

Numerical Integration of Stochastic Differential Equations

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Several numerical methods for treating stochastic differential equations are considered. Both the convergence in the mean square limit and the convergence of the moments is discussed and the generation of appropriate random numbers is treated. The necessity of simulations at various time steps with an extrapolation to time step zero is emphasized and demonstrated by a simple example.

KEY WORDS: Stochastic differential equations; numerical treatment; order of convergence; generation of random numbers.

1. INTRODUCTION

Dynamical quantities in complex physical systems are often governed by a set of stochastic differential equations,⁽¹⁻⁴⁾ which in the Ito interpretation may be written as

$$\dot{x}^i = f^i(x) + \sigma^{ij}(x) \eta_j(t) \quad (1.1)$$

Here $f^i(x)$ denotes the drift term and $\sigma^{ij}(x)$ the diffusion term, and the white noise $\eta_j(t)$ simulates the influence of the fast variables on the dynamical quantities x^i . According to the white noise properties, we have

$$\langle \eta_i(t) \rangle = 0 \quad (1.2a)$$

$$\langle \eta_i(t) \eta_j(t') \rangle = \delta_{ij} \delta(t - t') \quad (1.2b)$$

and all higher correlation functions are determined by the Gaussian character of the white noise.

Although the numerical integration of deterministic differential equations is a relatively clear and well-known problem, the analogous case for stochastic differential equations is more complicated and therefore has

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often led to some confusion and misunderstanding. There are already several papers in the mathematical literature on the numerical treatment of equations (1.1),⁽⁵⁻¹²⁾ but all of them tell little about realistic experience with the proposed algorithms, so that they are not of great help for the physicist interested in a clear and efficient method. The experience related in this paper has emerged from the study of stochastic equations in an applied physical science, the rheology of polymeric fluids, and the authors hope to have formulated a concise recipe for the physicist who wants to have a tool for treating stochastic equations.

In Section 2 we discuss the expansion of $x^i(t+h)$ in the time step h ; in Section 3 the convergence in the mean square sense and the convergence of the moments are introduced. In Section 4 various methods are studied and in Section 5 the practical calculation is presented with the extrapolation to $h \rightarrow 0$.

2. THE EXPANSION IN THE TIME STEP h

Since for brevity we will discuss only systems where drift and diffusion terms do not explicitly depend on time, we may assume that $x^i(t)$ is known at $t=0$ and that we are interested in $x^i(h)$ for $h>0$. Integration of (1.1) leads to

$$x^i(h) = x^i(0) + \int_0^h ds f^i(x(s)) + \int_0^h ds \sigma^{ij}(x(s)) \eta_j(s) \quad (2.1)$$

We expand drift and diffusion terms in (2.1) about $s=0$ by using (2.1) again, in order to get (with $f_{,k} = \partial f / \partial x_k$)

$$\begin{aligned} x^i(h) &= x^i(0) + \int_0^h ds f^i \left(x^k(0) + \int_0^s du f^k(x(u)) + \int_0^s du \sigma^{kl}(x(u)) \eta_l(u) \right) \\ &\quad + \int_0^h ds \sigma^{ij} \left[x^k(0) + \int_0^s du f^k(x(u)) + \int_0^s du \sigma^{kl}(x(u)) \eta_l(u) \right] \eta_j(s) \\ &= x^i(0) + hf^i(x(0)) + \sigma^{ij}(x(0)) \int_0^h ds \eta_j(s) \\ &\quad + f^i_{,k}(x(0)) \int_0^h ds \left[\int_0^s du f^k(x(u)) + \int_0^s du \sigma^{kl}(x(u)) \eta_l(u) \right] \\ &\quad + \frac{1}{2} f^i_{,kl}(x(0)) \int_0^h ds \left[\int_0^s du \sigma^{km}(x(u)) \eta_m(u) \right] \left[\int_0^s du \sigma^{ln}(x(u)) \eta_n(u) \right] \\ &\quad + \sigma^{ij}_{,k}(x(0)) \int_0^h ds \left[\int_0^s du f^k(x(u)) + \int_0^s du \sigma^{kl}(x(u)) \eta_l(u) \right] \eta_j(s) \\ &\quad + \dots \end{aligned} \quad (2.2)$$

Instead of using (2.1) yet again for expressing $x(u)$, we will approximate it by $x(0)$. Then the following terms involving the noise term $\eta_j(s)$ appear:

$$\begin{aligned} W_i(h) &= \int_0^h ds \eta_i(s) \\ C_{ij}(h) &= \int_0^h ds W_i(s) \eta_j(s) \\ F_i(h) &= \int_0^h ds W_i(s) \\ G_{ij}(h) &= \int_0^h ds W_i(s) W_j(s) \end{aligned} \tag{2.3}$$

The order of the terms in (2.3) can be easily determined by a dimensional argument. The dimension of η is $\text{sec}^{-1/2}$ and therefore we have

$$\begin{aligned} W_j(h) &= O(h^{1/2}), & C_{ij}(h) &= O(h) \\ F_i(h) &= O(h^{3/2}), & G_{ij}(h) &= O(h^2) \end{aligned} \tag{2.4}$$

Furthermore, if x^i is dimensionless, we get

$$[f^i] = \text{sec}^{-1}, \quad [\sigma^{ij}] = \text{sec}^{-1/2} \tag{2.5}$$

With the notation of (2.3) and the abbreviations

$$f^i := f^i(x(0)), \quad \sigma^{ij} := \sigma^{ij}(x(0)) \tag{2.6}$$

we obtain from (2.2) the expansion

$$\begin{aligned} x^i(h) &= x^i(0) + \sigma^{ij} W_j(h) + hf^i + f^i_{,k} \sigma^{kl} F_l(h) \\ &\quad + \frac{1}{2} f^i_{,kl} \sigma^{km} \sigma^{ln} G_{mn}(h) + \frac{1}{2} h^2 f^i_{,k} f^k + O(h^{5/2}) \end{aligned} \tag{2.7a}$$

in the case of additive noise (where derivatives of σ^{ij} are zero) and

$$x^i(h) = x^i(0) + \sigma^{ij} W_j(h) + hf^i + \sigma^{ij}_{,k} \sigma^{kl} C_{lj}(h) + O(h^{3/2}) \tag{2.7b}$$

in the multiplicative case.

Equations (2.7a) and (2.7b) are the basis of all further considerations and we will see that higher expansions in h are not necessary from a practical point of view. Because $W_i(h)$ and $F_i(h)$ are linear functionals of $\eta_i(s)$, they are also Gaussian random numbers. In the following the first and second moments of the quantities in (2.3) are needed. They can easily be calculated; we obtain

$$\begin{aligned}
\langle W_i(h) \rangle &= 0, & \langle W_i(h) W_j(h) \rangle &= h\delta_{ij} \\
\langle C_{ij}(h) \rangle &= 0, & \langle C_{ij}(h) C_{kl}(h) \rangle &= \frac{1}{2}h^2\delta_{ik}\delta_{jl} \\
\langle F_i(h) \rangle &= 0, & \langle F_i(h) F_j(h) \rangle &= \frac{1}{3}h^3\delta_{ij} \\
\langle G_{ij}(h) \rangle &= \frac{1}{2}h^2\delta_{ij}, & \langle G_{ij}(h) G_{kl}(h) \rangle &= O(h^4)
\end{aligned} \tag{2.8}$$

and

$$\begin{aligned}
\langle W_i(h) C_{jk}(h) \rangle &= 0 \\
\langle W_i(h) F_j(h) \rangle &= \frac{1}{2}h^2\delta_{ij}
\end{aligned} \tag{2.9}$$

3. CONVERGENCE IN THE MEAN SQUARE LIMIT AND OF THE MOMENTS

In a numerical method an expansion like (2.7a) or (2.7b) is approximated by a polynomial in $h^{1/2}$. For a deterministic differential equation the order of this polynomial can be chosen as high as one likes in order to obtain a corresponding accuracy within one time step. In the expansions (2.7a) and (2.7b) for stochastic differential equations, however, there appear nonlinear functionals (e.g., C_{ij} and G_{ij}) of the white noise. The simulation of these quantities is not known or may be prohibitively expensive. Therefore the aim cannot be to invent a method that is very accurate for one time step. Confined to algorithms of relatively low order, one will be forced to calculate the quantities of interest for various time steps and then extrapolate to time step zero. With this in mind one should find the algorithm that is simplest for calculating the quantities for finite time steps and for the extrapolation as well.

The convergence in the mean square limit will be measured by the behavior of

$$R(h) = \langle [x^i(h) - \bar{x}^i(h)]^2 \rangle \tag{3.1}$$

for $h \rightarrow 0$, where $\bar{x}^i(h)$ is an approximation of the full expansion (2.7a) or (2.7b) by a numerical algorithm. If $R(h) \rightarrow 0$ holds for $h \rightarrow 0$, then one calls such a method "convergent in the mean square limit."⁽¹³⁾ The quality of the convergence in the mean square limit plays a major role in problems where one has to look at the trajectory itself; for example, the simulation of the mean first passage time, the distribution of extrema, and also if the system (1.1) is confined by reflecting barriers.

This convergence in the mean square limit has to be distinguished from the convergence for the moments. If one writes

$$x^i(h) = D^i(h) + S^i(h) \tag{3.2}$$

where $D^i(h)$ contains the deterministic terms of the right-hand side of (2.7a) or (2.7b) and $S^i(h)$ the stochastic ones, then one gets

$$\begin{aligned} \langle [x^i(h)]^n \rangle &= \langle [D^i(h) + S^i(h)]^n \rangle = [D^i(h)]^n + n[D^i(h)]^{n-1} \langle S^i(h) \rangle \\ &+ \binom{n}{2} [D^i(h)]^{n-2} \langle [S^i(h)]^2 \rangle + \dots \end{aligned} \quad (3.3)$$

With

$$\begin{aligned} S^i(h) &= \sigma^{ij} W_j(h) + \sigma^{ij}{}_{,k} \sigma^{kl} C_{lj}(h) + f^i{}_{,k} \sigma^{kl} F_l(h) \\ &+ \frac{1}{2} f^i{}_{,kl} \sigma^{km} \sigma^{lm} G_{mn}(h) \end{aligned} \quad (3.4)$$

one obtains with (2.8) and (2.9)

$$\begin{aligned} \langle S^i(h) \rangle &= \frac{1}{4} h^2 f^i{}_{,kl} \sigma^{km} \sigma^{lm} + O(h^3, h^2) \\ \langle S^i(h) S^j(h) \rangle &= h \sigma^{ik} \sigma^{jk} + \frac{1}{2} h^2 \sigma^{ik} \sigma^{lk} f^j{}_{,l} \\ &+ \frac{1}{2} h^2 \sigma^{jk} \sigma^{lk} f^i{}_{,l} + O(h^3, h^2) \\ \langle S^i(h) S^j(h) S^k(h) \rangle &= O(h^3, h^2) \\ \langle [S^i(h)]^4 \rangle &= 3h^2 (\sigma^{ij})^4 + O(h^3, h^2) \\ \langle [S^i(h)]^5 \rangle &= O(h^3, h^2) \end{aligned} \quad (3.5)$$

where we have neglected all terms $O(h^3)$ in the additive case and $O(h^2)$ in the multiplicative case and $(\sigma^{ij})^4$ stands for a specific product of four σ^{ij} . The $D^i(h)$ always contains a term $O(h^0)$. An algorithm with

$$\bar{x}^i(h) = \bar{D}^i(h) + \bar{S}^i(h) \quad (3.6)$$

leads to

$$\begin{aligned} \langle [\bar{x}^i(h)]^n \rangle &= \langle [\bar{D}^i(h) + \bar{S}^i(h)]^n \rangle = [\bar{D}^i(h)]^n + n[\bar{D}^i(h)]^{n-1} \langle \bar{S}^i(h) \rangle \\ &+ \binom{n}{2} [\bar{D}^i(h)]^{n-2} \langle [\bar{S}^i(h)]^2 \rangle + \dots \end{aligned} \quad (3.7)$$

If the expansions (3.3) and (3.7) coincide up to terms h^2 , $D^i(h)$ and $\bar{D}^i(h)$ should as well, and $\langle [\bar{S}^i(h)]^n \rangle$ ($n = 1, 2, \dots$) should give rise to the same terms up to order h^2 as written in (3.5).

If all moments are approximated with a specific order of convergence, this is also true for every expectation value $m = \langle g(x^i) \rangle$ of a function of the process.

4. THE VARIOUS METHODS

In this section the simplest methods are discussed. Their convergence in the mean square limit and of the moments is determined. The optimal strategy for generating suitable random numbers is also given.

4.1. The Euler Method

The Euler method is defined by

$$\bar{x}^i(h) = x^i(0) + f^i(x(0))h + \sigma^{ij}(x(0)) W_j(h) \quad (4.1a)$$

i.e.,

$$D^i(h) = x^i(0) + f^i h, \quad S^i(h) = \sigma^{ij} W_j(h) \quad (4.1b)$$

One immediately concludes from (2.7a), (2.8), and (4.1a) that

$$R(h) = \langle [x^i(h) - \bar{x}^i(h)]^2 \rangle = O(h^3) \quad (4.2)$$

in the additive noise case, but

$$R(h) = O(h^2) \quad (4.3)$$

for multiplicative noise, because now the term with the functional $C_j(h)$ has to be taken into account. The integration over a finite time interval $(0, t_1)$ yields a total error $R(t) = O(h^2)$ for additive noise and $R(t) = O(h)$ for multiplicative noise.⁽¹¹⁾

For the moments we obtain

$$\langle [\bar{x}^i(h)]^n \rangle = \langle [x^i(h)]^n \rangle + O(h^2) \quad (4.4)$$

because the only term of order h in $\langle [S^i(h)]^n \rangle$ ($n = 1, 2, \dots$), namely the term in $\langle S^i(h) S^j(h) \rangle$,

$$\begin{aligned} \langle S^i(h) S^j(h) \rangle &= \langle [\sigma^{ik} W_k(h) + \dots][\sigma^{jl} W_l(h) + \dots] \rangle \\ &= \sigma^{ik} \sigma^{jk} h \end{aligned} \quad (4.5)$$

is reproduced by $\bar{S}^i(h)$.

An integration over a finite time interval $(0, t_1)$ will involve N time steps, where $N \sim 1/h$. Hence, the error accumulated during the time interval is one order less than the one-time-step error. In conclusion, for the Euler method the convergence of the moments for a finite time interval $(0, t_1)$ is

of the order h , and this is true for the additive case and for the multiplicative case as well.

All of the methods introduced in this section need random numbers that are functionals of the Wiener process, especially $W_i(h)$. The correct numerical simulation of $W_i(h)$ could be done by taking uncorrelated, Gaussian-distributed random numbers with variance h . Such a method is, for example, the Box–Muller algorithm,⁽¹⁴⁾ but this one needs for every two random numbers a logarithm and a square root. However, one can immediately see from (4.5) that when treating moments with the Euler algorithm it is sufficient to take an arbitrary random variable $\tilde{W}_i(h)$ where only the first three moments are correct

$$\begin{aligned} \langle \tilde{W}_i(h) \rangle &= 0 \\ \langle \tilde{W}_i(h) \tilde{W}_j(h) \rangle &= \delta_{ij} h \\ \langle \tilde{W}_i(h) \tilde{W}_j(h) \tilde{W}_k(h) \rangle &= 0 \end{aligned} \tag{4.6}$$

without getting a worse order of convergence. Taking random numbers R that are uniformly distributed on the interval $(0, 1)$ (which are normally produced by a random number generator implemented on a computer), one can get such simple random numbers $\tilde{W}_i(h)$ through

$$\tilde{W}_i(h) = (12h)^{1/2}(R - 0.5) \tag{4.7}$$

In comparison with taking Gaussian random numbers, this saves a great deal of computing time, although this has no influence on the order of convergence.

4.2. The Milshtein Method^(6,7)

To get a $O(h^3)$ convergence of $R(h)$ in the multiplicative case one has to simulate $C_{ij}(h)$ correctly. In the univariate case the functional $C(h)$ can be calculated immediately in order to get

$$C(h) = \int_0^h ds W(s) \eta(s) = \frac{1}{2} [W^2(h) - h] \tag{4.8}$$

Therefore the Milshtein method can be formulated (unfortunately in the univariate case only)

$$\begin{aligned} \bar{x}(h) &= x(0) + f(x(0))h - \frac{1}{2}\sigma'(x(0))\sigma(x(0))h \\ &+ \sigma(x(0))W(h) + \frac{1}{2}\sigma'(x(0))\sigma(x(0))W^2(h) \end{aligned} \tag{4.9}$$

Obviously we now have in the multiplicative case as well

$$R(h) = \langle [x(h) - \bar{x}(h)]^2 \rangle = O(h^3) \quad (4.10)$$

but the same convergence of the moments as for the Euler method in (4.4). This method is often used in the literature^(4,15) as a higher order method, but this is only true for the convergence in the mean square limit.

4.3. The Heun Method

We want to discuss the Heun method only explicitly for the case of additive noise. This method is defined as

$$\bar{x}^i(h) = x^i(0) + \frac{1}{2}[f^i(x(0)) + f^i(\xi(h))]h + \sigma^{ij}W_j(h) \quad (4.11a)$$

with

$$\xi^i(h) = x^i(0) + f^i(x(0))h + \sigma^{ij}W_j(h) \quad (4.11b)$$

Expanding the term $f^i(\xi(h))$, one gets

$$\begin{aligned} \bar{x}^i(h) &= x^i(0) + f^i h + \sigma^{ij}W_j(h) + \frac{1}{2}f^i_{,k} h[f^k h + \sigma^{kl}W_l(h)] \\ &\quad + \frac{1}{4}f^i_{,kl} h[f^k h + \sigma^{km}W_m(h)][f^l h + \sigma^{ln}W_n(h)] \\ &= x^i(0) + f^i h + \sigma^{ij}W_j(h) + \frac{1}{2}hf^i_{,k} \sigma^{kl}W_l(h) \\ &\quad + \frac{1}{2}h^2 f^i_{,k} f^k + \frac{1}{4}hf^i_{,kl} \sigma^{km} \sigma^{ln} W_m(h) W_n(h) + O(h^{5/2}) \end{aligned} \quad (4.12)$$

This is exactly formula (2.7a), where the terms $F_i(h)$ and $G_{mn}(h)$ are replaced by simpler (local) expressions in $W(h)$ with the same first moment, namely

$$\begin{aligned} F_i(h) &\text{ by } \tilde{F}_i(h) = \frac{1}{2}W_i(h)h \\ G_{mn}(h) &\text{ by } \tilde{G}_{mn}(h) = \frac{1}{2}hW_m(h)W_n(h) \end{aligned} \quad (4.13)$$

But the higher moments are not equal,

$$\langle \tilde{F}_i(h) \tilde{F}_j(h) \rangle = \langle \tilde{F}_i(h) F_j(h) \rangle = \frac{1}{4}h^3 \delta_{ij} \quad [\neq \langle F_i(h) F_j(h) \rangle] \quad (4.14)$$

However,

$$\langle W_i(h) \tilde{F}_j(h) \rangle = \langle W_i(h) F_j(h) \rangle = \frac{1}{2}h^2 \delta_{ij} \quad (4.15)$$

Hence we have

$$\begin{aligned} R(h) &= \langle \{ \sigma^{kl} f^i_{,k} (F_l(h) - \tilde{F}_l(h)) \\ &\quad + \frac{1}{2} \sigma^{km} \sigma^{ln} [G_{mn}(h) - \tilde{G}_{mn}(h)] \}^2 \rangle + O(h^4) \\ &= O(h^3) \end{aligned} \quad (4.16)$$

Therefore, the convergence in the mean square sense is of the same order as in the Euler method. But looking at the convergence of the moments, we now obtain

$$\begin{aligned} \bar{D}^i(h) &= x^i(0) + f^i h + \frac{1}{2} h^2 f^i_{,k} f^k \\ \bar{S}^i(h) &= \sigma^{ij} W_j(h) + f^i_{,k} \sigma^{kl} \tilde{F}_l(h) + \frac{1}{2} f^i_{,kl} \sigma^{km} \sigma^{ln} \tilde{G}_{mn}(h) \end{aligned} \tag{4.17}$$

and therefore

$$\begin{aligned} \langle \bar{S}^i(h) \rangle &= \frac{1}{4} h^2 f^i_{,kl} \sigma^{km} \sigma^{ln} + O(h^3) \\ \langle \bar{S}^i(h) \bar{S}^j(h) \rangle &= h \sigma^{ik} \sigma^{jk} + \frac{1}{2} h^2 \sigma^{ik} \sigma^{lk} f^j_{,l} \\ &\quad + \frac{1}{2} h^2 \sigma^{jk} \sigma^{lk} f^i_{,l} + O(h^3) \\ \langle \bar{S}^i(h) \bar{S}^j(h) \bar{S}^k(h) \rangle &= O(h^3) \\ \langle [\bar{S}^i(h)]^4 \rangle &= 3h^2 (\sigma^{ij})^4 + O(h^3) \end{aligned} \tag{4.18}$$

which are equal up to the order h^2 with the moments $\langle [S^i(h)]^n \rangle$ ($n=1, \dots, 4$). Since also $\bar{D}^i(h)$ coincides with $D^i(h)$ up to the order h^2 , the Heun method converges as

$$\langle [x^i(h)]^n \rangle - \langle [\bar{x}^i(h)]^n \rangle = O(h^3) \tag{4.19a}$$

and for a finite time step

$$\langle [x^i(t)]^n \rangle - \langle [\bar{x}^i(t)]^n \rangle = O(h^2) \tag{4.19b}$$

To obtain (4.18), we have used that also the fourth and fifth moments of $W_i(h)$ are Gaussian

$$\langle [W_i(h)]^4 \rangle = 3h^2, \quad \langle [W_i(h)]^5 \rangle = 0 \tag{4.20}$$

This cannot only be achieved by true Gaussian random numbers, but for example also by

$$\tilde{W}_i(h) = \begin{cases} -(3h)^{1/2} & \text{if } R < 1/6 \\ 0 & \text{if } 1/6 \leq R < 5/6 \\ +(3h)^{1/2} & \text{if } 5/6 \leq R \end{cases} \tag{4.21}$$

where R is a uniformly distributed random number on the interval $(0, 1)$.

In the multiplicative case the Heun method only has the same order of convergence in the mean square limit and of the moments as the simpler Euler method.

4.4. Other Methods

The Euler and Heun methods are in the deterministic case the lowest versions of the more general Runge-Kutta algorithms. However, taking a higher order Runge-Kutta scheme and simply adding a Gaussian random number does not lead to any reasonable stochastic algorithm, because this does not take care of the functionals C_{ij} , F_i, \dots . Therefore, one gets only the convergence already achieved by the Euler and Heun methods.

No method has in the multivariate and multiplicative case an error in the *mean square limit* as $R(t) = O(h^2)$, because it is not possible to simulate the functional $C_{ij}(h)$ correctly in this case. One possibility to improve the convergence behavior is to take weakly colored noise instead of white noise and then extrapolate to the white noise case. This can be done, e.g., by

$$\dot{x}^i = f^i(x) + \sigma^{ij}(x) z_j(t) \quad (4.22a)$$

where $z_j(t)$ is some colored noise from an Ornstein–Uhlenbeck process

$$\dot{z}_j(t) = (1/\tau)[-z_j(t) + \eta_j(t)] \quad (4.22b)$$

Equations (4.22a) and (4.22b) together are a $2N$ -dimensional stochastic differential equation with additive noise. This one can be treated with one of the above methods (preferably the Euler method), having now also a convergence in the mean square limit as $R(t) = O(h^2)$. This phenomena was already observed by Fox *et al.*⁽⁴⁾ (see their Figs. 13 and 15). One should note that the stochastic differential equation (4.22b) converges in the limit of white noise ($\tau \rightarrow 0$) to its Stratonovich interpretation, which can, however, easily be transferred into the Ito form.

For the other situations (additive or univariate multiplicative noise) there are also no methods with a better order of convergence in the mean square limit than the one obtained already by the methods introduced above (except in some very special cases) because of the nonlinear functionals $F_i(h)$, $G_{ij}(h), \dots$, which also cannot be numerically simulated.⁽¹¹⁾

The limits for the convergence of the *moments* are not so strict, because one needs only some properties about the moments of the functionals $C_{ij}(h)$, $G_{ij}(h), \dots$; it may be possible to formulate higher order methods. An example of such an algorithm was introduced by Klauder and Petersen,⁽¹²⁾ but this rather complicated method converges better only for the first two moments in the multiplicative case. However, we suppose that the expense in taking a higher order algorithm is not worthwhile, especially if one keeps in mind that one always gets a statistical error from the finite number of realizations and one has to extrapolate to $h \rightarrow 0$ anyhow. If one is only interested in moments of the process, it is not necessary to use colored noise.

5. PRACTICAL CONSEQUENCES

5.1. Discussing of the Errors

Treating stochastic differential equations by numerical methods, one will have two major contributions to the error, namely a statistical one due to the finite number of realizations and another one from the time discretization. The statistical error can be estimated as follows: Let N be the number of realizations and $M^{(i)}$ the result of the i th simulation. Then the average over all realizations,

$$m = \frac{1}{N} \sum_{i=1}^N M^{(i)} \quad (5.1)$$

is an estimation for the desired result. But m as well as $M^{(i)}$ are stochastic variables with a specific distribution. As is well known, the n th cumulants of the m -distribution and the M -distribution are related by

$$\kappa_n(m) = \frac{1}{N^{n-1}} \kappa_n(M) \quad (5.2)$$

The moments

$$\langle M^k \rangle = \frac{1}{N} \sum_{i=1}^N (M^{(i)})^k \quad (5.3)$$

we need for calculating these can easily be calculated at the same time with $m = \langle M \rangle$. In most cases the higher cumulants $\kappa_n(m)$ ($n > 2$) will come out to be very small because of the factors N in the denominator in (5.2), and the m -distribution is Gaussian to a very good approximation. We therefore need to specify it only by its width $\kappa_2(m)$, and denoting the interval

$$(m - [\kappa_2(m)]^{1/2}, m + [\kappa_2(m)]^{1/2}) \quad (5.4)$$

as the result of the simulation, meaning that the exact value lies with probability 0.68 within this range.

The error due to the time discretization cannot be estimated by one simulation alone. One has to make simulations at different time steps in order to get an idea about this error. Since one knows from the above calculations the order of the convergence of the method chosen, one is able to fit an appropriate curve through the simulation results for the different time steps and to extrapolate to $h=0$. The benefit of this procedure is mostly that one can control and nearly eliminate the error occurring from the time discretization. Furthermore, one may choose greater time steps.

Our experience shows that one can save a factor 2–5 of computing time, while obtaining a more reliable result than by simulating only once with a smaller time step and taking this result as the final one.

Summarizing, the following numerical strategy will be the most efficient one: Choosing a method with a known convergence behavior, one performs simulations with different (not too small) time steps h . Then one fits a polynomial of appropriate order to the results, which is a well known procedure.⁽¹⁶⁾ For the above methods this polynomial is of the form

$$f(h) = a_0 + a_1 h \quad (5.5a)$$

or

$$f(h) = a_0 + a_2 h^2 \quad (5.5b)$$

If some time steps are too great, only a relatively bad fit through the points with error bars is possible. Then the results for the greater time steps should be discarded in order to get a better fit.

The value of a_0 and its error may be declared as the result extrapolated to time step $h = 0$.

5.2. An Example

The strategy presented in the previous section will now be demonstrated with a simple example, the stochastic Ginzburg–Landau equation

$$\begin{aligned} \dot{x} &= \alpha x - x^3 + \sigma x \eta(t) && \text{(Stratonovich interpretation)} \\ \dot{x} &= (\alpha + \frac{1}{2}\sigma^2)x - x^3 + \sigma x \eta(t) && \text{(Ito interpretation)} \end{aligned} \quad (5.6)$$

with a parameter α .⁽¹⁵⁾

The aim of our simulation was the determination of the second moment at $t = 5$ when starting at $x(0) = 1$ with the parameters $\alpha = \sigma = 2$. The simulation was done with $N = 100,000$ realizations and different time steps. We used the Euler method, the Milshtein method, the Heun method (though not discussed for the multiplicative case), and the method proposed by Klauder and Petersen.⁽¹²⁾ The latter has difficulties arising from the natural boundary of the system at $x = 0$ and did not yield any useful result. The results of the other three methods are shown in Fig. 1. One clearly sees the linear order of convergence of all three methods and one also observes that the results at the smallest time step ($h = 0.01$) are still four to eight standard deviations from the exact value. Therefore a

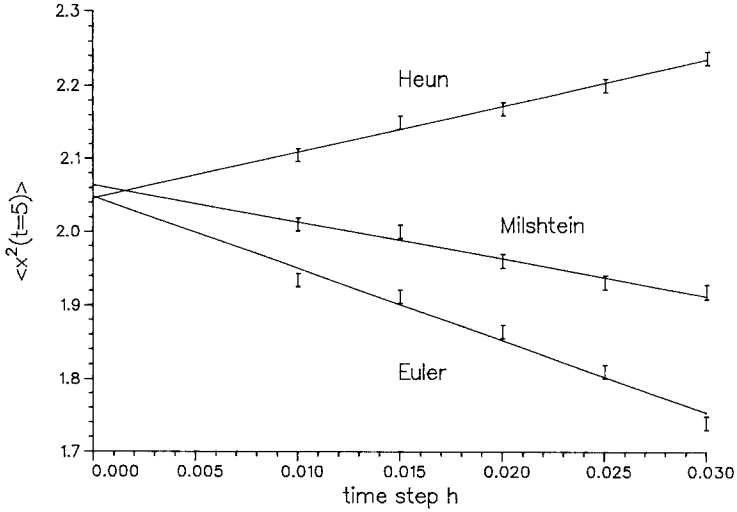


Fig. 1. The numerical simulation of the stochastic Ginzburg–Landau equation obtained from $N = 100,000$ realizations with the Euler, Milshtein, and Heun methods.

linear extrapolation is necessary. With such an extrapolation we get the following results:

	$\langle x^2(t=5) \rangle$	
Euler method	2.048 ± 0.012	
Milshtein method	2.064 ± 0.013	(5.7)
Heun method	2.046 ± 0.012	

All three results are compatible. We can also conclude from our results that the second moment at $t = 5$ is significantly above the stationary value, which is

$$\langle x^2 \rangle_{\text{stat}} = \alpha = 2 \tag{5.8}$$

For this example the Euler method is the appropriate one because the other methods need more computing time and do not yield any better result.

An example where the convergence of the trajectories (convergence in the mean square limit) is the major problem occurs when treating mean first passage time problems numerically. With normal methods one gets only a convergence as $O(h^{1/2})$. This is treated in a forthcoming article,⁽¹⁷⁾ where it is also shown how to overcome this bad order of convergence.

6. CONCLUSIONS

The considerations of this paper show that stochastic differential equations need a more sophisticated numerical treatment than do deterministic ones. But by taking the proposed strategy, one is able to get satisfactory results in moderate computing time. The main requirement is that one knows the convergence order of the chosen method and uses this to extrapolate to $h = 0$, eliminating the error due to the time discretization.

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