CERTAIN PROBLEMS WITH THE APPLICATION OF STOCHASTIC DIFFUSION PROCESSES FOR THE DESCRIPTION OF CHEMICAL ENGINEERING PHENOMENA. NUMERICAL SIMULATION OF ONE-DIMENSIONAL DIFFUSION PROCESS

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Some problems are analyzed arising when a numerical simulation of a random motion of a large ensemble of diffusing particles is used to approximate the solution of a one-dimensional diffusion equation. The particle motion is described by means of a stochastic differential equation. The problems emerging especially when the diffusion coefficient is a function of spatial coordinate are discussed. The possibility of simulation of various kinds of stochastic integral is demonstrated. It is shown that the application of standard numerical procedures commonly adopted for ordinary differential equations may lead to erroneous results when used for solution of stochastic differential equations. General conclusions are verified by numerical solution of three stochastic differential equations with different forms of the diffusion coefficient.
Key words: Stochastic modelling; Diffusion process; Stochastic differential equation.

Mass or heat transfer within a flowing liquid is commonly described by means of partial differential equations of parabolic type written, e.g., in the form

$$\frac{\partial b}{\partial t} + \nabla \bullet (\boldsymbol{v} b) - D \, \nabla \bullet \nabla \, b = 0 \quad , \tag{1}$$

where b denotes the transferred quantity (e.g., mass of a component or enthalpy), $\boldsymbol{v}$ is the liquid velocity vector and D denotes the intensity of relative motion (diffusion) of the transferred quantity within the moving liquid. Coefficient D in Eq. (*1*) is considered to be a constant scalar quantity. A source of the transferred quantity is not considered in Eq. (*1*).

Equations formally identical to Eq. (*1*) are commonly adopted in the theory of stochastic processes for the description of evolution of a so-called transitive probability density function $f(\boldsymbol{x};t|\,\boldsymbol{y};t_0)$ of spatially three-dimensional stochastic process $\boldsymbol{X}(t)$:

$$f(\boldsymbol{x};t|\,\boldsymbol{y};t_0) = \frac{\partial^3}{\partial x_1 \partial x_2 \partial x_3} P\,\{X_1 \leq x_1;\, X_2 \leq x_2;\, X_3 \leq x_3|\, \boldsymbol{X}(t_0) = \boldsymbol{y}\,\}\ , \qquad (2)$$

where $t > t_0$ and $X_i \equiv X_i(t)$, (i = 1, 2, 3).

The process $\boldsymbol{X}(t)$ can be considered, e.g., as a radius-vector describing stochastic trajectory of a diffusing molecule. This analogy was analyzed in recent paper[1] including the possibility that the diffusion coefficient can be treated as the second-order tensor with coordinates varying both in space and time.

If the transitive probability density function $f(\boldsymbol{x};t|\,\boldsymbol{y};t_0)$ of the stochastic process $\boldsymbol{X}(t)$ is a solution of Eq. (*1*), then it can be proved[2,3] that the process $\boldsymbol{X}(t)$ is generated by the following stochastic differential equation

$$\mathrm{d}\boldsymbol{X}(t) = \boldsymbol{v}\,\mathrm{d}t + \sqrt{2D}\,\mathrm{d}\boldsymbol{W}(t)\ . \qquad (3)$$

Symbol $\boldsymbol{W}(t)$ denotes the three-dimensional Wiener process. The individual coordinates of the process $\boldsymbol{W}(t)$ can be formally considered as integrals of the white-noise process[2,3]. The second term on the right-hand side of Eq. (*3*) therefore describes the effects of random factors acting on the diffusing molecule. The first term on the right-hand side expresses the dynamics of the deterministic part (i.e. the mean value) of process $\boldsymbol{X}(t)$. Coefficient $\boldsymbol{v}$ in Eq. (*3*) is commonly called the drift coefficient. It can be a deterministic function of the process $\boldsymbol{X}(t)$ and also explicit function of time.

The integration of the second term on the right-hand side of Eq. (*3*) becomes problematic when diffusion coefficient D is a function of $\boldsymbol{X}(t)$ or even of $\boldsymbol{W}(t)$. Two distinct definitions of the so-called stochastic integral of diffusion term $\sqrt{2D}\,\mathrm{d}\boldsymbol{W}(t)$ in Eq. (*3*) are reported in literature[2,3]: the Ito stochastic integral and the Stratonovich one. These two definitions yield different forms of the diffusion equation (Eq. (*1*)) when diffusion coefficient D is a function of position. The problem of proper formulation of the diffusion term in transport (balance) equations was analyzed also in chemical engineering literature[4].

In one of our previous papers[5], the definition of the stochastic integral was generalized and a set of stochastic integrals was introduced. The Ito and Stratonovich integrals are particular elements of this set. A so-called transport stochastic integral was defined yielding diffusion term in Eq. (*1*) in the form commonly adopted for the description of diffusion processes.

Stochastic differential equations (SDEs) in the form of Eq. (*3*) were used for the modelling of various chemical-engineering processes, including the modelling of flow chemical reactors[6–8], description of the mass and heat transfer in fluidized beds[9,10], modelling of a turbulent diffusion[11–13] and chemical reaction in a turbulent flow[14], and simulation of mixing the sand particles in a rotating drum mixer[15]. The equations of the same type were also adopted in physics, biology and chemistry, e.g., for the modelling of evolution of the chirality of organic molecules[16] and for the simulation of the prey-predator systems[17,18]. Remarkable attention was devoted to modelling the noise-induced phase transitions in systems exposed to a fluctuating environment, e.g., in a population of growing cancer cells[19–22].

A solution of SDE (*3*) is represented by a (vector) stochastic function of time $\boldsymbol{X}(t)$ under the assumption that the initial distribution of this function is given (formally we can write it as $\lim_{t \to t_0} \boldsymbol{X}(t) = \boldsymbol{X}_0$). Then the distribution of process $\boldsymbol{X}(t)$ at any subsequent time instant $t > t_0$ can be determined if Eq. (*3*) can be solved analytically. It is, however, usually possible only for very simple forms of coefficients $\boldsymbol{v}$ and D and for one-dimensional (scalar) problems.

The transitive probability density function (TPDF) describing the distribution of random variable $\boldsymbol{X}(t)$ at each time instant t under the given initial distribution at initial time instant t_0 (cf. Eq. (*2*)) represents the complete probabilistic description of solution of Eq. (*3*) as the stochastic process generated by Eq. (*3*) is of the Markov type[2,3]. The TPDF can be, in certain cases, gained by solving the corresponding Kolmogorov equation (cf. Eq. (*1*)) with the appropriate boundary and initial conditions. In many cases of practical interest, however, it is only possible to solve the Kolmogorov equation for the stationary probability density function (i.e., for $t \to \infty$) and very often it is not possible to solve the Kolmogorov equation analytically at all and even not by numerical methods. Simplified methods[23,24] yielding, however, only few of all of the statistical parameters (e.g., mean value and variance) of the process $\boldsymbol{X}(t)$ can be adopted under such circumstances. These simplified methods cannot be used for the simulation of transition states of the process.

A possible way of obtaining the solution of SDEs consists in the simulation of a large number of individual trajectories of the process $\boldsymbol{X}(t)$ using the stochastic differential equation(s) governing the process and the subsequent estimation of the TPDF or at least of some of its statistical parameters (e.g., moments) applying standard procedures to the ensemble of simulated trajectories of $\boldsymbol{X}(t)$ at selected values of t.

Hybrid computers can be used as efficient and fast solvers for SDEs (refs[11,12,19–21]). The analog part of the computer (an integrator) serves for the simulation of individual realizations of the process $\boldsymbol{X}(t)$. The Wiener process $\boldsymbol{W}(t)$ is obtained by analog integration of the white-noise process generated by means of an electrical noise generator with a sufficient band-width. The digital part of the hybrid computer is used for the sampling of the process $\boldsymbol{X}(t)$ and for an evaluation of required numerical outputs. The applicability of hybrid computers is somewhat restricted due to the limited ability of analog function generators to approximate arbitrary mathematical functions occurring in SDEs. The possibility of modelling various kinds of boundary conditions is also limited. The solution of SDEs obtained using the analog computer corresponds to the Stratonovich definition of the stochastic integral[2,3,11,12,19–21].

Another way of obtaining the individual trajectories of process ***X***(*t*) governed by SDE in the form of Eq. (*3*) consists in direct numerical solution of Eq. (*3*) using an appropriate numerical integration routine. One application of this routine yields single trajectory (random realization) of the process ***X***(*t*). Repeating this procedure many times results in ensemble of trajectories which can be used for the estimation of statistical parameters of the process ***X***(*t*) (refs[8–12,15,16]). Recently Laso[25] has published a valuable review paper on numerical solution of SDEs. A way of modelling of all kinds of boundary conditions has been presented. However, only the Ito definition of stochastic integral and constant drift term have been considered. Petersen[26] reviewed some algorithms for numerical solution of SDEs and published a new one (suitable also for multivariate problems) and tested it with several example SDEs.

Details of numerical methods used for the simulation of trajectories ***X***(*t*) are not usually reported in literature. Therefore, the aim of this paper is to present here our experience with the application of certain numerical procedure to solving the stochastic differential equations of diffusion type (cf. Eq. (*3*)). We restrict ourselves to the one-dimensional problems and to the SDEs involving the diffusion coefficient being a function of the spatial coordinate. These equations bring the most serious problems to be solved by numerical methods. A shortened version of this paper has been presented recently[27].

THEORETICAL

The stochastic differential equation generating the one-dimensional (scalar) diffusion process ***X***(*t*) (i.e., the equation describing random walk of a diffusing particle on the line) can be written in the form

$$\mathrm{d}X(t) = v[X(t),t]\,\mathrm{d}t + G[X(t),t]\,\mathrm{d}W(t)\ . \tag{4}$$

Both coefficients *v* and *G* can generally be functions of the instantaneous particle position and, occasionally, explicitly also of time. The integral form of Eq. (*4*) is[28]

$$X(t) - X(0) = \int_0^t v[X(s),s]\,\mathrm{d}s + \int_0^t G[X(s),s]\,\mathrm{d}W(s)\ . \tag{5}$$

The first integral on the right-hand side of Eq. (*5*) is a common integral in the Riemann sense. The second one (of the Stieltjes type) is denoted as the stochastic integral and is defined by the relation[5,28]

$$\int_c^d G[X(s),s]\,\mathrm{d}W(s) = \lim_{n\to\infty} \sum_{i=0}^{n-1} G[X(t_i) + \alpha\Delta X_i, t_i + \alpha k]\,\Delta W_i\ , \qquad [0 \le \alpha \le 1]\ , \tag{6}$$

where t_i are the equidistantly placed time instants resulted from the discretization of the time axis with step k. ΔW_i and ΔX_i are increments of the Wiener process and the process $X(t)$, respectively

$$\begin{aligned} k &= t_{i+1} - t_i \\ \Delta W_i &= W(t_{i+1}) - W(t_i) \\ \Delta X_i &= X(t_{i+1}) - X(t_i) \\ i &= 0, 1, 2, \ldots, n-1 \ , \end{aligned} \tag{7}$$

where $t_0 = c$ and $t_n = d$.

In the definition of the Riemann integral, parameter α can take an arbitrary value within the given bounds (see Eq. (*6*)), i.e., the position of abscissa αk within interval $\langle t_i, t_{i+1} \rangle$ can be also arbitrary. This is not true for the stochastic integral; in this case coefficient G is a function of process $X(t)$ itself. The solution of Eq. (*4*) – the process $X(t)$ – depends on the way, stochastic integral (*6*) is defined by, i.e., on the value of α. In the following text, the distinct solutions of Eq. (*4*) depending on the actual definition of the stochastic integral will be distinguished by the superscript, e.g., $X^{\alpha}(t)$.

The distinct types of the stochastic integral are related by the equation[2,3,29]

$$X^{\alpha}(t) = X^{\beta}(t) + (\alpha - \beta) \int_0^t G[X^{\beta}(s),s] \frac{\partial}{\partial X} [G(x,s)|_{x=X^{\beta}(s)}] \, \mathrm{d}s \ , \tag{8}$$

where the integral is of the Riemann kind. Equation (*6*) defines an infinite set of stochastic integrals depending on the value of α. However, the only three stochastic integrals are of practical interest:

1. For $\alpha = 0$, Eq. (*6*) defines the Ito stochastic integral (ISI). The ISI is considered as the mathematically rigorous definition of the stochastic integral because the integrand function G and the Wiener process increment ΔW are mutually stochastically independent[2–4,28].

2. For $\alpha = 1/2$, Eq. (*6*) defines the Stratonovich stochastic integral (SSI). The SSI is considered to be a natural way of stochastic processes integration governing real dynamical systems. Results of analog computer simulations confirm this statement[11,12,19–21].

3. For $\alpha = 1$, a so-called transport stochastic integral (TSI) was introduced[5] applicable to the description of systems involving the diffusional mass or heat transport.

In this case, coefficient G is a function of the spatial coordinate, three different forms of the diffusion equation for the TPDF are obtained for the above values of parameter α.

General form of the diffusion equation for a one-dimensional stochastic diffusion process $X^\alpha(t)$ may be written as follows[5]

$$\frac{\partial f^\alpha}{\partial t} + \frac{\partial}{\partial x}\,[v(x,t)f^\alpha] + \alpha\,\frac{\partial}{\partial x}\left[f^\alpha G(x,t)\,\frac{\partial}{\partial x}\,G(x,t)\right] - \frac{1}{2}\,\frac{\partial^2}{\partial x^2}\left[G^2(x,t)f^\alpha\right] = 0 \ , \qquad (9)$$

where $f^\alpha = f^\alpha(x;t|y)$ is the TPDF describing the process $X^\alpha(t)$. The solution of Eq. (*9*) can be used (if available) for the check of results of numerical simulations of SDEs.

The only initial condition, i.e., the value of stochastic process $X(t)$ at $t = 0$ (cf. Eq. (*5*)), is necessary for solution of Eq. (*4*). Throughout this paper, the initial condition is considered as a non-random constant, i.e.

$$X(0) = x_0 \ . \qquad (10)$$

The corresponding initial condition for Eq. (*9*) has a form of the Dirac δ-function

$$\lim_{t\to 0} f^\alpha = \delta(y - x_0) \ . \qquad (11)$$

Two boundary conditions have to be further supplied for the solution of Eq. (*9*). A distribution of the process $X(t)$ over the whole real axis x is commonly considered in the probability theory yielding the boundary conditions in the form

$$\lim_{x\to -\infty} f^\alpha = \lim_{x\to +\infty} f^\alpha = 0 \ . \qquad (12)$$

When the process $X(t)$ can take only positive values, the above boundary conditions usually have the form

$$\lim_{x\to 0+} f^\alpha = \lim_{x\to +\infty} f^\alpha = 0 \ . \qquad (13)$$

A distribution of the process $X(t)$ over the interval of the finite length is usually considered in chemical engineering problems, e.g., when processes within a closed equipment are to be modelled. The mass fluxes at boundaries of the closed system (i.e. at the ends of considered interval) have zero value

$$\lim_{x\to x_1+} j^\alpha(x;t) = \lim_{x\to x_2-} j^\alpha(x;t) = 0 \ , \qquad (14)$$

where flux j^α is defined (cf. Eq. (*9*)) as

$$j^\alpha(x;t) = v(x;t)\, f^\alpha + \frac{\alpha}{2} f^\alpha \frac{\partial}{\partial x}\left[G^2(x,t)\right] - \frac{1}{2}\frac{\partial}{\partial x}\left[G^2(x,t) f^\alpha\right] . \qquad (15)$$

Boundary conditions (*14*) are replaced with the conditions of the reflecting boundaries at the ends of the considered interval during numerical simulation of the SDEs (the trajectory of the simulated stochastic process reflects back into the interval when reaching the boundary). This approach was successfully adopted in our previous paper[15] dealing with the description of solid particles blending in a rotating horizontal drum mixer.

In the following, the above approach to numerical solution of SDEs will be applied to several test examples.

NUMERICAL EXPERIMENTS

Numerical Solution of SDEs

The basic principle of the approach to numerical solution of the diffusion SDEs having form of Eq. (*4*) adopted in this paper was described in one of previous papers[15] dealing exclusively with the evaluation of the Ito stochastic integral. Here we expand this approach to evaluation of the other kinds of stochastic integral.

The numerical solution of the SDEs consists in replacement of original equation (*4*) with the finite difference approximation

$$\begin{aligned} \Delta X_i^\alpha &= v(X_i^\alpha, t_i)k + G(X_i^\alpha + \alpha\, \Delta X_i^\alpha, t_i + \alpha k) N_{01}\sqrt{k} \\ X_{i+1}^\alpha &= X_i^\alpha + \Delta X_i^\alpha \\ X_i^\alpha &= X^\alpha(t_i)\ , \end{aligned} \qquad (16)$$

where term $N_{01}\sqrt{k}$ approximates the Wiener process increment over time interval k, N_{01} is the standardized Gaussian distributed random number. These numbers were generated using a method of backward interpolation of the Gaussian distribution function[30]. Great care should be taken of the selection of the generator of uniformly distributed pseudo-random numbers serving as input data for the interpolating procedure. The standard pseudo-random numbers generating functions implemented in programming languages showed not to be applicable. Throughout simulations presented in this paper, thoroughly tested procedure RAN2 from ref.[31] was used.

Form of the first term on the right-hand side of Eq. (*16*) implies that the deterministic part of the process $X(t)$ increment is evaluated according to the Euler integration scheme[32].

The evaluation of increment ΔX_i^α according to Eq. (*16*) repeats recursively for $i = 1, 2, 3,\ldots$ with given initial value x_0 for sufficiently large number of process trajectories N. A histogram of ΔX_i^α values obtained by sorting into h bins represents an approximation of the transitive probability density function $f^\alpha(x,t_i \mid x_0)$ at the given time instant t_i.

There is not, probably, any general procedure available for a priori estimation of a value of N yielding the required accuracy of the approximation of transitive probability density. Computations described in literature[11–14,16,20–22,25,26] operates with number of trajectories within the interval of $5 \,.\, 10^3$–$1.25 \,.\, 10^5$. The upper limit was imposed predominantly by computational power of the computer used.

The evaluation of increment ΔX_i^α is quite simple for zero value of α (i.e., for Ito integral). Equation (*16*) is generally a non-linear equation with respect to increment ΔX_i^α in case of $\alpha > 0$. Any usual numerical method for solving non-linear equations can be used for its solution with the Ito increment ΔX_i^0 as an initial guess. Preliminary tests with various forms of function $G[X^\alpha(t)]$ in Eq. (*16*) proved that 3 or 4 Newton iterations are sufficient to yield ΔX_i^α with relative precision within the interval of 10^{-3}–10^{-6}.

Due to the large amount of numerical operations involved in evaluating ΔX_i^α, an estimation procedure for reasonable size of integration time step k is highly desirable. The following procedure was adopted throughout computations presented in this paper:

The mean square value of the Ito increment (for zero drift velocity, i.e. $v = 0$) is given by

$$s_i = G(X_i)\sqrt{k} \qquad (17)$$

as a value of standard deviation of random numbers N_{01} is equal to unity. Then the relation for the maximum time step size is

$$k_{\max} \leq \left[\frac{s_{\mathrm{ir}}\, L}{G(X_i)}\right]^2 , \qquad (18)$$

where $s_{\mathrm{ir}} = s_i/L$ is the mean square value of stochastic increment related to interval length L. By choosing an acceptable value of s_{ir} (e.g., $s_{\mathrm{ir}} = 0.1$, i.e., the trajectory is allowed to cross 10% of the length L in one time step), one obtains an estimate of possible time step from Eq. (*18*). For functions $G(X)$ considered in this paper we gained dimensionless time step size estimates within the range of about 10^{-2}–10^{-4}. The time step size estimated by this procedure, however, does not provide convergence of the iteration procedure evaluating the increment ΔX_i^α if very large number N_{01} is generated.

Then the iteration loop has to be interrupted, and the evaluation of the increment is repeated with new number N_{01}. Large values of N_{01} occur very seldomly (depending on random number generator actually used). Tests proved that less than 0.5% of the total number of iteration loops does not converge. A reduction of $s_{i\,\mathrm{r}}$ lowers the number of unsuccessful iterations, however, no statistically significant increase of accuracy of SDE solution was observed.

The deterministic term (drift) $v[X(t),t]$ of Eq. (*4*) was integrated using either the Euler method (cf. Eq. (*16*)) or the second-order Runge–Kutta method (in the case of nonlinear drift term).

So-called reflecting boundaries were considered for trajectory $X(t)$ at both ends of the interval considered. The trajectory reflection at the boundary was simulated as in earlier paper[15]. The same method was used, e.g., by Laso[25].

The computations reported throughout this paper were performed either on IBM 3081 computer or AT 386 PC.

Test SDEs

The procedure for numerical solution of SDEs described in the previous section was tested using three particular forms of stochastic differential equations of diffusion type – cf. Eq. (*4*). The example equations were chosen with respect to the possibility of finding an analytical solution of the corresponding diffusion (Kolmogorov, Fokker–Planck) equation.

A. SDE with the Linear Drift Term

$$\mathrm{d}X = q\Phi X\,\mathrm{d}t + \sqrt{(a^2 + X^2)\Phi}\;\mathrm{d}W(t)\ , \qquad (19)$$

where a, q and Φ are constants. A kind of Eq. (*19*) was used by Seinfeld and Lapidus[4] as an example documenting the possibility of finding an analytical solution of SDE (for $\Phi = 1$ and $q = 1/2$). Constant Φ is a time scaling factor, therefore we considered $\Phi = 1\ \mathrm{s}^{-1}$ in our simulations. It was proved (see Appendix A) that the analytical solution of diffusion equation (Eq. (*A5*)) corresponding to SDE (*19*) is identical for all kinds of stochastic integral (i.e., for all values of α within interval $\langle 0,1\rangle$) supposing

$$q = \frac{1}{2} - \alpha\ . \qquad (20)$$

With reflecting boundaries at $x_1 = 0$ and $x_2 = L$ and with initial condition $X(0) = x_0$, the solution is

$$f(x;t|\,x_0) = \frac{1}{K\sqrt{a^2+x^2}}\left[1 + 2\sum_{n=1}^{\infty}\exp\left(-\frac{\Phi t n^2\pi^2}{2K^2}\right)\cos\left(\frac{M}{K}\right)\cos\left(\frac{M_0}{K}\right)\right] , \qquad (21)$$

where K = arcsinh (L/a), $M = n\pi$ arcsinh (x/a) and $M_0 = n\pi$ arcsinh (x_0/a). Stationary solution $f_s(x)$ of SDE (*19*)

$$f_s(x) = \lim_{x\to+\infty} f(x;t|\,x_0) \qquad (22)$$

can also be found for all values of q and all kinds of stochastic integral (condition (*20*) may not be fulfilled in this case)

$$f_s(x) = C(a^2 + x^2)^{q+\alpha-1} \ . \qquad (23)$$

Integration constant C is defined by the condition

$$\int_{x_1}^{x_2} f_s(x)\,\mathrm{d}x = 1 \ . \qquad (24)$$

Figures 1 and 2 depict results of numerical solution of Eq. (*19*) at several time instants for two different values of parameter a. The stochastic term of Eq. (*19*) was integrated

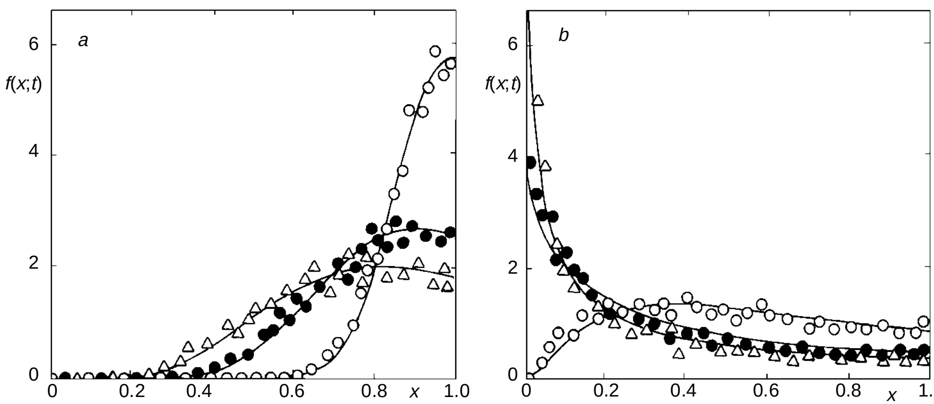

FIG. 1

Comparison of numerical solution of Eq. (*19*) with analytical solution (*21*) for Ito stochastic integral. Parameters: q = 0.5, a = 0.05, x_0 = 1, x_1 = 0, x_2 = L = 1, α = 0, N = 6 000, h = 50, k = 0.001; numerical solution (points), analytical solution (lines); *a* ❍ t = 0.02, ● t = 0.10, Δ t = 0.20; *b* ❍ t = 1.0, ● t = 4.0, Δ t = 7.0 (all parameter and variable values are given in arbitrary time and length units) according to Ito definition ($\alpha = 0$). With respect to Eq. (*20*), it is necessary to use $q = 1/2$ to make the comparison of Eq. (*19*) with Eq. (*21*) possible. TPDF according to Eq. (*21*) is compared with all three kinds of numerical integrals of the stochastic term in Eq. (*19*) in Figs 3 and 4. Figure 5 shows the stationary solutions of Eq. (*19*) without deterministic (drift) term, i.e., for $q = 0$. Reflecting boundaries were considered at $x_1 = -1$ and $x_2 = 1$. Equations (*23*) and (*24*) yield the stationary solutions

$$f_s^I(x) = \frac{1}{2\,\mathrm{arctg}\,(1/a)(a^2 + x^2)}\ , \qquad (\alpha = 0, q = 0)$$
$$f_s^S(x) = \frac{1}{2\,\mathrm{arcsinh}\,(1/a)\sqrt{a^2 + x^2}}\ , \qquad (\alpha = 1/2, q = 0) \qquad (25)$$
$$f_s^T = \frac{1}{2}\ , \qquad (\alpha = 1, q = 0)\ ,$$

depicted in Fig. 5.

B. SDE with the Nonlinear Drift Term

$$\mathrm{d}X = (-\kappa X^3 + \lambda X^2 - QX + R)\,\mathrm{d}t + \sigma X^2\,\mathrm{d}W(t)\ . \qquad (26)$$

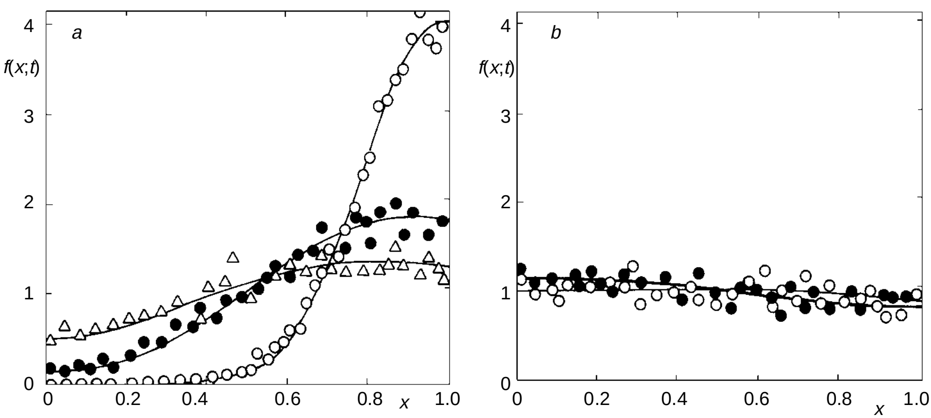

FIG. 2

Comparison of numerical solution of Eq. (*19*) with analytical solution (*21*) for Ito stochastic integral. Parameters: $q = 0.5$, $a = 1.0$, $x_0 = 1$, $x_1 = 0$, $x_2 = L = 1$, $N = 6\,000$, $h = 50$, $k = 0.001$, $\alpha = 0$; numerical solution (points), analytical solution (lines); *a* ❍ $t = 0.02$, ● $t = 0.10$, Δ $t = 0.20$; *b* ❍ $t = 1.0$, ● $t = 4.0$, heavy line: stationary solution according to Eq. (*23*) (analytical solution for $t = 4.0$ is not shown) (all parameter and variable values are given in arbitrary time and length units)

This equation was used for description of the tumor cell population dynamics[19–22]. Symbols κ, λ, Q, R and σ denote parameters of the population. The process $X(t)$ generated by Eq. (*26*) possesses either unimodal or bimodal stationary probability density function depending on parameter values and the kind of stochastic integral used (see Appendix A):

$$f_s^{\alpha}(x) = \frac{C^{\alpha}}{x^{2[2(1-\alpha)+\kappa/\sigma^2]}} \exp\left[\frac{2}{\sigma^2}\left(-\frac{\lambda}{x} + \frac{Q}{2x^2} - \frac{R}{3x^3}\right)\right] , \qquad (27)$$

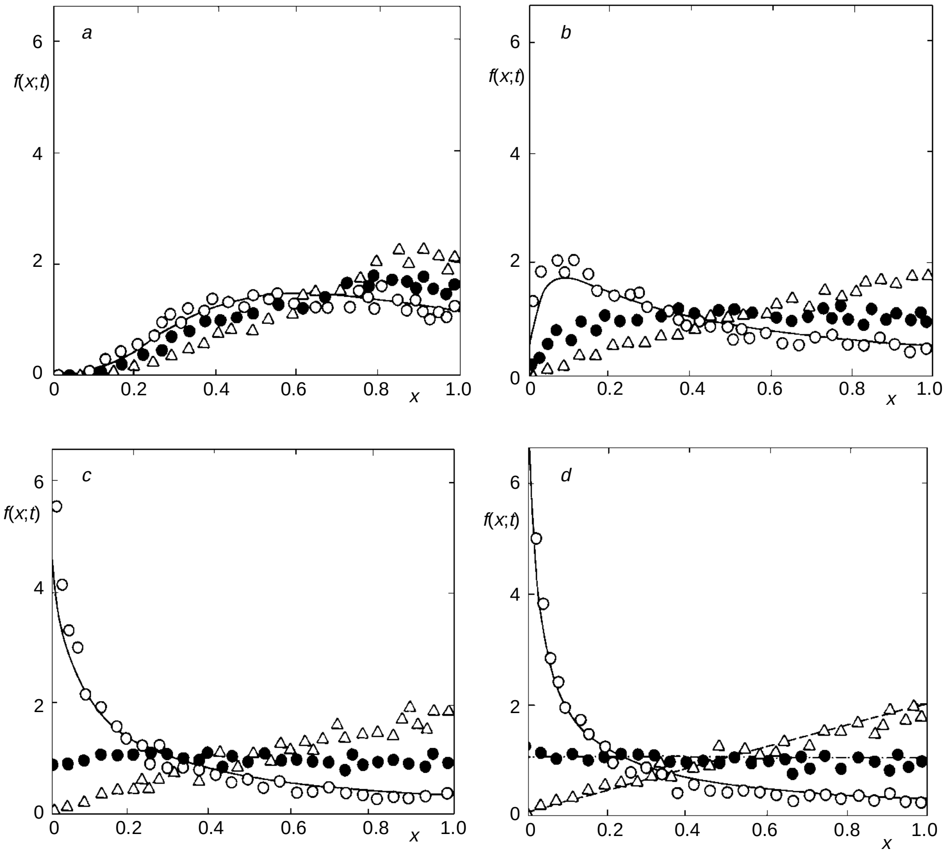

FIG. 3

Comparison of numerical solution of Eq. (*19*) with analytical solution (*21*) for various kinds of stochastic integral. Parameters: q = 0.5, a = 0.01, x_0 = 1, x_1 = 0, x_2 = L = 1, N = 6 000, h = 50, k = 0.001; *a* t = 0.5, *b* t = 2.5, *c* t = 5.0, *d* t = 7.0; ❍ Ito stochastic integral (α = 0), ● Stratonovich stochastic integral (α = 1/2), Δ transport stochastic integral (α = 1); —— analytical solution of Eq. (*19*) for α = 0, – · – · – stationary solution according to Eq. (*23*) for α = 1/2, — — — stationary solution according to Eq. (*23*) for α = 1 (all parameter and variable values are given in arbitrary time and length units) where C^{α} is the normalization factor and α again defines a kind of stochastic integral. The numerically obtained stationary solution of Eq. (*26*) together with function (*27*) confined to positive spatial half-axis are depicted in Fig. 6.

C. SDE with the Stochastic Term Being Explicit Function of Time

$$\mathrm{d}X = g\left[\frac{1 - \exp(-\Phi t)}{\Phi}\right]^{1/2} \mathrm{d}W(t) \qquad (28)$$

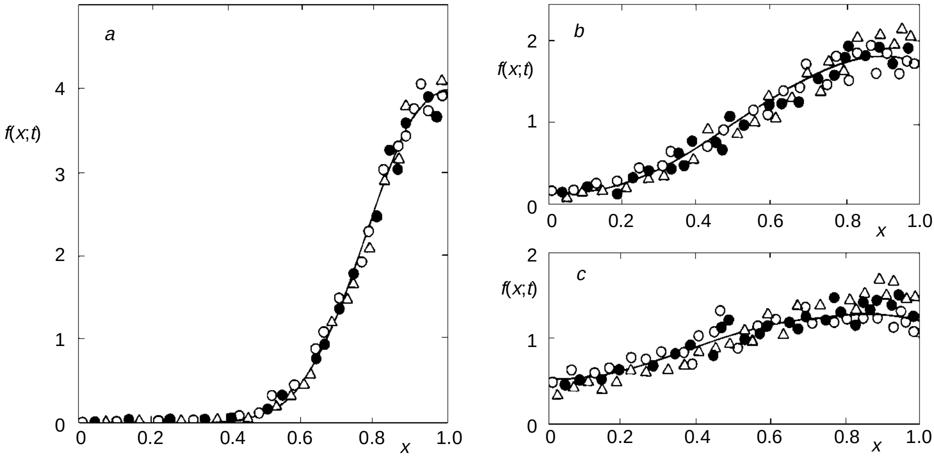

FIG. 4

Comparison of numerical solution of Eq. (*19*) with analytical solution (*21*) for various kinds of stochastic integral. Parameters: $q = 0.5$, $a = 1$, $x_0 = 1$, $x_1 = 0$, $x_2 = L = 1$, $N = 6\,000$, $h = 50$, $k = 0.001$; *a* $t = 0.02$, *b* $t = 0.1$, *c* $t = 0.20$; ❍ Ito stochastic integral ($\alpha = 0$), ● Stratonovich stochastic integral ($\alpha = 1/2$), Δ transport stochastic integral ($\alpha = 1$); —— analytical solution of Eq. (*19*) for $\alpha = 0$ (all parameter and variable values are given in arbitrary time and length units)

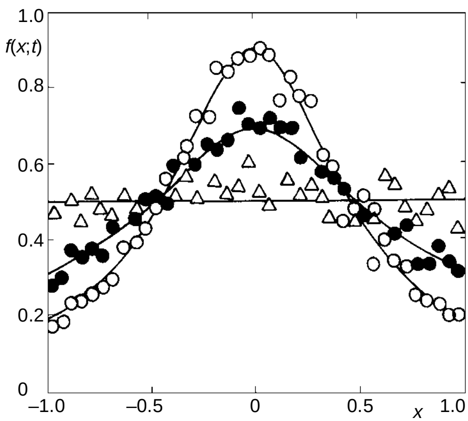

FIG. 5

Stationary solutions of Eq. (*19*) without drift term for different kinds of stochastic integral. Parameters: $q = 0$, $a = 1.0$, $x_0 = 0$, $x_1 = -1$, $x_2 = +1$, $N = 10\,000$, $h = 40$, $k = 0.001$, $t = 10$; lines: analytical solutions (*23*); numerical solutions: ❍ Ito stochastic integral, ● Stratonovich stochastic integral, Δ transport stochastic integral (all parameter and variable values are given in arbitrary time and length units)

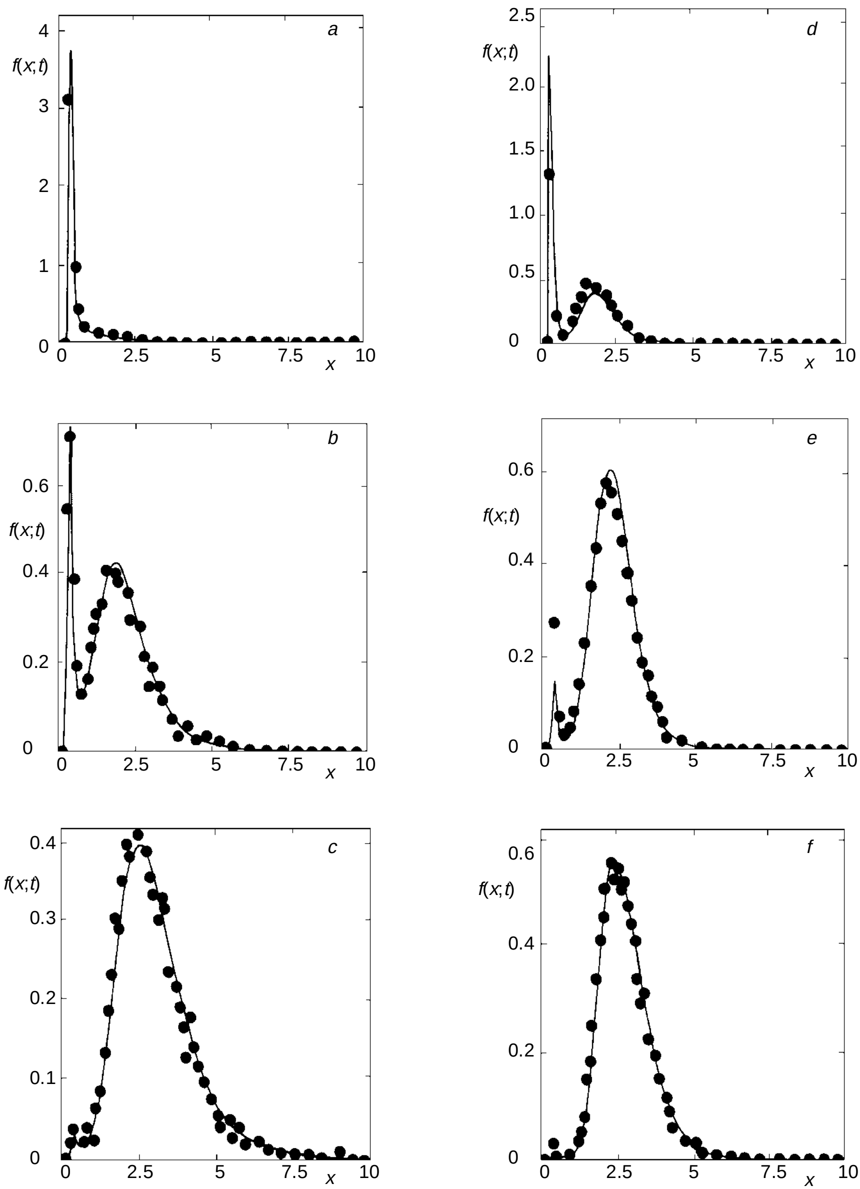

FIG. 6

Comparison of numerical stationary solution of Eq. (*26*) with analytical stationary solution (*27*) for various kinds of stochastic integral. Parameters: $\kappa = 1$, $\lambda = 3.6$, $Q = 3.0$, $R = 0.7$, $\sigma = 0.4$ (*a*, *b*, and *c*), $\sigma = 0.3$ (*d*, *e*, and *f*), $N = 6\ 000$, $h = 100$, $k = 0.001$; *a*, *d* Ito stochastic integral ($\alpha = 0$), *b*, *e* Stratonovich stochastic integral ($\alpha = 1/2$); *c*, *f* transport stochastic integral ($\alpha = 1$); —— analytical stationary solution (*27*); ● numerical stationary solution (all parameter and variable values are given in arbitrary time and length units)

This SDE generates the same stochastic diffusional process $X(t)$ with the Gaussian distribution for all kinds of stochastic integration. The time evolution of variance of the process $X(t)$ is (cf. Appendix A)

$$\sigma^2(t) = \left(\frac{g}{\Phi}\right)^2 [\Phi t - 1 + \exp(-\Phi t)] \; . \qquad (29)$$

It was proved earlier[33] that relation (*29*) results from modelling the diffusional motion of particles having distributed velocities. That model was shown to be an improvement of the conventional diffusional models considering time independent diffusion coefficient at the beginning of the process.

As far as only the confirmation of independence of the process $X(t)$ generated by Eq. (*28*) on the kind of stochastic integration used was required the variance of the process $X(t)$ was evaluated solely as a function of time. The process $X(t)$ was considered to be defined over interval $\langle -L,+L \rangle$ with initial value $x_0 = 0$. With respect to the spatial symmetry of the process $X(t)$, the estimate of its variance is given by the relation

$$[s_x^\alpha(t)]^2 = \sum_{j=1}^{N} \frac{[X_j^\alpha(t)]^2}{N-1} \; , \qquad (30)$$

where X_j^α denotes individual trajectories of $X(t)$ for the given value of α. In Appendix A it is shown that variance $\sigma_x^2(t)$ for any value of α is given by the relation

$$\sigma_x^2(t) = L^2 \left[\frac{1}{3} + \frac{4}{\pi^2} \sum_{m=1}^{\infty} \frac{(-1)^m}{m^2} \exp\left(-\frac{2\sigma^2(t) m^2 \pi^2}{L^2} \right) \right] , \qquad (31)$$

where $\sigma^2(t)$ is given by Eq. (*29*). Function $\sigma_x^2(t)$ according to Eq. (*31*) is compared with estimate $[s_x^\alpha(t)]^2$ (see Eq. (*30*)) in Fig. 7 for all kinds of the stochastic integral.

RESULTS AND DISCUSSION

As far as only particular problems concerning the numerical solution of SDEs are addressed in this paper, the only qualitative (graphical) comparison of numerical and analytical solutions of test SDEs is used instead of more sophisticated statistical tests.

Figures 5 and 6 show a good agreement of stationary numerical solutions of Eqs (*19*) and (*26*) both for uni- and bimodal distributions. The Newton method using the Ito increment as an initial guess was adopted for evaluating ΔX_i^α in case of the Stratonovich stochastic integral. The results confirm applicability of this approach. The maximum time step size estimation according to Eq. (*18*) is applicable despite its certain incorrectness. This is documented in Figs 1–6 by a fairly good agreement of numerical solutions of SDEs and analytical solutions of the corresponding Kolmogorov diffusion equations. The differences among the Ito, Stratonovich and transport integral of the same SDE are shown in Figs 3–6. These differences are negligible for low time values (due to identical initial distribution) and they become remarkable at high values of time. Figure 7 illustrates that all the kinds of stochastic integration yield the same solution for SDEs with stochastic term independent of the process $X(t)$ itself.

All the kinds of the stochastic integral can be numerically simulated by the numerical procedure described in this paper. Solutions unavailable by analytical methods can be therefore gained, see Figs 3 and 4. However, it is necessary to perform a preliminary analysis of each particular SDE with respect to the performance of the iterative procedure for ΔX_i^α evaluation with various values of problem parameters and time step size. This iterative procedure is somewhat time-consuming, therefore, more powerful computers are to be used, e.g., with parallel processing[13,25,26], or transformation (*8*) of the Stratonovich or transport integral to Ito one can be adopted (with $\beta = 0$).

It has to be pointed out that the application of common numerical methods (Runge–Kutta methods, Merson method, etc.) for the integration of SDEs may yield erroneous results. Let us consider Eq. (*4*) in a simplified form (without drift term $v[X(t),t]$) and with the diffusion coefficient being a function only of the evaluated process

$$\mathrm{d}X^\alpha(t) = G[X^\alpha(t)]\,\mathrm{d}W(t) \quad . \tag{32}$$

Only the Ito integral of Eq. (*32*) will be considered, therefore the superscript α will be omitted in the following text. Eqs (*16*) simplify to

$$X_{i+1} = X_i + G(X_i)H \quad , \tag{33}$$

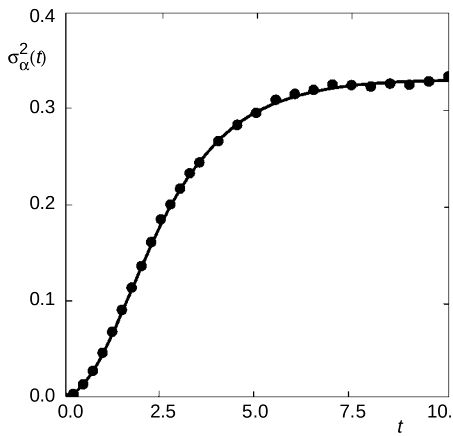

FIG. 7
Time evolution of variance of stochastic process $X(t)$ generated by SDE (*28*). Parameters: $\Phi = 1$, $g = 0.35$, $N = 8\,192$, $h = 100$, $k = 0.001$, $x_0 = 0$, $x_1 = -1$, $x_2 = +1$, $L = 2$; —— analytical solution (*31*), ● variance estimate according to Eq. (*29*) for all kinds of stochastic integral (all parameter and variable values are given in arbitrary time and length units)

where $H = \sqrt{k}N_{01}$. Equation (*33*) is formally identical with the Euler method formula for ODEs solution. An improvement of this method are Runge–Kutta methods of the second order[32], e.g., the Heun method or the modified Euler method. Formal application of these methods leads to the equation

$$X_{i+1} = X_i + (1 - \omega)G(X_i))H + \omega HG[X_i + HG(X_i)/(2\omega)] \ , \tag{34}$$

with ω = 1/2 for the Heun method and ω = 1 for the modified Euler method. It is shown in Appendix B that the application of Euler method yields the Ito solution (α = 0) of the SDE and both the Heun and the modified Euler method yield the Stratonovich solution, i.e., the solution of Eq. (*32*) for α = 1/2. This conclusion was proved by numerical

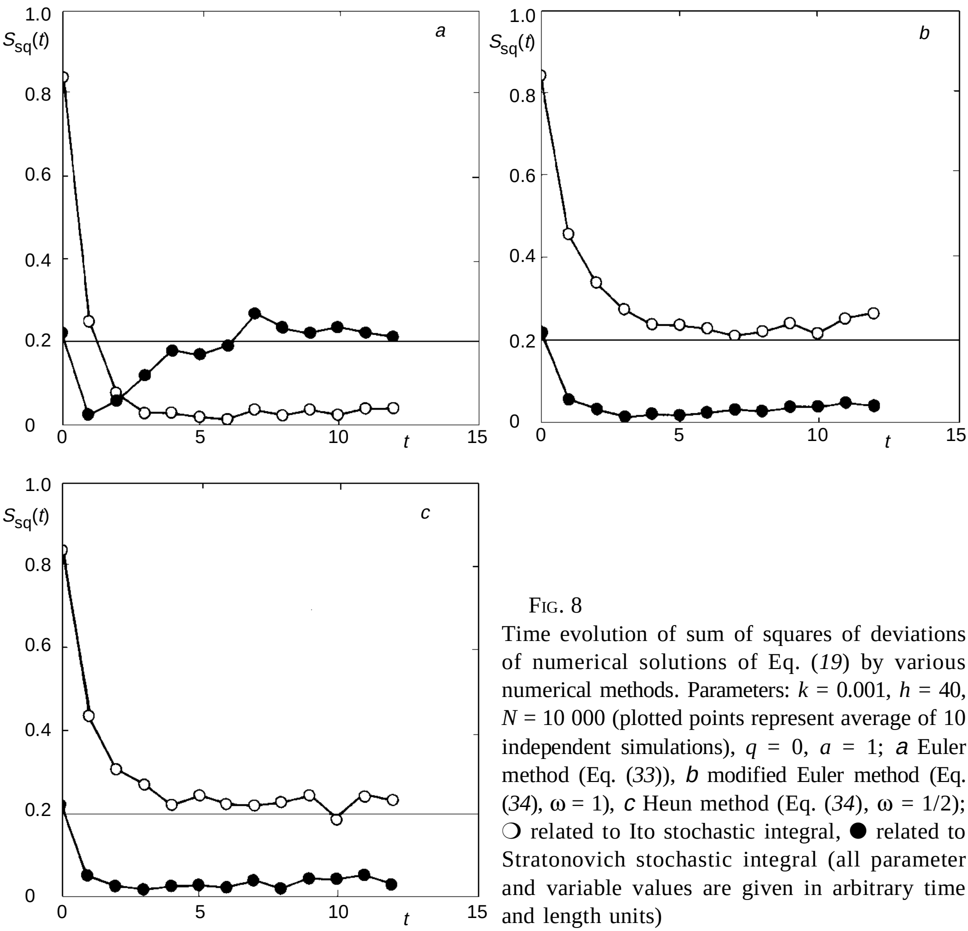

FIG. 8
Time evolution of sum of squares of deviations of numerical solutions of Eq. (*19*) by various numerical methods. Parameters: k = 0.001, h = 40, N = 10 000 (plotted points represent average of 10 independent simulations), q = 0, a = 1; *a* Euler method (Eq. (*33*)), *b* modified Euler method (Eq. (*34*), ω = 1), *c* Heun method (Eq. (*34*), ω = 1/2); ❍ related to Ito stochastic integral, ● related to Stratonovich stochastic integral (all parameter and variable values are given in arbitrary time and length units)

solution of Eq. (*19*) using q = 0 and considering the reflecting boundaries at $x = \pm 1$. Uniform distribution was considered as the initial condition

$$\lim_{t\to 0+} f(x;t|\,x_0) = f(x_0) = \begin{cases} 1/2 & \text{for } |\,x_0| \le 1 \\ 0 & \text{for } |\,x_0\,| > 1 \end{cases} \quad . \tag{35}$$

The results of numerical simulation were compared with the stationary probability density functions, i.e. with the first two of Eqs (*25*). Figure 8 shows the time evolution of the sum of squares of deviations between numerical and analytical solution:

$$S_{\mathrm{sq}}(t) = \sum_{i=1}^{h} \left[\frac{n_i(t)}{n} - \int_{(i-1)/h}^{i/h} f_{\mathrm{s}}^{\alpha}(x)\,\mathrm{d}x \right]^2 \quad . \tag{36}$$

Symbol h denotes the number of bins, n_i/n is the relative count of trajectories in the i-th bin at time t. The horizontal line in Fig. 8 shows sum of squares of deviations between $f_{\mathrm{s}}^{\mathrm{I}}(x)$ and $f_{\mathrm{s}}^{\mathrm{S}}(x)$ and the course of lines confirms the above conclusion.

CONCLUSIONS

The simple first-order numerical iterative procedure was developed for the solution of stochastic differential equations for diffusion processes. The procedure makes it possible to perform all kinds of stochastic integration by changing single parameter. The method enables to find an approximate numerical solution of partial differential equation of diffusional type by solving the corresponding stochastic differential equations.

The method makes it possible to solve problems with space- and time-varying diffusivities and various kinds of boundary conditions. The accuracy of the method can be varied within a wide range by selection of a number of trajectories generated and proper time step size.

It was shown by theoretical analysis and proved by numerical simulations that the formal application of common numerical procedures of higher orders for the numerical solution of ordinary differential equations can yield erroneous results (another kind of stochastic integral than requested can be obtained) when applied to the numerical solution of stochastic differential equations. More sophisticated methods of second order (reviewed, e.g., by Petersen[26]) require abundant computational effort compared with the simple algorithm presented in this paper.

APPENDIX A

Analytical Solution of Diffusion Equations Corresponding to the Example SDEs

First we shall prove that Eq. (*9*) has a simple analytical solution for zero drift velocity v, $\alpha = 1/2$ and coefficient G being independent of time. After multiplying Eq. (*9*) by G and after rearrangements, the following relation results

$$\frac{\partial p}{\partial t} - \frac{1}{2} G(x) \frac{\partial}{\partial x}\left[G(x)\frac{\partial p}{\partial x}\right] = 0, \quad (p \equiv fG(x)) \quad . \tag{A1}$$

After substituting

$$y = \int \frac{\mathrm{d}x}{G(x)}\,, \quad t = \tau \quad , \tag{A2}$$

the simple diffusion equation is obtained

$$\frac{\partial p}{\partial \tau} - \frac{1}{2}\frac{\partial^2 p}{\partial y^2} = 0 \quad . \tag{A3}$$

Solution of this equation exposed to reflecting boundaries at $y_1 = 0$ and $y_2 = K$ can be written as[34]

$$\begin{aligned} p(y;\tau|\, y_0) &= \frac{1}{\sqrt{2\pi\tau}} \sum_{-\infty}^{+\infty} \left\{ \exp\left[-\frac{(y - y_0 + 2nK)^2}{2\tau}\right] + \exp\left[-\frac{(y + y_0 + 2nK)^2}{2\tau}\right]\right\} = \\ &= \frac{1}{K}\left[1 + 2\sum_{n=1}^{+\infty} \exp\left(-\frac{\tau n^2 \pi^2}{2K^2}\right) \cos\left(\frac{n\pi y}{K}\right) \cos\left(\frac{n\pi y_0}{K}\right)\right] \quad . \end{aligned} \tag{A4}$$

This result will be used for evaluating TPDF f of SDE (*19*):

A) A comparison of Eqs(*4*) and (*9*) proves that the Kolmogorov diffusion equation corresponding to SDE (*19*) has form

$$\frac{\partial f^\alpha}{\partial t} + q\Phi \frac{\partial}{\partial x}(xf^\alpha) + \alpha\Phi \frac{\partial}{\partial x}(xf^\alpha) - \frac{1}{2}\frac{\partial^2}{\partial x^2}\left[(a^2 + x^2) f^\alpha\right] = 0 \quad . \tag{A5}$$

Using Eq. (*20*), we can obtain the following relation valid for all values of α (it will be, therefore, omitted in the following text)

$$\frac{\partial f}{\partial t}-\frac{1}{2}\frac{\partial}{\partial x}\left\{\sqrt{a^2+x^2}\,\frac{\partial}{\partial x}\left[\sqrt{a^2+x^2}\,f\right]\right\}=0\ . \qquad (A6)$$

After substituting the particular form of function G in Eq. (*A2*), we obtain transformations

$$y=\int_0^x\frac{\mathrm{d}z}{\sqrt{a^2+z^2}}=\operatorname{arcsinh}\left(\frac{x}{a}\right)=\ln\left(\frac{\sqrt{a^2+x^2}+x}{a}\right)$$
$$\tau=\Phi t\ . \qquad (A7)$$

In this way, the solution given by Eq. (*21*) was obtained.

B) Diffusion equation corresponding to SDE (*26*) has the form

$$\frac{\partial f^{\alpha}}{\partial t}+\frac{\partial}{\partial x}\left[\left(R-Qx+\lambda x^2-\kappa x^3\right)f^{\alpha}\right]+2\alpha\frac{\partial}{\partial x}(x^3f^{\alpha})-\frac{\sigma^2}{2}\frac{\partial^2}{\partial x^2}(x^4f^{\alpha})=0\ . \qquad (A8)$$

Stationary solution of this equation for $x \geq 0$ is given by Eq. (*27*). Values of constants C^{α} have to be evaluated numerically.

C) Diffusion equation corresponding to SDE (*28*), whose stochastic term is an explicit function of time, can be written in the simple form (for any value of α)

$$\frac{\partial f}{\partial t}-\frac{g^2}{\Phi}\left[1-\exp(-\Phi t)\right]\frac{\partial^2 f}{\partial x^2}=0\ . \qquad (A9)$$

As in Eq. (*A7*) we put

$$y=x\ ,$$
$$\tau=\frac{g^2}{\Phi}\int_0^t\left[1-\exp(-\Phi s)\right]\mathrm{d}s=\left(\frac{g}{\Phi}\right)^2\left[\Phi t-1+\exp(-\Phi t)\right]\ , \qquad (A10)$$

(cf. Eq. (*29*)) and finally we obtain Eq. (*A3*) with $p(y,\tau\,|\,y_0)=f(x;t\,|\,x_0)$. The solution for reflecting boundaries at $x_1=-L$ and $x_2=+L$ together with initial condition $\delta(x-x_0)=\delta(x)$ is

$$f(x;t|0)=\frac{1}{2L}\left\{1+2\sum_{n=1}^{+\infty}\exp\left(-\frac{2\tau n^2\pi^2}{L^2}\right)\cos\left(\frac{n\pi x}{L}\right)\right\}\ . \qquad (A11)$$

The above function is even and mean value of x is therefore zero. Variance of x is simply given by

$$\sigma_x^2(t) = 2 \int_0^L x^2 f(x;t|0)\, \mathrm{d}x \quad . \tag{A12}$$

After performing integration, one gets Eq. (*31*).

APPENDIX B

Formal Application of the Second-Order Runge–Kutta Methods to the Numerical Solution of SDEs

Let us consider SDE (*4*) without deterministic (drift) term $v[X(t),t]$ and with stochastic term not being an explicit function of time

$$\mathrm{d}X(t) = G(X(t))\, \mathrm{d}W(t) \ , \quad [X(t) = X^{\alpha}(t) \ , \quad \alpha = 0] \ , \tag{B1}$$

where $G = G(x)$ and its first derivative are continuous functions of x.

An analogous ordinary differential equation (ODE) can be formally written as

$$\mathrm{d}x(t) = G^{*}(x(t))\, \mathrm{d}t \ . \tag{B2}$$

The most simple numerical method for the solution of Eq. (*B2*) is the Euler method

$$x_{i+1} = x_i + kG^{*}(x_i) \ , \tag{B3}$$

with k denoting the integration step and $x_i = x(t_i)$. More accurate Runge–Kutta methods of second order are formulated in the following way[32]:

$$x_{i+1} = x_i + (1-\omega)kG^{*}(x_i) + \omega kG^{*}[x_i + (k/2\omega)G^{*}(x_i)] \ , \tag{B4}$$

where $\omega = 1/2$ defines the Heun method and $\omega = 1$ defines the modified Euler method. After expanding $G^{*}(x_i)$ in the last term on the right-hand side of Eq. (*B4*) in power series of k and dropping out higher-order terms, the following formula results

$$x_{i+1} = x_i + kG^*(x_i) + \frac{1}{2}k^2 G_x^*(x_i)G^*(x_i) + \mathrm{O}(k^3) \ , \qquad (B5)$$

where $G_x^* \equiv \mathrm{d}G^*(x)/\mathrm{d}x$. Equation (*B5*) with respect to Eqs (*B2*) and (*B3*) represents the Taylor expansion of $x(t_i + k)$ up to the second-order terms.

By applying the above approach to SDE, we obtain Eq. (*34*), i.e., the relation equivalent, with respect to accuracy, to the Taylor expansion (*B5*)

$$\Delta X(t) \approx G(X(t))\Delta W(t) + 0.5G_x(X(t))G(X(t))(\Delta W(t))^2 \ , \qquad (B6)$$

where $\Delta W(t) \approx H$.

The above relation is a finite difference approximation of SDE

$$\mathrm{d}X(t) = G(X(t)\ \mathrm{d}W(t) + 0.5G_x(X(t))G(X(t))\ \mathrm{d}t \ , \qquad (B7)$$

as $\mathrm{d}W^2(t) = \mathrm{d}t$ (cf., e.g.[35]). Equation (*B7*) obviously differs from Eq. (*B1*) and corresponds – with respect to Eq. (*8*) (for $\alpha = 1/2$ and $\beta = 0$) – to the Stratonovich form of SDE

$$\mathrm{d}X^\alpha(t) = G(X^\alpha(t))\ \mathrm{d}W(t) \ , \quad (\alpha = 1/2) \ . \qquad (B8)$$

SYMBOLS

a	constant in Eq. (*19*), m
b	general transferred (balanced) quantity
c	integration limit, s
C	integration constant
d	integration limit, s
D	diffusivity, $\mathrm{m^2\ s^{-1}}$
f	probability density function, $\mathrm{m^{-1}}$, $\mathrm{m^{-3}}$
G	diffusion coefficient in Eq. (*4*), $\mathrm{m\ s^{-1/2}}$
g	constant in Eq. (*28*), $\mathrm{m\ s^{-1}}$
h	number of bins
H	stochastic time step, $\mathrm{s^{1/2}}$
i	time step index
j	one-dimensional diffusional flux, $\mathrm{s^{-1}}$
K	dimensionless length of interval
k	time step, s
L	length of interval, m
M	constant in Eq. (*21*)

M_0	constant in Eq. (*21*)
N	number of trajectories (particles)
N_{01}	pseudo-random numbers with $N(0,1)$ distribution
n	number of steps
P	probability
q	constant in Eq. (*19*)
Q	parameter in Eq. (*26*), s^{-1}
R	constant in Eq. (*26*), m s^{-1}
s	mean square deviation, m
S_{sq}	sum of squares of deviations
t	time, s
$\boldsymbol{v}$	velocity vector, m s^{-1}
v	drift velocity in Eq. (*4*), m s^{-1}
$\boldsymbol{W}$	three-dimensional Wiener process, $s^{1/2}$
W	one-dimensional Wiener process, $s^{1/2}$
$\boldsymbol{x}$	position vector, m
$\boldsymbol{X}(t)$	position vector of a randomly moving particle, m
$X(t)$	stochastic process (particle position), m
y	initial position, m
$\boldsymbol{y}$	position vector, m
α	constant defining kind of stochastic integral
β	constant defining kind of stochastic integral
Φ	scale of time, s^{-1}
κ	constant in Eq. (*26*), m^{-2} s^{-1}
λ	constant in Eq. (*26*), m^{-1} s^{-1}
σ	constant in Eq. (*26*), m^{-1} $s^{-1/2}$
σ^2	variance, m^2
Subscripts	
i	i-th time step
0	related to initial time instant
r	relative quantity
s	steady state
x	related to x-axis
1	related to beginning of interval
2	related to end of interval
Superscripts	
I	Ito stochastic integral ($\alpha = 0$)
S	Stratonovich stochastic integral ($\alpha = 1/2$)
T	transport stochastic integral ($\alpha = 1$)
α	kind of stochastic integral
β	kind of stochastic integral

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