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Numerical integration of stochastic differential equations with variable diffusivity

I T Drummond, A Hoch and R R Horgan

Department of Applied Mathematics and Theoretical Physics, University of Cambridge, Silver Street, Cambridge CB3 9EW, UK

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Abstract. We construct two-stage second-order algorithms for integrating stochastic differential equations with variable diffusivity in one and higher dimensions.

1. Introduction

The numerical simulation of diffusion processes is important in a number of different fields. Recently Greensite and Helfand (Helfand 1979, Greensite and Helfand 1981) presented Runge-Kutta algorithms for the integration of stochastic differential equations appropriate to the case of constant diffusivity. Similar methods were developed independently by Drummond *et al* (1984, 1986) and applied to the problem of turbulent diffusion of scalar and magnetic fields and to the stochastic quantisation of $\lambda\Phi^4$ field theory.

However there are interesting problems such as the flow of fluids through non-uniform media (Collins 1961, Scheidegger 1974) which can be simulated by diffusion processes where the diffusivity depends on position. These are examples of so-called multiplicative noise problems. With the intention of applying it to the simulation of processes of the above type we have formulated an appropriate second-order Runge-Kutta algorithm for the relevant stochastic differential equation.

Our algorithm, which is of a two-stage type, does not deal with the most general case where an arbitrary drift field is included along with the diffusion process. Klauder and Petersen (1985) have proposed such an algorithm for the general case. However we have found that it does not work with complete accuracy as a second-order algorithm. Mil'shtein (1974) has also discussed higher-order methods for stochastic differential equations but his approach does not lead to algorithms which satisfy our criteria.

In § 2 we derive the Runge-Kutta integration procedure for a one-dimensional diffusion equation with variable diffusivity and demonstrate that it is correct to $O(\Delta t^2)$ at each step. In § 3 the results are illustrated by a simple example which can be worked out analytically and simulated numerically. We also examine a case where a straightforward analytical approach is not possible.

The algorithm for a multidimensional problem without drift is derived in § 4. It requires a slightly different treatment from the one-dimensional case because of the more complicated tensor structures which appear. The algorithm is applied to a simple model and the dependence of the systematic error on the time step is examined. We finish with some brief comments on future work.

2. Diffusion in one dimension

Rather than study the stochastic differential equation directly, we will base our analysis on the corresponding diffusion equation. In this section we study an equation of the form

$$\frac{\partial P}{\partial t}=\frac{\partial}{\partial x}\kappa(x)\frac{\partial P}{\partial x} \tag{2.1}$$

where $\kappa(x)$ is the position-dependent diffusivity and $P(x, t)$ is a probability distribution in x for each time t.

The time development of $P(x, t)$ can be viewed in two ways. First, we write

$$P(x, t+\Delta t)=\exp(\Delta t H)P(x, t) \tag{2.2}$$

where the operator H is given by

$$H=\frac{\partial}{\partial x}\kappa(x)\frac{\partial}{\partial x}. \tag{2.3}$$

Second, we introduce the kernel function $K(x', t'; x, t)$ which is the probability distribution in x' at t', conditioned so that $x'=x$ at $t'=t$. We then have

$$P(x', t+\Delta t)=\int \mathrm{d}x\, K(x', t+\Delta t; x, t)P(x, t). \tag{2.4}$$

If we set $x'=x+\xi$, then $K(x+\xi, t+\Delta t; x, t)$ is a narrow distribution in ξ with mean and variances both $O(\Delta t)$. We denote this distribution by $F(\xi)$, suppressing its dependence on x, t and Δt. Our procedure is to choose a prescription for $F(\xi)$ such that the result of (2.2) for $P(x, t+\Delta t)$ is reproduced to any given order in Δt. In this paper we work to $O(\Delta t^2)$.

In order to match the stochastic step ξ to (2.2) it is convenient to consider the time evolution of the expectation value $\langle f\rangle_t$ of a function $f(x)$, where

$$\langle f\rangle_t=\int \mathrm{d}x\, f(x)P(x, t). \tag{2.5}$$

We have from (2.2)

$$\langle f\rangle_{t+\Delta t}=\int \mathrm{d}x\, f(x)(1+\Delta t H+\tfrac{1}{2}\Delta t^2H^2)P(x, t)+O(\Delta t^3). \tag{2.6}$$

That is, using (2.3) for H,

$$\langle f\rangle_{t+\Delta t}=\int \mathrm{d}x\, f(x)[1+\Delta t(-\partial\kappa'+\partial^2\kappa)+\tfrac{1}{2}\Delta t^2(-\partial(\kappa\kappa'''+\kappa'\kappa'')$$
$$+\partial^2(3\kappa\kappa''+2\kappa'^2)-\partial^3(4\kappa'\kappa)+\partial^4\kappa^2)]P(x, t)+O(\Delta t^3) \tag{2.7}$$

where $\kappa'\equiv \mathrm{d}\kappa/\mathrm{d}x$, etc, and $\partial\equiv\partial/\partial x$.

From our alternative point of view

$$\langle f\rangle_{t+\Delta t}=\int \mathrm{d}x\, \mathrm{d}x'\, f(x')K(x', t+\Delta t; x, t)P(x, t) \tag{2.8}$$

i.e.

$$\langle f\rangle_{t+\Delta t}=\int \mathrm{d}x\,\mathrm{d}\xi f(x+\xi)F(\xi)P(x,t). \tag{2.9}$$

Since $F(\xi)$ is a narrow distribution we can expand $f(x+\xi)$ in a Taylor series:

$$\langle f\rangle_{t+\Delta t}=\int \mathrm{d}x\,P(x,t)(1+\bar{\xi}\partial+\tfrac{1}{2}\overline{\xi^2}\partial^2+\tfrac{1}{6}\overline{\xi^3}\partial^3+\tfrac{1}{24}\overline{\xi^4}\partial^4)f(x)+\mathrm{O}(\Delta t^3) \tag{2.10}$$

where

$$\overline{\xi^n}=\int \mathrm{d}\xi\,\xi^n F(\xi). \tag{2.11}$$

Finally integrating by parts, we find

$$\langle f\rangle_{t+\Delta t}=\int \mathrm{d}x f(x)(1-\partial\bar{\xi}+\tfrac{1}{2}\partial^2\overline{\xi^2}-\tfrac{1}{6}\partial^3\overline{\xi^3}+\tfrac{1}{24}\partial^2\overline{\xi^4})P(x,t)+\mathrm{O}(\Delta t^3). \tag{2.12}$$

If we compare (2.12) with (2.7) we see we must choose $F(\xi)$ so that

$$\bar{\xi}=\kappa'\Delta t+\tfrac{1}{2}(\kappa\kappa'''+\kappa'\kappa'')\Delta t^2 \tag{2.13}$$

$$\overline{\xi^2}=2\kappa\Delta t+(3\kappa\kappa''+2\kappa'^2)\Delta t^2 \tag{2.14}$$

$$\overline{\xi^3}=12\kappa\kappa'\Delta t^2 \tag{2.15}$$

$$\overline{\xi^4}=12\kappa^2\Delta t^2 \tag{2.16}$$

where we have neglected terms $\mathrm{O}(\Delta t^3)$ including all the higher moments.

Note that to $\mathrm{O}(\Delta t)$ it is sufficient to set

$$\xi=\Delta x=\kappa'\Delta t+(2\kappa\Delta t)^{1/2}\eta \tag{2.17}$$

where η is a Gaussian random variable of zero mean and unit variance. Our partial differential equation is therefore equivalent to an Ito-type stochastic differential equation of the form

$$\dot{x}=\kappa'(x)+(2\kappa(x))^{1/2}w(t) \tag{2.18}$$

where w is the standard white noise term.

The next step is to formulate a prescription for ξ which reproduces the above expectation values. We use a two-stage prescription of the same type as Klauder and Petersen (1985). We introduce two intermediate positions:

$$y_1=x+\alpha_1\kappa'\Delta t+\beta_1(\kappa\Delta t)^{1/2}\eta \tag{2.19}$$

$$y_2=x+\alpha_2\kappa'\Delta t+\beta_2(\kappa\Delta t)^{1/2}\eta \tag{2.20}$$

and a final position

$$x\equiv x+\xi=x+\alpha_{21}\kappa'\Delta t+\beta_{21}(\kappa\Delta t)^{1/2}\eta+\alpha_{22}\kappa'(y_2)\Delta t+\beta_{22}(\kappa(y_1)\Delta t)^{1/2}\zeta \tag{2.21}$$

where η and ζ are two independent Gaussian random variables of zero mean and unit variance. We omit the argument of κ when it is the original point x. If we expand in powers of $\Delta t^{1/2}$ we find

$$\begin{aligned}\xi={}&\kappa^{1/2}(\beta_{21}\eta+\beta_{22}\zeta)\Delta t^{1/2}+\kappa'(\alpha_{21}+\alpha_{22}+\tfrac{1}{2}\beta_1\beta_{22}\eta\zeta)\Delta t\\&+\left(\kappa^{1/2}\kappa''(\alpha_{22}\beta_2\eta+\tfrac{1}{4}\beta_1^2\eta^2\zeta)+\frac{1}{2}\frac{\kappa'^2}{\kappa^{1/2}}(\alpha_1-\tfrac{1}{4}\beta_1^2\eta^2)\zeta\right)\Delta t^{3/2}\\&+(\kappa''\kappa'\alpha_2\alpha_{22}+\tfrac{1}{2}\kappa'''\kappa\beta_2^2\eta^2)\Delta t^2+\mathrm{O}(\zeta\Delta t^2).\end{aligned} \tag{2.22}$$

On averaging over the two Gaussian random variables we obtain the results:

$$\bar{\xi}=\kappa'(\alpha_{21}+\alpha_{22})\Delta t+(\alpha_2\alpha_{22}\kappa''\kappa'+\tfrac{1}{2}\kappa'''\kappa\beta_2^2\alpha_{22})\Delta t^2 \tag{2.23}$$

$$\overline{\xi^2} = \kappa(\beta_{21}^2 + \beta_{22}^2)\Delta t + [\kappa'^2(1+\alpha_1\beta_{22}^2) + \kappa\kappa''(2\alpha_{22}\beta_{21}\beta_2 + \tfrac{1}{2}\beta_1^2\beta_{22}^2)]\Delta t^2 \tag{2.24}$$

$$\overline{\xi^3} = 3\kappa'\kappa(\beta_{21}^2 + \beta_{22}^2 + \beta_{21}\beta_1\beta_{22}^2)\Delta t^2 \tag{2.25}$$

$$\overline{\xi^4} = 3\kappa^2(\beta_{21}^2 + \beta_{22}^2)^2\Delta t^2. \tag{2.26}$$

Comparing these results with the requirements of (2.13)-(2.16) we obtain the conditions

$$\alpha_{22} + \alpha_{21} = 1 \tag{2.27}$$

$$\alpha_{22}\alpha_2 = \tfrac{1}{2} \tag{2.28}$$

$$\alpha_{22}\beta_2^2 = 1 \tag{2.29}$$

$$\beta_{21}^2 + \beta_{22}^2 = 2 \tag{2.30}$$

$$\beta_{22}^2\alpha_1 = 1 \tag{2.31}$$

$$2\alpha_{22}\beta_{21}\beta_2 + \tfrac{1}{2}\beta_1\beta_{22}^2 = 3 \tag{2.32}$$

$$\beta_{21}\beta_1\beta_{22}^2 = 2. \tag{2.33}$$

These equations are satisfied by

$$\begin{array}{llll} \alpha_{22} = \tfrac{1}{4} & \beta_{22} = 1 & \alpha_1 = 1 & \beta_1 = 2 \\ \alpha_{21} = \tfrac{3}{4} & \beta_{21} = 1 & \alpha_2 = 2 & \beta_2 = 2. \end{array} \tag{2.34}$$

When the Klauder–Petersen ansatz (1985) is applied to this problem it gives an incorrect answer for condition (2.15) in which the factor 12 is replaced by 6. In the next section we consider particular examples of $\kappa(x)$ and compare our results with theoretical predictions.

3. One-dimensional examples

An interesting case to consider because of its theoretical tractability is one where the diffusivity has a simple quadratic dependence on position, i.e.

$$\kappa(x) = a + bx^2 \tag{3.1}$$

with a and b both positive. If we set

$$f_n = \langle x^n \rangle \tag{3.2}$$

then (2.1) implies that $\{f_n\}$ satisfy simple differential equations. Thus

$$\dot{f}_n = n(n-1)af_{n-2} + n(n+1)bf_n. \tag{3.3}$$

In particular we have

$$\begin{aligned} \dot{f}_1 &= 2bf_1 \\ \dot{f}_2 &= 2a + 6bf_2 \\ \dot{f}_3 &= 6af_1 + 12bf_3. \end{aligned} \tag{3.4}$$

For the particular case where the initial distribution is $\delta(x - x_0)$, we obtain the solutions

$$\begin{aligned} f_1 &= x_0 \exp(2bt) \\ f_2 &= \left(x_0^2 + \frac{1}{3}\frac{a}{b}\right)\exp(6bt) - \frac{1}{3}\frac{a}{b} \\ f_3 &= \left(x_0^3 + \frac{3}{5}\frac{a}{b}x_0\right)\exp(12bt) - \frac{3}{5}\frac{a}{b}x_0\exp(2bt). \end{aligned} \tag{3.5}$$

Using the algorithm developed in the previous section we have carried out a simulation of this problem on the ICL DAP at Queen Mary College, London, a parallel processor which allows us to deal simultaneously with the paths of 4096 particles. The statistical errors which we quote are derived from samples of between 8×10^6 and 4×10^7 particle paths.

Figure 1 shows a comparison between our simulation and the above theoretical results for the case $x_0=1$, $a=1$, $b=\frac{1}{12}$, and a choice of $\Delta t=0.16$. The results are clearly satisfactory, the statistical error being too small to show on the graph. However, since even a first-order algorithm will yield good results for sufficiently small time steps, the crucial issue is the dependence of the *systematic* error on Δt.

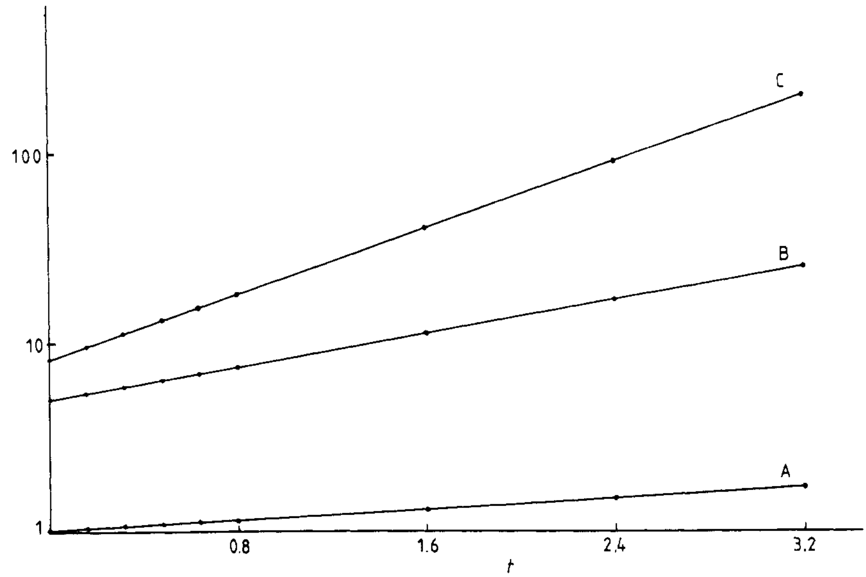


Figure 1. Comparison between theory (cf (3.1) and (3.5)) and simulation for $a=1$, $b=\frac{1}{12}$ and $x_0=1$. The graphs show the dependence on time of (A) f_1, (B) f_2+4 and (C) $f_3+\frac{36}{5}f_1$. These combinations are chosen to make the theoretical predictions (shown by the full lines) to be pure exponential. The dots representing the simulation are much larger than the errors.

In the present case we can analyse this question exactly because the moments $\{f_n\}$, as they develop in the discrete time series appropriate to the simulation, satisfy simple difference equations analogous to the differential equations of the continuous case. For example, if x_p is the position of the particle after p steps, then

$$x_{p+1}=x_p+\xi_p \tag{3.6}$$

where ξ_p is chosen according to the prescription of § 2. Using a bar to denote the average over the ξ_p ensemble we see that

$$\bar{x}_{p+1}=x_p+\bar{\xi}_p. \tag{3.7}$$

Hence, taking account of the specific form of $\kappa(x_p)$ specified in (3.1) and using (2.13) we find

$$\bar{x}_{p+1}=x_p(1+2b\Delta t+2b^2\Delta t^2+\mathrm{O}(\Delta t^3)). \tag{3.8}$$

Averaging now over all steps we find

$$f_1(p+1)=f_1(p)(1+2b\Delta t+2b^2\Delta t^2+\mathrm{O}(\Delta t^3)) \tag{3.9}$$

where $f_1(p)=\langle x_p\rangle$. It is convenient to rewrite this result in the form

$$f_1(p+1)=f_1(p)\exp(2b\Delta t)(1+\mathrm{O}(\Delta t^3)). \tag{3.10}$$

The solution, given that all particles start at x_0, is

$$f_1(p)=x_0\exp(2pb\Delta t)(1+\mathrm{O}(p\Delta t^3)) \tag{3.11}$$

where the correction $\mathrm{O}(p\Delta t^3)$ is a reasonable estimate for an upper bound to the actual error $\Sigma_{q=1}^{p}\mathrm{O}(\Delta t^3)$. Setting $t=p\Delta t$, we have

$$f_1(t)=x_0\exp(2bt)(1+\mathrm{O}(t\Delta t^2)). \tag{3.12}$$

The calculation of the second moment begins with

$$\overline{x_{p+1}^2}=x_p^2+2x_p\bar{\xi}_p+\overline{\xi_p^2} \tag{3.13}$$

and using (2.13) and (2.14) yields

$$\overline{x_{p+1}^2}=x_p^2(1+6b\Delta t+18b^2\Delta t^2+\mathrm{O}(\Delta t^3))+a(2\Delta t+6b\Delta t^2)+\mathrm{O}(\Delta t^3). \tag{3.14}$$

Averaging over all the steps we find

$$f_2(p+1)=f_2(p)\exp(6b\Delta t)(1+\mathrm{O}(\Delta t^3))+\frac{1}{3}\frac{a}{b}(\exp(6b\Delta t)-1)+\mathrm{O}(\Delta t^3) \tag{3.15}$$

where we have also rearranged the Δt series into obvious exponential form. Equation (3.15) can be recast as

$$\left(f_2(p+1)+\frac{1}{3}\frac{a}{b}\right)=\left(f_2(p)+\frac{1}{3}\frac{a}{b}\right)\exp(6b\Delta t)(1+\mathrm{O}(\Delta t^3)) \tag{3.16}$$

with the solution

$$f_2(p)=\left(x_0^2+\frac{1}{3}\frac{a}{b}\right)\exp(6bt)(1+\mathrm{O}(t\Delta t^2))-\frac{1}{3}\frac{a}{b}. \tag{3.17}$$

Third moments can be dealt with similarly though the calculation is a bit more complicated. Thus

$$\overline{x_{p+1}^3}=x_p^3+3x_p^2\overline{\xi_p}+3x_p\overline{\xi_p^2}+\overline{\xi_p^3}. \tag{3.18}$$

Using (2.13)-(2.15) we find

$$\overline{x_{p+1}^3}=x_p^3(1+12b\Delta t+72b^2\Delta t^2+\mathrm{O}(\Delta t^3))+x_p(6a\Delta t+42ab\Delta t^2+\mathrm{O}(\Delta t^3)). \tag{3.19}$$

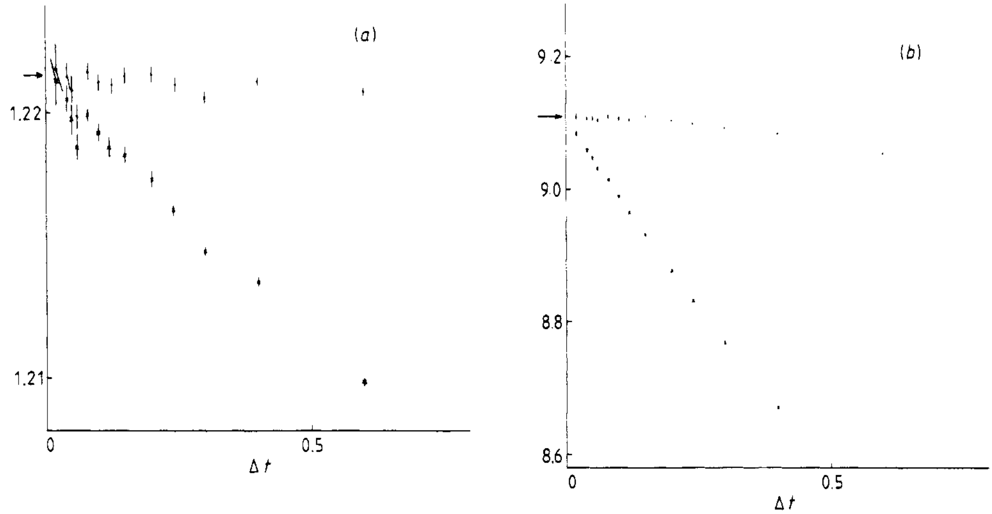
If we now average over all the steps and use the solution of the differential equation for guidance we obtain

$$f_3(p+1)+\frac{3}{5}\frac{a}{b}f_1(p+1)=\left(f_3(p)+\frac{3}{5}\frac{a}{b}f_1(p)\right)\exp(12b\Delta t)(1+\mathrm{O}(\Delta t^3)) \tag{3.20}$$

and hence that

$$f_3(t)+\left(x_0^3+\frac{3}{5}\frac{a}{b}x_0\right)\exp(12bt)(1+\mathrm{O}(t\Delta t^2))-\frac{3}{5}\frac{a}{b}x_0\exp(2bt)(1+\mathrm{O}(t\Delta t^2)). \tag{3.21}$$

In all these cases the error at given t is proportional to Δt^2. Note that at each stage it was important that the moments of ξ_p be included correctly with error $\mathrm{O}(\Delta t^3)$. In particular, to estimate $f_3(t)$ it is necessary to include $\overline{\xi_p^3}$ correct to this order. This is the point at which the Klauder–Petersen algorithm goes wrong.



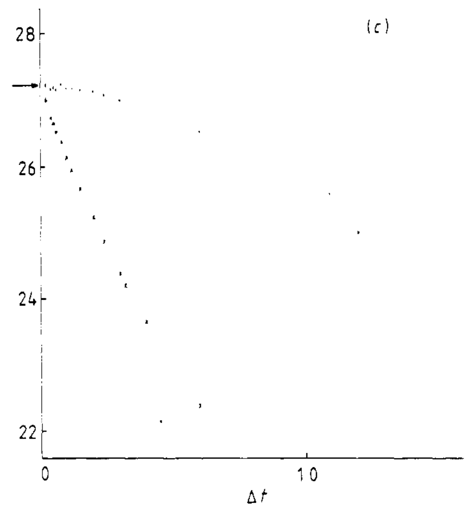


Figure 2. The first three moments of x for $t = 1.2$ plotted against Δt for $\kappa(x)$ given in (3.1) with $a = 1$, $b = \frac{1}{12}$ and $x_0 = 1$. The graphs are (a) f_1, (b) f_2 and (c) f_3. The results of the first-order scheme are signified by crosses and those of the second-order scheme by dots.

In figure 2 we show for the first three moments the dependence of the systematic error on Δt for $t = 1.2$. The results of the second-order algorithm are compared with those of the first-order version. The latter clearly shows an error proportional to Δt at small Δt, while the former shows a Δt^2 behaviour as predicted.

The corresponding results for the first two moments for the case

$$\kappa(x) = 2 + \sin x \tag{3.22}$$

are shown in figure 3. Again the contrast between the first- and second-order algorithms is evident.

4. Higher-dimensional case

In this section we study the diffusion equation

$$\partial P/\partial t = \partial_i \kappa(\boldsymbol{x}) \partial_i P. \tag{4.1}$$

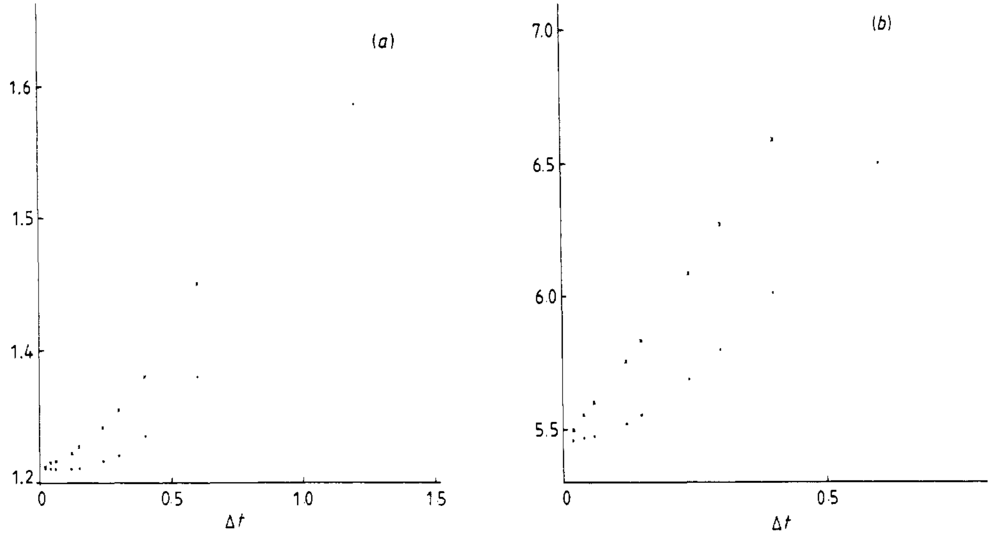


Figure 3. The first two moments of x for $t=1.2$ plotted against Δt for $\kappa(x)$ given in (3.22) with $x_0=1$. The graphs are (*a*) first moment and (*b*) second moment. The results of the first-order scheme are signified by crosses and those of the second-order scheme by dots.

It is possible to generalise this equation by replacing the scalar diffusivity $\kappa(\boldsymbol{x})$ with a diffusivity tensor. However, even the simpler version in (4.1) exhibits features not present in the one-dimensional case already discussed. It also has interesting applications to the theory of random media and is therefore of importance on its own account.

The stochastic differential equation corresponding to (4.1) is

$$\dot{x}_i = \kappa_i(\boldsymbol{x}) + (2\kappa(\boldsymbol{x}))^{1/2} w_i(t) \tag{4.2}$$

where the $w_i(t)$ are independent white noise processes:

$$\langle w_i(t) w_j(t')\rangle = \delta_{ij}\delta(t-t') \tag{4.3}$$

and

$$\kappa_i(\boldsymbol{x}) = \partial_i \kappa(\boldsymbol{x}). \tag{4.4}$$

Further indices attached to $\kappa(\boldsymbol{x})$ indicate the appropriate multiple derivative.

Following an analysis along the lines of the one-dimensional case we find that we can approximate the solutions to (4.1) or (4.2) correctly to $O(\Delta t^2)$ by a sequence of discrete steps $x_i \to x_i + \xi_i$ where ξ_i is drawn from an ensemble which satisfies

$$\overline{\xi_i} = \kappa_i \Delta t + \tfrac{1}{2}(\kappa_l \kappa_{li} + \kappa\kappa_{ill})\Delta t^2 \tag{4.5}$$

$$\overline{\xi_i\xi_j} = 2\kappa\delta_{ij}\Delta t + [\kappa_i\kappa_j + 2\kappa\kappa_{ij} + \delta_{ij}(\kappa_l^2 + \kappa\kappa_{ll})]\Delta t^2 \tag{4.6}$$

$$\overline{\xi_i\xi_j\xi_k} = 4(\delta_{ij}\kappa\kappa_k + \delta_{jk}\kappa\kappa_i + \delta_{ki}\kappa\kappa_j)\Delta t^2 \tag{4.7}$$

$$\overline{\xi_i\xi_j\xi_k\xi_l} = 4\kappa^2(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})\Delta t^2. \tag{4.8}$$

Note that, although these results reduce to (2.13)–(2.17) in one dimension, in general they exhibit a complicated tensor structure containing distinct terms which coincide in one dimension. It is for this reason that our prescription for the step ξ_i contains more parameters than its one-dimensional equivalent.

Our ansatz for ξ_i utilises *three* intermediate points. Thus

$$y_i^{(a)} = x_i + \alpha_a \kappa_i \Delta t + \beta_a (\kappa \Delta t)^{1/2} \eta_i \tag{4.9}$$

$a = 1, 2, 3$, with the final step given by

$$\xi_i = \alpha_{21} \kappa_i \Delta t + \beta_{21} (\kappa \Delta t)^{1/2} \eta_i + \alpha_{22} \kappa_i (y^{(1)}) \Delta t + \beta_{22} (\kappa (y^{(2)}) \Delta t)^{1/2} \zeta_i + \gamma_{22} (\kappa (y^{(3)}) \Delta t)^{1/2} \zeta_i \tag{4.10}$$

and η_i and ζ_i are independent Gaussian random variables with zero mean and unit variance.

To $O(\Delta t^2)$ we have

$$\begin{aligned}\xi_i = {} & \kappa^{1/2} (\beta_{21} \eta_i + (\beta_{22} + \gamma_{22}) \zeta_i) \Delta t^{1/2} + [(\alpha_{21} + \alpha_{22}) \kappa_i + \tfrac{1}{2} (\beta_{22} \beta_2 + \gamma_{22} \beta_3) \kappa_j \eta_j \zeta_i] \Delta t \\ & + \{\alpha_{22} \beta_1 \kappa^{1/2} \kappa_{ij} \eta_j + [\tfrac{1}{2} (\beta_{22} \alpha_2 + \gamma_{22} \alpha_3) \kappa_j^2 / \kappa^{1/2} \\ & + \tfrac{1}{4} (\beta_{22} \beta_2^2 + \gamma_{22} \beta_3^2) (\kappa^{1/2} \kappa_{jk} - \tfrac{1}{2} \kappa_j \kappa_k / \kappa^{1/2}) \eta_j \eta_k] \zeta_i\} \Delta t^{3/2} \\ & + (\alpha_{22} \alpha_1 \kappa_{ij} \kappa_j + \tfrac{1}{2} \beta_1^2 \kappa \kappa_{ijk} \eta_j \eta_k) \Delta t^2 + O(\zeta_i \Delta t^2).\end{aligned} \tag{4.11}$$

We then obtain the results

$$\overline{\xi_i} = (\alpha_{21} + \alpha_{22}) \kappa_i \Delta t + (\alpha_{22} \alpha_1 \kappa_{ij} \kappa_j + \tfrac{1}{2} \kappa \kappa_{ijj} \alpha_{22} \beta_1^2) \Delta t^2 \tag{4.12}$$

$$\begin{aligned}\overline{\xi_i \xi_j} = {} & \kappa (\beta_{21}^2 + (\beta_{22} + \gamma_{22})^2) \delta_{ij} \Delta t + \{(\alpha_{21} + \alpha_{22})^2 \kappa_i \kappa_j + 2 \alpha_{22} \beta_1 \beta_{21} \kappa \kappa_{ij} \\ & + [(\beta_{22} + \gamma_{22}) (\beta_{22} \alpha_2 + \gamma_{22} \alpha_3) + \tfrac{1}{4} (\beta_{22} \beta_2 + \gamma_{22} \beta_3)^2 \\ & - \tfrac{1}{4} (\beta_{22} + \gamma_{22}) (\beta_{22} \beta_2^2 + \gamma_{22} \beta_3^2)] \kappa_l^2 \delta_{ij} \\ & + \tfrac{1}{2} (\beta_{22} + \gamma_{22}) (\beta_{22} \beta_2^2 + \gamma_{22} \beta_3^2) \kappa \kappa_{ll} \delta_{ij}\} \Delta t^2\end{aligned} \tag{4.13}$$

$$\begin{aligned}\overline{\xi_i \xi_j \xi_k} = {} & [(\beta_{21}^2 + (\beta_{22} + \gamma_{22})^2) (\alpha_{21} + \alpha_{22}) + \beta_{21} (\beta_{22} + \gamma_{22}) (\beta_{22} \beta_2 + \gamma_{22} \beta_3)] \\ & \times \kappa (\kappa_i \delta_{jk} + \ldots) \Delta t^2.\end{aligned} \tag{4.14}$$

The remaining equation does not yield new information.

Comparing these results with (4.5)-(4.7) we find

$$\alpha_{21} + \alpha_{22} = 1 \tag{4.15}$$

$$\alpha_{22} \alpha_1 = \tfrac{1}{2} \tag{4.16}$$

$$\alpha_{22} \beta_1^2 = 1 \tag{4.17}$$

$$\alpha_{22} \beta_1 \beta_{21} = 1 \tag{4.18}$$

$$(\beta_{22} + \gamma_{22}) (\beta_{22} \alpha_2 + \gamma_{22} \alpha_3) + \tfrac{1}{4} (\beta_{22} \beta_2 + \gamma_{22} \beta_3)^2 - \tfrac{1}{4} (\beta_{22} + \gamma_{22}) (\beta_{22} \beta_2^2 + \gamma_{22} \beta_3^2) = 1 \tag{4.19}$$

$$\beta_{21}^2 + (\beta_{22} + \gamma_{22})^2 = 2 \tag{4.20}$$

$$(\beta_{22} + \gamma_{22}) (\beta_{22} \beta_2^2 + \gamma_{22} \beta_3^2) = 2 \tag{4.21}$$

$$\beta_{21} (\beta_{22} + \gamma_{22}) (\beta_{22} \beta_2 + \gamma_{22} \beta_3) = 2. \tag{4.22}$$

These equations do not have a unique solution but are satisfied by

$$\begin{array}{lll} \alpha_{22} = 1 & \beta_{22} = \tfrac{1}{2}(\sqrt{2} + 1) & \gamma_{22} = -\tfrac{1}{2}(\sqrt{2} - 1) \\ \alpha_{21} = 0 & \beta_{21} = 1 & \\ \alpha_1 = \tfrac{1}{2} & \beta_1 = 1 & \\ \alpha_2 = \tfrac{1}{2} & \beta_2 = \sqrt{2} & \\ \alpha_3 = \tfrac{1}{2} & \beta_3 = -\sqrt{2}. & \end{array} \tag{4.23}$$

In figure 4 we show the results for the systematic error in various moments, when κ has the form

$$\kappa(x, y) = 4 + \sin x + \sin y \tag{4.24}$$

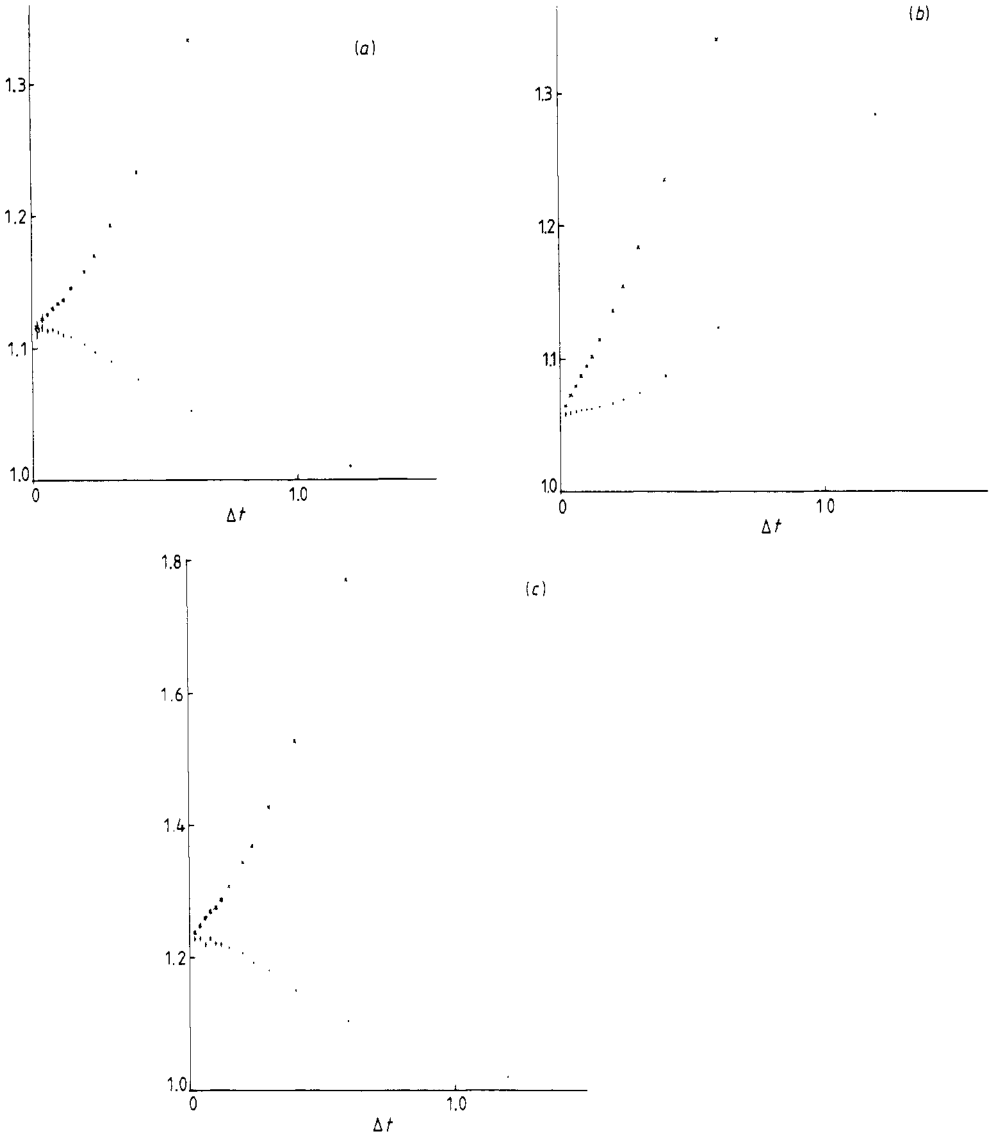


Figure 4. Three moments for the two-dimensional problem for $t = 1.2$ plotted against Δt for $\kappa(x, y)$ given in (4.24) with $x_0 = y_0 = 1$. The graphs are (a) $\langle x \rangle$, (b) $\langle x^2 \rangle$ and (c) $\langle xy \rangle$. The results of the first-order scheme are signified by crosses and those of the second-order scheme by dots.

the initial distribution being $\delta(x-1)\delta(y-1)$. Clearly the first-order algorithm reveals the expected linear dependence on Δt while the error for the second-order algorithm is proportional to Δt^2 at low Δt.

5. Conclusions

We have constructed an effective second-order algorithm for integrating stochastic differential equations with a position-dependent diffusivity. Because of the complexity of its tensor structure the high-dimensional algorithm required three intermediate evaluation points per step as opposed to the two points which were sufficient for the simpler one-dimensional case.

One limitation of our algorithm is that it is confined to cases where the diffusivity is a scalar function. Clearly it is of great interest to extend it to deal with tensor diffusivities. Another limitation is the absence of drift. We suspect that this is the more difficult of the two limitations to overcome. It might be that a three-stage algorithm is required in order to achieve steps correct to $O(\Delta t^2)$ in the presence of drift. In any case it is obviously important to construct higher-order algorithms.

References

Collins R E 1961 *Flow of Fluids Through Porous Materials* (New York: Van Nostrand Reinhold)
Drummond I T, Duane S and Horgan R R 1984 *J. Fluid Mech.* **138** 75
—— 1986 *Stochastic Quantisation and Φ^4-Field Theory. DAMTP preprint*
Drummond I T and Horgan R R 1986 *J. Fluid Mech.* **163** 425
Greensite H S and Helfand E 1981 *Bell Syst. Tech. J.* **60** 1927
Helfand E 1979 *Bell Syst. Tech. J.* **58** 2289
Klauder J R and Petersen W P 1985 *Numerical Integration of Multiplative-Noise Stochastic Differential Equations. AT&T Bell Labs. preprint*
Mil'shtein G N 1974 *Theor. Prob. Appl. SIAM* **19** 557
Scheidegger A E 1974 *The Physics of Flow through Porous Media* (Toronto: University of Toronto Press)