Modern methods of direct numerical simulations of transfer processes in random media

I V Derevich, A K Klochkov
Moscow State Technical University by N.E. Bauman (BMSTU), 2-ya Baumanskaya Str. 5 (main Building), Moscow, Russian Federation 105005
DerevichIgor@bmstu.ru

Abstract. The paper considers the methods of direct numerical investigation of the behaviour of dynamical systems of explosive type under the influence of random noise. Dynamical systems are described by a system of nonstationary ordinary differential equations (ODE). The dynamics of the system, taking into account random noise, is described by a system of stochastic ordinary differential equations (SODE). The paper provides an overview of modern algorithms based on modifications of Runge–Kutta integration methods. The features of the analysis of weak and strong convergence of the SODE integration methods are described. Methods for generating random noise with complex temporal structure (color noise) are described. The method of numerical solution of the system of SODE is used to generate random color noise. Examples of the study of the influence of random noise on biological and mechanical systems of explosive type are presented. It is shown that random noises acting on such systems qualitatively change the character of their behaviour.

1. Introduction
Transfer processes in natural phenomena, in biology, in a large number of technical applications are usually accompanied by random noises [1, 2]. Dynamical systems are described by a system of nonstationary ordinary differential equations. The inclusion of random noise in the dynamics equations leads to a fundamentally new type of stochastic ordinary differential equations. We do not use popular Monte Carlo methods, the inclusion of which in the algorithm for solving ODE systems and generating random noise of a given structure is difficult. The proposed methods of direct numerical modeling are based on modern methods for solving systems of stochastic ordinary differential equations (SODE) [3, 4]. Methods of direct numerical simulation allow us to identify qualitatively new features of the behavior of dynamic systems under the influence of random noise.

2. Algorithms for numerical integration of SODE
The dynamics of a random parameter $X(t)$ is represented by the Langevin equation

$$\frac{dX(t)}{dt} = A(X(t), t) + B(X(t), t)\xi(t) \quad X(0) = X_0$$

(1)

where $A(x, t), B(x, t)$ are deterministic functions; which is the delta time-correlated in time random Gaussian process (white noise)

$$\langle \xi(t')\xi(t''\rangle = \delta(t' - t'') \quad \langle \xi(t) \rangle = 0 \quad \langle \xi^2 \rangle = 1 \quad \xi(t) \sim N(0,1)$$
2.1. Multistage Runge Kutta methods for SODE

For the stochastic equation (1), the multistage \((s\)-stage) algorithm is written as follows

\[
x_i = x_n + \Delta t \sum_{j=1}^{s} R_{ij} A(x_j, t_{n}) + \Xi \sum_{j=1}^{s} \hat{R}_{ij} B(x_j, t_{n})
\]

\[
X_{n+1} = X_n + \Delta t \sum_{j=1}^{s} r_{ij} A(x_j, t_{n}) + \Xi \sum_{j=1}^{s} \hat{r}_{ij} B(x_j, t_{n})
\]

\[\Xi = \sqrt{\Delta t \xi} \]

Here the expressions for the matrices \(R_{ij}, \hat{R}_{ij}\) and vectors \(r_{ij}, \hat{r}_{ij}\) can be found, for example, in [3, 4]; \(\xi\) is random numbers generated by a computer, distributed according to the Gauss law with zero mean value and unit variance.

2.2. Analysis of strong and weak convergence of SODE integration methods

Due to the fractal structure of random curves, which are the solution of SODE, a comparison of the exact and numerical solutions can be carried out only at selected points. Let us present the results of the analysis on the example of a stochastic equation that has analytical solution \(X_{\text{ex}}(t)\)

\[
dX(t) = \lambda X(t) dt + \mu X(t) dW(t) \quad X(0) = X_0 \quad X_{\text{ex}}(t) = X_0 \exp \left\{ \left( \lambda - \mu^2/2 \right) t + \mu W(t) \right\}
\]

Figure 1 illustrates the result of numerical integration of SODE. The method has a strong convergence of order \(\gamma\) if there is a constant \(C\) that the condition is true

\[e_s = \left| X_n - X_{\text{ex}}(t_n) \right| \leq C \Delta t^\gamma\]

Here \(\langle \ldots \rangle\) denotes averaging over an ensemble of turbulent fluctuations.

The method has weak order \(\sigma\) convergence if there is a constant \(C\)

\[e_w = \left| X_n - \langle X_{\text{ex}}(t_n) \rangle \right| \leq C \Delta t^\sigma\]

Figure 2 shows the results of numerical experiments on the study of strict and weak convergence.

**Figure 1.** Numerical (lines) and exact solution of SODE (points). The dotted line shows the solution without noise.

**Figure 2.** Illustration of the strong and weak convergence of the SODE integration method using the modernized Runge-Kutta algorithm.
3. Generating random noise of a complex temporal structure

In the canonical Langevin equation, the source of the random behaviour of the system is white noise. White noise has infinite energy and is a rough approximation of real random processes. The generation of random processes with a given time structure (color noise) is possible based on the solution of stochastic differential equations.

3.1. A random process with an exponentially decaying autocorrelation function

We will write the system of stochastic equations for the newly generated process \( U(t) \) and \( V(t) \) in the following form

\[
\frac{dU}{dt} = \frac{1}{T}(\xi - U) \quad U(0) = U_0
\]

\[
\frac{dV}{dt} = \frac{1}{\tau}(U - V) \quad V(0) = V_0
\]

Here \( \xi(t) \) is delta-correlated in time random process (white noise); for the observation time \( t \geq \max(T, \tau) \) the dependence on the initial conditions disappears and the processes \( U, V \) become statistically stationary.

The correlation of a random process \( U(t) \) and \( V(t) \) has the form

\[
\langle U(t') U(t'') \rangle = \langle U^2 \rangle \Psi_U(t'' - t')
\]

\[
\langle V(t') V(t'') \rangle = \langle V^2 \rangle \Psi_V(t'' - t')
\]

Here \( \langle U^2 \rangle \), \( \langle V^2 \rangle \) are dispersions of random processes.

The analytical solution of equation (3) and equation (4) can be found by methods of spectral analysis of random processes [5]. The autocorrelation function of a random process \( U(t) \) decays exponentially in time. The process \( U(t) \) is not differentiable, while the process \( V(t) \) is differentiable.

Figure 3. Autocorrelation functions and the ratio of dispersion. Points are the results of numerical modeling; curves are analytical formulas.

Figure 3 represents the result of comparison of numerical integration of the SODU system with equation (3) and equation (4) and analytical calculations.

3.2. Random processes of a complex temporal structure

Stochastic differential equations are effective in creating random multiscale processes. We will illustrate this by the example of a system of two conjugate equations

\[
\frac{dU^{(a)}}{dt} = \frac{1}{T^{(a)}}(\xi^{(a)} - \chi^{(a)} U^{(b)} - U^{(a)})
\]

\[
\frac{dU^{(b)}}{dt} = \frac{1}{T^{(b)}}(\xi^{(b)} + \chi^{(a)} U^{(a)} - U^{(b)})
\]

Here \( \chi^{(a)} > 0, \chi^{(b)} > 0 \) are coefficients of mutual influence of random processes \( U^{(a)}(t), U^{(b)}(t) \); \( T^{(a)}, T^{(b)} \) are temporary macroscales; \( \xi^{(a)}(t), \xi^{(b)}(t) \) are installed independent sources of chaotic movement (white noise) \( \langle \xi^{(a)}(t) \rangle = \langle \xi^{(b)}(t) \rangle = 0 \).
We determine the correlation of random processes $U^{(\alpha)}(t), U^{(\beta)}(t)$ as
\[ \langle U^{(\alpha)}(t') U^{(\beta)}(t^*) \rangle = \psi^{(\alpha \beta)}(t' - t^*) \]

Stochastic equations (5) and equations (6) are integrated numerically. Figure 4 illustrates a satisfactory agreement between the results of direct numerical stimulation and analytical results.

Figure 4. The correlation function of a random process and the mutual correlation processes. Points are the results of direct numerical modeling; curves are analytical formulas.

Let us consider a random process $V(t)$ in which the source is synthesized noise $U^{(\alpha)}(t) + U^{(\beta)}(t)$
\[ \frac{dV}{dt} = \frac{1}{\tau} U^{(\alpha)} + U^{(\beta)} - V \]  \hfill (7)

As a result of numerical integration of equation (5), equation (6), and equation (7), we obtain the dependence of the autocorrelation function and the dispersion of a random process $V(t)$ on the parameter $\tau$ (Figure 5).

Figure 5. Comparison of the results of direct numerical simulation (points) with analytical solutions (curves) for the autocorrelation function and the dispersion of the process $V(t)$.

4. Examples of simulating technical and biological systems

In this section we will present examples of direct numerical simulation of the influence of random noise on transfer processes in biological and technical systems.

4.1. Random movement of a particle in a bimodal potential

The particle moves in a random velocity field of the medium in a bimodal potential. This simple model is promising for describing not only technical devices, but also for modeling complex biological processes at the cellular level [6, 7]. The equation system for the random trajectory of a particle $X(t)$ and the velocity fluctuation of the carrier medium $U(t)$ has the form
\[ \frac{dX}{dt} = G(X(t)) U(t) - \frac{d\Xi(X)}{dX} \bigg|_{X=X(t)} \]  \hfill (8)
Figure 6. The potential of the force field and the random trajectories of the particle. Examples of deterministic trajectories are shown.

Figure 6 shows the distribution of the force field potential and examples of deterministic and random particle trajectories. Unlike deterministic trajectories, which certainly fall into the position of potential minima, random trajectories migrate from one minimum to another.

Figure 7. Empirical PDF (histograms) and the solution of the equation for PDF (lines). The dashed line shows the position of the maximum of the initial PDF.

The numerical solution of equation (3) and equation (9) illustrates the dynamics of transformation of an initially non-equilibrium probability density function (PDF) into an equilibrium PDF (Figure 7). It can be seen that random noise qualitatively changes the behavior of the system in comparison with the deterministic case. It can be seen that, regardless of the initial coordinate of the particle, the stationary distribution of the PDF will have a bimodal structure.

4.2. The effect of random migration on the growth of the concentration of pathogenic virus

The equation of the growth of virus concentration in the body of an individual \( X(t) \), taking into account the random change in the concentration of the virus in the surrounding atmosphere \( \tilde{U}(t) \), has the form [8]

\[
\frac{dX(t)}{dt} = \alpha X(t) \left[ X(t) - 1 \right] + \frac{\tilde{U}(t) - X(t)}{T} \quad \tilde{U}(t) = U_0 + U(t) \quad U_0 = \langle \tilde{U}(t) \rangle \quad X(0) = X_0
\]

Here \( U_0 \) is an average concentration of the virus in the atmosphere; \( T \) is a characteristic time of diffusion and transport of the virus to the organs of its intensive reproduction.

Fluctuations in the concentration of the virus \( U(t) \) in the atmosphere are caused by random relative movement of individuals in the group. There is a critical concentration inside the body, exceeding which leads to an explosive increase in the concentration of the virus in the body. Equation (3) and equation (9) were numerically integrated.

Figure 8. Examples of random realizations of the virus concentration in the body when the virus concentration in the atmosphere is below the critical value. Dashed lines - analytical results.
It follows from Figure 8 that fluctuations in the concentration of the virus in the atmosphere can lead to the intensive development of a disease, even if the average concentration of the virus in the atmosphere is significantly lower than the critical value.

4.3. Influence of surroundings temperature fluctuations on the thermal explosion of a particle

The equation for the temperature of a particle with an exothermic chemical reaction in the environment with temperature fluctuations has the form [9]

$$\frac{d\Theta(t)}{dt} = \frac{1}{\tau} \left[ U(t) - \Theta(t) \right] + \frac{QA}{c} \exp \left( -\frac{E_{act}}{R\Theta(t)} \right) \Theta(0) = \Theta_0 \quad \tilde{U}(t) = U_0 + U(t) \quad (10)$$

Here $A$ is the rate of chemical reaction; $Q$ is the thermal effect of reaction; $R$ is the universal gas constant; $E_{act}$ is the activation energy of the reaction; $c$ is the heat capacity of the particle; $U_0$ is the averaged temperature of the surroundings; $U(t)$ represents temperature fluctuations.

There is a critical temperature, exceeding which always leads to a thermal explosion (Figure 9). The integration of equation (3) and equation (10) illustrates the random trajectories of the particle temperature leading to a thermal explosion. Note that a thermal explosion in a deterministic theory is impossible if the initial temperature of the particle is below the critical temperature.

5. Conclusions

A method for integrating systems of stochastic differential equations based on modernized Runge-Kutta algorithms is presented. The criteria for evaluating the effectiveness of algorithms are described. Systems of stochastic differential equations are used to generate color noise with a complex temporary structure. Qualitatively new effects under the influence of color noise on dynamic systems of a biological and technical nature are illustrated. In random fields, nonlinear dynamic systems of the explosive type lose stability under initial conditions that are far from critical values in the deterministic case.

Acknowledgments

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