ESAM 346
Modeling and Computation in Science and Engineering

Winter 2005

Hermann Riecke

Problem Set 4

February 27, 2005 Due Friday, March 4, 2005

In this homework you develop two codes for stochastic differential equations, study their behavior and apply them to a quite abstract model of an activated reaction. You will have to average over a reasonable number of realizations of the noise, which may take a while. You may therefore want to alot more time for the computation for this homework than in previous assignments.

Consider the scalar stochastic differential equation

$$dy = F(y)\,dt + g(y)\,dW \tag{1}$$

where dW is the increment of the Wiener process.

1. Write a code that gives a *strong* approximation to (1) using the

   (a) forward Euler scheme

   (b) forward Milstein scheme.

   For each scheme measure for a given realization $W(t)$ of the Wiener process the final value $y(t_{max})$ and the time-averaged values

   $$\bar{y} \equiv \frac{1}{t_{max}} \int_0^{t_{max}} y(t)\,dt$$

   and

   $$\bar{y^2} \equiv \frac{1}{t_{max}} \int_0^{t_{max}} y(t)^2\,dt$$

   of the position and the square of the position[1]. For the convergence tests measure the error in the strong sense of $y(t_{max})$ in terms of the change of $y(t_{max})$ when Δt is changed by a factor of 2,

   $$E_s\left(y(t_{max});\Delta t)\right) = \langle \Big| y_{\Delta t}(t_{max}) - y_{\Delta t/2}(t_{max}) \Big| \rangle_W \tag{2}$$

   where $\langle ... \rangle_W$ denotes the average over different realizations of the Wiener process. Note that for this error the realizations of the Wiener process have to be the same for $y_{\Delta t}(t_{max})$ and for $y_{\Delta t/2}(t_{max})$. For the quantities $\bar{y}$ and $\bar{y^2}$ measure the error in the weak sense,

   $$E_w\left(\bar{y};\Delta t\right) = \Big| \langle \bar{y}_{\Delta t} \rangle_W - \langle \bar{y}_{\Delta t/2} \rangle_W \Big| \tag{3}$$

   The increments ΔW are drawn from a Gaussian distribution with variance Δt.

2. Use your two codes to test the convergence of these two schemes as Δt is decreased. Do this for two choices of F and g:

[1] The time-averaged values are simply the mean of the vectors y_i and y_i^2, respectively.

(a)

$$F(y) \quad = \quad -2Ay + B \qquad g(y) = 1$$

with $t_{max} = 10$, $A = 5$, $B = 0.1$ and initial condition $y(0) = 0.02$. Vary the number of time steps from 2^6 to 2^{13} by factors of 2. When varying Δt do not forget to adapt the realization of the Wiener process to the time step to make sure that you are implementing the same realization at a different temporal resolution. Thus, generate first a realization corresponding to the smallest Δt and when you *increase* Δt add the appropriate increments of the realization to obtain the realization at the coarser temporal grid.
Show in a log-log plot the error for $y(t_{max})$ in the strong approximation as defined in (2) and the error for $\bar{y}$ and for $\bar{y^2}$ in the weak approximation as defined in (3) as a function of Δt. In order to get meaningful results for the slope in those plots you may have to take $M = 100$ or larger (you will notice that $\bar{y}$ gives the largest scatter and you may not be able to get good results for its convergence).
How do the convergence rates for the three quantities compare with the results expected based on the theoretical truncation error of the scheme? Do the convergence rates obtained with the Milstein scheme differ from those obtained with the Euler scheme?

(b) For

$$F(y) = -2Ay + B \qquad g(y) = y$$

follow the same procedure with the same values of the parameters as in part 2a. How do the convergence rates compare with the theoretical predictions and with the results from part 2a? Do the convergence rates obtained with the Milstein scheme differ from those obtained with the Euler scheme?

3. Now consider a particle in a double-minimum potential

$$V(y) = A(y-1)^2(y+1)^2 - By$$

which results in the force

$$F(y) \quad = \quad -\frac{dV}{dy} = -2A\left((y-1)(y+1)^2 + (y-1)^2(y+1)\right) + B$$

on the particle. Here $A = 2$ and $g(y) = 1$. As initial condition for all runs take $y(0) = 0$. Depending on the external field B the minimum at $y = 1$ or the minimum at $y = -1$ has lower potential energy V. The position y could be considered as an abstract model characterizing the state of an activated chemical reaction

$$C + D \longleftrightarrow CD$$

with the two minima corresponding to the states $C + D$ and CD, respectively. Depending on the parameter B, which in the particle picture corresponds to an external field, one or the other of the two states has lower energy. For the probability to find the system in a state with energy E one expects for a thermal system a Boltzmann distribution

$$P(E) \propto e^{-\frac{E}{k_B T}}, \tag{4}$$

where T is the temperature and k_B the Boltzmann constant.
Run your code to $t_{max} = 500$ with $\Delta t = 0.025$. To test the expectation (4) vary B from $B = -1$ to $B = +1$ in 5 steps and measure the number N^+ of realizations for which $y(t_{max}) > 0$ and the number N^- for which $y(t_{max}) < 0$. Plot $\ln(N^+/N^-)$ as a function

of the difference ΔE between the energies corresponding to the two minima of the potential[2]. Do you get a linear dependence on B? How is the slope of the line related to the temperature in this model system?

[2]Thus, you assume that the particle is almost all of the time in one of the two minima and you take $V(\pm 1)$ rather than $V(y(t_{max}))$ as the energy of the particle.