A Gentle Introduction to the Integration of Stochastic Differential Equations

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Abstract. A gentle introduction to the simulation of stochastic differential equations is presented, with particular attention to the simulation of rare fluctuations, a topic of interest in the light of recent theoretical work on optimal paths. The "best algorithm" and some problems connected to the treatment of the boundaries will be discussed.

1 Introduction

A common denominator of the papers contained in this book is the presence of stochastic processes, introduced to model a variety of different physical situations. Unfortunately, the most common situation is that the stochastic model cannot be exactly solved: then, one typically turns to simulations, analogue or digital, of the system of interest. A very complete review of analogue techniques has recently appeared, and the interested reader is referred to it for further details [1]. We concentrate here on digital simulations, with particular emphasis on simulations of rare fluctuations. Rare fluctuations are fluctuations which bring the stochastic system very far from the phase space which the system explores most of the time. It is possible to relate the happening of a rare fluctuation to some building up of an activation energy (one can think of the energy necessary to overcome a potential barrier, like in a chemical reaction). The nature of rare fluctuations is such that we should have algorithms which correctly explore the tails of the distribution functions; we should be able to stop in a correct way our simulation when the rare fluctuation hits a prescribed boundary in phase space; we should optimise, if possible, our algorithms to situations when the system lacks detailed balance; and, finally, we should have pseudo random number generators fast and very reliable, able to provide us with very long random sequences. We will address all these problems in this paper. For further comments and references, the interested reader can consult, among others, [2–5].

2 The Basic Algorithm

A stochastic differential equation has the generic form

$$\dot{x}_i = f_i(x) + g_i(x)\xi(t), \quad \langle \xi(t) \rangle = 0, \quad \langle \xi(t)\xi(s) \rangle = \delta(t-s),$$

(1)
where we assume that the stochastic process $\xi$ is Gaussian and that only one stochastic forcing is present. In the following, we call $h$ the integration time step, and we use Stratonovich calculus [4]. A simple minded approach to solve Eq. 1 is to formally integrate it, then to use a Taylor expansion around the point $t = 0$, to find recursively the various contributions [6]. Restricting the discussion to a one dimensional case, the equation has the form

$$\dot{x} = f(x) + g(x)\xi(t)$$  \hspace{1cm} (2)

A formal integration yields

$$x(h) - x(0) = \int_0^h (f(x(t)) + g(x(t))\xi(t)) \, dt$$  \hspace{1cm} (3)

Let us define

$$f_0 \equiv f(x(0)) \quad g'_0 \equiv \frac{\partial g(x(t))}{\partial x(t)} \bigg|_{x=x(0)}$$

and so on. By Taylor expansion it is meant that the functions are expanded as $f_t = f_0 + (x(t) - x(0))f'_0 + \ldots$. The simple minded lowest order in $h$ seems to be

$$x(h) - x(0) = \int_0^h (f_0 + g_0\xi(t)) \, dt = hf_0 + g_0\int_0^h \xi(t) \, dt.$$  \hspace{1cm} (4)

We will see that this is not the correct lowest order in $h$. For the moment, note that on the r.h.s. there is a so called “stochastic integral”

$$Z_1(h) \equiv \int_0^h \xi(t) \, dt$$  \hspace{1cm} (5)

which is the integral over the time range $(0, h)$ of the stochastic process $\xi(t)$. This integral is a stochastic variable, and the integration amounts at adding up some gaussian variables: as such, $Z_1(h)$ is itself a Gaussian variable, or, in other words, its probability distribution is a Gaussian distribution. This implies that the probability distribution of $Z_1(h)$ is determined once the average and the standard deviation of the distribution are known. A simple minded numerical integrator would then be, at each time step: generate a random gaussian variable, with appropriate average and standard deviation (to “simulate” the stochastic integral); substitute the stochastic integral on the r.h.s. of Eq. 4 with this random variable; integrate the equation using any standard integrator valid for deterministic differential equations. How can we work out the statistical properties of $Z_1(h)$? As we mentioned, we only need its average and its standard deviation. Using $\langle \ldots \rangle$ to indicate statistical averages,

$$\langle Z_1 \rangle = \int_0^h \langle \xi(s) \rangle ds = 0$$  \hspace{1cm} (6)

$$\langle Z_1^2(h) \rangle = \int_0^h \int_0^h \langle \xi(s)\xi(t) \rangle dsdt = \int_0^h \int_0^h \delta(t-s)dsdt = \int_0^h ds = h.$$  \hspace{1cm} (7)