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Sigal Gottlieb
Chi-Wang Shu
Eitan Tadmor

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Department of Mathematics
University of California, Los Angeles
Los Angeles, CA. 90095-1555

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Sigal Gottlieb* Chi-Wang Shu† and Eitan Tadmor‡

ABSTRACT

In this paper we review and further develop a class of high order time discretizations for semi-discrete methods, so called methods of lines for the approximate solution of partial differential equations. Termed TVD (Total Variation Diminishing) time discretizations before, this class of high order time discretization methods preserves the strong stability properties of first order Euler time stepping and has proved very useful especially in solving hyperbolic partial differential equations. The new developments in this paper include the construction of optimal explicit Strong Stability Preserving (SSP) linear Runge-Kutta methods, their application to the question of strong stability of coercive approximations, a systematic study of explicit SSP multi-step methods for nonlinear problems, and the study of the SSP property of implicit Runge-Kutta and multi-step methods.

Key Words: Strong stability preserving, Runge-Kutta methods, multi-step methods, high order accuracy, time discretization

AMS(MOS) subject classification: 65M20, 65L06

*Department of Mathematics, University of Massachusetts, Dartmouth, Massachusetts 02747 and Division of Applied Mathematics, Brown University, Providence, Rhode Island 02912. E-mail: sgottlieb@umassd.edu. Research supported by ARO grant DAAG55-97-1-0318 and NSF grant ECS-9627849.

†Division of Applied Mathematics, Brown University, Providence, Rhode Island 02912. E-mail: shu@cfm.brown.edu. Research supported by ARO grant DAAG55-97-1-0318, NSF grants DMS-9804985, ECS-9906606 and INT-9601084, NASA Langley grant NAG-1-2070 and Contract NAS1-97046 while this author was in residence at ICASE, NASA Langley Research Center, Hampton, VA 23681-2199, and AFOSR grant F49620-99-1-0077.

‡Department of Mathematics, University of California Los Angeles, Los Angeles, California 90095. E-mail: tadmor@math.ucla.edu. Research supported by NSF Grant No. DMS97-06827 and ONR Grant No. N00014-1-J-1076.

Contents

1 Introduction

It is a common practice in solving time dependent Partial Differential Equations (PDEs) to first discretize the spatial variables to obtain a semi-discrete method of lines scheme. This is then an Ordinary Differential Equation (ODE) system in the time variable which can be discretized by an ODE solver. A relevant question here is stability. For problems with smooth solutions, usually a linear stability analysis is adequate. For problems with discontinuous solutions, however, such as solutions to hyperbolic problems, a stronger measure of stability is usually required.

In this paper we review and further develop a class of high order, Strong Stability Preserving (SSP) time discretization methods for the semi-discrete method of lines approximations of PDEs. This class of time discretization methods was first developed in [19] and [18] and was termed TVD (Total Variation Diminishing) time discretizations. It was further developed in [6]. The idea is to *assume* that the first order forward Euler time discretization of the method of lines ODE is strongly stable under a certain norm, when the time step Δt is suitably restricted, and then try to find a higher order time discretization (Runge-Kutta or multi-step) that preservers strong stability for the same norm, perhaps under a different time step restriction. In [19] and [18], the relevant norm was the total variation norm: the

Euler forward time discretization of the method of lines ODE was assumed TVD, hence the class of high order time discretization developed there was termed TVD time discretizations. This terminology was kept also in [6]. In fact, the essence of this class of high order time discretizations lies in its ability to preserve the strong stability in the same norm as the first order forward Euler version, hence "strong stability preserving", or SSP, time discretization is a more suitable term which will be used in this paper.

We begin this paper by discussing explicit SSP methods. We first give, in §2, a brief introduction for the setup and basic properties of these methods. We then move in §3, to our new results on optimal SSP Runge-Kutta methods of arbitrary order of accuracy for *linear* ODEs suitable for solving PDEs with linear spatial discretizations. This is used to prove strong stability for a class of well posed problems $u_t = L(u)$ where the operator L is linear and coercive, improving and simplifying the proofs for the results in [13]. We review and further develop the results in [19], [18] and [6] for nonlinear SSP Runge-Kutta methods in §4 and multi-step methods in §5. Section 6 of this paper contains our new results on implicit SSP schemes. It starts with a numerical example showing the necessity of preserving the strong stability property of the method, then it moves on to the analysis of the rather disappointing negative results about the non-existence of SSP implicit Runge-Kutta or multi-step methods of order higher than one. Concluding remarks are given in §7.

2 Explicit SSP methods

2.1 Why SSP methods?

Explicit SSP methods were developed in [19] and [18] (termed TVD time discretizations there) to solve systems of ODEs

$$\frac{d}{dt}u = L(u), \tag{2.1}$$

resulting from a method of lines approximation of the hyperbolic conservation law,

$$u_t = -f(u)_x, \tag{2.2}$$

where the spatial derivative, $f(u)_x$, is discretized by a TVD finite difference or finite element approximation, e.g. [8], [16], [20], [2], [9]; consult [21] for a recent overview. Denoted by $-L(u)$, it is assumed that the spatial discretization has the property that when it is combined with the first order forward Euler time discretization,

$$u^{n+1} = u^n + \Delta t L(u^n), \tag{2.3}$$

then, for a sufficiently small time step dictated by the CFL condition,

$$\Delta t \leq \Delta t_{FE}, \tag{2.4}$$

the Total Variation (TV) of the one-dimensional discrete solution $u^n := \sum_j u_j^n 1_{\{x_{j-\frac{1}{2}} \leq x \leq x_{j+\frac{1}{2}}\}}$ does not increase in time, i.e., the following, so called TVD property, holds

$$TV(u^{n+1}) \leq TV(u^n), \qquad TV(u^n) := \sum_j |u_{j+1}^n - u_j^n|. \tag{2.5}$$

The objective of the high order Strong Stability Preserving (SSP) Runge-Kutta or multistep time discretization, is to preserve the strong stability property (2.5) while achieving higher order accuracy in time, perhaps with a modified CFL restriction (measured here with a CFL coefficient, c)

$$\Delta t \leq c\,\Delta t_{FE}. \tag{2.6}$$

In [6] we gave numerical evidence to show that oscillations may occur when using a linearly stable, high-order method which lacks the strong stability property, even if the same spatial discretization is TVD when combined with the first-order forward Euler time-discretization. The example is illustrative so we reproduce it here. We consider a scalar conservation law, the familiar Burgers' equation

$$u_t + \left(\frac{1}{2}u^2\right)_x = 0 \tag{2.7}$$

with a Riemann initial data:

$$u(x,0) = \begin{cases} 1, & \text{if } x \leq 0 \\ -0.5, & \text{if } x > 0. \end{cases} \tag{2.8}$$

The spatial discretization is obtained by a second order MUSCL [12], which is TVD for forward Euler time discretization under suitable CFL restriction.

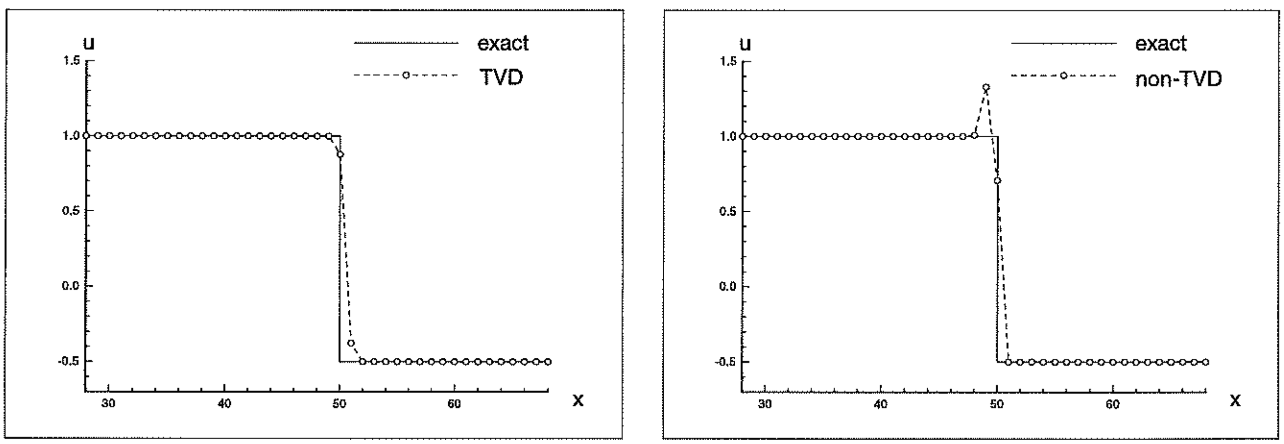

Figure 2.1: Second order TVD MUSCL spatial discretization. Solution after the shock moves 50 mesh points. Left: SSP time discretization; Right: non SSP time discretization.

In Fig. 2.1, we show the result of using a SSP second order Runge-Kutta method for the time discretization (left), and that of using a non SSP second order Runge-Kutta method (right). We can clearly see that the non SSP result is oscillatory (there is an overshoot).

This simple numerical example illustrates that it is safer to use a SSP time discretization for solving hyperbolic problems. After all, they do not increase the computational cost and have the extra assurance of provable stability.

As we have already mentioned above, the high-order SSP methods discussed here are not restricted to preserving (or non increasing of –) the total variation. Our arguments below rely on convexity, hence these properties hold for *any* norm. Consequently, SSP methods have a wide range of applicability, as they can be used to ensure stability in an arbitrary norm, once the forward Euler time discretization is shown to be strongly stable*, i.e., $\|u^n + \Delta t L(u^n)\| \leq \|u^n\|$. For linear examples we refer to [7], where weighted L^2-strong stability is preserved for higher order discretizations of spectral schemes are discussed. For nonlinear scalar conservation laws in several space dimensions, the TVD property is ruled out for high resolution schemes; instead, strong stability in the maximum norm is sought. Applications of L^∞-SSP higher-order discretization can be found in [3],[9] for discontinuous Galerkin and central schemes. Finally, we note that since our arguments below are based on convex decompositions of high-order methods in terms of the first-order Euler method, any convex function will be preserved by such high-order time discretizations. In this context we refer, for example, to the cell entropy stability property of high order schemes studied in [17],[15].

2.2 SSP Runge-Kutta methods

In [19], a general m stage Runge-Kutta method for (2.1) is written in the form:

$$\begin{aligned} u^{(0)} &= u^n, \\ u^{(i)} &= \sum_{k=0}^{i-1} \left(\alpha_{i,k} u^{(k)} + \Delta t \beta_{i,k} L(u^{(k)}) \right), \quad \alpha_{i,k} \geq 0, \qquad i = 1, ..., m \\ u^{n+1} &= u^{(m)}. \end{aligned} \tag{2.9}$$

Clearly, if all the $\beta_{i,k}$'s are nonnegative, $\beta_{i,k} \geq 0$, then since by consistency $\sum_{k=0}^{i-1} \alpha_{i,k} = 1$, it follows that the intermediate stages in (2.9), $u^{(i)}$, amount to convex combinations of forward Euler operators, with Δt replaced by $\frac{\beta_{i,k}}{\alpha_{i,k}} \Delta t$, We thus conclude

Lemma 2.1 *[19]. If the forward Euler method (2.3) is strongly stable under the CFL restriction (2.4), $\|u^n + \Delta t L(u^n)\| \leq \|u^n\|$, then the Runge-Kutta method (2.9) with $\beta_{i,k} \geq 0$ is SSP, $\|u^{n+1}\| \leq \|u^n\|$, provided the following CFL restriction (2.6) is fulfilled,*

$$\Delta t \leq c \Delta t_{FE}, \quad c = \min_{i,k} \frac{\alpha_{i,k}}{\beta_{i,k}}. \tag{2.10}$$

If some of the $\beta_{i,k}$'s are negative, we need to introduce an associated operator $\tilde{L}$ corresponding to stepping *backward* in time. The requirement for $\tilde{L}$ is that it approximates the same spatial derivative(s) as L, but that the strong stability property holds $\|u^{n+1}\| \leq \|u^n\|$, (– either with respect to the TV or another relevant norm), for first order Euler scheme, solved backward in time, i.e.,

$$u^{n+1} = u^n - \Delta t \tilde{L}(u^n) \tag{2.11}$$

This can be achieved for hyperbolic conservation laws, for example, by solving the backward in time version of (2.2),

$$u_t = f(u)_x. \tag{2.12}$$

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.

*By the notion of strong stability we refer to the fact that there is no temporal growth, as opposed to the general notion of stability which allows a *bounded* temporal growth, $\|u^n\| \leq Const \cdot \|u^0\|$ with any arbitrary constant, possibly $Const > 1$.

Lemma 2.2 *[19]. If the forward Euler method combined with the spatial discretization L in (2.3) is strongly stable under the CFL restriction (2.4), $\|u^n + \Delta t L(u^n)\| \leq \|u^n\|$, and if Euler's method solved backward in time in combination with the spatial discretization $\tilde{L}$ in (2.11) is also strongly stable under the CFL restriction (2.4), $\|u^n - \Delta t \tilde{L}(u^n)\| \leq \|u^n\|$, then the Runge-Kutta method (2.9) is SSP, $\|u^{n+1}\| \leq \|u^n\|$, under the CFL restriction (2.6),*

$$\Delta t \leq c\Delta t_{FE}, \quad c = \min_{i,k} \frac{\alpha_{i,k}}{|\beta_{i,k}|}, \tag{2.13}$$

provided $\beta_{i,k}L$ is replaced by $\beta_{i,k}\tilde{L}$ whenever $\beta_{i,k}$ is negative.

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 $\beta_{i,k}$ as much as possible. However, as shown in [6] it is not always possible to avoid negative $\beta_{i,k}$.

2.3 SSP multi step methods

SSP multi-step methods of the form:

$$u^{n+1} = \sum_{i=1}^{m} \left(\alpha_i u^{n+1-i} + \Delta t \beta_i L(u^{n+1-i}) \right), \qquad \alpha_i \geq 0, \tag{2.14}$$

were studied in [18]. Since $\sum \alpha_i = 1$, it follows that u^{n+1} is given by a convex combination of forward Euler solvers with suitably scaled Δt's, and hence, similar to our discussion for Runge-Kutta methods we arrive at the following lemma.

Lemma 2.3 *[18]. If the forward Euler method combined with the spatial discretization L in (2.3) is strongly stable under the CFL restriction (2.4), $\|u^n + \Delta t L(u^n)\| \leq \|u^n\|$, and if Euler's method solved backward in time in combination with the spatial discretization $\tilde{L}$ in (2.11) is also strongly stable under the CFL restriction (2.4), $\|u^n - \Delta t \tilde{L}(u^n)\| \leq \|u^n\|$, then the multi-step method (2.14) is SSP $\|u^{n+1}\| \leq \|u^n\|$, under the CFL restriction (2.6),*

$$\Delta t \leq c\Delta t_{FE}, \quad c = \min_{i} \frac{\alpha_i}{|\beta_i|}, \tag{2.15}$$

provided $\beta_i L(\cdot)$ is replaced by $\beta_i \tilde{L}(\cdot)$ whenever β_i is negative.

3 Linear SSP Runge-Kutta methods of arbitrary order

3.1 SSP Runge-Kutta methods with optimal CFL condition

In this section we present a class of optimal (in the sense of CFL number) SSP Runge-Kutta methods of any order for the ODE (2.1) where L is *linear*. With a linear L being realized as finite dimensional matrix we denote, $L(u) = Lu$. We will first show that the m-stage, m-th order SSP Runge-Kutta method can have, at most, CFL coefficient $c = 1$ in (2.10). We then proceed to construct optimal SSP linear Runge-Kutta methods.

Proposition 3.1 *Consider the family of m-stage, m-th order SSP Runge-Kutta methods (2.9) with nonnegative coefficients $\alpha_{i,k}$ and $\beta_{i,k}$. The maximum CFL restriction attainable for such methods is the one dictated by the forward Euler scheme,*

$$\Delta t \leq \Delta t_{FE}$$

i.e., (2.6) holds with maximal CFL coefficient $c = 1$.

Proof. We consider the special case where L is linear, and prove that even in this special case the maximum CFL coefficient c attainable is 1. Any m-stage method (2.9), for this linear case, can be rewritten as:

$$u^{(i)} = \left(1 + \sum_{k=0}^{i-1} A_{i,k}(\Delta t L)^{k+1}\right) u^{(0)}, \qquad i = 1, ..., m.$$

where

$$A_{1,0} = \beta_{1,0}, \qquad A_{i,0} = \sum_{k=1}^{i-1} \alpha_{i,k} A_{k,0} + \sum_{k=0}^{i-1} \beta_{i,k},$$

$$A_{i,k} = \sum_{j=k+1}^{i-1} \alpha_{i,j} A_{j,k} + \sum_{j=k}^{i-1} \beta_{i,j} A_{j,k-1}, \qquad k = 1, ..., i-1.$$

In particular, using induction, it is easy to show that the last two terms of the final stage can be expanded as

$$\begin{aligned} A_{m,m-1} &= \prod_{l=1}^{m} \beta_{l,l-1} \\ A_{m,m-2} &= \sum_{k=2}^{m} \beta_{k,k-2} \left(\prod_{l=k+1}^{m} \beta_{l,l-1}\right)\left(\prod_{l=1}^{k-2} \beta_{l,l-1}\right) + \sum_{k=1}^{m} \alpha_{k,k-1} \left(\prod_{l=1, l\neq k}^{m} \beta_{l,l-1}\right). \end{aligned}$$

For a m-stage, m-th order linear Runge-Kutta scheme $A_{m,k} = \frac{1}{(k+1)!}$. Using $A_{m,m-1} = \prod_{l=1}^{m} \beta_{l,l-1} = \frac{1}{m!}$, we can rewrite

$$A_{m,m-2} = \sum_{k=1}^{m} \frac{\alpha_{k,k-1}}{m!\beta_{k,k-1}} + \sum_{k=2}^{m} \beta_{k,k-2} \left(\prod_{l=k+1}^{m} \beta_{l,l-1}\right)\left(\prod_{l=1}^{k-2} \beta_{l,l-1}\right).$$

With the non negative assumption on $\beta_{i,k}$'s and the fact $A_{m,m-1} = \prod_{l=1}^{m} \beta_{l,l-1} = \frac{1}{m!}$ we have $\beta_{l,l-1} > 0$ for all l. For the CFL coefficient $c \geq 1$ we must have $\frac{\alpha_{k,k-1}}{\beta_{k,k-1}} \geq 1$ for all k. Clearly, $A_{m,m-2} = \frac{1}{(m-1)!}$ is possible under these restrictions only if $\beta_{k,k-2} = 0$ and $\frac{\alpha_{k,k-1}}{\beta_{k,k-1}} = 1$ for all k, in which case the CFL coefficient $c \leq 1$. ∎

We remark that the conclusion of Proposition 3.1 is valid only if the m stage Runge-Kutta method is m-th order accurate. In [18], we constructed an m stage, first order SSP Runge-Kutta method with a CFL coefficient $c = m$ which is suitable for steady state calculations.

The proof above also suggests a construction for the optimal linear m stage, m-th order SSP Runge-Kutta methods.

Proposition 3.2 *The class of m stage schemes given (recursively) by:*

$$\begin{aligned} u^{(i)} &= u^{(i-1)} + \Delta t L u^{(i-1)}, \qquad i = 1, ..., m-1 \\ u^{(m)} &= \sum_{k=0}^{m-2} \alpha_{m,k} u^{(k)} + \alpha_{m,m-1} \left(u^{(m-1)} + \Delta t L u^{(m-1)} \right), \end{aligned} \tag{3.1}$$

where $\alpha_{1,0} = 1$ *and*

$$\begin{aligned} \alpha_{m,k} &= \frac{1}{k} \alpha_{m-1,k-1}, \qquad k = 1, ..., m-2 \\ \alpha_{m,m-1} &= \frac{1}{m!}, \qquad \alpha_{m,0} = 1 - \sum_{k=1}^{m-1} \alpha_{m,k} \end{aligned} \tag{3.2}$$

is an m-order linear Runge-Kutta method which is SSP with CFL coefficient $c = 1$,

$$\Delta t \leq \Delta t_{FE}.$$

Proof. The first order case is forward Euler, which is first order accurate, and SSP with CFL coefficient $c = 1$ by definition. The other schemes will be SSP with a CFL coefficient $c = 1$ by construction, as long as the coefficients are nonnegative.

We now show that scheme (3.1)-(3.2) is m-th order accurate when L is linear. In this case clearly

$$u^{(i)} = (1 + \Delta t L)^i u^{(0)} = \left(\sum_{k=0}^{i} \frac{i!}{k!(i-k)!} (\Delta t L)^k \right) u^{(0)}, \qquad i = 1, ..., m-1,$$

hence scheme (3.1)-(3.2) results in

$$u^{(m)} = \left(\sum_{j=0}^{m-2} \alpha_{m,j} \sum_{k=0}^{j} \frac{j!}{k!(j-k)!} (\Delta t L)^k + \alpha_{m,m-1} \sum_{k=0}^{m} \frac{m!}{k!(m-k)!} (\Delta t L)^k \right) u^{(0)}.$$

Clearly, by (3.2), the coefficient of $(\Delta t L)^{m-1}$ is $\alpha_{m,m-1} \frac{m!}{(m-1)!} = \frac{1}{(m-1)!}$, the coefficient of $(\Delta t L)^m$ is $\alpha_{m,m-1} = \frac{1}{m!}$, and the coefficient of $(\Delta t L)^0$ is

$$\frac{1}{m!} + \sum_{j=0}^{m-2} \alpha_{m,j} = 1.$$

It remains to show that, for $1 \leq k \leq m-2$, the coefficient of $(\Delta t L)^k$ is equal to $\frac{1}{k!}$:

$$\frac{1}{k!(m-k)!} + \sum_{j=k}^{m-2} \alpha_{m,j} \frac{j!}{k!(j-k)!} = \frac{1}{k!}. \tag{3.3}$$

This will be shown by induction. Thus we assume (3.3) is true for m, then for $m+1$ we have, for $0 \leq k \leq m-2$, the coefficient of $(\Delta t L)^{k+1}$ is equal to

$$\frac{1}{(k+1)!(m-k)!} + \sum_{j=k+1}^{m-1} \alpha_{m+1,j} \frac{j!}{(k+1)!(j-k-1)!}$$

$$
\begin{aligned}
&= \frac{1}{(k+1)!}\left(\frac{1}{(m-k)!} + \sum_{l=k}^{m-2} \alpha_{m+1,l+1}\frac{(l+1)!}{(l-k)!}\right) \\
&= \frac{1}{(k+1)!}\left(\frac{1}{(m-k)!} + \sum_{l=k}^{m-2} \frac{1}{(l+1)}\alpha_{m,l}\frac{(l+1)!}{(l-k)!}\right) \\
&= \frac{1}{(k+1)!}\left(\frac{1}{(m-k)!} + \sum_{l=k}^{m-2} \alpha_{m,l}\frac{l!}{(l-k)!}\right) \\
&= \frac{1}{(k+1)!}.
\end{aligned}
$$

where in the second equality we used (3.2) and in the last equality we used the induction hypothesis (3.3). This finishes the proof.

Finally, we show that all the α's are nonnegative. Clearly $\alpha_{2,0} = \alpha_{2,1} = \frac{1}{2} > 0$. If we assume $\alpha_{m,j} \geq 0$ for all $j = 0, ..., m-1$, then

$$
\alpha_{m+1,j} = \frac{1}{j}\alpha_{m,j-1} \geq 0, \qquad j = 1, ..., m-1; \qquad \alpha_{m+1,m} = \frac{1}{(m+1)!} \geq 0,
$$

and, by noticing that $\alpha_{m+1,j} \leq \alpha_{m,j-1}$ for all $j = 1, ..., m$, we have

$$
\alpha_{m+1,0} = 1 - \sum_{j=1}^{m} \alpha_{m+1,j} \geq 1 - \sum_{j=1}^{m} \alpha_{m,j-1} = 0. \blacksquare
$$

As the m stage, m-th order linear Runge-Kutta method is unique, we have in effect proved this unique m stage, m-th order linear Runge-Kutta method is SSP under CFL coefficient $c = 1$. If L is nonlinear, scheme (3.1)-(3.2) is still SSP under CFL coefficient $c = 1$, but it is no longer m-th order accurate. Notice that all but the last stage of these methods are simple forward Euler steps.

We note in passing the examples of the ubiquitous third- and forth-order Runge-Kutta methods, which admit the following convex – and hence SSP decompositions

$$
\sum_{k=0}^{3} \frac{1}{k!}(\Delta t L)^k = \frac{1}{3} + \frac{1}{2}(I + \Delta t L) + \frac{1}{6}(I + \Delta t L)^3 \tag{3.4}
$$

$$
\sum_{k=0}^{4} \frac{1}{k!}(\Delta t L)^k = \frac{3}{8} + \frac{1}{3}(I + \Delta t L) + \frac{1}{4}(I + \Delta t L)^2 + \frac{1}{24}(I + \Delta t L)^4 \tag{3.5}
$$

We list, in Table 3.1, the coefficients $\alpha_{m,j}$ of these optimal methods in (3.2) up to $m = 8$.

order m	$\alpha_{m,0}$	$\alpha_{m,1}$	$\alpha_{m,2}$	$\alpha_{m,3}$	$\alpha_{m,4}$	$\alpha_{m,5}$	$\alpha_{m,6}$	$\alpha_{m,7}$
1	1							
2	$\frac{1}{2}$	$\frac{1}{2}$						
3	$\frac{1}{3}$	$\frac{1}{2}$	$\frac{1}{6}$					
4	$\frac{3}{8}$	$\frac{1}{3}$	$\frac{1}{4}$	$\frac{1}{24}$				
5	$\frac{11}{30}$	$\frac{3}{8}$	$\frac{1}{6}$	$\frac{1}{12}$	$\frac{1}{120}$			
6	$\frac{53}{144}$	$\frac{11}{30}$	$\frac{3}{16}$	$\frac{1}{18}$	$\frac{1}{48}$	$\frac{1}{720}$		
7	$\frac{103}{280}$	$\frac{53}{144}$	$\frac{11}{60}$	$\frac{3}{48}$	$\frac{1}{72}$	$\frac{1}{240}$	$\frac{1}{5040}$	
8	$\frac{2119}{5760}$	$\frac{103}{280}$	$\frac{53}{288}$	$\frac{11}{180}$	$\frac{1}{64}$	$\frac{1}{360}$	$\frac{1}{1440}$	$\frac{1}{40320}$

Table 3.1: Coefficients $\alpha_{m,j}$ of the SSP methods (3.1)-(3.2)

3.2 Application to coercive approximations

We now apply the optimal linear SSP Runge-Kutta methods to coercive approximations. We consider the linear system of ODEs of the general form, with possibly variable, time-dependent coefficients,

$$\frac{d}{dt}u(t) = L(t)u(t). \tag{3.6}$$

As an example we refer to [7], where the far-from-normal character of the spectral differentiation matrices defies the straightforward von-Neumann stability analysis when augmented with high-order time discretizations.

We begin our stability study for Runge-Kutta approximations of (3.6) with the first-order forward-Euler scheme (with $\langle \cdot, \cdot \rangle$ denoting the usual Euclidean inner product)

$$u^{n+1} = u^n + \Delta t_n L(t^n) u^n,$$

based on variable time-steps, $t^n := \sum_{j=0}^{n-1} \Delta t_j$. Taking L^2 norms on both sides one finds

$$|u^{n+1}|^2 = |u^n|^2 + 2\Delta t_n Re\langle L(t^n)u^n, u^n\rangle + (\Delta t_n)^2 |L(t^n)u^n|^2,$$

and hence strong stability holds, $|u^{n+1}| \le |u^n|$, provided the following restriction on the time step, Δt_n, is met,

$$\Delta t_n \le -2Re\langle L(t^n)u^n, u^n\rangle / |L(t^n)u^n|^2.$$

Following Levy and Tadmor [13] we therefore make the

Assumption 3.1 *(Coercivity). The operator $L(t)$ is (uniformly) coercive in the sense that there exists $\eta(t) > 0$ such that*

$$\eta(t) := \inf_{|u|=1} -\frac{Re\langle L(t)u, u\rangle}{|L(t)u|^2} > 0. \tag{3.7}$$

We conclude that for coercive L's, the forward Euler scheme is strongly stable, $\|I + \Delta t_n L(t^n)\| \leq 1$, if and only if

$$\Delta t_n \leq 2\eta(t^n).$$

In a generic case, $L(t^n)$ represents a spatial operator with a coercivity-bound $\eta(t^n)$, which is proportional to some power of the smallest spatial scale. In this context the above restriction on the time-step amounts to the celebrated Courant-Friedrichs-Levy (CFL) stability condition. Our aim is to show that the general m stage, m-th order accurate Runge-Kutta scheme is strongly stable under the *same* CFL condition.

Remark. Observe that the coercivity constant, η, is an upper bound in the size of L; indeed, by Cauchy-Schwartz, $\eta(t) \leq |L(t)u| \cdot |u|/|L(t)u|^2$ and hence

$$\|L(t)\| = \sup_u \frac{|L(t)u|}{|u|} \leq \frac{1}{\eta(t)}. \tag{3.8}$$

To make one point we consider the fourth-order Runge-Kutta approximation of (3.6)

$$\begin{aligned}
k^1 &= L(t^n)u^n && (3.9)\\
k^2 &= L(t^{n+\frac{1}{2}})(u^n + \frac{\Delta t_n}{2}k^1) && (3.10)\\
k^3 &= L(t^{n+\frac{1}{2}})(u^n + \frac{\Delta t_n}{2}k^2) && (3.11)\\
k^4 &= L(t^{n+1})(u^n + \Delta t_n k^3) && (3.12)\\
u^{n+1} &= u^n + \frac{\Delta t_n}{6}\left[k^1 + 2k^2 + 2k^3 + k^4\right]. && (3.13)
\end{aligned}$$

Starting with second-order and higher the Runge-Kutta intermediate steps depend on the time variation of $L(\cdot)$, and hence we require a minimal smoothness in time, making

Assumption 3.2 *(Lipschitz regularity). We assume that $L(\cdot)$ is Lipschitz. Thus, there exists a constant $K > 0$ such that*

$$\|L(t) - L(s)\| \leq \frac{K}{\eta(t)}|t - s|. \tag{3.14}$$

We are now ready to make our main result, stating

Proposition 3.3 *Consider the coercive systems of ODEs, (3.6)-(3.7), with Lipschitz continuous coefficients (3.14). Then the fourth-order Runge-Kutta scheme (3.9-3.13) is stable under CFL condition,*

$$\Delta t_n \leq 2\eta(t^n), \tag{3.15}$$

and the following estimate holds

$$|u^n| \leq e^{3Kt_n}|u^0|. \tag{3.16}$$

Remark. The result along these lines was introduced by Levy and Tadmor [13, Main Theorem], stating the strong stability of the constant coefficients s-order Runge-Kutta scheme under CFL condition $\Delta t_n \leq C_s \eta(t^n)$. Here we improve in both simplicity and generality. Thus, for example, the previous bound of $C_4 = 1/31$ [13, Theorem 3.3] is now improved to a practical time-step restriction with our uniform $C_s = 2$.

Proof. We proceed in two steps. We first freeze the coefficients at $t = t^n$, considering (here we abbreviate $L^n = L(t^n)$)

$$j^1 = L^n u^n \tag{3.17}$$

$$j^2 = L^n(u^n + \frac{\Delta t_n}{2} j^1) \equiv L^n(I + \frac{\Delta t_n}{2} L^n) u^n \tag{3.18}$$

$$j^3 = L^n(u^n + \frac{\Delta t_n}{2} j^2) \equiv L^n \left[I + \frac{\Delta t_n}{2} L^n (I + \frac{\Delta t_n}{2} L^n) \right] u^n \tag{3.19}$$

$$j^4 = L^n(u^n + \Delta t_n j^3) \tag{3.20}$$

$$v^{n+1} = u^n + \frac{\Delta t_n}{6} \left[j^1 + 2j^2 + 2j^3 + j^4 \right]. \tag{3.21}$$

Thus, $v^{n+1} = P_4(\Delta t_n L^n) u^n$, where following (3.5)

$$P_4(\Delta t_n L^n) := \frac{3}{8} I + \frac{1}{3}(I + \Delta t L) + \frac{1}{4}(I + \Delta t L)^2 + \frac{1}{24}(I + \Delta t L)^4.$$

Since the CFL condition (3.15) implies the strong stability of forward-Euler, i.e. $\|I + \Delta t_n L^n\| \leq 1$, it follows that $\|P_4(\Delta t_n L^n)\| \leq 3/8 + 1/3 + 1/4 + 1/24 = 1$. Thus,

$$|v^{n+1}| \leq |u^n|. \tag{3.22}$$

Next, we turn to include the time dependence. We need to measure the difference between the exact and the 'frozen' intermediate values – the k's and the j's. We have

$$k^1 - j^1 = 0 \tag{3.23}$$

$$k^2 - j^2 = \left[L(t^{n+\frac{1}{2}}) - L(t^n) \right] (I + \frac{\Delta t_n}{2} L^n) u^n \tag{3.24}$$

$$k^3 - j^3 = L(t^{n+\frac{1}{2}}) \frac{\Delta t_n}{2} (k^2 - j^2) + \left[L(t^{n+\frac{1}{2}}) - L(t^n) \right] \frac{\Delta t_n}{2} j^2 \tag{3.25}$$

$$k^4 - j^4 = L(t^{n+1}) \Delta t_n (k^3 - j^3) + \left[L(t^{n+1}) - L(t^n) \right] \Delta t_n j^3. \tag{3.26}$$

Lipschitz continuity (3.14) and the strong stability of forward-Euler imply

$$|k^2 - j^2| \leq \frac{K \cdot \Delta t_n}{2\eta(t^n)} |u^n| \leq K |u^n|. \tag{3.27}$$

Also, since $\|L^n\| \leq \frac{1}{\eta(t^n)}$, we find from (3.18) that $|j^2| \leq |u^n|/\eta(t^n)$, and hence (3.25) followed by (3.27) and the CFL condition (3.15) imply

$$\begin{aligned} |k^3 - j^3| &\leq \frac{\Delta t_n}{2\eta(t^n)} |k^2 - j^2| + \frac{K \cdot \Delta t_n}{2\eta(t^n)} \cdot \frac{\Delta t_n}{2\eta(t^n)} |u^n| \leq \\ &\leq 2K \left(\frac{\Delta t_n}{2\eta(t^n)} \right)^2 |u^n| \leq 2K |u^n|. \end{aligned} \tag{3.28}$$

Finally, since by (3.19) j^3 does not exceed, $|j^3| < \frac{1}{\eta(t^n)}(1+\frac{\Delta t_n}{2\eta(t^n)})|u^n|$, we find from (3.26) followed by (3.28) and the CFL condition (3.15),

$$\begin{aligned}|k^4 - j^4| &\le \frac{\Delta t_n}{\eta(t^n)}|k^3 - j^3| + \frac{K\cdot\Delta t_n}{\eta(t^n)}\cdot\frac{\Delta t_n}{\eta(t^n)}\left(1+\frac{\Delta t_n}{2\eta(t^n)}\right)|u^n| \\ &\le K\left(\left(\frac{\Delta t_n}{\eta(t^n)}\right)^3 + \left(\frac{\Delta t_n}{\eta(t^n)}\right)^2\right)|u^n| \le 12K|u^n|.\end{aligned} \tag{3.29}$$

We conclude that u^{n+1},

$$u^{n+1} = v^{n+1} + \frac{\Delta t_n}{6}\left[2(k^2-j^2) + 2(k^3-j^3) + (k^4-j^4)\right],$$

is upper bounded by, consult, (3.22), (3.27)-(3.29),

$$\begin{aligned}|u^{n+1}| &\le |v^{n+1}| + \frac{\Delta t_n}{6}\left[2K|u^n| + 4K|u^n| + 12K|u^n|\right] \\ &\le (1+3K\Delta t_n)|u^n|\end{aligned}$$

and the result (3.16) follows. ■

4 Nonlinear SSP Runge-Kutta methods

In the previous section we derived SSP Runge-Kutta methods for linear spatial discretizations. As explained in the introduction, SSP methods are often required for nonlinear spatial discretizations. Thus, most of the research to date has been in the derivation of SSP methods for nonlinear spatial discretizations. In [19], schemes up to third order were found to satisfy the conditions in Lemma 2.1 with CFL coefficient $c = 1$. In [6] it was shown that all four stage, fourth order Runge-Kutta methods with positive CFL coefficient c in (2.13) must have at least one negative $\beta_{i,k}$, and a method which seems optimal was found. For large scale scientific computing in three space dimensions, storage is usually a paramount consideration. We review the results presented in [6] about strong stability preserving properties among such low storage Runge-Kutta methods.

4.1 Nonlinear methods of second, third and fourth order

Here we review the optimal (in the sense of CFL coefficient and the cost incurred by $\tilde{L}$ if it appears) SSP Runge-Kutta methods of m-stage, m-th order, for $m = 2, 3, 4$, written in the form (2.9).

Proposition 4.1 *[6]. If we require $\beta_{i,k} \ge 0$, then an optimal second order SSP Runge-Kutta method (2.9) is given by*

$$\begin{aligned}u^{(1)} &= u^n + \Delta t L(u^n) \\ u^{n+1} &= \frac{1}{2}u^n + \frac{1}{2}u^{(1)} + \frac{1}{2}\Delta t L(u^{(1)}),\end{aligned} \tag{4.1}$$

with a CFL coefficient $c = 1$ in (2.10). An optimal third order SSP Runge-Kutta method (2.9) is given by

$$\begin{aligned} u^{(1)} &= u^n + \Delta t L(u^n) \\ u^{(2)} &= \frac{3}{4}u^n + \frac{1}{4}u^{(1)} + \frac{1}{4}\Delta t L(u^{(1)}) \\ u^{n+1} &= \frac{1}{3}u^n + \frac{2}{3}u^{(2)} + \frac{2}{3}\Delta t L(u^{(2)}), \end{aligned} \tag{4.2}$$

with a CFL coefficient $c = 1$ in (2.10).

In the fourth order case we proved in [6] that we cannot avoid the appearance of negative $\beta_{i,k}$:

Proposition 4.2 *[6]. The four stage, fourth order SSP Runge Kutta scheme (2.9) with a nonzero CFL coefficient c in (2.13) must have at least one negative $\beta_{i,k}$.*

We thus must settle for finding an efficient fourth order scheme containing $\tilde{L}$, which maximizes the operation cost measured by $\frac{c}{4+i}$, where c is the CFL coefficient (2.13) and i is the number of $\tilde{L}$s. This way we are looking for a SSP method which reaches a fixed time T with a minimal number of evaluations of L or $\tilde{L}$. The best method we could find in [6] is:

$$\begin{aligned} u^{(1)} &= u^n + \frac{1}{2}\Delta t L(u^n) \\ u^{(2)} &= \frac{649}{1600}u^{(0)} - \frac{10890423}{25193600}\Delta t \tilde{L}(u^n) + \frac{951}{1600}u^{(1)} + \frac{5000}{7873}\Delta t L(u^{(1)}) \\ u^{(3)} &= \frac{53989}{2500000}u^n - \frac{102261}{5000000}\Delta t \tilde{L}(u^n) + \frac{4806213}{20000000}u^{(1)} \\ &\quad -\frac{5121}{20000}\Delta t \tilde{L}(u^{(1)}) + \frac{23619}{32000}u^{(2)} + \frac{7873}{10000}\Delta t L(u^{(2)}) \\ u^{n+1} &= \frac{1}{5}u^n + \frac{1}{10}\Delta t L(u^n) + \frac{6127}{30000}u^{(1)} + \frac{1}{6}\Delta t L(u^{(1)}) + \frac{7873}{30000}u^{(2)} + \frac{1}{3}u^{(3)} + \frac{1}{6}\Delta t L(u^{(3)}) \end{aligned} \tag{4.3}$$

with a CFL coefficient $c = 0.936$ in (2.13). 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 (4.3) is an optimal 4 stage, 4th order SSP Runge-Kutta method.

4.2 Low storage methods

For large scale scientific computing in three space dimensions, storage is usually a paramount consideration. Therefore low storage Runge-Kutta methods [22], [1], which only require 2 storage units per ODE variable, may be desirable. Here we review the results presented in [6] concerning strong stability preserving properties among such low storage Runge-Kutta methods.

The general low-storage Runge-Kutta schemes can be written in the form [22], [1]:

$$\begin{aligned} u^{(0)} &= u^n, \quad du^{(0)} = 0, \\ du^{(i)} &= A_i du^{(i-1)} + \Delta t L(u^{(i-1)}), \ i = 1, \dots, m, \\ u^{(i)} &= u^{(i-1)} + B_i du^{(i)}, \qquad i = 1, \dots, m, \qquad B_1 = c, \\ u^{n+1} &= u^{(m)}, \end{aligned} \tag{4.4}$$

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

Following Carpenter and Kennedy [1], the best SSP third order method found by numerical search in [6] is given by the system

$$\begin{aligned} z_1 &= \sqrt{36c^4 + 36c^3 - 135c^2 + 84c - 12}, & z_2 &= 2c^2 + c - 2 \\ z_3 &= 12c^4 - 18c^3 + 18c^2 - 11c + 2, & z_4 &= 36c^4 - 36c^3 + 13c^2 - 8c + 4 \\ z_5 &= 69c^3 - 62c^2 + 28c - 8, & z_6 &= 34c^4 - 46c^3 + 34c^2 - 13c + 2 \end{aligned}$$

$$B_2 = \frac{12c(c-1)(3z_2 - z_1) - (3z_2 - z_1)^2}{144c(3c-2)(c-1)^2}, \quad B_3 = \frac{-24(3c-2)(c-1)^2}{(3z_2 - z_1)^2 - 12c(c-1)(3z_2 - z_1)}$$

$$A_2 = \frac{-z_1(6c2 - 4c + 1) + 3z_3}{(2c+1)z_1 - 3(c+2)(2c-1)^2}, \quad A_3 = \frac{-z_1 z_4 + 108(2c-1)c^5 - 3(2c-1)z_5}{24z_1 c(c-1)^4 + 72cz_6 + 72c^6(2c-13)}$$

with $c = 0.924574$, resulting in a CFL coefficient $c = 0.32$ in (2.6). This is of course less optimal than (4.2) in terms of CFL coefficient, but the low storage form is useful for large scale calculations. Carpenter and Kennedy [1] have also given classes of five stage, fourth order low storage Runge-Kutta methods. We have been unable to find SSP methods in that class with positive $\alpha_{i,k}$ and $\beta_{i,k}$. A low-storage method with negative $\beta_{i,k}$ cannot be made SSP, as $\tilde{L}$ cannot be used without destroying the low storage property.

4.3 Hybrid multi-step Runge-Kutta methods

Hybrid multi-step Runge-Kutta methods (e.g. [10] and [14]) are methods which combine the properties of Runge-Kutta and multi-step methods. We explore the 2-step, 2-stage method:

$$u^{n+\frac{1}{2}} = \alpha_{21}u^n + \alpha_{20}u^{n-1} + \Delta t\left(\beta_{20}L(u^{n-1}) + \beta_{21}L(u^n)\right), \qquad \alpha_{2k} \ge 0, \tag{4.5}$$

$$\begin{aligned} u^{n+1} &= \alpha_{30}u^{n-1} + \alpha_{31}u^{n+\frac{1}{2}} + \alpha_{32}u^n + \\ &\quad + \Delta t\left(\beta_{30}L(u^{n-1}) + \beta_{31}L(u^{n+\frac{1}{2}}) + \beta_{32}L(u^n)\right), \qquad \alpha_{3k} \ge 0. \end{aligned} \tag{4.6}$$

Clearly, this method is SSP under the CFL coefficient (2.10) if $\beta_{i,k} \ge 0$. We could also consider the case allowing negative $\beta_{i,k}$'s, using instead (2.13) for the CFL coefficient and replacing $\beta_{i,k}L$ by $\beta_{i,k}\tilde{L}$ for the negative $\beta_{i,k}$'s.

For third order accuracy, we have a 3 parameter family (depending on c, α_{30} and α_{31}):

$$\begin{aligned} \alpha_{20} &= 3c^2 + 2c^3 \\ \beta_{20} &= c^2 + c^3 \\ \alpha_{21} &= 1 - 3c^2 - 2c^3 \end{aligned}$$

$$
\begin{aligned}
\beta_{21} &= c+2c^2+c^3 \\
\beta_{30} &= \frac{2+2\alpha_{30}-3c+3\alpha_{30}c+\alpha_{31}c^3}{6(1+c)} \\
\beta_{31} &= \frac{5-\alpha_{30}-3\alpha_{31}c^2-2\alpha_{31}c^3}{6c+6c^2} \\
\alpha_{32} &= 1-\alpha_{31}-\alpha_{30} \\
\beta_{32} &= \frac{-5+\alpha_{30}+9c+3\alpha_{30}c-3\alpha_{31}c^2-\alpha_{31}c^3}{6c}.
\end{aligned}
\tag{4.7}
$$

The best method we were able to find is given by $c = 0.4043$, $\alpha_{30} = 0.0605$ and $\alpha_{31} = 0.6315$, and has a CFL coefficient $c \approx 0.473$. Clearly, this is not as good as the optimal third order Runge-Kutta method (4.2) with CFL coefficient $c = 1$. We would hope that a fourth order scheme with a large CFL coefficient could be found, but unfortunately this is not the case as is proven in the following

Proposition 4.3 *There are no fourth order schemes (4.5) with all nonnegative* $\alpha_{i,k}$.

Proof. The fourth order schemes are given by a two parameter family depending on c, α_{30} and setting α_{31} in (4.7) with

$$\alpha_{31} = \frac{-7-\alpha_{30}+10c-2\alpha_{30}c}{c^2(3+8c+4c^2)}.$$

The requirement $\alpha_{21} \geq 0$ enforces, consult (4.7), $c \leq \frac{1}{2}$. The further requirement $\alpha_{20} \geq 0$ yields $-\frac{3}{2} \leq c \leq \frac{1}{2}$. α_{31} has a positive denominator and a negative numerator for $-\frac{1}{2} < c < \frac{1}{2}$, and its denominator is 0 when $c = -\frac{1}{2}$ or $c = -\frac{3}{2}$, thus we require $-\frac{3}{2} \leq c < -\frac{1}{2}$. In this range, the denominator of α_{31} is negative, hence we also require its numerator to be negative, which translates to $\alpha_{30} \leq \frac{-7+10c}{1+2c}$. Finally, we would require $\alpha_{32} = 1-\alpha_{31}-\alpha_{30} \geq 0$, which translates to $\alpha_{30} \geq \frac{c^2(2c+1)(2c+3)+7-10c}{(2c+1)(2c-1)(c+1)^2}$. The two restrictions on α_{30} gives us the following inequality:

$$\frac{-7+10c}{1+2c} \geq \frac{c^2(2c+1)(2c+3)+7-10c}{(2c+1)(2c-1)(c+1)^2},$$

which, in the range of $-\frac{3}{2} \leq c < -\frac{1}{2}$, yields $c \geq 1$ — a contradiction. ■

5 Linear and nonlinear multi-step methods

In this section we review and further study SSP explicit multi-step methods (2.14), which were first developed in [18]. These methods are r-th order accurate if

$$
\begin{aligned}
\sum_{i=1}^{m} \alpha_i &= 1 \\
\sum_{i=1}^{m} i^k \alpha_i &= k\left(\sum_{i=1}^{m} i^{k-1}\beta_i\right), \qquad k = 1, \ldots, r.
\end{aligned}
\tag{5.1}
$$

We first prove a proposition which sets the minimum number of steps in our search for SSP multi-step methods.

Proposition 5.1 *For $m \geq 2$, there is no m step, m-th order SSP method with all non-negative β_i, and there is no m step SSP method of order $(m+1)$.*

Proof. By the accuracy condition (5.1), we clearly have for an r-order accurate method

$$\sum_{i=1}^{m} p(i)\alpha_i = \sum_{i=1}^{m} p'(i)\beta_i, \tag{5.2}$$

for any polynomial $p(x)$ of degree at most r satisfying $p(0) = 0$.

When $r = m$, we could choose

$$p(x) = x(m-x)^{m-1}$$

Clearly $p(i) \geq 0$ for $i = 1, ..., m$, equality holds only for $i = m$. On the other hand, $p'(i) = m(1-i)(m-i)^{m-2} \leq 0$, equality holds only for $i = 1$ and $i = m$. Hence (5.2) would have a negative right side and a positive left side and would not be an inequality, if all α_i and β_i are non-negative, unless the only nonzero entries are α_m, β_1 and β_m. In this special case we have $\alpha_m = 1$, and $\beta_1 = 0$ to get a positive CFL coefficient c in (2.15). The first two order conditions in (5.1) now leads to $\beta_m = m$ and $2\beta_m = m$, which cannot be simultaneously satisfied.

When $r = m+1$, we could choose

$$p(x) = \int_0^x q(t)dt, \qquad q(t) = \prod_{i=1}^{m}(i-t). \tag{5.3}$$

Clearly $p'(i) = q(i) = 0$ for $i = 1, ..., m$. We also claim (and prove below) that all the $p(i)$'s, $i = 1, \ldots, m$, are positive. With this choice of p in (5.2), its right hand side vanishes, while the left hand side is strictly positive if all $\alpha_i \geq 0$ — a contradiction.

We conclude with the proof of the

Claim. $\quad p(i) = \int_0^i q(t)dt > 0, \qquad q(t) := \prod_{i=1}^{m}(i-t)$.

Indeed, $q(t)$ oscillates between being positive on the even intervals $I_0 = (0,1), I_2 = (2,3), \ldots$ and being negative on the odd intervals, $I_1 = (1,2), I_3 = (3,4), \ldots$. The positivity of the $p(i)$'s for $i \leq (m+1)/2$ follows since the integral of $q(t)$ over each pair of consecutive intervals is positive, at least for the first $[(m+1)/2]$ intervals,

$$\begin{aligned} p(2k+2) - p(2k) &= \int_{I_{2k}} |q(t)|dt - \int_{I_{2k+1}} |q(t)|dt = \int_{I_{2k}} - \int_{I_{2k+1}} |(1-t)(2-t)\ldots(m-t)|dt = \\ &= \int_{I_{2k}} |(1-t)(2-t)\ldots(m-1-t)| \times (|(m-t)| - |t|)dt > 0, \qquad 2k+1 \leq (m+1)/2. \end{aligned}$$

For the remaining intervals we note the symmetry of $q(t)$ w.r.t. the midpoint $(m+1)/2$, i.e., $q(t) = (-1)^m q(m+1-t)$ which enables us to write for $i > (m+1)/2$

$$\begin{aligned} p(i) &= \int_0^{(m+1)/2} q(t)dt + (-1)^m \int_{(m+1)/2}^{i} q(m+1-t)dt = \\ &= \int_0^{(m+1)/2} q(t)dt + (-1)^m \int_{m+1-i}^{(m+1)/2} q(t')dt'. \end{aligned} \tag{5.4}$$

Thus, if m is odd then $p(i) = p(m+1-i) > 0$ for $i > (m+1)/2$. If m is even, then the second integral on the right of (5.4) is positive for odd i's, since it starts with a positive integrand on the even interval, I_{m+1-i}. And finally, if m is even and i is odd then second integral starts with a negative contribution from its first integrand on the odd interval, I_{m+1-i}, while the remaining terms which follow cancel in pairs as before; a straightforward computation shows that this first negative contribution is compensated by the positive gain from the first pair, i.e.,

$$p(m+2-i) > \int_0^2 q(t)dt + \int_{m+1-i}^{m+2-i} q(t)dt > 0, \qquad m \text{ even}, \ i \text{ odd}.$$

This concludes the proof of our claim. ■

We remark that [4] contains a result which states that there are no linearly stable m step, $(m+1)$-th order method when m is odd. When m is even such linearly stable methods exist but would require negative α_i. This is consistent with our result.

In the remainder of this section we will discuss optimal m step, m-th order SSP methods (which must have negative β_i according to Proposition 5.1 and m step, $(m-1)$-th order SSP methods with positive β_i.

For two step, second order SSP methods, a scheme was given in [18] with a CFL coefficient $c = \frac{1}{2}$ (Scheme 1 in Table 5.1). We prove this is optimal in terms of CFL coefficients.

Proposition 5.2 *For two step, second order SSP methods, the optimal CFL coefficient c in (2.15) is $\frac{1}{2}$.*

Proof. The accuracy condition (5.1) can be explicitly solved to obtain a one parameter family of solutions

$$\alpha_2 = 1 - \alpha_1, \qquad \beta_1 = 2 - \frac{1}{2}\alpha_1, \qquad \beta_2 = -\frac{1}{2}\alpha_1.$$

The CFL coefficient c is a function of α_1 and it can be easily verified that the maximum is $c = \frac{1}{2}$ achieved at $\alpha_1 = \frac{4}{5}$. ■

We move on to three step, second order methods. It is now possible to have SSP schemes with positive α_i and β_i. One such method is given in [18] with a CFL coefficient $c = \frac{1}{2}$ (Scheme 2 in Table 5.1). We prove this is optimal in CFL coefficient in the following proposition. We remark that this multi-step method has the same efficiency as the optimal two stage, second order Runge-Kutta method (4.1). This is because there is only one L evaluation per time step here, compared with two L evaluations in the two stage Runge-Kutta method. Of course, the storage requirement here is larger.

Proposition 5.3 *If we require $\beta_i \geq 0$, then the optimal three step, second order method has a CFL coefficient $c = \frac{1}{2}$.*

Proof. The coefficients of the three step, second order method are given by,

$$\alpha_1 = \frac{1}{2}(6 - 3\beta_1 - \beta_2 + \beta_3), \qquad \alpha_2 = -3 + 2\beta_1 - 2\beta_3, \qquad \alpha_3 = \frac{1}{2}(2 - \beta_1 + \beta_2 + 3\beta_3).$$

For CFL coefficient $c > \frac{1}{2}$ we need $\frac{\alpha_k}{\beta_k} > \frac{1}{2}$ for all k. This implies

$$\begin{aligned} 2\alpha_1 > \beta_1 &\Rightarrow 6 - 4\beta_1 - \beta_2 + \beta_3 > 0 \\ 2\alpha_2 > \beta_2 &\Rightarrow -6 + 4\beta_1 - \beta_2 - 4\beta_3 > 0 \end{aligned}$$

This means that

$$\beta_2 - \beta_3 < 6 - 4\beta_1 < -\beta_2 - 4\beta_3 \qquad \Rightarrow \qquad 2\beta_2 < -3\beta_3.$$

Thus, we would have a negative β. ■

We remark that if more steps are allowed, then the CFL coefficient can be improved. Scheme 3 in Table 5.1 is a four step, second order method with positive α_i and β_i and a CFL coefficient $c = \frac{2}{3}$.

We now move to three step, third order methods. In [18] we gave a three step, third order method with a CFL coefficient $c \approx 0.274$ (Scheme 4 in Table 5.1). A computer search gives a slightly better scheme (Scheme 5 in Table 5.1) with a CFL coefficient $c \approx 0.287$.

Next we move on to four step, third order methods. It is now possible to have SSP schemes with positive α_i and β_i. One example was given in [18] with a CFL coefficient $c = \frac{1}{3}$ (Scheme 6 in Table 5.1). We prove this is optimal in CFL coefficient in the following proposition. We remark again that this multi-step method has the same efficiency as the optimal three stage, third order Runge-Kutta method (4.2). This is because there is only one L evaluation per time step here, compared with three L evaluations in the three stage Runge-Kutta method. Of course, the storage requirement here is larger.

Proposition 5.4 *If we require $\beta_i \geq 0$, then the optimal four step, third order method has a CFL coefficient $c = \frac{1}{3}$.*

Proof. The coefficients of the four step, third order method are given by,

$$\begin{aligned} \alpha_1 &= \frac{1}{6}(24 - 11\beta_1 - 2\beta_2 + \beta_3 - 2\beta_4), \qquad \alpha_2 = -6 + 3\beta_1 - \frac{1}{2}\beta_2 - \beta_3 + \frac{3}{2}\beta_4, \\ \alpha_3 &= 4 - \frac{3}{2}\beta_1 + \beta_2 + \frac{1}{2}\beta_3 - 3\beta_4, \qquad \alpha_4 = \frac{1}{6}(-6 + 2\beta_1 - \beta_2 + 2\beta_3 + 11\beta_4). \end{aligned}$$

For a CFL coefficient $c > \frac{1}{3}$ we need $\frac{\alpha_k}{\beta_k} > \frac{1}{3}$ for all k. This implies:

$$\begin{aligned} 24 - 13\beta_1 - 2\beta_2 + \beta_3 - 2\beta_4 > 0, \qquad -36 + 18\beta_1 - 5\beta_2 - 6\beta_3 + 9\beta_4 > 0, \\ 24 - 9\beta_1 + 6\beta_2 + \beta_3 - 18\beta_4 > 0, \qquad -6 + 2\beta_1 - \beta_2 + 2\beta_3 + 9\beta_4 > 0. \end{aligned}$$

Combining these (9 times the first inequality plus 8 times the second plus 3 times the third) we get:

$$-40\beta_2 - 36\beta_3 > 0,$$

which implies a negative β. ■

We again remark that if more steps are allowed, the CFL coefficient can be improved. Scheme 7 in Table 5.1 is a five step, third order method with positive α_i and β_i and a CFL coefficient $c = \frac{1}{2}$. Scheme 8 in Table 5.1 is a six step, third order method with positive α_i and β_i and a CFL coefficient $c = 0.567$.

We now move on to four step, fourth order methods. In [18] we gave a four step, fourth order method (Scheme 9 in Table 5.1) with a CFL coefficient $c \approx 0.154$. A computer search gives a slightly better scheme with a CFL coefficient $c \approx 0.159$, Scheme 10 in Table 5.1. If we allow two more steps, we can improve the CFL coefficient to $c = 0.245$, Scheme 11 in Table 5.1.

#	steps m	order r	CFL c	α_i	β_i
1	2	2	$\frac{1}{2}$	$\frac{4}{5}, \frac{1}{5}$	$\frac{8}{5}, -\frac{2}{5}$
2	3	2	$\frac{1}{2}$	$\frac{3}{4}, 0, \frac{1}{4}$	$\frac{3}{2}, 0, 0$
3	4	2	$\frac{2}{3}$	$\frac{8}{9}, 0, 0, \frac{1}{9}$	$\frac{4}{3}, 0, 0, 0$
4	3	3	0.274	$\frac{4}{7}, \frac{2}{7}, \frac{1}{7}$	$\frac{25}{12}, -\frac{20}{21}, \frac{37}{84}$
5	3	3	0.287	$\frac{2973}{5000}, \frac{351}{1250}, \frac{623}{5000}$	$\frac{1297}{625}, -\frac{49}{50}, \frac{1087}{2500}$
6	4	3	$\frac{1}{3}$	$\frac{16}{27}, 0, 0, \frac{11}{27}$	$\frac{16}{9}, 0, 0, \frac{4}{9}$
7	5	3	$\frac{1}{2}$	$\frac{25}{32}, 0, 0, 0, \frac{7}{32}$	$\frac{25}{16}, 0, 0, 0, \frac{5}{16}$
8	6	3	0.567	$\frac{108}{125}, 0, 0, 0, 0, \frac{17}{125}$	$\frac{36}{25}, 0, 0, 0, 0, \frac{6}{25}$
9	4	4	0.154	$\frac{29}{72}, \frac{7}{24}, \frac{1}{4}, \frac{1}{18}$	$\frac{481}{192}, -\frac{1055}{576}, \frac{937}{576}, -\frac{197}{576}$
10	4	4	0.159	$\frac{1989}{5000}, \frac{2893}{10000}, \frac{517}{2000}, \frac{34}{625}$	$\frac{601613}{240000}, -\frac{1167}{640}, \frac{130301}{80000}, -\frac{82211}{240000}$
11	6	4	0.245	$\frac{747}{1280}, 0, 0, 0, \frac{81}{256}, \frac{1}{10}$	$\frac{237}{128}, 0, 0, 0, \frac{165}{128}, -\frac{3}{8}$
12	5	4	0.021	$\frac{1557}{32000}, \frac{1}{32000}, \frac{1}{120}, \frac{2063}{48000}, \frac{9}{10}$	$\frac{5323561}{2304000}, \frac{2659}{2304000}, \frac{904987}{2304000}, \frac{1567579}{768000}, 0$
13	5	5	0.077	$\frac{1}{4}, \frac{1}{4}, \frac{7}{24}, \frac{1}{6}, \frac{1}{24}$	$\frac{185}{64}, -\frac{851}{288}, \frac{91}{24}, -\frac{151}{96}, \frac{199}{576}$
14	5	5	0.085	$\frac{1}{4}, \frac{13}{50}, \frac{8}{25}, \frac{7}{50}, \frac{3}{100}$	$\frac{52031}{18000}, -\frac{26617}{9000}, \frac{1412}{375}, -\frac{14407}{9000}, \frac{6161}{18000}$
15	6	5	0.130	$\frac{7}{20}, \frac{3}{10}, \frac{4}{15}, 0, \frac{7}{120}, \frac{1}{40}$	$\frac{291201}{108000}, -\frac{198401}{86400}, \frac{88063}{43200}, 0, -\frac{17969}{43200}, \frac{73061}{432000}$

Table 5.1: SSP multi-step methods (2.14)

Next we move on to five step, fourth order methods. It is now possible to have SSP schemes with positive α_i and β_i. The solution can be written in the following five parameter family:

$$\alpha_5 = 1 - \alpha_1 - \alpha_2 - \alpha_3 - \alpha_4, \qquad \beta_1 = \frac{1}{24}\left(55 + 9\alpha_2 + 8\alpha_3 + 9\alpha_4 + 24\beta_5\right),$$

$$\beta_2 = \frac{1}{24}\left(5 - 64\alpha_1 - 45\alpha_2 - 32\alpha_3 - 37\alpha_4 - 96\beta_5\right),$$

$$\beta_3 = \frac{1}{24}\left(5 + 32\alpha_1 + 27\alpha_2 + 40\alpha_3 + 59\alpha_4 + 144\beta_5\right),$$
$$\beta_4 = \frac{1}{24}\left(55 - 64\alpha_1 - 63\alpha_2 - 64\alpha_3 - 55\alpha_4 - 96\beta_5\right).$$

We can clearly see that to get $\beta_2 \geq 0$ we would need $\alpha_1 \leq \frac{5}{64}$, and also $\beta_1 \geq \frac{55}{24}$, hence the CFL coefficient cannot exceed $c \leq \frac{\alpha_1}{\beta_1} \leq \frac{3}{88} \approx 0.034$. A computer search gives a scheme (Scheme 12 in Table 5.1) with a CFL coefficient $c = 0.021$. The significance of this scheme is that it disproves the believe that SSP schemes of order four or higher must have negative β and hence must use $\tilde{L}$ (see Proposition 4.2 for Runge-Kutta methods). However, the CFL coefficient here is probably too small for the scheme to be of much practical use.

We finally look at five step, fifth order methods. In [18] a scheme with CFL coefficient $c = 0.077$ is given (Scheme 13 in Table 5.1). A computer search gives us a scheme with a slightly better CFL coefficient $c \approx 0.085$, Scheme 14 in Table 5.1. Finally, by increasing one more step, one could get [18] a scheme with CFL coefficient $c = 0.130$, Scheme 15 in Table 5.1.

We list in Table 5.1 the multi-step methods studied in this section.

6 Implicit SSP methods

6.1 Implicit TVD stable scheme

Implicit methods are useful in that they typically eliminate the step-size restriction (CFL) associated with stability analysis. For many applications, the backward-Euler method possesses strong stability properties that we would like to preserve in higher order methods. For example, it is easy to show a version of Harten's lemma [8] for the TVD property of implicit backward-Euler method:

Lemma 6.1 *(Harten). The following implicit backward-Euler method*

$$u_j^{n+1} = u_j^n + \Delta t\left[C_{j+\frac{1}{2}}\left(u_{j+1}^{n+1} - u_j^{n+1}\right) - D_{j-\frac{1}{2}}\left(u_j^{n+1} - u_{j-1}^{n+1}\right)\right] \tag{6.1}$$

where $C_{j+\frac{1}{2}}$ and $D_{j-\frac{1}{2}}$ are functions of u^n and/or u^{n+1} at various (usually neighboring) grid points satisfying

$$C_{j+\frac{1}{2}} \geq 0, \qquad D_{j-\frac{1}{2}} \geq 0, \tag{6.2}$$

is TVD in the sense of (2.5) for arbitrary Δt.

Proof. Taking a spatial forward difference in (6.1) and moving terms one gets

$$\begin{aligned} &\left[1 + \Delta t\left(C_{j+\frac{1}{2}} + D_{j+\frac{1}{2}}\right)\right]\left(u_{j+1}^{n+1} - u_j^{n+1}\right) \\ = \;& u_{j+1}^n - u_j^n + \Delta t C_{j+\frac{3}{2}}\left(u_{j+2}^{n+1} - u_{j+1}^{n+1}\right) + \Delta t D_{j-\frac{1}{2}}\left(u_j^{n+1} - u_{j-1}^{n+1}\right). \end{aligned}$$

Using the positivity of C and D in (6.2) one gets

$$\begin{aligned} &\left[1 + \Delta t\left(C_{j+\frac{1}{2}} + D_{j+\frac{1}{2}}\right)\right]\left|u_{j+1}^{n+1} - u_j^{n+1}\right| \\ \leq \;& \left|u_{j+1}^n - u_j^n\right| + \Delta t C_{j+\frac{3}{2}}\left|u_{j+2}^{n+1} - u_{j+1}^{n+1}\right| + \Delta t D_{j-\frac{1}{2}}\left|u_j^{n+1} - u_{j-1}^{n+1}\right|, \end{aligned}$$

which, upon summing over j would yield the TVD property (2.5). ■

Another example is the cell entropy inequality for the square entropy, satisfied by the discontinuous Galerkin method of arbitrary order of accuracy in any space dimensions, when the time discretization is by a class of implicit time discretization including backward-Euler and Crank-Nicholson, again without any restriction on the time step Δt [11].

As in Section 2 for explicit methods, here we would like to discuss the possibility of designing higher order implicit methods which share the strong stability properties of backward-Euler, without any restriction on the time step Δt.

Unfortunately, we are not as lucky in the implicit case. Let us look at a simple example of second order implicit Runge-Kutta methods:

$$\begin{aligned} u^{(1)} &= u^n + \beta_1 \Delta t L(u^{(1)}) \\ u^{n+1} &= \alpha_{2,0} u^n + \alpha_{2,1} u^{(1)} + \beta_2 \Delta t L(u^{n+1}), \end{aligned} \tag{6.3}$$

Notice that we have only a single implicit L term for each stage and no explicit L terms, in order to avoid time step restrictions necessitated by the strong stability of explicit schemes. However, since the explicit $L(u^{(1)})$ term is contained indirectly in the second stage through the $u^{(1)}$ term, we do not lose generality in writing the schemes as the form in (6.3) except for the absence of the $L(u^n)$ terms in both stages.

To simplify our example we assume L is linear. Second order accuracy requires the coefficients in (6.3) to satisfy

$$\alpha_{2,1} = \frac{1}{2\beta_1(1-\beta_1)}, \qquad \alpha_{2,0} = 1 - \alpha_{2,1}, \qquad \beta_2 = \frac{1-2\beta_1}{2(1-\beta_1)}. \tag{6.4}$$

To obtain a SSP scheme out of (6.4) we would require $\alpha_{2,0}$ and $\alpha_{2,1}$ to be non-negative. We can clearly see that this is impossible as $\alpha_{2,1}$ is in the range $[4, +\infty)$ or $(-\infty, 0)$.

We will use the following simple numerical example to demonstrate that a non SSP implicit method may destroy the non-oscillatory property of the backward-Euler method, despite the same underlying non-oscillatory spatial discretization. We solve the simple linear wave equation

$$u_t = u_x \tag{6.5}$$

with a step-function initial condition:

$$u(x,0) = \begin{cases} 1, & \text{if } x \le 0 \\ 0, & \text{if } x > 0 \end{cases} \tag{6.6}$$

u_x in (6.5) is approximated by the simple first order upwind difference:

$$L(u)_j = \frac{1}{\Delta x}\left(u_{j+1} - u_j\right).$$

The backward-Euler time discretization

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

for this problem is unconditionally TVD according to Lemma 6.1. We can see on the left of Fig. 6.1 that the solution is monotone. However, if we use (6.3)-(6.4) with $\beta_1 = 2$ (which results in positive $\beta_2 = \frac{3}{2}$, $\alpha_{2,0} = \frac{5}{4}$ but a negative $\alpha_{2,1} = -\frac{1}{4}$) as the time discretization, we can see on the right of Fig. 6.1, that the solution is oscillatory.

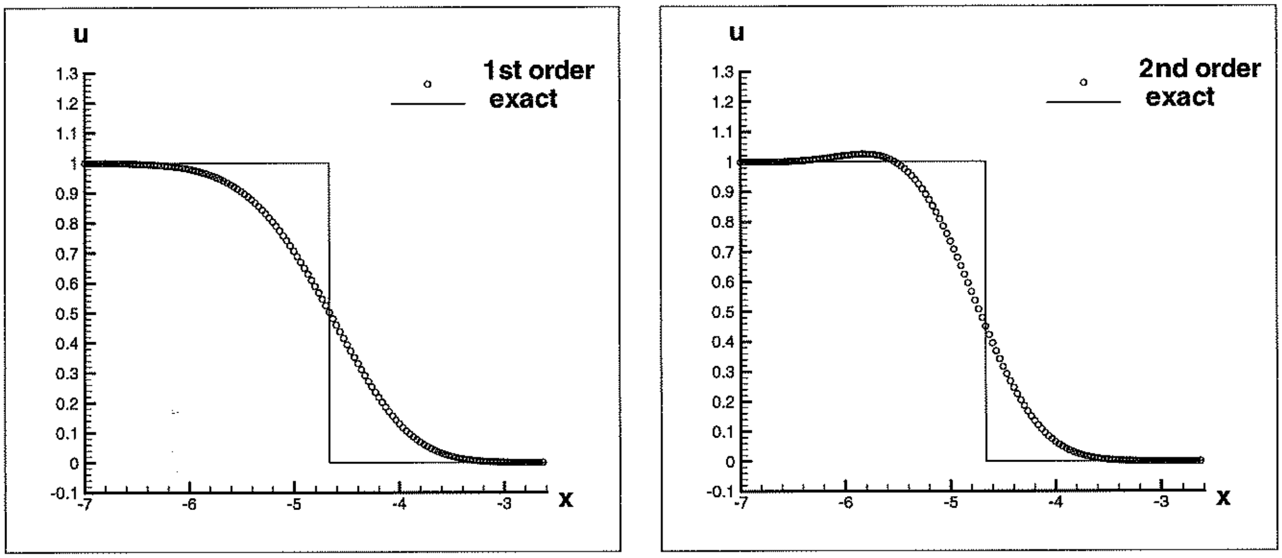

Figure 6.1: First order upwind spatial discretization. Solution after 100 time steps at CFL number $\frac{\Delta t}{\Delta x} = 1.4$. Left: first order backward-Euler time discretization; Right: non SSP second order implicit Runge-Kutta time discretization (6.3)-(6.4) with $\beta_1 = 2$.

In the next two subsections we discuss he rather disappointing negative results about the non-existence of high order SSP Runge-Kutta or multi-step methods.

6.2 Implicit Runge-Kutta methods

A general implicit Runge-Kutta method for (2.1) can be written in the form

$$\begin{aligned} u^{(0)} &= u^n, \\ u^{(i)} &= \sum_{k=0}^{i-1} \alpha_{i,k} u^{(k)} + \Delta t \beta_i L(u^{(i)}), \quad \alpha_{i,k} \geq 0, \qquad i = 1, ..., m \\ u^{n+1} &= u^{(m)}. \end{aligned} \tag{6.7}$$

Notice that we have only a single implicit L term for each stage and no explicit L terms. This is to avoid time step restrictions for strong stability properties of explicit schemes. However, since explicit L terms are contained indirectly beginning at the second stage from u of the previous stages, we do not lose generality in writing the schemes as the form in (6.7) except for the absence of the $L(u^{(0)})$ terms in all stages. If these $L(u^{(0)})$ terms are included, we would be able to obtain SSP Runge-Kutta methods under restrictions on Δt similar to explicit methods.

Clearly, if we assume that the first order implicit Euler discretization

$$u^{n+1} = u^n + \Delta t L(u^{n+1}) \tag{6.8}$$

is unconditionally strongly stable, $\|u^{n+1}\| \le \|u^n\|$, then (6.7) would be unconditionally strongly stable under the same norm provided $\beta_i > 0$ for all i. If β_i becomes negative, (6.7) would still be unconditionally strongly stable under the same norm if $\beta_i L$ is replaced by $\beta_i \tilde{L}$ whenever the coefficient $\beta_i < 0$, with $\tilde{L}$ approximates the same spatial derivative(s) as L, but is unconditionally strongly stable for first order implicit Euler, backward in time:

$$u^{n+1} = u^n - \Delta t \tilde{L}(u^{n+1}) \tag{6.9}$$

As before, this can again be achieved, for hyperbolic conservation laws, by solving (2.12), the negative in time version of (2.2). Numerically, the only difference is the change of upwind direction.

Unfortunately, we have the following negative result which completely rules out the existence of SSP implicit Runge-Kutta schemes (6.7) of order higher than one.

Proposition 6.1 *If (6.7) is at least second order accurate, then $\alpha_{i,k}$ cannot be all non-negative.*

Proof. We prove that the statement holds even if L is linear. In this case second order accuracy implies

$$\sum_{k=0}^{i-1} \alpha_{i,k} = 1, \qquad X_m = 1, \qquad Y_m = \frac{1}{2} \tag{6.10}$$

where X_m and Y_m can be recursively defined as

$$X_1 = \beta_1, \qquad Y_1 = \beta_1^2, \qquad X_m = \beta_m + \sum_{i=1}^{m-1} \alpha_{m,i} X_i, \qquad Y_m = \beta_m X_m + \sum_{i=1}^{m-1} \alpha_{m,i} Y_i. \tag{6.11}$$

We now show that, if $\alpha_{i,k} \ge 0$ for all i and k, then

$$X_m - Y_m < \frac{1}{2}, \tag{6.12}$$

which is clearly a contradiction to (6.10). In fact, we use induction on m to prove

$$(1-a)X_m - Y_m < c_m (1-a)^2 \qquad \text{for any real number } a, \tag{6.13}$$

where

$$c_1 = \frac{1}{4}, \qquad c_{i+1} = \frac{1}{4(1-c_i)}. \tag{6.14}$$

It is easy to show that (6.14) implies

$$\frac{1}{4} = c_1 < c_2 < \cdots < c_m < \frac{1}{2}. \tag{6.15}$$

We start with the case $m = 1$. Clearly,

$$(1-a)X_1 - Y_1 = (1-a)\beta_1 - \beta_1^2 \le \frac{1}{4}(1-a)^2 = c_1(1-a)^2$$

for any a. Now assume (6.13)-(6.14), hence also (6.15), is valid for all $m < k$, for $m = k$ we have

$$\begin{aligned}(1-a)X_k - Y_k &= (1-a-\beta_k)\beta_k + \sum_{i=1}^{k-1} \alpha_{k,i}\left[(1-a-\beta_k)X_i - Y_i\right] \\ &\leq (1-a-\beta_k)\beta_k + c_{k-1}(1-a-\beta_k)^2 \\ &\leq \frac{1}{4(1-c_{k-1})}(1-a)^2 \\ &= c_k(1-a)^2\end{aligned}$$

where in the first equality we used (6.11), in the second inequality we used (6.10) and the induction hypothesis (6.13) and (6.15), and the third inequality is a simple maximum of a quadratic function in β_k. This finishes the proof. ■

We remark that the proof of Proposition 6.1 can be simplified, using existing ODE results in [5], if all β_i's are non-negative or all β_i's are non-positive. However, the case containing both positive and negative β_i's cannot be handled by existing ODE results, as L and $\tilde{L}$ do not belong to the same ODE.

6.3 Implicit multi-step methods

For our purpose, a general implicit multi-step method for (2.1) can be written in the form

$$u^{n+1} = \sum_{i=1}^{m} \alpha_i u^{n+1-i} + \Delta t \beta_0 L(u^{n+1}), \quad \alpha_i \geq 0. \tag{6.16}$$

Notice that we have only a single implicit L term and no explicit L terms. This is to avoid time step restrictions for norm properties of explicit schemes. If explicit L terms are included, we would be able to obtain SSP multi-step methods under restrictions on Δt similar to explicit methods.

Clearly, if we assume that the first order implicit Euler discretization (6.8) is unconditionally strongly stable under a certain norm, then (6.16) would be unconditionally strongly stable under the same norm provided that $\beta_0 > 0$. If β_0 is negative, (6.16) would still be unconditionally strongly stable under the same norm if L is replaced by $\tilde{L}$.

Unfortunately, we have the following negative result which completely rules out the existence of SSP implicit multi-step schemes (6.16) of order higher than one.

Proposition 6.2 *If (6.16) is at least second order accurate, then α_i cannot be all non-negative.*

Proof. Second order accuracy implies

$$\sum_{i=1}^{m} \alpha_i = 1, \qquad \sum_{i=1}^{m} i\alpha_i = \beta_0, \qquad \sum_{i=1}^{m} i^2\alpha_i = 0. \tag{6.17}$$

The last equality in (6.17) implies that α_i cannot be all non-negative. ■

7 Concluding Remarks

We have systematically studied strong stability preserving, or SSP, time discretization methods, which preserve strong stability of the forward Euler (for explicit methods) or the backward Euler (for implicit methods) first order time discretizations. Runge-Kutta and multi-step methods are both investigated. The methods listed here can be used for method of lines numerical schemes for partial differential equations, especially for hyperbolic problems.

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