmark this second-order algorithm.

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