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An integration factor method for stochastic and stiff reaction–diffusion systems

Catherine Ta, Dongyong Wang, Qing Nie *

Department of Mathematics, University of California, Center for Mathematical and Computational Biology, Center for Complex Biological Systems, Irvine, CA 92697, USA

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ABSTRACT

Stochastic effects are often present in the biochemical systems involving reactions and diffusions. When the reactions are stiff, existing numerical methods for stochastic reaction diffusion equations require either very small time steps for any explicit schemes or solving large nonlinear systems at each time step for the implicit schemes. Here we present a class of semi-implicit integration factor methods that treat the diffusion term exactly and reaction implicitly for a system of stochastic reaction–diffusion equations. Our linear stability analysis shows the advantage of such methods for both small and large amplitudes of noise. Direct use of the method to solving several linear and nonlinear stochastic reaction–diffusion equations demonstrates good accuracy, efficiency, and stability properties. This new class of methods, which are easy to implement, will have broader applications in solving stochastic reaction–diffusion equations arising from models in biology and physical sciences.

1. Introduction

Complex patterns can be extensively found in nature, from the skin of zebrafish to the disposition of feather buds in chicks and hair follicles in mice. Often, those patterns are created by biochemical reactions along with diffusions of the molecules in a cellular or multi-cellular systems [1]. Such biological systems, which may be described in reaction–diffusion equations, are constantly subjected to stochastic effects such as noises and environmental perturbations. The stochastic effects on the biochemical reactions at the single-cell level can result in heterogeneous responses of cellular populations and influence their behaviors [2]. Previous studies on stochasticity reveal the adaptation of biological systems to noise, which can be characterized by the systems' strategies to combat noise, whether by attenuating or exploiting it [2,3]. For example, spatial stochastic effects help to either prompt the tight localization of proteins or enhance the response to the directional change of a moving pheromone input, resulting in a more robust cell polarization [4]; and the boundary of gene expression domains is sharpened as a result of gene-switching prompted by intracellular noise [5]. It has become increasingly important to incorporate these stochastic effects into the reaction–diffusion equations for better understanding of biological systems.

One can describe a biological system in terms of the following stochastic reaction–diffusion equations:

$$\frac{\partial U}{\partial t} = a\frac{\partial^2 U}{\partial x^2} + f(U) + g(U)\dot{W}(x,t) \tag{1}$$

* Corresponding author.
E-mail address: qnie@uci.edu (Q. Nie).

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where $\dot{W}(x,t)$ is a standard two-dimensional Wiener process.

One typical way of solving Eq. (1) numerically is to apply central difference first to the diffusion and then use the temporal explicit scheme to solve the subsequent system [6], such as using the explicit Euler method [7] or the two, three, and four-stage explicit Runge Kutta schemes for the system containing additive noise and one-dimensional Wiener process in [8]. Another common approach is using the Galerkin projection of the stochastic partial differential equation (SPDE) and then applying the numerical scheme to a finite-dimensional version of the SPDE. For example, Exponential Time Differencing (ETD) scheme may be applied to the Galerkin projection of the SPDE [9,10]. One other such example is the Lord and Rougemont scheme, which is derived through Galerkin projection and an integrating factor approach [11]. This scheme is most effective for SPDE with Gevrey regularity, and more improvement may be made on such schemes by taking advantage of the Itô–Taylor expansion [11].

While explicit temporal schemes may be directly implemented for various spatial discretization, including finite element and Galerkin methods [12], to deal with the stability constraint associated with the diffusions, one can treat the diffusion term implicitly, while treating other terms explicitly [6] such as implicit Euler and Crank–Nicolson schemes [7]. Higher order methods [13] can be achieved using Galerkin projection and the linear-implicit versions of strong Taylor schemes [10]. Non-uniform time discretization on Brownian motion can also be obtained for implicit Euler scheme [14].

Stochastic stiffness arises from large differences in the magnitudes of Lyapunov exponents [15], resulting in the presence of different time scales. As in the deterministic case, explicit methods face step-size constraint when used to solve stiff stochastic systems [16]. The time-step constraint can be improved with the modification of the stochastic term by adding more terms from the Itô–Taylor expansion for higher order of accuracy and stability. One of the most well-known schemes stemmed from this construction is the Milstein scheme [15]. Treating the stochastic term implicitly is also one of the popular approaches [17–20], albeit computationally expensive. Hence, a class of explicit methods known as Chebyshev methods are derived, which have better mean-square stability than explicit Euler method and are not as computationally expensive as implicit methods [21]. A combination of different numerical schemes into one method can also be seen, such as the case of the Composite Euler scheme [22]. For this scheme, at each temporal step, the stochastic differential equation is either solved by implicit Euler method or semi-implicit Euler method. The Composite method has similar order of convergence 1/2 to the Euler Maruyama method but better stability.

Most of the methods mentioned so far are derived to combat the stochastic stiffness through the improvement of the stochastic term, which can be costly and not as effective if the stiffness only occurs in the deterministic term. In such case, methods that treat the deterministic term implicitly while keeping an explicit treatment of the stochastic term are preferred [18]. Here, we propose a new approach to the problem of stiffness caused by the deterministic term, more specifically the reaction term in Eq. (1). The approach is based on the semi-Implicit Integration Factor (IIF) methods [23–26], which has been found to be effective for the stiff reaction–diffusion equations with better stability constraints imposed on the time steps associated with both reaction and diffusion. In this approach, the time-step constraint for the diffusion term arising due to the inverse of the eigenvalues of the diffusion matrix, which can be large in magnitude, is resolved by treating the linear diffusion term exactly using Integration Factor (IF) methods. Such treatment results in an exponential function of the diffusion term and an integral of the nonlinear reaction term, which is then treated using implicit approach through the Lagrange interpolation to deal with its stiffness. Appropriate choices of approximation schemes lead to decoupling on the treatment for the diffusions and reactions such that one only needs to solve nonlinear systems with the size of the original PDEs. The IIF methods also have exceptional stability properties and its second-order version is absolutely stable. For higher-dimensional problems, the compact IIF (cIIF) method [24] is a great improvement on computational efficiency without altering the stability properties of the IIF methods [23].

In this paper, we exploit the simple structure of the IIF methods as well as their desirable stability properties and efficiency for solving the system in Eq. (1). Because of the nice decoupling properties in the IIF method, we will treat the deterministic diffusion and reaction terms in a similar fashion [23], while dealing with the stochastic term explicitly as in the Euler Maruyama method [27]. We compare this approach with similarly constructed schemes whose main difference is in the treatment of the deterministic part of the equation, which can be approximated using ETD, Crank–Nicolson, or Implicit Euler methods. When all of the properties such as order of accuracy, mean errors, and stability region are taken into consideration, the new approach shows many advantages. We also take advantage of the low computational cost of the cIIF methods to similarly construct a stochastic method that can be applied to higher-dimensional problems. The paper is organized as followed. We first present the construction of the method for systems with additive noise or multiplicative noise, along with linear stability analysis and their comparisons with several other methods. Next, we compare the new method with other methods on linear SODEs and SPDEs on their orders of accuracy and stability constraints. Then, we use this approach to study a nonlinear activator–substrate system of two diffusion species and lastly, make our conclusion.

2. Implicit integration factor methods

2.1. Construction of general method

We consider the stiff reaction–diffusion equation with spatial white noise below:

$$\frac{\partial U}{\partial t} = a\frac{\partial^2 U}{\partial x^2} + f(U) + g(U)\frac{\partial^2 W}{\partial x \partial t} \tag{2}$$