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Nonstandard explicit third-order Runge-Kutta method with positivity property

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Abstract

When one solves differential equations, modeling physical phenomena, it is of great importance to take physical constraints into account. More precisely, numerical schemes have to be designed such that discrete solutions satisfy the same constraints as exact solutions. Based on general theory for positivity, with an explicit third-order Runge-Kutta method (we will refer to it as RK3 method) positivity is not ensured when applied to the inhomogeneous linear systems and the same result is regained on nonlinear positivity for this method. Here we mean by positivity that the nonnegativity of the components of the initial vector is preserved. Nonstandard finite differences (NSFDs) schemes can improve the accuracy and reduce computational costs of traditional finite difference schemes. In addition to NSFDs produce numerical solutions which also exhibit essential properties of solution. In this paper, we investigate the positivity property for nonstandard RK3 method when applied to the numerical solution of special nonlinear initial value problems (IVPs) for ordinary differential equations (ODEs). We obtain new results for positivity which are important in practical applications. We provide some numerical examples to illustrate our results.

Keywords: Positivity; Initial value problems; Advection equation; Bergers' equation; Runge-Kutta methods.
2010 MSC: Primary 65L05; Secondary 65L06, 65L20, 65M20.

1. Introduction

Systems of partial differential equations (PDEs) and ordinary differential equations (ODEs) are used extensively in the modeling of many physical, biological and economic applications. They constitute

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a central component in applied mathematics and their numerical simulations are fundamental importance in gaining the correct qualitative and quantitative information on the systems. Numerical methods based on finite difference approximations, Taylor series expansion, and interpolation, such as Euler, Runge-Kutta and Adams methods are widely used, e.g, [4, 5]. Traditionally, important requirements in this context are, the investigation of the consistency of the discrete scheme with the original differential equation and linear stability analysis for problems with smooth solutions. These requirements are important, because they guarantee convergence of the discrete solution to the exact one, but the essential qualitative properties of the solution are not transferred to the numerical solution. Thus, the stated disadvantage might be catastrophic. One way of avoiding this disadvantage is to employ finite difference schemes that are nonstandard in the sense of Mickens' [1, 15] definition. Nonstandard finite difference techniques were developed empirically for solving practical problems in applied sciences and in engineering, e.g., [9]. As mentioned above one of the main advantages of the NSFDs that in addition to the usual properties of consistency, stability and hence convergence, they produce numerical solutions which also exhibit essential properties of solution. Special nonlinear stability properties indicated by fixed points and their stability, oscillatory, conservation of energy, positivity, boundedness, and elementary stability, have received extensive attention in the design of qualitatively stable NSFDs[8, 9, 10, 16]. In this paper we deal with the numerical solution (using NSFD schemes) of initial value problems, for positive first-order and systems of ODEs, which can be written in the form

$$\frac{d}{dt}U(t) = F(U(t)), \quad (t \geq 0), \qquad\qquad U(0) = U_0, \tag{1.1}$$

where U may be a single function or a vector of functions of length k mapping $[t_0, T) \to \mathcal{C}^k$ and the corresponding F a single function or a vector of functions of length k mapping $([t_0, T), \mathcal{C}^k) \to \mathcal{C}^k$. Discretization of the continuous differential equation, or beginning instead with a difference equation, we define $t_n = t_0 + n\Delta t$, where Δt is a positive step size, and say that the discretized version of the function U at time t_n is $U_n \approx U(t_n)$. Then the discretized version of Eq.(1.1) becomes

$$\mathcal{D}_{\Delta t}U_n = \mathcal{F}_n(F, U_n), \tag{1.2}$$

where $\mathcal{D}_{\Delta t}U_n$ represents the discretized version of $\frac{d}{dt}U(t)$ and $\mathcal{F}_n(F, U_n)$ approximates $F(U(t_n))$ at time t_n. We define the nonstandard one-step finite-difference method as follows.

Definition 1.1. (Anguelov and Lubuma [1]) Method (1.2) is called a nonstandard finite-difference method if at least one of the following conditions is met:

• In the discrete derivatives $\mathcal{D}_{\Delta t}U_n$ the traditional denominator Δt is replaced by a nonnegative function $\varphi(\Delta t)$ such that

$$\varphi(\Delta t) = \Delta t + O(\Delta t^2) \;\; as \;\; 0 < \Delta t \to 0. \tag{1.3}$$

• Nonlinear terms in $F(U(t))$ are approximated in a nonlocal way, i.e. by a suitable function of several points of the mesh.

There are many problems of practical interest that can be medelled by positive ODEs. For example, in electrical engineering, where the charge transport in semiconductor devices is usually described by a convection-diffusion equation. Here the charge transport is described in terms of charge carrier densities, which should be non-negative. Similar reasoning holds for the modeling of chemical reactions or semi-discrete form of advection-diffusion equations. Also, in financial applications e.g. the computation of the fair price of an option, it is a natural demand that the resulting numerical approximations, should be non-negative. Further more, a negative value may cause under shoots or over shoots near a steep gradient. Therefor, we need to construct positivity preserving schemes that avoid unrealistic negative values for the solution. One possibility are NSFDs. As our numerical method, we consider the nonstandard RK3 method,

$$\begin{aligned}
U_{n_1} &= U_n, \\
U_{n_2} &= U_n + \tfrac{1}{3}\varphi(\Delta t)F(t_n, U_{n_1}), \\
U_{n_3} &= U_n + \tfrac{2}{3}\varphi(\Delta t)F(t_n + \tfrac{1}{3}\varphi(\Delta t), U_{n_2}) \\
U_{n+1} &= U_n + \varphi(\Delta t)(\tfrac{1}{4}F(t_n, U_{n_1}) + \tfrac{3}{4}F(t_n + \tfrac{2}{3}\varphi(\Delta t), U_{n_3})).
\end{aligned} \tag{1.4}$$

In the literature, we can find several papers devoted to discussing positivity property (e.g., [3, 6, 7, 8, 9, 11, 14, 18]). Positivity results have been presented for some Runge-Kutta methods by Hundsdorfer et al[7]. Based on these results, with standard RK3 method positivity is not ensured when applied to the inhomogeneous linear systems and the same result is regained on nonlinear positivity for this method. Usually, *step size coefficients* γ are determined such that monotonicity, in the sense of mentioned in [8, 9, 17, 19], is present for all Δt with $0 < \Delta t \leq \gamma\tau_0$ ($\tau_0 > 0$ is a maximal step size such that $\|v + \Delta t F(t, v)\| \leq \|v\|$ for all t, $0 < \Delta t \leq \tau_0$ and $v \in \mathbb{R}^m$). General monotonicity of Runge-Kutta methods presented in [17] shows that the maximal step size coefficient γ for standard RK3, is equal to 0. Monotonicity-preserving methods, can prevent the occurrence of negative values where even very small negative values are unacceptable, as for example, in the advective transport of chemical species see e.g. [2]. On the other hand, monotonicity with step size coefficient γ implies positivity with the same step size coefficient, see [11].

Applying the nonstandard RK3 method to special nonlinear ODEs (positive semi-discrete systems arising 1D and 2D advection test problems and Bergers' equation with limited third-order upwind-biased spatial discretization), it is observed that the stepsize restriction here, is comparable to the stepsize restriction for the explicit trapezoidal rule and explicit midpoint method with respect to positivity(see e.g. [12]). Such a result will be confirmed in Figures 1-3. From this practical point of view, the question arises whether it is theoretically possible to have positivity preservation for the nonstandard RK3 method. To answer this question, nonstandard RK3 is applied to a special ODEs, and some results are achieved theoretically that coincide with numerical experiments. Here, we focus on positivity and for nonstandard RK3.

In the second section, general positivity results are presented for standard RK3 method. In the third section, the main positivity results are obtained for nonstandard RK3 method. The numerical results obtained are then compared in fourth section with respect to positivity. Both one and two-dimensional linear scalar advection equations and Bergers' equation are used as test cases.

2. General results on positivity for RK3 method

In this section, we study the general positivity for RK3 method. In many papers, one starts from an assumption about F which, $\tau_0 \geq 0$, to be the maximal step size such that positivity holds for the forward Euler method, i.e.,

$$U + \Delta t F(t, U) \geq 0 \ \text{(for all } t \text{ and } U \geq 0),$$

whenever $0 < \Delta t \leq \tau_0$ and $U \in \mathbb{R}^m$. As we can see in [7], diagonally implicit Runge-Kutta methods can be written as follows:

$$\begin{aligned}
v_i &= \textstyle\sum_{j=0}^{i-1} \Big(p_{ij} + q_{ij}\Delta t F(t_n + c_{j+1}\Delta t, v_j)\Big) + s_i \Delta t F(t_n + c_{i+1}\Delta t, v_i), \\
v_0 &= U_n,
\end{aligned} \tag{2.1}$$

for $i = 1, \ldots, s$, and finally set $U_{n+1} = v_s$. Here p_{ij}, q_{ij} and c_i are parameters defining the method. If $\sum_{j=0}^{i-1} p_{ij} = 1$ and $q_s = 0$, this is just another way of writing the s-stage diagonally implicit form of general Runge-Kutta method. If $s_i = 0$ for all indices i, the method is explicit. This form is theoretically convenient because the whole process in Runge-Kutta methods is written in terms of linear combinations of scaled forward and backward Euler steps.

We shall determine the step size coefficients γ, such that the positivity is valid for (2.1) under the step size restriction $\Delta t \leq \gamma\tau_0$. Following an idea of Shu-Osher [18] if all parameters p_{ij}, q_{ij} and s_i with $0 \leq j < i \leq s$ are non-negative, then method (2.1) will be positive under the step size restriction $\Delta t \leq \min_{0 \leq j < i \leq s}(p_{ij}/q_{ij})\tau_0$. Since RK3 rule can not be written as convex combinations of Euler steps, with non-negative coefficients p_{ij}, q_{ij}, therefore, we have an empty positivity interval ($\gamma = 0$) for this method . A proof for the non-existence of coefficients $p_{ij}, q_{ij} \geq 0$ is given in [18].

General monotonicity results have been obtained in [17]. In that paper it has been shown that the obtained step size coefficient ($\gamma = 0$) is necessary for monotonicity in the maximum norm. It follows that the Shu-Osher form (2.1) is optimal.

3. Main results

In this section, we obtain the largest step size for nonstandard RK3 method for which the corresponding numerical approximations are non-negative (component-wise non-negative) with arbitrary non-negative initial vector. The new results are determined, whenever the underlying ODE possesses the related positivity preserving property. Let us consider

$$U_i' = \frac{s_i\big(U(t)\big)}{\Delta x}\big(U_{i-1}(t) - U_i(t)\big)\ ,\ i = 1, 2\ldots, m, \tag{3.1}$$

with the nonlinear function $s_i(U)$ satisfying

$$s_i(U) \geq 0 \quad \text{for any vector } U, \tag{3.2}$$

and $\Delta x = \frac{1}{m},\ U = [U_1, U_2, \ldots, U_m]^T,\ U_0 = U_m$. This special semi-discrete system arises from a linear advection problem after discretization using a flux limiter. Assuming (3.2) and Lipschitz continuity for s_i in (3.1) with respect to U, this nonlinear system is positive (see [11]).

In the following we assume that there is a maximal step size $\tau_0 > 0$ under which positivity holds for the forward Euler method,

$$U + \varphi(\Delta t)\frac{s_i(U)}{\Delta x}\big(U_{i-1} - U_i\big) \geq 0, \qquad \text{for all } 0 < \Delta t \leq \tau_0,\ U \geq 0,$$

and we shall determine γ such that the positivity is valid for (1.4) under the step size restriction $\Delta t \leq \gamma\tau_0$. Applying of (1.4) to (3.1) with $\zeta_i^l = \varphi(\Delta t)\frac{s_i(U_l)}{\Delta x}$, $l = n_1, n_2, n_3$ and $i = 1, 2, \ldots, m$, gives

$$(U_{n_2})_i = U_i^n + \tfrac{1}{3}\varphi(\Delta t)\tfrac{s_i(U_l)}{\Delta x}(U_{i-1}^n - U_i^n) = U_i^n + \tfrac{1}{3}\zeta_i^{n_1}(U_{i-1}^n - U_i^n),$$

$$\begin{aligned}(U_{n_3})_i &= U_i^n + \tfrac{2}{3}\varphi(\Delta t)\tfrac{s_i(U_l)}{\Delta x}((U_{n_2})_{i-1} - (U_{n_2})_i)\\ &= \tfrac{2}{9}\zeta_{i-1}^{n_1}\zeta_i^{n_2}U_{i-2}^n + \big(\tfrac{2}{3}\zeta_i^{n_2} - \tfrac{2}{9}\zeta_i^{n_2}\zeta_{i-1}^{n_1} - \tfrac{2}{9}\zeta_i^{n_2}\zeta_i^{n_1}\big)U_{i-1}^n\\ &\quad + \big(1 - \tfrac{2}{3}\zeta_i^{n_2} + \tfrac{2}{9}\zeta_i^{n_2}\zeta_i^{n_2}\big)U_i^n,\end{aligned}$$

where $U_i^n \approx U(x_i, t_n)$ as mentioned above is the fully discrete approximation. Therefore, we have

$$U_i^{n+1} = U_i^n + \frac{1}{4}\zeta_i^{n_1}(U_{i-1}^n - U_i^n) + \frac{3}{4}\zeta_i^{n_3}\big((U_{n_3})_{i-1} - (U_{n_3})_i\big),$$

after substituting and by rearranging

$$\begin{aligned}
U_i^{n+1} = &\Big(1 - \tfrac{1}{4}\zeta_i^{n_1} - \tfrac{3}{4}\zeta_i^{n_3}\big(1 - \tfrac{2}{3}\zeta_i^{n_2} + \tfrac{2}{9}\zeta_i^{n_2}\zeta_i^{n_1}\big)\Big)U_i^n \\
&+\Big(\tfrac{1}{4}\zeta_i^{n_1} + \tfrac{3}{4}\zeta_i^{n_3}\big(1 - \tfrac{2}{3}\zeta_{i-1}^{n_2} + \tfrac{2}{9}\zeta_{i-1}^{n_2}\zeta_{i-1}^{n_1} - \tfrac{2}{3}\zeta_i^{n_2} + \tfrac{2}{9}\zeta_i^{n_2}\zeta_{i-1}^{n_1} + \tfrac{2}{9}\zeta_i^{n_2}\zeta_i^{n_1}\big)\Big)U_{i-1}^n \\
&+\tfrac{3}{4}\zeta_i^{n_3}\big(\tfrac{2}{3}\zeta_{i-1}^{n_2} - \tfrac{2}{9}\zeta_{i-1}^{n_2}\zeta_{i-2}^{n_1} - \tfrac{2}{9}\zeta_{i-1}^{n_2}\zeta_{i-1}^{n_1} - \tfrac{2}{9}\zeta_i^{n_2}\zeta_{i-1}^{n_1}\big)U_{i-2}^n \\
&+\tfrac{1}{6}\zeta_i^{n_3}\zeta_{i-2}^{n_1}\zeta_{i-1}^{n_2}U_{i-3}^n.
\end{aligned} \tag{3.3}$$

Theorem 3.1. Sufficient for scheme (1.4) applied to (3.1), to be positive is $0 \leq \varphi(\Delta t)\frac{s_i(U)}{\Delta x} \leq \gamma, \gamma = 1$, for all $U \in \mathbb{R}^m$ and $i = 1, 2, \ldots, m$.

Proof . From (3.3) it is enough to show that

$$\begin{aligned}
A &= (1 - \tfrac{2}{3}\zeta_i^{n_2} + \tfrac{2}{9}\zeta_i^{n_2}\zeta_i^{n_1}) \geq 0, \\
B &= (1 - \tfrac{2}{3}\zeta_{i-1}^{n_2} + \tfrac{2}{9}\zeta_{i-1}^{n_2}\zeta_{i-1}^{n_1} - \tfrac{2}{3}\zeta_i^{n_2} + \tfrac{2}{9}\zeta_i^{n_2}\zeta_{i-1}^{n_1} + \tfrac{2}{9}\zeta_i^{n_2}\zeta_i^{n_1}) \geq 0, \\
C &= (\tfrac{2}{3}\zeta_{i-1}^{n_2} - \tfrac{2}{9}\zeta_{i-1}^{n_2}\zeta_{i-2}^{n_1} - \tfrac{2}{9}\zeta_{i-1}^{n_2}\zeta_{i-1}^{n_1} - \tfrac{2}{9}\zeta_i^{n_2}\zeta_{i-1}^{n_1}) \geq 0.
\end{aligned} \tag{3.4}$$

Considering A and B as functions of multi-variables, our goal is to find the global minimum of these three functions. Since the functions A and B are algebraic, to find critical points, we set the partial derivatives equal to 0 and solved for variables. It can be shown that there is no interior critical point and the global minimum occurs only at corner points. After evaluation functions A and B one can easily find that the global minimum is 0 and, therefore this concludes the sufficiency of $\gamma = 1$ for A and B to be non-negative. It is fair to say that for the last inequality in (3.4) we have no formal proof. But, we have conclusive numerical evidence: we computed values U_n with the Math Toolbox software of Matlab and found for random independent uniform $(0, 1)$ variables ζ_i^l, $l = n_1, n_2, n_3$, that U_n rounded to 16 decimal digits equals precisely 1 (for final time $t_f = 5$). Combining this result with $(A, B \geq 0)$ conclude the theorem. □

4. Test cases

In this section we perform numerical experiments to demonstrate the performance of the classical fourth-order method with respect to positivity developed in the previous section. Several test cases were run to assess the performance of this positivity-preserving flux-limited scheme. The cases include one and two dimensional linear advection test problems and Bergers' equation.

Test case1: 1D scalar linear advection equation

First we have considered the scalar linear advection equation in one dimension

$$U_t + U_x = 0, \quad 0 < x < 1, \quad t > 0,$$

with a periodic boundary condition. We have discretized in space on uniformly distributed grid points $x_i = i\Delta x$, and $\Delta x = \frac{1}{500}$ by means of the flux form

$$U_i'(t) = \frac{1}{\Delta x}\Big(F_{i-\frac{1}{2}}\big(t, U(t)\big) - F_{i+\frac{1}{2}}\big(t, U(t)\big)\Big), \quad F_{i\pm\frac{1}{2}}\big(t, U\big) = U_{i\pm\frac{1}{2}} \quad i = 1, 2, \ldots, 500,$$

where the values $U_{i\pm1/2}$ are defined at the cell boundaries $x_{i\pm1/2}$. With the third-order upwind-biased flux we have

$$F_{i+\frac{1}{2}}(t, U) = \frac{1}{6}\big(-U_{i-1} + 5U_i + 2U_{i+1}\big) = \big(U_i + (\frac{1}{3} + \frac{1}{6}\theta_i)(U_{i+1} - U_i)\big), \tag{4.1}$$

where θ_i is the ratio

$$\theta_i = \frac{U_i - U_{i-1}}{U_{i+1} - U_i} \qquad i = 1, 2, \ldots, 500.$$

The general discretization (4.1) written out in full gives

$$U_i' == \frac{1}{\Delta x}\Big(1 - \psi(\theta_{i-1}) + \frac{1}{\theta_i}\psi(\theta_i)\Big)\big(U_{i-1} - U_i\big) \qquad i = 1, 2, \ldots, 200,$$

with the *limiter function* ψ, here

$$\psi(\theta) = \max\Big(0, \min\big(1, \frac{1}{3} + \frac{1}{6}\theta, \theta\big)\Big). \tag{4.2}$$

This limiter function was introduced by Koren [10]. The numerical solution for method (1.4) is shown in Figure 1, with $\varphi(\Delta t) = 1 - e^{-\Delta t}$ and block initial profile: $U_0(x, t) = 1$ for $0.3 \leq x \leq 0.7$ and 0 otherwise. Our final time is $t_f = 1$. It has used the number steps $N = 400, 450, 500, 550, 600$ and this leads to values of $\Delta t \simeq 0.0025, 0.0022, 0.002, 0.0018, 0.0018$ and the Courant (CFL) numbers $\nu = \frac{\Delta t}{\Delta x} = \frac{500}{N} \simeq 1.25, 1.1111, 1, 0.9091, 0.8333$. It can be seen easily that nonstandard RK3 performs well up to CFL numbers =1 but it's results quickly deteriorate when applied with larger CFL numbers.

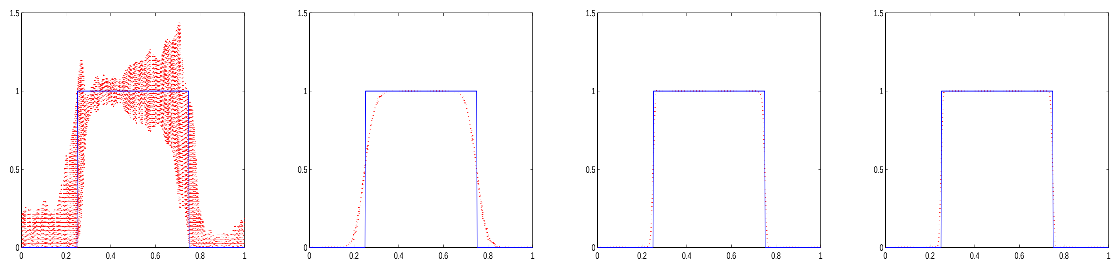

Figure 1: Numerical solutions obtained by nonstandard RK3. From left, with N=400, 425, 450, 500 time steps.

Table 1 gives some numerical solutions with $\varphi(\Delta t) = 1 - e^{-\Delta t}$ and two initial profiles, viz. the peaked function $U_0(x, t) = sin^{100}(\pi x)$ and above mentioned block function. Furthermore, in order to characterize positivity, the value of the smallest component of the solutions is given. The corresponding biggest component of the solutions shows that the positivity may also imply a maximum principle ($\min_i U_i^0 \leq U_i^n \leq \max_i U_i^0$ for all $n \geq 1$). Practical experience indicates that the smallest number N is needed to achieve positivity with the peaked function, for nonstandard RK3, is equal to 500. In the case of block function, we see little difference for this method with respect to positivity.

Table 1: Results for the scalar linear advection. N denotes the number of time steps.

	1D advection with smooth profile		1D advection with non-smooth profile	
N	$\min_{i,n}(U_i^n)$	$\max_{i,n}(U_i^n)$	$\min_{i,n}(U_i^n)$	$\max_{i,n}(U_i^n)$
400	-0.0256e+000	1.0309e+000	-0.1104e+000	1.1104e+000
450	1.3509e-203	1.0002	-0.0390	1.0391
500	1.3349e-203	0.9998	-0.0219	1.0219
550	1.3461e-203	0.9995	-0.0181	1.0181
600	1.3723e-203	0.9995	0.0063	1.0063

With the block function nonstandard method, is free from negative values for $N > 550$. Considering, an approximate solution positive if the smallest component is greater than -10^{-25}, nonstandard method perform well up to CFL numbers = 1 but their results quickly deteriorates when applied with larger and larger CFL numbers.

Test case 2: Scalar Burgers' equation

The second test case consists of the scaler Burgers' equation

$$\frac{\partial}{\partial t}U(x,t) + \frac{\partial}{\partial x}\Big(\frac{1}{2}U^2(x,t)\Big) = 0 \qquad t \geq 0, \quad -\infty < x < \infty,$$

with the initial conditions set to:

$$U(x,0) = \begin{cases} 1 & 0.3 \leq x < 0.7, \\ 0 & \text{otherwise.} \end{cases}$$

With the third-order upwind-biased flux we have

$$F_{i+\frac{1}{2}}(t,U) = \frac{1}{12}(-U_{i-1}^2 + 5U_i^2 + 2U_{i+1}^2) = \frac{1}{2}(U_i^2 + (\frac{1}{3} + \frac{1}{6}\eta_i)(U_{i+1}^2 - U_i^2), \tag{4.3}$$

where η_i is the ratio

$$\eta_i = \frac{U_i^2 - U_{i-1}^2}{U_{i+1}^2 - U_i^2} \quad i = 1, 2, \ldots, 500. \tag{4.4}$$

The general discretization (4.3) written out in full gives

$$U_i' = \frac{1}{2\Delta x}\Big(1 - \psi(\eta_{i-1}) + \frac{1}{\eta_i}\psi(\eta_i)\Big)(U_{i-1}^2 - U_i^2) \quad i = 1, 2, \ldots, 500,$$

with the same limiter function ψ in (4.2). It is fair to say that for $U_{n+1} \geq 0$, we have no formal proof (our interest for future research), but we have conclusive numerical evidence (see Table 2) which shows that positivity holds for (1.4). Our final time is $t_f = 0.25$.

Also, the resulting nonlinear semi-discrete system (4.4) was integrated in time with the classical fourth-order method and Courant number $\frac{\Delta t}{\Delta x}$ equal to $\frac{1}{2}$. We get a nice total variation diminishing (TVD) property in the sense that

$$\|U_{n+1}\|_{TV} \leq \|U_n\|_{TV}, \quad n = 0, 1, 2, \ldots .$$

Here for vectors $v = (v_i)$ the seminorm $\|v\|_{TV} = TV(v)$ is defined by

$$TV(v) = \sum_i \mid v_{i+1} - v_i \mid .$$

Table 2: Results for Burgers' equation. N denotes the number of time steps.

	Burgers' equation with smooth profile		Burgers' equation with non-smooth profile	
N	$\min_{i,n}(U_i^n)$	$\max_{i,n}(U_i^n)$	$\min_{i,n}(U_i^n)$	$\max_{i,n}(U_i^n)$
150	-2.9515e+181	2.7251e+181	-Inf	+Inf
175	0.0000	1.3506	-4.4119e+089	5.0665e+089
200	0.0000	1.0775	0.0000	1.2106
225	0.0000	1.0558	0.0000	1.1306
250	0.0000	1+3e-006	0.0000	1+6e-005

TVD assures that global undershoot and overshoot cannot occur. The evolution of the total variation of U_N ($\| U_N \|_{TV}$, $N = \frac{T}{\Delta t}$) is shown in Figure 2 with $\varphi(\Delta t) = 1 - e^{-\Delta t}$ for the output times $T = 1, 2, \ldots, 15$, revealing a decreasing. On several occasions it has been mentioned that absence of oscillations which are localized under and overshoots implies the positivity (see e.g. [7, 12, 13]).

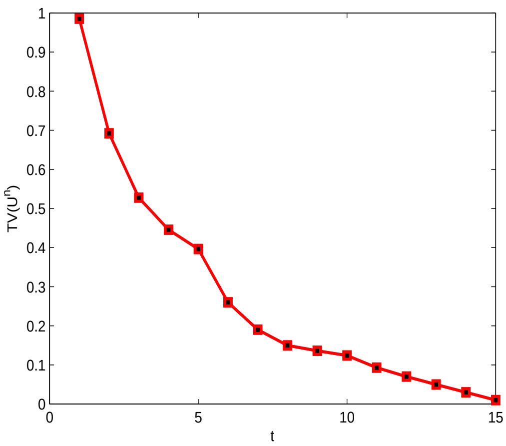

Figure 2: Values of $\| U_N \|_{TV}$ for $T = 1, 2, \ldots, 5$.

Test case 3: 2D advection equation

In the third test case, we deal with the numerical solution of the 2-dimensional advetion equation, defined by

$$U_t + aU_x + bU_y = 0,$$

on the unit square with constant $a, b = 1$. The initial profile is a cylinder with height 1, centered at $(0.25, 0.25)$ with radius 0.1. Our final time is $t_f = 0.5$, and at the inflow boundaries, homogeneous Dirichlet conditions are imposed. Spatial discretization with one-dimensional limiters are also common for two-dimensional advection problem in two spatial directions. Therefore, the semi-discrete system here can be written as

$$U'_{ij}(t) = \alpha_{ij}(U(t))\big(U_{i-1,j}(t) - U_{ij}(t)\big) + \beta_{ij}(U(t))\big(U_{i,j-1}(t) - U_{ij}(t)\big),$$

with nonlinear functions α_{ij},β_{ij} satisfying

$$0 \leq \alpha_{ij}(U) \leq \frac{2}{\Delta x}, \quad 0 \leq \beta_{ij}(U) \leq \frac{2}{\Delta y},$$

where Δx and Δy being the mesh width in the x-direction and y-direction, respectively. For more details see [6, p. 307]. In Figure 3, some numerical results have been shown on a 50×50 grid for the classical fourth-order method. For the solution the qualitative behaviour and temporal accuracy is good with this method for the CFL numbers ≤ 0.25. Furthermore, we found that there are no global undershoots or overshoots for this Runge-Kutta method. Our final time is taken as $t_f = 0.5$ and $\varphi(\Delta t) = 1 - e^{-\Delta t}$.

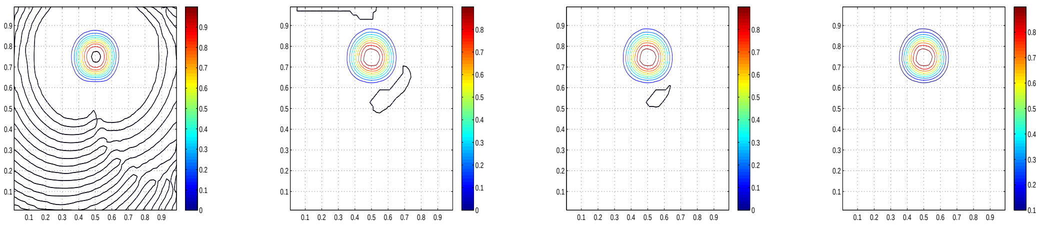

Figure 3: Advection for the cylinder profile on a 50×50 grid. From left, solutions for the nonstandard RK3, time stepping with 25, 35, 50, 80 time steps, respectively. Corresponding Courant numbers are 1, 0.7, 0.5, 0.3. Contour lines at levels 0.1, 0.2,. . .,0.9.

5. Conclusion

Schemes preserving the positivity are great importance in practice. Such schemes can be employed to prevent the occurrence of negative values where even very small negative values are unacceptable. In Theorem 1, we have derived sufficient condition for the nonstandard RK3 method with respect to positivity, for the model $U_t + U_x = 0$, with the limiter (4.2), spatial periodicity $U(x \pm 1, t = U(x,t)$ and two initial profiles, viz. the smooth function $U_0(x,t) = \sin^{100}(\pi x)$ and the nonsmooth function $U_0(x,t) = 1$ for $0.3 \leq x \leq 0.7$ and 0 otherwise. Also, we studied the sufficient condition on positivity for the nonstandard RK3 method with Bergers' equation and 2D advection test equation, exprimentally . We think, the necessity of non-zero interval of positivity, $\gamma > 0$ can be demonstrated. This is still being investigated and is not yet ready for reporting. Further, a future work can be to establish the TVD property of nonstandard RK3 method, since as mentioned in fourth section we have numerical evidences show that this method is free of spurious oscillations around discontinuities, when applied to the special nonlinear positive systems.

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