A Strong Stability Preserving Analysis for Multistage Two-Derivative Time-Stepping Schemes Based on Taylor Series Conditions.

Zachary Grant\textsuperscript{1,*}, Sigal Gottlieb\textsuperscript{1}, David C. Seal\textsuperscript{2}
\textsuperscript{1}Department of Mathematics, University of Massachusetts, Dartmouth
\textsuperscript{2}Department of Mathematics, U.S. Naval Academy.

Abstract

High order strong stability preserving (SSP) time discretizations are often needed to ensure the nonlinear non-inner-product strong stability properties of spatial discretizations specially designed for the solution of hyperbolic PDEs. Multiderivative time-stepping methods have recently been increasingly used for evolving hyperbolic PDEs, and the strong stability properties of these methods are of new interest. In our prior work we explored time discretizations that preserve the strong stability properties of spatial discretizations coupled with forward Euler and a second derivative formulation. However, many spatial discretizations do not satisfy strong stability properties when coupled with this second derivative formulation, but rather with a more natural Taylor series formulation. In this work we demonstrate sufficient conditions for a two-derivative multistage method to preserve the strong stability properties of spatial discretizations in a forward Euler and Taylor series formulation. We call these strong stability preserving (SSP) Taylor series (TS) methods. We also prove that the maximal order of SSP TS methods is $p = 6$, and define an optimization procedure that allows us to find such SSP methods. Several types of these methods are presented and their efficiency compared. Finally, These methods are tested on several PDEs to demonstrate the benefit of these SSP TS methods, the need for the SSP property, and the sharpness of the SSP time-step in many cases.

1 Introduction

The solution to a hyperbolic conservation law

\[ U_t + f(U)_x = 0, \]  

may develop sharp gradients or discontinuities, which results in significant challenges to the numerical simulation of such problems. To ensure that it can handle the presence of a discontinuity, a spatial discretization is carefully designed to satisfy some nonlinear non-inner-product stability properties, such as total variation diminishing, maximum norm preserving, or positivity preserving properties, for example. The development of high order spatial discretizations that can handle discontinuities is a major research area [6, 16, 28, 30, 35, 46, 47, 48, 4, 49, 54].

When the partial differential equation (1) is semi-discretized we obtain the ordinary differential equation (ODE)

\[ u_t = F(u), \]  

(2)

(where $u$ is a vector of approximations to $U$). This formulation is often referred to as a method of lines (MOL) formulation, and has the advantage of decoupling the spatial and time-discretizations. The spatial
discretizations designed to handle discontinuities ensure that when the semi-discretized equation (2) is evolved using a forward Euler method

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

where $u^n$ is a discrete approximation to $U$ at time $t^n$) the numerical solution satisfies the desired strong stability property, such as total variation stability or positivity. If the desired nonlinear non-inner-product stability property such as a norm, semi-norm, or convex functional, is represented by $\| \cdot \|$, the spatial discretization satisfies the monotonicity property

$$\|u^n + \Delta t F(u^n)\| \leq \|u^n\|,$$

(4)

under the time-step restriction

$$0 \leq \Delta t \leq \Delta t_{FE}.$$  

(5)

In practice, in place of the first order time discretization (3), we typically require a higher-order time integrator, that preserves the strong stability property

$$\|u^{n+1}\| \leq \|u^n\|,$$

(6)

perhaps under a modified time-step restriction. Strong stability preserving (SSP) time-discretizations were developed to address this need. SSP multistep and Runge–Kutta methods satisfy the strong stability property (6) for any function $F$, any initial condition, and any convex functional $\| \cdot \|$ under some time-step restriction, provided only that (4) is satisfied.

Recently, there has been interest in exploring the SSP properties of multi-stage multiderivative methods. Multistage multiderivative methods were first considered in [33, 51, 45, 40, 41, 21, 22, 31, 34, 3], and recently have been explored for use with partial differential equations (PDEs) [39, 50, 29, 36, 9]. These methods have a form similar to Runge–Kutta methods but use an additional derivative $U_{tt} \approx \ddot{F}$ to allow for higher order. The SSP properties of these methods were discussed in [5, 32]. In [5], a method was defined as SSP if it satisfies the strong stability property (6) for any function $F$, any initial condition, and any convex functional $\| \cdot \|$ under some time-step restriction, provided that (4) is satisfied for any $\Delta t \leq \Delta t_{FE}$ and an additional condition of the form

$$\|u^n + \Delta t^2 \ddot{F}(u^n)\| \leq \|u^n\|$$

is satisfied for any $\Delta t \leq \tilde{K} \Delta t_{FE}$. These conditions allow us to find a wide variety of SSP time-discretizations, but they limit the type of spatial discretization that can be used in this context.

In this paper, we present a different approach to the SSP analysis, which is more along the lines of the idea in [32]. For this analysis, we use, as before, the forward Euler base condition (4), but add to it a Taylor series condition of the form

$$\|u^n + \Delta t F(u^n) + \frac{1}{2} \Delta t^2 \ddot{F}(u^n)\| \leq \|u^n\|$$

that holds for any $\Delta t \leq K \Delta t_{FE}$. Compared to those studied in [5], this pair of base conditions allows for more flexibility in the choice of spatial discretizations (such as the methods that satisfy a Taylor series condition in [10, 37, 7, 39]), at the cost of more limited variety of time discretizations. The goal of this paper is to study a class of methods that is suitable for use with existing spatial discretizations, and present
families of such methods that are optimized for the relationship between the forward-Euler time-step $\Delta t_{FE}$ and the Taylor series timestep $K\Delta t_{FE}$.

In the following subsections we describe SSP multistep and multistage time discreizations and explain multistage two derivative methods. We then motivate the need for methods that preserve the nonlinear stability properties of the forward Euler and Taylor series base conditions. In Section 2 we formulate the SSP optimization problem for finding two-derivative methods which can be written as the convex combination of forward Euler and Taylor series steps with the largest allowable time-step, which we will later use to find optimized methods. In Subsection 2.2 we prove that there are order barriers associated with two derivative methods that preserve the properties of forward Euler and Taylor series steps with a positive time-step. In Section 2.3 we present the SSP coefficients of the optimized methods we obtain. The methods themselves can be downloaded from our github repository \[14\]. In Section 3 we demonstrate how these methods perform on specially selected test cases, and in Section 4 we present our conclusions.

1.1 SSP methods

It is well-known \[42, 13\] that some multi-step and Runge–Kutta methods can be decomposed into convex combinations of forward Euler steps, so that any convex functional property satisfied by (4) will be preserved by these higher-order time discretizations. If we re-write the s-stage explicit Runge–Kutta method in the form \[43\],

\[
\begin{align*}
  y^{(0)} &= u^n, \\
  y^{(i)} &= \sum_{j=0}^{i-1} \left( \alpha_{i,j} y^{(j)} + \Delta t \beta_{i,j} F(y^{(j)}) \right), \quad i = 1, ..., s \\
  u^{n+1} &= y^{(s)}
\end{align*}
\]

(7)

it is clear that if all the coefficients $\alpha_{i,j}$ and $\beta_{i,j}$ are non-negative, and provided $\alpha_{i,j}$ is zero only if its corresponding $\beta_{i,j}$ is zero, then each stage can be written as a convex combination of forward Euler steps of the form (3), and be bounded by:

\[
\|y^{(i)}\| \leq \sum_{j=0}^{i-1} \left( \alpha_{i,j} \|y^{(j)}\| + \Delta t \beta_{i,j} \|F(y^{(j)})\| \right) \\
\leq \sum_{j=0}^{i-1} \alpha_{i,j} \|y^{(j)}\| + \Delta t \sum_{j=0}^{i-1} \beta_{i,j} \|F(y^{(j)})\| \\
\leq \sum_{j=0}^{i-1} \alpha_{i,j} \|y^{(j)}\|
\]

under the condition $\frac{\beta_{i,j}}{\alpha_{i,j}} \Delta t \leq \Delta t_{FE}$. By the consistency condition $\sum_{j=0}^{i-1} \alpha_{i,j} = 1$, we now have $\|u^{n+1}\| \leq \|u^n\|$, under the condition

\[
\Delta t \leq C \Delta t_{FE} \quad \text{where} \quad C = \min_{i,j} \frac{\alpha_{i,j}}{\beta_{i,j}}
\]

(8)

where if any of the $\beta$s are equal to zero, the corresponding ratios are considered infinite.

If a method can be decomposed into such a convex combination of (3), with a positive value of $C > 0$ then the method is called strong stability preserving (SSP), and the value $C$ is called the SSP coefficient.
SSP methods guarantee the strong stability properties of any spatial discretization, provided only that these properties are satisfied when using the forward Euler method. The convex combination approach guarantees that the intermediate stages in a Runge–Kutta method satisfy the desired strong stability property as well. The convex combination approach clearly provides a sufficient condition for preservation of strong stability. Moreover, it has also been shown that this condition is necessary [11, 12, 17, 18].

Second and third order explicit Runge–Kutta methods [43] and later fourth order methods [44, 23] were found that admit such a convex combination decomposition with $C > 0$. However, it has been proven that explicit Runge–Kutta methods with positive SSP coefficient cannot be more than fourth-order accurate [27, 38].

The time-step restriction (8) is comprised of two distinct factors: (1) the term $\Delta t_{FE}$ that is a property of the spatial discretization, and (2) the SSP coefficient $C$ that is a property of the time-discretization. Research on SSP time-stepping methods for hyperbolic PDEs has primarily focused on finding high-order time discretizations with the largest allowable time-step $\Delta t \leq C \Delta t_{FE}$ by maximizing the SSP coefficient $C$ of the method.

Higher order methods can also be obtained by adding more steps (e.g. linear multistep methods) or more derivatives (Taylor series methods). Multistep methods that are SSP have been found [13], and explicit multistep SSP methods exist of very high order $p > 4$, but have severely restricted SSP coefficients [13]. These approaches can be combined with Runge–Kutta methods to obtain methods with multiple steps, and stages. Explicit multistage multistage methods that are SSP and have order $p > 4$ have been developed as well [24, 1].

### 1.2 Multistage two derivative methods

In this work, we consider explicit multistage two-derivative time integrators as applied to the numerical solution of hyperbolic conservation laws. Using the ODEs (2) resulting from the spatial discretization of a hyperbolic PDE of the form (1), we define the one-stage, two-derivative building block method $u^{n+1} = u^n + \alpha \Delta t F(u^n) + \beta \Delta t^2 \dot{F}(u^n)$ where $\alpha \geq 0$ and $\beta \geq 0$ are the coefficients of the method. This method can be at most second order, with coefficients $\alpha = 1$ and $\beta = \frac{1}{2}$: the well-known second-order Taylor series method.

Higher order explicit methods can be obtained by and adding more stages:

$$y^{(i)} = u^n + \Delta t \sum_{j=1}^{i-1} a_{ij} F(y^{(j)}) + \Delta t^2 \sum_{j=1}^{i-1} \hat{a}_{ij} \dot{F}(y^{(j)}), \quad i = 2, \ldots, s$$

$$u^{n+1} = u^n + \Delta t \sum_{j=1}^{s} b_j F(y^{(j)}) + \Delta t^2 \sum_{j=1}^{i-1} \hat{b}_j \dot{F}(y^{(j)}),$$

where $y^{(1)} = u^n$. The coefficients can be put into matrix vector form, where

$$A = \begin{pmatrix} 0 & 0 & \vdots & 0 \\ a_{21} & 0 & \vdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ a_{s1} & a_{s2} & \vdots & 0 \end{pmatrix}, \quad \hat{A} = \begin{pmatrix} 0 & 0 & \vdots & 0 \\ \hat{a}_{21} & 0 & \vdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ \hat{a}_{s1} & \hat{a}_{s2} & \vdots & 0 \end{pmatrix}, \quad b = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_s \end{pmatrix}, \quad \hat{b} = \begin{pmatrix} \hat{b}_1 \\ \hat{b}_2 \\ \vdots \\ \hat{b}_s \end{pmatrix}.$$
We also define additional vectors \( c = A e \) and \( \hat{c} = \hat{A} e \), where \( e \) is a vector of ones.

As in our prior work \([5]\), we focus on using multistage two-derivative methods as time integrators for evolving hyperbolic PDEs in time. For our purposes, the operator \( F \) is obtained by a spatial discretization of the term \( U_t = -f(U)_x \) to obtain the system \( u_t = F(u) \). Instead of computing the second derivative term \( \dot{F} \) directly from the definition of the spatial discretization \( F \), we employ the Cauchy-Kowalevskaya procedure which uses the PDE (1) to replace the time derivatives by the spatial derivatives, and discretize these in space. If the term \( F(u) \) is computed using a conservative spatial discretization \( D_x \) applied to the flux:

\[
F(u) = -D_x(f(u)),
\]

then we approximate

\[
F(u)_t = u_{tt} \approx U_{tt} = -f(U)_{xt} = -(f(U))_t_x = -(f'(U)U_t)_x \approx -\hat{D}_x (f'(u)u_t),
\]

where a (potentially different) spatial differentiation operator \( \hat{D}_x \) is used. Although these two approaches are different, the differences between them are of high order in space, so that in practice, as long as the spatial errors are smaller than the temporal errors, we see the correct order of accuracy in time, as shown in \([5]\).

1.3 Motivation for the new base conditions for SSP analysis

In \([5]\) we considered multistage two-derivative methods and developed sufficient conditions for strong stability preservation for these methods. We showed that explicit SSP methods within this class can break this well-known order barrier for explicit Runge–Kutta methods. In that work we considered two derivative methods that preserve the strong stability property satisfied by a function \( F \) under a convex functional \( \| \cdot \| \), provided that the conditions:

Forward Euler condition: \( \| u^n + \Delta t F(u^n) \| \leq \| u^n \| \) for \( \Delta t \leq \Delta t_{FE} \),

and

Second derivative condition: \( \| u^n + \Delta t^2 \dot{F}(u^n) \| \leq \| u^n \| \) for \( \Delta t \leq \hat{K} \Delta t_{FE} \),

where \( K \) is a scaling factor that compares the stability condition of the second derivative term to that of the forward Euler term. While the forward Euler condition is characteristic of all SSP methods (and has been justified by the observation that it is the circle contractivity condition in \([11]\)), the second derivative condition was chosen over the Taylor series condition:

Taylor series condition: \( \| u^n + \Delta t F(u^n) + \frac{1}{2} \Delta t^2 \dot{F}(u^n) \| \leq \| u^n \| \) for \( \Delta t \leq K \Delta t_{FE} \),

because it is more general. If the forward Euler (12) and second derivative (13) conditions are both satisfied, then the Taylor series condition (14) will be satisfied as well. Furthermore, some methods of interest and importance in the literature cannot be written using a Taylor series decomposition, most notably the unique two-stage fourth order method

\[
y^{(1)} = u^n + \frac{1}{2} \Delta t F(u^n) + \frac{1}{8} \Delta t^2 \dot{F}(u^n)
\]

\[
u^{n+1} = u^n + \Delta t F(u^n) + \frac{1}{6} \Delta t^2 \dot{F}(u^n) + \frac{1}{3} \Delta t^2 \dot{F}(y^{(1)})
\]
which appears commonly in the literature on this subject \cite{29, 36, 9}. For these reasons, it made sense to consider the pair of base conditions (12) and (13) first. If a spatial discretization satisfies (12) and (13) it will also satisfy (14), so that the base conditions considered in \cite{5} allow for the most general time-discretizations.

However, as we will see in the example below, there are spatial discretizations for which the second derivative condition (13) is not satisfied but the forward Euler condition (12) and the Taylor series condition (14) are both satisfied. In such cases, the methods derived in \cite{5} may not preserve the strong stability properties of such spatial discretizations. The existence of such spatial discretization is the main motivation for the current work, in which we re-examine the strong stability properties of the MDRK method (9) using the base conditions (12) and (14). This approach increases our flexibility in the choice of spatial discretization, allowing the formulation of time discretization that are SSP for a wide variety of spatial discretizations with desirable nonlinear non-inner-product stability properties. Of course, this enhanced flexibility in the choice of spatial discretization is expected to result in limitations on the time-discretization (e.g. the two-stage fourth order method method is not SSP in this sense).

To illustrate the need for time-discretizations that preserve the strong stability properties of spatial discretizations that satisfy (12) and (14), but not (13), consider the one-way wave equation

\[ U_t = U_x \]

(here \( f(U) = U \)) where \( F \) is defined by the first-order upwind method

\[ F(u^n)_j := \frac{1}{\Delta x} (u^n_{j+1} - u^n_j) \approx U_x(x_j), \quad (17) \]

and \( \hat{F} \) is computed by simply applying the differentiation operator twice (note that \( f'(U) = 1 \))

\[ \hat{F} := \frac{1}{\Delta x^2} (u^n_{j+2} - 2u^n_{j+1} + u^n_j). \quad (18) \]

We note that when computed this way, the spatial discretization \( F \) coupled with forward Euler satisfies the total variation diminishing condition:

\[ \|u^n + \Delta t F(u^n)\|_{TV} \leq \|u^n\|_{TV} \quad \text{for} \quad \Delta t \leq \Delta x, \quad (19) \]

while the Taylor series term using \( F \) and \( \hat{F} \) satisfies the strong stability condition

\[ \|u^n + \Delta t F(u^n) + \frac{1}{2} \Delta t^2 \hat{F}(u^n)\|_{TV} \leq \|u^n\|_{TV} \quad \text{for} \quad \Delta t \leq \Delta x. \quad (20) \]

In other words, these spatial discretizations satisfy the conditions (12) and (14) with \( K = 1 \), in the total variation semi-norm. However, (13) is not satisfied. The methods derived in \cite{5} do not guarantee the preservation of the total variation diminishing property of the numerical solution for this spatial discretization, because (18) does not satisfy the second derivative condition (13) in the total variation semi-norm. Our goal in the current work is to develop time discretizations that will preserve the desired strong stability properties (e.g. the total variation diminishing property) when using spatial discretizations such as the upwind approximation (18) that satisfy (12) and (14) but do not require that (13) be satisfied.

In this work we develop two-derivative multistage methods of the form (9) that can be written as convex combinations of forward Euler and Taylor series terms, and so preserve the convex functional properties
satisfied by these two terms. We can easily see that when spatial discretizations \( F \) and \( \dot{F} \) that satisfy (12) and (14) are coupled with such a time-stepping method, then the strong stability condition

\[
\| u^{n+1} \| \leq \| u^n \|
\]

will be preserved, perhaps under a different time-step condition

\[
\Delta t \leq C \Delta t_{FE}.
\]  

(21)

If a method can be decomposed in such a way, with \( C > 0 \) we say that it is SSP. It is important to distinguish these methods, which are convex combinations on (12) and (14) from the ones in [5] which are convex combinations on (12) and (13). When necessary to make this distinction clear, we will refer to the methods in this work as TS methods and the methods in our previous work as MSRK methods.

In the next section, we define an optimization problem that will allow us to find methods of the form (9) that can be decomposed into convex combinations of forward Euler and Taylor series terms, that preserve the strong stability properties (12) and (14) with the largest possible SSP coefficient \( C \).

2 Optimized methods

2.1 Formulating the SSP optimization problem

We consider the system of ODEs

\[
u_t = F(u)
\]  

(22)

resulting from a semi-discretization of the hyperbolic conservation law (1) such that \( F \) satisfies the forward Euler (first derivative) condition (12)

**Forward Euler condition:** \( \| u^n + \Delta t F(u^n) \| \leq \| u^n \| \) for \( \Delta t \leq \Delta t_{FE} \),

for the desired stability property indicated by the convex functional \( \| \cdot \| \).

The methods we are interested in also require an appropriate approximation to the second derivative in time

\[\dot{F} \approx u_{tt}.\]

We assume in this work that this second derivative operator satisfies an additional condition of the form (14)

**Taylor series condition:** \( \| u^n + \Delta t F(u^n) + \frac{1}{2} \Delta t^2 \dot{F}(u^n) \| \leq \| u^n \| \) for \( \Delta t \leq K \Delta t_{FE} \),

in the same convex functional \( \| \cdot \| \), where \( K \) is a scaling factor that compares the stability condition of the Taylor series term to that of the forward Euler term.

We wish to show that given conditions (12) and (14), the multi-derivative method (9) satisfies the desired monotonicity condition under a given time-step. This is easier if we re-write the method (9) in an equivalent matrix-vector form

\[
y = eu^n + \Delta t SF(y) + \Delta t^2 \dot{S} \dot{F}(y),
\]  

(23)
where $y = (y^{(1)}, y^{(2)}, \ldots, y^{(s)}, u^{n+1})^T$, 

$$S = \begin{bmatrix} A & 0 \\ b^T & 0 \end{bmatrix} \quad \text{and} \quad \hat{S} = \begin{bmatrix} \hat{A} & 0 \\ \hat{b}^T & 0 \end{bmatrix}$$

and $e$ is a vector of ones. As in prior SSP work, we require that all the coefficients in $S$ and $\hat{S}$ be non-negative. This allows us to easily establish sufficient conditions for a method of this form to be SSP.

**Theorem 1.** Given spatial discretizations $F$ and $\hat{F}$ that satisfy (12) and (14), a two-derivative multi-stage method of the form (23) preserves the strong stability property $\|u^{n+1}\| \leq \|u^n\|$ under the time-step restriction $\Delta t \leq r\Delta t_{FE}$ if it satisfies the conditions

$$
\begin{align*}
&\left(I + rS + \frac{2r^2}{K^2} (1 - K) \hat{S}\right)^{-1} e \geq 0 \\
r \left(I + rS + \frac{2r^2}{K^2} (1 - K) \hat{S}\right)^{-1} \left(S - \frac{2r}{K} \hat{S}\right) \geq 0 \\
&\frac{2r^2}{K^2} \left(I + rS + \frac{2r^2}{K^2} (1 - K) \hat{S}\right)^{-1} \hat{S} \geq 0
\end{align*}
$$

for some $r > 0$. In the above conditions, the inequalities are understood component-wise.

**Proof.** We begin with the method

$$y = eu^n + \Delta t SF(y) + \Delta t^2 \hat{S} \hat{F}(y),$$

and add the terms $rS\hat{y}$ and $2\hat{r}(\hat{r} - r)\hat{S}\hat{y}$ to both sides to obtain

$$
\begin{align*}
(I + rS + 2\hat{r}(\hat{r} - r)\hat{S})y &= u^n e + r(S - 2\hat{S}) \left(y + \frac{\Delta t}{r} F(y)\right) \\
&+ 2\hat{r}^2 \hat{S} \left(y + \frac{\Delta t}{r} F(y) + \frac{\Delta t^2}{2\hat{r}^2} \hat{F}(y)\right), \\
y &= R(eu^n) + P \left(y + \frac{\Delta t}{r} F(y)\right) + Q \left(y + \frac{\Delta t}{r} F(y) + \frac{\Delta t^2}{2\hat{r}^2} \hat{F}(y)\right),
\end{align*}
$$

where

$$R = \left(I + rS + 2\hat{r}(\hat{r} - r)\hat{S}\right)^{-1}, \quad P = rR \left(S - 2\hat{S}\right), \quad Q = 2\hat{r}^2 R \hat{S}.$$ 

If the elements of $P$, $Q$, and $Re$ are all non-negative, and if $(R + P + Q) e = e$, then these three terms describe a convex combination of terms which are SSP, and the resulting value is SSP as well

$$\|y\| \leq R\|eu^n\| + P\|y + \frac{\Delta t}{r} F(y)\| + Q\|y + \frac{\Delta t}{r} F(y) + \frac{\Delta t^2}{2\hat{r}^2} \hat{F}(y)\|.$$

under the time-step restrictions $\Delta t \leq r\Delta t_{FE}$ and $\Delta t \leq K\hat{r}\Delta t_{FE}$. In such cases, the optimal time-step is given by the minimum of the two. In the cases we encounter here, this minimum occurs when these two values are set equal, so we require $r = K\hat{r}$. Conditions (24a)-(24c) now ensure that $P \geq 0$, $Q \geq 0$, and $Re \geq 0$ component-wise for $\hat{r} = \frac{r}{K}$, and so the method preserves the strong stability condition $\|u^{n+1}\| \leq \|u^n\|$ under the time-step restriction $\Delta t \leq r\Delta t_{FE}$.

\[\square\]
This theorem gives us the conditions for the method (23) to be SSP for any time-step $\Delta t \leq r \Delta t_{FE}$. Following [5, 13, 23, 25] we now formulate a search for optimal SSP two-derivative methods as:

Find the coefficient matrices $S$ and $\hat{S}$ that maximize the value of $C = \max r$

such that the relevant order conditions (summarized in Appendix A) and the SSP conditions (24a)-(24b) are all satisfied.

To accomplish this, we develop and use a MATLAB optimization code [14] (similar to Ketcheson’s code [26]) for finding optimal two-derivative multistage methods that preserve the SSP properties (12) and (14). The SSP coefficients of the optimized SSP multistage two-derivative methods of order up to $p = 6$ (for different values of $K$) are presented in Section 2.3. However, before we present the optimal methods we present the theoretical results on the allowable order of multistage multi-derivative methods that are SSP in the sense of Theorem 1 above.

2.2 Order barriers

Explicit SSP Runge–Kutta methods with $C > 0$ are known to have an order barrier of four, while the implicit methods have a barrier of six [13]. This follows from the fact that the order $p$ of irreducible methods with nonnegative coefficients depends on the stage order $q$ such that

$$q \geq \left\lfloor \frac{p - 1}{2} \right\rfloor.$$ 

For explicit Runge–Kutta methods the first stage is a forward Euler step, so $q = 1$ and thus $p \leq 4$, whereas for implicit Runge–Kutta methods the first stage is at most of order two, so that $q = 2$ and thus $p \leq 6$.

For two-derivative multistage methods, where the SSP condition is defined based on the forward Euler (12) and Taylor series (14) conditions in the section above, we find that similar results hold. A stage order of $q = 2$ is possible for explicit two-derivative methods (unlike explicit Runge–Kutta methods) because the first stage can be second order, i.e., a Taylor series method. However, since the first stage can be no greater than second order we have a bound on the stage order $q \leq 2$, which results in an order barrier of $p \leq 6$ for these methods. In the following results we establish these order barriers.

**Lemma 1.** Given a method of the form (9) which can be decomposed into a convex combination of the base conditions (12) and (14), we observe that if $b_j = 0$ then the corresponding $\hat{b}_j = 0$.

Proof. In any method (9) that can be decomposed into a convex combination of forward Euler and Taylor series terms, the appearance of a second derivative term $\dot{F}$ can only happen as part of a Taylor series term. This tells us that the $\dot{F}$ must be accompanied by the corresponding $F$, meaning that whenever we have a nonzero $\hat{a}_{ij}$ or $\hat{b}_j$ term, the corresponding $a_{ij}$ or $b_j$ term must be nonzero.

**Lemma 2.** Any method of the form (9) that can be written as a convex combination of the forward Euler formula (12) and the Taylor series formula (14) can also be written as a convex combination of the forward Euler formula (12) and the second derivative formula (13).

Proof. We can easily see that any Taylor series step can be rewritten as a convex combination of the forward Euler formula (12) and the second derivative formula (13):

$$u^n + \Delta t F(u^n) + \frac{1}{2} \Delta t^2 \dot{F}(u^n) = \alpha \left( u^n + \frac{\Delta t}{\alpha} F(u^n) \right) + (1 - \alpha) \left( u^n + \frac{1}{2(1 - \alpha)} \Delta t^2 \dot{F}(u^n) \right),$$

9
for any $0 < \alpha < 1$. Clearly then, if a method can be decomposed into a convex combination of (12) and (14), and in turn (14) can be decomposed into a convex combination of (12) and (13), then the method itself can be written as a convex combination of (12) and (13).

**Remark 1.** This result is simply a recognition that the methods found in this paper are a subset of the methods in our previous paper [5]. The difference between the methods we found in [5] and the methods in this work is that while the methods in [5] require that the conditions (12) and (13) are satisfied, our new methods will still satisfy the strong stability conditions even if the second derivative condition (13) is not satisfied, as long as (12) and (14) are.

**Lemma 3.** Any method of the form (9) that can be written as a convex combination of (12) and (13) must satisfy the (componentwise) condition

$$b + \hat{b} > 0.$$  

**Proof.** This result is due to Higueras [19], who performed SSP analysis on additive Runge–Kutta methods of the form

\[
y^{(i)} = u^n + \Delta t \sum_{j=1}^{s} a_{ij} F(y^{(j)}) + \Delta t \sum_{j=1}^{s} \hat{a}_{ij} G(y^{(j)}), \quad i = 1, \ldots, s \tag{25}
\]

\[
u^{n+1} = u^n + \Delta t \sum_{j=1}^{s} b_j F(y^{(j)}) + \Delta t \sum_{j=1}^{s} \hat{b}_j G(y^{(j)}),
\]

for solving the ODE $u' = F(u) + G(u)$. Higueras showed that if a method (25) can be decomposed into a convex combination of forward Euler type steps

$$u^n + \frac{\Delta t}{r} F(u^n) \quad \text{and} \quad u^n + \frac{\Delta t}{\hat{r}} G(u^n)$$

(for some non-negative $r$ and $\hat{r}$) then it must have $b + \hat{b} > 0$. In our case, we simply let $G = \Delta t F$ and the result follows.

**Corollary 1.** Any method of the form (9) that can be written as a convex combination of (12) and (14) must satisfy the (componentwise) condition

$$b > 0.$$  

**Proof.** Any method (9) that can be written as a convex combination of (12) and (14) can also be written as a convex combination of (12) and (13), according to Lemma 2. Applying Lemma 3 we obtain the condition $b + \hat{b} > 0$, componentwise. Now, Lemma 1 tells us that if any component $b_j = 0$ then its corresponding $\hat{b}_j = 0$, so that $b_j + \hat{b}_j > 0$ for each $j$ implies that $b_j > 0$ for each $j$.

**Theorem 2.** A method of the form (9) with order $p \geq 5$ which can be decomposed into a convex combination of the base conditions (12) and (14), must satisfy the stage order $q = 2$ condition

$$\tau_2 = Ac + \hat{c} - \frac{1}{2} c^2 = 0 \tag{26}$$

where the term $c^2$ is a component-wise squaring.
Proof. A method of order \( p \geq 5 \) must satisfy the 17 order conditions presented in the Appendix A. Three of those necessary conditions are
\[
\begin{align*}
& b^T c^4 + 4\hat{b}^T c^3 = \frac{1}{5} & (27a) \\
& b^T (c^2 \odot Ac) + b^T (c^2 \odot \hat{c}) + \hat{b}^T c^3 + 2\hat{b}^T (c \odot Ac) + 2\hat{b}^T (c \odot \hat{c}) = \frac{1}{10} & (27b) \\
& b^T (Ac \odot Ac) + 2b^T (\hat{c} \odot Ac) + b^T c^2 + 2\hat{b}^T (c \odot Ac) + 2\hat{b}^T (c \odot \hat{c}) = \frac{1}{20} & (27c)
\end{align*}
\]

From this, we find that the following linear combination of these equations gives
\[
\frac{1}{4} (27a) - (27b) + (27c) = b^T \left( Ac + \hat{c} - \frac{1}{2}c^2 \right)^2 = b^T \tau_2^2 = 0
\]
(once again, the squaring here is component-wise). Given the strict component-wise positivity of the vector \( b \) according to Corollary 1 and the non-negativity of \( \tau_2^2 \), this condition becomes \( \tau_2 = 0 \). \( \square \)

**Theorem 3.** A method of the form (9) which can be decomposed into a convex combination of the base conditions (12) and (14), cannot have order \( p = 7 \).

**Proof.** This proof is similar to the proof of Theorem 2. The complete list of additional order conditions for seventh order is lengthy and beyond the scope of this work. However, only three of these conditions are needed for this proof. These are:
\[
\begin{align*}
& b^T c^6 + 6bc^5 = \frac{1}{7} & (28a) \\
& b^T (Ac^2 \odot c^3) + 2b^T (\hat{Ac} \odot c^3) + 3\hat{b}^T (Ac^2 \odot c^2) + 6\hat{b}^T (\hat{Ac} \odot c^2) = \frac{1}{21} & (28b) \\
& b^T (Ac^2 \odot Ac^2) + 4\hat{b}^T (\hat{Ac} \odot Ac^2) + 4\hat{b}^T (\hat{Ac} \odot \hat{Ac}) + 4\hat{b}^T (\hat{Ac} \odot c^2) + 2\hat{b}^T (Ac^2 \odot c^2) = \frac{1}{63} & (28c)
\end{align*}
\]

Combining these three equations we have:
\[
\frac{1}{9} (28a) - \frac{2}{3} (28b) + (28c) = b^T \left( Ac^2 + \hat{Ac} - \frac{1}{3}c^3 \right)^2 = 0.
\]

From this we see that any seventh order method of the form (9) which admits a decomposition of a convex combination of (12) and (14), must satisfy the stage order \( q = 3 \) condition
\[
\tau_3 = \left( Ac^2 + \hat{Ac} - \frac{1}{3}c^3 \right) = 0.
\]

However, as noted above, the first stage of the explicit two-derivative multistage method (9) has the form
\[
u^n + a_{21} \Delta t F(u^n) + \hat{a}_{21} \Delta t^2 \hat{F}(u^n)
\]
which can be at most of second order. This means that the stage order of explicit two-derivative multistage methods can be at most \( q = 2 \), and so the \( \tau_3 = 0 \) condition cannot be satisfied. Thus, the result of the theorem follows. \( \square \)

\( ^1 \)In this work we use \( \odot \) to denote component-wise multiplication.
2.3 Optimal methods

We considered three types of methods:

(M1) Methods that have the general form (9) with no simplifications.

(M2) Methods that are constrained to satisfy the stage order two \((q = 2)\) requirement (26):

\[ \tau_2 = Ac + \hat{c} - \frac{1}{2}c^2 = 0. \]

(M3) Methods that satisfy the stage order two \((q = 2)\) (26) requirement and require only \(\dot{F}(u^n)\), so they have only one second derivative evaluation. This is equivalent to requiring that all values in \(\hat{A}\) and \(\hat{b}\), except those on the first column of the matrix and the first element of the vector, be zero.

We refer to the methods by type, number of stages, order of accuracy, and value of \(K\). For example, a method of type (M1) with \(s = 5\) and \(p = 4\), optimized for the value of \(K = 1.5\) would be referred to as M1(5,4,1.5) or as SSP TS M1(5,4,1.5). For comparison, we refer to methods from [5] that are SSP in the sense that they preserve the properties of the spatial discretization coupled with (12) and (13) as MSMD(s,p,k) methods.

![Figure 1](image_url)

Figure 1: The SSP coefficient \(C\) of fourth order M1 and M2 methods with \(s = 3, 4, 5\) stages plotted against the value of \(K\). The open stars indicate methods of type (M1) while the filled circles are methods of type (M2). Filled stars are (M1) markers overlaid with (M2) markers indicating close if not equal SSP coefficients.
2.3.1 Fourth Order Methods

Using the optimization approach described above, we find fourth order methods with $s = 3, 4, 5$ stages for a range of $K = 0.1, ..., 2.0$. In Figure 1 we show the SSP coefficients of methods of type (M1) and (M2) with $s = 3, 4, 5$ (in blue, red, green) plotted against the value of $K$. The open stars indicate methods of type (M1) while the filled circles are methods of type (M2). Filled stars are (M1) markers overlaid with (M2) markers indicating close if not equal SSP coefficients.

**Three Stage Methods:** Three stage methods with fourth order accuracy exist, and all these have stage order two ($q = 2$), so they are all of type (M2). Figure 1 shows the SSP coefficients of these methods in blue. The (M3) methods have an SSP coefficient

$$C = \begin{cases} \frac{2K}{K+1} & \text{for } K \leq 1 \\ 1 & \text{for } K \geq 1. \end{cases}$$

For the case where $K \geq 1$ we obtain the following optimal (M3) scheme with an SSP coefficient $C = 1$:

$$y^{(1)} = u^n$$
$$y^{(2)} = u^n + \Delta t F(y^{(1)}) + \frac{1}{2} \Delta t^2 \dot{F}(y^{(1)})$$
$$y^{(3)} = u^n + \frac{1}{2} \Delta t \left( 14F(y^{(1)}) + 4F(y^{(2)}) \right) + \frac{2}{3} \Delta t^2 \ddot{F}(y^{(1)})$$
$$u^{n+1} = u^n + \frac{1}{3} \Delta t \left( 17F(y^{(1)}) + 4F(y^{(2)}) + 27F(y^{(3)}) \right) + \frac{1}{21} \Delta t^2 \dddot{F}(y^{(1)})$$

When $K \leq 1$ we have to modify the coefficients accordingly to obtain the maximal value of $C$ as defined above. Here we provide the non-zero coefficients for this family of M3(3,4,K) as a function of $K$:

$$a_{21} = \frac{K+1}{2}, \quad b_1 = \frac{3K^2 - 9K + 22K^2 + 50K^2 + 30K^2 + 21K + 11}{3(K-3)^2(K+1)^3}, \quad \hat{a}_{21} = \frac{(K+1)^2}{8}$$
$$a_{31} = \frac{(K+1)(-K^3 - 3K^2 + 14K + 3)}{2(K+2)^3}, \quad b_2 = \frac{2K}{3(K+1)}, \quad \hat{a}_{31} = \frac{K(-K^2 + 2K + 3)^2}{8(K+2)^3}$$
$$a_{32} = \frac{(K+1)(K-3)^2}{2(K+2)^3}, \quad b_3 = \frac{3K^2 + 3K^2 + 2K + 1}{6(K-3)(K+1)}, \quad \hat{b}_1 = -\frac{3K^2 + 3K^2 + 2K + 1}{6(K-3)(K+1)}.$$

In Table 1 we compare the SSP coefficient of three stage fourth order methods of type (M2) and (M3) for a selection of values of $K$. Clearly, the (M3) methods have a much smaller SSP coefficient than the (M2) methods. However, a better measure of efficiency is the *effective SSP coefficient* computed by normalizing for the number of function evaluations required, which is $2s$ for the (M2) methods, and $s + 1$ for the (M3) methods. If we consider the effective SSP coefficient, we find that while the (M2) methods are more efficient for the larger values of $K$, for smaller values of $K$ the (M3) methods are more efficient.

**Four Stage Methods:** While four stage fourth order explicit SSP Runge-Kutta methods do not exist, four stage fourth order SSP two-derivative Runge-Kutta methods do. Four stage fourth order methods do not necessarily satisfy the stage order two ($q = 2$) condition. These methods have a more nuanced behavior: for very small $K < 0.2$, the optimized SSP methods have stage order $q = 1$. For $0.2 < K < 1.6$ the optimized SSP methods have stage order $q = 2$. Once $K$ becomes larger again, for $K \geq 1.6$, the optimized SSP methods are once again of stage order $q = 1$. However, the difference in the SSP coefficients is very small (so small it does not show on the graph) so the (M2) methods can be used without significant loss of efficiency.
| K       | 0.1  | 0.2  | 0.5  | 1.0  | 1.5  | 2.0  |
|---------|------|------|------|------|------|------|
| M2      | C    | 0.1995 | 0.3953 | 0.9757 | 1.8789 | 2.4954 | 2.7321 |
|         | C_{eff} | 0.0333 | 0.0659 | 0.1626 | 0.3131 | 0.4159 | 0.4553 |
| M3      | C    | 0.1818 | 0.3333 | 0.6667 | 1.0000 | 1.0000 | 1.0000 |
|         | C_{eff} | 0.0454 | 0.0833 | 0.1667 | 0.2500 | 0.2500 | 0.2500 |

Table 1: SSP coefficients of three stage fourth order methods.

| K       | 0.1  | 0.2  | 0.3  | .5   | 1.0  | 1.5  | 1.6  | 1.8  | 2.0  |
|---------|------|------|------|------|------|------|------|------|------|
| M1      | C    | 0.4400 | 0.6921 | 0.9662 | 1.5617 | 2.6669 | 3.4735 | 3.5607 | 3.6759 |
|         | C_{eff} | 0.0550 | 0.0865 | 0.1208 | 0.1952 | 0.3334 | 0.4342 | 0.451 | 0.4955 |
| M2      | C    | 0.3523 | 0.6569 | 0.9662 | 1.5617 | 2.6669 | 3.4735 | 3.5301 | 3.5850 |
|         | C_{eff} | 0.0440 | 0.0821 | 0.1208 | 0.1952 | 0.3334 | 0.4342 | 0.4413 | 0.4841 |
| M3      | C    | 0.3381 | 0.6102 | 0.8407 | 1.2174 | 1.8181 | 2.0596 | 2.0793 | 2.1093 |
|         | C_{eff} | 0.0676 | 0.1220 | 0.1681 | 0.2435 | 0.3636 | 0.4119 | 0.4159 | 0.4206 |

Table 2: SSP coefficients of four stage fourth order methods.

| K       | 0.1  | 0.2  | 0.3  | .5   | .6   | .7   | 1.0  | 1.5  | 2.0  |
|---------|------|------|------|------|------|------|------|------|------|
| M1      | C    | 1.5256 | 1.5768 | 1.6563 | 2.0934 | 2.4472 | 2.7819 | 3.5851 | 4.4371 |
|         | C_{eff} | 0.1526 | 0.1577 | 0.1656 | 0.2093 | 0.2447 | 0.2782 | 0.3585 | 0.4437 |
| M2      | C    | 0.5876 | 1.0003 | 1.3319 | 2.0934 | 2.4472 | 2.7819 | 3.5381 | 4.3629 |
|         | C_{eff} | 0.0588 | 0.1000 | 0.1332 | 0.2093 | 0.2447 | 0.2782 | 0.3538 | 0.4363 |
| M3      | C    | 0.5631 | 0.9296 | 1.2057 | 1.6551 | 1.8554 | 2.0300 | 2.4407 | 2.8748 |
|         | C_{eff} | 0.0939 | 0.1549 | 0.2009 | 0.2758 | 0.3092 | 0.3383 | 0.4068 | 0.4791 |

Table 3: SSP coefficients of five stage fourth order methods.
As seen in Table 2, the methods with the special structure (M3) have smaller SSP coefficients. But when we look at the effective SSP coefficient we notice that, once again, for smaller $K$ they are more efficient. Table 2 shows that the (M3) methods are more efficient when $K \leq 1.5$, and remain competitive for larger values of $K$.

It is interesting to consider the limiting case, $M2(4,4,\infty)$, in which the Taylor series formula is unconditionally stable (i.e., $K = \infty$). This provides us with an upper bound of the SSP coefficient for this class of methods by ignoring any time step constraint coming from condition (14). A four stage fourth order method that is optimal for $K = \infty$ is:

\[
\begin{align*}
y^{(1)} & = u^n \\
y^{(2)} & = u^n + \frac{1}{4} \Delta t F(y^{(1)}) + \frac{1}{72} \Delta t^2 \dot{F}(y^{(1)}) \\
y^{(3)} & = u^n + \frac{1}{4} \Delta t \left( F(y^{(1)}) + F(y^{(2)}) \right) + \frac{1}{72} \Delta t^2 \left( \dot{F}(y^{(1)}) + \dot{F}(y^{(2)}) \right) \\
y^{(4)} & = u^n + \frac{1}{4} \Delta t \left( F(y^{(1)}) + F(y^{(2)}) + F(y^{(3)}) \right) + \frac{1}{72} \Delta t^2 \left( \dot{F}(y^{(2)}) + 2\dot{F}(y^{(3)}) \right) \\
u^{n+1} & = u^n + \frac{1}{4} \Delta t \left( F(y^{(1)}) + F(y^{(2)}) + F(y^{(3)}) + F(y^{(4)}) \right) \\
& \quad + \frac{1}{288} \Delta t^2 \left( 5\dot{F}(y^{(1)}) + 12\dot{F}(y^{(2)}) + 3\dot{F}(y^{(3)}) + 16\dot{F}(y^{(4)}) \right).
\end{align*}
\]

This method has SSP coefficient $C = 4$, with effective SSP coefficient $C_{\text{eff}} = \frac{1}{2}$. This method also has stage order $q = 2$. This method is not intended to be useful in the SSP context but gives us an idea of the limiting behavior: i.e., what the best possible value of $C$ could be if the Taylor series condition had no constraint ($K = \infty$). We observe in Table 2 that the SSP coefficient of the M2(4,4,K) method is within 10% of this limiting $C$ for values of $K = 2$.

**Five Stage Methods**: The optimized five stage fourth order methods have stage order $q = 2$ for the values of $0.5 \leq K \leq 7$, and otherwise have stage order $q = 1$. The SSP coefficients of these methods are shown in the green line in Figure 1, and the SSP and effective SSP coefficients for all three types of methods are compared in Table 3. We observe that these methods have higher effective SSP coefficients than the corresponding four stage methods.

### 2.3.2 Fifth Order Methods

While fifth order explicit SSP Runge-Kutta methods do not exist, the addition of a second derivative which satisfies the Taylor Series condition allows us to find explicit SSP methods of fifth order. For fifth order, we have the result (in Section 2.2 above) that all methods must satisfy the stage order $q = 2$ condition, so we consider only (M2) and (M3) methods. In Figure 2 we show the SSP coefficients of M2(s,5,K) methods for $s = 4, 5, 6$.

**Four Stage Methods**: Four stage fifth order methods exist, and their SSP coefficients are shown in blue in Figure 2. We were unable to find M3(4,5,K) methods, possibly due to the paucity of available coefficients for this form.

**Five Stage Methods**: The SSP coefficient of the five stage M2 methods can be seen in red in Figure 2. We observe that the SSP coefficient of the M2(5,5,K) methods plateaus with respect to $K$. As shown in Table 4, methods with the form (M3) have a significantly smaller SSP coefficient than that of (M2).
However, the effective SSP coefficient is more informative here, and we see that the (M3) methods are more efficient for small values of $K \leq 0.5$, but not for larger values.

**Six Stage Methods:** The SSP coefficient of the six stage M2 methods can be seen in green in Figure 2. In Table 4 we compare the SSP coefficients and effective SSP coefficients of (M2) and (M3) methods. As in the case above, the methods with the form (M3) have a significantly smaller SSP coefficient than that of (M2), and the SSP coefficient of the (M3) methods plateaus with respect to $K$. However, the effective SSP coefficient shows that the (M3) methods are more efficient for small values of $K \leq 0.7$, but not for larger values.

### Table 4: SSP coefficients and effective SSP coefficients of fifth order methods.

| K   | 0.1 | 0.2 | 0.3 | 0.5 | 1.0 | 1.5 | 1.6 | 1.8 | 2.0 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| M2(5,5) | $C$ | 0.3802 | 0.7448 | 1.0892 | 1.6877 | 2.9281 | 3.8102 | 3.8479 | 3.8879 | 3.8971 |
|      | $C_{\text{eff}}$ | 0.0380 | 0.0745 | 0.1089 | 0.1688 | 0.2928 | 0.3810 | 0.3848 | 0.3888 | 0.3897 |
| M3(5,5) | $C$ | 0.3298 | 0.5977 | 0.8186 | 1.0625 | 1.0625 | 1.0625 | 1.0625 | 1.0625 | 1.0625 |
|      | $C_{\text{eff}}$ | 0.0550 | 0.0996 | 0.1364 | 0.1771 | 0.1771 | 0.1771 | 0.1771 | 0.1771 | 0.1771 |
| M2(6,5) | $C$ | 0.5677 | 1.0230 | 1.4581 | 2.2102 | 3.8749 | 4.9201 | 5.0002 | 5.0903 | 5.1301 |
|      | $C_{\text{eff}}$ | 0.0473 | 0.0852 | 0.1215 | 0.1842 | 0.3229 | 0.4100 | 0.4167 | 0.4242 | 0.4275 |
| M3(6,5) | $C$ | 0.5398 | 0.9370 | 1.2592 | 1.6914 | 1.8208 | 1.8208 | 1.8208 | 1.8208 | 1.8208 |
|      | $C_{\text{eff}}$ | 0.0771 | 0.1339 | 0.1799 | 0.2416 | 0.2601 | 0.2601 | 0.2601 | 0.2601 | 0.2601 |

### Table 5: SSP coefficients and effective SSP coefficients of sixth order SSP TS methods.

| K   | 0.1 | 0.2 | 0.3 | 0.5 | 1.0 | 1.5 | 2.0 |
|-----|-----|-----|-----|-----|-----|-----|-----|
| M2(5,6) | $C$ | 0.1441 | 0.2280 | 0.2780 | 0.3242 | 0.3500 | 0.3536 | 0.3555 |
|      | $C_{\text{eff}}$ | 0.0144 | 0.0228 | 0.0278 | 0.0324 | 0.0350 | 0.0354 | 0.0355 |
| M2(6,6) | $C$ | 0.2944 | 0.5157 | 0.6725 | 0.9044 | 1.5225 | 2.0002 | 2.1966 |
|      | $C_{\text{eff}}$ | 0.0245 | 0.0430 | 0.0560 | 0.0754 | 0.1269 | 0.1667 | 0.1831 |
| M2(7,6) | $C$ | 0.3981 | 0.7158 | 0.9734 | 1.4217 | 2.0376 | 2.5648 | 2.7794 |
|      | $C_{\text{eff}}$ | 0.0284 | 0.0511 | 0.0695 | 0.1016 | 0.1455 | 0.1832 | 0.1985 |
| M3(7,6) | $C$ | 0.3547 | 0.6007 | 0.8059 | 0.8941 | 0.8947 | 0.8947 | 0.8947 |
|      | $C_{\text{eff}}$ | 0.0443 | 0.0751 | 0.1007 | 0.1118 | 0.1118 | 0.1118 | 0.1118 |
| M3(8,6) | $C$ | 0.5495 | 0.9754 | 1.2882 | 1.6435 | 1.7369 | 1.7369 | 1.7369 |
|      | $C_{\text{eff}}$ | 0.0611 | 0.1084 | 0.1431 | 0.1826 | 0.1930 | 0.1930 | 0.1930 |

### 2.3.3 Sixth Order Methods

As shown in Section 2.2, the highest order of accuracy this class of methods can obtain is $p = 6$, and these methods must satisfy (26). We find sixth order methods with $s = 5, 6, 7$ stages of type (M2). As to methods with the special structure M3, we are unable to find methods with $s \leq p$, but we find M3(7,6,K) methods and M3(8,6,K) methods. In the first six rows of Table 5 we compare the SSP and effective SSP coefficients of the (M2) methods with $s = 5, 6, 7$ stages. In the last four rows of Table 5 we compare the SSP coefficients and effective SSP coefficients for sixth order methods with $s = 7, 8$ stages. Figure 3 shows...
the SSP coefficients of the optimized (M3) methods for seven and eight stages, which clearly plateau with respect to $K$ (as can be seen in the tables as well). For the sixth order methods, it is clear that M3(8,6,K) methods are most efficient for all values of $K$.

2.4 Comparison with existing methods

First, we wish to compare the methods in this work to those in our prior work [5]. If a spatial discretization satisfies the forward Euler condition (12) and the second derivative condition (13) it will also satisfy the Taylor series condition (14), with

$$K = \tilde{K} \left( \sqrt{\tilde{K}^2 + 2} - \tilde{K} \right).$$

In this case, it is preferable to use the MDRK methods in [5]. However, in the case that the second derivative condition (13) is not satisfied for any value of $\tilde{K} > 0$, or if the Taylor series condition is independently satisfied with a larger $K$ than would be established from the two conditions, i.e., $K > \tilde{K} \left( \sqrt{K^2 + 2} - \tilde{K} \right)$, then it may be preferable to use one of the TS methods derived in this work.

Next, we wish to compare the methods in this work to those in [32], which was the first paper to consider an SSP property based on the forward Euler and Taylor series base conditions. The approach used in our work is somewhat similar to that in [32] where the authors consider building time integration schemes which can be composed as convex combinations of forward Euler and Taylor series time steps, where they aim to find methods which are optimized for the largest SSP coefficients. However, there are several differences between our approach and the one of [32], which results in the fact that in this paper we are able to find more methods, of higher order, and with better SSP coefficients. In addition, in the present work we find and prove an order barrier for SSP methods of the TS type.

The first difference between our approach and the approach in [32] is that we allow computations of $\dot{F}$ of the intermediate values, rather than only $\dot{F}(u^n)$. Another way of saying this is that we consider methods that are not of type M3, while the methods considered in [32] are all of type M3. In some cases, when we restrict our search to M3 methods and $K = 1$, we find methods with the same SSP coefficient.
as in [32]. For example, HBT34 matches our M3(3,4,1) method with an SSP coefficient of \( C = 1 \), HBT44 matches our M3(4,4,1) method with \( C = \frac{20}{17} \), HBT54 matches our M3(5,4,1) method with \( C = 2.441 \), and HBT55 matches our M3(5,5,1) method with an SSP coefficient of \( C = 1.062 \). While methods of type M3 have their advantages, they are sometimes sub-optimal in terms of efficiency, as we point out in the tables above.

The second difference between the SSP TS methods in this paper and the methods in [32] is that in [32] only one method of order \( p > 4 \) is reported, while we have many fifth and sixth order methods of various types and stages, optimized for a variety of \( K \) values.

The most fundamental difference between our approach and the approach in [32] is that our methods are optimized for the relationship between the forward Euler restriction and the Taylor series restriction while the time step restriction in the methods of [32] is defined as the most restrictive of the forward Euler and Taylor series time step conditions. Respecting the minimum of the two cases will still satisfy the nonlinear stability property, but this approach does not allow for a balance between the restrictions considered, which can lead to severely more restrictive conditions. In our approach we use the relationship between the two time-step restrictions to select optimal methods. For this reason, the methods we find have larger allowable time-steps in many cases. To understand this a little better consider the case where the forward Euler condition is

\[
\Delta t_{FE} \leq \Delta x
\]

and the Taylor series condition is

\[
\Delta t_{TS} \leq \frac{1}{2} \Delta x.
\]

In the approach used in [32], the base time step restriction is then \( \Delta t_{\text{max}} = \max\{\Delta t_{FE}, \Delta t_{TS}\} \leq \frac{1}{2} \Delta x \). The HBT23 method in [32] is a third order scheme with 2 stages which has an SSP coefficient of \( C = 1 \), so the allowable time-step with this scheme will be the same \( \Delta t \leq C \Delta t_{\text{max}} \leq \frac{1}{2} \Delta x \). On the other hand, using our optimal M2(2,3,5) scheme, which has an SSP coefficient \( C = .75 \), the allowable time step is \( \Delta t \leq C \Delta t_{FE} \leq \frac{3}{4} \Delta x \), a 50\% increase. This is not only true when \( K < 1 \): consider the case where \( \Delta t_{FE} \leq \frac{1}{2} \Delta x \) and \( \Delta t_{TS} \leq \Delta x \). Once again the HBT23 method in [32] will have a time step restriction of \( \Delta t \leq C \Delta t_{\text{max}} \leq \frac{1}{2} \Delta x \), while our M2(2,3,2) method has an SSP coefficient \( C = 1.88 \), so that the overall time step restriction would be \( \Delta t \leq \frac{1.88}{2} \Delta x = .94 \Delta x \), which is 88\% larger. Even when the two base conditions are the same (i.e., \( K = 1 \)) and we have \( \Delta t_{FE} \leq \Delta x \) and \( \Delta t_{TS} \leq \Delta x \), the HBT23 method in [32] gives an allowable time-step of \( C = 1 \) while our M2(2,3,1) has an SSP coefficient \( C = 1.5 \), so that our method allows a time-step that is 50\% larger. These simple cases demonstrate that our methods, which are optimized for the value of \( K \), will usually allow a larger SSP coefficient than the methods obtained in [32].

### 3 Numerical Tests

We wish to test our methods on what are now considered standard benchmark tests in the SSP community. In this subsection we preview our results, which we then present in more detail throughout the remainder of the section.

First, in the tests in Examples 1 we focus on how the strong stability properties of these methods are observed in practice, by considering the total variation of the numerical solution. We focus on two scalar PDEs: the linear advection equation and Burgers’ equation, using simple first order spatial discretizations which are known to satisfy a total variation diminishing property over time for the forward Euler and Taylor series building blocks. We want to ensure that our numerical approximation to these solutions observe similar properties as long as the predicted SSP time step restriction, \( \Delta t \leq C \Delta t_{FE} \), is respected. These

\[\text{These efficiency measures do not account for the fact that the methods in [32] are of type M3 and so require fewer funding evaluations. Correcting for this, our methods are still 10-40\% more efficient.}\]
scalar one-dimensional partial differential equations are chosen for their simplicity so we may understand the behavior of the numerical solution, but the discontinuous initial conditions may lead to instabilities if standard time discretization techniques are employed. Our tests show that the methods we design here preserve these properties as expected by the theory.

In Example 2, we extend the results from Example 1 to the case where we use the higher order weighted essentially non-oscillatory (WENO) method, which is not provably TVD but gives results that have very small increases in total variation. We demonstrate that our methods out-perform other methods, such as the MDRK methods in [5], and that non-SSP methods that are standard in the literature do not preserve the TVD property for any time-step.

In many of these examples we are concerned with the total variation diminishing property. To measure the sharpness of the SSP condition we compute the maximal observed rise in total variation over each step, defined by

$$\max_{0 \leq n \leq N-1} \left( ||u^{n+1}||_{TV} - ||u^n||_{TV} \right),$$

as well as the maximal observed rise in total variation over each stage, defined by

$$\max_{1 \leq j \leq s} \left( ||y^{(j+1)}||_{TV} - ||y^{(j)}||_{TV} \right),$$

where $y^{(s+1)}$ corresponds to $u^{n+1}$. The quantity of interest is the time-step $\Delta t_{obs}$, or the SSP coefficient $C_{obs} = \frac{\Delta t_{obs}}{\Delta t_{FE}}$ at which this rise becomes significant, as defined by a maximal increase of $10^{-10}$.

It is important to notice that the SSP TS methods we designed depend on the value of $K$ in (14). However, in practice we often do not know the exact value of $K$. In Example 3 we investigate what happens when we use spatial discretizations with a given value of $K$ with time discretization methods designed for an incorrect value of $K$. We conclude that although in some cases a smaller step-size is required, for methods of type M3 there is generally no adverse result from selecting the wrong value of $K$.

**Remark 2. On the numerical implementation of the second derivative.** Multi-derivative methods utilize higher order temporal derivatives to achieve the higher order of accuracy. We compute this higher order information by utilizing the Cauchy-Kowalevskaya procedure as done in [5, 39, 50], which use the PDE to represent the higher order time derivatives in terms of spatial operators.

In our case the spatial discretization is performed as follows: at each iteration we take the known value $u^n$ and compute the flux $f(u^n) = u^n$ in the linear case and $f(u^n) = \frac{1}{2} (u^n)^2$ for Burgers’ equation. Now to compute the spatial derivative $f(u^n)_x$ we use an operator $D$ and compute

$$u^n_t = f(u^n)_x \rightarrow u^n_t = D(f(u^n)).$$

In the numerical examples below the differential operator $D$ will represent, depending on the problem, a first order upwind finite difference scheme and the fifth order finite difference WENO method [20]. In our scalar test cases $f'(u)$ does not change sign, so we avoid flux splitting.

Now we have the approximation to $U_t$ at time $t^n$, and wish to compute the approximation to $U_{tt}$. For the linear advection problem, this is very straightforward as $U_{tt} = U_{xx}$. To compute this, we take $u_x$ as computed before, and differentiate it again. For Burgers’ equation, we have $U_{tt} = -(UU_t)_x$. We take the approximation to $U_t$ that we obtained above, and we multiply it by $u^n$, then differentiate in space once again. In pseudocode, the calculation takes the form:

$$u^n_{tt} = (f'(u^n)u^n)_x \rightarrow u^n_{tt} = \hat{D}(f'(u^n)u^n);$$
Using these, we can now construct our two building blocks

**Forward Euler** \( u^{n+1} = u^n + \Delta t u^n_t, \)

**Taylor series** \( u^{n+1} = u^n + \Delta t u^n_t + \frac{1}{2} \Delta t^2 u^n_{tt}. \)

In choosing the spatial discretizations \( D \) and \( \tilde{D} \) it is important that these building blocks satisfy (12) and (14), respectively, in the desired convex functional \( \| \cdot \|. \)

In Example 4 we investigate the increased flexibility in the choice of spatial discretization that results from relying on the (12) and (14) base conditions. As we saw in the remark above, the only constraint in the choice of differentiation operators \( D \) and \( \tilde{D} \) is that the resulting building blocks must satisfy the monotonicity conditions (12) and (14) in the desired convex functional \( \| \cdot \|. \) As noted above, this constraint is less restrictive than requiring that (12) and (13) are satisfied: any spatial discretizations for which (12) and (13) are satisfied will also satisfy (14). However, there are some spatial discretizations that satisfy (12) and (14) that do not satisfy (13). In Example 4 we find that choosing spatial discretizations that satisfy (12) and (14) but not (13) allows for larger time-steps before the rise in total variation. And finally, in Example 5, we demonstrate the positivity preserving behavior of our methods when applied to a nonlinear system of equations.

### 3.1 TVD first order finite difference approximations

In this section we use first order spatial discretizations, that are provably total variation diminishing (TVD), coupled with a variety of time-stepping methods. We look at the maximal rise in total variation.

**Example 1a: Linear advection.** As a first test case, we consider a linear advection problem

\[ U_t - U_x = 0, \quad (31) \]

on a domain \( x \in [-1, 1], \) with step-function initial conditions

\[ u_0(x) = \begin{cases} 
1 & \text{if } -\frac{1}{2} \leq x \leq \frac{1}{2}, \\
0 & \text{otherwise},
\end{cases} \quad (32) \]

and periodic boundary conditions. This simple example is chosen as our experience has shown [13] that this problem often demonstrates the sharpness of the SSP time-step.

For the spatial discretization we use a first order forward difference for the first and second derivative:

\[ F(u^n)_j := \frac{u^n_{j+1} - u^n_j}{\Delta x} \approx U_x(x_j), \quad \text{and} \quad \tilde{F}(u^n)_j := \frac{u^n_{j+2} - 2u^n_{j+1} + u^n_j}{\Delta x^2} \approx U_{xx}(x_j). \]

These spatial discretizations satisfy:

**Forward Euler condition** \( u^{n+1}_j = u^n_j + \frac{\Delta t}{\Delta x} (u^n_{j+1} - u^n_j) \) is TVD for \( \Delta t \leq \Delta x, \)

and

**Taylor series condition** \( u^{n+1}_j = u^n_j + \frac{\Delta t}{\Delta x} (u^n_{j+1} - u^n_j) + \frac{1}{2} \left( \frac{\Delta t}{\Delta x} \right)^2 (u^n_{j+2} - 2u^n_{j+1} + u^n_j) \) is TVD for \( \Delta t \leq \Delta x. \)
So that \( \Delta t_{FE} = \Delta x \) and in this case we have \( K = 1 \) in (14). Note that the second derivative discretization used above \textit{does not} satisfy the \textbf{Second Derivative} condition (13), so that most of the methods we devised in [5] do not guarantee strong stability preservation for this problem.

For all of our simulations for this example, we use a fixed grid of \( M = 601 \) points, for a grid size \( \Delta x = \frac{1}{600} \), and a time-step \( \Delta t = \lambda \Delta x \) where we vary \( \lambda \) from \( \lambda = 0 \) until beyond the point where the TVD property is violated. We step each method forward by \( N = 50 \) time-steps and compare the performance of the various time-stepping methods constructed earlier in this work, for \( K = 1 \). We define the observed SSP coefficient \( C_{obs} \) as the multiple of \( \Delta t_{FE} \) for which the maximal rise in total variation exceeds \( 10^{-10} \).

We verify that the observed values of \( \Delta t_{FE} \) and \( K \) match the predicted values, and test this problem to see how well the observed SSP coefficient \( C_{obs} \) matches the predicted SSP coefficient \( C_{pred} \) for the fourth, fifth, and sixth order methods. The results are listed in the left-hand columns of Table 6.

**Example 1b: Burgers’ equation** We repeat the example above with all the same parameters but for the problem

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

on \( x \in (-1, 1) \). Here we use the spatial derivatives:

\[
F(u^n)_j = \frac{f_j^n - f_{j-1}^n}{\Delta x} \approx f(U)_x(x_j),
\]

| Linear Advection | \( C_{pred} \) | \( C_{obs} \) | \( C_{eff}^{pred} \) | \( C_{eff}^{obs} \) |
|------------------|-----------------|-----------------|---------------------|---------------------|
| FE               | 1.0000          | 1.0000          | 1.00                | 1.00                |
| TS               | 1.0000          | 1.0000          | 0.50                | 0.50                |
| M2(3,4,1)        | 1.8788          | 1.8788          | 0.31                | 0.31                |
| M3(3,4,1)        | 1.0000          | 1.0000          | 0.25                | 0.25                |
| M2(4,4,1)        | 2.6668          | 2.6668          | 0.33                | 0.33                |
| M3(4,4,1)        | 1.8181          | 1.8181          | 0.36                | 0.36                |
| M2(5,4,1)        | 3.5381          | 3.6291          | 0.35                | 0.35                |
| M3(5,4,1)        | 2.4406          | 2.4406          | 0.40                | 0.40                |
| M2(4,5,1)        | 2.1864          | 2.2239          | 0.27                | 0.27                |
| M2(5,5,1)        | 2.9280          | 3.1681          | 0.29                | 0.31                |
| M3(5,5,1)        | 1.0625          | 1.5436          | 0.17                | 0.25                |
| M2(6,5,1)        | 3.8749          | 3.8749          | 0.32                | 0.32                |
| M3(6,5,1)        | 1.8207          | 2.0003          | 0.26                | 0.28                |
| M2(5,6,1)        | 0.3500          | 1.9398          | 0.03                | 0.19                |
| M2(6,6,1)        | 1.5225          | 2.3548          | 0.12                | 0.19                |
| M2(7,6,1)        | 2.1150          | 2.3695          | 0.15                | 0.19                |
| M3(7,6,1)        | 0.8946          | 1.2893          | 0.11                | 0.16                |
| M3(8,6,1)        | 1.7369          | 1.9861          | 0.19                | 0.21                |

| Burgers’ | \( C_{pred} \) | \( C_{obs} \) | \( C_{eff}^{pred} \) | \( C_{eff}^{obs} \) |
|----------|-----------------|-----------------|---------------------|---------------------|
| FE       | 1.0000          | 1.0000          | 1.00                | 1.00                |
| TS       | 1.0000          | 1.0000          | 0.50                | 0.50                |
| M2(3,4,1) | 1.8788          | 1.8788          | 0.31                | 0.31                |
| M3(3,4,1) | 1.0000          | 1.0000          | 0.25                | 0.25                |
| M2(4,4,1) | 2.6668          | 2.6668          | 0.33                | 0.33                |
| M3(4,4,1) | 1.8181          | 1.8181          | 0.36                | 0.36                |
| M2(5,4,1) | 3.5381          | 3.6102          | 0.35                | 0.35                |
| M3(5,4,1) | 2.4406          | 2.4406          | 0.40                | 0.40                |
| M2(4,5,1) | 2.1864          | 2.2130          | 0.27                | 0.27                |
| M2(5,5,1) | 2.9280          | 3.1009          | 0.29                | 0.31                |
| M3(5,5,1) | 1.0625          | 1.5436          | 0.17                | 0.25                |
| M2(6,5,1) | 3.8749          | 3.8749          | 0.32                | 0.32                |
| M3(6,5,1) | 1.8207          | 2.0003          | 0.26                | 0.28                |
| M2(5,6,1) | 0.3500          | 1.9239          | 0.03                | 0.19                |
| M2(6,6,1) | 1.5225          | 2.2875          | 0.12                | 0.19                |
| M2(7,6,1) | 2.1150          | 2.3189          | 0.15                | 0.16                |
| M3(7,6,1) | 0.8946          | 1.2893          | 0.11                | 0.16                |
| M3(8,6,1) | 1.7369          | 1.9734          | 0.19                | 0.21                |

Table 6: Example 1: \( C_{pred} \) and \( C_{obs} \) for M2 and M3 methods.
and
\[ F(u^n)_j = f(u^n)_j F(u^n)_j - f'(u^n_{j-1}) F(u^n)_{j-1} \approx (f'(U) f(U) x(x_j)). \]

The results are quite similar to those of the linear advection equation in Example 1a, as can be seen in the right-hand columns of Table 6.

The results from these two studies show that the SSP TS methods provide a reliable guarantee of the allowable time-step for which the method preserves the strong stability condition in the desired norm. For methods of order \( p = 4 \), we observe that the SSP coefficient is sharp: the predicted and observed values of the SSP coefficient are identical for all the fourth order methods tested. For methods of higher order (\( p = 5, 6 \)) the observed SSP coefficient is often significantly higher than the minimal value guaranteed by the theory.

### 3.2 Example 2: Weighted essentially non-oscillatory (WENO) approximations

In this section we re-consider the nonlinear Burgers’ equation (33)
\[ U_t + \left( \frac{U^2}{2} \right)_x = 0, \]
on \( x \in (-1, 1) \). We use the step function initial conditions (32), and periodic boundaries. We use \( M = 201 \) points in the spatial domain, so that \( \Delta x = \frac{1}{100} \), and we step forward for \( N = 50 \) time-steps and measure the maximal rise in total variation for each case.

For the spatial discretization, we use the fifth order finite difference WENO method in space, as this is a high order method that can handle shocks. Recall that the motivation for the development of SSP multi-stage multi-derivative time-stepping is for use in conjunction with high order methods for problems with shocks. Ideally, the specially designed spatial discretizations satisfy (12) and (14). Although the weighted essentially non-oscillatory (WENO) methods do not have a theoretical guarantee of this type, in practice we observe that these methods do control the rise in total variation, as long as the step-size is below a certain threshold.

Below, we refer to the WENO method on a flux with \( f'(u) \geq 0 \) as WENO\(^+\) and to the corresponding method on a flux with \( f'(u) \leq 0 \) as WENO\(^-\). Because \( f'(u) \) is strictly non-negative in this example, we do not need to use flux splitting, and use \( D = \text{WENO}^+ \). For the second derivative we have the freedom to use \( D = \text{WENO}^+ \) or \( D = \text{WENO}^- \). In this example, we use \( D = D = \text{WENO}^+ \). In Example 4 below we show that this is more efficient.

In Figure 4 on the left, we compare the performance of our SSP TS M3(7,5,1) and SSP TS M2(4,5,1) methods, which both have eight function evaluations per time-step, and our SSP TS M3(5,5,1), which has six function evaluations per time-step, to the SSP MDRK(3,5,2) in [5] and non-SSP RK(6,5) Dormand-Prince method [8], which also have six function evaluations per time-step. We note that we use the SSP MDRK(3,5,2) (designed for \( K = 2 \)) because this method performs best compared to other MDRK methods designed for different values of \( K \). Clearly, the non-SSP method is not safe to use on this example. The M3 methods are most efficient, allowing the largest time-step per function evaluation before the total variation begins to rise.

This conclusion is also the case for the sixth order methods. In Figure 4 on the right, we compare our M3(9,6,1) and M2(5,6,1) methods, which both have ten function evaluations per time-step, and our M3(7,6,1), which has eight function evaluations per time-step, to the MDRK(4,6,1) and non-SSP RK(8,6)
method given in Verner’s paper table [52], which also have eight function evaluations per time-step. Clearly, the non-SSP method is not safe to use on this example. The M3 methods are most efficient, allowing the largest time-step per function evaluation before the total variation begins to rise.

This example demonstrates the need for SSP methods: classical non-SSP methods do not control the rise in total variation. We also observe that the methods of type M3 are efficient, and may be the preferred choice of methods for use in practice.

3.3 Example 3: Testing methods designed with various values of $K$

In general, the value of $K$ is not exactly known for a given problem, so we cannot choose a method that is optimized for the correct $K$. We wish to investigate how methods with different values of $K$ perform for a given problem. In this example, we re-consider the linear advection equation (31)

$$U_t = U_x$$

with step function initial conditions (32), and periodic boundary conditions on $x \in (-1,1)$. We use the fifth order WENO method with $M = 201$ points in the spatial domain, so that $\Delta x = \frac{1}{100}$, and we step forward for $N = 50$ time-steps and measure the maximal rise in total variation for each case. Using this example, we investigate how time-stepping methods optimized for different $K$ values perform on the linear advection with finite difference spatial approximation test case above, where it is known that $K = 1$. We use a variety of fifth and sixth order methods, designed for $0.1 \leq K \leq 2$ and give the value of $\lambda = \frac{\Delta t}{\Delta x}$ for which the maximal rise in total variation becomes large, when applied to the linear advection problem.

In Figure 5 (left) we give the observed value (solid lines) of $\lambda$ for a number of methods, M2(4,5,K), M2(5,5,K), M2(6,5,K), M3(5,5,K), and M3(6,5,K), and the corresponding predicted value (dotted lines) that a method designed for $K = 1$ should give. In Figure 5 (right) we repeat this study with sixth order
methods $M2(5,6,K)$, $M2(6,6,K)$, $M3(7,6,K)$, and $M3(8,6,K)$. We observe that while choosing the correct $K$ value can be beneficial, and is certainly important theoretically, in practice using methods designed for different $K$ values often makes little difference, particularly when the method is optimized for a value close to the correct $K$ value. For the sixth order methods in particular, the observed values of the SSP coefficient are all larger than the predicted SSP coefficient.

3.4 Example 4: The benefit of different base conditions

In [5] we use the choice of $D = WENO^+$ followed by $\tilde{D} = WENO^-$ by analogy to the first order finite difference for the linear advection case $U_t = U_x$, where we use a differentiation operator $D^+$ followed by the downwind differentiation operator $D^-$ to produce a centered difference for the second derivative. In fact, this approach makes sense for these cases because it respects the properties of the flux for the second derivative and consequently satisfies the second derivative condition (13). However, if we simply wish the Taylor series formulation to satisfy a TVD-like condition, so we are free to use the same operator ($WENO^+$ or $WENO^-$, as appropriate) twice, and indeed this gives a larger allowable $\Delta t$.

In Figure 6 we show how using the repeated upwind discretization $D = WENO^-$ and $\tilde{D} = WENO^-$ (solid lines) which satisfy the Taylor Series Condition (14) but not the second derivative condition (13) to approximate the higher order derivative allows for a larger time-step than the spatial discretizations (dashed lines) used in 9. We see that for the fifth order methods the rise in total variation always occurs for larger $\lambda$ for the solid lines ($\tilde{D} = D = WENO^-$) than for the dashed lines ($D = WENO^-$ and $\tilde{D} = WENO^+$), even for the method designed in [5] to be SSP for the second case but not the first case. For the sixth order methods the results are almost that same, though the MDRK(4,6,1) method that is SSP for base conditions of the type in [5] performs identically in both cases. These results demonstrate the additional flexibility afforded by requiring that the methods only satisfy (12) and (14) but not necessarily.
Figure 6: Example 4: The maximal rise in total variation (on y-axis) for values of $\lambda$ (on the x-axis). Simulations using the repeated upwind discretization $D = WENO^-$ and $\tilde{D} = WENO^-$ (solid lines) are more efficient than those using $D = WENO^-$ and $\tilde{D} = WENO^+$ (dashed lines). This demonstrates the enhanced SSP time-step afforded by these methods.

(13) results in methods that are more efficient in practice in that larger time-steps are allowed.

3.5 Example 5: Nonlinear Shallow Water Equations

As a final test case we consider the shallow water equations, where we are concerned with the preservation of positivity in the numerical solution. The shallow water equations [2] are a non-linear system of hyperbolic conservation laws defined by

$$
\begin{align*}
\left(\begin{array}{c}
h \\
(hv)\end{array}\right)_t + \left(\begin{array}{c}
hv^2 + \frac{1}{2}gh^2 \\
(hv^2 + \frac{1}{2}gh^2)_x
\end{array}\right) &= \left(\begin{array}{c}
0 \\
0
\end{array}\right),
\end{align*}
$$

where $h(x,t)$ denotes the water height at location $x$ and time $t$, $v(x,t)$ the water velocity, $g$ is the gravitational constant, and $U = (h, hv)^T$ is the vector of unknown conserved variables. In our simulations, we set $g = 1$. To discretize this problem, we use the standard Lax-Friedrich’s flux

$$
\hat{f}_{j-1/2} := \frac{1}{2} (f(u_j) + f(u_{j-1})) - \frac{\alpha}{2} (u_j - u_{j-1}), \quad \alpha = \max_j \left\{ |v_j \pm \sqrt{h_j}| \right\},
$$

and define the (conservative) approximation to the first derivative as

$$
f(U(x_j))_x \approx \frac{1}{\Delta x} \left( \hat{f}_{j+1/2} - \hat{f}_{j-1/2} \right).$$

We discretize the spatial grid $x \in (0,1)$ with $M = 201$ points. To approximate the second derivative, we start with element-wise first derivative $u_{j,t} := -\frac{1}{\Delta x^2} \left( \hat{f}_{j+1/2} - \hat{f}_{j-1/2} \right)$, and then approximate the second
Table 7: The predicted and observed values of $\lambda = \alpha \frac{\Delta t}{\Delta x}$ for which positivity of the height of the water is preserved in the shallow water equations in Example 5.

| Method         | $\lambda_{\text{pred}}$ | $\lambda_{\text{obs}}$ | Method         | $\lambda_{\text{pred}}$ | $\lambda_{\text{obs}}$ |
|----------------|--------------------------|-------------------------|--------------------------|--------------------------|-------------------------|
| Forward Euler  | 1.00000                  | 1.01058                 | Taylor series            | 1.00000                  | 1.02598                 |
| Dormand Prince | 0.00000                  | 0.00000                 | nonSSPRK(8,6)            | 0.00000                  | 0.00000                 |
| MDRK(3,5,2)    | 0.92727                  | 1.03176                 | MDRK(4,6,1)              | 0.78538                  | 1.07803                 |
| M2(4,5,1)      | 2.18648                  | 3.01005                 | M2(5,6,1)                | 0.35001                  | 2.48411                 |
| M3(5,5,1)      | 1.06253                  | 1.78593                 | M3(7,6,1)                | 0.89468                  | 1.64084                 |
| M3(6,5,1)      | 1.82079                  | 2.12579                 | M3(9,6,1)                | 2.59860                  | 3.03387                 |

In problems such as the shallow water equations, the non-negativity of the numerical solution is important as a height of $h < 0$ is not physically meaningful, and the system loses hyperbolicity when the height becomes negative. For a positivity preserving test case, we consider a Riemann problem with no initial velocity, but with a wet and a dry state [2, 53]:

$$(h, v)^T = \begin{cases} (10, 0)^T & x \leq 0.5, \\ (0, 0)^T & x > 0.5. \end{cases}$$

In our numerical simulations, we focus on the impact of the numerical scheme on the positivity preservation of the solver for the the water height $h(x, t)$. This quantity is of interest from a numerical perspective because if the height $h(x, t) < 0$ for any $x$ or $t$, the code will crash due to square-root of height.

In Table 7 we compare the positivity preservation time-step of a variety of numerical time integrators. We consider the fifth order SSP TS methods M2(4,5,1), M3(5,5,1), and M3(6,5,1), and compare their performance to the SSP MDRK(3,5,2) method in [5], and the non-SSP Dormand Prince method. We also consider the sixth order SSP TS methods M2(5,6,1), M3(7,6,1), and M3(9,6,1), as well as the MDRK(4,6,1) from [5] and the non-SSPRK(8,6) method. Positivity of the water height is measure at each stage for a total of $N = 60$ time-steps. We report the largest allowable value of $\lambda = \frac{\alpha \Delta t}{\Delta x}$ (which is the maximal wavespeed for the domain) for which the solution remains positive. In Table 7 we show that all of our SSP TS methods preserve the positivity of the solution for values larger than those guaranteed by the theory $\lambda_{\text{obs}} > \lambda_{\text{pred}}$, and that even for the SSP MSRK methods there is a large region of values $\lambda_{\text{obs}}$ for which the solution remains positive. However, the non-SSP methods permit no positive time step that retains positivity of the solution, highlighting the importance of SSP methods.

4 Conclusions

In [5] we introduced a formulation and base conditions to extend the SSP framework to multi-stage multi-derivative time-stepping methods. While this choice of base conditions we used in [9] gives us more flexibility
in finding SSP time stepping schemes, it limits the flexibility in the choice of the spatial discretization. In the current paper we introduce an alternative SSP formulation based on the conditions (12) and (14) and investigate SSP time integrators that preserve the strong stability properties (12) and (14). These base conditions are relevant because some commonly used spatial discretizations may not satisfy the second derivative condition (13) which we required in [5], but do satisfy the Taylor series condition (14). This approach decreases the flexibility in our choice of time discretization because some time discretizations that can be decomposed into convex combinations of (12) and (13) cannot be decomposed into convex combinations of (12) and (14). However, it increases the flexibility in our choice of spatial discretizations, as we may now consider spatial methods that satisfy (12) and (14) but not (13). In the numerical tests we showed that this increased flexibility allowed for more efficient simulations in several cases.

In this paper, we proved that explicit SSP methods which preserve the strong stability properties of (12) and (14), called explicit strong stability preserving Taylor series (SSP TS) methods, have a maximum obtainable order of $p = 6$. Next we formulated the proper optimization procedure to generate SSP TS methods. Within this new class we were able to organize our schemes into three sub categories that reflect the different simplifications used in the optimization. We obtained methods up to and including order $p = 6$ thus breaking the SSP order barrier for explicit SSP Runge-Kutta methods. Our numerical tests show that the SSP TS methods perform as expected, preserving the strong stability properties satisfied by the base conditions (12) and (14) under the predicted time-step conditions. Our simulations demonstrate the the sharpness of the SSP condition in some cases, and the need for SSP time-stepping methods in simulations where the spatial discretization is specially designed to satisfy certain nonlinear non-inner-product stability properties such as total variation diminishing (TVD) and positivity. Furthermore the numerical results indicate that the added freedom in the choice of spatial discretization results in larger allowable time steps. The SSP TS methods described in this work can be downloaded from [14].

**Acknowledgements.** The work of D.C. Seal was supported in part by the Naval Academy Research Council. The work of S. Gottlieb and Z.J. Grant was supported by the AFOSR grant #FA9550-15-1-0235.
A Order Conditions

Any method of the form (9) must satisfy the order conditions for all \( p \leq P \) to be of order \( P \).

\[
\begin{align*}
p = 1 & \quad b^T e = 1 \\
p = 2 & \quad b^T c + \tilde{b}^T e = \frac{1}{2} \\
p = 3 & \quad b^T c^2 + 2\tilde{b}^T c = \frac{1}{3} \\
& \quad b^T Ac + b^T \hat{c} + \tilde{b}^T c = \frac{1}{6} \\
p = 4 & \quad b^T c^3 + 3\tilde{b}^T c^2 = \frac{1}{4} \\
& \quad b^T (c \odot Ac) + b^T (c \odot \hat{c}) + \tilde{b}^T c^2 + b^T Ac + \tilde{b}^T \hat{c} = \frac{1}{8} \\
& \quad b^T Ac^2 + 2b^T \hat{A}c + \tilde{b}^T c^2 = \frac{1}{12} \\
& \quad b^T A^2c + b^T A\hat{c} + b^T \hat{A}c + \tilde{b}^T Ac + \tilde{b}^T \hat{c} = \frac{1}{24} \\
p = 5 & \quad b^T c^4 + 4\tilde{b}^T c^3 = \frac{1}{5} \\
& \quad b^T (c^2 \odot Ac) + b^T (c^2 \odot \hat{c}) + \tilde{b}^T c^3 + 2\tilde{b}^T (c \odot Ac) + 2\tilde{b}^T (c \odot \hat{c}) = \frac{1}{10} \\
& \quad b^T (c \odot Ac^2) + 2b^T (c \odot \hat{A}c) + \tilde{b}^T c^3 + b^T Ac^2 + 2\tilde{b}^T \hat{A}c = \frac{1}{15} \\
& \quad b^T (c \odot A^2c) + b^T (c \odot Ac) + b^T (c \odot \hat{A}c) + \tilde{b}^T (c \odot Ac) + \tilde{b}^T A^2c + b^T A\hat{c} + b^T \hat{A}c = \frac{1}{30} \\
& \quad b^T (Ac \odot Ac) + 2b^T (\hat{c} \odot Ac) + b^T \hat{c}^2 + 2\tilde{b}^T (c \odot Ac) + 2\tilde{b}^T (c \odot \hat{c}) = \frac{1}{20} \\
& \quad b^T Ac^3 + 3b^T A\hat{c}^2 + \tilde{b}^T c^3 = \frac{1}{20} \\
& \quad b^T A(c \odot Ac) + b^T A(c \odot \hat{c}) + b^T A\hat{c}^2 + b^T \hat{A}Ac + b^T \hat{A}\hat{c} + b^T (c \odot Ac) + b^T (c \odot \hat{c}) = \frac{1}{40} \\
& \quad b^T A^2c^2 + 2b^T A\hat{A}c + b^T A\hat{c}^2 + b^T \hat{A}c^2 + 2\tilde{b}^T \hat{A}c = \frac{1}{60} \\
& \quad b^T A^3c + b^T A^2\hat{c} + b^T A\hat{A}c + b^T A\hat{A}\hat{c} + b^T \hat{A}c^2 + b^T \hat{A}c + b^T \hat{A}\hat{c} = \frac{1}{120}
\end{align*}
\]
\[ p = 6 \]
\[ b^T c^3 + 5b^T c^4 = \frac{1}{6} \]
\[ b^T (c^3 \circ Ac) + 3b^T (c^2 \circ Ac) + b^T c^4 + b^T (c^3 \circ c) + 3b^T (c^2 \circ c) = \frac{1}{12} \]
\[ b^T (c^2 \circ Ac^2) + 2b^T (c \circ Ac^2) + 2b^T \left( c^2 \circ \hat{A}c \right) + b^T c^4 + 4b^T \left( c \circ \hat{A}c \right) = \frac{1}{18} \]
\[ b^T (c \circ Ac^3) + 3b^T \left( c \circ \hat{A}c^2 \right) + b^T Ac^3 + 3b^T \hat{A}c^2 + b^T c^4 = \frac{1}{24} \]
\[ b^T Ac^4 + 4b^T \hat{A}c^3 + b^T c^4 = \frac{1}{30} \]
\[ b^T (c^2 \circ A^2c) + 2b^T (c \circ A^2c) + b^T \left( c^2 \circ Ac \right) + b^T \left( c^2 \circ Ac \right) + 2b^T (c \circ Ac) \]
\[ + 2b^T \left( c \circ \hat{A}c \right) + b^T \left( c^2 \circ c \right) = \frac{1}{36} \]
\[ b^T (c^2 \circ A^2c^2) + b^T A^2c^2 + b^T \left( c \circ Ac^2 \right) + b^T \left( c \circ Ac^2 \right) + 2b^T \left( c \circ A\hat{A}c \right) + b^T \hat{A}c^2 + 2b^T A\hat{A}c \]
\[ + 2b^T \left( c \circ \hat{A}c \right) = \frac{1}{72} \]
\[ b^T A^2c^3 + b^T Ac^3 + b^T \hat{A}c^3 + 3b^T A\hat{A}c^2 + 3b^T \hat{A}c^2 = \frac{1}{120} \]
\[ b^T (c \circ Ac \circ Ac) + b^T \left( Ac \circ Ac \right) + b^T \left( Ac \circ Ac \right) + b^T \left( c \circ A \left( c \circ c \right) \right) + b^T \left( c \circ Ac \right) + b^T \left( c \circ \hat{A}c^2 \right) \]
\[ + b^T \hat{A}Ac + b^T A \left( c \circ c \right) + b^T \left( Ac \circ \hat{A}c \right) + b^T \hat{A}c^2 + b^T c^2 \circ c + 2b^T \hat{A}c = \frac{1}{48} \]
\[ b^T A \left( c^2 \circ Ac \right) + b^T A \left( c^2 \circ c \right) + b^T \left( c^2 \circ Ac \right) + 2b^T \left( \hat{A}c \circ Ac \right) + b^T \hat{A}c^3 + 2b^T \left( \hat{A}c \circ \hat{c} \right) \]
\[ + b^T \left( c^2 \circ c \right) = \frac{1}{60} \]
\[ b^T \left( Ac \circ Ac \right) + b^T \left( c \circ Ac \right) + \hat{b}^T \left( c \circ Ac \right) + b^T \hat{A}c^2 + 2b^T \left( Ac \circ \hat{A}c \right) + 2b^T \hat{A}c^2 + 2b^T \left( c \circ \hat{A}c \right) = \frac{1}{90} \]
\[ b^T \left( c \circ A^3c \right) + b^T A^3c + b^T \left( c \circ A^2c \right) + b^T \left( c \circ \hat{A}c \right) + b^T \left( c \circ A\hat{A}c \right) + b^T \left( c \circ A^2c \right) + b^T \hat{A}Ac \]
\[ + b^T A\hat{A}c + b^T A^3c + b^T \left( c \circ \hat{A}c \right) + b^T C\hat{A}c + b^T C\hat{A}c + b^T \hat{A}c = \frac{1}{144} \]
\[ b^T \left( Ac \circ A^2c \right) + b^T \left( Ac \circ \hat{A}c \right) + b^T \left( Ac \circ Ac \right) + b^T \left( Ac \circ Ac \right) + b^T \hat{A}A^2c + b^T \left( c \circ A^2c \right) \]
\[ + b^T \left( \hat{A}c \circ \hat{c} \right) + b^T \hat{A}Ac + b^T \left( c \circ c \right) + b^T \hat{A}c^3 + b^T \hat{A}c + b^T \left( c \circ c \right) = \frac{1}{180} \]
\[ b^T \left( A^2 \circ c \circ Ac \right) + b^T \left( A^2 \circ c \circ c \right) + b^T \hat{A}Ac + b^T A\hat{A}Ac + b^T \hat{A} \left( c \circ Ac \right) + b^T A \left( c \circ Ac \right) + b^T A\hat{A}c \]
\[ + b^T \hat{A} \left( c \circ c \right) + b^T A \left( c \circ c \right) + b^T \hat{A}c^3 + b^T \hat{A}Ac + b^T \hat{A}c = \frac{1}{240} \]
\[ b^T A^3c^2 + b^T A^2c^2 + b^T A\hat{A}Ac^2 + b^T A\hat{A}Ac^2 + 2b^T A^2c + b^T Ac^2 + 2b^T Ac^2 + 2b^T A\hat{A}Ac + 2b^T A^2c = \frac{1}{360} \]
\[ b^T \left( c \circ Ac \circ Ac \right) + b^T \left( Ac \circ Ac \right) + 2b^T \left( c \circ \hat{c} \circ Ac \right) + 2b^T \left( c^2 \circ Ac \right) + 2b^T \left( \hat{c} \circ Ac \right) + 2b^T \left( c^2 \circ \hat{c} \right) \]
\[ + b^T \left( c \circ c^2 \right) + b^T c^2 = \frac{1}{24} \]
\begin{align*}
&b^T (Ac \odot A^2c) + b^T (\hat{c} \odot A^2c) + \hat{b}^T (c \odot A^2c) + \hat{b}^T (Ac \odot Ac) + b^T (Ac \odot \hat{Ac}) \\
&+ 2\hat{b}^T (\hat{c} \odot Ac) + b^T (\hat{c} \odot \hat{Ac}) + \hat{b}^T (c \odot \hat{Ac}) + b^T (c \odot Ac) + \hat{b}^T \hat{c}^2 = \frac{1}{72} \\
&b^T (Ac \odot Ac^2) + b^T (\hat{c} \odot Ac^2) + \hat{b}^T (c \odot Ac^2) + \hat{b}^T (Ac \odot c^2) + 2b^T (Ac \odot \hat{Ac}) + \hat{b}^T (\hat{c} \odot c^2) \\
&+ 2b^T (\hat{c} \odot \hat{Ac}) + 2\hat{b}^T (c \odot \hat{Ac}) = \frac{1}{36} \\
&b^T A (Ac \odot Ac) + 2b^T A (\hat{c} \odot Ac) + 2b^T \hat{A} (c \odot Ac) + \hat{b}^T (Ac \odot Ac) + 2\hat{b}^T (\hat{c} \odot Ac) + 2b^T \hat{A} (c \odot \hat{c}) \\
&+ b^T \hat{c}^2 + \hat{b}^T \hat{c}^2 = \frac{1}{120} \\
&b^T A^4c + b^T A^3\hat{c} + b^T A^2\hat{Ac} + b^T \hat{A} \hat{Ac} + b^T \hat{A} A^2c + \hat{b}^T A^3c + b^T A^2\hat{c} + b^T \hat{A} \hat{Ac} + b^T A^2\hat{c}
&+ b^T \hat{A}^2c + \hat{b}^T A\hat{Ac} + \hat{b}^T \hat{A}Ac + \hat{b}^T \hat{A}\hat{c} = \frac{1}{720}
\end{align*}
B Coefficients of selected methods

All the time-stepping methods in this work can be downloaded as Matlab files from [14]. In this appendix we present selected methods.

**SSP TS M2(4,5,1)**: This method has $\mathcal{C} = 2.18648$

\[
\begin{align*}
a_{21} &= 4.280141748183123e-01 & a_{55} &= 3.779563241192044e-01 & a_{21} &= 6.12029259553491e-02 & b_1 &= 3.456442194983256e-01 \\
a_{31} &= 3.17436442211321e-01 & a_{31} &= 2.06815938961376e-02 & b_2 &= 1.551487425849178e-01 \\
a_{32} &= 1.032647478325804e-01 & \hat{a}_{32} &= 2.361437143530821e-02 & b_3 &= 3.45893244735502e-01 \\
a_{41} &= 3.280547501426051e-01 & a_{41} &= 1.869435227642530e-02 & b_4 &= 1.533137931832064e-01 \\
a_{42} &= 9.334228125655676e-02 & \hat{a}_{42} &= 2.134532206271365e-02 & \hat{b}_2 &= 3.226836941745746e-02 \\
a_{43} &= 4.134096583922347e-01 & a_{43} &= 9.453767556809974e-02 & \hat{b}_3 &= 7.49019151289183e-02 \\
          &                           &                                      & \hat{b}_4 &= 3.50594848132897e-02
\end{align*}
\]

**SSP TS M3(8,6,1)**: This method has $\mathcal{C} = 1.7369$

\[
\begin{align*}
a_{21} &= 3.498630949258150e-01 & a_{65} &= 3.779563241192044e-01 & a_{21} &= 6.12029259553491e-02 & b_1 &= 1.921063160949869e-02 \\
a_{31} &= 2.253295269463227e-01 & a_{71} &= 2.148681581922796e-01 & a_{31} &= 4.358605297856505e-03 \\
a_{32} &= 1.807161013759724e-01 & a_{72} &= 1.533420472452636e-01 & a_{41} &= 1.236333816692593e-03 \\
a_{41} &= 2.071695605568409e-01 & a_{73} &= 1.813808417863181e-02 & a_{51} &= 1.402456855983780e-03 \\
a_{42} &= 4.100178308548576e-02 & a_{74} &= 7.994387176143736e-02 & a_{61} &= 1.548804492637956e-02 \\
a_{43} &= 1.306253212278126e-01 & a_{75} &= 1.630752796649391e-01 & a_{61} &= 1.927179349665056e-01 \\
a_{51} &= 1.667117585911237e-01 & a_{76} &= 2.48409380616690e-01 & a_{61} &= 7.457643792836319e-02 \\
a_{52} &= 2.00966799616593e-02 & a_{81} &= 2.036762412289922e-01 & b_1 &= 1.927179349665056e-01 \\
a_{53} &= 6.402490521280881e-02 & a_{82} &= 1.456707401767411e-01 & b_2 &= 7.457643792836319e-02 \\
a_{54} &= 2.821909187189924e-01 & a_{83} &= 2.379744031395224e-02 & b_3 &= 1.097549250079706e-01 \\
a_{61} &= 1.49314192375556e-01 & a_{84} &= 1.04877345557326e-01 & b_4 &= 1.166274027628658e-01 \\
a_{62} &= 1.319303489675465e-02 & a_{85} &= 2.139668745571685e-01 & b_5 &= 1.862061970475841e-01 \\
a_{63} &= 4.203095914776495e-02 & a_{86} &= 6.560681670556633e-02 & b_6 &= 1.088089628270683e-01 \\
a_{64} &= 1.852522020371737e-01 & a_{87} &= 1.520556075200664e-01 & b_7 &= 4.414821350738243e-02 \\
          &                           &                                      & b_8 &= 1.671599259522612e-01 \\
          &                           &                                      & \hat{b}_1 &= 1.156518516980132e-02
\end{align*}
\]
References

[1] C. Bresten, S. Gottlieb, Z. Grant, D. Higgs, D. I. Ketcheson, and A. Németh, Strong stability preserving multistep Runge-Kutta methods, Mathematics of Computation, 86 (2017), pp. 747–769.

[2] S. Bunya, E. J. Kubatko, J. J. Westerink, and C. Dawson, A wetting and drying treatment for the Runge-Kutta discontinuous Galerkin solution to the shallow water equations, Comput. Methods Appl. Mech. Engrg., 198 (2009), pp. 1548–1562.

[3] R. P. K. Chan and A. Y. J. Tsai, On explicit two-derivative Runge-Kutta methods, Numerical Algorithms, 53 (2010), pp. 171–194.

[4] J. B. Cheng, E. F. Toro, S. Jiang, and W. Tang, A sub-cell WENO reconstruction method for spatial derivatives in the ADER scheme, Journal of Computational Physics 251 (2013), pp. 53 - 80.

[5] A. Christlieb, S. Gottlieb, Z. Grant, and D. C. Seal, Explicit strong stability preserving multistage two-derivative time-stepping schemes, Journal of Scientific Computing, 68 (2016), pp. 914–942.

[6] B. Cockburn and C.-W. Shu, TVB Runge-Kutta local projection discontinuous Galerkin finite element method for conservation laws II: general framework, Mathematics of Computation 52 (1989), pp. 411–435.

[7] V. Daru and C. Tenaud, High order one-step monotonicity-preserving schemes for unsteady compressible flow calculations, Journal of Computational Physics 193 (2004), pp. 563–594.

[8] J. R. Dormand and P. J. Prince, A family of embedded Runge-Kutta formulae, Journal of Computational and Applied Mathematics, 6 (1980), pp. 19–26.

[9] Z. Du and J. Li, A Hermite WENO reconstruction for fourth order temporal accurate schemes based on the GRP solver for hyperbolic conservation laws, Journal of Computational Physics 355 (2018), pp. 385–396

[10] M. Dumbser, O. Zanotti, A. Hidalgo, and D. S. Balsara, ADER-WENO finite volume schemes with space-time adaptive mesh refinement, Journal of Computational Physics 248 (2013), pp. 257 - 286.

[11] L. Ferracina and M. N. Spijker, Stepsize restrictions for the total-variation-diminishing property in general Runge–Kutta methods, SIAM Journal of Numerical Analysis, 42 (2004), pp. 1073–1093.

[12] ______, An extension and analysis of the Shu–Osher representation of Runge–Kutta methods, Mathematics of Computation, 249 (2005), pp. 201–219.

[13] S. Gottlieb, D. I. Ketcheson, and C.-W. Shu, Strong Stability Preserving Runge–Kutta and Multistep Time Discretizations, World Scientific Press, 2011.

[14] S. Gottlieb, Z. J. Grant, D. C. Seal, Explicit SSP multistage two-derivative methods with Taylor series base conditions. https://github.com/SSPmethods/SSPTSmethods.

[15] Z. J. Grant, Explicit SSP multistage two-derivative SSP optimization code. https://github.com/SSPmethods/SSPMultiStageTwoDerivativeMethods, February 2015.

[16] A. Harten, High resolution schemes for hyperbolic conservation laws, Journal of Computational Physics 49 (1983), pp. 357–393.
[17] I. Higuera, *On strong stability preserving time discretization methods*, Journal of Scientific Computing, 21 (2004), pp. 193–223.

[18] ———, *Representations of Runge–Kutta methods and strong stability preserving methods*, SIAM Journal On Numerical Analysis, 43 (2005), pp. 924–948.

[19] I. Higuera, *Strong stability for additive Runge–Kutta methods*, SIAM Journal on Numerical Analysis, 44 (2006), pp. 1735–1758.

[20] G.-S. Jiang and C.-W. Shu, *Efficient implementation of weighted ENO schemes*, J. Comput. Phys., 126 (1996), pp. 202–228.

[21] K. Kastlunger and G. Wanner, *On Turan type implicit Runge-Kutta methods*, Computing (Arch. Elektron. Rechnen), 9 (1972), pp. 317–325.

[22] K. H. Kastlunger and G. Wanner, *Runge Kutta processes with multiple nodes*, Computing (Arch. Elektron. Rechnen), 9 (1972), pp. 9–24.

[23] D. I. Ketcheson, *Highly efficient strong stability preserving Runge–Kutta methods with low-storage implementations*, SIAM Journal on Scientific Computing, 30 (2008), pp. 2113–2136.

[24] D. I. Ketcheson, S. Gottlieb, and C. B. Macdonald, *Strong stability preserving two-step Runge-Kutta methods*, SIAM Journal on Numerical Analysis, (2012), pp. 2618–2639.

[25] D. I. Ketcheson, C. B. Macdonald, and S. Gottlieb, *Optimal implicit strong stability preserving Runge–Kutta methods*, Applied Numerical Mathematics, 52 (2009), p. 373.

[26] D. I. Ketcheson, M. Parsani, and A. J. Ahmadia, *RK-Opt: software for the design of Runge–Kutta methods*, version 0.2. [https://github.com/ketch/RK-opt](https://github.com/ketch/RK-opt).

[27] J. F. B. M. Kraaijevanger, *Contractivity of Runge–Kutta methods*, BIT, 31 (1991), pp. 482–528.

[28] A. Kurganov and E. Tadmor, *New high-resolution schemes for nonlinear conservation laws and convection-diffusion equations*, Journal of Computational Physics 160 (2000), pp. 241–282.

[29] J. Li and Z. Du, *A two-stage fourth order time-accurate discretization for Lax-Wendroff type flow solvers I. hyperbolic conservation laws*, SIAM J. Sci. Computing, 38 (2016) pp. 3046–3069.

[30] X.-D. Liu, S. Osher and T. Chan, *Weighted essentially non-oscillatory schemes*, Journal of Computational Physics 115 (1994), pp. 200–212.

[31] T. Mitsui, *Runge-Kutta type integration formulas including the evaluation of the second derivative*. i., Publications of the Research Institute for Mathematical Sciences, 18 (1982), pp. 325–364.

[32] T. Nguyen-Ba, H. Nguyen-Thu, T. Giordano, and R. Vailancourt, *One-step strong-stability-preserving Hermite-Birkhoff-Taylor methods*, Scientific Journal of Riga Technical University, 45 (2010), pp. 95–104.

[33] N. Obreschkoff, *Neue quadraturformeln*, Abh. Preuss. Akad. Wiss. Math.-Nat. Kl., 4 (1940).

[34] H. Ono and T. Yoshida, *Two-stage explicit Runge-Kutta type methods using derivatives*, Japan Journal of Industrial and Applied Mathematics, 21 (2004), pp. 361–374.

[35] S. Osher and S. Chakravarthy, *High resolution schemes and the entropy condition*, SIAM Journal on Numerical Analysis 21(1984), pp. 955–984.

[36] L. Pan, K. Xu, Q. Li, and J. Li, *An efficient and accurate two-stage fourth-order gas-kinetic scheme for the Euler and Navier–Stokes equations*, Journal of Computational Physics 326 (2016), pp. 197–221.
[37] J. Qiu, M. Dumbser, and C.-W. Shu, *The discontinuous Galerkin method with Lax–Wendroff type time discretizations*, Computer Methods in Applied Mechanics and Engineering 194 (2005), pp. 4528–4543.

[38] S. J. Ruuth and R. J. Spiteri, *Two barriers on strong-stability-preserving time discretization methods*, Journal of Scientific Computing, 17 (2002), pp. 211–220.

[39] D. C. Seal, Y. Guclu, and A. J. Christlieb, *High-order multiderivative time integrators for hyperbolic conservation laws*, Journal of Scientific Computing, 60 (2014), pp. 101–140.

[40] H. Shintani, *On one-step methods utilizing the second derivative*, Hiroshima Mathematical Journal, 1 (1971), pp. 349–372.

[41] ———, *On explicit one-step methods utilizing the second derivative*, Hiroshima Mathematical Journal, 2 (1972), pp. 353–368.

[42] C.-W. Shu, *Total-variation diminishing time discretizations*, SIAM Journal on Scientific and Statistical Computing, 9 (1988), pp. 1073–1084.

[43] C.-W. Shu and S. Osher, *Efficient implementation of essentially non-oscillatory shock-capturing schemes*, Journal of Computational Physics, 77 (1988), pp. 439–471.

[44] R. J. Spiteri and S. J. Ruuth, *A new class of optimal high-order strong-stability-preserving time discretization methods*, SIAM J. Numer. Anal., 40 (2002), pp. 469–491.

[45] D. D. Stancu and A. H. Stroud, *Quadrature formulas with simple Gaussian nodes and multiple fixed nodes*, Mathematics of Computation, 17 (1963), pp. 384–394.

[46] P.K. Sweby, *High resolution schemes using flux limiters for hyperbolic conservation laws*, SIAM Journal on Numerical Analysis 21 (1984), pp. 995–1011.

[47] E. Tadmor, *Approximate solutions of nonlinear conservation laws* in Advanced Numerical Approximation of Nonlinear Hyperbolic Equations, Lectures Notes from CIME Course Cetraro, Italy, 1997, Number 1697 in Lecture Notes in Mathematics. Springer-Verlag, 1998.

[48] E. Toro and V.A. Titarev, *Solution of the generalized Riemann problem for advection–reaction equations*, Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences 458 (2002), pp. 271–281.

[49] E.F. Toro and V.A. Titarev, *Derivative Riemann solvers for systems of conservation laws and ADER methods*, Journal of Computational Physics 212 (2006), pp. 150–165.

[50] A. Y. J. Tsai, R. P. K. Chan, and S. Wang, *Two-derivative Runge–Kutta methods for PDEs using a novel discretization approach*, Numerical Algorithms, 65 (2014), pp. 687–703.

[51] P. Turán, *On the theory of the mechanical quadrature*, Acta Universitatis Szegediensis. Acta Scientiarum Mathematicarum, 12 (1950), pp. 30–37.

[52] J. Verner, *Explicit rungeKutta methods with estimates of the local truncation error*, SIAM Journal on Numerical Analysis, 15 (2014), pp. 772–790.

[53] Y. Xing, X. Zhang, and C.-W. Shu, *Positivity-preserving high order well-balanced discontinuous Galerkin methods for the shallow water equations*, Advances in Water Resources, 33 (2010), pp. 1476–1493.

[54] X. Zhang and C.-W. Shu, *On Maximum-principle-satisfying High Order Schemes for Scalar Conservation Laws*, Journal of Computational Physics 229 (2010), pp. 3091–3120.