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TOTAL VARIATION DIMINISHING RUNGE-KUTTA SCHEMES

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ABSTRACT. In this paper we further explore a class of high order TVD (total variation diminishing) Runge-Kutta time discretization initialized in a paper by Shu and Osher, suitable for solving hyperbolic conservation laws with stable spatial discretizations. We illustrate with numerical examples that non-TVD but linearly stable Runge-Kutta time discretization can generate oscillations even for TVD (total variation diminishing) spatial discretization, verifying the claim that TVD Runge-Kutta methods are important for such applications. We then explore the issue of optimal TVD Runge-Kutta methods for second, third and fourth order, and for low storage Runge-Kutta methods.

1. INTRODUCTION

In this paper we further explore a class of high order TVD (total variation diminishing) Runge-Kutta time discretization initialized in [12]. For related work of multi-step type see [11]. The method is used to solve a system of ODEs:

$$u_t = L(u) \tag{1.1}$$

with suitable initial conditions, resulting from a method of lines approximation to a hyperbolic conservation law:

$$u_t = -f(u)_x \tag{1.2}$$

where the spatial derivative $f(u)_x$ is approximated by a TVD finite difference or finite element approximation (e.g. [4], [8], [13], [2]), denoted by $-L(u)$, which has the property that the total variation of the numerical solution:

$$TV(u) = \sum_j |u_{j+1} - u_j| \tag{1.3}$$

does not increase

$$TV(u^{n+1}) \le TV(u^n) \tag{1.4}$$

for a first order in time Euler forward stepping:

$$u^{n+1} = u^n + \Delta t L(u^n) \tag{1.5}$$

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under suitable restriction on Δt:

$$\Delta t \leq \Delta t_1. \tag{1.6}$$

The objective of the high order TVD Runge-Kutta time discretization, is to maintain the TVD property (1.4) while achieving higher order accuracy in time, perhaps with a different time step restriction than (1.6):

$$\Delta t \leq c\,\Delta t_1, \tag{1.7}$$

where c is termed the CFL coefficient for the high order time discretization.

The TVD high order time discretization is useful not only for TVD spatial discretizations, but also for TVB (total variation bounded) (e.g. [10]), or ENO (Essentially Non-Oscillatory) (e.g. [5], [12]), or other types of spatial discretizations for hyperbolic problems. It maintains stability in whatever norm, of the Euler forward first order time stepping, for the high order time discretization, under the time step restriction (1.7). For example, if it is used for multi-dimensional scalar conservation laws, for which TVD is not possible but maximum norm stability can be maintained for high order spatial discretizations plus forward Euler time stepping (e.g. [3]), then the same maximum norm stability can be maintained if TVD high order time discretization is used. As another example, if an entropy inequality can be proved for the Euler forward, then the same entropy inequality is valid under a high order TVD time discretization.

In [12], a general Runge-Kutta method for (1.1) is written in the form:

$$\begin{aligned} u^{(i)} &= \sum_{k=0}^{i-1} \left(\alpha_{ik} u^{(k)} + \Delta t \beta_{ik} L(u^{(k)}) \right), \qquad i = 1, ..., m, \\ u^{(0)} &= u^n, \qquad u^{(m)} = u^{n+1}. \end{aligned} \tag{1.8}$$

Clearly, if all the coefficients are nonnegative $\alpha_{ik} \geq 0$, $\beta_{ik} \geq 0$, then (1.8) is just a convex combination of Euler forward operators, with Δt replaced by $\frac{\beta_{ik}}{\alpha_{ik}}\Delta t$, since by consistency $\sum_{k=0}^{i-1} \alpha_{ik} = 1$. We thus have

Lemma 1.1 ([12])**.** *The Runge-Kutta method* (1.8) *is TVD under the CFL coefficient* (1.7)*:*

$$c = \min_{i,k} \frac{\alpha_{ik}}{\beta_{ik}}, \tag{1.9}$$

provided that $\alpha_{ik} \geq 0$*,* $\beta_{ik} \geq 0$*.* □

In [12], schemes up to third order were found to satisfy the conditions in Lemma 1.1 with CFL coefficient equal to 1.

If we only have $\alpha_{ik} \geq 0$ but β_{ik} might be negative, we need to introduce an adjoint operator $\tilde{L}$. The requirement for $\tilde{L}$ is that it approximates the same spatial derivative(s) as L, but is TVD (or stable in another relevant norm) for first order Euler, backward in time:

$$u^{n+1} = u^n - \Delta t \tilde{L}(u^n). \tag{1.10}$$

This can be achieved, for hyperbolic conservation laws, by solving the backward in time version of (1.2):

$$u_t = f(u)_x. \tag{1.11}$$

Numerically, the only difference is the change of upwind direction. Clearly, $\tilde{L}$ can be computed with the same cost as that of computing L. We then have the following lemma:

Lemma 1.2 ([12]). *The Runge-Kutta method* (1.8) *is TVD under the CFL coefficient* (1.7)*:*

$$c = \min_{i,k} \frac{\alpha_{ik}}{|\beta_{ik}|}, \tag{1.12}$$

provided that $\alpha_{ik} \geq 0$, and L is replaced by $\tilde{L}$ for negative β_{ik}. □

Notice that, if for the same k, both $L(u^{(k)})$ and $\tilde{L}(u^{(k)})$ must be computed, the cost as well as storage requirement for this k is doubled. For this reason, we would like to avoid negative β_{ik} as much as possible. In [12], two $\tilde{L}$'s were used to give a fourth order TVD Runge-Kutta method with a CFL coefficient $c = 0.87$. We will improve it in this paper, however unfortunately we also prove that all four stage, fourth order Runge-Kutta methods with positive CFL coefficient c in (1.12) must have at least one negative β_{ik}.

For large scale scientific computing in three space dimensions, storage is usually a paramount consideration. There are therefore the discussions about low storage Runge-Kutta methods [15], [1], which only require 2 storage units per ODE equation. We will consider in this paper TVD properties among such low storage Runge-Kutta methods.

In the next section, we will give numerical evidence to show that, even with a very nice second order TVD spatial discretization, if the time discretization is by a non-TVD but linearly stable Runge-Kutta method, the result may be oscillatory. Thus it would always be safer to use TVD Runge-Kutta methods for hyperbolic problems.

The investigation of TVD time discretization can also be carried out for the generalized Runge-Kutta methods (which have more than one step) in, e.g., [6] and [7]. We have performed this study but failed to find good (in terms of CFL coefficients and whether $\tilde{L}$ appears) TVD methods in this class. The result will not be discussed in this paper.

2. The necessity to use a TVD time stepping: A numerical example

In this section we will show a numerical example, using the standard minmod based MUSCL second order spatial discretization [14]. We will compare the results of TVD versus non-TVD second order Runge-Kutta time discretizations. The PDE is the simple Burgers equation

$$u_t + \left(\frac{1}{2}u^2\right)_x = 0 \tag{2.1}$$

with Riemann initial data:

$$u(x,0) = \begin{cases} 1, & \text{if } x \leq 0, \\ -0.5, & \text{if } x > 0, \end{cases} \tag{2.2}$$

$\left(\frac{1}{2}u^2\right)_x$ in (2.1) is approximated by the conservative difference

$$\frac{1}{\Delta x}\left(\hat{f}_{j+\frac{1}{2}} - \hat{f}_{j-\frac{1}{2}}\right),$$

where the numerical flux $\hat{f}_{j+\frac{1}{2}}$ is defined by

$$\hat{f}_{j+\frac{1}{2}} = h\left(u^-_{j+\frac{1}{2}}, u^+_{j+\frac{1}{2}}\right)$$

with

$$\begin{aligned} u^-_{j+\frac{1}{2}} &= u_j + \frac{1}{2} minmod(u_{j+1} - u_j, u_j - u_{j-1}), \\ u^+_{j+\frac{1}{2}} &= u_{j+1} - \frac{1}{2} minmod(u_{j+2} - u_{j+1}, u_{j+1} - u_j). \end{aligned}$$

The monotone flux h is the Godunov flux

$$h(u^-, u^+) = \begin{cases} \min_{u^- \le u \le u^+} \left(\frac{u^2}{2}\right), & \text{if } u^- \le u^+, \\ \max_{u^- \ge u \ge u^+} \left(\frac{u^2}{2}\right), & \text{if } u^- > u^+, \end{cases}$$

and the now standard *minmod* function is given by

$$minmod(a, b) = \frac{sign(a) + sign(b)}{2} \min(|a|, |b|).$$

It is easy to prove, by using Harten's Lemma [4], that the Euler forward time discretization with this second order MUSCL spatial operator is TVD under the CFL condition (1.6):

$$\Delta t \le \frac{\Delta x}{2 \max_j |u_j^n|}. \tag{2.3}$$

Thus $\Delta t = \frac{\Delta x}{2 \max_j |u_j^n|}$ will be used in all our calculations.

The TVD second order Runge-Kutta method we consider is the one given in [12]:

$$\begin{aligned} u^{(1)} &= u^n + \Delta t L(u^n), \\ u^{n+1} &= \frac{1}{2} u^n + \frac{1}{2} u^{(1)} + \frac{1}{2} \Delta t L(u^{(1)}), \end{aligned} \tag{2.4}$$

the non-TVD method we use is

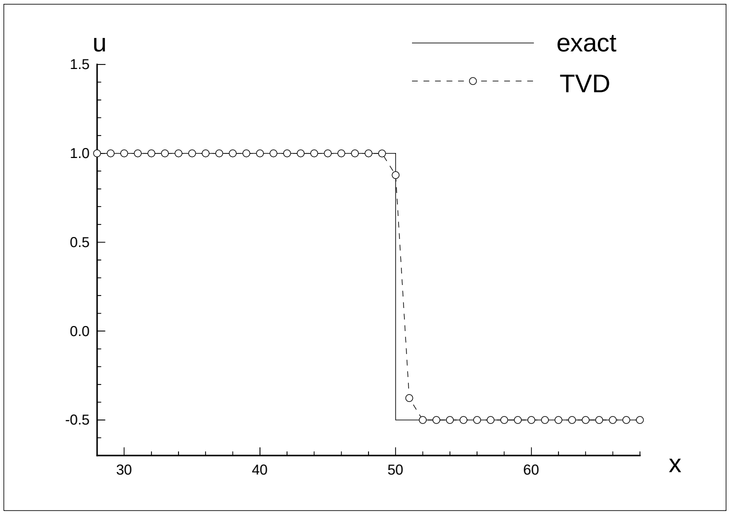
$$\begin{aligned} u^{(1)} &= u^n - 20 \Delta t L(u^n), \\ u^{n+1} &= u^n + \frac{41}{40} \Delta t L(u^n) - \frac{1}{40} \Delta t L(u^{(1)}). \end{aligned} \tag{2.5}$$

It is easy to verify that both methods are second order accurate in time. The second one (2.5) is however clearly non-TVD, since it has negative βs in both stages (i.e. it partially simulates backward in time with wrong upwinding).

If the operator L is linear (for example the first order upwind scheme applied to a linear PDE), then both Runge-Kutta methods (actually all the two stage, second order Runge-Kutta methods) yield identical results (the two stage, second order Runge-Kutta method for a linear ODE is unique). However, since our L is nonlinear, we may and do observe different results when the two Runge-Kutta methods are used.

In Figure 1 we show the result of the TVD Runge-Kutta method (2.4) and the non-TVD method (2.5), after the shock moves about 50 grids (400 time steps for the TVD method, 528 time steps for the non-TVD method). We can clearly see that the non-TVD result is oscillatory (there is an overshoot).

Such oscillations are also observed when the non-TVD Runge-Kutta method coupled with a second order TVD MUSCL spatial discretization is applied to a



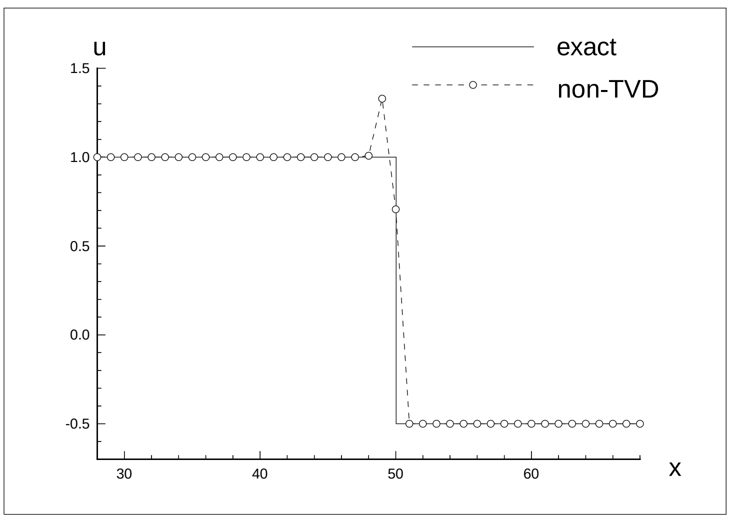


FIGURE 1. Second order TVD MUSCL spatial discretization. Solution after 500 time steps. Top: TVD time discretization (2.4); Bottom: non-TVD time discretization (2.5).

linear PDE ($u_t + u_x = 0$). Moreover, for some Runge-Kutta methods, if one looks at the intermediate stages, i.e. $u^{(i)}$ for $1 \leq i < m$ in (1.8), one observes even bigger oscillations. Such oscillations may render difficulties when physical problems are solved, such as the appearance of negative density and pressure for Euler equations of gas dynamics. On the other hand, the TVD Runge-Kutta method guarantees that each middle stage solution is also TVD.

This simple numerical test convinces us that it is much safer to use a TVD Runge-Kutta method for solving hyperbolic problems.

3. The optimal TVD Runge-Kutta methods of second, third and fourth order

In this section we will try to identify the optimal (in the sense of CFL coefficient and the cost incurred by $\tilde{L}$ if it appears) TVD Runge-Kutta methods of m-stage, m-th order, for $m = 2, 3, 4$, written in the form (1.8).

For second order $m = 2$, we can choose β_{10} and α_{21} as free parameters. The other coefficients are then given as [12]:

$$\left\{\begin{array}{l} \alpha_{10} = 1, \\ \alpha_{20} = 1 - \alpha_{21}, \\ \beta_{20} = 1 - \frac{1}{2\beta_{10}} - \alpha_{21}\beta_{10}, \\ \beta_{21} = \frac{1}{2\beta_{10}}. \end{array}\right. \tag{3.1}$$

Proposition 3.1. *If we require $\alpha_{ik} \geq 0$ and $\beta_{ik} \geq 0$, then the optimal second order TVD Runge-Kutta method* (1.8) *is given by*

$$\begin{aligned} u^{(1)} &= u^n + \Delta t L(u^n), \\ u^{n+1} &= \frac{1}{2}u^n + \frac{1}{2}u^{(1)} + \frac{1}{2}\Delta t L(u^{(1)}), \end{aligned} \tag{3.2}$$

with a CFL coefficient $c = 1$ in (1.9).

Proof. If we would like a CFL coefficient $c > 1$, then $\alpha_{10} = 1$ implies $\beta_{10} < 1$, which in turn implies $\frac{1}{2\beta_{10}} > \frac{1}{2}$. Also, $\alpha_{21} > \beta_{21} = \frac{1}{2\beta_{10}}$, which implies $\alpha_{21}\beta_{10} > \frac{1}{2}$. We thus have

$$\beta_{20} = 1 - \frac{1}{2\beta_{10}} - \alpha_{21}\beta_{10} < 1 - \frac{1}{2} - \frac{1}{2} = 0,$$

which is a contradiction. $\square$

For the third order case $m = 3$, the general Runge-Kutta method consists of a two parameter family as well as two special cases of one parameter families [9]. We can similarly prove the following proposition:

Proposition 3.2. *If we require $\alpha_{ik} \geq 0$ and $\beta_{ik} \geq 0$, then the optimal third order TVD Runge-Kutta method* (1.8) *is given by*

$$\begin{aligned} u^{(1)} &= u^n + \Delta t L(u^n), \\ u^{(2)} &= \frac{3}{4}u^n + \frac{1}{4}u^{(1)} + \frac{1}{4}\Delta t L(u^{(1)}), \\ u^{n+1} &= \frac{1}{3}u^n + \frac{2}{3}u^{(2)} + \frac{2}{3}\Delta t L(u^{(2)}), \end{aligned} \tag{3.3}$$

with a CFL coefficient $c = 1$ in (1.9).

Proof. The proof is more technical, and is given in the Appendix. $\square$

For the fourth order case $m = 4$, the general Runge-Kutta method again consists of a two parameter family as well as three special cases of one parameter families [9]. Unfortunately, this time we cannot avoid the appearance of negative β_{ik}:

Proposition 3.3. *The four stage, fourth order Runge-Kutta scheme* (1.8) *with a nonzero CFL coefficient c in* (1.12) *must have at least one negative β_{ik}.*

Proof. The proof is technical, and is given in the Appendix. $\square$

We thus must settle for finding an efficient solution containing $\tilde{L}$, which maximizes $\frac{c}{4+i}$, where c is the CFL coefficient (1.12) and i is the number of $\tilde{L}$s. This way we are looking for a TVD method which reaches a fixed time T with a minimal number of residue evaluations for L or $\tilde{L}$. We use a computer program and the help of optimization routines to achieve this goal. The following is the best method we can find:

(3.4)
$$\begin{aligned}
u^{(1)} &= u^n + \frac{1}{2}\Delta t L(u^n),\\
u^{(2)} &= \frac{649}{1600}u^{(0)} - \frac{10890423}{25193600}\Delta t\tilde{L}(u^n) + \frac{951}{1600}u^{(1)} + \frac{5000}{7873}\Delta t L(u^{(1)}),\\
u^{(3)} &= \frac{53989}{2500000}u^n - \frac{102261}{5000000}\Delta t\tilde{L}(u^n) + \frac{4806213}{20000000}u^{(1)}\\
&\quad - \frac{5121}{20000}\Delta t\tilde{L}(u^{(1)}) + \frac{23619}{32000}u^{(2)} + \frac{7873}{10000}\Delta t L(u^{(2)}),\\
u^{n+1} &= \frac{1}{5}u^n + \frac{1}{10}\Delta t L(u^n) + \frac{6127}{30000}u^{(1)} + \frac{1}{6}\Delta t L(u^{(1)}) + \frac{7873}{30000}u^{(2)}\\
&\quad + \frac{1}{3}u^{(3)} + \frac{1}{6}\Delta t L(u^{(3)})
\end{aligned}$$

with a CFL coefficient $c = 0.936$ in (1.12). Notice that two $\tilde{L}$s must be computed. The effective CFL coefficient, comparing with an ideal case without $\tilde{L}$s, is $0.936 \times \frac{4}{6} = 0.624$. Since it is difficult to solve the global optimization problem, we do not claim that (3.4) is the optimal 4 stage, 4th order TVD Runge-Kutta method.

4. The low storage TVD Runge-Kutta methods

For large scale scientific computing in three space dimensions, storage is usually a paramount consideration. There are therefore the discussions about low storage Runge-Kutta methods [15], [1], which only require 2 storage units per ODE variable. We will consider in this section TVD properties among such low storage Runge-Kutta methods.

The general low storage Runge-Kutta schemes can be written in the form [15], [1]:

$$\begin{aligned}
du^{(i)} &= A_i du^{(i-1)} + \Delta t L(u^{(i-1)}),\\
u^{(i)} &= u^{(i-1)} + B_i du^{(i)}, \qquad i = 1, ..., m,\\
u^{(0)} &= u^n,\ u^{(m)} = u^{n+1},\ A_0 = 0.
\end{aligned} \tag{4.1}$$

Only u and du must be stored, resulting in two storage units for each variable.

Carpenter and Kennedy [1] have classified all the three stage, third order ($m=3$) low storage Runge-Kutta methods, obtaining the following one parameter family:

$$
\begin{aligned}
z_1 &= \sqrt{36c_2^4+36c_2^3-135c_2^2+84c_2-12},\\
z_2 &= 2c_2^2+c_2-2,\\
z_3 &= 12c_2^4-18c_2^3+18c_2^2-11c_2+2,\\
z_4 &= 36c_2^4-36c_2^3+13c_2^2-8c_2+4,\\
z_5 &= 69c_2^3-62c_2^2+28c_2-8,\\
z_6 &= 34c_2^4-46c_2^3+34c_2^2-13c_2+2,\\
B_1 &= c_2,\\
B_2 &= \frac{12c_2(c_2-1)(3z_2-z_1)-(3z_2-z_1)^2}{144c_2(3c_2-2)(c_2-1)^2},\\
B_3 &= \frac{-24(3c_2-2)(c_2-1)^2}{(3z_2-z_1)^2-12c_2(c_2-1)(3z_2-z_1)},\\
A_2 &= \frac{-z_1(6c_2^2-4c_2+1)+3z_3}{(2c_2+1)z_1-3(c_2+2)(2c_2-1)^2},\\
A_3 &= \frac{-z_4z_1+108(2c_2-1)c_2^5-3(2c_2-1)z_5}{24z_1c_2(c_2-1)^4+72c_2z_6+72c_2^6(2c_2-13)}.
\end{aligned}
\tag{4.2}
$$

We convert this form into the form (1.8), by introducing three new parameters. Then we search for values of these parameters that would maximize the CFL restriction, again by a computer program. The result seems to indicate that

$$c_2 = 0.924574 \tag{4.3}$$

gives an almost best choice, with CFL coefficient $c=0.32$ in (1.9). This is of course less optimal than (3.3) in terms of CFL coefficients, however the low storage form is useful for large scale calculations.

Carpenter and Kennedy [1] have also given classes of 5 stage, 4th order low storage Runge-Kutta methods. We have been unable to find TVD methods in that class with positive α_{ik} and β_{ik}. Notice that $\tilde{L}$ cannot be used without destroying the low storage property, hence negative β_{ik} cannot be used here.

5. Concluding remarks

We have given a simple but illustrating numerical example to show that it is in general much safer to use a TVD Runge-Kutta method for hyperbolic problems. We then explore the optimal second, third and fourth order TVD Runge-Kutta methods. While for second and third order optimal methods are found with a CFL coefficient equal to one, for fourth order we simply give the best method we can find. A TVD third order low storage Runge-Kutta method is found, which uses only two storage units per equation and has a CFL coefficient equal to 0.32. Finally, we prove that general four stage fourth order Runge-Kutta methods cannot be TVD without introducing an adjoint operator $\tilde{L}$.

Appendix

In this appendix we prove Proposition 3.2 and Proposition 3.3.

We write the general 4 stage, 4th order Runge-Kutta method in the following standard form [9]:

$$
\begin{aligned}
u^{(1)} &= u^n + c_{10}L(u^n), \\
u^{(2)} &= u^n + c_{20}\Delta t L(u^n) + c_{21}\Delta t L(u^{(1)}), \\
u^{(3)} &= u^n + c_{30}\Delta t L(u^n) + c_{31}\Delta t L(u^{(1)}) + c_{32}\Delta t L(u^{(2)}), \\
u^{n+1} &= u^n + c_{40}\Delta t L(u^n) + c_{41}\Delta t L(u^{(1)}) + c_{42}\Delta t L(u^{(2)}) + c_{43}\Delta t L(u^{(3)}).
\end{aligned}
\tag{5.1}
$$

The relationship between the coefficients c_{ik} here and α_{ik} and β_{ik} in (1.8) is:

$$
\begin{aligned}
c_{10} &= \beta_{10}, \\
c_{20} &= \beta_{20} + \alpha_{21}\beta_{10}, \\
c_{21} &= \beta_{21}, \\
c_{30} &= \alpha_{32}\alpha_{21}\beta_{10} + \alpha_{31}\beta_{10} + \alpha_{32}\beta_{20} + \beta_{30}, \\
c_{31} &= \alpha_{32}\beta_{21} + \beta_{31}, \\
c_{32} &= \beta_{32}, \\
c_{40} &= \alpha_{43}\alpha_{32}\alpha_{21}\beta_{10} + \alpha_{43}\alpha_{32}\beta_{20} + \alpha_{43}\alpha_{31}\beta_{10} + \alpha_{42}\alpha_{21}\beta_{10}, \\
&\quad + \alpha_{41}\beta_{10} + \alpha_{42}\beta_{20} + \alpha_{43}\beta_{30} + \beta_{40}, \\
c_{41} &= \alpha_{43}\alpha_{32}\beta_{21} + \alpha_{42}\beta_{21} + \alpha_{43}\beta_{31} + \beta_{41}, \\
c_{42} &= \alpha_{43}\beta_{32} + \beta_{42}, \\
c_{43} &= \beta_{43}.
\end{aligned}
\tag{5.2}
$$

For a third order Runge-Kutta method, the general form (5.1) is similar without the last line (and with $u^{(3)}$ replaced by u^{n+1}). The relationship (5.2) also is similar without the last four lines for c_{40}, c_{41}, c_{42} and c_{43}.

Proof of Proposition 3.2. The general third order, three stage Runge-Kutta method in the form (5.1) is given by a two parameter family as well as by two special cases of one parameter families [9].

- **General Case:** If $\alpha_3 \neq \alpha_2$, $\alpha_3 \neq 0$, $\alpha_2 \neq 0$ and $\alpha_2 \neq \frac{2}{3}$:

$$
\begin{aligned}
c_{10} &= \alpha_2, \\
c_{20} &= \frac{3\alpha_2\alpha_3(1-\alpha_2) - \alpha_3^2}{\alpha_2(2-3\alpha_2)}, \\
c_{21} &= \frac{\alpha_3(\alpha_3-\alpha_2)}{\alpha_2(2-3\alpha_2)}, \\
c_{30} &= 1 + \frac{2-3(\alpha_2+\alpha_3)}{6\alpha_2\alpha_3}, \\
c_{31} &= \frac{3\alpha_3 - 2}{6\alpha_2(\alpha_3-\alpha_2)}, \\
c_{32} &= \frac{2-3\alpha_2}{6\alpha_3(\alpha_3-\alpha_2)}.
\end{aligned}
$$

Notice that $6\alpha_2 c_{21} c_{32} = 1$ and $c_{20} + c_{21} = \alpha_3$. If we want to have a CFL coefficient $c > 1$ in (1.9), we would need $\alpha_{ik} > \beta_{ik} \geq 0$ unless both of them are zeroes. This also implies that $c_{ik} \geq 0$ by (5.2). Also, notice that $c_{i,i-1} = \beta_{i,i-1} > 0$, for otherwise that stage is not necessary.

Now, $c_{10} = \beta_{10} < \alpha_{10} = 1$ and $c_{10} > 0$ imply $0 < \alpha_2 < 1$.

1. $\alpha_3 > \alpha_2$.
   $c_{21} \geq 0$ implies $\alpha_2 < \frac{2}{3}$, and $c_{31} \geq 0$ requires $\alpha_3 \geq \frac{2}{3}$.
   $\beta_{20} \geq 0$ and $\alpha_{21} > \beta_{21}$ imply $c_{20} \geq \alpha_{21}\beta_{10} > \beta_{21}\beta_{10}$, which is $\alpha_3 - c_{21} > c_{21}\alpha_2$, or $\frac{\alpha_3}{1+\alpha_2} > c_{21}$. So we must have
   $$\alpha_3 < \frac{3\alpha_2 - 2\alpha_2^2}{1+\alpha_2}.$$
   On the other hand, $\beta_{31} \geq 0$ requires $c_{31} \geq \alpha_{32}\beta_{21} > c_{32}c_{21} = \frac{1}{6\alpha_2}$, which is $3\alpha_3 - 2 > \alpha_3 - \alpha_2$, or
   $$\alpha_3 > 1 - \frac{1}{2}\alpha_2.$$
   Combining these two inequalities, we get $1 - \frac{1}{2}\alpha_2 < \frac{3\alpha_2 - 2\alpha_2^2}{1+\alpha_2}$, or $(2 - 3\alpha_2)(1 - \alpha_2) < 0$, which is a contradiction, since $2 - 3\alpha_2 > 0$ and $1 - \alpha_2 > 0$.
2. $\alpha_2 > \alpha_3$.
   $\alpha_3 = c_{20} + c_{21} > 0$ requires $\alpha_3 > 0$.
   $c_{32} > 0$ requires $\alpha_2 > \frac{2}{3}$, and $c_{31} \geq 0$ requires $\alpha_3 \leq \frac{2}{3}$.
   $c_{31} \geq \alpha_{32}\beta_{21} > c_{32}c_{21} = \frac{1}{6\alpha_2}$, which is
   $$\alpha_3 < 1 - \frac{1}{2}\alpha_2,$$
   $c_{20} \geq \alpha_{21}\beta_{10} > \beta_{21}\beta_{10}$ requires
   $$\alpha_3 > \frac{\alpha_2(3 - 2\alpha_2)}{1+\alpha_2}.$$
   Putting these two inequalities together, we have $\frac{\alpha_2(3-2\alpha_2)}{1+\alpha_2} < 1 - \frac{1}{2}\alpha_2$, which means $(2 - 3\alpha_2)(1 - \alpha_2) > 0$, a contradiction since $1 - \alpha_2 > 0$ and $2 - 3\alpha_2 < 0$.

- **Special Case I**: $\alpha_2 = \alpha_3 = \frac{2}{3}$. In this case
$$\begin{aligned}
c_{10} &= \frac{2}{3}, \\
c_{20} &= \frac{2}{3} - \frac{1}{4\omega_3}, \\
c_{21} &= \frac{1}{4\omega_3}, \\
c_{30} &= \frac{1}{4}, \\
c_{31} &= \frac{3}{4} - \omega_3, \\
c_{32} &= \omega_3.
\end{aligned}$$

$\beta_{31} \geq 0$ and $\alpha_{32} > \beta_{32} = c_{32}$ requires $c_{31} \geq \alpha_{32}\beta_{21} > c_{32}\beta_{21} = \frac{1}{4}$ which implies $\omega_3 < \frac{1}{2}$.

$\beta_{20} \geq 0$ and $\alpha_{21} > \beta_{21} = c_{21}$ requires $c_{20} \geq \alpha_{21}\beta_{10} > \frac{2}{3}c_{21}$, which means $\frac{2}{3} - \frac{1}{4\omega_3} > \frac{2}{3}\frac{1}{4\omega_3}$, for which we must have $\omega_3 > \frac{5}{8}$. A contradiction.

- **Special Case II**: $\alpha_3 = 0$. In this case the equations read

$$\begin{aligned} c_{10} &= \frac{2}{3}, \\ c_{20} &= \frac{1}{4\omega_3}, \\ c_{21} &= -\frac{1}{4\omega_3}, \\ c_{30} &= \frac{1}{4} - \omega_3, \\ c_{31} &= \frac{3}{4}, \\ c_{32} &= \omega_3. \end{aligned}$$

  Clearly c_{20} and c_{21} cannot be simultaneously nonnegative.
- **Special Case III**: $\alpha_2 = 0$. In this case the method is not third order. □

Proof of Proposition 3.3. Recall that all the α_{ik}'s must be nonnegative to satisfy our TVD criteria. From the relationship (5.2) between the coefficients of (5.1) and of (1.8), we can see that nonnegative β_{ik}'s imply nonnegative c_{ik}'s. We now show that we cannot have all nonnegative c_{ik}'s.

- **General Case**. If two parameters α_2 and α_3 are such that: $\alpha_2 \neq \alpha_3$, $\alpha_2 \neq 1$, $\alpha_2 \neq 0$, $\alpha_2 \neq \frac{1}{2}$, $\alpha_3 \neq 1$, $\alpha_3 \neq 0$, $\alpha_3 \neq \frac{1}{2}$, and $6\alpha_2\alpha_3 - 4(\alpha_2+\alpha_3) + 3 \neq 0$. Then the coefficients c_{ik} are [9]:
  $c_{10} = \alpha_2$, $c_{20} = \alpha_3 - c_{21}$, $c_{21} = \frac{\alpha_3(\alpha_3-\alpha_2)}{2\alpha_2(1-2\alpha_2)}$,
  $c_{30} = 1 - c_{31} - c_{32}$, $c_{31} = \frac{(1-\alpha_2)[\alpha_2+\alpha_3-1-(2\alpha_3-1)^2]}{2\alpha_2(\alpha_3-\alpha_2)[6\alpha_2\alpha_3-4(\alpha_2+\alpha_3)+3]}$,
  $c_{32} = \frac{(1-2\alpha_2)(1-\alpha_2)(1-\alpha_3)}{\alpha_3(\alpha_3-\alpha_2)[6\alpha_2\alpha_3-4(\alpha_2+\alpha_3)+3]}$,
  $c_{40} = \frac{1}{2} + \frac{1-2(\alpha_2+\alpha_3)}{12\alpha_2\alpha_3}$, $c_{41} = \frac{2\alpha_3-1}{12\alpha_2(\alpha_3-\alpha_2)(1-\alpha_2)}$, $c_{42} = \frac{(1-2\alpha_2)}{12\alpha_3(\alpha_3-\alpha_2)(1-\alpha_3)}$,
  $c_{43} = \frac{1}{2} + \frac{2(\alpha_2+\alpha_3)-3}{12(1-\alpha_2)(1-\alpha_3)}$.
  There are five possibilities to consider:
  1. $\alpha_2 < 0$ implies $c_{10} < 0$.
  2. $\alpha_3 > \alpha_2 > 0$ and $0 < \alpha_2 < \frac{1}{2}$:
     $c_{41} \geq 0$ requires $\alpha_3 > \frac{1}{2}$. $c_{20} \geq 0$ requires $\alpha_3 \leq 3\alpha_2 - 4\alpha_2^2 \leq \frac{9}{16}$. $c_{32} \geq 0$ and $c_{31} \geq 0$ require that $\alpha_2 \geq 2 - 5\alpha_3 + 4\alpha_3^2$. Since this is a decreasing function of α_3 when $\alpha_3 \leq \frac{9}{16}$, we obtain $\alpha_2 \geq 2 - 5(3\alpha_2 - 4\alpha_2^2) + 4(3\alpha_2 - 4\alpha_2^2)^2$. Rearranging, we find that $0 \geq 2((2\alpha_2-1)^2 + 4\alpha_2^2)\cdot(2\alpha_2-1)^2$, which is impossible.
  3. $\alpha_3 < \alpha_2$ and $\alpha_2 > \frac{1}{2}$:
     $c_{42} \geq 0$ requires $0 < \alpha_3 < 1$.
     We can only have $c_{32} \geq 0$ in one of two ways:
     (a) If $1 - \alpha_2 > 0$, and $6\alpha_2\alpha_3 - 4(\alpha_2+\alpha_3) + 3 > 0$.
     $c_{41} \geq 0$ requires $\alpha_3 < \frac{1}{2}$. Simple calculation yields $c_{30} = 1 - c_{31} - c_{32} = \frac{(2-6\alpha_2+4\alpha_2^2)+(-5+15\alpha_2-12\alpha_2^2)\alpha_3+(4-12\alpha_2+12\alpha_2^2)\alpha_3^2}{2\alpha_2\alpha_3(6\alpha_2\alpha_3-4(\alpha_2+\alpha_3)+3)}$, hence $c_{30} \geq 0$ requires

$$A + B\alpha_3 + C\alpha_3^2 \equiv (2-6\alpha_2+4\alpha_2^2) + (-5+15\alpha_2-12\alpha_2^2)\alpha_3 + (4-12\alpha_2+12\alpha_2^2)\alpha_3^2 \geq 0.$$

It is easy to show that, when $\frac{1}{2} < \alpha_2 < 1$, we have $A < 0$, $B < 0$ and $C > 0$. Thus, for $0 < \alpha_3 < \frac{1}{2}$, we have

$$A + B\alpha_3 + C\alpha_3^2 < \max\left(A, A + \frac{1}{2}B + \frac{1}{4}C\right) = \max\left(A, \frac{1}{2}(1-2\alpha_2)(1-\alpha_2)\right) < 0,$$

which is a contradiction.

(b) $\alpha_2 > 1$, and $6\alpha_2\alpha_3 - 4(\alpha_2+\alpha_3) + 3 < 0$.
$c_{31} \ge 0$ requires $\alpha_2 + \alpha_3 - 1 - (2\alpha_3 - 1)^2 \le 0$, which implies

$$(1-4\alpha_3)(1-\alpha_3) = 4\alpha_3^2 - 5\alpha_3 + 1 \ge \alpha_2 - 1 > 0.$$

Clearly, this is true only if $\alpha_3 < \frac{1}{4}$.
Now, $c_{40} \ge 0$ requires that $0 \le 6\alpha_2\alpha_3 - 2(\alpha_2+\alpha_3) + 1 = 2\alpha_3(3\alpha_2 - 1) + (1-2\alpha_2) \le \frac{1}{2}(3\alpha_2 - 1) + (1-2\alpha_2) = \frac{1}{2}(1-\alpha_2)$, an apparent contradiction.

4. $0 < \alpha_2 < \frac{1}{2}$ and $\alpha_3 < \alpha_2$: in this case we can see immediately that $c_{42} < 0$.
5. If $\frac{1}{2} < \alpha_2 < \alpha_3$, $c_{21} < 0$.

- If $6\alpha_2\alpha_3 - 4(\alpha_2+\alpha_3) + 3 = 0$, or if $\alpha_2 = 0$ or if $\alpha_3 = 1$, then this method is not fourth order [9].
- **Special Case I**. If $\alpha_2 = \alpha_3$ the method can be fourth order only if $\alpha_2 = \alpha_3 = \frac{1}{2}$. In this case [9] $c_{10} = \frac{1}{2}$, $c_{20} = \frac{1}{2} - \frac{1}{6w_3}$, $c_{21} = \frac{1}{6w_3}$, $c_{30} = 0$, $c_{31} = 1 - 3w_3$, $c_{32} = 3w_3$, $c_{40} = \frac{1}{6}$, $c_{41} = \frac{2}{3} - w_3$, $c_{42} = w_3$, $c_{43} = \frac{1}{6}$.

  Clearly we need to have $c_{42} = w_3 \ge 0$. To have $c_{31} = 1 - 3w_3 \ge 0$ and $c_{20} = \frac{1}{2} - \frac{1}{6w_3} \ge 0$, we require $w_3 = \frac{1}{3}$. This leads to the classical fourth order Runge-Kutta method. Clearly, then, $\alpha_{21} = \frac{c_{20} - \beta_{20}}{\beta_{10}} = -2\beta_{20}$. This is only acceptable if $\alpha_{21} = \beta_{20} = 0$. But $\beta_{21} = \frac{1}{2}$, so in the case where all β_{ik}'s are nonnegative, the CFL coefficient (1.12) is equal to zero.
- **Special Case II**. If $\alpha_2 = 1$, the method can be fourth order only if $\alpha_3 = \frac{1}{2}$. Then [9] $c_{10} = 1$, $c_{20} = \frac{3}{8}$, $c_{21} = \frac{1}{8}$, $c_{30} = 1 - c_{31} - c_{32}$, $c_{31} = -\frac{1}{12w_4}$, $c_{32} = \frac{1}{3w_4}$, $c_{40} = \frac{1}{6}$, $c_{41} = \frac{1}{6} - w_4$, $c_{42} = \frac{2}{3}$, $c_{43} = w_4$.

  In this case we want $c_{31} = -\frac{1}{12w_4} \ge 0$ which means $w_4 < 0$. But then $c_{43} = w_4 < 0$. So this case does not allow all nonnegative β_{ik}'s.
- **Special Case III**. If $\alpha_3 = 0$ the method can be fourth order only if $\alpha_2 = \frac{1}{2}$. Then [9] $c_{10} = \frac{1}{2}$, $c_{20} = -\frac{1}{12w_3}$, $c_{21} = \frac{1}{12w_3}$, $c_{30} = 1 - c_{31} - c_{32}$, $c_{31} = \frac{3}{2}$, $c_{32} = 6w_3$, $c_{40} = \frac{1}{6} - w_3$, $c_{41} = \frac{2}{3}$, $c_{42} = w_3$, $c_{43} = \frac{1}{6}$.

  Clearly, $c_{20} = -\frac{1}{12w_3} = -c_{21}$, one of these must be negative. Thus, this case does not allow all nonnegative β_{ik}'s, either. □

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