Available online at www.sciencedirect.com

ScienceDirect

Journal of Taibah University for Science 8 (2014) 186–198

Journal of Taibah University for Science

www.elsevier.com/locate/jtusci

Multidimensional Milstein scheme for solving a stochastic model for prebiotic evolution

Mostafa Zahri *

Department of Mathematics, Faculty of Sciences, University of Taibah, P.O. Box 30002, Madinah, Saudi Arabia

Received 5 July 2013; accepted 27 December 2013
Available online 10 January 2014

Abstract

A multi-dimensional system of stochastic differential equations is presented for modeling prebiotic evolution. The system consists of replication of several reacting species using activated monomers and inactivated residues. The stochastic effects are included in the system as excitations which can be caused by the prebiotic medium where the reactions are taking place. To numerically solve the considered system we consider a generalized Milstein method for multi-dimensional stochastic differential equations. A first-order accuracy is ensured in the approximation of double Itô integrals by using a truncation in the Fourier series expansion. To verify the accuracy of the proposed method we consider a system of two stochastic differential equations with known analytical solution. Numerical results are presented for a reduced prototype system of the prebiotic model.

MSC: 35R60; 35K57; 60H15; 65L06

Keywords: Stochastic differential equations; Prebiotic evolution; RNA-like molecules; Milstein method

After the discovery of the catalytic process of some RNA-like molecules (ribozymes) [2,7], the formation of prebiotic material has been subject of many theoretical an experimental studies, see [11,1] among others. These RNA-like molecules (also referred to as replicators) with unspecific catalytic capabilities could have formed ensemble of species, the so-called catalytic networks. It should be pointed out that, although the evolution of these catalytic networks has been extensively studied from a theoretical point of view over the last decades, most of the work has been focused on the analysis of their dynamics under deterministic input conditions [11,1,5]. Less attention has been given to the role of stochastic excitations on the behavior of these prebiotic models. However, it is well known that stochastic forces may play an important role on the dynamics of the biochemical systems. For instance, the stochastic forces may probably occur in the reaction medium known by the prebiotic soup, see [3] for more details. Therefore, it ought to be taken into account in the mathematical equations governing these models.

In this paper, we consider the problem of prebiotic evolution in one of the theoretical models proposed to study the behavior of catalytic networks [6]. This model is a closed system (only energy can be interchanged with the surroundings) where activated material (nucleotides) react to build up self-replicative

* Tel.: +966 599486488.
E-mail addresses: mzahri@taibahu.edu.sa, zahri@gmx.net
Peer review under responsibility of Taibah University.

ELSEVIER Production and hosting by Elsevier

1658-3655
http://dx.doi.org/10.1016/j.jtusci.2013.12.002

units following preestablished rules. These energy rich monomers are regenerated from the by-product of the reaction (obtained mainly as the result of the hydrolysis of self-replicative species) by means of a recycle mechanism (basically due to an external energy source, for example sunlight). The closure of the system directly imposes a selection pressure on the population. All these biochemical features can be mathematically modeled by a multi-dimensional system of deterministic ordinary differential equations with nonlinear kinetic reactions, see for example [4,6]. The spatial effects can also be incorporated into this model by introducing the diffusion operator in the ordinary differential equations resulting in a set of reaction–diffusion equations, compare [11,1]. To stabilize these partial differential equations, authors in [12] have added an additive noise into the system. In the present work, we propose a new technique to account for excitations from the prebiotic medium. The key idea is to introduce a stochastic diffusion matrix in the system of ordinary differential equations and transform this model to a system of stochastic differential equations. Here, we consider a drift term driven by both additive and multiplicative noises and it can be raised from uncertainties in catalytic coefficients or simply by excitations from the prebiotic medium. The main advantage of such approach comes from the fact that features of interest in random dynamics (*i.e.* random fixed points, random bifurcation, random attractors, etc.) are harder to describe in the framework of stochastic calculus than in the framework of classical deterministic calculus.

To numerically approximate the solutions of the proposed system, we apply a generalized Milstein method. The basic ingredients of this approach are the piecewise linear approximation by the Itô–Taylor expansion of the vector fields and the numerical integration of the resulting linear equation. Fourier series expansions are used to approximate double Itô integrals. In the case of stochastic differential equations, the Milstein method has been restricted either to the class of equations with additive noise terms or scalar equations with multiplicative noise. Therefore, the application of the Milstein method to cover wider classes of stochastic differential equations is an appealing challenge. In particular, the current study focuses in the class of stochastic differential equations driven by multiplicative noise. Numerical results are presented for a prototype system of four catalyzed selfreplicator species along with activated and inactivated residues. Phase-space portraits and strange attractors are also displayed.

This paper is organized as follows. In Section 1 we describe the model for prebiotic evolution. The Milstein method for multi-dimensional systems of stochastic differential equations is formulated in Section 2. In Section 3 we present numerical results for two accuracy test examples and for the reduced prebiotic model. Section 4 summarizes the paper with concluding remarks.

1. Stochastic model for prebiotic evolution

The model we consider in this paper consists on the replication of N reacting species $I_1, I_2, \ldots, I_N$ using activated monomers A and inactivated residues B according to the following reactions:

$$I_i + A \xrightarrow{\alpha_i} 2I_i, \tag{R1}$$

$$I_i + I_j + A \xrightarrow{k_{ji}} 2I_i + I_j, \tag{R2}$$

$$I_i \xrightarrow{\delta_i} B, \tag{R3}$$

$$B \xrightarrow{\gamma} A. \tag{R4}$$

These reaction steps have been used in pattern formation in a model proposed to study the behavior of catalytic networks in the RNA-like molecules, compare [11,1,5] among others. This notation is intended to be similar to that used in traditional chemistry for which the steps (R1) and (R2) mean:

(R1) Each specie I_i ($i = 1, \ldots, N$), in the presence of the substrate A, selfreplicates noncatalytically with a rate α_i.
(R2) Specie I_j ($j \neq i$) catalyzes the selfreplication of the species I_i with a rate k_{ji} in the presence of the substrate A.
(R3) Specie I_i degrades in B with a rate δ_i.
(R4) The product of the degradation B is recyclated in energy-high substrate A with a rate γ.

For more details on biochemical aspects of the considered model we refer the reader to [11,1,5] and further references are cited therein. The above set of reactions can be mathematically formulated based on deterministic ordinary differential equations (ODE). Thus, if we use the notations x_i, y and z to denote, respectively, the concentrations of the selfreplicator species I_i, the activated monomers A and the inactivated residues B then