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Stochastic Runge-Kutta Methods for Preserving Maximum Bound Principle of Semilinear Parabolic Equations. Part I: Gaussian Quadrature Rule

Yabing Sun[1] and Weidong Zhao[2,*]

[1] *College of Science, National University of Defense Technology, Changsha 410073, China.*
[2] *School of Mathematics, Shandong University, Jinan 250100, China.*

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Abstract. In this paper, we propose a class of stochastic Runge-Kutta (SRK) methods for solving semilinear parabolic equations. By using the nonlinear Feynman-Kac formula, we first write the solution of the parabolic equation in the form of the backward stochastic differential equation (BSDE) and then deduce an ordinary differential equation (ODE) containing the conditional expectations with respect to a diffusion process. The time semidiscrete SRK methods are then developed based on the corresponding ODE. Under some reasonable constraints on the time step, we theoretically prove the maximum bound principle (MBP) of the proposed methods and obtain their error estimates. By combining the Gaussian quadrature rule for approximating the conditional expectations, we further propose the first- and second-order fully discrete SRK schemes, which can be written in the matrix form. We also rigorously analyze the MBP-preserving and error estimates of the fully discrete schemes. Some numerical experiments are carried out to verify our theoretical results and to show the efficiency and stability of the proposed schemes.

AMS subject classifications: 35B50, 60H30, 65L06, 65M12

Key words: Semilinear parabolic equation, backward stochastic differential equation, stochastic Runge-Kutta scheme, MBP-preserving, error estimates.

1 Introduction

In this paper, we consider the following initial-boundary-value problem of a second-order semilinear parabolic partial differential equation (PDE):

*Corresponding author. *Email addresses:* `sunybly@163.com` (Y. Sun), `wdzhao@sdu.edu.cn` (W. Zhao)

$$\begin{aligned} &u_t = \frac{1}{2}\sigma\sigma^\top : \nabla^2 u + f(u), && (t,\boldsymbol{x}) \in (0,T] \times D, \\ &u(t,\cdot) \quad \text{is } D\text{-periodic}, && t \in [0,T], \\ &u(0,\boldsymbol{x}) = \varphi(\boldsymbol{x}), && \boldsymbol{x} \in \overline{D}, \end{aligned} \tag{1.1}$$

where $u(t,\boldsymbol{x})$ denotes the unknown function, $\nabla^2 u$ is the Hessian matrix of u with respect to $\boldsymbol{x}$, f is a nonlinear operator, $D=(0,a)^d \subset \mathbb{R}^d\,(d=1,2,3)$ is a hypercube domain, and the matrix $\sigma \in \mathbb{R}^{d\times d}$ is defined as

$$\sigma = \begin{pmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_d \end{pmatrix}, \quad \sigma_i \neq 0, \quad i=1,\ldots,d.$$

Since the matrix $A=\sigma\sigma^\top/2$ is symmetric and positive definite uniformly, it is well known that the semilinear parabolic equation (1.1) possesses the maximum bound principle [8]. The semilinear parabolic equation (1.1) can be used to describe the evolution of physical quantities, such as density, concentration and pressure, which only take values in a given range to be consistent with physical phenomena. Therefore, the MBP is an indispensable tool to study physical features of semilinear parabolic equations, including the aspects of mathematical analysis and numerical simulation. Up to now, great efforts have been made in developing MBP-preserving numerical methods for equations like (1.1), such as the stablized linear semi-implicit method [24, 25], the nonlinear second-order method [9, 10], the exponential time differencing method [7, 8], the integrating factor method [13, 16, 17], the exponential cut-off method [15, 29], and the exponential-SAV method [11, 12]. As for the spatial discretizations, a partial list includes the works for finite element method [2, 5, 15, 27, 28, 30], finite difference method [3, 4, 26], and finite volume method [21, 22]. Moreover, by using a regularized energy technique in their recent work [6], the authors studied the effect of noise on the MBP-preserving property and energy evolution property of numerical methods for parabolic stochastic partial differential equation with a logarithmic Flory-Huggins potential.

Note that the efficient spectral method can not be used to construct the MBP-preserving numerical schemes for the equations like (1.1), and to match the high temporal accuracy of the existing high order numerical schemes, the spatial size needs to be very small, which leads to heavy computational efforts. Thus, it is necessary to construct some numerical schemes with efficient spatial discretizations. On the other hand, Pardoux and Peng studied the existence and uniqueness of the backward stochastic differential equation in their pioneer work [20], and then by using the theory of BSDE, Peng [23] developed the nonlinear Feynman-Kac formula, which gives a probabilistic representation of the solution of the semilinear parabolic equation including the one like (1.1).

Motivated by such probabilistic interpretation, we are aim to construct a class of MBP-preserving stochastic Runge-Kutta methods for solving (1.1) avoiding to approximate the