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2-stage explicit total variation diminishing preserving Runge-Kutta methods

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Abstract In this paper, we investigate the total variation diminishing property for a class of 2-stage explicit Runge-Kutta methods of order two (RK2) when applied to the numerical solution of special nonlinear initial value problems (IVPs) for ODEs. Schemes preserving the essential physical property of diminishing total variation are of great importance in practice. Such schemes are free of spurious oscillations around discontinuities.

Keywords. Initial value problem, Method of Line, Total-variation-diminishing, Runge-Kutta methods.

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1. Introduction

The method of lines is a popular semidiscretization method for the solution of time-dependent partial differential equations (PDEs). A suitable discretization of the spatial variables (e.g. by finite differences, finite volumes, finite elements, or spectral methods) yields a set of ordinary differential equations (ODEs) with respect to time. Then, these ODEs can be integrated using standard time-stepping techniques such as linear multistep methods (LMMs), Runge-Kutta (RK) methods or general linear methods (GLMs). The numerical computation of solutions of nonlinear hyperbolic PDEs has proved, in fact, to be perhaps unexpectedly difficult. Discontinuities are likely to appear in the solution, and schemes which are accurate in smooth regions tend to produce spurious oscillations in the neighborhood of the discontinuities. These oscillations can be eliminated by the use of strongly dissipative first order accurate schemes, but these schemes severely degrade the accuracy and usually

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produce excessively smeared discontinuities. Hence, time integration methods based on nonlinear stability requirement are desirable. This type of methods originated with Shu [6] and Harten [2] and were originally called TVD (total variation diminishing) time discretizations. In this paper, we investigate the TVD property for a class of 2-stage explicit Runge-Kutta (RK2) methods of order two when applied to the numerical solution of special nonlinear initial value problems (IVPs) for ODEs.
Let us consider an initial value problem for a TVD system (The total variation is decreasing) of ODEs of type

$$U^{'}(t) = F(t, U(t)), \quad (t \geq 0), \quad U(0) = U_0. \tag{1.1}$$

Let a mesh $t_n = n\Delta t$, $n = 0, 1, ...$ in the time direction be given, $U_i^n \simeq U(x_i, t_n)$ and $U_n = [U_1^n, U_2^n, ..., U_m^n]^T \in \mathbb{R}^m$. Since (1.1) stands for a semidiscrete version of a conservation law as mentioned above, it is desirable that the (fully discrete) process be total variation diminishing (TVD) in the sense that

$$\|U_{n+1}\|_{TV} \leq \|U_n\|_{TV}, \quad n = 0, 1, 2, \ldots. \tag{1.2}$$

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

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

As our numerical method, we consider the following 2-stage explicit Runge-Kutta scheme

$$\begin{aligned} U_{n_1} &= U_n \\ U_{n_2} &= U_n + \kappa \Delta t F(t_n, U_{n_1}) \\ U_{n+1} &= U_n + \Delta t\big((1 - \tfrac{1}{2\kappa})F(t_n, U_{n_1}) + \tfrac{1}{2\kappa}F(t_n + \kappa\Delta t, U_{n_2})\big). \end{aligned} \tag{1.3}$$

If $\kappa = 1$, (1.3) gives the explicit trapezoidal method. With $\kappa = \frac{1}{2}$, we have the one-step explicit midpoint rule.
The rest of the paper is organized as follows. In Section 2 we give some preliminary settings and general result on TVD for Runge-Kutta methods. In Section 3, some results are obtained for RK2 methods. We have given some numerical results in Section 4.

2. General result on TVD

As many papers, we assume that there is a maximal step size $\tau^\star \geq 0$ such that TVD property holds for the forward Euler method i.e.,

$$\|v + \Delta t F(t, v)\|_{TV} \leq \|v\|_{TV} (\text{for all } v \in \mathbb{R}^n,\ t \geq 0,\ 0 < \Delta t \leq \tau^\star). \tag{2.1}$$

We shall determine step size coefficients $\gamma(\kappa)$, $\kappa > 0$ such that the TVD is valid for (2.1) under the step size restriction $\Delta t \leq \gamma(\kappa)\tau^{\star}$. The backward Euler method $U_{n+1} = U_n + \Delta t F(t_{n+1}, U_{n+1})$ is TVD under assumption (2.1) without any time step restriction [3]. Similar to positivity analysis [5], sufficient condition for the TVD can be derived for Runge-Kutta methods, by using properties known for the forward and backward Euler.
We consider the s-stage Runge-Kutta method in the special form
$v_0 = U_n$,
$v_i = \sum_{j=0}^{i-1}\Big(p_{ij}v_j + q_{ij}\Delta t F(t_n + \tilde{c}_j\Delta t, v_j)) + q_i \Delta t F(t_n + \tilde{c}_i \Delta t, v_i\Big), \quad i = 1, 2, ..., s,$
and finally set $U_{n+1} = v_s$. With non-negative parameters p_{ij}, q_{ij}, q_i, the method is TVD for general systems $U^{'}(t) = F(t, U(t))$, satisfying (2.1), under the step-size restriction

$$\Delta t \leq \tau^{\star} \min_{0 \leq j < i \leq s}(\frac{p_{ij}}{q_{ij}}). \tag{2.2}$$

For more details see [3, 6]. Following this idea, the last stage of (1.3) is written as

$$\begin{aligned} U_{n+1} = (1-\theta)U_n + (1 - \frac{1}{2\kappa} - \kappa\theta)\Delta t F(t_n, U_n) \\ + \theta U_{n_2} + \frac{1}{2\kappa}\Delta t F(t_n + \kappa\Delta t, U_{n_2}), \end{aligned} \tag{2.3}$$

with $0 \leq \theta \leq 1$ and $U_{n_2} = U_n + \kappa \Delta t F(U_{n_1})$. In accordance with the bound (2.2) TVD holds for (1.3) under step size restriction $\Delta t \leq \gamma\tau^{\star}$, where

$$\gamma(\kappa) = \min(\frac{1-\theta}{1 - \frac{1}{2\kappa} - \kappa\theta}, 2\kappa\theta).$$

Obviously, we are interested in largest $\gamma(\kappa)$ so that we will have better TVD properties of the scheme. With $\frac{1}{2} < \kappa < 1$ and $\kappa > 1$, the largest $\gamma(\kappa)$ obtain when $\theta = \frac{2\kappa^2 - 4\kappa + 1}{4\kappa^3 - 4\kappa^2}$ and $\theta = \frac{1}{2\kappa^2}$, respectively, and for $0 < \kappa < \frac{1}{2}$, since $1 - \frac{1}{2\kappa} < 0$, the largest $\gamma(\kappa)$ is 0. Therefore we have

$$\gamma(\kappa) = \begin{cases} 0, & 0 < \kappa < \frac{1}{2} \\ 2 - \frac{1}{\kappa}, & \frac{1}{2} \leq \kappa \leq 1 \\ \frac{1}{\kappa}, & \kappa > 1. \end{cases} \tag{2.4}$$

In accordance with the (2.4), the second-order explicit trapezoidal rule ($\kappa = 1$) satisfies the theoretical TVD condition with $\gamma(\kappa) = 1$ and TVD is not ensured ($\gamma(\kappa) = 0$) for the explicit midpoint rule. The question of whether similar result is possible for midpoint rule ($\gamma(\kappa) = 1$), seems not to have been considered in the literature thus far. To answer this question the class of RK2 in (1.3) which includes the explicit midpoint method and the explicit trapezoidal rule is applied to special nonlinear systems of ODE and some new results are achieved.

3. Main result

In this section, we derive straight for the sufficient condition for explicit trapezoidal method to be TVD. Applying of explicit trapezoidal method to (1.1) under assumption (2.1) we have

$$
\begin{aligned}
U_{n+1} &= U_n+\frac{1}{2}\Delta tF(t_n,U_n)+\frac{1}{2}\Delta tF(t_{n+1},\bar{U}_{n+1}),\ \bar{U}_{n+1}=U_n+\Delta tF(t_n,U_n),\\
U_{n+1} &= \frac{1}{2}U_n+\frac{1}{2}U_n+\frac{1}{2}\Delta tF(t_n,U_n)+\frac{1}{2}\Delta tF(t_{n+1},\bar{U}_{n+1}),\\
U_{n+1} &= \frac{1}{2}\big(U_n+\Delta tF(t_n,U_n)\big)+\frac{1}{2}U_n+\frac{1}{2}\Delta tF(t_{n+1},\bar{U}_{n+1}),\\
&= \frac{1}{2}U_n+\frac{1}{2}\big(\bar{U}_{n+1}+\Delta tF(t_{n+1},\bar{U}_{n+1})\big),
\end{aligned}
$$

and

$$
\begin{aligned}
\|U_{n+1}\|_{TV} =& \|\frac{1}{2}U_n+\frac{1}{2}\big(\bar{U}_{n+1}+\Delta F(t_{n+1},\bar{U}_{n+1})\big)\|_{TV}\\
&\leq \frac{1}{2}\|U_n\|_{TV}+\|\frac{1}{2}\big(\bar{U}_{n+1}+\Delta tF(t_{n+1},\bar{U}_{n+1})\big)\|_{TV},
\end{aligned}
$$

assumption (2.1) yielding

$$
\|\bar{U}_{n+1}+\Delta tF(t_{n+1},\bar{U}_{n+1})\|_{TV}\leq\|\bar{U}_{n+1}\|_{TV},
$$

therefore

$$
\|U_{n+1}\|_{TV}\leq\frac{1}{2}\|U_n\|_{TV}+\frac{1}{2}\|\bar{U}_{n+1}\|_{TV}\leq\frac{1}{2}\|U_n\|_{TV}+\frac{1}{2}\|U_n\|_{TV},
$$

and so $\|U_{n+1}\ |_{TV}\leq\|U_n\|_{TV}$ for any $\Delta t>0$. On the other hand, the trapezoidal method is TVD under assumption (2.1) without any time step restriction. This result coincide with (2.4) for explicit trapezoidal method ($\kappa=1$) which shows that the Shu-Osher form (2.3) is optimal.

In the following, the class of RK2 in (1.3) which includes the explicit midpoint method and the explicit trapezoidal rule, is applied to special nonlinear system of ODE and some results are achieved numerically. Let us consider

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

with the nonlinear function $q_i(U)$ satisfying $q_i(U)\geq 0$ for any vector U, and $\Delta x=\frac{1}{m}$, $U=[U_1,U_2,...,U_m]^T$, $U_0=U_m$. This special semi-discrete system arises from a linear advection problem ($u_t + u_x = 0$) after discretization using a flux limiter [3]. This nonlinear system is positive [5]. Application of (1.3) to (3.1) with $\nu_i^l = \Delta t \frac{q_i(U_l)}{\Delta x}$ and $l = n_1, n_2$ gives

$$(U_{n_2})_i = U_i^n + \kappa \Delta t \frac{q_i(U_{n_1})}{\Delta x}(U_{i-1}^n - U_i^n) = U_i^n + \kappa \nu_i^{n_1}(U_{i-1}^n - U_i^n),$$

$i = 1, 2, ..., m$, where $U_i^n \simeq U(x_i, t_n)$ as mentioned above is the fully discrete approximation. Therefore, we have

$$\begin{aligned} U_i^{n+1} = U_i^n &+ \frac{1}{2}\nu_i^{n_2}\nu_{i-1}^{n_1}(U_{i-2}^n - U_{i-1}^n) \\ &- \big(\tfrac{1}{2}\nu_i^{n_2}\nu_i^{n_1} - \tfrac{1}{2\kappa}\nu_i^{n_2} - \nu_i^{n_1}(1 - \tfrac{1}{2\kappa})\big)(U_{i-1}^n - U_i^n). \end{aligned}$$

By rearranging, we have

$$\begin{aligned} (U_{i+1}^{n+1} - U_i^{n+1}) =& (U_{i+1}^n - U_i^n) - \big((1 - \frac{1}{2\kappa})\nu_{i+1}^{n_1} + \frac{1}{2\kappa}\nu_{i+1}^{n_2} - \frac{1}{2}\nu_{i+1}^{n_2}\nu_{i+1}^{n_1})\big)U_{i+1}^n \\ &+ \big(- \frac{1}{2}\nu_i^{n_2}\nu_i^{n_1} + \frac{1}{2\kappa}\nu_i^{n_2} + (1 - \frac{1}{2\kappa})\nu_i^{n_1} - \frac{1}{2}\nu_{i+1}^{n_2}\nu_{i+1}^{n_1} + \frac{1}{2\kappa}\nu_{i+1}^{n_2} \\ &\quad - (1 - \frac{1}{2\kappa})\nu_{i+1}^{n_1} - \frac{1}{2}\nu_{i+1}^{n_2}\nu_i^{n_1}\big)U_i^n \\ &+ \big(\frac{1}{2}\nu_{i+1}^{n_2}\nu_i^{n_1} + \frac{1}{2}\nu_i^{n_2}\nu_i^{n_1} - \frac{1}{2\kappa}\nu_i^{n_2} \\ &\quad - (1 - \frac{1}{2\kappa})\nu_i^{n_1}\big)U_{i-1}^n - \frac{1}{2}\nu_i^{n_2}\nu_{i-1}^{n_1}U_{i-2}^n. \end{aligned}$$

It is fair to say that for $\|U_{n+1}\|_{TV} \leq \|U_n\|_{TV}$, we have no formal proof (our interest for future research), but we have conclusive numerical evidence in Section 4 which shows that TVD property holds for (1.3) with $\kappa \geq \frac{1}{2}$.

4. Numerical results

In this section, at first we consider advection equation

$$U_t + U_x = 0, \qquad (t > 0 \text{ and } 0 < x < 1),$$

with periodic boundary conditions. We have discretized in space on uniformly distributed grid points $x_i = i\Delta x$, with $\Delta x = \frac{1}{200}$ by means of the flux form

$$\begin{aligned} U_i'(t) = &\frac{1}{\Delta x}(F_{i-\frac{1}{2}}(t, U(t)) - F_{i+\frac{1}{2}}(t, U(t)), F_{i\pm\frac{1}{2}}(t, U) \\ &= U_{i\pm\frac{1}{2}}, \qquad i = 1, 2, ..., 200, \end{aligned} \tag{4.1}$$

where the values $U_{i\pm\frac{1}{2}}$ are defined at the cell boundaries $x_{i\pm\frac{1}{2}}$. With the third-order upwind-biased flux [3] we have

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

where θ_i is the ratio

$$\theta_i = \frac{U_i - U_{i-1}}{U_{i+1} - U_i} \quad i = 1, 2, ..., 200.$$

The general discretization (4.1) written out in full gives

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

with the limiter function ψ, here

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

This limiter function was introduced by Koren [4]. The numerical solution for method (2.1) for $\kappa = 0.5, 0.75, 1, 1.5$ are shown in Figures 1-4, with block initial profile: $U_0(x, t) = 1$ for $0.3 < x < 0.7$ and 0 otherwise. Our final time is $t_f = 1$. For each of these schemes, it has used the number steps $N = 198, 200, 250$ and this leads to values of $\Delta t \simeq 0.0051, 0.0050, 0.0040$ and the Courant (CFL) numbers $\nu = \frac{\Delta t}{\Delta x} = \frac{200}{N} \simeq 1.0101, 1, 0.8$. It can be seen easily from the Figure 1 and Figure 3 that midpoint method and trapezoidal rule perform well up to CFL numbers =1 but their results quickly deteriorate when applied with larger CFL numbers. Therefore, in practical sense these two methods are equally efficient with regard to TVD. With other RK2 methods ($\frac{1}{2} \leq \kappa \leq 1$), a similar behavior was observed (see Figure 2). The necessity of the step size restriction (2.4) was experimentally studied for several RK2 methods with $\kappa > 1$, (see Figure 4). In general it was found that the (2.4) is somewhat too strict.

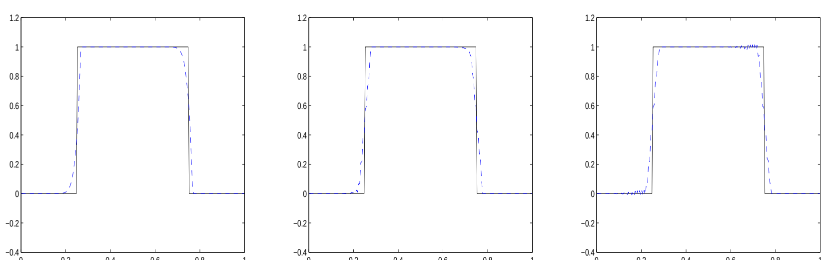

FIGURE 1. Numerical solutions obtained by midpoint rule ($\kappa = 0.5$). From left, with 250, 200, 198 time steps.

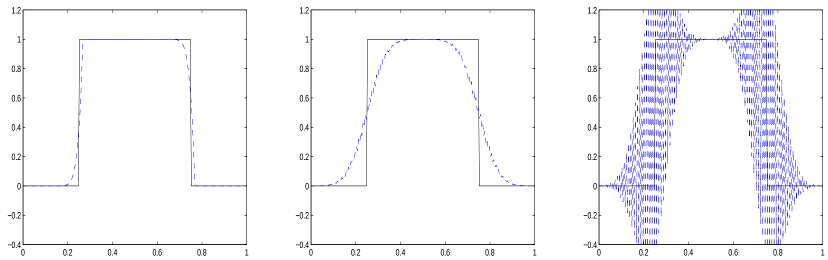

FIGURE 2. Numerical solutions obtained by RK2 ($\kappa = 0.75$). From left, with 250, 200, 198 time steps.

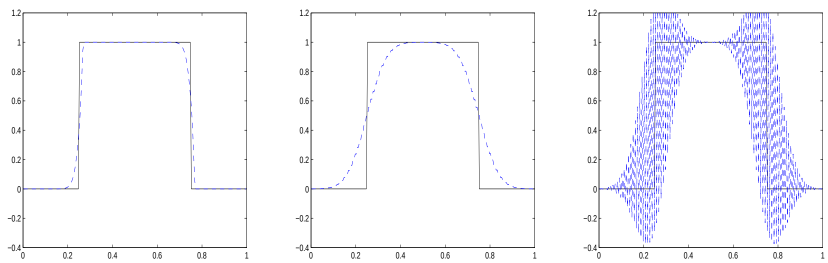

FIGURE 3. Numerical solutions obtained by trapezoidal rule. From left, with 250, 200, 198 time steps.

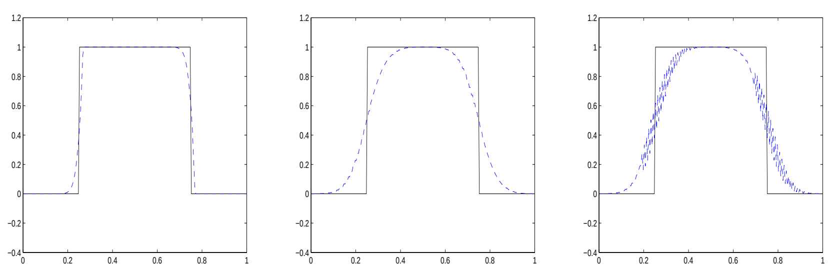

FIGURE 4. Numerical solutions for RK2 ($\kappa = 1.5$). From left, with 250, 200, 198 time steps.

Next we apply the RK2 to the Burger's equation

$$U_t + \left(\frac{1}{2}U^2\right)_x = 0,$$

with above mentioned block initial profile. With the third-order upwind-biased flux we have

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

where θ_i is the ratio

$$\theta_i = \frac{U_i^2-U_{i-1}^2}{U_{i+1}^2-U_i^2} \quad i=1,2,...,200.$$

The general discretization (4.1) written out in full gives

$$U_i' = \frac{1}{2\Delta x}\Big(1-\psi(\theta_{i-1})+\frac{1}{\theta_i}\psi(\theta_i)\Big)(U_{i-1}^2-U_i^2) \quad i=1,2,...,200, \quad (4.2)$$

with the limiter function ψ, here

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

The resulting nonlinear semi-discrete system (4.2) was integrated in time with the above four methods and Courant number $\frac{\Delta t}{\Delta x}$ equal to $\frac{1}{2}$. The behavior of the schemes is seen to be similar and we get a nice TVD behavior for all schemes. The evolution of the total variation of U_N ($\| U_N \|_{TV}$, $N=\frac{T}{\Delta t}$) is shown in Figure 5, for the output times $t=T$ with $T=1,2,...,5$ and $\kappa = 0.5, 0.75, 1, 1.5$, revealing a decreasing.

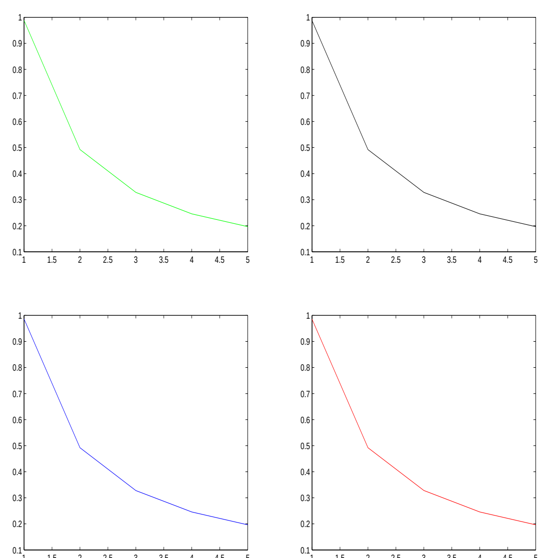

FIGURE 5. Values of $\| U_N \|_{TV}$ for $T=1,2,...,5$. From left, for $\kappa = 0.5, 0.75, 1, 1.5$.

5. Conclusions

Schemes preserving the TVD are great importance in practice. Such schemes are free of spurious oscillations around discontinuities. In this paper, we have investigated the TVD property for a class of 2-stage explicit Runge-Kutta methods of order two. A future work is to establish the TVD property of RK3, since we have numerical evidence that RK3 preserve the TVD of the solutions when applied to the special nonlinear TVD systems.

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