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

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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):

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

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 differential operators contained in the equation. To be more specific, we first represent the solution of (1.1) using an integral equation without containing any differential operator, but containing a conditional expectation with respect to a diffusion process. Then based on such integral equation, by combining the properties of the diffusion process and conditional expectation, we propose a class of explicit time semidiscrete SRK schemes up to fourth order. We rigorously prove the MBP-preserving of the proposed semidiscrete schemes and theoretically derive their sharp error estimates. Moreover, a class of fully discrete SRK schemes are constructed by approximating the conditional expectations in the semidiscrete schemes using the Gaussian quadrature rule. To show the MBP-preserving of the fully discrete SRK schemes, we write the fully discrete one-stage and two-stage SRK schemes in the matrix form by setting the number of quadrature points to be three and choosing an appropriate spatial mesh size. Then by using the property of the coefficient matrix, we prove their fully discrete MBP-preserving and error estimates in detail. Since the proposed fully discrete schemes can be written in the matrix form as the finite difference method, they are very simple in structure and can be implemented efficiently via the fast fourier transform (FFT) technique. Some numerical experiments including the convergence tests and long time simulations verify our theoretical conclusions and show the efficiency and stability of the proposed fully discrete schemes.

The rest of this paper is organized as follows. In Section 2, we present the probabilistic representation of the solution of (1.1) and give a probabilistic explanation for its MBP property. Based on such probabilistic representation, we propose a class of time semidiscrete SRK schemes for solving the Eq. (1.1), prove their MBP-preserving and derive their error estimates in Section 3. In Section 4, we further construct a class of fully discrete SRK schemes by approximating the conditional expectations in time semidiscete schemes using the Gaussian quadrature rule, and prove their MBP-preserving and error estimates. In Section 5, some numerical tests are carried out to verify our theoretical results, and we finally give some concluding remarks in Section 6.

2 The probabilistic interpretation of PDE

In this section, we introduce the probabilistic representation of the solution of semilinear parabolic equation (1.1) and present a probabilistic explanation for its MBP property.

2.1 The nonlinear Feynman-Kac formula

Let $(\Omega,\mathcal{F},\mathbb{F},P)$ be a filtered complete probability space with the filtration $\mathbb{F}=(\mathcal{F}_t)_{0\leq t\leq T}$ being generated by a d-dimensional Brownian motion $W=(W_t)_{0\leq t\leq T}$. Then we consider the following backward stochastic differential equation (BSDE) defined on $(\Omega,\mathcal{F},\mathbb{F},P)$:

$$Y_t=\varphi(X_T)+\int_t^T f(Y_r)dr-\int_t^T Z_r dW_r, \quad 0\leq t\leq T, \tag{2.1}$$

where $\{X_t, 0\leq t\leq T\}$ is a d-dimensional diffusion process defined by

$$X_t = X_0 + \sigma W_t$$

with $X_0 \in \mathcal{F}_0$ being the initial condition. A couple (Y_t, Z_t) is called an L^2-adapted solution of the BSDE (2.1) if it is $\mathcal{F}_t$-adapted, square integrable and satisfies (2.1). To give its probabilistic interpretation by using the above BSDE, we write (1.1) in the backward form as

$$\begin{aligned} &u_t + \frac{1}{2}\sigma\sigma^\top : \nabla^2 u + f(u) = 0, \quad && (t,\boldsymbol{x}) \in [0,T)\times D, \\ &u(T,\boldsymbol{x}) = \varphi(\boldsymbol{x}), && \boldsymbol{x}\in \overline{D}. \end{aligned} \tag{2.2}$$

Then the nonlinear Feynman-Kac formula in the following lemma [23, 31] reveals the relationship between the PDE (2.2) and the BSDE (2.1).

Lemma 2.1. *Assume that the functions f and φ are Lipschitz continuous, then the BSDE* (2.1) *admits a unique adapted solution (Y_t, Z_t) and the viscosity solution of the PDE* (2.2) *can be represented as*

$$u(t,\boldsymbol{x}) = Y_t^{t,\boldsymbol{x}}, \tag{2.3}$$

where $Y_t^{t,\boldsymbol{x}}$ is the value of Y_t with X_t starting from $(t,\boldsymbol{x})$. Conversely, if u is the classical solution of the PDE (2.2)*, then the solution of the BSDE* (2.1) *can be represented as*

$$Y_t = u(t,X_t), \quad Z_t = (\nabla u\sigma)(t,X_t), \tag{2.4}$$

which are the so called nonlinear Feynman-Kac formula.

Remark 2.1. Because of the maximum bound principle, the Lipschitz condition on the nonlinear term f is automatically satisfied in the above lemma, which is used to guarantee the existence and uniqueness of the solution of BSDEs [20]. Moreover, we point out that we can weaken the Lipschitz condition on f in the above lemma. For instance, under the monotonicity assumption on f, this condition is weakened to the polynomial growth in [1] and to an arbitrary growth in [19]. However, for presentational simplicity, we still assume the Lipschitz condition on f in this paper.

Remark 2.2. Note that the representation (2.3) only gives the viscosity solution of the PDE (2.2). To construct high order fully discrete Runge-Kutta schemes for solving (2.2) in theoretical level, we shall need some smoothness requirements for the solution u. Fortunately, when φ and f are smooth enough, the viscosity solution u becomes the classical solution. In fact, for $k=0,1,2,\ldots$, if $f\in C_b^{2+2k}$ and $\varphi\in C_b^{2+2k+\alpha}$ for some $\alpha\in(0,1)$, then $u\in C_b^{1+k,2+2k}$ (see [32]). Here C_b^l denotes the set of continuous differentiable functions $\phi(\boldsymbol{x})$ with uniformly bounded partial derivatives up to the l-th order and $C_b^{l+\alpha}$ is the set of functions in C_b^l whose l-th order derivative is Holder continuous with index α. Because of the maximum bound principle, such smoothness requirement is not hard to satisfy.

2.2 The maximum bound principle

In this subsection, we show that the maximum bound principle of the semilinear parabolic equation (2.2) is a direct result of the comparison theorem for BSDE. First, we recall the comparison theorem [14].

Theorem 2.1. *Let (Y_t^i,Z_t^i) for $i=1,2$ be the solutions of the following BSDEs:*

$$Y_t^i=\xi^i+\int_t^T f^i\left(Y_r^i\right)dr-\int_t^T Z_r^i dW_r,\quad 0\le t\le T,$$

respectively, where the functions $f^i:\mathbb{R}\to\mathbb{R}$ are Lipschitz continuous and the terminal conditions $\xi^i\in\mathcal{F}_T$ are square integrable random variables. Then if almost surely

$$\xi^1\ge\xi^2,\quad f^1\left(Y_t^2\right)\ge f^2\left(Y_t^2\right),$$

we have that almost surely for any time $t\in[0,T]$, $Y_t^1\ge Y_t^2$.

Theorem 2.2. *Assume that f and φ are Lipschitz continuous and there exists a positive constant ρ such that*

$$f(\rho)=f(-\rho)=0.$$

Then if $-\rho\le\varphi(\boldsymbol{x})\le\rho$ for any $\boldsymbol{x}\in\overline{D}$, the classical solution $u(t,\boldsymbol{x})$ of (2.2) *satisfies*

$$-\rho\le u(t,\boldsymbol{x})\le\rho,\quad \forall\,(t,\boldsymbol{x})\in[0,T]\times\overline{D}.$$

Proof. Take $f^1=f^2=f,\xi^1=\rho$ and $\xi^2=\varphi(X_T)$ in the comparison Theorem 2.1. Since $\varphi(\boldsymbol{x})\le\rho$ for any $\boldsymbol{x}\in\overline{D}$, we have $\xi^1\ge\xi^2$, and thus

$$Y_t^1\ge Y_t^2$$

almost surely. By using the conditions $\xi^1=\rho$ and $f(\rho)=0$, we get

$$\left(Y_t^1,Z_t^1\right)=(\rho,0).$$

Then by the fact $(Y_t^2,Z_t^2)=(Y_t,Z_t)$ and the nonlinear Feynman-Kac formula (2.4), we have

$$Y_t=u(t,X_t)\le\rho \tag{2.5}$$

almost surely.

Let $\Omega_0=\{\omega\in\Omega:Y_t(\omega)\le\rho\}$, then $P(\Omega_0)=1$. Define

$$B:=\{\boldsymbol{x}=X_t(\omega):\omega\in\Omega_0\}\subset\mathbb{R}^d.$$

Since $P(\Omega_0)=1$, we can prove that the complementary of B is a zero measure set, which means that when restricted on Ω_0 (i.e. $Y_t=u(t,X_t)\le\rho$), X_t can reach almost every point in $\mathbb{R}^d$ except a zero measurable set. Thus, X_t can reach almost every point in $\overline{D}$ when restricted on Ω_0. Then by (2.5), we get

$$u(t,\boldsymbol{x}) \le \rho \quad \text{almost everywhere in } \overline{D}.$$

By noting that u is the classical solution of (2.2), we obtain

$$u(t,\boldsymbol{x}) \le \rho, \quad \forall\, (t,\boldsymbol{x}) \in [0,T] \times \overline{D}.$$

Similarly, we have

$$u(t,\boldsymbol{x}) \ge -\rho, \quad \forall\, (t,\boldsymbol{x}) \in [0,T] \times \overline{D},$$

which completes the proof. □

It is worth noting that the condition $f(\rho)=f(-\rho)=0$ is satisfied by many semilinear parabolic equations. For example, the nonlinear function of the Allen-Cahn equation is the negative derivative of a given potential $F(u)$, that is,

$$f(u) = -F'(u).$$

Usually, we consider the Ginzburg-Landau potential

$$F(u) = \frac{1}{4}(u^2-1)^2,$$

and the Flory-Huggins potential

$$F(u) = \frac{\theta}{2}\left[(1+u)\ln(1+u) + (1-u)\ln(1-u)\right] - \frac{\theta_c}{2}u^2.$$

Then we obtain the corresponding odd function $f(u)$ as

$$f(u) = \begin{cases} u - u^3, & \text{Ginzburg-Landau potential,} \\ \dfrac{\theta}{2}\ln\dfrac{1-u}{1+u} + \theta_c u, & \text{Flory-Huggins potential.} \end{cases} \tag{2.6}$$

For the Ginzburg-Landau potential, the positive root of $f(u)$ is

$$\rho = 1.$$

For the Flory-Huggins potential, if we take $\theta = 0.8$ and $\theta_c = 1.6$, then the positive root of $f(u)$ is

$$\rho \approx 0.9575.$$

3 Stochastic Runge-Kutta schemes

In this section, based on the nonlinear Feynman-Kac formula, we develop a class of explicit stochastic Runge-Kutta (SRK) methods for solving the semilinear parabolic equation. To this end, we introduce the following uniform time partition:

$$t_n = n\Delta t, \quad n = 0,1,\ldots,N_t,$$

where $\Delta t = T/N_t$ with N_t being a given positive integer. For a positive integer s, let $\{a_{ij}, i,j = 0,\ldots,s\}$ and $\{c_i, i = 0,\ldots,s\}$ be real numbers satisfying $a_{ij} = 0$ for $i \le j$ and

$$\begin{cases} 0 = c_0 \le \cdots \le c_s = 1, \\ \displaystyle\sum_{j=0}^{i-1} a_{ij} = c_i, \quad i = 0,\ldots,s. \end{cases} \tag{3.1}$$

Then we can define the s intermediate times in the interval $[t_n, t_{n+1}]$ as

$$t_n^i = t_{n+1} - c_i \Delta t, \quad i = 0,\ldots,s,$$

and thus we have $t_n = t_n^s \le \cdots \le t_n^0 = t_{n+1}$.

3.1 The time semidiscrete schemes

To develop the time semidiscrete SRK schemes, for $n = 0,1,\ldots,N_t - 1$, we write the BSDE (2.1) as

$$Y_t = Y_{t_{n+1}} + \int_t^{t_{n+1}} f(Y_r)dr - \int_t^{t_{n+1}} Z_r dW_r. \tag{3.2}$$

By the nonlinear Feynman-Kac formula (2.4), the above equation can be written as

$$u(t,X_t) = u(t_{n+1}, X_{t_{n+1}}) + \int_t^{t_{n+1}} f\big(u(r,X_r)\big)dr - \int_t^{t_{n+1}} (\nabla u \sigma)(r,X_r)dW_r, \tag{3.3}$$

where u is the classical solution of (2.2). Let $\mathcal{M}_t$ be the σ-algebra generated by $\{X_r : 0 \le r \le t\}$, that is, $\mathcal{M}_t = \sigma\{X_0, W_r | 0 \le r \le t\}$. Then it holds that ([18, Theorem 5.21])

$$\mathcal{M}_t \subseteq \mathcal{F}_t, \quad 0 \le t \le T.$$

Since u is the classical solution of (2.2), it is measurable and thus

$$u(t,X_t) \in \mathcal{M}_t, \quad 0 \le t \le T.$$

Now we define the conditional expectation

$$\mathbb{E}_t^{X_t}[\cdot] = \mathbb{E}[\cdot | \mathcal{M}_t], \quad 0 \le t \le T,$$

and take $\mathbb{E}_t^{X_t}[\cdot]$ on both sides of (3.3), and then we obtain

$$u(t,X_t)=\mathbb{E}_t^{X_t}[u(t_{n+1},X_{t_{n+1}})]+\int_t^{t_{n+1}}\mathbb{E}_t^{X_t}\left[f\left(u(r,X_r)\right)\right]dr. \tag{3.4}$$

By taking $t=t_n^i$ in (3.4) for $i=0,\ldots,s$, we get

$$u\left(t_n^i,X_{t_n^i}\right)=\mathbb{E}_{t_n^i}^{X_{t_n^i}}\left[u\left(t_{n+1},X_{t_{n+1}}\right)\right]+\int_{t_n^i}^{t_{n+1}}\mathbb{E}_{t_n^i}^{X_{t_n^i}}\left[f\left(u(r,X_r)\right)\right]dr, \quad i=0,\ldots,s-1, \tag{3.5}$$

$$u\left(t_n,X_{t_n}\right)=\mathbb{E}_{t_n}^{X_{t_n}}\left[u\left(t_{n+1},X_{t_{n+1}}\right)\right]+\int_{t_n}^{t_{n+1}}\mathbb{E}_{t_n}^{X_{t_n}}\left[f\left(u(r,X_r)\right)\right]dr. \tag{3.6}$$

Based on the Eqs. (3.5) and (3.6), we derive the following two reference equations:

$$\bar{u}\left(t_n^i,X_{t_n^i}\right)=\mathbb{E}_{t_n^i}^{X_{t_n^i}}[u(t_{n+1},X_{t_{n+1}})]+\Delta t\sum_{j=0}^{i-1}a_{ij}\mathbb{E}_{t_n^i}^{X_{t_n^i}}\left[f\left(\bar{u}\left(t_n^j,X_{t_n^j}\right)\right)\right], \quad i=0,\ldots,s-1, \tag{3.7}$$

$$u(t_n,X_{t_n})=\mathbb{E}_{t_n}^{X_{t_n}}[u(t_{n+1},X_{t_{n+1}})]+\Delta t\sum_{i=0}^{s-1}a_{si}\mathbb{E}_{t_n}^{X_{t_n}}\left[f\left(\bar{u}\left(t_n^i,X_{t_n^i}\right)\right)\right]+R_n, \tag{3.8}$$

where $\bar{u}(t_n^0,X_{t_n^0})=u(t_{n+1},X_{t_{n+1}})$ for $i=0$ and R_n is the local truncation error.

Let $u_n(\boldsymbol{x})$ and $u_n^{(i)}(\boldsymbol{x})$ be the approximations for the solution $u(t,\boldsymbol{x})$ of (2.2) at times t_n and t_n^i, respectively. Based on the reference equations (3.7) and (3.8), by removing the local truncation error term R_n, we get the following explicit time semidiscrete s-stage SRK scheme for solving (2.2) in Butcher form:

$$u_n^{(0)}(X_{t_{n+1}})=u_{n+1}(X_{t_{n+1}}), \tag{3.9a}$$

$$u_n^{(i)}(X_{t_n^i})=\mathbb{E}_{t_n^i}^{X_{t_n^i}}[u_{n+1}(X_{t_{n+1}})]+\Delta t\sum_{j=0}^{i-1}a_{ij}\mathbb{E}_{t_n^i}^{X_{t_n^i}}\left[f\left(u_n^{(j)}\left(X_{t_n^j}\right)\right)\right], \quad i=1,\ldots,s, \tag{3.9b}$$

$$u_n(X_{t_n})=u_n^{(s)}(X_{t_n}). \tag{3.9c}$$

3.2 The Shu-Osher form

To construct the MBP-preserving schemes, we write the SRK scheme (3.9) in Shu-Osher form. To this end, we let $\{\alpha_{ij}\}$ be the nonnegative coefficients satisfying

$$\sum_{j=0}^{i-1}\alpha_{ij}=1, \quad i=1,\ldots,s.$$

For notational simplicity, we denote

$$u_n=u_n(X_{t_n}), \quad u_n^{(i)}=u_n^{(i)}(X_{t_n^i}).$$

Then by using the following property of the conditional expectation:

$$\mathbb{E}_t^{X_t}\left[\mathbb{E}_s^{X_s}[\cdot]\right]=\mathbb{E}\left[\mathbb{E}[\cdot|\mathcal{M}_s]\middle|\mathcal{M}_t\right]=\mathbb{E}[\cdot|\mathcal{M}_t]=\mathbb{E}_t^{X_t}[\cdot],\quad \forall 0\le t\le s\le T,$$

we can rewrite the Eq. (3.9b) as

$$\begin{aligned}
u_n^{(i)}&=\mathbb{E}_{t_n^i}^{X_{t_n^i}}[u_{n+1}]+\Delta t\sum_{j=0}^{i-1}a_{ij}\mathbb{E}_{t_n^i}^{X_{t_n^i}}\left[f\left(u_n^{(j)}\right)\right]\\
&=\sum_{j=0}^{i-1}\alpha_{ij}\mathbb{E}_{t_n^i}^{X_{t_n^i}}\left[\mathbb{E}_{t_n^j}^{X_{t_n^j}}[u_{n+1}]\right]+\Delta t\sum_{j=0}^{i-1}a_{ij}\mathbb{E}_{t_n^i}^{X_{t_n^i}}\left[f\left(u_n^{(j)}\right)\right]\\
&=\sum_{j=0}^{i-1}\alpha_{ij}\mathbb{E}_{t_n^i}^{X_{t_n^i}}\left[\mathbb{E}_{t_n^j}^{X_{t_n^j}}[u_{n+1}]+\Delta t\sum_{k=0}^{j-1}a_{jk}\mathbb{E}_{t_n^j}^{X_{t_n^j}}\left[f\left(u_n^{(k)}\right)\right]-\Delta t\sum_{k=0}^{j-1}a_{jk}\mathbb{E}_{t_n^j}^{X_{t_n^j}}\left[f\left(u_n^{(k)}\right)\right]\right]\\
&\quad+\Delta t\sum_{j=0}^{i-1}a_{ij}\mathbb{E}_{t_n^i}^{X_{t_n^i}}\left[f\left(u_n^{(j)}\right)\right]\\
&=\sum_{j=0}^{i-1}\alpha_{ij}\mathbb{E}_{t_n^i}^{X_{t_n^i}}\left[u_n^{(j)}-\Delta t\sum_{k=0}^{j-1}a_{jk}\mathbb{E}_{t_n^j}^{X_{t_n^j}}\left[f\left(u_n^{(k)}\right)\right]\right]+\Delta t\sum_{j=0}^{i-1}a_{ij}\mathbb{E}_{t_n^i}^{X_{t_n^i}}\left[f\left(u_n^{(j)}\right)\right],
\end{aligned}$$

that is,

$$\begin{aligned}
u_n^{(i)}&=\sum_{j=0}^{i-1}\alpha_{ij}\mathbb{E}_{t_n^i}^{X_{t_n^i}}\left[u_n^{(j)}\right]-\Delta t\sum_{j=0}^{i-1}\sum_{k=0}^{j-1}\alpha_{ij}a_{jk}\mathbb{E}_{t_n^i}^{X_{t_n^i}}\left[f\left(u_n^{(k)}\right)\right]+\Delta t\sum_{j=0}^{i-1}a_{ij}\mathbb{E}_{t_n^i}^{X_{t_n^i}}\left[f\left(u_n^{(j)}\right)\right]\\
&=\sum_{j=0}^{i-1}\alpha_{ij}\mathbb{E}_{t_n^i}^{X_{t_n^i}}\left[u_n^{(j)}\right]-\Delta t\sum_{k=0}^{i-1}\sum_{j=k+1}^{i-1}\alpha_{ij}a_{jk}\mathbb{E}_{t_n^i}^{X_{t_n^i}}\left[f\left(u_n^{(k)}\right)\right]+\Delta t\sum_{k=0}^{i-1}a_{ik}\mathbb{E}_{t_n^i}^{X_{t_n^i}}\left[f\left(u_n^{(k)}\right)\right]\\
&=\sum_{j=0}^{i-1}\alpha_{ij}\mathbb{E}_{t_n^i}^{X_{t_n^i}}\left[u_n^{(j)}\right]+\Delta t\sum_{j=0}^{i-1}\left(a_{ij}-\sum_{k=j+1}^{i-1}\alpha_{ik}a_{kj}\right)\mathbb{E}_{t_n^i}^{X_{t_n^i}}\left[f\left(u_n^{(j)}\right)\right].
\end{aligned}$$

Define the coefficients $\{\beta_{ij}\}$ as

$$\beta_{ij}=a_{ij}-\sum_{k=j+1}^{i-1}\alpha_{ik}a_{kj},\quad i=1,\ldots,s, \tag{3.10}$$

and we have

$$\begin{aligned}
u_n^{(i)}&=\sum_{j=0}^{i-1}\alpha_{ij}\mathbb{E}_{t_n^i}^{X_{t_n^i}}\left[u_n^{(j)}\right]+\Delta t\sum_{j=0}^{i-1}\beta_{ij}\mathbb{E}_{t_n^i}^{X_{t_n^i}}\left[f\left(u_n^{(j)}\right)\right]\\
&=\sum_{j=0}^{i-1}\mathbb{E}_{t_n^i}^{X_{t_n^i}}\left[\alpha_{ij}u_n^{(j)}+\Delta t\beta_{ij}f\left(u_n^{(j)}\right)\right],
\end{aligned}$$

which leads to the following SRK scheme in Shu-Osher form:

$$
\begin{aligned}
&u_n^{(0)}(X_{t_{n+1}})=u_{n+1}(X_{t_{n+1}}),\\
&u_n^{(i)}(X_{t_n^i})=\sum_{j=0}^{i-1}\mathbb{E}_{t_n^i}^{X_{t_n^i}}\left[\alpha_{ij}u_n^{(j)}\left(X_{t_n^j}\right)+\Delta t\beta_{ij}f\left(u_n^{(j)}\left(X_{t_n^j}\right)\right)\right],\quad i=1,\dots,s,\\
&u_n(X_{t_n})=u_n^{(s)}(X_{t_n}).
\end{aligned}
$$

Since $\{X_{t_n^i}\}$ are random variables taking values in $\mathbb{R}^d$, we take $X_{t_n^i}=\boldsymbol{x}\in\mathbb{R}^d$ to obtain

$$
\begin{aligned}
u_n^{(i)}(\boldsymbol{x})&=\sum_{j=0}^{i-1}\mathbb{E}_{t_n^i}^{\boldsymbol{x}}\left[\alpha_{ij}u_n^{(j)}\left(X_{t_n^j}\right)+\Delta t\beta_{ij}f\left(u_n^{(j)}\left(X_{t_n^j}\right)\right)\right]\\
&=\sum_{j=0}^{i-1}\mathbb{E}\left[\alpha_{ij}u_n^{(j)}\left(X_{t_n^j}^{t_n^i,\boldsymbol{x}}\right)+\Delta t\beta_{ij}f\left(u_n^{(j)}\left(X_{t_n^j}^{t_n^i,\boldsymbol{x}}\right)\right)\right],
\end{aligned}
$$

where

$$
X_{t_n^j}^{t_n^i,\boldsymbol{x}}=\boldsymbol{x}+\sigma\left(W_{t_n^j}-W_{t_n^i}\right). \tag{3.11}
$$

Then we get the time semidiscrete s-stage SRK scheme for solving (2.2) as

$$
\begin{aligned}
&u_n^{(0)}(\boldsymbol{x})=u_{n+1}(\boldsymbol{x}),\\
&u_n^{(i)}(\boldsymbol{x})=\sum_{j=0}^{i-1}\mathbb{E}\left[\alpha_{ij}u_n^{(j)}\left(X_{t_n^j}^{t_n^i,\boldsymbol{x}}\right)+\Delta t\beta_{ij}f\left(u_n^{(j)}\left(X_{t_n^j}^{t_n^i,\boldsymbol{x}}\right)\right)\right],\quad i=1,\dots,s,\\
&u_n(\boldsymbol{x})=u_n^{(s)}(\boldsymbol{x}).
\end{aligned} \tag{3.12}
$$

Remark 3.1. Note that $u_n^{(i)}(\boldsymbol{x})$ in (3.12) can be viewed as a convex combination of the Euler substeps

$$
\mathbb{E}\left[u_n^{(j)}\left(X_{t_n^j}^{t_n^i,\boldsymbol{x}}\right)+\Delta t\frac{\beta_{ij}}{\alpha_{ij}}f\left(u_n^{(j)}\left(X_{t_n^j}^{t_n^i,\boldsymbol{x}}\right)\right)\right],
$$

which is very similar to the integrating factor Runge-Kutta (IFRK) scheme in [13] except that the exponential integrating factor in IFRK scheme is now replaced by the mathematical expectation operator in our scheme.

Remark 3.2. The expectation $\mathbb{E}[u(r,X_r^{t,\boldsymbol{x}})]$ with $t\le r$ can be written as

$$
\begin{aligned}
\mathbb{E}\left[u\left(r,X_r^{t,\boldsymbol{x}}\right)\right]&=\mathbb{E}\left[u\left(r,\boldsymbol{x}+\sigma(W_r-W_t)\right)\right]\\
&=\frac{1}{(2\pi)^{\frac{d}{2}}}\int_{\mathbb{R}^d}u\left(r,\boldsymbol{x}+\boldsymbol{r}_1\sigma\sqrt{r-t}\right)e^{-\frac{|\boldsymbol{r}_1|^2}{2}}d\boldsymbol{r}_1,
\end{aligned}
$$

and thus the regularity of the above expectation with respect to t is passed to the regularity of the solution u.

3.3 The time semidiscrete MBP

In this subsection, we shall show the MBP-preserving of the time semidiscrete SRK scheme (3.12). To this end, we assume that the nonlinear function f satisfies the following conditions:

$$\exists r_0^+>0 \quad \text{such that} \quad |\xi+rf(\xi)|\le\rho, \quad \forall \xi\in[-\rho,\rho], \quad \forall r\in\left(0,r_0^+\right], \tag{3.13}$$

$$\exists r_0^->0 \quad \text{such that} \quad |\xi-rf(\xi)|\le\rho, \quad \forall \xi\in[-\rho,\rho], \quad \forall r\in\left(0,r_0^-\right]. \tag{3.14}$$

The above conditions are satisfied by many semilinear parabolic equations. Taking the Allen-Cahn equation as an example, when we consider the Ginzburg-Landau potential, it holds that [13]

$$r_0^+=\frac{1}{2}, \quad r_0^-=1, \tag{3.15}$$

and when we consider the Flory-Huggins potential, it holds that

$$r_0^+=\frac{1-\rho^2}{\theta-\theta_c(1-\rho^2)}, \quad r_0^-=\frac{1}{\theta_c-\theta}. \tag{3.16}$$

We also assume that α_{ij} is zero only if its corresponding β_{ij} is zero. Then each stage in (3.12) can be rearranged into a convex combination of forward Euler steps

$$u_n^{(i)}(\boldsymbol{x})=\sum_{j=0}^{i-1}\alpha_{ij}\mathbb{E}\left[u_n^{(j)}\left(X_{t_n^j}^{t_n^i,\boldsymbol{x}}\right)+\Delta t\frac{\beta_{ij}}{\alpha_{ij}}f\left(u_n^{(j)}\left(X_{t_n^j}^{t_n^i,\boldsymbol{x}}\right)\right)\right].$$

Theorem 3.1. *Assume that f satisfies* (3.13) *and* (3.14)*, then if $\|u_{n+1}\|_{L^\infty}\le\rho$, the solution u_n obtained from* (3.12) *satisfies $\|u_n\|_{L^\infty}\le\rho$, provided that*

$$\Delta t\le\mathcal{C}r_0^+, \quad \mathcal{C}=\min_{i,j}\frac{\alpha_{ij}}{\beta_{ij}}, \tag{3.17}$$

when β_{ij} are all nonnegative, or satisfies

$$\Delta t\le\mathcal{C}\min\{r_0^+,r_0^-\}, \quad \mathcal{C}=\min_{i,j}\frac{\alpha_{ij}}{|\beta_{ij}|}, \tag{3.18}$$

whenever there is a negative β_{ij}.

Proof. Since $\|u_{n+1}\|_{L^\infty}\le\rho$, we can suppose that $\|u_n^{(j)}\|_{L^\infty}\le\rho$ for all $j\le i-1$. For the i-th stage, we have

$$\begin{aligned}\|u_n^{(i)}\|_{L^\infty}&=\left\|\sum_{j=0}^{i-1}\alpha_{ij}\mathbb{E}\left[u_n^{(j)}\left(X_{t_n^j}^{t_n^i,\boldsymbol{x}}\right)+\Delta t\frac{\beta_{ij}}{\alpha_{ij}}f\left(u_n^{(j)}\left(X_{t_n^j}^{t_n^i,\boldsymbol{x}}\right)\right)\right]\right\|_{L^\infty}\\&\le\sum_{j=0}^{i-1}\alpha_{ij}\left\|\mathbb{E}\left[u_n^{(j)}\left(X_{t_n^j}^{t_n^i,\boldsymbol{x}}\right)+\Delta t\frac{\beta_{ij}}{\alpha_{ij}}f\left(u_n^{(j)}\left(X_{t_n^j}^{t_n^i,\boldsymbol{x}}\right)\right)\right]\right\|_{L^\infty}.\end{aligned}$$

By combining with the conditions (3.13), (3.14), (3.17) and (3.18), we deduce

$$
\begin{aligned}
&\left\|\mathbb{E}\left[u_n^{(j)}\left(X_{t_n^j}^{t_n^i,x}\right)+\Delta t\frac{\beta_{ij}}{\alpha_{ij}}f\left(u_n^{(j)}\left(X_{t_n^j}^{t_n^i,x}\right)\right)\right]\right\|_{L^\infty}\\
=&\sup_{x\in\overline{D}}\left|\mathbb{E}\left[u_n^{(j)}\left(X_{t_n^j}^{t_n^i,x}\right)+\Delta t\frac{\beta_{ij}}{\alpha_{ij}}f\left(u_n^{(j)}\left(X_{t_n^j}^{t_n^i,x}\right)\right)\right]\right|\\
\le&\mathbb{E}\left[\sup_{x\in\overline{D}}\left|u_n^{(j)}\left(X_{t_n^j}^{t_n^i,x}\right)+\Delta t\frac{\beta_{ij}}{\alpha_{ij}}f\left(u_n^{(j)}\left(X_{t_n^j}^{t_n^i,x}\right)\right)\right|\right]\\
\le&\mathbb{E}\left[\sup_{x\in\overline{D}}\left|u_n^{(j)}(x)+\Delta t\frac{\beta_{ij}}{\alpha_{ij}}f\left(u_n^{(j)}(x)\right)\right|\right]\\
=&\mathbb{E}\left[\left\|u_n^{(j)}+\Delta t\frac{\beta_{ij}}{\alpha_{ij}}f\left(u_n^{(j)}\right)\right\|_{L^\infty}\right]\le\mathbb{E}[\rho]=\rho,
\end{aligned}
$$

which leads to

$$
\|u_n^{(i)}\|_{L^\infty}\le\sum_{j=0}^{i-1}\alpha_{ij}\rho=\rho.
$$

Then by induction, we get $\|u_n\|_{L^\infty}\le\rho$, which completes the proof. □

Remark 3.3. It is worth noting that the conditions used in the above theorem are the same as the ones of [13, Theorem 3.1], which indicates that the SRK scheme is MBP-preserving if and only if the IFRK scheme is MBP-preserving with the same coefficients. Hence, one can propose some specific time semidiscrete MBP-preserving SRK schemes up to fourth order by choosing exactly the same coefficients of the MBP-preserving IFRK schemes presented in [13,17].

3.4 The time semidiscrete error estimate

We write the time semidiscrete SRK scheme (3.12) in Butcher form

$$
\begin{aligned}
&u_n^{(0)}(x)=u_{n+1}(x),\\
&u_n^{(i)}(x)=\mathbb{E}\left[u_{n+1}\left(X_{t_{n+1}}^{t_n^i,x}\right)\right]+\Delta t\sum_{j=0}^{i-1}a_{ij}\mathbb{E}\left[f\left(u_n^{(j)}\left(X_{t_n^j}^{t_n^i,x}\right)\right)\right],\quad i=1,\ldots,s,\\
&u_n(x)=u_n^{(s)}(x).
\end{aligned}
\tag{3.19}
$$

Suppose that the SRK scheme (3.12) is p-th order with $1\le p\le s$ and then we have the following error estimate for (3.19).

Theorem 3.2. *Let u_n be the numerical solution obtained from the SRK scheme* (3.19) *with $u_{N_t}(\boldsymbol{x})=\varphi(\boldsymbol{x})$. Assume that $\|\varphi\|_{L^\infty}\le\rho$ and the exact solution u of* (2.2) *satisfies $u\in C_b^{p+1,2p+2}$. Then under the conditions in Theorem* 3.1*, we get*

$$\|u(t_n,\cdot)-u_n\|_{L^\infty}\le C_1\left(e^{\tilde{C}s(T-t_n)}-1\right)(\Delta t)^p,\quad n=0,\ldots,N_t,$$

where $\tilde{C}=\max_{|\xi|\le\rho}|f'(\xi)|$ and the constant $C_1>0$ is independent of Δt.

Proof. Take $X_{t_n^i}=\boldsymbol{x}$ and $X_{t_n}=\boldsymbol{x}$ in (3.7) and (3.8), respectively, and we obtain

$$\bar{u}\left(t_n^i,\boldsymbol{x}\right)=\mathbb{E}\left[u\left(t_{n+1},X_{t_{n+1}}^{t_n^i,\boldsymbol{x}}\right)\right]+\Delta t\sum_{j=0}^{i-1}a_{ij}\mathbb{E}\left[f\left(\bar{u}\left(t_n^j,X_{t_n^j}^{t_n^i,\boldsymbol{x}}\right)\right)\right],\quad i=0,\ldots,s-1, \tag{3.20}$$

$$u(t_n,\boldsymbol{x})=\mathbb{E}\left[u\left(t_{n+1},X_{t_{n+1}}^{t_n,\boldsymbol{x}}\right)\right]+\Delta t\sum_{i=0}^{s-1}a_{si}\mathbb{E}\left[f\left(\bar{u}\left(t_n^i,X_{t_n^i}^{t_n,\boldsymbol{x}}\right)\right)\right]+R_n, \tag{3.21}$$

where the local truncation error term R_n satisfies

$$\max_{0\le n\le N_t-1}\|R_n\|_{L^\infty}\le C(\Delta t)^{p+1},$$

where C is a positive constant independent of Δt. Since $\|\varphi\|_{L^\infty}\le\rho$, we have

$$\|u(t_{n+1},\cdot)\|_{L^\infty}\le\rho.$$

Then by using the similar approach in Theorem 3.1, we prove

$$\left\|\bar{u}\left(t_n^i,\cdot\right)\right\|_{L^\infty}\le\rho,\quad i=1,\ldots,s-1.$$

Now we define the numerical errors of the scheme (3.19) as

$$e_n(\boldsymbol{x})=u(t_n,\boldsymbol{x})-u_n(\boldsymbol{x}),\quad e_n^{(i)}(\boldsymbol{x})=\bar{u}\left(t_n^i,\boldsymbol{x}\right)-u^{(i)}(\boldsymbol{x}),\quad i=0,\ldots,s-1.$$

By combining the equations in (3.19)-(3.21), we get

$$\begin{aligned}
e_n^{(i)}(\boldsymbol{x})&=\mathbb{E}\left[e_{n+1}\left(X_{t_{n+1}}^{t_n^i,\boldsymbol{x}}\right)\right]+\Delta t\sum_{j=0}^{i-1}a_{ij}\mathbb{E}\left[f\left(\bar{u}\left(t_n^j,X_{t_n^j}^{t_n^i,\boldsymbol{x}}\right)\right)-f\left(u_n^{(j)}\left(X_{t_n^j}^{t_n^i,\boldsymbol{x}}\right)\right)\right],\\
e_n(\boldsymbol{x})&=\mathbb{E}\left[e_{n+1}\left(X_{t_{n+1}}^{t_n,\boldsymbol{x}}\right)\right]+\Delta t\sum_{i=0}^{s-1}a_{si}\mathbb{E}\left[f\left(\bar{u}\left(t_n^i,X_{t_n^i}^{t_n,\boldsymbol{x}}\right)\right)-f\left(u_n^{(i)}\left(X_{t_n^i}^{t_n,\boldsymbol{x}}\right)\right)\right]+R_n.
\end{aligned}$$

Then by the fact that $0\le a_{ij}\le c_i\le 1$ and $\|u_n^{(i)}\|_{L^\infty}\le\rho$, we deduce

$$\begin{aligned}
\|e_n^{(i)}\|_{L^\infty}&\le\mathbb{E}\left[\left\|e_{n+1}\left(X_{t_{n+1}}^{t_n^i,\cdot}\right)\right\|_{L^\infty}\right]+\Delta t\sum_{j=0}^{i-1}\mathbb{E}\left[\left\|f\left(\bar{u}\left(t_n^j,X_{t_n^j}^{t_n^i,\cdot}\right)\right)-f\left(u_n^{(j)}\left(X_{t_n^j}^{t_n^i,\cdot}\right)\right)\right\|_{L^\infty}\right]\\
&\le\mathbb{E}\left[\|e_{n+1}\|_{L^\infty}\right]+\Delta t\sum_{j=0}^{i-1}\mathbb{E}\left[\left\|f\left(\bar{u}\left(t_n^j,\cdot\right)\right)-f\left(u_n^{(j)}(\cdot)\right)\right\|_{L^\infty}\right]\\
&\le\|e_{n+1}\|_{L^\infty}+\tilde{C}\Delta t\sum_{j=0}^{i-1}\|e_n^{(j)}\|_{L^\infty},
\end{aligned}$$

which indicates that $\|e_n^{(0)}\|_{L^\infty}\le\|e_{n+1}\|_{L^\infty}$. We claim that $\|e_n^{(j)}\|_{L^\infty}\le(1+\tilde{C}\Delta t)^j\|e_{n+1}\|_{L^\infty}$, for all $j=0,\dots,s-1$. Indeed, we assume that

$$\big\|e_n^{(j)}\big\|_{L^\infty}\le(1+\tilde{C}\Delta t)^j\|e_{n+1}\|_{L^\infty},\quad j=0,\dots,i-1.$$

Then by induction, we get

$$\begin{aligned}\big\|e_n^{(i)}\big\|_{L^\infty}&\le\|e_{n+1}\|_{L^\infty}+\tilde{C}\Delta t\sum_{j=0}^{i-1}(1+\tilde{C}\Delta t)^j\|e_{n+1}\|_{L^\infty}\\&=(1+\tilde{C}\Delta t)^i\|e_{n+1}\|_{L^\infty},\quad i=0,\dots,s-1,\end{aligned}$$

which leads to

$$\begin{aligned}\|e_n\|_{L^\infty}&\le\|e_{n+1}\|_{L^\infty}+\tilde{C}\Delta t\sum_{i=0}^{s-1}\big\|e_n^{(i)}\big\|_{L^\infty}+\|R_n\|_{L^\infty}\\&\le\|e_{n+1}\|_{L^\infty}+\tilde{C}\Delta t\sum_{i=0}^{s-1}(1+\tilde{C}\Delta t)^i\|e_{n+1}\|_{L^\infty}+C(\Delta t)^{p+1}\\&=(1+\tilde{C}\Delta t)^s\|e_{n+1}\|_{L^\infty}+C(\Delta t)^{p+1}\\&\le(1+\tilde{C}\Delta t)^{(N_t-n)s}\|e_{N_t}\|_{L^\infty}+C(\Delta t)^{p+1}\sum_{k=0}^{N_t-n-1}(1+\tilde{C}\Delta t)^{ks}\\&\le\frac{C}{\tilde{C}s}(\Delta t)^p\big((1+\tilde{C}\Delta t)^{(N_t-n)s}-1\big)\\&\le C_1(\Delta t)^p\big(e^{\tilde{C}s(T-t_n)}-1\big),\end{aligned}$$

where the constant $C_1=C/\tilde{C}s$. □

Remark 3.4. According to Remark 2.2, when $f\in C_b^{2p+2}$ and $\varphi\in C_b^{2p+2+\alpha}$ for some $\alpha\in(0,1)$, we can guarantee the condition $u\in C_b^{p+1,2p+2}$ in the above theorem.

4 The fully discrete SRK schemes

To construct the fully discrete schemes, we set $h=a/N_x$ for a given even integer N_x and introduce the following mesh D_h of the domain $D=(0,a)^d$ as

$$D_h=\{\boldsymbol{x}_k=h\boldsymbol{k},\ 1\le k_i\le N_x,\ i=1,\dots,d\},$$

where $\boldsymbol{k}\in\mathbb{N}^d$ denotes a multi-index.

4.1 The fully discrete schemes

The key point to construct the fully discrete SRK schemes is how to approximate the expectations in the time semidiscrete schemes. For simplicity of representation, we let $v:\mathbb{R}^d\to\mathbb{R}$ denote some given smooth functions and write the expectations in (3.12) in the following general form:

$$\mathbb{E}\left[v\left(X_r^{t,x}\right)\right],\quad 0\le t\le r\le T.$$

Now we take $d=2$ for example to illustrate how to approximate the above expectation. Without loss of generality, we assume that $\sigma_i=\sigma>0$ for $i=1,\ldots,d$. Since

$$X_r^{t,x}=\boldsymbol{x}+\sigma(W_r-W_t)$$

and $W_t=(W_t^1,\ldots,W_t^d)^\top$ with $W_t^i\overset{iid}{\sim}N(0,t)$, we let ξ and ξ' be two independent standard normal random variables to deduce

$$\begin{aligned}\mathbb{E}\left[v\left(X_r^{t,x}\right)\right]&=\mathbb{E}\left[v\left(\boldsymbol{x}+\sigma(W_r-W_t)\right)\right]\\&=\mathbb{E}\left[v\left(x_1+\sigma\sqrt{r-t}\xi,x_2+\sigma\sqrt{r-t}\xi'\right)\right]\\&=\frac{1}{2\pi}\int_{\mathbb{R}}\int_{\mathbb{R}}v\left(x_1+r_1\sigma\sqrt{r-t},x_2+r_2\sigma\sqrt{r-t}\right)e^{-\frac{r_1^2+r_2^2}{2}}dr_1dr_2\\&=\frac{1}{\pi}\int_{\mathbb{R}}\int_{\mathbb{R}}v\left(x_1+r_1\sigma\sqrt{2(r-t)},x_2+r_2\sigma\sqrt{2(r-t)}\right)e^{-r_1^2-r_2^2}dr_1dr_2.\end{aligned}\tag{4.1}$$

Now we use the following Gauss-Hermite quadrature rule to approximate the integral in the above equation:

$$\int_{\mathbb{R}}g(x)e^{-x^2}dx=\sum_{p=1}^{M}\omega_pg(a_p)+R(g,M),\tag{4.2}$$

where $g:\mathbb{R}\to\mathbb{R}$ is a given smooth function, the positive integer M is the number of quadrature points, $\{a_p\}_{p=1}^M$ are the roots of the Hermite polynomial $H_M(x)$ of degree M, $\{\omega_p\}_{p=1}^M$ are the corresponding weights, and $R(g,M)$ is the truncation error with

$$R(g,M)=\frac{M!\sqrt{\pi}}{2^M(2M)!}g^{(2M)}(\bar{x})\quad\text{for some}\quad\bar{x}\in\mathbb{R}.\tag{4.3}$$

Then by applying the Gaussian quadrature rule (4.2) to (4.1), we obtain

$$\mathbb{E}\left[v\left(X_r^{t,x}\right)\right]=\mathbb{E}_M\left[v\left(X_r^{t,x}\right)\right]+R_M(v),$$

where the approximation $\mathbb{E}_M[v(X_r^{t,x})]$ is defined as

$$\mathbb{E}_M\left[v\left(X_r^{t,x}\right)\right]=\frac{1}{\pi}\sum_{p_1=1}^{M}\sum_{p_2=1}^{M}w_{p_1}w_{p_2}v\left(x_1+a_{p_1}\sigma\sqrt{2(r-t)},x_2+a_{p_2}\sigma\sqrt{2(r-t)}\right),\tag{4.4}$$

and $R_M(v)$ is the truncation error. If $v\in C_b^{2M}(\mathbb{R}^2)$, then by (4.3), it holds that

$$|R_M(v)|\le C\sigma^{2M}(r-t)^M, \tag{4.5}$$

where C is a positive constant depending on M and the upper bounds of the derivatives of v. On the other hand, when calculating the approximation $\mathbb{E}_M[v(X_r^{t,\boldsymbol{x}_k})]$ for a given grid point $\boldsymbol{x}_k=(x_1^k,x_2^k)$, the used points $(x_1^k+a_{p_1}\sigma\sqrt{2(r-t)},x_2^k+a_{p_2}\sigma\sqrt{2(r-t)})$ may not belong to D_h. Thus, we need to approximate the values of v at those points by using some interpolation methods based on the values of v on the grid points. Let $\hat{v}$ denote the corresponding interpolation polynomial. Then for any grid point $\boldsymbol{x}_k$, we define the approximation of $\mathbb{E}[v(X_r^{t,\boldsymbol{x}_k})]$ as

$$\mathbb{E}_M^h\left[v\left(X_r^{t,\boldsymbol{x}_k}\right)\right]=\frac{1}{\pi}\sum_{p_1=1}^{M}\sum_{p_2=1}^{M}w_{p_1}w_{p_2}\hat{v}\left(x_1+a_{p_1}\sigma\sqrt{2(r-t)},x_2+a_{p_2}\sigma\sqrt{2(r-t)}\right).$$

Now by using the above approximation for expectation in the time semidiscrete scheme, we construct the fully discrete scheme. Let $u_{n,k}^{(i)}$ and $u_{n,k}$ denote the approximation values of $u(t_n^i,\boldsymbol{x}_k)$ and $u(t_n,\boldsymbol{x}_k)$, respectively. Then we get the following fully discrete SRK scheme:

$$\begin{aligned}
&u_{n,k}^{(0)}=u_{n+1,k},\\
&u_{n,k}^{(i)}=\sum_{j=0}^{i-1}\mathbb{E}_M^h\left[\alpha_{ij}u_{n,k}^{(j)}+\Delta t\beta_{ij}f\left(u_{n,k}^{(j)}\right)\right],\quad i=1,\dots,s,\\
&u_{n,k}=u_{n,k}^{(s)}.
\end{aligned} \tag{4.6}$$

4.2 The fully discrete MBP

Note that the fully discrete SRK scheme (4.6) needs the interpolation method to approximate expectation, which can be very time consuming and may lead to the MBP not preserved. To construct some efficient MBP-preserving fully discrete SRK schemes, we consider the following time semidiscrete first-order one-stage SRK (SRK1) scheme:

$$u_n(\boldsymbol{x})=\mathbb{E}\left[u_{n+1}\left(X_{t_{n+1}}^{t_n,\boldsymbol{x}}\right)+\Delta t f\left(u_{n+1}\left(X_{t_{n+1}}^{t_n,\boldsymbol{x}}\right)\right)\right], \tag{4.7}$$

and the second-order two-stage SRK (SRK2) scheme with $c_1=1$

$$\begin{aligned}
u_n^{(1)}(\boldsymbol{x})&=\mathbb{E}\left[u_{n+1}\left(X_{t_{n+1}}^{t_n,\boldsymbol{x}}\right)+\Delta t f\left(u_{n+1}\left(X_{t_{n+1}}^{t_n,\boldsymbol{x}}\right)\right)\right],\\
u_n(\boldsymbol{x})&=\mathbb{E}\left[\alpha_{20}u_{n+1}\left(X_{t_{n+1}}^{t_n,\boldsymbol{x}}\right)+\Delta t\beta_{20}f\left(u_{n+1}\left(X_{t_{n+1}}^{t_n,\boldsymbol{x}}\right)\right)\right]\\
&\quad+\alpha_{21}u_n^{(1)}(\boldsymbol{x})+\Delta t\beta_{21}f\left(u_n^{(1)}(\boldsymbol{x})\right).
\end{aligned} \tag{4.8}$$

The key point is that all the expectations in the above two schemes can be written as $\mathbb{E}[v(X_{t_{n+1}}^{t_n,\boldsymbol{x}})]$, which can be approximated without using the interpolation methods when choosing appropriate quadrature points number M and mesh size h. We first take $d=1$ to illustrate this approximation. For $d=1$, we have

$$\mathbb{E}_M\left[v\left(X_{t_{n+1}}^{t_n,\boldsymbol{x}}\right)\right]=\frac{1}{\sqrt{\pi}}\sum_{p=1}^{M}w_p v\left(\boldsymbol{x}+a_p\sigma\sqrt{2\Delta t}\right).$$

When we take $M=3$, it holds that

$$(a_1,a_2,a_3)=\sqrt{\frac{3}{2}}(-1,0,1),\quad (w_1,w_2,w_3)=\frac{\sqrt{\pi}}{6}(1,4,1),$$

and thus

$$\mathbb{E}_3\left[v\left(X_{t_{n+1}}^{t_n,\boldsymbol{x}}\right)\right]=\frac{1}{6}\Big(v\big(\boldsymbol{x}-\sigma\sqrt{3\Delta t}\big)+4v(\boldsymbol{x})+v\big(\boldsymbol{x}+\sigma\sqrt{3\Delta t}\big)\Big).$$

Then by letting

$$h=\sigma\sqrt{3\Delta t},$$

we obtain

$$\mathbb{E}_3\left[v\left(X_{t_{n+1}}^{t_n,\boldsymbol{x}_k}\right)\right]=\frac{1}{6}\big(v(\boldsymbol{x}_{k-1})+4v(\boldsymbol{x}_k)+v(\boldsymbol{x}_{k+1})\big),$$

which is similar to the approximation of $v''(\boldsymbol{x}_k)$ using the central difference method. Then we can write the corresponding fully discrete schemes of (4.7) and (4.8) in the matrix forms by defining

$$G_3=\frac{1}{6}\begin{pmatrix}4 & 1 & & & 1\\ 1 & 4 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & 4 & 1\\ 1 & & & 1 & 4\end{pmatrix}.$$

Let $\boldsymbol{u}_{n,h}$ (or $\boldsymbol{u}_{n,h}^{(i)}$) $\in\mathbb{R}^{N_x^d}$ be the vector of $u_{n,k}$ (or $u_{n,k}^{(i)}$) ordered lexicographically, and then we get the fully discrete SRK1 scheme

$$\boldsymbol{u}_{n,h}=G\big(\boldsymbol{u}_{n+1,h}+\Delta t f(\boldsymbol{u}_{n+1,h})\big), \tag{4.9}$$

and the fully discrete SRK2 scheme

$$\begin{aligned}&\boldsymbol{u}_{n,h}^{(1)}=G\big(\boldsymbol{u}_{n+1,h}+\Delta t f(\boldsymbol{u}_{n+1,h})\big),\\ &\boldsymbol{u}_{n,h}=G\big(\alpha_{20}\boldsymbol{u}_{n+1,h}+\Delta t\beta_{20}f(\boldsymbol{u}_{n+1,h})\big)+\alpha_{21}\boldsymbol{u}_{n,h}^{(1)}+\Delta t\beta_{21}f\big(\boldsymbol{u}_{n,h}^{(1)}\big),\end{aligned} \tag{4.10}$$

where the matrix G is defined by

$$G=\begin{cases}G_3, & d=1,\\ G_3\otimes G_3, & d=2,\\ G_3\otimes G_3\otimes G_3, & d=3.\end{cases} \tag{4.11}$$

Now we show the MBP-preserving of the fully discrete schemes (4.9) and (4.10). Let $\|\cdot\|_\infty$ be the vector or matrix maximum norm, then we deduce

$$\|G\|_\infty = \max_i \sum_{j=1}^{N_x^d} G_{ij} = 1. \tag{4.12}$$

Theorem 4.1. *Assume that f satisfies the condition* (3.13)*, then if $\|\boldsymbol{u}_{n+1,h}\|_\infty \le \rho$, the solution $\boldsymbol{u}_{n,h}$ obtained from* (4.9) *satisfies $\|\boldsymbol{u}_{n,h}\|_\infty \le \rho$, provided that*

$$\Delta t \le r_0^+. \tag{4.13}$$

Proof. Since $\|\boldsymbol{u}_{n+1,h}\|_\infty \le \rho$, then by using (3.13) and (4.13), we get

$$\|\boldsymbol{u}_{n,h}\|_\infty \le \|G\|_\infty \|\boldsymbol{u}_{n+1,h} + \Delta t f(\boldsymbol{u}_{n+1,h})\|_\infty \le \rho,$$

which completes the proof. □

Theorem 4.2. *Assume that f satisfies the conditions* (3.13) *and* (3.14)*, then if $\|\boldsymbol{u}_{n+1,h}\|_\infty \le \rho$, the solution $\boldsymbol{u}_{n,h}$ obtained from* (4.10) *satisfies $\|\boldsymbol{u}_{n,h}\|_\infty \le \rho$, provided that*

$$\Delta t \le \mathcal{C} r_0^+, \quad \mathcal{C} = \min_{i,j} \frac{\alpha_{ij}}{\beta_{ij}}, \tag{4.14}$$

when β_{ij} are all nonnegative, or satisfies

$$\Delta t \le \mathcal{C} \min\{r_0^+, r_0^-\}, \quad \mathcal{C} = \min_{i,j} \frac{\alpha_{ij}}{|\beta_{ij}|}, \tag{4.15}$$

whenever there is a negative β_{ij}.

Proof. Since $\|\boldsymbol{u}_{n+1,h}\|_\infty \le \rho$, then by Theorem 4.1, we know that

$$\big\|\boldsymbol{u}_{n,h}^{(1)}\big\|_\infty \le \rho. \tag{4.16}$$

Then by using (4.16) and the conditions in the theorem, we deduce

$$\begin{aligned}
\|\boldsymbol{u}_{n,h}\|_\infty &\le \|G\|_\infty \|\alpha_{20}\boldsymbol{u}_{n+1,h} + \Delta t \beta_{20} f(\boldsymbol{u}_{n+1,h})\|_\infty + \big\|\alpha_{21}\boldsymbol{u}_{n,h}^{(1)} + \Delta t \beta_{21} f\big(\boldsymbol{u}_{n,h}^{(1)}\big)\big\|_\infty \\
&\le \alpha_{20} \left\|\boldsymbol{u}_{n+1,h} + \Delta t \frac{\beta_{20}}{\alpha_{20}} f(\boldsymbol{u}_{n+1,h})\right\|_\infty + \alpha_{21} \left\|\boldsymbol{u}_{n,h}^{(1)} + \Delta t \frac{\beta_{21}}{\alpha_{21}} f\left(\boldsymbol{u}_{n,h}^{(1)}\right)\right\|_\infty \\
&\le \alpha_{20}\rho + \alpha_{21}\rho = \rho,
\end{aligned}$$

which completes the proof. □

Remark 4.1. Note that we supposed that $\sigma_i = \sigma$ is a constant when constructing the above MBP-preserving fully discrete schemes. Nevertheless, if σ_i is not a constant, we can also obtain the MBP-preserving fully discrete SRK schemes (4.9) and (4.10) by taking different mesh sizes in different dimensions, that is, we only need to take

$$h_i = \sigma_i \sqrt{3\Delta t}, \quad i = 1, \ldots, d,$$

where h_i denotes the mesh size in the i-th dimension.

4.3 The fully discrete error estimate

In this subsection, we analyze the spatial errors of the fully discrete schemes (4.9) and (4.10), and further give their error estimates. Denote by $\boldsymbol{U}_n^{(i)}$ and $\boldsymbol{U}_n$ the restrictions of $u_n^{(i)}(\boldsymbol{x})$ and $u_n(\boldsymbol{x})$ on the mesh D_h, respectively. Then the terminal condition in (4.9) and (4.10) is set to be

$$\boldsymbol{u}_{N_t,h}=\boldsymbol{U}_{N_t}.$$

Theorem 4.3. *Let $u_n(\boldsymbol{x})$ and $\boldsymbol{u}_{n,h}$ be the numerical solutions obtained from the semidiscrete SRK1 scheme* (4.7) *with $u_{N_t}(\boldsymbol{x})=\varphi(\boldsymbol{x})$ and the fully discrete SRK1 scheme* (4.9) *with $\boldsymbol{u}_{N_t,h}=\boldsymbol{U}_{N_t}$, respectively. Assume that $\|\varphi\|_{L^\infty}\leq\rho$ and u_n satisfies $u_n\in C_b^6$. Then under the conditions in Theorem* 4.1*, we get*

$$\|\boldsymbol{U}_n-\boldsymbol{u}_{n,h}\|_\infty\leq C_2\sigma^6\big(e^{\tilde{C}(T-t_n)}-1\big)(\Delta t)^2,\quad n=0,\ldots,N_t, \tag{4.17}$$

where $\tilde{C}=\max_{|\xi|\leq\rho}|f'(\xi)|$ and the constant $C_2>0$ is independent of Δt.

Proof. Define the spatial errors of the scheme (4.9) as

$$\boldsymbol{v}_n=\boldsymbol{U}_n-\boldsymbol{u}_{n,h},\quad n=0,\ldots,N_t.$$

Since $\boldsymbol{U}_n$ is the restriction of $u_n(\boldsymbol{x})$, it satisfies

$$\boldsymbol{U}_n=G\big(\boldsymbol{U}_{n+1}+\Delta t f(\boldsymbol{U}_{n+1})\big)+r_n, \tag{4.18}$$

where r_n is the error generated by approximating expectations. Similar to (4.5), we obtain

$$\|r_n\|_\infty\leq C\sigma^6(\Delta t)^3, \tag{4.19}$$

where C is a positive constant independent of Δt. By using (4.9) and (4.18), we get

$$\boldsymbol{v}_n=G\big(\boldsymbol{v}_{n+1}+\Delta t\big(f(\boldsymbol{U}_{n+1})-f(\boldsymbol{u}_{n+1,h})\big)\big)+r_n.$$

Combining with the conditions in the theorem and Theorems 3.1 and 4.1, we have

$$\|\boldsymbol{U}_n\|_\infty\leq\rho,\quad \|\boldsymbol{u}_{n,h}\|_\infty\leq\rho,$$

which leads to

$$\begin{aligned}
\|\boldsymbol{v}_n\|_\infty&\leq\|G\|_\infty\big\|\boldsymbol{v}_{n+1}+\Delta t\big(f(\boldsymbol{U}_{n+1})-f(\boldsymbol{u}_{n+1,h})\big)\big\|_\infty+\|r_n\|_\infty\\
&\leq\|\boldsymbol{v}_{n+1}\|_\infty+\tilde{C}\Delta t\|\boldsymbol{v}_{n+1}\|_\infty+\|r_n\|_\infty\\
&\leq(1+\tilde{C}\Delta t)\|\boldsymbol{v}_{n+1}\|_\infty+C\sigma^6(\Delta t)^3\\
&\leq(1+\tilde{C}\Delta t)^{N_t-n}\|\boldsymbol{v}_{N_t}\|_\infty+C\sigma^6(\Delta t)^3\sum_{k=0}^{N_t-n-1}(1+\tilde{C}\Delta t)^k\\
&\leq C\sigma^6(\Delta t)^3\frac{(1+\tilde{C}\Delta t)^{N_t-n}-1}{\tilde{C}\Delta t}\\
&\leq C_2\sigma^6(\Delta t)^2\big(e^{\tilde{C}(T-t_n)}-1\big),
\end{aligned} \tag{4.20}$$

where the constant $C_2=C/\tilde{C}$. □

Remark 4.2. According to Remark 2.2, when $f\in C_b^6$ and $\varphi\in C_b^{6+\alpha}$ for some $\alpha\in(0,1)$, we have $u\in C_b^{3,6}$, and thus we can ensure the condition $u_n\in C_b^6$ in the above theorem.

Now we turn to the fully discrete SRK2 scheme (4.10), which can be written in the Butcher form

$$\begin{aligned} \boldsymbol{u}_{n,h}^{(1)} &= G\big(\boldsymbol{u}_{n+1,h}+\Delta t f(\boldsymbol{u}_{n+1,h})\big),\\ \boldsymbol{u}_{n,h} &= G\big(\boldsymbol{u}_{n+1,h}+\Delta t a_{20} f(\boldsymbol{u}_{n+1,h})\big)+\Delta t a_{21} f\big(\boldsymbol{u}_{n,h}^{(1)}\big). \end{aligned} \tag{4.21}$$

Since $\boldsymbol{U}_n^{(1)}$ and $\boldsymbol{U}_n$ are restrictions of $u_n^{(1)}(\boldsymbol{x})$ and $u_n(\boldsymbol{x})$, it holds that

$$\begin{aligned} \boldsymbol{U}_n^{(1)} &= G\big(\boldsymbol{U}_{n+1}+\Delta t f(\boldsymbol{U}_{n+1})\big)+r_n^{(1)},\\ \boldsymbol{U}_n &= G\big(\boldsymbol{U}_{n+1}+\Delta t a_{20} f(\boldsymbol{U}_{n+1})\big)+\Delta t a_{21} f\big(\boldsymbol{U}_n^{(1)}\big)+r_n, \end{aligned} \tag{4.22}$$

where $r_n^{(1)}$ and r_n are the errors generated by approximating expectations.

Theorem 4.4. *Let $u_n(\boldsymbol{x})$ and $\boldsymbol{u}_{n,h}$ be the numerical solutions obtained from the semidiscrete SRK2 scheme* (4.8) *with $u_{N_t}(\boldsymbol{x})=\varphi(\boldsymbol{x})$ and the fully discrete SRK2 scheme* (4.21) *with $\boldsymbol{u}_{N_t,h}=\boldsymbol{U}_{N_t}$, respectively. Assume that $\|\varphi\|_{L^\infty}\le\rho$ and u_n satisfies $u_n\in C_b^6$. Then under the conditions in Theorem* 4.2*, we get*

$$\|\boldsymbol{U}_n-\boldsymbol{u}_{n,h}\|\le C_3\sigma^6\big(e^{2\tilde{C}(T-t_n)}-1\big)(\Delta t)^2, \tag{4.23}$$

where $\tilde{C}=\max_{|\xi|\le\rho}|f'(\xi)|$ and the constant $C_3>0$ is independent of Δt.

Proof. Define the spatial errors of the scheme (4.21) as

$$\boldsymbol{v}_n=\boldsymbol{U}_n-\boldsymbol{u}_{n,h},\quad \boldsymbol{v}_n^{(1)}=\boldsymbol{U}_n^{(1)}-\boldsymbol{u}_{n,h}^{(1)},\quad n=0,\ldots,N_t.$$

Then by using (4.21) and (4.22), we have

$$\begin{aligned} \boldsymbol{v}_n^{(1)} &= G\big(\boldsymbol{v}_{n+1}+\Delta t\big(f(\boldsymbol{U}_{n+1})-f(\boldsymbol{u}_{n+1,h})\big)\big)+r_n^{(1)},\\ \boldsymbol{v}_n &= G\big(\boldsymbol{v}_{n+1}+\Delta t a_{20}\big(f(\boldsymbol{U}_{n+1})-f(\boldsymbol{u}_{n+1,h})\big)\big)\\ &\quad +\Delta t a_{21}\big(f\big(\boldsymbol{U}_n^{(1)}\big)-f\big(\boldsymbol{u}_{n,h}^{(1)}\big)\big)+r_n. \end{aligned} \tag{4.24}$$

Combining with the conditions in the theorem and Theorems 3.1 and 4.2, we get

$$\big\|\boldsymbol{U}_n^{(1)}\big\|_\infty\le\rho,\quad \|\boldsymbol{U}_n\|_\infty\le\rho,\quad \big\|\boldsymbol{u}_{n,h}^{(1)}\big\|_\infty\le\rho,\quad \|\boldsymbol{u}_{n,h}\|_\infty\le\rho,$$

which leads to

$$\begin{aligned} \big\|\boldsymbol{v}_n^{(1)}\big\|_\infty &\le \|G\|_\infty\big\|\boldsymbol{v}_{n+1}+\Delta t\big(f(\boldsymbol{U}_{n+1})-f(\boldsymbol{u}_{n+1,h})\big)\big\|_\infty+\big\|r_n^{(1)}\big\|_\infty\\ &\le \|\boldsymbol{v}_{n+1}\|_\infty+\tilde{C}\Delta t\|\boldsymbol{v}_{n+1}\|_\infty+\big\|r_n^{(1)}\big\|_\infty, \end{aligned}$$

$$\begin{aligned}
\|\boldsymbol{v}_n\|_\infty &\leq \|G\|_\infty \big\|\boldsymbol{v}_{n+1} + \Delta t a_{20}\big(f(\boldsymbol{U}_{n+1}) - f(\boldsymbol{u}_{n+1,h})\big)\big\|_\infty \\
&\quad + \Delta t a_{21} \big\|f\big(\boldsymbol{U}_n^{(1)}\big) - f\big(\boldsymbol{u}_{n,h}^{(1)}\big)\big\|_\infty + \|r_n\|_\infty \\
&\leq \|\boldsymbol{v}_{n+1}\|_\infty + \tilde{C}\Delta t \|\boldsymbol{v}_{n+1}\|_\infty + \tilde{C}\Delta t \big\|\boldsymbol{v}_n^{(1)}\big\|_\infty + \|r_n\|_\infty \\
&\leq (1+\tilde{C}\Delta t)\|\boldsymbol{v}_{n+1}\|_\infty + \tilde{C}\Delta t\big((1+\tilde{C}\Delta t)\|\boldsymbol{v}_{n+1}\|_\infty + \big\|r_n^{(1)}\big\|_\infty\big) + \|r_n\|_\infty \\
&= (1+\tilde{C}\Delta t)^2 \|\boldsymbol{v}_{n+1}\|_\infty + \tilde{C}\Delta t \big\|r_n^{(1)}\big\|_\infty + \|r_n\|_\infty.
\end{aligned}$$

Similar to (4.5), we obtain

$$\big\|r_n^{(1)}\big\|_\infty \leq C\sigma^6 (\Delta t)^3, \quad \|r_n\|_\infty \leq C\sigma^6 (\Delta t)^3,$$

where C is a positive constant independent of Δt. Then we deduce

$$\begin{aligned}
\|\boldsymbol{v}_n\|_\infty &\leq (1+\tilde{C}\Delta t)^2 \|\boldsymbol{v}_{n+1}\|_\infty + (1+\tilde{C}\Delta t) C\sigma^6 (\Delta t)^3 \\
&\leq (1+\tilde{C}\Delta t)^{2(N_t-n)} \|\boldsymbol{v}_{N_t}\|_\infty + C\sigma^6 (\Delta t)^3 (1+\tilde{C}\Delta t) \sum_{k=0}^{N_t-n-1} (1+\tilde{C}\Delta t)^{2k} \\
&\leq C\sigma^6 (\Delta t)^3 (1+\tilde{C}\Delta t) \frac{(1+\tilde{C}\Delta t)^{2(N_t-n)} - 1}{\tilde{C}\Delta t(2+\tilde{C}\Delta t)} \\
&\leq C_3 \sigma^6 (\Delta t)^2 \big(e^{2\tilde{C}(T-t_n)} - 1\big),
\end{aligned}$$

where the constant $C_3 = C/\tilde{C}$. □

Now by combining Theorems 3.2, 4.3 and 4.4, we give the error estimates of the fully discrete SRK schemes (4.9) and (4.10). Let $\boldsymbol{u}(t_n)$ denote the restriction of $u(t,\boldsymbol{x})$ on the mesh D_h. Then by noticing the fact that $p=1$ for the SRK1 scheme and $p=2$ for the SRK2 scheme, we have the following theorems.

Theorem 4.5. *Let $u(t,\boldsymbol{x})$ be the exact solution of* (2.2) *and $\boldsymbol{u}_{n,h}$ be the numerical solution obtained from the fully discrete SRK1 scheme* (4.9) *with $\boldsymbol{u}_{N_t,h} = \boldsymbol{u}(T)$. Assume that $\|\varphi\|_{L^\infty} \leq \rho$ and u satisfies $u \in C_b^{2,6}$. Then under the conditions in Theorem* 4.1*, we get*

$$\|\boldsymbol{u}(t_n) - \boldsymbol{u}_{n,h}\|_\infty \leq C\big(e^{\tilde{C}(T-t_n)} - 1\big)\big(\Delta t + \sigma^6 (\Delta t)^2\big),$$

where $\tilde{C} = \max_{|\xi|\leq\rho} |f'(\xi)|$ and the constant $C>0$ is independent of Δt.

Theorem 4.6. *Let $u(t,\boldsymbol{x})$ be the exact solution of* (2.2) *and $\boldsymbol{u}_{n,h}$ be the numerical solution obtained from the fully discrete SRK2 scheme* (4.10) *with $\boldsymbol{u}_{N_t,h} = \boldsymbol{u}(T)$. Assume that $\|\varphi\|_{L^\infty} \leq \rho$ and u satisfies $u \in C_b^{3,6}$. Then under the conditions in Theorem* 4.2*, we get*

$$\|\boldsymbol{u}(t_n) - \boldsymbol{u}_{n,h}\|_\infty \leq C\big(e^{2\tilde{C}(T-t_n)} - 1\big)\big((\Delta t)^2 + \sigma^6 (\Delta t)^2\big),$$

where $\tilde{C} = \max_{|\xi|\leq\rho} |f'(\xi)|$ and the constant $C>0$ is independent of Δt.

Remark 4.3. Theorems 4.3 and 4.4 indicate that the spatial errors of the fully discrete schemes (4.9) and (4.10) can match their temporal errors and can even be neglected when σ is close to zero. For example, for the Allen-Cahn equation, its interface parameter $\epsilon=\sigma/\sqrt{2}$ is usually a small number and thus the spatial errors of (4.9) and (4.10) can be neglected for solving Allen-Cahn equation even for the large time step size such as $\Delta t=\mathcal{O}(1)$.

5 Numerical experiments

Let us consider the reaction-diffusion equation in the backward form

$$u_t+\epsilon^2\Delta u+f(u)=0,\quad \boldsymbol{x}\in D=(0,1)^d,\quad t\in[0,T) \tag{5.1}$$

with the terminal condition $u(T,\boldsymbol{x})=\varphi(\boldsymbol{x})$ and subject to the periodic boundary condition. In this case, we have

$$\frac{1}{2}\sigma^2=\epsilon^2.$$

Let $F(u)$ be a given potential function with $F'(u)=-f(u)$, then (5.1) can be seen as the gradient flow of the energy functional

$$E(u)=\int_D\left(\frac{\sigma^2}{4}|\nabla u|^2+F(u)\right)d\boldsymbol{x}.$$

We shall use the SRK1 scheme (4.9) and the SRK2 scheme (4.10) to solve (5.1). For the SRK2 scheme, we choose $\alpha_{20}=\alpha_{21}=1/2$, $\beta_{20}=0$ and $\beta_{21}=1/2$, that is

$$\begin{aligned}
&\boldsymbol{u}_{n,h}^{(1)}=G\big(\boldsymbol{u}_{n+1,h}+\Delta t f(\boldsymbol{u}_{n+1,h})\big),\\
&\boldsymbol{u}_{n,h}=G\left(\boldsymbol{u}_{n+1,h}+\frac{1}{2}\Delta t f(\boldsymbol{u}_{n+1,h})\right)+\frac{1}{2}\Delta t f\big(\boldsymbol{u}_{n,h}^{(1)}\big).
\end{aligned} \tag{5.2}$$

Then we deduce $\mathcal{C}=1$ in Theorem 3.1 and the constraint for Δt becomes

$$\Delta t\le r_0^+, \tag{5.3}$$

where

$$r_0^+=\begin{cases}0.5, & \text{Ginzburg-Landau potential,}\\ 0.125, & \text{Flory-Huggins potential}\end{cases}$$

with $\theta=0.8$ and $\theta_c=1.6$ in Flory-Huggins potential as shown in (3.15) and (3.16).

5.1 Convergence tests

In this subsection, we test the convergence rates of the fully discrete schemes (4.9) and (5.2) with Ginzburg-Landau potential, that is,

$$f(u)=u-u^3. \tag{5.4}$$

We take $T=1.0$ and set the terminal condition as

$$\varphi(x,y)=0.2\sin(2\pi x)\sin(2\pi y)+0.1.$$

In our experiments, we shall choose $\sigma=0.02, 0.1$ and 0.5. We calculate the numerical solutions at $t=0$ with $\Delta t=1/(3k^2)$ for $k=2,4,\ldots,20$ and regard the approximations of the IFRK4 scheme [13] with $\Delta t=1/(3\times 50^2)$ as the benchmark solution, where the Fourier collocation method with $h=1/128$ is used for spatial discretization.

To compare the accuracy of the SRK2 scheme (5.2) with other second-order schemes, we also use the IFRK2 scheme [13] and the ETDRK2 scheme [7] to solve (5.1) with the same time steps. For the IFRK2 and ETDRK2 schemes, the central finite difference method with $h=1/128$ is used for the spatial discretization. The maximum norm errors and the convergence rates for different schemes with various values of σ are presented in Tables 1-4, respectively.

From the results listed in Tables 1-4, we come to the following conclusions:

- The fully discrete SRK1 scheme (4.9) and the fully discrete SRK2 scheme (5.2) can respectively achieve the expected first-order and second-order convergence rates for different values of σ, which are consistent with our theoretical results.
- The errors of the SRK2 scheme (5.2) are almost the same as the ones of the IFRK2 and ETDRK2 schemes, which shows that the proposed SRK2 scheme can achieve the same accuracy as the other two existing explicit second-order schemes.

Table 1: Errors and convergence rates of the SRK1 scheme.

N_t	$\sigma=0.02$		$\sigma=0.1$		$\sigma=0.5$	
	Error	Rate	Error	Rate	Error	Rate
3×2^2	1.050E-02	0.000	1.033E-02	0.000	9.072E-03	0.000
3×4^2	2.692E-03	0.982	2.651E-03	0.981	2.354E-03	0.973
3×6^2	1.202E-03	0.994	1.185E-03	0.993	1.053E-03	0.991
3×8^2	6.773E-04	0.997	6.675E-04	0.997	5.940E-04	0.996
3×10^2	4.338E-04	0.998	4.275E-04	0.998	3.806E-04	0.997
3×12^2	3.014E-04	0.999	2.970E-04	0.999	2.645E-04	0.998
3×14^2	2.215E-04	0.999	2.183E-04	0.999	1.944E-04	0.999
3×16^2	1.696E-04	0.999	1.672E-04	0.999	1.489E-04	0.999
3×18^2	1.340E-04	1.000	1.321E-04	1.000	1.176E-04	0.999
3×20^2	1.086E-04	1.000	1.070E-04	1.000	9.529E-05	0.999

Table 2: Errors and convergence rates of the SRK2 scheme.

N_t	$\sigma=0.02$		$\sigma=0.1$		$\sigma=0.5$	
	Error	Rate	Error	Rate	Error	Rate
3×2^2	3.041E-04	0.000	2.980E-04	0.000	3.240E-04	0.000
3×4^2	1.985E-05	1.968	1.937E-05	1.972	2.110E-05	1.970
3×6^2	3.954E-06	1.990	3.853E-06	1.991	4.192E-06	1.993
3×8^2	1.254E-06	1.995	1.222E-06	1.996	1.329E-06	1.997
3×10^2	5.145E-07	1.997	5.012E-07	1.997	5.449E-07	1.998
3×12^2	2.483E-07	1.998	2.418E-07	1.998	2.629E-07	1.999
3×14^2	1.341E-07	1.999	1.306E-07	1.999	1.419E-07	1.999
3×16^2	7.862E-08	1.999	7.657E-08	1.999	8.322E-08	1.999
3×18^2	4.909E-08	1.999	4.781E-08	1.999	5.196E-08	1.999
3×20^2	3.221E-08	1.999	3.137E-08	1.999	3.409E-08	2.000

Table 3: Errors and convergence rates of the IFRK2 scheme.

N_t	$\sigma=0.02$		$\sigma=0.1$		$\sigma=0.5$	
	Error	Rate	Error	Rate	Error	Rate
3×2^2	3.041E-04	0.000	2.957E-04	0.000	3.155E-04	0.000
3×4^2	1.985E-05	1.968	1.923E-05	1.971	2.057E-05	1.969
3×6^2	3.953E-06	1.990	3.826E-06	1.991	4.091E-06	1.992
3×8^2	1.254E-06	1.995	1.214E-06	1.996	1.297E-06	1.996
3×10^2	5.145E-07	1.997	4.976E-07	1.997	5.320E-07	1.998
3×12^2	2.483E-07	1.998	2.401E-07	1.998	2.567E-07	1.998
3×14^2	1.341E-07	1.999	1.297E-07	1.999	1.386E-07	1.999
3×16^2	7.861E-08	1.999	7.603E-08	1.999	8.126E-08	1.999
3×18^2	4.909E-08	1.999	4.747E-08	1.999	5.074E-08	1.999
3×20^2	3.221E-08	1.999	3.115E-08	1.999	3.329E-08	2.000

Table 4: Errors and convergence rates of the ETDRK2 scheme.

N_t	$\sigma=0.02$		$\sigma=0.1$		$\sigma=0.5$	
	Error	Rate	Error	Rate	Error	Rate
3×2^2	3.031E-04	0.000	2.451E-04	0.000	3.228E-04	0.000
3×4^2	1.979E-05	1.969	1.603E-05	1.968	2.153E-05	1.953
3×6^2	3.941E-06	1.990	3.192E-06	1.990	4.294E-06	1.988
3×8^2	1.250E-06	1.995	1.013E-06	1.995	1.363E-06	1.994
3×10^2	5.128E-07	1.997	4.155E-07	1.997	5.592E-07	1.997
3×12^2	2.475E-07	1.998	2.005E-07	1.998	2.699E-07	1.998
3×14^2	1.336E-07	1.999	1.083E-07	1.999	1.458E-07	1.998
3×16^2	7.836E-08	1.999	6.349E-08	1.999	8.547E-08	1.999
3×18^2	4.893E-08	1.999	3.964E-08	1.999	5.337E-08	1.999
3×20^2	3.211E-08	1.999	2.601E-08	1.999	3.502E-08	1.999

5.2 Tests for MBP preservation

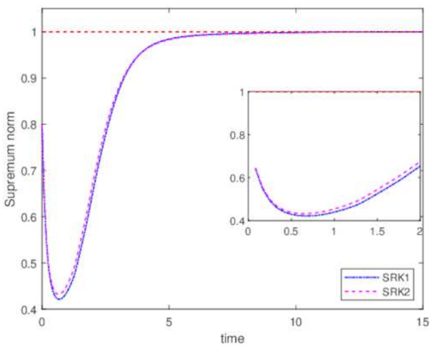
In this subsection, we test the MBP-preserving property of the SRK schemes (4.9) and (5.2). To this end, we simulate the processes of the coarsening dynamics with $\sigma=0.02$ and $\sigma=0.1$ for the Ginzburg-Landau potential with $f(u)$ defined by (5.4) and the Flory-Huggins potential with

$$f(u)=\frac{\theta}{2}\ln\frac{1-u}{1+u}+\theta_c u, \quad \theta=0.8, \quad \theta_c=1.6. \tag{5.5}$$

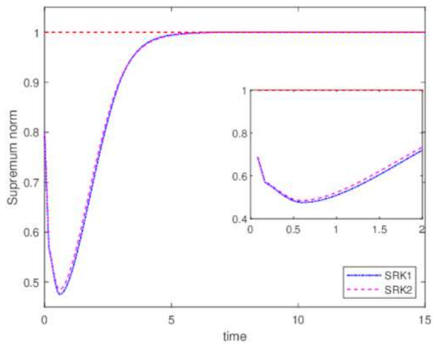
The initial data is generated by the uniform distribution on $(-0.8,0.8)$. We use the schemes (4.9) and (5.2) with the uniform time step size $\Delta t=1/(3\times 2^2)$, close to the upper bound of the time step size for the Flory-Huggins potential in (5.3). Then by using the spatial mesh size $h=\sigma\sqrt{3\Delta t}$, we obtain

$$h=\begin{cases} 0.05 & \text{for} \quad \sigma=0.1, \\ 0.01 & \text{for} \quad \sigma=0.02. \end{cases}$$

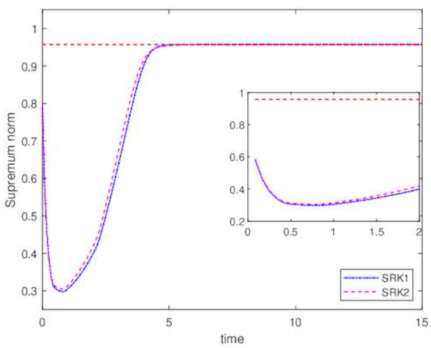
Fig. 1 plots the evolutions of the supremum norms of the numerical solutions. The red dash horizontal line shows the theoretical upper bound ρ of the numerical solutions.



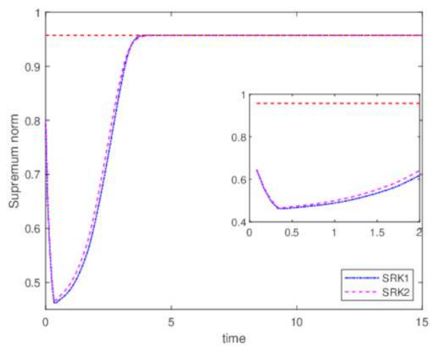
(a) Ginzburg-Landau, $\sigma=0.1$



(b) Ginzburg-Landau, $\sigma=0.02$



(c) Flory-Huggins, $\sigma=0.1$



(d) Flory-Huggins, $\sigma=0.02$

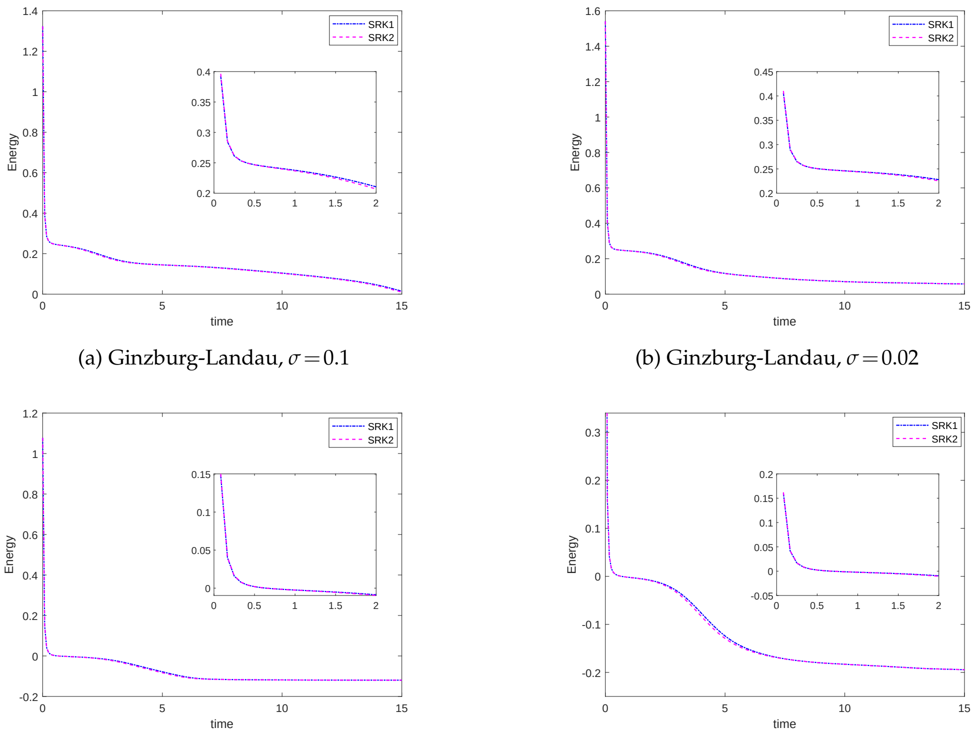
Figure 1: Evolutions of the supremum norms.

It can be observed that for the both kinds of nonlinear terms, the supremum norms of the numerical solutions with different values of σ are always bounded by the theoretical values. Fig. 2 plots the evolutions of the energies of the numerical solutions, which show that the schemes (4.9) and (5.2) are energy stable in the discrete sense.

Next, we simulate the evolutions of a shrinking bubble in 2D governed by (5.1) for the Flory-Huggins potential with $f(u)$ defined by (5.5). We take $\sigma=0.02$ in our simulation and the terminal bubble is given by

$$\varphi(x,y)=\begin{cases} 0.95, & \text{if} \quad (x-0.5)^2+(y-0.5)^2\leq 0.1, \\ -0.95, & \text{otherwise}. \end{cases}$$

The SRK2 scheme (5.2) is adopted, and the time step size is set to be $\Delta t=1/(3\times 2^2)$ and thus the mesh size $h=0.01$. Fig. 3 presents the evolutions of the bubble at times $t=100k$, $k=1,2,\ldots,6$, respectively. Fig. 4 shows the cross-section view with $y=0.5$ of the initial value (left) and the evolutions (right). Throughout the evolution, the bubble gets smaller and smaller until it ultimately disappears at around $t=248$. We present the evolutions of supremum norm (left) and energy (right) in Fig. 5, which again verify the MBP-preserving and the energy-decreasing of the scheme (5.2).



(a) Ginzburg-Landau, $\sigma=0.1$

(b) Ginzburg-Landau, $\sigma=0.02$

(c) Flory-Huggins, $\sigma=0.1$

(d) Flory-Huggins, $\sigma=0.02$

Figure 2: Evolutions of the energies.

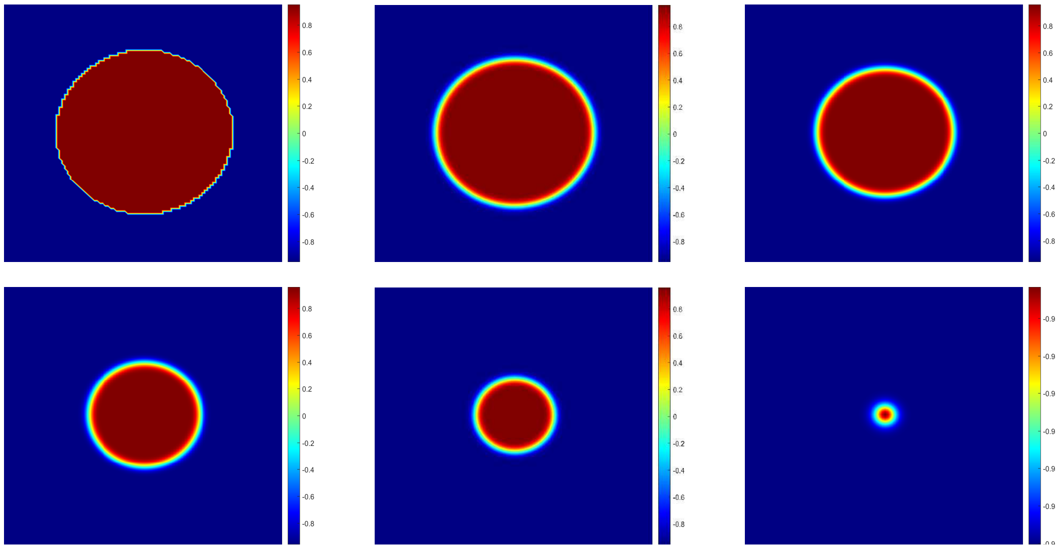


Figure 3: The snapshots of the evolution at $t = 0,50,100,150,200,250$, respectively (left to right and top to bottom), for the 2D shrinking bubble.

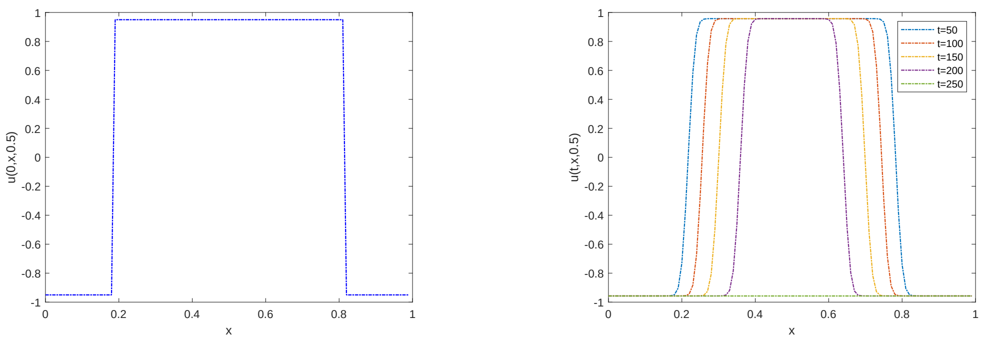


Figure 4: The cross-section views with $y = 0.5$ of the initial value (left) and the evolutions (right).

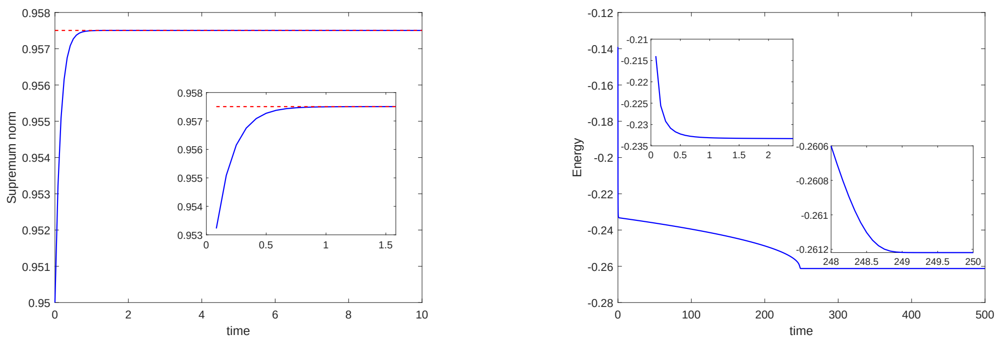


Figure 5: Evolutions of the supremum norm (left) and the energy (right) for the 2D shrinking bubble.

5.3 The coarsening dynamics

In this subsection, we shall use the SRK2 scheme (5.2) to simulate the 2D and 3D coarsening dynamics of the Eq. (5.1) for the Flory-Huggins potential with a random initial data ranging from -0.8 to 0.8.

First, we simulate the 2D coarsening dynamics with $\sigma = 0.02$ and $T = 1000$. The time step size is set to be $\Delta t = 1/(3\times 2^2)$ with the corresponding mesh size $h = 0.01$. Using a laptop with a twelve-core Intel 2.60 GHz and 64 GB memory, the calculations are performed by MATLAB software. The CPU time for the computation is about 7.93 seconds. Fig. 6 presents the evolutions of the phase structures at $t = 4, 6, 10, 30, 100$, and 300, respectively. The simulated dynamics begins with a random state and towards the homogeneous steady state of constant ρ, which is reached after about $t = 340$ in our simulation. The evolutions of the supremum norms and the energies are also plotted in Fig. 7, which

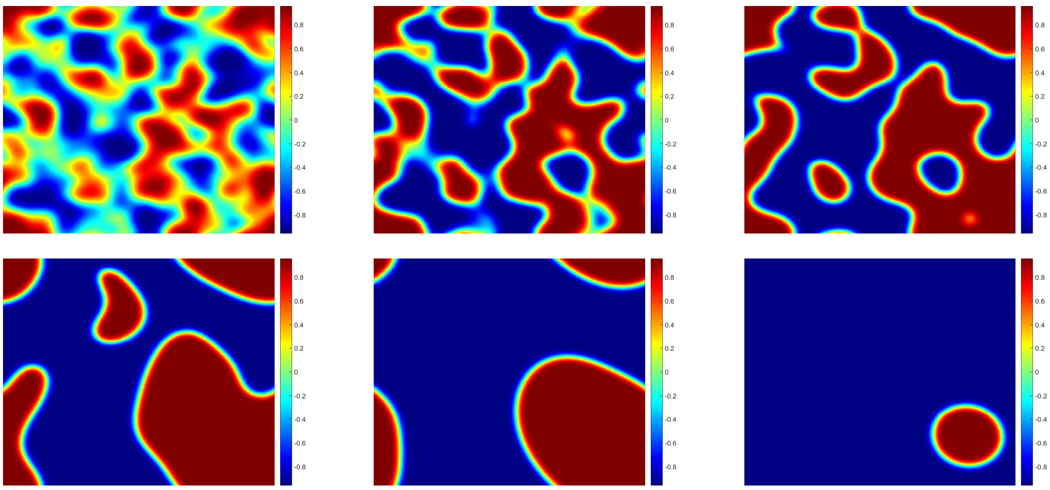


Figure 6: The snapshots of the evolution at t=4,6,10,30,100,300, respectively (left to right and top to bottom), for the 2D coarsening dynamics.

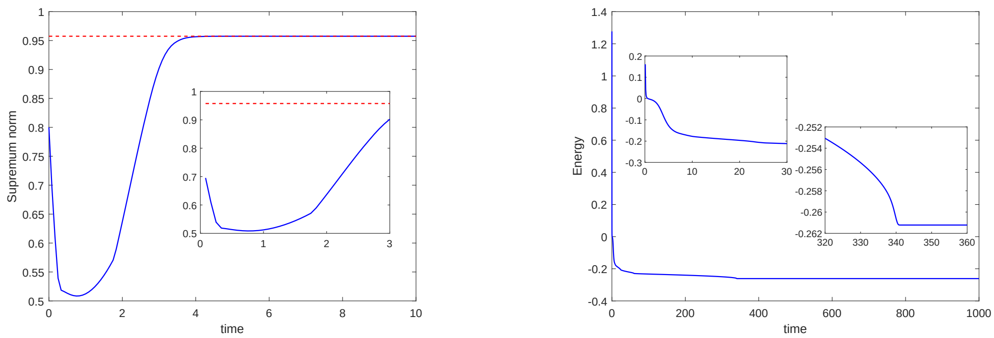


Figure 7: Evolutions of the supremum norm (left) and the energy (right) for the 2D coarsening dynamics.

show that the energy decreases monotonically and the MBP is perfectly preserved so that the solution is always located in $[-\rho,\rho]$.

Next, we simulate the 3D coarsening dynamics with $\sigma=0.02$ and $T=500$. The CPU time for running the SRK2 scheme is around 5.71 minutes. Fig. 8 shows the evolutions of the zero-isosurface of the numerical solutions given by the SRK2 scheme. Similar to the 2D case, the simulated dynamics begins with a random state and reaches the steady state of constant ρ around $t=373$. Fig. 9 plots the evolutions of the supremum norms and the energies, where the MBP is preserved and the energy decreases in time.

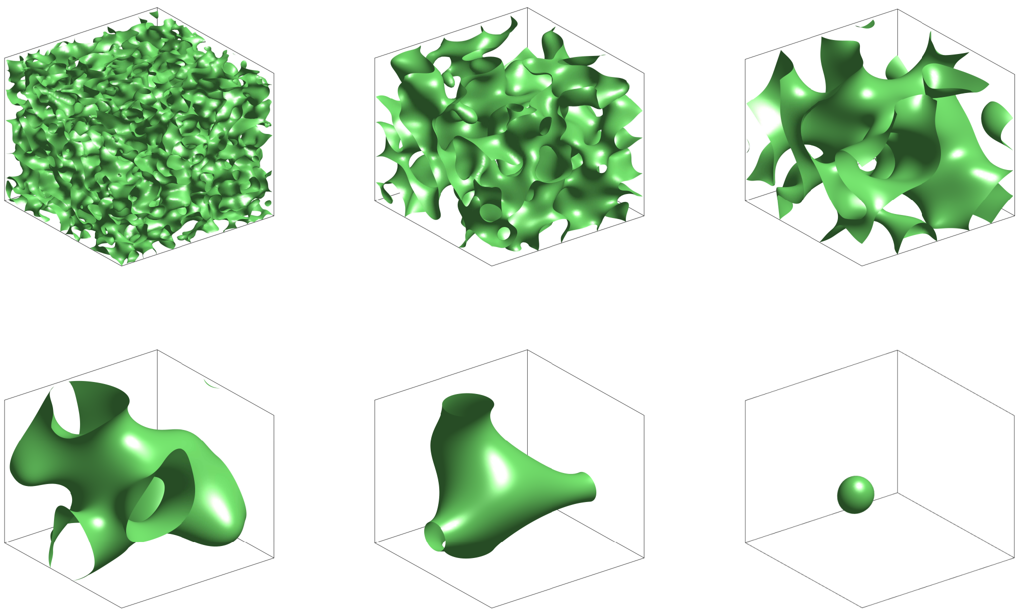


Figure 8: The snapshots of the evolution at $t=2,10,40,100,240,360$, respectively (left to right and top to bottom), for the 3D coarsening dynamics.

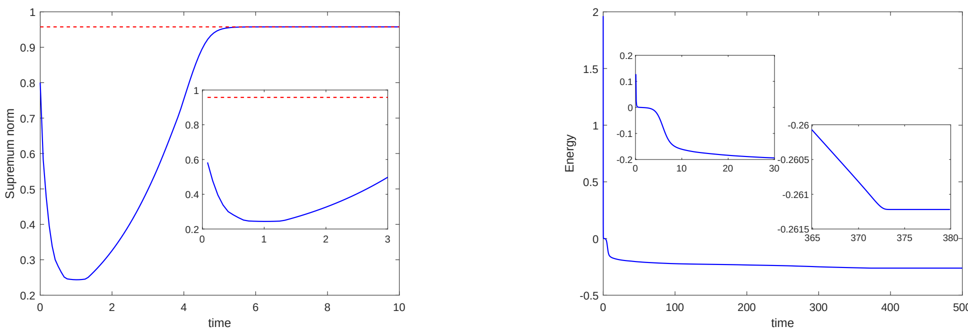


Figure 9: Evolutions of the supremum norm (left) and the energy (right) for the 3D coarsening dynamics.

6 Conclusions

In this paper, we proposed a class of stochastic Runge-Kutta schemes (SRK) for solving the semilinear parabolic equations by using their probabilistic representation via BSDEs. We theoretically proved the MBP-preserving and error estimates of the proposed time semidiscrete SRK schemes. By choosing the three-point Gaussian quadrature rule in the fully discrete schemes, we constructed the fully discrete MBP-preserving first-order SRK1 scheme and second-order SRK2 scheme. Their MBP-preserving and error estimates are also rigorously analyzed. Some numerical experiments are carried out to verify the theoretical results, and to show the efficiency and stability of the proposed schemes. In our future work, we will consider to propose the fully discrete MBP-preserving stochastic Runge-Kutta schemes up to fourth order by using the Sinc quadrature rule for the approximation of the conditional expectation.

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