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Strong Stability-Preserving High-Order Time Discretization Methods*

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Abstract. In this paper we review and further develop a class of strong stability-preserving (SSP) high-order time discretizations for semidiscrete method of lines approximations of partial differential equations. Previously termed TVD (total variation diminishing) time discretizations, these high-order time discretization methods preserve the strong stability properties of first-order Euler time stepping and have proved very useful, especially in solving hyperbolic partial differential equations. The new developments in this paper include the construction of optimal explicit SSP linear Runge–Kutta methods, their application to the strong stability of coercive approximations, a systematic study of explicit SSP multistep methods for nonlinear problems, and the study of the SSP property of implicit Runge–Kutta and multistep methods.

Key words. strong stability preserving, Runge–Kutta methods, multistep methods, high-order accuracy, time discretization

AMS subject classifications. 65M20, 65L06

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1. Introduction. It is a common practice in solving time-dependent partial differential equations (PDEs) to first discretize the spatial variables to obtain a semidiscrete 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 concerns 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.

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In this paper we review and further develop a class of high-order strong stability-preserving (SSP) time discretization methods for the semidiscrete method of lines approximations of PDEs. These time discretization methods were first developed in [20] and [19] and were called TVD (total variation diminishing) time discretizations. This class of methods 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 to try to find a higher order time discretization (Runge–Kutta or multistep) that maintains strong stability for the same norm, perhaps under a different time step restriction. In [20] and [19], the relevant norm was the total variation norm: the forward Euler time discretization of the method of lines ODE was assumed to be TVD, hence the class of high-order time discretization developed there was termed *TVD time discretization*. This terminology was also used in [6]. In fact, the essence of this class of high-order time discretizations lies in its ability to maintain the strong stability in the same norm as the first-order forward Euler version, hence *SSP time discretization* is a more suitable term, which we will use in this paper.

We begin this paper by discussing explicit SSP methods. We first give, in section 2, a brief introduction to the setup and basic properties of the methods. We then move, in section 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 [20], [19], and [6] for nonlinear SSP Runge–Kutta methods in section 4 and for multistep methods in section 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 concerning the nonexistence of SSP implicit Runge–Kutta or multistep methods of order higher than 1. Concluding remarks are given in section 7.

2. Explicit SSP Methods.

2.1. Why SSP Methods? Explicit SSP methods were developed in [20] and [19] (termed TVD time discretizations there) to solve systems of ODEs

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

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

$$(2.2) \quad u_t = -f(u)_x,$$

where the spatial derivative, $f(u)_x$, is discretized by a TVD finite difference or finite element approximation; see, e.g., [8], [16], [21], [2], [9], and consult [22] 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,

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

then, for a sufficiently small time step dictated by the Courant–Friedrichs–Levy (CFL) condition,

$$(2.4) \quad \Delta t \leq \Delta t_{FE},$$

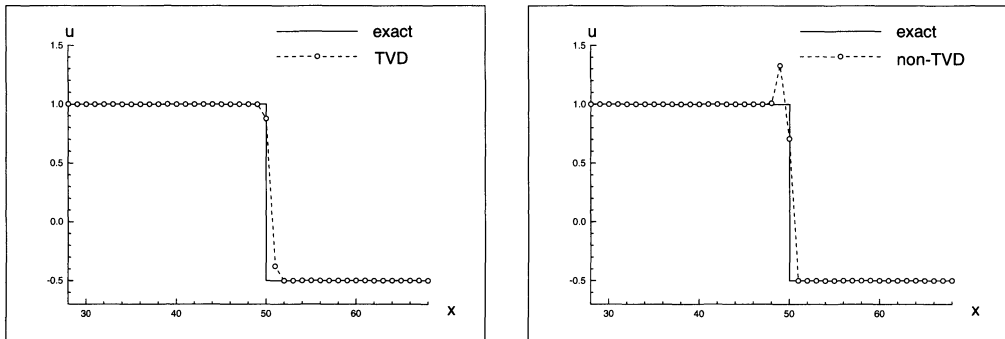


Fig. 2.1 Second-order TVD MUSCL spatial discretization. Solution after the shock moves 50 mesh points. Left: SSP time discretization; right: non-SSP time discretization.

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:

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

The objective of the high-order SSP Runge–Kutta or multistep time discretization is to maintain 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)

$$(2.6) \quad \Delta t \leq c \Delta t_{FE}.$$

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

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

with Riemann initial data

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

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

In Figure 2.1, we show the result of using an 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 an 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 (not increasing) the TV. 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,¹ i.e., $\|u^n + \Delta t L(u^n)\| \leq \|u^n\|$. For linear examples we refer to [7], where weighted L^2 SSP higher order discretizations of spectral schemes were 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 for discontinuous Galerkin and central schemes can be found in [3] and [9]. 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] and [15].

We remark that the strong stability assumption for the forward Euler $\|u^n + \Delta t L(u^n)\| \leq \|u^n\|$ can be relaxed to the more general stability assumption $\|u^n + \Delta t L(u^n)\| \leq (1 + O(\Delta t))\|u^n\|$. This general stability property will also be preserved by the high-order SSP time discretizations. The total variation bounded (TVB) methods discussed in [18] and [2] belong to this category. However, if the forward Euler operator is not stable, the framework in this paper cannot be used to determine whether a high-order time discretization is stable or not.

2.2. SSP Runge–Kutta Methods. In [20], a general m -stage Runge–Kutta method for (2.1) is written in the form

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

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 with the following lemma.

LEMMA 2.1 (see [20]). *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:*

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

¹By 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, $\|u^n\| \leq \text{Const} \cdot \|u^0\|$, with any arbitrary constant, possibly $\text{Const} > 1$.

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 approximate the same spatial derivative(s) as L , but that the strong stability property hold with $\|u^{n+1}\| \leq \|u^n\|$ (with respect to either the TV or another relevant norm) for the first-order Euler scheme solved backward in time, i.e.,

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

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

$$(2.12) \quad u_t = f(u)_x.$$

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 2.2 (see [20]). *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),*

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

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 the 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 Multistep Methods.

SSP multistep methods of the form

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

were studied in [19]. 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 (see [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 multistep method (2.14) is SSP, $\|u^{n+1}\| \leq \|u^n\|$, under the CFL restriction (2.6),*

$$(2.15) \quad \Delta t \leq c \Delta t_{FE}, \quad c = \min_i \frac{\alpha_i}{|\beta_i|},$$

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 a 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

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

where

$$\begin{aligned} A_{1,0} &= \beta_{1,0}, & A_{i,0} &= \sum_{k=1}^{i-1} \alpha_{i,k} A_{k,0} + \sum_{k=0}^{i-1} \beta_{i,k}, \\ A_{i,k} &= \sum_{j=k+1}^{i-1} \alpha_{i,j} A_{j,k} + \sum_{j=k}^{i-1} \beta_{i,j} A_{j,k-1}, & k &= 1, \dots, i-1. \end{aligned}$$

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 an 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 nonnegative 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 $c \leq 1$. \square

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 [19], 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*

$$(3.1) \quad u^{(i)} = u^{(i-1)} + \Delta t L u^{(i-1)}, \quad i = 1, \dots, m-1,$$

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

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

$$(3.2) \quad \alpha_{m,k} = \frac{1}{k} \alpha_{m-1,k-1}, \quad k = 1, \dots, m-2,$$

$$\alpha_{m,m-1} = \frac{1}{m!}, \quad \alpha_{m,0} = 1 - \sum_{k=1}^{m-1} \alpha_{m,k}$$

is an m th-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

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

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 $\frac{1}{k!}$:

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

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

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

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 $j = 0, \dots, m-1$, then

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

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

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

As the m -stage, m th-order linear Runge–Kutta method is unique, we have in effect proved that 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 fourth-order Runge–Kutta methods, which admit the following convex, and hence SSP, decompositions:

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

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

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

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

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	$\frac{2119}{5760}$	$\frac{103}{280}$	$\frac{53}{288}$	$\frac{11}{180}$	$\frac{1}{64}$	$\frac{1}{360}$	$\frac{1}{1440}$	$\frac{1}{40320}$

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,

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

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

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

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

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

Following Levy and Tadmor [13] we therefore make the following assumption.

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

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

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 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

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

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

$$(3.9) \quad k^1 = L(t^n)u^n,$$

$$(3.10) \quad k^2 = L(t^{n+\frac{1}{2}}) \left(u^n + \frac{\Delta t_n}{2} k^1 \right),$$

$$(3.11) \quad k^3 = L(t^{n+\frac{1}{2}}) \left(u^n + \frac{\Delta t_n}{2} k^2 \right),$$

$$(3.12) \quad k^4 = L(t^{n+1})(u^n + \Delta t_n k^3),$$

$$(3.13) \quad u^{n+1} = u^n + \frac{\Delta t_n}{6} [k^1 + 2k^2 + 2k^3 + k^4].$$

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 the following assumption.

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

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

We are now ready to make our main result, stating the following proposition.

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*

$$(3.15) \quad \Delta t_n \leq 2\eta(t^n),$$

and the following estimate holds:

$$(3.16) \quad |u^n| \leq e^{3Kt_n} |u^0|.$$

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 $L^n = L(t^n)$)

$$(3.17) \quad j^1 = L^n u^n,$$

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

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

$$(3.20) \quad j^4 = L^n (u^n + \Delta t_n j^3),$$

$$(3.21) \quad v^{n+1} = u^n + \frac{\Delta t_n}{6} [j^1 + 2j^2 + 2j^3 + j^4].$$

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

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

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,

$$(3.22) \quad |v^{n+1}| \leq |u^n|.$$

Next, we 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

$$(3.23) \quad k^1 - j^1 = 0,$$

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

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

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

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

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

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

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

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),

$$(3.29) \quad |k^4 - j^4| \leq \frac{\Delta t_n}{\eta(t^n)}|k^3 - j^3| + \frac{K \cdot \Delta t_n}{\eta(t^n)} \cdot \frac{\Delta t_n}{\eta(t^n)} \left(1 + \frac{\Delta t_n}{2\eta(t^n)}\right) |u^n|$$

$$\leq K \left(\left(\frac{\Delta t_n}{\eta(t^n)} \right)^3 + \left(\frac{\Delta t_n}{\eta(t^n)} \right)^2 \right) |u^n| \leq 12K|u^n|.$$

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))

$$|u^{n+1}| \leq |v^{n+1}| + \frac{\Delta t_n}{6} \left[2K|u^n| + 4K|u^n| + 12K|u^n| \right]$$

$$\leq (1 + 3K\Delta t_n)|u^n|$$

and the result (3.16) follows. \square

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

$$(4.1) \quad u^{(1)} = u^n + \Delta t L(u^n),$$

$$u^{n+1} = \frac{1}{2}u^n + \frac{1}{2}u^{(1)} + \frac{1}{2}\Delta t L(u^{(1)}),$$

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

$$(4.2) \quad u^{(1)} = u^n + \Delta t L(u^n),$$

$$u^{(2)} = \frac{3}{4}u^n + \frac{1}{4}u^{(1)} + \frac{1}{4}\Delta t L(u^{(1)}),$$

$$u^{n+1} = \frac{1}{3}u^n + \frac{2}{3}u^{(2)} + \frac{2}{3}\Delta t L(u^{(2)}),$$

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 $\beta_{i,k}$, as demonstrated in the following proposition.

PROPOSITION 4.2 (see [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 an SSP method that 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

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

with a CFL coefficient $c = 0.936$ in (2.13). Notice that two \tilde{L} 's must be computed. The effective CFL coefficient, compared 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 four stage, fourth-order SSP Runge–Kutta method.

4.2. Low Storage Methods. Storage is usually an important consideration for large scale scientific computing in three space dimensions. Therefore, low-storage Runge–Kutta methods [23], [1], which only require two storage units per ODE variable, may be desirable. Here we review the results presented in [6] concerning SSP properties among such low-storage Runge–Kutta methods.

The general low-storage Runge–Kutta schemes can be written in the form [23], [1]

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

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

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

$$\begin{aligned}
B_2 &= \frac{12c(c-1)(3z_2 - z_1) - (3z_2 - z_1)^2}{144c(3c-2)(c-1)^2}, \\
B_3 &= \frac{-24(3c-2)(c-1)^2}{(3z_2 - z_1)^2 - 12c(c-1)(3z_2 - z_1)}, \\
A_2 &= \frac{-z_1(6c^2 - 4c + 1) + 3z_3}{(2c+1)z_1 - 3(c+2)(2c-1)^2}, \\
A_3 &= \frac{-z_1z_4 + 108(2c-1)c^5 - 3(2c-1)z_5}{24z_1c(c-1)^4 + 72cz_6 + 72c^6(2c-13)},
\end{aligned}$$

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 Multistep Runge–Kutta Methods. Hybrid multistep Runge–Kutta methods (e.g., [10], [14]) are methods that combine the properties of Runge–Kutta and multistep methods. We explore the two-step, two-stage method

$$(4.5) \quad u^{n+\frac{1}{2}} = \alpha_{21}u^n + \alpha_{20}u^{n-1} + \Delta t (\beta_{20}L(u^{n-1}) + \beta_{21}L(u^n)), \quad \alpha_{2k} \geq 0,$$

$$u^{n+1} = \alpha_{30}u^{n-1} + \alpha_{31}u^{n+\frac{1}{2}} + \alpha_{32}u^n$$

$$(4.6) \quad + \Delta t (\beta_{30}L(u^{n-1}) + \beta_{31}L(u^{n+\frac{1}{2}}) + \beta_{32}L(u^n)), \quad \alpha_{3k} \geq 0.$$

Clearly, this method is SSP under the CFL coefficient (2.10) if $\beta_{i,k} \geq 0$. 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 three-parameter family (depending on c , α_{30} , and α_{31}):

$$\begin{aligned}
\alpha_{20} &= 3c^2 + 2c^3, \\
\beta_{20} &= c^2 + c^3, \\
\alpha_{21} &= 1 - 3c^2 - 2c^3, \\
\beta_{21} &= c + 2c^2 + c^3, \\
(4.7) \quad \beta_{30} &= \frac{2 + 2\alpha_{30} - 3c + 3\alpha_{30}c + \alpha_{31}c^3}{6(1+c)}, \\
\beta_{31} &= \frac{5 - \alpha_{30} - 3\alpha_{31}c^2 - 2\alpha_{31}c^3}{6c + 6c^2}, \\
\alpha_{32} &= 1 - \alpha_{31} - \alpha_{30}, \\
\beta_{32} &= \frac{-5 + \alpha_{30} + 9c + 3\alpha_{30}c - 3\alpha_{31}c^2 - \alpha_{31}c^3}{6c}.
\end{aligned}$$

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 hoped 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.

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) to be

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

The requirement $\alpha_{21} \geq 0$ enforces (see (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} give 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. \square

5. Linear and Nonlinear Multistep Methods. In this section we review and further study SSP explicit multistep methods (2.14), which were first developed in [19]. These methods are r th-order accurate if

$$(5.1) \quad \sum_{i=1}^m \alpha_i = 1, \\ \sum_{i=1}^m i^k \alpha_i = k \left(\sum_{i=1}^m i^{k-1} \beta_i \right), \quad k = 1, \dots, r.$$

We first prove a proposition that sets the minimum number of steps in our search for SSP multistep methods.

PROPOSITION 5.1. *For $m \geq 2$, there is no m -step, m th-order SSP method with all nonnegative 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 th-order accurate method

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

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 $i = 1, \dots, m$, and equality holds only for $i = m$. On the other hand, $p'(i) = m(1-i)(m-i)^{m-2} \leq 0$, and 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 nonnegative, 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 lead to $\beta_m = m$ and $2\beta_m = m$, which cannot be simultaneously satisfied.

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

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

Clearly $p'(i) = q(i) = 0$ for $i = 1, \dots, m$. We also claim (and prove below) that all the $p(i)$'s, $i = 1, \dots, m$, 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 following claim.

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

Indeed, $q(t)$ oscillates between being positive on the even intervals $I_0 = (0, 1)$, $I_2 = (2, 3)$, \dots , and being negative on the odd intervals, $I_1 = (1, 2)$, $I_3 = (3, 4)$, \dots . 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 $\lfloor (m+1)/2 \rfloor$ intervals,

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

$$2k+1 \leq (m+1)/2.$$

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

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

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 the second integral starts with a negative contribution from its first integrand on the odd interval I_{m+1-i} , while the remaining terms that follow cancel in pairs as before. A straightforward computation shows that this first negative contribution is compensated for by the positive gain from the first pair, i.e.,

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

This concludes the proof of our claim. \square

Table 5.1 *SSP multistep methods (2.14).*

#	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	$\frac{7}{20}, \frac{3}{10}, \frac{4}{15}, 0, \frac{7}{120}, \frac{1}{40}$	$\frac{291201}{108000}, -\frac{198401}{86400}, \frac{88063}{43200}, 0, -\frac{17969}{43200}, \frac{73061}{432000}$

We remark that [4] contains a result stating that there are no linearly stable m -step, $(m+1)$ st-order methods 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, $(m-1)$ st-order SSP methods with positive β_i .

For two-step, second-order SSP methods, a scheme was given in [19] 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

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

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 $\alpha_1 = \frac{4}{5}$. \square

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 [19] with a CFL coefficient $c = \frac{1}{2}$ (scheme 2 in Table 5.1). We prove this is optimal in the CFL coefficient in the following proposition. We remark that this multistep 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

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

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

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

Thus, we would have a negative β . \square

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 [19] 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 [19] with a CFL coefficient $c = \frac{1}{3}$ (scheme 6 in Table 5.1). We prove this is optimal in the CFL coefficient in the following proposition. We remark again that this multistep 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

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

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

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

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 . \square

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 [19] 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).

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 as the following five-parameter family:

$$\begin{aligned}\alpha_5 &= 1 - \alpha_1 - \alpha_2 - \alpha_3 - \alpha_4, & \beta_1 &= \frac{1}{24} (55 + 9\alpha_2 + 8\alpha_3 + 9\alpha_4 + 24\beta_5), \\ \beta_2 &= \frac{1}{24} (5 - 64\alpha_1 - 45\alpha_2 - 32\alpha_3 - 37\alpha_4 - 96\beta_5), \\ \beta_3 &= \frac{1}{24} (5 + 32\alpha_1 + 27\alpha_2 + 40\alpha_3 + 59\alpha_4 + 144\beta_5), \\ \beta_4 &= \frac{1}{24} (55 - 64\alpha_1 - 63\alpha_2 - 64\alpha_3 - 55\alpha_4 - 96\beta_5).\end{aligned}$$

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 belief 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 [19] 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 [19], a scheme with CFL coefficient $c = 0.130$, scheme 15 in Table 5.1.

We list in Table 5.1 the multistep 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 methods.

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

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

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

$$(6.2) \quad C_{j+\frac{1}{2}} \geq 0, \quad D_{j-\frac{1}{2}} \geq 0,$$

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

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

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

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

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

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 that 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:

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

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

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

To obtain an SSP scheme from (6.4) we would require $\alpha_{2,0}$ and $\alpha_{2,1}$ to be nonnegative. 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 nonoscillatory property of the backward Euler method, despite the same underlying nonoscillatory spatial discretization. We solve the simple linear wave equation

$$(6.5) \quad u_t = u_x$$

with a step-function initial condition:

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

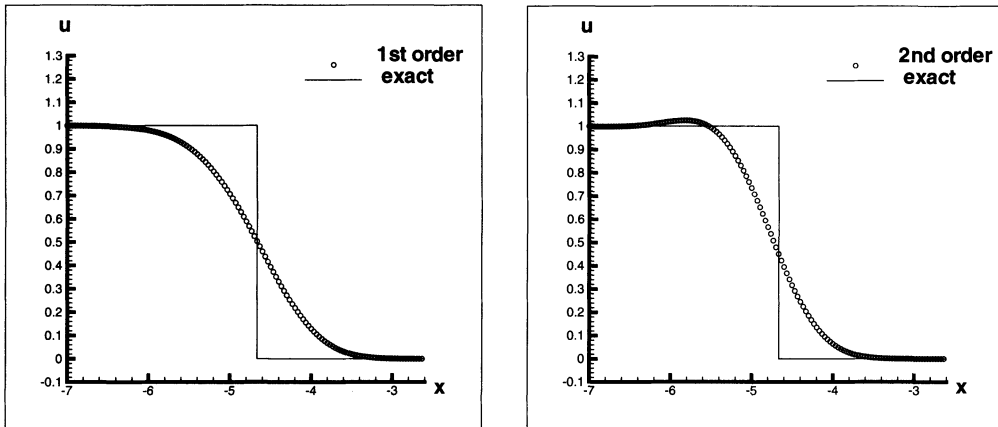


Fig. 6.1 First-order upwind spatial discretization. Solution after 100 time steps at CFL number $\frac{\Delta t}{\Delta x} = 1.4$. Left: First-order backward Euler time discretization; right: non-SSP second-order implicit Runge-Kutta time discretization (6.3)–(6.4) with $\beta_1 = 2$.

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

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

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 Figure 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 Figure 6.1 that the solution is oscillatory.

In the next two subsections we discuss the rather disappointing negative results about the nonexistence of high-order SSP Runge–Kutta or multistep methods.

6.2. Implicit Runge–Kutta Methods. A general implicit Runge–Kutta method for (2.1) can be written in the form

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

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

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

is unconditionally strongly stable, $\|u^{n+1}\| \leq \|u^n\|$, 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:

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

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 1.

PROPOSITION 6.2. *If (6.7) is at least second-order accurate, then $\alpha_{i,k}$ cannot be all nonnegative.*

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

$$(6.10) \quad \sum_{k=0}^{i-1} \alpha_{i,k} = 1, \quad X_m = 1, \quad Y_m = \frac{1}{2},$$

where X_m and Y_m can be recursively defined as

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

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

$$(6.12) \quad X_m - Y_m < \frac{1}{2},$$

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

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

where

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

It is easy to show that (6.14) implies

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

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

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

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

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

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

We remark that the proof of Proposition 6.2 can be simplified, using existing ODE results in [5], if all β_i 's are nonnegative or all β_i 's are nonpositive. 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 Multistep Methods. For our purpose, a general implicit multistep method for (2.1) can be written in the form

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

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 multistep 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 were replaced by \tilde{L} .

Unfortunately, we have the following negative result which completely rules out the existence of SSP implicit multistep schemes (6.16) of order higher than 1.

PROPOSITION 6.3. *If (6.16) is at least second-order accurate, then α_i cannot be all nonnegative.*

Proof. Second order accuracy implies

$$(6.17) \quad \sum_{i=1}^m \alpha_i = 1, \quad \sum_{i=1}^m i\alpha_i = \beta_0, \quad \sum_{i=1}^m i^2\alpha_i = 0.$$

The last equality in (6.17) implies that α_i cannot be all nonnegative. \square

7. Concluding Remarks. We have systematically studied SSP time discretization methods, which preserve stability, in any norm, of the forward Euler (for explicit methods) or the backward Euler (for implicit methods) first-order time discretizations. Runge–Kutta and multistep methods are both investigated. The methods listed here can be used for method of lines numerical schemes for PDEs, especially for hyperbolic problems.

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