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A Generalized Second-Order Positivity-Preserving Numerical Method for Non-Autonomous Dynamical Systems with Applications

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Abstract

In this work, we propose a generalized, second-order, nonstandard finite difference (NSFD) method for non-autonomous dynamical systems. The proposed method combines the NSFD framework with a new non-local approximation of the right-hand side function. This method achieves second-order convergence and unconditionally preserves the positivity of solutions for all step sizes. Especially, it avoids the restrictive conditions required by many existing positivity-preserving, second-order NSFD methods. The method is easy to implement and computationally efficient. Numerical experiments, including an improved NSFD scheme for an SIR epidemic model, confirm the theoretical results. Additionally, we demonstrate the method's applicability to nonlinear partial differential equations and boundary value problems with positive solutions, showcasing its versatility in real-world modeling.

Keywords: Nonstandard finite difference, Positivity-preserving, Non-local approximation, Epidemic Models, Non-autonomous dynamical systems.
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1. Introduction

Various important processes and phenomena in real-world situations can be modeled mathematically by non-autonomous dynamical systems of the form:

$$y'(t) = F(t, y(t)), \quad y(0) = y_0 \in \mathbb{R}^n, \tag{1.1}$$

where $y(t) = [y_1(t), y_2(t), \dots, y_n(t)]^\top : \mathbb{R} \to \mathbb{R}^n$ is an unknown function that must be determined as the solution; $F(t, y) = [F_1(t, y), F_2(t, y), \dots, F_n(t, y)]^\top : \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}^n$ satisfies conditions that guarantee the existence and uniqueness of solutions to (1.1) [4, 15, 28, 40].

For these dynamical systems, the positivity of the solutions can be considered as the most common and important characteristic [4, 28, 40]. This characteristic can be easily investigated by a simple necessary and sufficient condition (see [22, Lemma 1] and [40, Proposition B.7]): The solution of (1.1) admits the set $\mathbb{R}^n_+ = \{(y_1, y_2, \dots, y_n) \in \mathbb{R}^n | y_1 \geq 0, \ y_2 \geq 0, \dots, y_n \geq 0\}$ as a positively invariant set if and only if

$$F_i(t, y)|_{y_i=0} := F_i(t, y_1, \dots, y_{i-1}, 0, y_{i+1}, \dots y_n) \geq 0 \tag{1.2}$$

for $i = 1, 2, \dots, n$ and $(t, y) \in \mathbb{R}_+ \times \mathbb{R}^n_+$.

Numerical methods that preserve the positivity of solutions to (1.1) are essential in both theory and practice (see, for instance, [22, 23, 30, 31, 32, 33, 34]). Nonstandard finite difference (NSFD) schemes,

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which were first introduced by Mickens in the 1980s [30, 31, 32, 33, 34], have become an efficient approach to the positivity-preserving problem of numerical methods. Specifically, NSFD schemes have the ability to preserve not only the positivity of the solutions but also other qualitative dynamical properties for all step sizes [30, 31, 32, 33, 34, 38, 39]. However, NSFD schemes typically achieve only first-order accuracy. For this reason, high-order NSFD schemes for dynamical systems governed by nonlinear ordinary differential equations (ODEs), mainly second-order schemes, have been intensively studied in recent years (see [1, 2, 10, 16, 17, 18, 19, 20, 25] and references therein). These NSFD schemes are derived from methodology of Mickens [30, 31, 32, 33, 34] with a non-local approximation for the right-hand side functions and renormalization of the denominator functions.

Second-order NSFD methods have been developed for one-dimensional dynamical systems (see, e.g., [16, 17, 18, 25]). For multi-dimensional dynamical systems, Alalhareth et al. [1] have been developed the approach used in [43] to construct second-order modified positive and elementary stable (SOPESN) NSFD methods for n-dimensional autonomous differential equations. These SOPESN methods were subsequently employed in [3] to numerically solve a mathematical model of nutrient recycling and dormancy in a chemostat. In a recent work [20], the authors have used a nonlocal approximation with right-hand side function weights and nonstandard denominator functions to construct a second-order and dynamically consistent NSFD method for a general Rosenzweig-MacArthur predator-prey model. Recently, Conte et al. [10] have derived a general procedure to obtain unconditionally positive second-order NSFD methods. Furthermore, adding parameters to these schemes for each particular problem allows one to determine the optimal parameter values to guarantee positivity, elementary stability, and minimization of the local truncation error.

Inspired by the importance of positivity-preserving numerical methods, this work proposes a straightforward method for constructing second-order positivity-preserving numerical methods for system (1.1). Throughout this paper, we will consider the system (1.1) under the condition (1.2).

It is not difficult to show that for each $1 \leq i \leq n$:

- if $F_i(t, y)|_{y_i=0} = 0$ and $y_i(0) = 0$, then $y_i(t) = 0$ for all $t \geq 0$ is the unique solution;
- if $F_i(t, y)|_{y_i=0} = 0$ and $y_i(0) > 0$, then $y_i(t) > 0$ for all $t > 0$;
- if $F_i(t, y)|_{y_i=0} > 0$ and $y_i(0) > 0$, then $y_i(t) > 0$ for all $t > 0$;
- if $F_i(t, y)|_{y_i=0} > 0$ and $y_i(0) = 0$, then there exists $t_0 > 0$ such that $y_i(t) > 0$ for all $t \geq t_0$.

Consequently, without loss of generality, we can consider (1.1) with strictly positive solutions, that is for each i

$$y_i(0) > 0 \Longrightarrow y_i(t) > 0 \quad \text{for} \quad t > 0. \tag{1.3}$$

In other words, the system (1.1) admits the interior $\text{int}(\mathbb{R}^n_+)$ of $\mathbb{R}^n_+$ as a positively invariant set. Therefore, our goal is to develop second-order numerical methods that possess the property

$$y_i(0) > 0 \Longrightarrow y_i^k > 0 \quad \text{for all} \quad k = 1, 2, \dots \quad \text{and} \quad \Delta t > 0, \tag{1.4}$$

where $\Delta t > 0$ is the step size and y_i^k is the intended approximation of $y_i(t^k)$ with $t^k = k\Delta t$ for $k = 1, 2, \dots$.

Based on a representation theorem [12, Theorem 10], it is important to note that the system (1.1) can be represented in the form

$$y_i'(t) = f_i(t, y) - y_i\, g_i(t, y), \quad i = 1, 2, \dots, n \tag{1.5}$$

where f_i and g_i are two functions from $\mathbb{R}_+ \times \text{int}\left(\mathbb{R}^n_+\right) \to \mathbb{R}_+$.

From now on, we will work with (1.5) instead of (1.1). Using the approaches used in [1, 2] and [10], one can obtain second-order positivity-preserving schemes for (1.1). However, as will be discussed in Section 2, the resulting NSFD schemes require a strict and indispensable condition (Condition (2.10)), which limits their applicability in computations. In contrast, the NSFD method proposed in this work relaxes this condition. As a result, its computational implementation is straightforward. It is well-known that Runge-Kutta methods only guarantee the positivity preserving property in many situations if the step size is smaller than a positivity step size threshold (see, e.g., [22, 23]). However, the constructed NSFD method is positivity-preserving regardless of the chosen step size. In other words, it is unconditionally positive.

The paper is organized as follows. In Section 2, we apply the well-known approaches proposed in [1, 2] and [10] to obtain second-order positivity-preserving NSFD schemes for (1.5), thereby identifying a strict and indispensable condition (Condition (2.10)) imposed on the resulting NSFD schemes. In Section 3, we construct and analyze a generalized second-order positivity-preserving NSFD method for which the condition (2.10) is relaxed. In Section 4, we conduct a set of numerical experiments to support and illustrate the theoretical results. In these experiments, we consider a modified Susceptible-Infected-Removed (SIR) model [6] as a test problem. An important consequence is that the dynamically consistent NSFD scheme for the SIR model, constructed very recently in [27], is improved. Finally, in Sections 5 and 6, we apply the constructed NSFD method to solve some classes of partial differential equations (PDEs) and boundary value problems (BVPs) with positive solutions. The last section includes some concluding remarks and discussions.

2. NSFD Schemes Based on Well-Known Approaches

In this section, we apply the NSFD methods constructed in [1, 2] and [10] to obtain second-order NSFD positivity-preserving NSFD schemes for (1.5).

First, applying the approach in [2] leads to the following NSFD scheme for (1.5):

$$\frac{y_i^{k+1} - y_i^k}{\phi_i(\Delta t, t^k, y^k)} = f_i(t^k, y_i^k) - y_i^{k+1} g_i(t^k, y_i^k), \tag{2.1}$$

where $\phi_i(.)$ is a function satisfying

$$\begin{aligned} &\phi_i(\Delta_t, t, y) > 0 \quad \text{for all} \quad \Delta t > 0, \quad (t, y) \in \mathbb{R}_+ \times \text{int}(\mathbb{R}_+^n), \\ &\phi_i(\Delta_t, t, y) = \Delta t + \mathcal{O}(\Delta t^2) \quad \text{as} \quad \Delta t \to 0. \end{aligned} \tag{2.2}$$

The system (2.1) can be written in the form

$$y_i^{k+1} = \frac{y_i^k + \phi_i\, f_i(t^k, y^k)}{1 + \phi_i\, g_i(t^k, y^k)}. \tag{2.3}$$

This implies that (2.1) preserves the positivity of the solutions for all $\Delta t > 0$. Note that first-order NSFD schemes for a general class of two ODEs constructed [11] and for a n-dimensional productive-destructive systems [44] can be derived from (2.3) with $\phi_i = \phi$ for all $i = 1, 2, \dots n$.

A condition ensuring the second-order accuracy of (2.1) is determined via Taylor's expansion theorem as follows (see [2]).

Lemma 2.1. *Assume that the denominator functions ϕ_i ($i = 1, 2, \dots, n$) satisfy* (2.2)*. Then, the truncated error of* (2.1) *is $\mathcal{O}(\Delta t^3)$ as $\Delta t \to 0$ whenever*

$$\frac{\partial^2 \phi_i}{\partial \Delta t^2}(0, t, y) = 2g_i(t, y) + \frac{1}{F_i(t, y)}\left(\frac{\partial F_i}{\partial t}(t, y) + \sum_{j=1}^{n} \frac{\partial F_i}{\partial y_j}(t, y)\, F_j(t, y)\right) \tag{2.4}$$

for all $t \geq 0$, $y \in \text{int}(\mathbb{R}_+^n)$ such that $F_i(t, y) \neq 0$, where $F_i(t, y) = f_i(t, y) + y_i\, g(t, y)$ is the right-hand side function of the i-th equation of (1.1)*.*

Next, we apply the approach used in [1] (as well as in [2]) to obtain a second-order and positive NSFD scheme for (1.1). The resulting NSFD scheme is given by

$$\frac{y_i^{k+1} - y_i^k}{\phi_i(\Delta t, t^k, y^k)} = w_i^k F_i(t^k, y^k), \tag{2.5}$$

where

$$w_i^k := \begin{cases} 1, & \text{if} \quad F_i(t^k, y^k) \geq 0, \\ \dfrac{y_i^{k+1}}{y_i^k}, & \text{if} \quad F_i(t^k, y^k) < 0, \end{cases}$$

and $\phi_i(.)$ are functions satisfying (2.2).

The following result is proven based on the proof of [2, Theorem 3.2.1] (see also [1]).

Lemma 2.2. *Assume that the denominator functions ϕ_i $(i = 1, 2, \dots, n)$ satisfy* (2.2)*. Then, the truncated error of* (2.1) *is $\mathcal{O}(\Delta t^3)$ as $\Delta t \to 0$ whenever*

$$\frac{\partial^2 \phi_i}{\partial \Delta t^2}(0, t, y) = \begin{cases} \dfrac{1}{F_i(t, y)}\left(\dfrac{\partial F_i}{\partial t}(t, y) + \displaystyle\sum_{j=1}^{n} \dfrac{\partial F_i}{\partial y_j}(t, y) F_j(t, y)\right) & \text{if} \quad F_i(t, y) \geq 0, \\ 2\dfrac{F_i(t, y)}{y_i^2} - \dfrac{1}{F_i(t, y) y_i^2}\displaystyle\sum_{j=1}^{n}\left(\dfrac{\partial F_i}{\partial t}(t, y) + \displaystyle\sum_{j=1}^{n} \dfrac{\partial F_i}{\partial y_j}(t, y) F_j(t, y)\right) & \text{if} \quad F_i(t, y) < 0 \end{cases} \tag{2.6}$$

for all $t \geq 0$, $y \in \mathrm{int}(\mathbb{R}_+^n)$ such that $F_i(t, y) \neq 0$, where $F_i(t, y)$ is the right-hand side function of the i-th equation of (1.1)*.*

We now construct another positivity-preserving and second-order NSFD scheme for (1.1), based on the α-NSFD method recently formulated in [10]. The resulting NSFD scheme is given by

$$\frac{y_i^{k+1} - y_i^k}{\phi_i(\Delta t, t^k, y^k)} = F_i(t^k, y^k) - \alpha^i \frac{y_i^{k+1} - y_i^k}{y_i^k} F_{i-}(t^k, y^k), \tag{2.7}$$

where the right-side functions $F_i = F_{i+} + F_{i-}$ are split into a positive F_+ term and a negative F_{i-} term; α^i are non-negative real numbers for $i = 1, 2, \dots, n$.

Applying (2.7) to (1.5) yields

$$\frac{y_i^{k+1} - y_i^k}{\phi_i(\Delta t, t^k, y^k)} = F_i(t^k, y^k) - \alpha^i \frac{y_i^{k+1} - y_i^k}{y_i^k} y_i^k g_i(t^k, y^k). \tag{2.8}$$

Note that (2.8) reduces to (2.1) if $\alpha^i = 1$. Furthermore, we deduce from [10, Theorem 3] that (2.9) preserves the positivity of the solutions of (1.5) if $\alpha^i \geq F_i(t^k, y^k)/(y_i^k g_i(t^k, y^k))$ for all $t_k \geq 0$ and $y^k \in \mathrm{int}(\mathbb{R}_+^n)$. A condition for (1.1) to be second-order accurate was given in [10, Theorem 4]. Based on this, we obtain the following lemma.

Lemma 2.3. *Assume that the denominator functions ϕ_i $(i = 1, 2, \dots, n)$ satisfy* (2.2)*. Then, the truncated error of* (2.1) *is $\mathcal{O}(\Delta t^3)$ as $\Delta t \to 0$ provided that*

$$\frac{\partial \phi_i}{\partial \Delta t}(0, t, y) = 2\alpha^i\, g_i(t, y) + \frac{1}{F_i(t, y)}\left(\frac{\partial F_i}{\partial t}(t, y) + \sum_{j=1}^{n} \frac{\partial F_i}{\partial y_j}(t, y)\, F_j(t, y)\right) \tag{2.9}$$

for all $t \geq 0$, $y \in \mathrm{int}(\mathbb{R}_+^n)$ such that $F_i(t, y) \neq 0$, where $F_i(t, y)$ is the right-hand side function of the i-th equation of (1.1)

Remark 2.4. Consistency is a local property of one-step schemes, such as the NSFD schemes (2.1), (2.5), and (2.7). Using the well-known result that the convergence order can follow from the consistency order [5], we obtain the NSFD schemes convergence of order 2 from the second-order consistent ones.

Remark 2.5. Lemmas 2.1–2.3 provide the conditions for the NSFD schemes to be convergent of order 2. However, it is easy to see a strict and indispensable condition for the NSFD schemes (2.1), (2.5) and (2.7) is

$$F_i(t^k, y^k) \neq 0 \quad \text{for all} \quad k \geq 0 \quad \text{and} \quad i = 1, 2, \dots, n. \tag{2.10}$$

This condition can be removed for 1-D dynamical systems [16, 17, 18, 25]; however, it limits the applicability of the corresponding NSFD schemes for computing solutions to multi-dimensional dynamical systems. To illustrate this, we consider the following simple system

$$y_1' = F_1(t, y_1, y_2) := t^2(y_1 - a)^2 + t^4(y_2 - b)^4,$$
$$y_2' = F_2(t, y_1, y_2) := t^4(y_1 - c)^2 + t^2(y_2 - d)^2,$$

subject to the initial data: $y_1(0) > 0$ and $y_2(0) > 0$, where a, b, c, d are positive real numbers. If at a certain iteration k ($k \geq 0$) we obtain $y_1^k = a, y_2^k = b$, then $F_1(t^k, y_1^k, y_2^k) = 0$; consequently, the condition (2.10) is violated. The same can be said if $y_1^k = c, y_2^k = d$ for some $k \geq 0$. For autonomous dynamical systems, (2.4), (2.6) and (2.9) are not satisfied if there exists an approximation y^k belonging to the nullclines of the dynamical systems under consideration.

The NSFD scheme (2.5) requires determining the sign of the right-hand side function at each iteration step to choose w_i^k. Similarly, the NSFD scheme (2.9) requires choosing the value of α^i at each iteration step.

3. Construction of New Second-Order Positivity-Preserving NSFD Method

In this section, we will construct a generalized, second-order, positivity-preserving NSFD method that relaxes the condition (2.10).

For any function u from $\text{int}(\mathbb{R}_+^m)$ to $\mathbb{R}_+$, we define

$$\mathcal{D}(u) = \{(u_+, u_-) | u_+, u_- : \text{int}(\mathbb{R}_+^m) \to \mathbb{R}; u_+, u_- \geq 0, u_+ - u_- = u\}.$$

It is easy to see that $\mathcal{D}(u)$ is not empty. Indeed, the following are elements of $\mathcal{D}(u)$:

$$\left(u_+ = \frac{u + |u|}{2},\ u_- = -\frac{u - |u|}{2}\right), \quad (u_+ = u^2 + 1 + u,\ u_- = u^2 + 1), \quad (e^u + u,\ e^u).$$

We propose the following NSFD model for (1.5)

$$\frac{y_i^{k+1} - y_i^k}{\phi_i(\Delta t, t^k, y^k)} = f_i(t^k, y^k) - y_i^{k+1} g_i(t^k, y^k) + \varphi_i(\Delta t, t^k, y^k)\left(A_i(t^k, y^k) - \frac{y_i^{k+1}}{y_i^k} B_i(t^k, y^k)\right), \tag{3.1}$$

where

- $\phi_i(.)$ ($i = 1, 2, \ldots, n$) are denominator functions satisfying (2.2);
- $A_i(.)$ and $B_i(.)$ ($i = 1, 2, \ldots, n$) are functions from $\mathbb{R}_+ \times \text{int}(\mathbb{R}_+^n)$ to $\mathbb{R}_+$, which will be determined so that the NSFD scheme is convergent of order 2;
- $\varphi_i(\Delta t)$ ($i = 1, 2, \ldots, n$) are functions of Δt that satisfy

$$\begin{aligned} &\varphi_i(\Delta t) > 0 \quad \text{for all} \quad \Delta t > 0, \\ &\varphi_i'(0) := \kappa_i > 0. \end{aligned} \tag{3.2}$$

First, we investigate the positivity of solutions to the system (3.1).

Theorem 3.1. *If $A_i(t, y)$ and $B_i(t, y)$ ($i = 1, 2, \ldots, n$) satisfy $A_i(t, y) \geq 0$ and $B_i(t, y) \geq 0$ for all $(t, y) \in \mathbb{R}_+ \times \text{int}(\mathbb{R}_+^n)$, then the model* (3.1) *admits the set* $\text{int}(\mathbb{R}_+^n)$ *as a positively invariant set for all $\Delta t > 0$. In other words, the NSFD method* (3.1) *preserves the positivity of the solution to the dynamical system* (1.1) *for all finite values of the step size.*

Proof. We must prove that $y^k \in \mathrm{int}(\mathbb{R}^n_+)$ for $k > 0$ whenever $y^0 = y(0) \in \mathrm{int}(\mathbb{R}^n)$. Indeed, we transform (3.1) into the explicit form

$$y_i^{k+1} = \frac{y_i^k + \phi_i\, f_i(t^k, y^k) + \phi_i\, \varphi_i\, A_i(t^k, y^k)}{1 + \phi_i\, g_i(t^k, y^k) + \phi_i\, \varphi_i\, B_i(t^k, y^k)/y_i^k} = \frac{(y_i^k)^2 + \phi_i\, y_i^k\, f_i(t^k, y^k) + \phi_i\, \varphi_i\, y_i^k\, A_i(t^k, y^k)}{1 + \phi_i\, y_i^k\, g_i(t^k, y^k) + \phi_i\, \varphi_i\, B_i(t^k, y^k)}, \tag{3.3}$$

which implies that $y_i^{k+1} > 0$ if $y_i^k > 0$. Therefore, by mathematical induction, we obtain the desired conclusion. The proof is complete. □

We will now determine the conditions under which the NSFD method (3.1) is convergent of order 2. To this end, let us denote

$$v_i(t, y) = \frac{\partial F_i}{\partial t}(t, y) + \sum_{j=1}^{n} \frac{\partial F_i}{\partial y_j}(t, y)\, F_j(t, y), \quad i = 1, 2, \ldots, n \tag{3.4}$$

Theorem 3.2. *Assume that the following conditions hold for $i = 1, 2, \ldots, n$:*

- *$\phi_i(\Delta t, t, y)$ are denominator functions with the property that*

$$\frac{\partial^2 \phi_i}{\partial \Delta t^2}(0, t, y) = 2g_i(t, y) \tag{3.5}$$

  for all $(t, y) \in \mathbb{R}_+ \times \mathrm{int}(\mathbb{R}^n_+)$.
- *$\varphi_i(\Delta t)$ satisfy (3.2);*
- *(A_i, B_i) is an element of the set $\mathcal{D}(v_i/(2\kappa_i))$.*

Then, the NSFD method (3.1) satisfies (1.4) and its truncated error is $\mathcal{O}(\Delta t^3)$ as $\Delta t \to 0$.

Proof. First, the positivity of the approximate solutions generated by (3.1) is a direct consequence of Theorem 3.1. To analyze the truncated error, we rewrite (3.3) in the form

$$y_i^{k+1} := V_i(\Delta t, t^k, y_i^k, y^k) = y_i^k + \frac{\phi_i\, F_i(t^k, y^k) + \phi_i\, \varphi_i\, \big(A_i(t^k, y^k) - B_i(t^k, y^k)\big)}{1 + \phi_i\, g_i(t^k, y^k) + \phi_i\, \varphi_i\, B_i(t^k, y^k)/y_i^k}.$$

By some simple manipulations, we obtain

$$\begin{aligned}
&V_i(0, t^k, y_i^k, y^k) = y_i^k,\\
&\frac{\partial V_i}{\partial \Delta t}(0, t^k, y_i^k, y^k) = F_i(t^k, y^k),\\
&\frac{\partial^2 V_i}{\partial \Delta t^2}(0, t^k, y_i^k, y^k) = F_i(t^k, y^k)\left[\frac{\partial^2 \phi_i}{\partial \Delta t^2}(0, t^k, y^k) - 2g_i(t^k, y^k)\right] + 2\kappa_i\, \big(A_i(t^k, y^k) - B_i(t^k, y^k)\big).
\end{aligned} \tag{3.6}$$

On the other hand, applying Taylor's expansion for $y_i(t)$ yields

$$\begin{aligned}
y_i(t^k + \Delta t) &= y_i(t^k) + y_i'(t^k)\Delta t + \frac{1}{2} y_i''(t^k)\Delta t^2\\
&= y_i(t^k) + F_i\big(t^k, y(t^k)\big)\Delta t + \frac{1}{2} v_i\big(t^k, y_i(t^k)\big)\Delta t^2 + \mathcal{O}(\Delta t^3),
\end{aligned} \tag{3.7}$$

where v_i is defined in (3.4). It follows from (3.5) and (3.6) that

$$\begin{aligned}
y_i^{k+1} &= V_i(\Delta t, t^k, y_i^k, y^k)\\
&= V_i(0, t^k, y_i^k, y^k) + \frac{\partial V_i}{\partial \Delta t}(0, t^k, y_i^k, y^k)\Delta t + \frac{1}{2}\frac{\partial^2 V_i}{\partial \Delta t^2}(0, t^k, y_i^k, y^k)\Delta t^2 + \mathcal{O}(\Delta t^3)\\
&= y_i^k + F_i(t^k, y^k)\Delta t + 2\kappa_i\, \big(A_i(t^k, y^k) - B_i(t^k, y^k)\big)\Delta t^2 + \mathcal{O}(\Delta t^3).
\end{aligned} \tag{3.8}$$

From (3.7), (3.8) and $(A_i, B_i) \in \mathcal{D}(v_i/(2\kappa_i))$, we obtain

$$y_i^{k+1} - y_i(t^{k+1}) = \mathcal{O}(\Delta t^3).$$

This is the desired conclusion. The proof is complete. □

Remark 3.3. Theorem 3.2 provides a second-order and positivity-preserving NSFD method for (1.1) but it does not require the condition (2.10). A suitable denominator function that satisfies the condition of Theorem 3.2 is

$$\phi_i(\Delta t, t, y) = \begin{cases} \dfrac{e^{2g_i(t,y)\Delta t} - 1}{2g_i(t,y)} & \text{if} \quad g_i(t,y) > 0, \\ \Delta t \quad \text{if} \quad g_i(t,y) = 0. \end{cases} \tag{3.9}$$

Since $g_i(t, y) \geq 0$, another denominator function can be

$$\phi_i(\Delta t, t, y) = g_i(t, y)\Delta t^2 + \Delta t, \tag{3.10}$$

which is simpler that (3.9). The functions defined in (3.9) and (3.10) are not bounded as $\Delta t \to \infty$. A denominator function that is bounded as $t \to \infty$ is given by

$$\begin{aligned} &\phi(\Delta t, t, y) = \frac{\gamma_1(t,y)\Delta t + \gamma_2(t,y)\Delta t^2}{\gamma_3(t,y) + \gamma_4(t,y)\Delta t^3}, \quad \gamma_i(t,y) > 0, \\ &\gamma_1(t,y) = \gamma_3(t,y), \quad \frac{\gamma_2(t,y)}{\gamma_3(t,y)} = g(t,y), \quad m > 2, \end{aligned} \tag{3.11}$$

which is suitable when large step sizes are used to observe the behaviour of the dynamical system over long time periods.

In general, the values of the denominator functions ϕ_i are updated at each iteration step. However, if the functions g_i are identical constants, that is $g_i(t, y) = g_i$, then the denominator functions do not require an update at each iteration step. Assume that the functions F_i $(i = 1, 2, \ldots, n)$ have the property that there exists $\alpha_i > 0$ such that

$$F_i(t, y) + \alpha_i y_i \geq 0 \quad \text{for all} \quad t \geq 0, y \in \text{int}(\mathbb{R}^n_+). \tag{3.12}$$

Many differential equation models have this property (see [4, 22, 23, 40]). Hoang [21] constructed a generalized NSFD method preserving the positivity of the solutions and the local dynamics of autonomous dynamical systems with the property (3.12).

Systems that satisfy (3.12) can written in the form

$$y_i' = f_i(t, y) - y_i g_i(t, y), \quad f_i(t, y) = \big(F_i(t, y) + \alpha_i y_i\big), \quad g_i(t, y) = \alpha_i. \tag{3.13}$$

Therefore, (3.1) provides a second-order positivity-preserving NSFD method for which the denominator functions in the form (3.9)-(3.11) do not require updating values at each iteration step.

4. Numerical Simulation of an SIR Epidemic Model

In this section, we perform numerical experiments to support and illustrate the theoretical results. These experiments consider a mathematical epidemiological model.

We consider a modified Susceptible-Infected-Removed (SIR) model [6] as a test problem, which reads

$$\begin{aligned} &y_1'(t) = -\frac{by_1(t)y_2(t)}{y_1(t) + y_2(t)}, \quad y_1(0) > 0, \\ &y_2'(t) = \frac{by_1(t)y_2(t)}{y_1(t) + y_2(t)} - cy_2(t), \quad y_2(0) > 0, \\ &y_3'(t) = cy_2(t), \quad y_3(0) \geq 0, \end{aligned} \tag{4.1}$$

where b and c are positive real numbers; $y_1(t)$, $y_2(t)$ and $y_3(t)$ represent the number of susceptible individuals infected individuals and removed individuals at the time t, respectively. We refer the readers to [6] for more details of (4.1).

In a recent work [27], Lemos-Silva et al. applied the Mickens' methodology [30, 31, 32, 33, 34] to obtain an NSFD model of the following form:

$$\begin{aligned}\frac{y_1^{k+1}-y_1^k}{\Delta t} &= -\frac{by_1^{k+1}y_2^k}{y_1^k+y_2^k},\\ \frac{y_2^{k+1}-y_2^k}{\Delta t} &= \frac{by_1^{k+1}y_2^k}{y_1^k+y_2^k}-cy_2^{k+1},\\ \frac{y_3^{k+1}-y_3^k}{\Delta t} &= cy_2^{k+1}.\end{aligned} \tag{4.2}$$

Notably, the exact solution of (4.2) has been explicitly determined in [27, Theorem 1]. Previously, Bohner et al. [7] had proposed a new method for finding the exact solution of (4.1), considering not only constant b, c but also variable coefficients $b, c\colon \mathbb{R}_+ \to \mathbb{R}_+$.

In this example, we will consider (4.1) with variable coefficients. Since the total population $N(t) = y_1(t)+y_2(t)+y_3(t)$ is constant for $t \geq t_0$, it is sufficient to consider the first two equations of (4.1):

$$\begin{aligned}y_1'(t) &= -\frac{b(t)y_1(t)y_2(t)}{y_1(t)+y_2(t)}, \quad y_1(0)>0,\\ y_2'(t) &= \frac{b(t)y_1(t)y_2(t)}{y_1(t)+y_2(t)} - c(t)y_2(t), \quad y_2(0)>0.\end{aligned} \tag{4.3}$$

We now apply the NSFD method (3.1) to (4.3). First, we decompose the right-hand side function of (4.3) as follows:

$$\begin{aligned}F_1(t,y) &= -\frac{b(t)y_1y_2}{y_1+y_2}, \quad f_1(t,y)=0, \quad g_1(t,y) = -\frac{b(t)y_2}{y_1+y_2},\\ F_2(t,y) &= \frac{b(t)y_1y_2}{y_1+y_2} - c(t)y_2, \quad f_2(t,y) = \frac{b(t)y_1y_2}{y_1+y_2}, \quad g_2(y) = -c(t)\end{aligned} \tag{4.4}$$

By simple calculations, we obtain

$$\begin{aligned}v_1(t,y) &= -\frac{b'y_1y_2}{y_1+y_2} + \frac{b^2y_1y_2^3}{(y_1+y_2)^3} - \frac{b^2y_1^3y_2}{(y_1+y_2)^3} + \frac{bcy_1^2y_2}{(y_1+y_2)^2},\\ 2\kappa_1A_1(t,y) &= -\frac{(b')_-y_1y_2}{y_1+y_2} + \frac{b^2y_1y_2^3}{(y_1+y_2)^3} + \frac{bcy_1^2y_2}{(y_1+y_2)^2},\\ 2\kappa_1B_1(t,y) &= \frac{(b')_+y_1y_2}{y_1+y_2} + \frac{b^2y_1^3y_2}{(y_1+y_2)^3}, \quad \big((b')_+,(b')_-\big)\in\mathcal{D}(b'),\\ v_2(t,y) &= \frac{b'y_1y_2}{y_1+y_2} - c'y_2 - \frac{b^2y_1y_2^3}{(y_1+y_2)^3} + \frac{b^2y_1^3y_2}{(y_1+y_2)^3} - \frac{bcy_1^2y_2}{(y_1+y_2)^2} - \frac{bcy_1y_2}{y_1+y_2} + c^2y_2,\\ 2\kappa_2A_2(t,y) &= \frac{(b')_+y_1y_2}{y_1+y_2} - (c')_-y_2 + \frac{b^2y_1^3y_2}{(y_1+y_2)^3} + c^2y_2, \quad \big((c')_+,(c)'_-\big)\in\mathcal{D}(c'),\\ 2\kappa_2B_2 &= \frac{(b')_-y_1y_2}{y_1+y_2} - (c')_+y_2 - \frac{b^2y_1y_2^3}{(y_1+y_2)^3} - \frac{bcy_1^2y_2}{(y_1+y_2)^2} - \frac{bcy_1y_2}{y_1+y_2}.\end{aligned} \tag{4.5}$$

Once the 4-tuple $(\phi_1, \phi_2, \varphi_1, \varphi_2)$ is chosen, (4.4) and (4.5) define a second-order positivity-preserving NSFD scheme for (4.3). In the numerical examples reported below, we will use some NSFD schemes derived from (4.4) and (4.5), that utilize the functions ϕ_i and φ_i given in Table 1.

Table 1: NSFD schemes derived from (4.4) and (4.5) ($\tau > 0$)

NSFD scheme	ϕ_1	ϕ_2	φ_1	φ_2
2dPNSFD1	$g_1(t,y)\Delta t^2 + \Delta t$	$g_2(t,y)\Delta t^2 + \Delta t$	Δt	Δt
2dPNSFD2	$\dfrac{e^{2g_1(t,y)\Delta t} - 1}{2g_1(t,y)}$	$\dfrac{e^{2g_2(t,y)\Delta t} - 1}{2g_2(t,y)}$	Δt	Δt
2dPNSFD3	$\dfrac{\Delta t + g_1(t,y)\Delta t^2}{1 + \Delta t^3}$	$\dfrac{\Delta t + g_2(t,y)\Delta t^2}{1 + \Delta t^3}$	$1 - e^{-\tau\Delta t}$	$1 - e^{-\tau\Delta t}$

Assume that $b(t)$ and $c(t)$ are bounded for $t \geq 0$, that is, there exist c^* and b^* such that

$$\max_{t\geq 0} b(t) = b^* > 0, \quad \max_{t\geq 0} b(t) = c^* > 0. \tag{4.6}$$

Then, (4.3) can be rewritten as

$$\begin{aligned} y_1' &= \left(b^* y_1 - \frac{b(t)y_1y_2}{y_1 + y_2}\right) - b^* y_1, \\ y_2' &= \left(\frac{b(t)y_1y_2}{y_1 + y_2} - c(t)y_2 + c^* y_2\right) - c^* y_2. \end{aligned} \tag{4.7}$$

Then, the right-hand side function of (4.7) can be decomposed in the form

$$\begin{aligned} f_1(t,y) &= b^* y_1 - \frac{b(t)y_1y_2}{y_1 + y_2}, \quad g_1(t,y) = b^*, \\ f_2(t,y) &= \left(\frac{b(t)y_1y_2}{y_1 + y_2} - c(t)y_2 + c^* y_2\right), \quad g_2(t,y) = c^*. \end{aligned} \tag{4.8}$$

Therefore, once the 4-tuple $(\phi_1, \phi_2, \varphi_1, \varphi_2)$ is determined, (4.5) and (4.8) define a second-order positivity-preserving NSFD scheme for (4.3). We consider the following NSFD schemes derived from (4.5) and (4.8) with the functions ϕ_i and φ_i in Table 2

Table 2: NSFD schemes derived from (4.5) and (4.8) ($\tau > 0$)

NSFD scheme	ϕ_1	ϕ_2	φ_1	φ_2
2dPNSFD4	$b^*\Delta t^2 + \Delta t$	$c^*\Delta t^2 + \Delta t$	Δt	Δt
2dPNSFD5	$\dfrac{e^{2b^*\Delta t} - 1}{2b^*}$	$\dfrac{e^{2c^*\Delta t} - 1}{2c^*}$	Δt	Δt
2dPNSFD6	$\dfrac{e^{2b^*\Delta t} - 1}{2b^*}$	$\dfrac{e^{2c^*\Delta t} - 1}{2c^*}$	$1 - e^{-\tau\Delta t}$	$1 - e^{-\tau\Delta t}$

Next, we consider (4.3) with (see [7])

$$b(t) = 1/(1+t), \quad c(t) = 2/(2+t), \quad y_1(0) = 0.8, \quad y_2(0) = 0.2.$$

The exact solution is given by [7]:

$$\begin{aligned} y_1(t) &= y_1(0)\frac{(y_2(0)/y_1(0)) + 1 + t}{\big[(y_2(0)/y_1(0) + 1\big](t+1)}, \\ y_2(t) &= y_2(0)\frac{(y_2(0)/y_1(0)) + 1 + t}{\big[(y_2(0)/y_1(0) + 1\big](t+1)^2}. \end{aligned}$$

Note that $b'(t), c'(t) < 0$ for $t \geq 0$. Hence, we choose $(b')_+ = 0$ and $(c')_+ = 0$ in (4.5). On the other hand, $b(t)$ and $c(t)$ satisfy (4.6) with $b^* = 1$ and $c^* = 2$.

We now compare global errors (err) at $T = 1$ and rates of convergence (ROC) estimated from the NSFD schemes: 2ndNSFD1, 2ndNSFD2, 2ndNSFD3, 2ndNSFD4, 2ndNSFD5 and 2ndNSFD6 and (4.2). The results are reported in Tables 3–6. In these tables, the quantities err and ROC are computed similarly to [5, Example 4.1].

$$\begin{aligned} err(\Delta t) &= |y_1^N - y_1(t_N)| + |y_2^N - y_2(t_N)|, \quad t_N = 1, \quad \Delta t = \frac{1}{N}, \\ ROC &= \log_{\left(\frac{\Delta t_1}{\Delta t_2}\right)} \left(\frac{err(\Delta t_1)}{err(\Delta t_2)}\right). \end{aligned}$$

Additionally, the graphs of the errors obtained from the second-order NSFD scheme 2ndNSFD2 and the first-order NSFD scheme (4.2) with $\Delta t = 0.01$ over $[0, 1]$ are depicted in Figure 1.

The results in Tables 2–5 show that all second-order NSFD schemes 2ndNSFD1, 2ndNSFD2, 2ndNSFD3, 2ndNSFD4, 2ndNSFD5 and 2ndNSFD6 are convergent of order 2, whereas (4.2) is convergent only order 1. Furthermore, the errors of the second-order NSFD schemes depend on the decomposition of the right-hand side function and the chosen 4-tuple $(\phi_1, \phi_2, \varphi_1, \varphi_2)$. This leads to the problem of optimizing the errors of the second-order NSFD schemes.

Table 3: Computed errors and ROC of the 2ndNSFD1 and 2ndNSFD2 schemes

Δt	2ndPNSFD1 err	2ndPNSFD1 rate	2ndPNSFD2 err	2ndPNSFD2 rate
0.5	6.559410475124927e-002		6.094269133987174e-002	
0.25	1.781929796473945e-002	1.8801	1.337060657340174e-002	2.1884
10^{-1}	3.275021538910197e-003	1.8487	2.110852617736816e-003	2.0146
10^{-2}	3.365172105951331e-005	1.9882	1.971819766188876e-005	2.0296
10^{-3}	3.366450123387654e-007	1.9998	1.954409423743364e-007	2.0039
10^{-4}	3.366496442724909e-009	2.0000	1.952614056555113e-009	2.0004
10^{-5}	3.368197387665362e-011	1.9998	1.954746087218240e-011	1.9995
10^{-6}	5.451750162421831e-013	1.7909	3.052558206206868e-013	1.8064

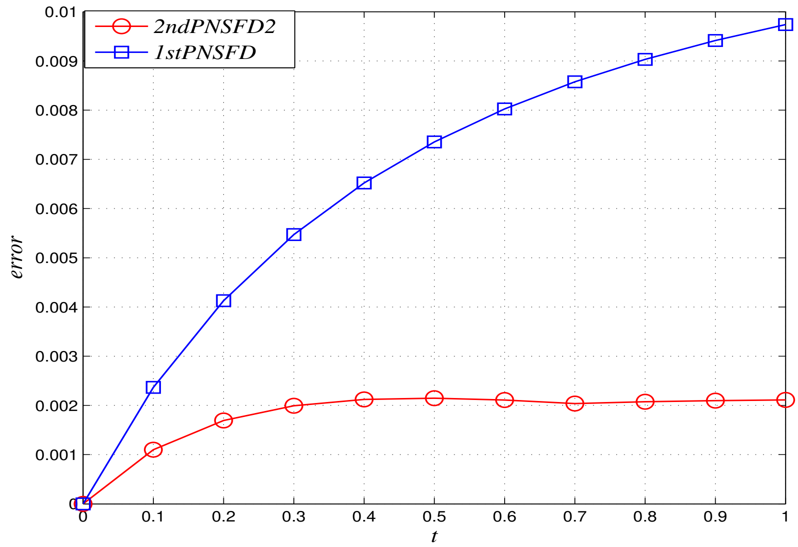

Figure 1: Errors obtained from the second-order and first-order NSFD schemes with $\Delta t = 0.01$.

Table 4: Computed errors and ROC of 2ndNSFD3 ($\tau = 5$) and 2ndNSFD4 schemes

Δt	2ndPNSFD3 err	2ndPNSFD3 rate	2ndPNSFD4 err	2ndPNSFD4 rate
0.5	6.944878986451183e-002		7.902791685990487e-002	
0.25	1.644040274307838e-002	2.0787	2.262044634310900e-002	1.8047
10^{-1}	2.314507864212931e-003	2.1397	3.725237331228468e-003	1.9685
10^{-2}	2.233206780007102e-005	2.0155	4.118012549277073e-005	1.9565
10^{-3}	2.220343807701752e-007	2.0025	4.161038818784046e-007	1.9955
10^{-4}	2.219014763604754e-009	2.0003	4.164809150331017e-009	1.9996
10^{-5}	2.825792377869618e-011	1.8950	4.781298967859726e-011	1.9400
10^{-6}	2.506370111454714e-012	1.0521	8.942110940601822e-012	0.7281

Table 5: Computed errors and ROC of the 2ndNSFD5 and 2ndNSFD6 schemes ($\tau = 5$)

Δt	2ndPNSFD5 err	2ndPNSFD5 rate	2ndPNSFD6 err	2ndPNSFD6 rate
0.5	3.095702263303372e-002		2.508826597831147e-002	
0.25	1.271590524117193e-002	1.2836	8.484925721237491e-003	1.5640
10^{-1}	2.564051674735432e-003	1.7476	1.583635745764422e-003	1.8319
10^{-2}	2.849100598348309e-005	1.9542	1.715684442334109e-005	1.9652
10^{-3}	2.874830316440535e-007	1.9961	1.728584778509790e-007	1.9967
10^{-4}	2.877374796761423e-009	1.9996	1.729869816835539e-009	1.9997
10^{-5}	2.876071603097330e-011	2.0002	7.268394219828167e-012	2.3766
10^{-6}	5.016959070403004e-013	1.7584	2.456840286768625e-012	0.4711

Table 6: Computed errors and ROC of the first-order NSFD (4.2)

Δt	1stNSFD err	1stNSFD rate
0.5	4.272727272727273e-002	
0.25	2.312169312169320e-002	0.8859
10^{-1}	9.738562091503381e-003	0.9437
10^{-2}	1.006246214038789e-003	0.9858
10^{-3}	1.009623162852857e-004	0.9985
10^{-4}	1.009962301373735e-005	0.9999
10^{-5}	1.009996232648192e-006	1.0000
10^{-6}	1.010000383189214e-007	1.0000

Before concluding this section, we will examine the dynamic behavior of the numerical solution generated by the second-order NSFD method using large step sizes. To this end, we use the 2ndPNSFD3 scheme to simulate the dynamics of (4.3) over $[0, 100]$ and then, compare the numerical solution obtained with those generated by the explicit Euler (first-order) and trapezoidal (second-order) methods (see [5]). The solutions are depicted in Figures 2 and 3. Clearly, the 2ndPNSFD3 scheme preserves the dynamical behavior of the continuous model. In contrast, the explicit Euler and trapezoidal schemes produce negative approximations that are negative and differ from the exact solution.

Remark 4.1. The NSFD schemes (2.1), (2.5) and (2.9) are only applicable for the SIR model (4.3) when

$$\big(b(t_k) - c(t_k)\big)\, y_1^k \neq c(t_k)\, y_2^k, \quad k \geq 0.$$

5. Second-Order Positivity-Preserving NSFD Method Applied to Nonlinear PDEs

In this section, we present an application of the constructed numerical method (2.1) in solving a class of nonlinear PDEs whose solutions are positive.

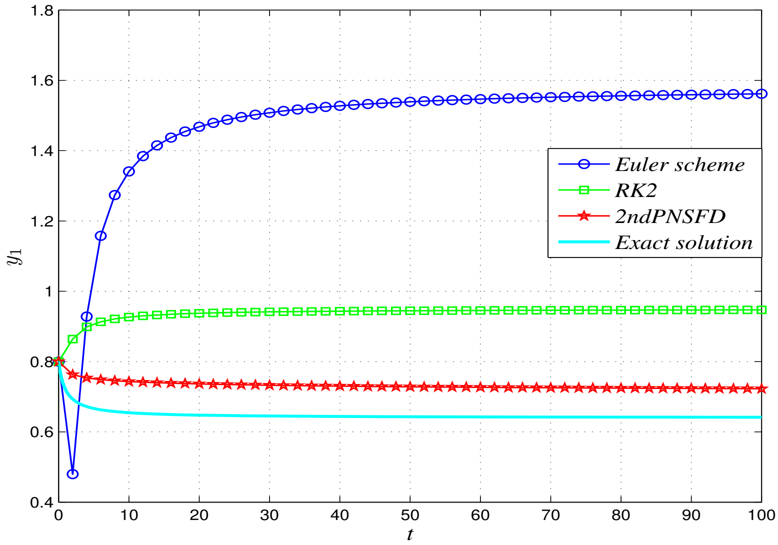

Figure 2: Approximate solutions for the y_1-components generated by the second-order NSFD scheme and two standard numerical schemes.

Many important phenomena and processes arising in mechanics, physics, chemistry, biology, ecology, finance, environment, etc. can be modeled mathematically by nonlinear PDEs (see, e.g., [4, 37]). The solutions of these PDEs often possess essential properties; the most notable of these is the positivity of the solutions. Therefore, constructing numerical methods that preserve the positivity of PDEs is important but not simple in general (see, e.g., [13, 30, 31, 32, 33, 34, 35, 36, 38, 39]).

We now consider a class of nonlinear PDEs of the form

$$\frac{\partial u(x,t)}{\partial t} + C(u)\frac{\partial u(x,t)}{\partial x} = D(u)\frac{\partial^2 u(x,t)}{\partial x^2} + f(u), \quad a \le x \le b, \quad 0 \le t \le T, \tag{5.1}$$

associated with the boundary conditions

$$u(a,t) = a(t), \quad u(b,t) = b(t), \quad 0 \le t \le T \tag{5.2}$$

and the initial condition

$$u(x,0) = u_0(x), \quad a \le x \le b. \tag{5.3}$$

In (5.1)–(5.3), $C(u)$, $D(u)$, $f(u)$, $a(t)$, $b(t)$ and $u_0(x)$ are functions that satisfy conditions necessary to guarantee unique, positive solutions to the problem (5.1)-(5.3) on $[a,b] \times [0,T]$. The following theorem provides a condition for the solutions of (5.1)–(5.3) to be positive.

Theorem 5.1. *Assume that* $C(u)$, $D(u)$, $f(t,u)$, $a(t)$, $b(t)$ *and* $u_0(x)$ *satisfy conditions that guarantee that the solutions to the PDE model* (5.1)-(5.3) *exist and are unique. Then,* $u(t,x) \ge 0$ *for* $(x,t) \in [a,b] \times [0,T]$ *if*

$$\begin{aligned} &C(0) \ge 0, \quad D(0) \ge 0, \quad f(0) \ge 0,\\ &a(t) \ge 0, \quad b(t) \ge 0, \quad t \in [0,T],\\ &u_0(x) \ge 0, \quad x \in [a,b]. \end{aligned}$$

Proof. To prove the theorem, we first use the *method of lines* (MOL) [5, 42] to discretize (5.1)-(5.3) with respect to the space variable. To do so, we fix a regular partition $a = x_0 < x_1 < \ldots < x_M = b$ of

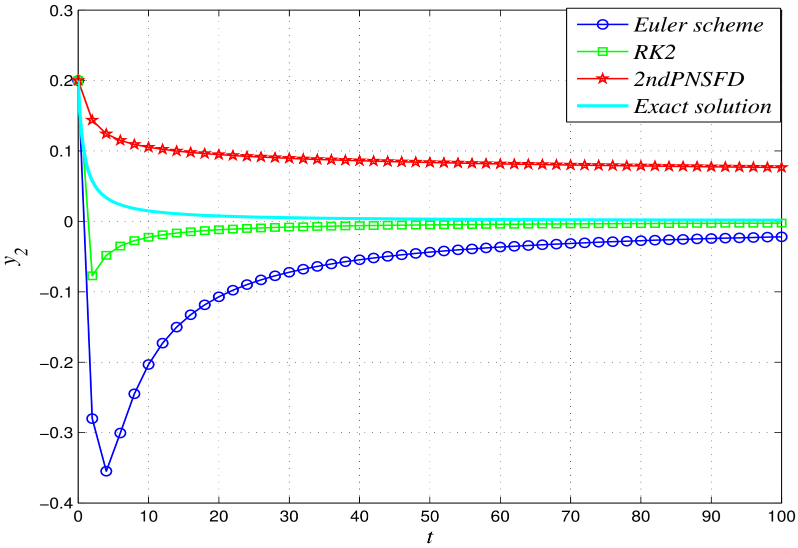

Figure 3: Approximate solutions for the y_2-components generated by the second-order NSFD scheme and two standard numerical schemes.

$[a, b]$ with a step size $\Delta x = (b-a)/M$ and denote by $u_i(t)$ the approximate the value of $u(x,t)$ at (x_i, t) for $i = 0, 1, \ldots, M$. In these terms, the partial derivatives with respect to x are approximated by finite difference quotients as follows:

$$\begin{aligned}\frac{\partial u(x,t)}{\partial x} &\approx \frac{u_i(t) - u_{i-1}(t)}{\Delta x}\\ \frac{\partial^2 u(x,t)}{\partial x^2} &\approx \frac{u_{i+1}(t) - 2u_i(t) + u_{i-1}(t)}{(\Delta x)^2}, \quad i = 1, 2, \ldots M-1.\end{aligned} \tag{5.4}$$

Consequently, we obtain a system of ODEs for $u_i(t)$ $(i = 1, 2, \ldots, M-1)$:

$$\begin{aligned}&u_i'(t) = -C\big(u_i(t)\big)\frac{u_i(t) - u_{i-1}(t)}{\Delta x} + D\big(u_i(t)\big)\frac{u_{i+1}(t) - 2u_i(t) + u_{i-1}(t)}{(\Delta x)^2} + f\big(u_i(t)\big),\\ &u_i(0) = u_0(x_i).\end{aligned} \tag{5.5}$$

Note that $u_0(t) = a(t) \geq 0$ and $u_N(t) = b(t) \geq 0$. It follows from (5.5) that

$$u_i'|_{u_i=0} = C(0)u_{i-1} + D(0)\frac{u_{i+1} + u_{i-1}}{(\Delta x)^2} + f(0).$$

Therefore, if $C(0), D(0), f(0) \geq 0$ then $u_i'\big|_{u_i=0} \geq 0$ for $u_{i+1}, u_{i-1} \geq 0$. By using [23, Lemma 2] and [40, Proposition B.7], we conclude that the set $\mathbb{R}_+^{M-1}$ is a positively invariant set of the system (5.5).

Conversely, the space discretization (5.5) is convergent (see [42]), that is, $u_i(t) \to u\,(t, x_i)$ as $\Delta x \to 0$. Therefore, we conclude that $u(t, x) \geq 0$ for $t \in [0, T]$ and $x \in [a, b]$. The proof is complete. □

By using suitable forms of the 3-tuple $C(u), D(u)$ and $f(u)$, we can obtain a huge variety of highly important PDEs models. Below, we mention some mathematical models represented by (5.1).

- If we take $C = 0, D > 0$ and define $f(u) = u(1-u)(\alpha - u)$ with $0 \leq \alpha \leq 1$, we obtain the Fitzhugh-Nagumo equation

$$\frac{\partial u(x,t)}{\partial t} = D(u)\frac{\partial^2 u(x,t)}{\partial x^2} + u(1-u)(\alpha - u), \tag{5.6}$$

which arises in population genetics. More details of this model are provided in [14].

- In the case $C = 0, D > 0$, and the function f is given by $f(u) = \alpha u + \beta u^m$ with $\alpha, \beta, m \neq 1$, we obtain the Kolmogorov-Petrovskii-Piskunov (KPP) equation:

$$\frac{\partial u(x,t)}{\partial t} + C(u)\frac{\partial u(x,t)}{\partial x} = D(u)\frac{\partial^2 u(x,t)}{\partial x^2} + \alpha u + \beta u^m, \tag{5.7}$$

  which arises in heat and mass transfer, combustion theory, biology, and ecology. More details about the equation can be found in [29]. An explicit positivity-preserving finite-difference scheme for (5.7) was constructed in [13].

- If $C = 0, D > 0$ and $f(u) = u(1 - u^\tau)$ with $\tau > 1$, then (5.1) generates the Fisher-Kolmogorov equation with applications in biology, see [37]

$$\frac{\partial u(x,t)}{\partial t} = D(u)\frac{\partial^2 u(x,t)}{\partial x^2} + u\left(1 - u^\tau\right). \tag{5.8}$$

  In the case $C, D > 0$ and $f(u) = \lambda_1 u - \lambda_2 u^2$, where λ_1 and λ_2 are both positive, (5.1) becomes the Fisher PDE

$$\frac{\partial u(x,t)}{\partial t} = D(u)\frac{\partial^2 u(x,t)}{\partial x^2} + \lambda_1 u - \lambda_2 u^2. \tag{5.9}$$

  This equation was considered in [35], in which a positivity-preserving NSFD scheme was constructed.

- Especially, if $D > 0$, $C(u) = u$ and $f(u) = u(1 - u)$, we obtain from (5.1) the Fisher PDE having nonlinear diffusion:

$$\frac{\partial u(x,t)}{\partial t} + u\frac{\partial u(x,t)}{\partial x} = D\frac{\partial^2 u(x,t)}{\partial x^2} + u(1 - u). \tag{5.10}$$

  This equation was considered in [36], in which a positivity-preserving NSFD scheme was formulated.

In this section, we consider (5.1)–(5.3) with strictly positive solutions:

$$u(x,t) > 0 \quad \text{for all} \quad (x,t) \in [a,b] \times [0,T].$$

In order to obtain a positivity-preserving numerical scheme, we apply the second-order NSFD method (3.1) for (5.5). For this purpose, we rewrite the system (5.5) in the form

$$\begin{aligned}
u_i'(t) &= -\big[C_+(u_i) - C_-(u_i)\big]\frac{u_i(t) - u_{i-1}(t)}{\Delta x} \\
&\quad + \big[D_+(u_i) - D_-(u_i)\big]\frac{u_{i+1}(t) - 2u_i(t) + u_{i-1}(t)}{(\Delta x)^2} + f_i(u_i) - u_i g_i(u_i), \\
&\quad (C_+, C_-) \in \mathcal{D}(C), \quad (D_+, D_-) \in \mathcal{D}(D), \quad (f_i, u_i g_i) \in \mathcal{D}(f(u_i)), \\
u_i(0) &= u_0\left(x_i\right),
\end{aligned} \tag{5.11}$$

or equivalently,

$$u_i' := \mathcal{F}_i(u) = F_i(u) - u_i G_i(u), \tag{5.12}$$

where $u = [u_1 \;\; u_2 \;\; \dots \;\; u_{M-1}]^\top$ and

$$\begin{aligned}
F_i(u) &= C_-(u_i)\frac{u_i}{\Delta x} + C_+(u_i)\frac{u_{i-1}}{\Delta x} + D_+(u_i)\frac{u_{i+1} + u_{i-1}}{(\Delta x)^2} + D_-(u_i)\frac{2u_i}{\Delta x^2} + f_i(u_i), \\
G_i(u) &= \frac{C_+(u_i)}{\Delta x} + \frac{C_-(u_i)}{u_i}\frac{u_{i-1}}{\Delta x} + D_-(u_i)\frac{u_{i+1} + u_{i-1}}{u_i \Delta x^2} + g_i(u_i).
\end{aligned}$$

We then obtain a second-order, positivity-preserving numerical scheme for the original PDE model (5.1)–(5.3)by applying the NSFD method (3.1) to (5.12).

Remark 5.2. The NSFD schemes constructed in [35] for the Fisher PDE (5.9) and in [13] for the KPP model (5.7) are essentially applications of the NSFD methodology to the resulting ODE systems obtained by applying the MOL to the PDE models. Therefore, they only achieve first-order convergence with respect to Δt. The second-order positivity-preserving NSFD method (3.1) is generally applicable not only for (5.12) but also to ODE systems obtained by applying the MOL to PDEs. Thus, it is useful for solving several PDE models with positive solutions.

6. Second-Order Positivity-Preserving NSFD Method Applied to BVPs

This section introduces the application of the constructed NSFD method to solving nonlinear BVPs whose solutions are positive.

It is well-known that both linear and nonlinear shooting methods for BVPs lead to solving systems of ODEs [5, 9]. Therefore, the NSFD method (3.1) can be used to solve the resulting ODE systems. To illustrate this observation, we consider a class of nonlinear BVPs of the form:

$$u''(t) + \lambda f(u(t)) = 0, \quad 0 \leq t \leq L, \quad u(0) = u(L) = 0, \tag{6.1}$$

which models certain physical problems [26], where

- $f(w) > 0$ for $w > 0$;
- $\lambda > 0$ is a physical parameter

Laetsch [26] investigated the values of λ for which the BVP (6.1) admits positive solutions, as well as how the behavior of these solutions changes with respect to λ. One of the main results addresses the case in which f is a convex function of w satisfying $f(w) > 0$ for $w > 0$. We refer the reader to [26] for a more detailed discussion of these findings.

A particularly important special case of the BVP (6.1) is the Bratu equation [8]:

$$u''(t) = -\lambda e^{u(t)}, \quad 0 \leq t \leq 1,$$

subject to the boundary condition

$$u(0) = u(1) = 0.$$

This equation has many important theoretical and practical applications, and it is widely used as a benchmark to verify the reliability and efficiency of various approximation methods (see, e.g., [24, 41] and references therein).

We now assume that the solutions to (6.1) exist. To apply the constructed second-order NSFD method (3.1), we first use the solutions' symmetry to transform the problem of solving (6.1) into the problem of solving a sequence of ODEs with positive solutions. Any solution of (6.1) is symmetric about the point $t = L/2$, that is $u(t) = u(L/2 - t)$ for $0 \leq t \leq L$ [26]; hence, we only need to consider (6.1) on the interval $[0, L/2]$. On this interval, it is easy to verify that

- $u(t) > 0$ for $0 < t \leq L/2$;
- $u'(t) > 0$ for $0 < t < L/2$;
- $u'(L/2) = 0$ and therefore, $\max_{0 \leq t \leq L} u(t) = u(L/2)$.

As a result, we transform (6.1) to the following system of ODEs:

$$\begin{aligned} u' &= v, \quad u(0) = 0, \\ v' &= -\lambda f(u), \quad v(0) = s > 0, \end{aligned} \tag{6.2}$$

where the first slope s is determined such that $v'(L/2) = 0$. (6.2) can be rewritten in the form (1.5) as follows:

$$\begin{aligned} y_1' &= f_1(y_1, y_2) - y_1 g_1(y_1, y_2), \\ y_2' &= f_2(y_1, y_2) - y_2 g_2(y_1, y_2), \end{aligned} \tag{6.3}$$

where

$$\begin{aligned} &y_1 = u, \quad y_2 = v, \\ &f_1(y_1, y_2) = y_2, \quad g_1(y_1, y_2) = 0, \\ &f_2(y_1, y_2) = 0, \quad g_2(y_1, y_2) = -\lambda \frac{f(y_1)}{y_2}. \end{aligned}$$

We obtain positive approximate solutions with second-order accuracy by applying the NSFD method (3.1) to (6.3). The solution of the BVP is obtained by solving a sequence of initial value problems, for which the initial slope is determined via the equation $y_2(s, L/2) = 0$.

7. Concluding Remarks and Discussions

In this work, we we have proposed a simple and efficient approach for constructing a generalized, second-order, positivity-preserving numerical method for non-autonomous dynamical systems. This method is based on a new non-local approximation of the right-hand side function combined with the normalization of denominator functions. Notably, the constructed method does not require the strict and indispensable conditions imposed by some well-known second-order positivity-preserving NSFD methods. Therefore, a computational implementation is straightforward.

Important applications of the constructed NSFD method are also provided, and numerical experiments are carried out to support and illustrate the theoretical results. As a result, the NSFD scheme for the SIR epidemic model constructed in [27] has been improved. Additionally, applications of the constructed second-order positivity-preserving NSFD method to solving classes of PDEs and BVPs that arise in real-world situations have been introduced and analyzed.

In the near future, we will expand upon the present approach and the results obtained in this work to study the construction of higher-order, dynamically consistent numerical methods for differential equation models with complex dynamics. Additionally, the practical applications of the proposed methods will be of particular interest.

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CRediT authorship contribution statement

Manh Tuan Hoang: Writing – review & editing, Writing – original draft, Visualization, Validation, Supervision, Software, Resources, Project administration, Methodology, Investigation, Formal analysis, Data curation, Conceptualization, Funding acquisition.

Mathias Ehrhardt: Writing – review & editing, Writing – original draft, Visualization, Validation, Supervision, Software, Resources, Project administration, Methodology, Investigation, Formal analysis, Data curation, Conceptualization, Funding acquisition.

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