Stochastic Runge-Kutta algorithms. I. White noise

Rebecca L. Honeycutt
David Taylor Research Center, Code 1945, Bethesda, Maryland 20084-5000
(Received 6 June 1991)

A higher-order algorithm for the numerical integration of one-variable, additive, white-noise equations is developed. The method of development is to extend standard deterministic Runge-Kutta algorithms to include stochastic terms. The ability of the algorithm to generate proper correlation properties is tested on the Ornstein-Uhlenbeck process, showing higher accuracy even with longer step size.

PACS number(s): 05.40.+j, 02.50.+s, 02.60.+y

I. INTRODUCTION

Since analytic solutions cannot be found for stochastic differential equations, complete analysis of the equations require numerical simulations [1–5]. These simulations are most commonly done with a first-order Euler-type algorithm. For higher accuracy we have developed a method of extending deterministic Runge-Kutta algorithms to include stochastic terms [6]. These extensions are developed first for white-noise equations. Following the same line of development, part II of this work develops similar algorithms for differentiating colored-noise equations. Both the white- and colored-noise algorithms are tested to show improved accuracy over the standard methods.

We will now consider the one-variable, additive, white-noise equation [7]

$$\dot{x}=f(x)+g_w(t)\ , \tag{1.1}$$

where $g_w(t)$ is Gaussian white noise with properties

$$\langle g_w(t)\rangle=0 \tag{1.2a}$$

and

$$\langle g_w(t)g_w(t')\rangle=2D\delta(t-t')\ . \tag{1.2b}$$

II. EXPANSION OF x

For a general stochastic differential equation such as (1.1), algorithms can be developed by obtaining an expression for $x(\Delta t)$ in the following manner. Integrate (1.1) from $t=0$ to Δt to obtain

$$x(\Delta t)=x_0+\int_0^{\Delta t}f(x(t'))dt'+\int_0^{\Delta t}g_w(t')dt'\ . \tag{2.1}$$

Define

$$\Gamma_0(t)\equiv\int_0^t g_w(t')dt'\ , \tag{2.2a}$$

$$\Gamma_i(t)\equiv\int_0^t\Gamma_{i-1}(t')dt',\quad i=1,2,3,\dots\ . \tag{2.2b}$$

Inserting the above expressions along with the Taylor expansion for f about x_0 into (2.1) yields

$$x(\Delta t)=x_0+\Gamma_0(\Delta t)+\Delta t f+\cdots+\frac{1}{i!}f^{(i)}\int_0^{\Delta t}(x'-x_0)^i dt'+\cdots\ , \tag{2.3}$$

where the derivatives of f are evaluated at x_0, and x' indicates $x(t')$. Inserting (2.3) into itself repeatedly, while neglecting terms of order higher than Δt^4, results in the following expansion of $x(\Delta t)$:

$$\begin{aligned}x(\Delta t)=x_0&+\Delta t f+\tfrac{1}{2}\Delta t^2 ff^{(1)}\\&+\tfrac{1}{6}\Delta t^3(ff^{(1)2}+f^2f^{(2)})\\&+\tfrac{1}{24}\Delta t^4(ff^{(1)3}+4f^2f^{(1)}f^{(2)}+f^3f^{(3)})+R(\Delta t)\ ,\end{aligned} \tag{2.4}$$

where $R(\Delta t)$ is the stochastic portion of $x(\Delta t)$. After integration by parts has been performed, many terms of $R(\Delta t)$ can be combined yielding the following expression for $R(\Delta t)$ [6]:

$$\begin{aligned}R(\Delta t)=&\,\Gamma_0(\Delta t)+f^{(1)}\Gamma_1(\Delta t)+\tfrac{1}{2}f^{(2)}\int_0^{\Delta t}\Gamma_0^2+\left[\tfrac{1}{6}f^{(3)}\int_0^{\Delta t}\Gamma_0^3+ff^{(2)}[\Delta t\Gamma_1(\Delta t)-\Gamma_2(\Delta t)]+f^{(1)2}\Gamma_2(\Delta t)\right]\\&+\tfrac{1}{24}\left[12f^{(1)}f^{(2)}\left[\int_0^{\Delta t}(\Delta t-t')\Gamma_0^2+\Gamma_1^2(\Delta t)\right]+12ff^{(3)}\int_0^{\Delta t}t'\Gamma_0^2+f^{(4)}\int_0^{\Delta t}\Gamma_0^4\right]\\&+\Bigg\{f^{(1)3}\Gamma_3(\Delta t)+\tfrac{1}{2}ff^{(1)}f^{(2)}[\Delta t^2\Gamma_1(\Delta t)+2\Delta t\Gamma_2(\Delta t)-4\Gamma_3(\Delta t)]\\&\quad+\tfrac{1}{6}f^{(1)}f^{(3)}\left[\int_0^{\Delta t}(\Delta t-t')\Gamma_0^3+3\Gamma_1(\Delta t)\int_0^{\Delta t}\Gamma_0^2-3\int_0^{\Delta t}\left[\Gamma_0\int_0^{t'}\Gamma_0^2\right]\right]\\&\quad+\tfrac{1}{2}f^2f^{(3)}[\Delta t^2\Gamma_1(\Delta t)-2\Delta t\Gamma_2(\Delta t)+2\Gamma_3(\Delta t)]\end{aligned}$$

$$+\tfrac{1}{2}f^{(2)2}\int_0^{\Delta t}\left[\Gamma_0\int_0^{t'}\Gamma_0^2\right]+\tfrac{1}{6}ff^{(4)}\int_0^{\Delta t}(t'\Gamma_0^3)+\frac{1}{5!}f^{(5)}\int_0^{\Delta t}\Gamma_0^5\Bigg\}$$

$$+\tfrac{1}{24}\Bigg\{6f^{(1)2}f^{(2)}\left[\int_0^{\Delta t}(\Delta t-t')^2\Gamma_0^2+4\Gamma_1(\Delta t)\Gamma_2(\Delta t)\right]$$

$$+3ff^{(1)}f^{(3)}\left[2\int_0^{\Delta t}(2t'\Delta t-t'^2)\Gamma_0^2+\Delta t\,\Gamma_1^2(\Delta t)-\int_0^{\Delta t}\Gamma_1^2\right]$$

$$+6ff^{(2)2}\left[2\Delta t\,\Gamma_1^2(\Delta t)+2\int_0^{\Delta t}\Gamma_1^2-4\Gamma_1(\Delta t)\Gamma_2(\Delta t)+\int_0^{\Delta t}(\Delta t^2-t'^2)\Gamma_0^2\right]$$

$$+f^{(1)}f^{(4)}\left[\int_0^{\Delta t}(\Delta t-t')\Gamma_0^4+4\Gamma_1(\Delta t)\int_0^{\Delta t}\Gamma_0^3-4\int_0^{\Delta t}\left[\Gamma_0\int_0^{t'}\Gamma_0^3\right]\right]$$

$$+2f^{(2)}f^{(3)}\left[2\int_0^{\Delta t}\left[\Gamma_0\int_0^{t'}\Gamma_0^3\right]+3\int_0^{\Delta t}\left[\Gamma_0^2\int_0^{t'}\Gamma_0^2\right]\right]$$

$$+6f^2f^{(4)}\int_0^{\Delta t}t'^2\Gamma_0^2+ff^{(5)}\int_0^{\Delta t}t'\Gamma_0^4+\tfrac{1}{30}f^{(6)}\int_0^{\Delta t}\Gamma_0^6\Bigg\}\ . \tag{2.5}$$

In the development of algorithms to integrate stochastic differential equations, the deterministic portion of the algorithms are required to agree with (2.4). As well, the stochastic portion must agree with both the form and statistical properties of (2.5).

III. CORRELATION PROPERTIES OF $R(\Delta t)$

To determine the statistical properties of $R(\Delta t)$, those of the Γ's must first be determined. Since $g_w(t)$ is Gaussian and has a zero mean, the Γ's are also Gaussian with mean zero, i.e., $\langle\Gamma_i(\Delta t)\rangle=0$. To obtain the correlation properties of these variables it is helpful to rewrite (2.2b) in the following manner:

$$\Gamma_n(t_n)=\int_0^{t_n}dt_{n-1}\int_0^{t_{n-1}}dt_{n-2}\cdots\int_0^{t_2}dt_1\int_0^{t_1}dt_0\int_0^{t_0}g_w(\tau)d\tau\ . \tag{3.1}$$

The order of integration can be reversed by applying the identity

$$\int_0^a dt\int_0^t d\tau=\int_0^a d\tau\int_\tau^a dt$$

n times. This draws the noise term to the outermost integral. Performing the resulting inner integrations yields

$$\Gamma_n(t)=\int_0^t\frac{(t-\tau)^n}{n!}g_w(\tau)d\tau\ . \tag{3.2}$$

The correlation properties of the Γ's are then found to be

$$\langle\Gamma_m(t)\Gamma_n(s)\rangle=2D\frac{t^{m+1}}{m!}\sum_i\frac{(s-t)^{n-i}t^i}{i!(n-i)!(m+i+1)}\quad(t<s) \tag{3.3}$$

where i ranges from 0 to n. Applying this to (2.5), the mean and variance of $R(\Delta t)$ become [6]

$$\langle R(\Delta t)\rangle=\tfrac{1}{2}\Delta t^2Df^{(2)}+\tfrac{1}{6}\Delta t^3[D(3f^{(1)}f^{(2)}+2ff^{(3)})+D^2f^{(4)}]$$
$$+\tfrac{1}{24}\Delta t^4[D(7f^{(1)2}f^{(2)}+\tfrac{13}{2}ff^{(1)}f^{(3)}+7ff^{(2)2}+3f^2f^{(4)})+D^2(7f^{(1)}f^{(4)}+11f^{(2)}f^{(3)}+3ff^{(5)})+D^3f^{(6)}] \tag{3.4a}$$

and

$$\langle R^2(\Delta t)\rangle=2D\Delta t+2D\Delta t^2f^{(1)}+\tfrac{4}{3}\Delta t^3[D(f^{(1)2}+ff^{(2)})+D^2f^{(3)}]$$
$$+\Delta t^4[D(\tfrac{13}{6}ff^{(1)}f^{(2)}+\tfrac{1}{2}f^2f^{(3)}+\tfrac{2}{3}f^{(1)3})+D^2(5f^{(1)}f^{(3)}+\tfrac{11}{4}f^{(2)2}+ff^{(4)})+\tfrac{1}{2}D^3f^{(5)}]\ . \tag{3.4b}$$

IV. EXTENDING THE RUNGE-KUTTA METHODS

To integrate deterministic equations, Runge-Kutta methods (RK) [8] are standard. For the equation

$$\dot{x}=F(x)\ , \tag{4.1}$$

the RK algorithm of second order (RKII), which is commonly used, is

$$x(\Delta t)=x_0+\tfrac{1}{2}\Delta t(F_1+F_2)\ , \tag{4.2}$$

where

$$F_1=F(x_0)\ , \tag{4.3a}$$

$$F_2=F(x_0+\Delta tF_1)\ . \tag{4.3b}$$

If we try to integrate (1.1) by letting $F(x)=f(x)+g_w$, we quickly run into trouble. The quantity g_w cannot be generated since it has infinite variance. Therefore the standard RK cannot be used to integrate stochastic differential equations without some alterations. (This argument holds for higher-order RK algorithms as well).

A second option is to let $F(x)=f(x)$, and change (4.2) to

$$x(\Delta t)=x_0+\tfrac{1}{2}\Delta t(F_1+F_2)+\Gamma_0(\Delta t) . \tag{4.4}$$

This way, the noise term is brought into the equations as the integral of g_w, which has a finite variance. Expanding F_1 and F_2 and substituting into (4.4) results in the expansion

$$x(\Delta t)=x_0+\Delta t f+\tfrac{1}{2}\Delta t^2 f f^{(1)}+\Gamma_0(\Delta t) \tag{4.5}$$

to order Δt^2. As before, this is not a proper algorithm. Although the deterministic portion of (4.5) agrees with (2.4), the stochastic portion only agrees to order Δt. Therefore this is only a first-order algorithm, which implies that a more elaborate extension of the deterministic RK must be made in order to include the stochastic terms. In extending the deterministic RK to a stochastic RK the following structure is used:

$$x(\Delta t)=x_0+\tfrac{1}{2}\Delta t(F_1+F_2)+(2D\Delta t)^{1/2}\phi_0 , \tag{4.6}$$

where

$$F_1=f(x_0+(2D\Delta t)^{1/2}\phi_1) , \tag{4.7a}$$

$$F_2=f(x_0+\Delta t F_1+(2D\Delta t)^{1/2}\phi_2) . \tag{4.7b}$$

ϕ_0, ϕ_1, and ϕ_2 are random variables, each with zero mean and correlation properties that are determined later in this paper. The deterministic portion of the extension has been chosen to be the same as a typical deterministic RK algorithm. This choice is not required, but it simplifies the calculations since expansions of F_1 and F_2 will automatically yield the correct deterministic portions. Noise terms have been added to the arguments of f so that terms with multiples of Γ's and derivatives of $f(x)$ will be part of the expansions. The prefactor $(2D\Delta t)^{1/2}$ is inserted because $2D\Delta t$ is a time-dependent prefactor of all the terms of $\langle R^2(\Delta t)\rangle$, therefore preventing the ϕ's from having any time dependence.

Expanding F_1 and F_2 and inserting these expansions into (4.6) gives

$$x(\Delta t)=x_0+\Delta t f+\tfrac{1}{2}\Delta t^2 f f^{(1)}+R'(\Delta t) , \tag{4.8a}$$

where

$$\begin{aligned} R'(\Delta t)=&(2D\Delta t)^{1/2}\phi_0+\tfrac{1}{2}\Delta t(2D\Delta t)^{1/2}f^{(1)}(\phi_1+\phi_2)\\ &+\tfrac{1}{2}\Delta t^2 D f^{(2)}(\phi_1^2+\phi_2^2)\\ &+\tfrac{1}{2}\Delta t^2(2D\Delta t)^{1/2}[\tfrac{1}{3}D f^{(3)}(\phi_1^3+\phi_2^3)+f^{(1)2}\phi_1\\ &+\tfrac{1}{2}f f^{(2)}\phi_2] . \end{aligned} \tag{4.8b}$$

A comparison of (4.8a) and (4.8b) with (2.4) and (2.5), respectively, shows that the deterministic portions of these expressions agree, and that the stochastic portions have the same basic structure. In addition, we require the statistical properties of $R'(\Delta t)$ and $R(\Delta t)$ to agree. Consequently, the properties of the ϕ's are determined. The mean and variance of $R'(\Delta t)$ are

$$\langle R'(\Delta t)\rangle=\tfrac{1}{2}\Delta t^2 D f^{(2)}(\langle\phi_1^2\rangle+\langle\phi_2^2\rangle) \tag{4.9a}$$

and

$$\langle R'^2(\Delta t)\rangle=2D\Delta t\langle\phi_0^2\rangle+2D\Delta t^2 f^{(1)}\langle\phi_0(\phi_1+\phi_2)\rangle . \tag{4.9b}$$

The higher correlations of R' are zero to order Δt^2. Equating coefficients of (4.9) with (3.4) results in the following set of equations which must be satisfied:

$$\langle\phi_0^2\rangle=1 , \tag{4.10a}$$

$$\langle\phi_0(\phi_1+\phi_2)\rangle=1 , \tag{4.10b}$$

$$\langle\phi_1^2\rangle+\langle\phi_2^2\rangle=1 . \tag{4.10c}$$

Since there are three independent equations and three unknowns, one random variable ψ is enough to solve (4.6). Define ψ such that $\langle\psi\rangle=0$, $\langle\psi^2\rangle=1$, and $\phi_i=a_i\psi$. Substituting these expressions into Eq. (4.10) gives four possible sets of real solutions for the a_i's. To keep the famil-

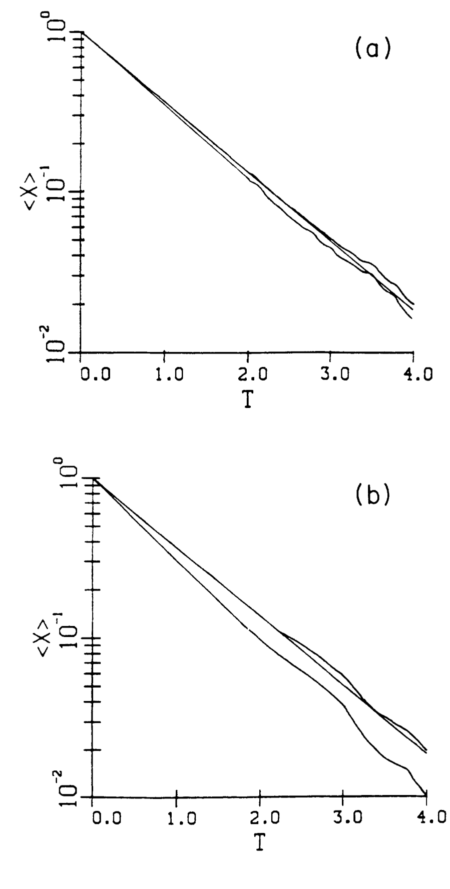

FIG. 1. The average value of x for the Ornstein-Uhlenbeck process. The straight line is the theoretical value, the upper curve is from the SRKII method, and the lower curve is from the Euler method. Both methods use 5000 realizations, noise strength $D=0.1$, correlation time $\lambda^{-1}=1.0$, initial value $x=1.0$, and time step (a) $\Delta t=0.1$ and (b) $\Delta t=0.25$.

iar structure of the deterministic RKII, we chose $a_0=1$, $a_1=r0$, and $a_2=1$. The resulting stochastic RKII (SRKII) method is

$$x(\Delta t)=x_0+\tfrac{1}{2}\Delta t(F_1+F_2)+(2D\Delta t)^{1/2}\psi \;, \tag{4.11}$$

with

$$F_1=f(x_0) \;, \tag{4.12a}$$

$$F_2=f(x_0+\Delta t F_1+(2D\Delta t)^{1/2}\psi) \;, \tag{4.12b}$$

where $\langle \psi \rangle=0$ and $\langle \psi^2 \rangle=1$.

To develop extensions of higher-order RK algorithms for white noise, the same technique can be applied.

V. ORNSTEIN-UHLENBECK PROCESS

In order to compare the accuracy of the Euler algorithm and the SRKII algorithm, we consider the Ornstein-Uhlenbeck process [9,10]. The defining equation for this system is

$$\dot{x}=-\lambda x+\lambda g_w(t) \;. \tag{5.1}$$

The properties considered are the average and the variance, which are

$$\langle x(t) \rangle = x(0)\exp(-\lambda t) \tag{5.2}$$

and

$$\langle x^2(t) \rangle = x^2(0)\exp(-2\lambda t)+D\lambda[1-\exp(-2\lambda t)] \;. \tag{5.3}$$

Both algorithms have been used to integrate (5.1). In all of the simulations, the same sequence of random numbers was used, and 5000 realizations were averaged over. The initial values are $D=0.1$, $\lambda=1.0$, and $x(0)=1.0$. The methods are compared for time steps of $\Delta t=0.1$ and 0.25. From the Figs. 1 and 2 it is clear that the SRKII method is more accurate than the Euler method, even when a larger time step is used on the SRKII method.

VI. CONCLUSION

Although we have only extended to a second-order RK algorithm, the same extension technique can be applied to higher-order algorithms. These algorithms should also yield more accuracy and the ability to use larger step sizes.

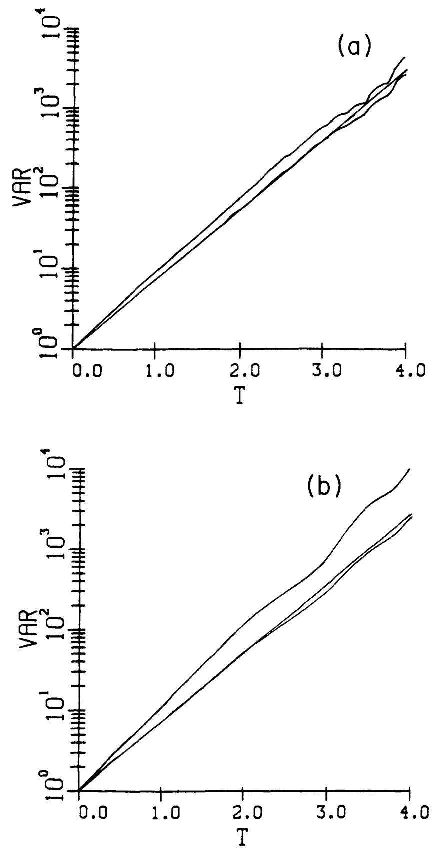

FIG. 2. The normalized variance of x for the Ornstein-Uhlenbeck process. The straight line is the theoretical value, the lower curve is from the SRKII method, and the upper curve is from the Euler method. The variables have the same values as in Fig. 1.

ACKNOWLEDGMENTS

I would like to thank the Physics Department at Georgia Institute of Technology where this work was done, and Ronald Fox for the many discussions over the past few years.

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