THE BELL SYSTEM TECHNICAL JOURNAL
Vol. 58, No. 10, December 1979
Printed in U.S.A.

Numerical Integration of Stochastic Differential Equations

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(Manuscript received June 28, 1979)

A procedure for numerical integration of a stochastic differential equation, by extension of the Runge-Kutta method, is presented. The technique produces results which are statistically correct to a given order in the time step. Second- and third-order approximations are explicitly displayed.

I. INTRODUCTION

Systematic work on numerical solution of stochastic differential equations (SDEs) seems not to have kept pace with the considerable analytical developments. This parallels the lag which existed between the analytical and numerical study of ordinary differential equations near the turn of the century (which is perhaps understandable in view of the difficulty of implementing even straightforward algorithms at the time). In the last few years, there has been a burst of activity in performing Brownian dynamics computer simulations[1] to gain insight into motions in complex physical systems. Little attention seems to have been paid, though, to the systematic development of the numerical techniques in most of these works.

In the present paper, the Runge-Kutta (RK) approximation for deterministic differential equations (DDEs) is extended to SDEs. Although we have not as yet explicitly considered other popular numerical schemes, we feel that the techniques utilized here should have wider applicability. For the sake of simplicity, several further restrictions are placed on the discussions in this paper. These, we believe, can ultimately be removed by fairly simple means.

(*i*) We shall work only with a single equation rather than a set of n equations. It has been explicitly verified that the second-order approximation carries over in a straightforward manner to sets (and in our studies of polymers[2] we used it for 600 simultaneous equations).

However, bear in mind Butcher's demonstration[3] that extra conditions arise with the RK method when one generalizes fifth-order (5_O) and higher schemes from single equations to sets.

(*ii*) We present explicit results only for low-order algorithms, second (2_O) and third (3_O) order, although the principles of higher order extensions will be written down.

(*iii*) Finally, we restrict attention to a simple SDE, which is of the general form occurring in Brownian motion theory. This is

$$dx/dt = f(x) + A(t), \tag{1}$$

where the $A(t)$ are Gaussianly distributed random variables with mean zero and covariance

$$\langle A(t)A(t')\rangle = \xi\delta(t - t') \tag{2}$$

(white noise). The extension to $f(x,t)$ appears to involve little new, but makes the presentation more cumbersome.

In Section II, we review the RK technique for DDEs. After defining more clearly what is meant by numerical solution of an SDE in Section III, we explicitly extend the 2_O RK method to SDEs and outline the generalization to any order. A 3_O RK scheme is presented in the appendix. Section IV is a brief discussion of the question of accuracy. The concluding remarks indicate areas for future studies.

Abbreviations used throughout the paper are listed in Table I.

II. SUMMARY OF THE RK APPROXIMATION FOR DDEs

To set the stage, it will be useful to review[4] briefly the application of the RK technique to the DDE

$$dx/dt = f(x). \tag{3}$$

Of course, this equation can be solved by quadrature, but not when x and f are vectors, or when f is a function of x and t (the RK procedure for the latter case is presented in most standard texts[4] and does not differ greatly from the case we are considering).

Begin by writing down the solution of eq. (3) as a series in the time step s:

$$x(s) = x_o + sf_o + \tfrac{1}{2}s^2 f_o f_o' + (\tfrac{1}{6})s^3(f_o f_o'^2 + f_o^2 f_o'') + \cdots, \tag{4}$$

Table I—Summary of abbreviations

SDE	Stochastic differential equation
DDE	Deterministic differential equation
RK	Runge-Kutta
k_O	kth order
l_S	l stages
m_G	m Gaussian random variables per step

where $f_o^{(n)}$ denotes the nth derivative of f evaluated at x_o. The aim of many numerical procedures is to present an algorithm which, when expanded in s, matches the series (4) to a given order, k, in s. Of course, merely evaluating eq. (4) will do that, but a further aim is to avoid the determination of derivatives of f. Thus, in the RK theory one goes from an initial condition x_o to $x(s)$ in l stages by the general procedure

$$g_1 = f(x_o),$$

$$g_2 = f(x_o + \beta_{21} s g_1),$$

$$g_3 = f(x_o + \beta_{31} s g_1 + \beta_{32} s g_2),$$

$$\cdots$$

$$g_l = f(x_o + \beta_{l1} s g_1 + \cdots + \beta_{l,l-1} s g_{l-1}), \tag{5}$$

$$x_s = x_o + s(A_1 g_1 + A_2 g_2 + \cdots + A_l g_l). \tag{6}$$

The $\frac{1}{2} l(l+1)$ parameters $A_1, \cdots, A_l, \beta_{21}, \cdots, \beta_{l,l-1}$ are to be selected so that an expansion of eq. (6) in powers of s matches Eq. (4) through order k. Only for $k \leq 4$ can a kth order (k_O) RK calculation be done in k stages (k_S). For $k \geq 5$, a larger number of stages than the order is necessary to provide enough parameters to match the true series.

In the $2_O 2_S$ RK, the parameters must satisfy

$$A_1 + A_2 = 1, \tag{7}$$

$$A_2 \beta_{21} = \tfrac{1}{2}. \tag{8}$$

This illustrates the common occurrence of less equations than parameters. The user then has the freedom to select some parameters (one in the present case) for convenience, or to achieve the smallest error estimates.[5]

III. GENERALIZATION OF RK METHOD TO SDEs

An SDE does not have a definite solution. When we say that we are numerically integrating an SDE, we mean that we are generating a statistically representative trajectory. Furthermore, as in numerical integration of a DDE, we are not going to generate the full trajectory, but only values of x at discrete times: $x(0)$, $x(s_1)$, $x(s_1 + s_2)$, $\cdots$. Let us be more specific. The stochastic process x (or set of processes) specified by eq. (1) is Markovian. Thus, the process is completely specified by the conditional probability density function $p(x, s \mid x_o)$, which gives the probability density of observing x at time s, given the value x_o of the variable at time zero. What we seek is a method of selecting a value x_s with statistics correct to kth order in s. By this, we

mean that the moments $\langle x_s^q \rangle$ are all correctly given to $O(s^k)$; i.e., there exists a sequence C_q such that for sufficiently small s

$$|\langle x_s^q \rangle_a - \langle x(s)^q \rangle_e| \leq C_q s^k, \tag{9}$$

for all positive integers q. The average $\langle\ \rangle_a$ is over the ensemble generated by the approximate process, while $\langle\ \rangle_e$ is over the exact process.

An approximation algorithm will involve generation of some random numbers. Naturally, if $p(x,s \mid x_o)$ is known, all that need be done is to generate a single uniformly distributed random number, u, for each step and solve the equation $p(x,s \mid x_o) = u$ for x. We shall see that a 1_O approximation is equivalent to linearizing f (since f'' does not enter until $O(s^2)$). For a linear SDE, $p(x,s \mid x_o)$ is a well-known Gaussian.[6] Use of this Gaussian as an approximate process has been suggested.[7,8] This is practical for a single variable x, but for a large set, the amount of matrix manipulation is overwhelming.

In the RK extension to be discussed, for each step of time s, m independent Gaussianly distributed variables, Z_i (or m sets, $\mathbf{Z}_i$), will be needed. These have

$$\langle Z_i \rangle = 0, \tag{10}$$

$$\langle Z_i Z_j \rangle = \delta_{ij}. \tag{11}$$

An approximation which requires m Z's will be said to be m-fold Gaussian, abbreviated m_G.

Now we shall present a parallel to the RK procedure for SDEs. Again begin by developing a "power series" expansion for the solution of the SDE (1):

$$dx/dt = f(x) + A(t). \tag{1}$$

This may be done by iteration and Taylor series expansion:

$$x(s) = x_o + \int_0^s ds_1 f\left\{x_o + \int_0^{s_1} ds_2 f[x_o + \cdots] + w_o(s_1)\right\} + w_o(s) \tag{12}$$

$$= x_o + s f_o + \frac{1}{2} s^2 f_o f_o' + \frac{1}{6} s^3 (f_o f_o'^2 + f_o^2 f_o'') + \cdots + S, \tag{13}$$

$$S = \{w_o(s)\} + \{f_o' w_1(s)\} + \left\{\frac{1}{2} f_o'' \int_0^s ds_1 w_o^2(s_1)\right\} + \left\{f_o'^2 w_2(s) + f_o f_o''[s w_1(s) - w_2(s)]\right\}$$

$$+\frac{1}{6}f_o'''\int_0^s ds_1 w_o^3(s_1)\Bigg\}$$

$$+\left\{\frac{1}{2}f_o'f_o''\int_0^s ds_1(s-s_1)w_o^2(s_1)+\frac{1}{2}f_of_o'''\int_0^s ds_1 s_1 w_o^2(s_1)\right.$$

$$\left.+\frac{1}{24}f_o^{(iv)}\int_0^s ds_1 w_o^4(s_1)\right\}+\cdots; \tag{14}$$

$$w_n(s)=\int_0^s ds_1 w_{n-1}(s_1),\quad n>0, \tag{15}$$

$$=\int_0^s ds_1\frac{(s-s_1)^n}{n!}A(s_1),\quad n\geq 0 \tag{16}$$

($w_o(s)$ is the Wiener process). The term S is a stochastic process. Its various parts, set off in braces, have orders in probability $s^{1/2}$, $s^{3/2}$, s^2, $s^{5/2}$, s^3, $\cdots$ (N.B.: there is no s^1 term). A stochastic variable v will be said to have an order s^k in probability if

$$|\langle v^q\rangle|\leq K_q s^{qk}, \tag{17}$$

for all positive integers q, a set of constants K_q, and sufficiently small s. The w_n are correlated Gaussian random variables with mean zero and covariances

$$\langle w_n(s)w_m(s)\rangle=\xi s^{n+m+1}/n!m!(n+m+1), \tag{18}$$

$$\langle w_o(s)w_o(t)\rangle=\xi\min(s,t).$$

$$\langle w_o(s)w_1(t)\rangle=\begin{cases}\frac{1}{2}\xi t^2, & t\leq s,\\ \frac{1}{2}\xi s(2t-s), & t\geq s,\end{cases} \tag{19}$$

$$\cdots$$

The statistics of the stochastic part of the trajectory are embodied in the moments of S which, from eqs. (18) to (20), are

$$\langle S\rangle=\tfrac{1}{4}s^2\xi f_o''+s^3\xi(\tfrac{1}{12}f_o'f_o''+\tfrac{1}{6}f_of_o'''+\tfrac{1}{24}\xi f_o^{(iv)})+\cdots, \tag{20}$$

$$\langle S^2\rangle=s\xi+s^2\xi f_o'+s^3\xi(\tfrac{2}{3}f_o'^2+\tfrac{2}{3}f_of_o''+\tfrac{1}{3}\xi f_o''')+\cdots, \tag{21}$$

$$\langle S^3\rangle=\tfrac{7}{4}s^3\xi^2 f_o''+\cdots. \tag{22}$$

For the expansion through $O(s^3)$, the terms of S nonlinear in the w's do not contribute to the moments $\langle S^4\rangle$ and higher. Thus, these moments are related to the second moment by the usual Gaussian formulas: $\langle S^4\rangle=3\langle S^2\rangle$, etc.; i.e., the cumulants vanish to $O(s^3)$. The point is that, if $\langle S^2\rangle$ is properly given, so will $\langle S^k\rangle$, $k\geq 4$, be. The aim of a k_O numerical scheme will be to match not only the nonstochastic

terms of the series solution for x, eq. (13), but also to match all the moments of the stochastic term.

We delay the presentation of the general extension of the RK approximation and first explicitly display a $2_O2_S1_G$ scheme. Consider the algorithm:

$$g_1 = f(x_o + s^{1/2}\xi^{1/2}\lambda_1 Z), \tag{23}$$

$$g_2 = f(x_o + s\beta g_1 + s^{1/2}\xi^{1/2}\lambda_2 Z), \tag{24}$$

$$x = x_o + s(A_1 g_1 + A_2 g_2) + s^{1/2}\xi^{1/2}\lambda_o Z. \tag{25}$$

Z is a single Gaussian random variable with mean zero and variance unity, generated for each time step s. Using these equations, x can be developed in power of $s^{1/2}$ to $O(s^2)$:

$$x = x_o + (A_1 + A_2)sf_o + A_2\beta s^2 f_o f_o'' + \cdots + \tilde{S}, \tag{26}$$

$$\tilde{S} = \lambda_o Z s^{1/2}\xi^{1/2} + (A_1\lambda_1 + A_2\lambda_2)Z s^{3/2}\xi^{1/2}f_o' + \tfrac{1}{2}(A_1\lambda_1^2 + A_2\lambda_2^2)Z^2 s^2 \xi f_o'' + \cdots . \tag{27}$$

The moments of $\tilde{S}$ through $O(s^2)$ are

$$\langle \tilde{S} \rangle = \tfrac{1}{2}(A_1\lambda_1^2 + A_2\lambda_2^2)s^2\xi f_o'' + \cdots \tag{28}$$

$$\langle \tilde{S}^2 \rangle = \lambda_o^2 s\xi + 2(A_1\lambda_1 + A_2\lambda_2)\lambda_o s^2 \xi f_o' \cdots . \tag{29}$$

To $O(s^2)$, the moments $\langle \tilde{S}^3 \rangle$ and higher involve only the linear terms of $\tilde{S}$, so they are Gaussianly related to $\langle \tilde{S}^2 \rangle$. Matching the deterministic part of eq. (26) to (13), eq. (28) to (20), and eq. (29) to (21), we find as equations for the parameters:

$$A_1 + A_2 = 1, \tag{30}$$

$$A_2\beta = \tfrac{1}{2}, \tag{31}$$

$$\lambda_o^2 = 1, \tag{32}$$

$$(A_1\lambda_1 + A_2\lambda_2)\lambda_o = \tfrac{1}{2}, \tag{33}$$

$$A_1\lambda_1^2 + A_2\lambda_2^2 = \tfrac{1}{2}. \tag{34}$$

The sign of λ_o is immaterial since it multiplies a symmetric random variable. There are five equations and six parameters. A convenient solution set is

$$A_1 = A_2 = \tfrac{1}{2}, \tag{35}$$

$$\beta = 1, \tag{36}$$

$$\lambda_o = 1, \tag{37}$$

and either

$$(\lambda_1 = 0, \lambda_2 = 1), \tag{38a}$$

or

$$(\lambda_1 = 1, \lambda_2 = 0). \tag{38b}$$

With this as background, the general procedure for constructing a $k_O l_S m_G$ approximation should be clear. Consider the m Gaussian random variables as a vector $\mathbf{Z} = (Z_1, Z_2, \cdots, Z_m)$. Also define $l + 1$ vectors of parameters, each of dimension m:

$$\begin{aligned}
\boldsymbol{\lambda}_o &= (\lambda_{o1}, 0, 0, \cdots) \\
\boldsymbol{\lambda}_1 &= (\lambda_{11}, \lambda_{12}, 0, \cdots) \\
&\cdots \\
\boldsymbol{\lambda}_l &= (\lambda_{l1}, \lambda_{l2}, \cdots, \lambda_{lm}).
\end{aligned} \tag{39}$$

The number of scalar λ parameters is $m(l - \frac{1}{2}m + \frac{3}{2})$. The generalization of the RK algorithm is

$$\begin{aligned}
g_1 &= f(x_o + s^{1/2}\xi^{1/2}\,\boldsymbol{\lambda}_1\cdot\mathbf{Z}), \\
g_2 &= f(x_o + s\beta_{21}g_1 + s^{1/2}\xi^{1/2}\,\boldsymbol{\lambda}_2\cdot\mathbf{Z}), \\
&\cdots \\
g_l &= f(x_o + s\beta_{l1}g_1 + \cdots + s\beta_{l,l-1}g_{l-1} + s^{1/2}\xi^{1/2}\,\boldsymbol{\lambda}_l\cdot\mathbf{Z}),
\end{aligned} \tag{40}$$

$$x = x_o + s(A_1g_1 + \cdots + A_lg_l) + s^{1/2}\xi^{1/2}\,\boldsymbol{\lambda}_o\cdot\mathbf{Z}. \tag{41}$$

The A's and β's are subject to the usual RK equations since, for $\xi = 0$, the DDE is recovered. The equations for the λ's are obtained by expanding eq. (41), in powers of $s^{1/2}$ to order s^k and separating off a stochastic term $\tilde{S}$. Each term of the moments of $\tilde{S}$ has the form of a product of a numerical coefficient, an integral power of s and of ξ, a product of powers of f_o and its derivatives, and a product of the A, β and λ parameters (the λ parameters enter only as dot products of the $\boldsymbol{\lambda}$ vectors). This term is equated to the term of the exact moments of S with the same powers of s, ξ, f_o, and derivatives of f_o [see eqs. (20) to (22)]. The result is a set of equations for the λ's, and the number of Gaussians must be chosen so that there are a sufficient number of parameters to satisfy these equations. One Gaussian will do for 2_O2_S, and two Gaussians for 3_O3_S (see the appendix).

IV. ACCURACY

The accuracy of a numerical scheme for integrating a DDE can be judged on the basis of its ability to determine trajectories for analytically soluble equations. The schemes for SDEs can only be judged on

a statistical basis. For example, the probability density, $p(x, t)$, for the random process x defined by eq. (1) satisfies the Fokker-Planck equation

$$\frac{dp}{dt} = -\frac{d}{dx}\left[f(x)p - \frac{1}{2}\xi\frac{d}{dx}p\right]. \tag{42}$$

This has a stationary solution

$$p_o(x) = N(\xi)\exp\left[2F(x)/\xi\right], \tag{43}$$

$$F(x) = \int^x f(x')dx', \tag{44}$$

$$1/N(\xi) = \int_{-\infty}^{\infty} \exp\left[2F(x')/\xi\right]dx' \tag{45}$$

(assuming that the density is normalizable). For a stable approximation scheme, the distribution of x will also approach a stationary probability density. One could attempt to test the overall "goodness of fit" of the observed to the theoretical density function.[9] An easier procedure is to assume that eq. (43) holds and to obtain an estimate of ξ, for instance by maximum likelihood estimation.[9] The estimated ξ is then compared with the exact ξ. We have used this technique and have clearly observed how the estimate improves with decreasing step size s. However, no systematic studies have been carried out yet to determine whether the error decreases as s^{k+1}.

In general, one is interested in the complete comparison of the transition probability $p(x, s \mid x_o)$ for the SDE and the numerical scheme. This is embodied in the spectral resolution, for the exact process and the approximation, of $p(x,s \mid x_o)$ regarded as an integral kernel. Here studies performed on exactly soluble systems would be of value.

A question related to accuracy is: How long a trajectory need one run to reduce statistical error in some property to acceptable levels? The answer depends on the time, τ, for decay of correlation of that property. New statistical information is only generated in a time of $O(\tau)$.[10] Therefore, a simulation of total time t will lead to a decrease of error like $(\tau/t)^{1/2}$. Some systems cannot be described in such a clear-cut fashion since they have a spectrum of relaxation times, some of which may be very long. In such cases, there may be an advantage in reinitializing the run to break correlations.

V. DIRECTIONS FOR FURTHER RESEARCH

The specific procedures displayed in this paper are illustrative of the manner in which standard numerical techniques can be extended

to stochastic differential equations. There are several general directions in which further research may be aimed.

5.1 More general SDEs

The numerical schemes should be directed toward more general SDEs. The extension to sets of equations has been mentioned. More general forms of SDEs than eq. (1) are

$$dx = f(x,t)dt + \phi(x, t)dw_0(t) \tag{46}$$

or

$$\frac{dx}{dt} = f(x, t, A(t)). \tag{47}$$

Another generalization is that A may be other than Gaussianly distributed. Also, in the physical literature there is increased attention being directed to stochastic integrodifferential equations, representing processes with memory, such as[11,12]

$$\frac{dx}{dt} = f(x) + \int_0^t d\tau K(\tau)x(t-\tau) + A(t), \tag{48}$$

$$\langle A(t)A(t+\tau)\rangle \propto K(\tau), \tag{49}$$

or more generally,[13]

$$\frac{dx}{dt} = f(x) + \int_0^t d\tau G[\tau, x(t-\tau)] + A, \tag{50}$$

with A and G related by a generalized fluctuation-dissipation theorem.

5.2 Other numerical schemes

It would be interesting to develop stochastic versions of other numerical schemes used for DDEs. One may raise the objection to any multistep procedure that it does violence to the Markovian nature of the process. One would have to reuse the random variables, Z_i, for several steps to eliminate the spurious memory to the desired order.

5.3 General principles

There are many matters, which are the standard fare of the deterministic numerical analyst, that should be placed in a stochastic context. The question of accuracy has been raised. Another is stability. A third question is that of step-by-step error estimation. An interesting problem arises in developing the analog of step-size adjustment and the criteria for when it is necessary. Imagine that such criteria exist

and a particularly large Z triggers the call for step-size adjustment. The new Z's that are generated should not be independent of the old Z's.

Finally, as a general problem, the matter of computational speed should be considered. To gather statistical data, long trajectories must be run, sometimes on systems of many degrees of freedom. It is urgent that there be an analysis of various procedures with respect to their relative speeds, for a given accuracy.

APPENDIX

$3_O3_S2_G$ Procedure

To carry out a 3_O procedure requires three stages and two Gaussian random variables. The explicit algorithm is eqs. (40) and (41) with $l = 3$. The parameters must satisfy the equations

$$A_1 + A_2 + A_3 = 1, \tag{51}$$

$$A_2\beta_{21} + A_3(\beta_{31} + \beta_{32}) = \tfrac{1}{2}, \tag{52}$$

$$A_2\beta_{21}^2 + A_3(\beta_{31} + \beta_{32})^2 = \tfrac{1}{3}, \tag{53}$$

$$A_3\beta_{32}\beta_{21} = \tfrac{1}{6}, \tag{54}$$

$$\lambda_{o1} = 1, \tag{55}$$

$$A_1\lambda_{11} + A_2\lambda_{21} + A_3\lambda_{31} = \tfrac{1}{2}, \tag{56}$$

$$A_1|\lambda_1|^2 + A_2|\lambda_2|^2 + A_3|\lambda_3|^2 = \tfrac{1}{2}, \tag{57}$$

$$A_1\lambda_{11}^2 + A_2\lambda_{21}^2 + A_3\lambda_{31}^2 = \tfrac{1}{3}, \tag{58}$$

$$A_1|\lambda_1|^2\lambda_{11} + A_2|\lambda_2|^2\lambda_{21} + A_3|\lambda_3|^2\lambda_{31} = \tfrac{1}{3}, \tag{59}$$

$$A_2\beta_{21}\lambda_{21} + A_3(\beta_{31} + B_{32})\lambda_{31} = \tfrac{1}{3} \tag{60}$$

$$|A_1\lambda_1 + A_2\lambda_2 + A_3\lambda_3|^2 + 2(A_2\beta_{21}\lambda_{11} + A_3\beta_{31}\lambda_{11} + A_3\beta_{32}\lambda_{21}) = \tfrac{2}{3}. \tag{61}$$

The first four equations are the usual ones for a 3_O RK approximation. They leave two degrees of freedom. A widely used solution is

$$A_1 = \tfrac{2}{9}, \quad A_2 = \tfrac{3}{9}, \quad A_3 = \tfrac{4}{9}; \tag{62}$$

$$\beta_{21} = \tfrac{1}{2}, \quad \beta_{31} = 0, \quad \beta_{32} = \tfrac{3}{4}. \tag{63}$$

With this set, the remaining seven equations can be solved for the λ parameters. The solution is

$$\lambda_{o1} = 1, \quad \lambda_{11} = 0, \quad \lambda_{21} = \tfrac{1}{2}, \quad \lambda_{31} = \tfrac{3}{4}. \tag{64}$$

There are four solutions for the λ_{l2}'s, two of which are complex. The real solutions are either

$$\begin{aligned} \lambda_{12} &= 0.245538, \\ \lambda_{22} &= -0.023225, \\ \lambda_{32} &= 0.544169, \end{aligned} \tag{65}$$

or

$$\begin{aligned} \lambda_{12} &= -1.34583, \\ \lambda_{22} &= 1.24987, \\ \lambda_{32} &= 0.385032. \end{aligned} \tag{66}$$

Solution (65) is probably superior because it uses less of the Z_2 process. (All the λ_{l1} and/or all the λ_{l2} may be reversed in sign as an acceptable solution, as is evident since they multiply symmetrically distributed random numbers.)

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