Strong Stability Preserving Integrating Factor Runge–Kutta Methods

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Abstract

Strong stability preserving (SSP) Runge–Kutta methods are often desired when evolving in time problems that have two components that have very different time scales. For problems with a linear component that is stiff and a nonlinear component that is not, integrating factor methods offer an attractive alternative to traditional time-stepping methods. However, the strong stability properties of integrating factor Runge–Kutta methods have not been established. In this work we show that it is possible to define explicit integrating factor Runge–Kutta methods that preserve the desired strong stability properties satisfied by each of the two components when coupled with forward Euler time-stepping, or even given weaker conditions. We define sufficient conditions for an explicit integrating factor Runge–Kutta method to be SSP, namely that they are based on explicit SSP Runge–Kutta methods with non-decreasing abscissas. We find such methods of up to fourth order and up to ten stages, analyze their SSP coefficients, and prove their optimality in a few cases. We test these methods to demonstrate their convergence and to show that the SSP time-step predicted by the theory is generally sharp, and that the non-decreasing abscissa condition is needed in our test cases. Finally, we show that on a typical total variation diminishing nonlinear test-case our new explicit SSP integrating factor Runge–Kutta methods out-perform the corresponding explicit SSP Runge–Kutta methods, implicit-explicit SSP Runge–Kutta methods, and some well-known exponential time differencing methods.

1 Introduction

Explicit strong stability preserving (SSP) Runge–Kutta methods were first developed in [12, 13] for use in conjunction with total variation diminishing (TVD) spatial discretizations for hyperbolic
conservation laws

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

with discontinuous solutions. These spatial discretizations of \( f(U)_x \) ensure that when the resulting semi-discretized system of ordinary differential equations (ODEs)

\[ u_t = F(u), \quad (1) \]

is evolved in time using the \textit{forward Euler method}, a strong stability property

\[ \|u^{n+1}\| = \|u^n + \Delta t F(u^n)\| \leq \|u^n\| \quad (2) \]

is satisfied, under some step size restriction

\[ 0 \leq \Delta t \leq \Delta t_{FE}. \quad (3) \]

These TVD spatial discretizations are designed to satisfy the strong stability property

\[ \|u^{n+1}\| \leq \|u^n\| \quad (4) \]

\textit{when coupled with the forward Euler time discretization}. However, in actuality a higher order time integrator is desired, for both accuracy and linear stability reasons. If we can re-write a higher order time discretization as a convex combination of forward Euler steps, we can ensure that any convex functional property \((4)\) that is satisfied by the forward Euler method will still be satisfied by the higher order time discretization, perhaps under a different time-step.

For example, we can write an \( s \)-stage explicit Runge–Kutta method as:

\[ u^{(0)} = u^n, \quad u^{(i)} = \sum_{j=0}^{i-1} (\alpha_{i,j} u^{(j)} + \Delta t \beta_{i,j} F(u^{(j)})), \quad i = 1, \ldots, s \quad (5) \]

\[ u^{n+1} = u^{(s)}. \]

Note that for consistency, we must have \( \sum_{j=0}^{i-1} \alpha_{i,j} = 1 \). If all the coefficients \( \alpha_{i,j} \) and \( \beta_{i,j} \) are non-negative, and a given \( \alpha_{i,j} \) is zero only if its corresponding \( \beta_{i,j} \) is zero, then each stage can be rearranged into a convex combination of forward Euler steps

\[ \|u^{(i)}\| = \left\| \sum_{j=0}^{i-1} (\alpha_{i,j} u^{(j)} + \Delta t \beta_{i,j} F(u^{(j)})) \right\| \leq \sum_{j=0}^{i-1} \alpha_{i,j} \left\| u^{(j)} + \Delta t \frac{\beta_{i,j}}{\alpha_{i,j}} F(u^{(j)}) \right\| \leq \|u^n\|, \]
where the final inequality follows from (2) and (3), provided that the time-step satisfies

$$\Delta t \leq \min_{i,j} \frac{\alpha_{i,j}}{\beta_{i,j}} \Delta t_{\text{FE}}. \tag{6}$$

(Note that if any of the $\beta$’s are equal to zero, the corresponding ratio is considered infinite).

It is clear from this example that whenever we can re-write an explicit Runge–Kutta method as a convex combination of forward Euler steps, the forward Euler condition (2) will be preserved by the higher-order time discretizations, under the time-step restriction $\Delta t \leq C \Delta t_{\text{FE}}$ where $C = \min_{i,j} \frac{\alpha_{i,j}}{\beta_{i,j}}$. As long as $C > 0$, the method is called strong stability preserving (SSP) with SSP coefficient $C$. We observe that in the original papers [12, 13], the term $\| \cdot \|$ in Equation (2) above represented the total variation semi-norm. In general, though, the strong stability preservation property holds for any semi-norm, norm, or convex functional, as determined by the design of the spatial discretization. The only requirements are that the forward Euler condition (2) holds, and that the time-discretization can be decomposed into a convex combination of forward Euler steps with $C > 0$, as above.

Clearly, this convex combination condition is a sufficient condition for strong stability preservation. In fact, it has been shown that it is also necessary for strong stability preservation [5, 9, 14]. This means that if a method cannot be decomposed into a convex combination of forward Euler steps, then we can always find some ODE with some initial condition such that the forward Euler condition is satisfied but the method does not satisfy the strong stability condition for any positive time-step [5].

It is not always possible to decompose a method into convex combinations of forward Euler steps where $C > 0$. In fact in [9, 11] it was shown that explicit SSP Runge–Kutta methods cannot exist for order $p > 4$. Furthermore, the value of $C$ determines in large part what the size of an allowable time-step will be, and so we seek methods that have the largest possible SSP coefficient. Of course, a more important quantity is the total cost of the time evolution, which is related to the allowable time step relative to the number of function evaluations at each time-step. To allow us to compare the efficiency of explicit methods of a given order, we define the effective SSP coefficient $C_{\text{eff}} = \frac{C}{s}$ where $s$ is the number of stages (typically the number of function evaluations). Unfortunately, all explicit $s$-stage Runge–Kutta methods have an SSP bound $C \leq s$, and therefore $C_{\text{eff}} \leq 1$ [5]. Even worse, this upper bound is not usually attained. However, many efficient explicit SSP Runge–Kutta methods have been found, as we discuss in Section 2.

In this work, we are interested in a semi-discretized problem of the form

$$u_t = Lu + N(u)$$

where $L$ is a linear operator that significantly restricts the time-step. This motivates our investigation of integrating factor methods, where the linear component $Lu$ is handled exactly, and then the
allowable time-step depends only upon the nonlinear component \( N(u) \). In this work, we discuss the conditions under which this process guarantees that the strong stability property (4) is preserved. In particular, we show that if we step the transformed problem forward using an SSP Runge–Kutta method where the abscissas (i.e. the time-levels approximated by each stage) are non-decreasing, we obtain a method that preserves the desired strong stability property.

The paper is structured as follows. In Section 2 we review some optimal explicit SSP Runge–Kutta methods of orders \( p \leq 4 \) and give the SSP coefficients and effective SSP coefficients of the optimal methods in this class. In Section 3 we describe explicit integrating factor (also known as Lawson type) Runge–Kutta (IFRK) methods [10]. We prove that when IFRK methods are based on explicit SSP Runge–Kutta methods with non-decreasing abscissas, they preserve the strong stability property. We also show an example that demonstrates that when using an IFRK method based on an explicit SSP Runge–Kutta method that has decreasing abscissas, the SSP property is violated. In Section 4 we formulate the optimization problem that will enable us to find optimal explicit SSP Runge–Kutta methods that have non-decreasing abscissas, and in Section 5 we present some optimal methods in this class and their SSP coefficients and effective SSP coefficients. We also prove the optimality of one of the methods in this class. In Section 6 we present numerical examples that show how our explicit SSP integrating factor Runge–Kutta (eSSPIFRK) methods perform on typical test cases compared to explicit, implicit-explicit (IMEX), and exponential time differencing (ETD) methods. In Section 7 we present our conclusions.

Note: The following acronyms and notations are used in this work:

| Acronym     | Description                                    |
|-------------|------------------------------------------------|
| IFRK        | integrating factor Runge–Kutta method.         |
| SSP         | strong stability preserving.                    |
| eSSPRK      | explicit SSP Runge–Kutta method.               |
| eSSPRK+     | explicit SSP Runge–Kutta method with non-decreasing abscissas. |
| eSSPIFRK    | explicit SSP integrating factor Runge–Kutta method. |
| (s,p)       | number of stages \( s \) and order \( p \).    |
| IMEX        | implicit-explicit additive method.             |
| ETD         | exponential time-differencing methods.         |

2 A review of explicit SSP Runge–Kutta methods

SSP Runge–Kutta methods guarantee the strong stability (in any norm, semi-norm, or convex functional) of the numerical solution of any ODE provided only that the forward Euler condition (2) is satisfied under a time step restriction (3). This requirement leads to severe restrictions on the allowable order of SSP methods, and the allowable time step \( \Delta t \leq C \Delta t_{FE} \). In this section, we review
some popular and efficient explicit SSP Runge–Kutta methods, and present the SSP coefficients of optimal methods of up to ten stages and fourth order.

In the original papers on SSP time-stepping methods (there called TVD time-stepping) [12, 13], the authors presented the first explicit SSP Runge–Kutta methods. These methods were second and third order with SSP coefficient $C = 1$ ($C_{\text{eff}} = \frac{1}{2}$ and $C_{\text{eff}} = \frac{1}{3}$, respectively), and were proven optimal [6]. We use the notation eSSPRK(s,p) to denote an explicit SSP Runge–Kutta method with $s$ stages and of order $p$.

**eSSPRK(2,2):**

\[
\begin{align*}
  u^{(1)} &= u^n + \Delta t F(u^n) \\
  u^{n+1} &= \frac{1}{2}u^n + \frac{1}{2} (u^{(1)} + \Delta t F(u^{(1)})),
\end{align*}
\]

**eSSPRK(3,3):**

\[
\begin{align*}
  u^{(1)} &= u^n + \Delta t F(u^n) \\
  u^{(2)} &= \frac{3}{4}u^n + \frac{1}{4} (u^{(1)} + \Delta t F(u^{(1)})) \\
  u^{n+1} &= \frac{1}{3}u^n + \frac{2}{3} (u^{(2)} + \Delta t F(u^{(2)})).
\end{align*}
\]

Method (8) has been extensively used and is known as the Shu-Osher method.

| $s$ | $p$ | 2   | 3   | 4   |
|-----|-----|-----|-----|-----|
| 1   | 2   | -   | -   | -   |
| 2   | 3.0000 | 2.0000 | -   | -   |
| 3   | 4.0000 | 2.6506 | 1.5082 |
| 4   | 5.0000 | 3.5184 | 2.2945 |
| 5   | 6.0000 | 4.2879 | 3.3209 |
| 6   | 7.0000 | 5.1071 | 4.1459 |
| 7   | 8.0000 | 6.0000 | 4.9142 |
| 8   | 9.0000 | 6.7853 | 6.0000 |

| $s$ | $p$ | 2   | 3   | 4   |
|-----|-----|-----|-----|-----|
| 1   | 2   | -   | -   | -   |
| 2   | 0.5000 | -   | -   | -   |
| 3   | 0.6667 | 0.3333 | -   | -   |
| 4   | 0.7500 | 0.5000 | -   | -   |
| 5   | 0.8000 | 0.5301 | 0.3016 |
| 6   | 0.8333 | 0.5864 | 0.3824 |
| 7   | 0.8571 | 0.6126 | 0.4744 |
| 8   | 0.8750 | 0.6384 | 0.5182 |
| 9   | 0.8889 | 0.6667 | 0.5460 |
| 10  | 0.9000 | 0.6785 | 0.6000 |

Table 1: SSP coefficients of the optimal eSSPRK(s,p) methods.

Table 2: Effective SSP coefficients of the optimal eSSPRK(s,p) methods.
No four stage fourth order explicit Runge–Kutta methods exist with a positive SSP coefficient [6, 11]. However, fourth order methods with more than four stages \((s > p)\) do exist.

**eSSPRK(5,4):** Found by Spiteri and Ruuth [15]

\[
\begin{align*}
    u^{(1)} &= u^n + 0.391752226571890\Delta t F(u^n) \\
    u^{(2)} &= 0.444370493651235u^n + 0.555629506348765u^{(1)} + 0.368410593050371\Delta t F(u^{(1)}) \\
    u^{(3)} &= 0.620101851488403u^n + 0.379898148511597u^{(2)} + 0.251891774271694\Delta t F(u^{(2)}) \\
    u^{(4)} &= 0.178079954393132u^n + 0.821920045606868u^{(3)} + 0.544974750228521\Delta t F(u^{(3)}) \\
    u^{n+1} &= 0.517231671970585u^{(2)} + 0.096059710526147u^{(3)} + 0.063692468666290\Delta t F(u^{(3)}) \\
    & \quad + 0.386708617503269u^{(4)} + 0.226007483236906\Delta t F(u^{(4)})
\end{align*}
\]

has \(C = 1.508\) \((C_{eff} = 0.302)\).

**eSSPRK(10,4):** Found by Ketcheson [8] \((C_{eff} = 0.6)\) that has a low-storage formulation:

\[
\begin{align*}
    u^{(1)} &= u^n + \frac{1}{6}\Delta t F(u^n) \\
    u^{(i+1)} &= u^{(i)} + \frac{1}{6}\Delta t F(u^{(i)}) \quad i = 1, 2, 3 \\
    u^{(5)} &= \frac{3}{5}u^n + \frac{2}{5} \left( u^{(4)} + \frac{1}{6}\Delta t F(u^{(4)}) \right) \\
    u^{(i+1)} &= u^{(i)} + \frac{1}{6}\Delta t F(u^{(i)}) \quad i = 5, 6, 7, 8 \\
    u^{n+1} &= \frac{1}{25}u^n + \frac{9}{25} \left( u^{(4)} + \frac{1}{6}\Delta t F(u^{(4)}) \right) + \frac{3}{5} \left( u^{(9)} + \frac{1}{6}\Delta t F(u^{(9)}) \right)
\end{align*}
\]

has \(C = 6\).

In Table 1 we present the SSP coefficients of optimal explicit SSP Runge–Kutta methods of up to \(s = 10\) stages and order \(p = 4\), and in Table 2 the corresponding effective SSP coefficients. Unfortunately, no methods of order \(p \geq 5\) with positive SSP coefficients can exist [9, 11].

### 3 Explicit SSP Runge–Kutta schemes for use with integrating factor methods

**Motivation:** We consider a problem of the form

\[
    u_t = Lu + N(u) \quad (9)
\]
with a linear constant coefficient component $Lu$ and a nonlinear component $N(u)$. The case we are interested in is when some strong stability condition is known for the forward Euler step of the nonlinear component $N(u)$

$$\|u^n + \Delta t N(u^n)\| \leq \|u^n\| \quad \text{for} \quad \Delta t \leq \Delta t_{FE}$$

while taking a forward Euler step using the linear component $Lu$ results in the strong stability condition

$$\|u^n + \Delta t Lu^n\| \leq \|u^n\| \quad \text{for} \quad \Delta t \leq \tilde{\Delta} t_{FE}$$

where $\tilde{\Delta} t_{FE} << \Delta t_{FE}$. In such cases, stepping forward using an explicit SSP Runge–Kutta method, or even an implicit-explicit (IMEX) SSP Runge–Kutta method will result in severe constraints on the allowable time-step.

An alternative methodology that may alleviate the restriction on the allowable time-step involves solving the linear part exactly using an integrating factor approach

$$e^{-Lt}u_t - e^{-Lt}Lu = e^{-Lt}N(u)$$

$$\left(e^{-Lt}u\right)_t = e^{-Lt}N(u).$$

A transformation of variables $w = e^{-Lt}u$ gives the ODE system

$$w_t = e^{-Lt}N(e^{Lt}w) = G(w),$$

which can then be evolved forward in time using, for example, an explicit Runge–Kutta method of the form (5). For each stage $u^{(i)}$, which corresponds to the solution at time $t_i = t^n + c_i \Delta t$ (where each $c_i$ is the abscissa of the method at the $i$th stage), the corresponding integrating factor Runge–Kutta method becomes

$$e^{-Lt_i}u^{(i)} = \sum_{j=0}^{i-1} \left( \alpha_{i,j} e^{-Lt_j}u^{(j)} + \Delta t \beta_{i,j} e^{-Lt_j}N(u^{(j)}) \right),$$

or

$$u^{(i)} = \sum_{j=0}^{i-1} \left( \alpha_{i,j} e^{L(t_i-t_j)}u^{(j)} + \Delta t \beta_{i,j} e^{L(t_i-t_j)}N(u^{(j)}) \right) = \sum_{j=0}^{i-1} \left( \alpha_{i,j} e^{L(c_i-c_j)\Delta t}u^{(j)} + \Delta t \beta_{i,j} e^{L(c_i-c_j)\Delta t}N(u^{(j)}) \right).$$

In the following results we establish the SSP properties of this approach.

\textbf{Theorem 1.} If a linear operator $L$ satisfies (11) for some value of $\tilde{\Delta} t_{FE} > 0$, then

$$\|e^{\tau L}u^n\| \leq \|u^n\| \quad \forall \tau \geq 0.$$  (13)
Proof. The Taylor series expansion of $e^z$ can be written as
\[
e^z = \sum_{j=0}^{\infty} \gamma_j(r) \left(1 + \frac{z}{r}\right)^j\] where $\gamma_j = \frac{r^j}{j!} e^{-r}$
where the coefficients $\gamma_j$ are clearly nonnegative for all values of $r \geq 0$. These coefficients sum to one because
\[
\sum_{j=0}^{\infty} \gamma_j = \sum_{j=0}^{\infty} \frac{r^j}{j!} e^{-r} = e^{-r} \sum_{j=0}^{\infty} \frac{r^j}{j!} = e^{-r} e^r = 1.
\]
Using this we can show that $e^{\tau L} u^n$ can be written as a convex combination of forward Euler steps with a modified time-step $\hat{\tau}$, so that
\[
\|e^{\tau L} u^n\| = \left\| \sum_{j=0}^{\infty} \gamma_j(r) \left(1 + \frac{\tau L}{r}\right)^j u^n \right\|
\leq \sum_{j=0}^{\infty} \gamma_j(r) \left\| \left(1 + \frac{\tau L}{r}\right)^j u^n \right\|
\leq \sum_{j=0}^{\infty} \gamma_j(r) \|u^n\| \leq \|u^n\| \text{ for any } 0 \leq \tau \leq r \Delta t_{FE}.
\]
As this is true for any value of $r \geq 0$, we have
\[
\|e^{\tau L} u^n\| \leq \|u^n\| \quad \forall \tau \geq 0.
\]
Note that a negative value of $\tau$ is not allowed here.

Note: The theorem above deals with the case that (11) is satisfied for some value of $\Delta t_{FE} > 0$. However, requiring $L$ to satisfy only condition (13) is sufficient for the integrating factor Runge–Kutta method to be SSP. In the following results, therefore, we only require the condition (13), which is a weaker condition than (11).

Lemma 1. Given a linear operator $L$ that satisfies (13) and a (possibly nonlinear) operator $N(u)$ that satisfies (10) for some value of $\Delta t_{FE} \geq 0$, we have
\[
\|e^{\tau L} (u^n + \Delta t N(u^n))\| \leq \|u^n\| \quad \forall \Delta t \leq \Delta t_{FE}, \quad \text{provided that } \tau \geq 0.
\] (14)
Proof. Separate the term $e^{\tau L} (u^n + \Delta t N(u^n))$ to two steps:
\[
y^{(1)} = u^n + \Delta t N(u^n)
y^{(2)} = e^{\tau L} y^{(1)}
\]
Clearly, from (13) we have
\[ \|y^{(2)}\| = \|e^{\tau L}y^{(1)}\| \leq \|y^{(1)}\| \]
for any \( \tau \geq 0 \). Now, from (10) we also have
\[ \|y^{(1)}\| = \|u^n + \Delta t N(u^n)\| \leq \|u^n\| \quad \forall \Delta t \leq \Delta t_{FE}. \]
Putting these two together we obtain the desired result. \( \square \)

The following theorem describes the conditions under which an integrating factor Runge–Kutta method is strong stability preserving.

**Theorem 2.** Given a linear operator \( L \) that satisfies (13) and a (possibly nonlinear) operator \( N(u) \) that satisfies (10) for some value of \( \Delta t_{FE} \geq 0 \), and a Runge–Kutta integrating factor method of the form
\[
\begin{align*}
u^{(0)} &= u^n, \\
u^{(i)} &= \sum_{j=0}^{i-1} e^{L(c_i-c_j)} \Delta t \left( \alpha_{i,j} u^{(j)} + \Delta t \beta_{i,j} N(u^{(j)}) \right), \quad i = 1, \ldots, s \\
u^{n+1} &= u^{(s)}
\end{align*}
\]
where \( 0 = c_1 \leq c_2 \leq \ldots \leq c_s \), then \( u^{n+1} \) obtained from (15) satisfies
\[ \|u^{n+1}\| \leq \|u^n\| \quad \forall \Delta t \leq C\Delta t_{FE}. \] (16)

**Proof.** We observe that for each stage of (15)
\[
\|u^{(i)}\| = \left\| \sum_{j=0}^{i-1} e^{L(c_i-c_j)} \Delta t \left( \alpha_{i,j} u^{(j)} + \Delta t \beta_{i,j} N(u^{(j)}) \right) \right\|
\leq \sum_{j=0}^{i-1} \|e^{L(c_i-c_j)} \Delta t \left( \alpha_{i,j} u^{(j)} + \Delta t \beta_{i,j} N(u^{(j)}) \right)\|
\leq \sum_{j=0}^{i-1} \alpha_{i,j} \left\| e^{L(c_i-c_j)} \Delta t \left( u^{(j)} + \Delta t \beta_{i,j} N(u^{(j)}) \right) \right\|
\]
where the last inequality follows from Corollary 1, as long as \( c_i - c_j \geq 0 \) and \( \Delta t \frac{\beta_{i,j}}{\alpha_{i,j}} \leq \Delta t_{FE} \). This establishes the result of the theorem. Furthermore, this proof ensures that these methods have internal stage strong stability as well, i.e. \( \|u^{(i+1)}\| \leq \|u^{(i)}\| \) at each stage \( i \) of the time-stepping, under the same time-step restriction. \( \square \)
Note: It is possible to preserve the strong stability property even with decreasing abscissas, provided that whenever the term $c_i - c_j$ is negative, the operator $L$ is replaced by an operator $\tilde{L}$ that satisfies the condition

$$\|e^{-\tau\tilde{L}}u^n\| \leq \|u^n\| \quad \forall \tau \geq 0.$$  

For hyperbolic partial differential equations, this is accomplished by using the spatial discretization that is stable for downwind problem. This approach is similar to the one employed in the classical SSP literature, where negative coefficients $\beta_{i,j}$ may be allowed if the corresponding operator is replaced by a downwinded operator.

**Example:** To demonstrate the practical importance of this theorem, consider the partial differential equation

$$u_t + 5u_x + \left(\frac{1}{2}u^2\right)_x = 0 \quad u(0, x) = \begin{cases} 1, & \text{if } 0 \leq x \leq 1/2 \\ 0, & \text{if } x > 1/2 \end{cases}$$

on the domain $[0, 1]$ with periodic boundary conditions. We discretize the spatial grid with $N = 400$ and use a first-order upwind difference to semi-discretize the linear term, and a fifth order WENO finite difference for the nonlinear terms. For the time discretization, we use the integrating factor method based on the explicit eSSPRK(3,3) Shu-Osher method (8):

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

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

$$u^{n+1} = \frac{1}{3} e^{L \Delta t}u^n + \frac{2}{3} e^{\frac{1}{2}L \Delta t}u^{(2)} + \frac{2}{3} e^{\frac{1}{2}L \Delta t} \Delta tN(u^{(2)}). \quad (17)$$

The appearance of exponentials with negative exponents is due to the fact that (8) has decreasing abscissas. For comparison we also use an IFRK(3,3) method based on an explicit SSP Runge–Kutta method with non-decreasing abscissas, denoted eSSPRK$^+$ (3, 3) (which we be presented in (21))

$$u^{(1)} = \frac{1}{2} e^{\frac{1}{2}L \Delta t}u^n + \frac{1}{2} e^{\frac{1}{2}L \Delta t} \left(u^n + \frac{4}{3} \Delta tN(u^n)\right)$$

$$u^{(2)} = \frac{2}{3} e^{\frac{1}{2}L \Delta t}u^n + \frac{1}{3} \left(u^{(1)} + \frac{4}{3} \Delta tN(u^{(1)})\right)$$

$$u^{n+1} = \frac{59}{128} e^{L \Delta t}u^n + \frac{15}{128} e^{L \Delta t} \left(u^n + \frac{4}{3} \Delta tN(u^n)\right) + \frac{27}{64} e^{\frac{1}{2}L \Delta t} \left(u^{(2)} + \frac{4}{3} \Delta tN(u^{(2)})\right). \quad (18)$$

The eSSPRK$^+$ (3, 3) method this integrating factor is based on has SSP coefficient $C = \frac{3}{4}$, which is smaller than the $C = 1$ of the Shu-Osher method (8), due to the restriction on the non-decreasing
Figure 1: Total variation behavior of the evolution over 25 time-steps using the integrating factor methods (17) (blue dots) and (18) (red stars). On the x-axis is the value of $\lambda = \frac{\Delta t}{\Delta x}$, on the y-axis is $\log_{10}$ of the maximal rise in TV.

Theorem 2 above tells us that the IFRK method (18) will be SSP while the IFRK method (17) based on the Shu-Osher method (8) will not be.

We selected different values of $\Delta t$ and used each one to evolve the solution 25 time steps using the IFRK methods (17) and (18). We calculated the maximal rise in total variation over each stage for 25 time steps. In Figure 1 we show the $\log_{10}$ of the maximal rise in total variation vs. the value of $\lambda = \frac{\Delta t}{\Delta x}$ of the evolution using (17) (in blue) and using (18) (in red). We observe that the results from method (17) have a large maximal rise in total variation even for very small values of $\lambda$, while the results from (18) maintain a small maximal rise in total variation up to $\lambda \approx 0.8$.

This example clearly illustrates that basing an IFRK method on an explicit SSP Runge–Kutta method is not enough to ensure the preservation of a strong stability property. In this case, we must use the non-decreasing abscissa condition in Theorem (2) to ensure that the strong stability property is preserved.

4 Formulating the optimization problem

Our aim is to find eSSPRK(s,p) methods which have non-decreasing abscissas and the largest possible SSP coefficient $C$. We denote these methods eSSPRK$^+(s, p)$. These methods can then be used to produce an integrating factor method (15) that has a guarantee of nonlinear stability, as we showed in Section 3 above. Following the approach developed by Ketcheson [8], we formulate an optimization
problem similar to the one used for explicit SSP Runge-Kutta methods [5] but with one additional constraint.

Although the C is most easily seen in Shu-Osher form, constructing the optimization problem is easier when the method is written in Butcher form:

\[
\begin{align*}
  u^{(i)} &= u^n + \Delta t \sum_{j=1}^{i-1} a_{ij} F(u^{(j)}) \quad (1 \leq i \leq s) \\
  u^{n+1} &= u^n + \Delta t \sum_{j=1}^{s} b_j F(u^{(j)}).
\end{align*}
\]

We can put all the \(a_{ij}\) values into a matrix \(A\) and all the \(b_j\) into a vector \(b\). Then we define the vector of abscissas \(c = Ae\), where \(e\) is the vector of ones of the appropriate length. We rewrite (19) in vector form

\[
Y = eu^n + \Delta t SF(Y)
\]

where \(S\) is the square matrix defined by:

\[
S = \begin{pmatrix} A & 0 \\ b^T & 0 \end{pmatrix}.
\]

We add \(rSY\) to each side to obtain

\[
(I + rS) Y = eu^n + rS \left( Y + \frac{\Delta t}{r} F(Y) \right) \Rightarrow Y = R(eu^n) + P \left( Y + \frac{\Delta t}{r} F(Y) \right),
\]

for \(R = (I + rS)^{-1}\) and \(P = rRS\). Clearly, if \(Re\) and \(P\) have all non-negative components, we have a convex combination of forward Euler steps. Therefore, the strong stability property (4) will be preserved under the modified time-step restriction \(\Delta t \leq r\Delta t_{FE}\).

As discussed in [5], the goal is to maximize the value of \(r\) subject to the constraints

\[
\begin{align*}
  (I + rS)^{-1} e &\geq 0 \quad \text{(20a)} \\
  r (I + rS)^{-1} S &\geq 0 \quad \text{(20b)} \\
  \tau_k(A, b) &= 0 \text{ for } k = 1, \ldots, P, \quad \text{(20c)}
\end{align*}
\]

Where in the inequalities are all component wise and \(\tau_k\) in (20c) are the order conditions.

In addition to the constraints (20a) – (20c), we must also add the condition that the abscissas are non-decreasing

\[
c_1 \leq c_2 \leq \cdots \leq c_s \leq 1.
\]

Solving this optimization problem will generate an explicit SSP Runge–Kutta method with coefficients \(A\) and \(b\) such that the abscissas are non-decreasing, with a SSP coefficient \(C = r\).
4.1 Order conditions

The equality constraints (20c) for the optimization problem above come from the order conditions. Below are the order conditions for methods up to fourth order.

\[ b^T e = 1 \]

In addition to this condition second order methods must also satisfy:

\[ b^T c = \frac{1}{2} \]

There are two more order conditions required to obtain third order:

\[ b^T (c \cdot c) = \frac{1}{3}, \quad b^T Ac = \frac{1}{6} \]

For fourth order four additional conditions must be satisfied:

\[ b^T (c \cdot c \cdot c) = \frac{1}{4}, \quad b^T (c \cdot Ac) = \frac{1}{8}, \quad b^T A (c \cdot c) = \frac{1}{12}, \quad b^T A^2 c = \frac{1}{24} \]

Note that \((a \cdot b)\) denotes element-wise multiplication. We do not present the order conditions past fourth order since there are no explicit SSP Runge–Kutta methods greater than fourth order.

5 Optimal methods

The optimization problem above was implemented in MATLAB and used to find optimal eSSPRK+ methods of up to ten stages and fourth order. These methods have non-decreasing abscissas and so can be used as a basis for explicit SSP integrating factor Runge–Kutta (eSSPIFRK) methods.

The SSP coefficients and effective SSP coefficients of the optimal eSSPRK+ methods are listed in Tables 3 and 4. The SSP coefficients of this family of methods are compared to those of the optimal eSSPRK methods with no constraint on the abscissas in Figure 2, where the circles indicate the SSP coefficient of the optimal explicit SSPRK methods while the lines are the SSP coefficients of the optimal explicit SSPRK+ methods.

We observe that the optimal second order methods we found have the same SSP coefficients as the previously known SSP Runge–Kutta methods. This is not surprising as the abscissas of those optimal methods are non-decreasing, so our optimization routine found the previously known optimal methods. These eSSPRK+(s,2) methods have SSP coefficient \(\mathcal{C} = s - 1\) and effective SSP coefficient
| s  | 2   | 3   | 4   |
|----|-----|-----|-----|
| 1  | -   | -   | -   |
| 2  | 1.0000 | -   | -   |
| 3  | 2.0000 | 0.7500 | -   |
| 4  | 3.0000 | 1.8182 | -   |
| 5  | 4.0000 | 2.6351 | 1.3466 |
| 6  | 5.0000 | 3.5184 | 2.2738 |
| 7  | 6.0000 | 4.2857 | 3.0404 |
| 8  | 7.0000 | 5.1071 | 3.8926 |
| 9  | 8.0000 | 6.0000 | 4.6048 |
| 10 | 9.0000 | 6.7853 | 5.2997 |

Table 3: SSP coefficients of the optimal eSSPRK+(s,p) methods.

| s  | 2   | 3   | 4   |
|----|-----|-----|-----|
| 1  | -   | -   | -   |
| 2  | 0.5000 | -   | -   |
| 3  | 0.6667 | 0.2500 | -   |
| 4  | 0.7500 | 0.4545 | -   |
| 5  | 0.8000 | 0.5270 | 0.2693 |
| 6  | 0.8333 | 0.5864 | 0.3790 |
| 7  | 0.8571 | 0.6122 | 0.4343 |
| 8  | 0.8750 | 0.6384 | 0.4866 |
| 9  | 0.8889 | 0.6667 | 0.5116 |
| 10 | 0.9000 | 0.6785 | 0.5300 |

Table 4: Effective SSP coefficients of the optimal eSSPRK+(s,p) methods.

In Section 5.1 we give the coefficients for these methods in both Shu-Osher form and Butcher form and show that the abscissas are indeed non-decreasing.

In the third order case, the additional requirement that the abscissas be non-decreasing results in smaller SSP coefficients than the typical explicit SSP Runge–Kutta methods. For example, the optimal eSSPRK(3,3) Shu-Osher method (8) has SSP coefficient $C = 1$ while the optimal eSSPRK+(3,3) method has SSP coefficient $C = \frac{3}{4}$, as we will prove in Section 5.2. This loss in the SSP coefficient is also evident for the eSSPRK+(4,3) method ($C = \frac{20}{17}$) compared to the eSSPRK(4,3) method ($C = 2$). However, as we add more stages the impact of the additional requirement of non-decreasing abscissas becomes negligible and the SSP coefficients of the eSSPRK+(s,3) methods are very close to those of the standard eSSPRK(s,3) methods, as seen in Figure 2.

In the fourth order case, the SSP coefficient of the optimal eSSPRK+(4) are certainly smaller than those of the corresponding eSSPRK methods. In fact, this does not significantly improve as we increase the number of stages. Notably, the optimal eSSPRK(10,4) method found by Ketcheson [8] has an SSP coefficient of $C = 6$ while the corresponding eSSPRK+(10,4) method has SSP coefficient $C = 5.3$, a reduction of over 10%. An exception to this is the optimal eSSPRK+(6,4) method in which the non-descreasing abscissa requirement results in only a 1% reduction of the SSP coefficient compared to the eSSPRK(6,4).
5.1 Optimal second order explicit SSP Runge–Kutta methods with non-decreasing abscessas

We mentioned above that the optimal eSSPRK(s,2) methods have non-decreasing coefficients. In this section we review these methods, first presented in [7], and show that the abscessas are in fact increasing. These methods can be written in Shu-Osher form:

\[
\begin{align*}
    u^{(0)} &= u^n \\
    u^{(i)} &= u^{(i-1)} + \frac{\Delta t}{s-1} F(u^{(i-1)}), \quad i = 1, \ldots, s-1 \\
    u^{(s)} &= \frac{1}{s} u^0 + \frac{s-1}{s} \left( u^{(s-1)} + \frac{\Delta t}{s-1} F(u^{(s-1)}) \right) \\
    u^{n+1} &= u^{(s)}.
\end{align*}
\]
In Butcher form, this becomes

\[
A = \begin{bmatrix}
0 & 0 & 0 & \ldots & 0 & 0 \\
\frac{1}{s-1} & 0 & 0 & \ldots & 0 & 0 \\
\vdots & \vdots & \ddots & \ddots & \vdots & \vdots \\
\frac{1}{s-1} & \frac{1}{s-1} & \frac{1}{s-1} & \frac{1}{s-1} & 0 & 0 \\
\end{bmatrix}, \quad \mathbf{b}^T = \begin{bmatrix}
\frac{1}{s-1} \\
\frac{1}{s-1} \\
\vdots \\
\frac{1}{s-1} \\
\end{bmatrix}, \quad \text{and the abscissas } \mathbf{c} = \begin{bmatrix}
0 \\
\frac{1}{s-1} \\
\vdots \\
\frac{s-2}{s-1} \\
\frac{1}{s} \\
\end{bmatrix}.
\]

Clearly, these optimal explicit SSP Runge–Kutta methods have increasing abscissas, and are therefore suitable use with an integrating factor approach to create eSSPIFRK methods.

### 5.2 Optimal third order explicit SSP Runge–Kutta methods with non-decreasing abscissas

**Theorem 3.** The eSSPRK\(^+(3,3)\) method given by

\[
\begin{align*}
\mathbf{u}^{(1)} &= \frac{1}{2} u^n + \frac{1}{2} \left( u^n + \frac{4}{3} \Delta t F(u^n) \right) \\
\mathbf{u}^{(2)} &= \frac{2}{3} u^n + \frac{1}{3} \left( \mathbf{u}^{(1)} + \frac{4}{3} \Delta t F(\mathbf{u}^{(1)}) \right) \\
\mathbf{u}^{n+1} &= \frac{59}{128} u^n + \frac{15}{128} \left( \mathbf{u}^{(1)} + \frac{4}{3} \Delta t F(\mathbf{u}^{(1)}) \right) + \frac{27}{64} \left( \mathbf{u}^{(2)} + \frac{4}{3} \Delta t F(\mathbf{u}^{(2)}) \right) 
\end{align*}
\]

is strong stability preserving with SSP coefficient \(C = \frac{3}{4}\) and is optimal among all eSSPRK\(^+(3,3)\) methods.

**Proof.** This method is given in its canonical Shu-Osher form. Clearly, we have a convex combination of forward Euler steps with time-step \(\frac{4}{3} \Delta t\) and so this method is SSP with \(C = \frac{3}{4}\).

To show that this is optimal among all possible eSSPRK\(^+(3,3)\) methods, we follow along the lines of the proof in [5]. We assume that \(C > \frac{3}{4}\), which means that \(\frac{\alpha_{ij}}{\beta_{ij}} > \frac{3}{4}\) or

\[
\alpha_{ij} > \frac{3}{4} \beta_{ij} \quad \text{for any } i, j,
\]

and proceed with a proof by contradiction.

First, recall that we can transform between the Shu-Osher coefficients \(\alpha, \beta\) and the Butcher array coefficients \(A\) and \(b\) as follows:

\[
\begin{align*}
\alpha_{21} &= \beta_{10}, \quad \alpha_{31} = \beta_{20} + \alpha_{21} \beta_{10}, \quad \alpha_{32} = \beta_{21} \\
b_1 &= \alpha_{32} \alpha_{21} \beta_{10} + \alpha_{31} \beta_{10} + \alpha_{32} \beta_{20} + \beta_{30}, \quad b_2 = \alpha_{32} \beta_{21} + \beta_{31}, \quad b_3 = \beta_{32} \\
c_1 &= 0, \quad c_2 = a_{21}, \quad c_3 = a_{31} + a_{32}.
\end{align*}
\]
Note that for the method to be SSP, the coefficients must all be non-negative. If the abscissas are non-decreasing, there are two possible cases: \( c_2 = c_3 = \frac{2}{3} \) and \( c_2 < c_3 \). We consider each of these cases separately.

**[Case (a)]** If the abscissas are equal, they must be \( c_2 = c_3 = \frac{2}{3} \). The coefficients in this case satisfy

\[
a_{21} = \frac{2}{3}, \quad a_{31} = \frac{2}{3} - \frac{1}{4\omega}, \quad a_{32} = \frac{1}{4\omega}, \quad b_1 = \frac{1}{4}, \quad b_2 = \frac{3}{4} - \omega, \quad b_3 = \omega
\]

for parameter \( \omega \). The assumption that \( \alpha_{ij} > \frac{3}{4}\beta_{ij} \) and the non-negativity assumption on the coefficients results in

\[
b_2 = \alpha_{32}\beta_{21} + \beta_{31} \geq \alpha_{32}\beta_{21} > \frac{3}{4}\beta_{32}\beta_{21} = \frac{3}{4}b_3a_{32} = \frac{3}{16} \implies \omega < \frac{9}{16}.
\]

On the other hand,

\[
a_{31} = \beta_{20} + \alpha_{21}\beta_{10} \geq \alpha_{21}\beta_{10} > \frac{3}{4}\beta_{21}a_{21} = \frac{3}{4}a_{32}a_{21} = \frac{3}{4} \frac{2}{4} \frac{3}{4} = \frac{1}{8\omega}
\]

so that

\[
\frac{2}{3} - \frac{1}{4\omega} > \frac{1}{8\omega} \implies \omega > \frac{9}{16},
\]

which contradicts the bound on \( \omega \) above.

**[Case (b)]** If the two abscissas are not equal, and we require non-decreasing abscissas, we must have \( c_2 < c_3 \). In this case, the coefficients are given by a two parameter system, where the parameters are the abscissas \( c_2 \) and \( c_3 \).

\[
a_{21} = c_2, \quad a_{31} = \frac{3c_2c_3(1 - c_2) - c_3^2}{c_2(2 - 3c_2)}, \quad a_{32} = \frac{c_3(c_3 - c_2)}{c_2(2 - 3c_2)}
\]

\[
b_1 = 1 + \frac{2 - 3(c_2 + c_3)}{6c_2c_3}, \quad b_2 = \frac{3c_3 - 2}{6c_2(c_3 - c_2)}, \quad b_3 = \frac{2 - 3c_2}{6c_3(c_3 - c_2)}.
\]

The first stage has a value \( \alpha_{10} = 1 \), so we must have \( \beta_{10} < \frac{4}{3} \). The requirement that \( c_2 < c_3 \) and that both \( b_2 \) and \( b_3 \) are non-negative gives

\[
b_2 = \frac{3c_3 - 2}{6c_2(c_3 - c_2)} \geq 0 \implies c_3 \geq \frac{2}{3}
\]

\[
b_3 = \frac{2 - 3c_2}{6c_3(c_3 - c_2)} \geq 0 \implies c_2 \leq \frac{2}{3}
\]
Now begin with \( a_{31} = \beta_{20} + \alpha_{21} \beta_{10} \), and recall that \( \alpha_{21} > \frac{3}{4} \beta_{21} \) and \( \beta_{10} = a_{21} = c_2 \) and \( \beta_{21} = a_{32} \), so that

\[
a_{31} > \frac{3}{4} \beta_{21} c_2 = \frac{3}{4} a_{32} c_2 \implies c_3 - a_{32} > \frac{3}{4} a_{32} c_2 \implies c_3 > a_{32} \left(1 + \frac{3}{4} c_2\right) \implies a_{32} < \frac{c_3}{1 + \frac{3}{4} c_2}.
\]

Using the definition of \( a_{32} \), this means

\[
\frac{c_3 (c_3 - c_2)}{c_2 (2 - 3c_2)} < \frac{c_3}{(1 + \frac{3}{4} c_2)} \implies c_3 < \frac{3c_2 - \frac{9}{4} c_2^2}{(1 + \frac{3}{4} c_2)}.
\]

Next, we look use the fact that \( \beta_{31} \geq 0 \) to obtain

\[
b_2 = \alpha_{32} \beta_{21} + \beta_{31} \geq \alpha_{32} \beta_{21} > \frac{3}{4} b_3 a_{32} \implies a_{32} < \frac{4 b_2}{3 b_3} = \frac{4 c_3 (3c_3 - 2)}{3 c_2 (2 - 3c_2)}.
\]

Now we use \( a_{32} = \frac{c_3 (c_3 - c_2)}{c_2 (2 - 3c_2)} \) to conclude that

\[
\frac{c_3 (c_3 - c_2)}{c_2 (2 - 3c_2)} < \frac{4 c_3 (3c_3 - 2)}{3 c_2 (2 - 3c_2)} \implies c_3 > \frac{1}{3} c_2 + \frac{8}{9}.
\]

We now have two statements that need to be simultaneously true

\[
c_3 < \frac{3c_2 - \frac{9}{4} c_2^2}{(1 + \frac{3}{4} c_2)} \quad \text{and} \quad c_3 > \frac{1}{3} c_2 + \frac{8}{9}
\]

which means that we must have

\[
-\frac{1}{3} c_2 + \frac{8}{9} < \frac{3c_2 - \frac{9}{4} c_2^2}{(1 + \frac{3}{4} c_2)} \implies (3c_2 - 2)^2 < 0
\]

however this is a contradiction because \((3c_2 - 2)^2\) is always greater than or equal to zero. This means that our original assumption was not correct, and that if \( c_2 < c_3 \) we cannot have \( C > \frac{3}{4} \).

### 5.3 Recommended SSP Runge–Kutta methods for use with integrating factor methods

The optimal second order methods eSSPRK\(^+(s,2)\) listed above have a nice low storage form and a general formula. However, for the optimal third and fourth order methods, we do not have a general formula for the optimal methods. In this section we list a few of the optimal eSSPRK\(^+(s,3)\) and
eSSPRK\(^+(s,4)\) methods. The coefficients of all the methods we found can be downloaded as .mat files from our github repository [4].

**eSSPRK\(^+(4,3)\)** This method has rational coefficients and sparse Shu-Osher matrices that lead to a low-storage implementation:

\[
\begin{align*}
  u^{(1)} &= u^n + \frac{11}{20} \Delta t F(u^n) \\
  u^{(2)} &= \frac{3}{8} u^n + \frac{5}{8} \left( u^{(1)} + \frac{11}{20} \Delta t F(u^{(1)}) \right) \\
  u^{(3)} &= \frac{4}{9} u^n + \frac{5}{9} \left( u^{(2)} + \frac{11}{20} \Delta t F(u^{(2)}) \right) \\
  u^{(4)} &= \frac{111}{1331} u^n + \frac{260}{1331} \left( u^n + \frac{11}{20} \Delta t F(u^n) \right) + \frac{960}{1331} \left( u^{(3)} + \frac{11}{20} \Delta t F(u^{(3)}) \right)
\end{align*}
\]

The abscissas are \(c_1 = 0, c_2 = \frac{11}{20}, c_3 = c_4 = \frac{11}{16}\). This method has SSP coefficient \(C = \frac{20}{11}\).

**eSSPRK\(^+(9,3)\)** This method has \(C = 6\) and features rational coefficients and sparse Shu-Osher matrices that lead to a low-storage implementation:

\[
\begin{align*}
  u^{(0)} &= u^n \\
  u^{(i)} &= u^{(i-1)} + \frac{1}{6} \Delta t F(u^{(i-1)}) \quad \text{for } i = 1, \ldots, 4 \\
  u^{(5)} &= \frac{1}{5} u^n + \frac{4}{5} \left( y^{(4)} + \frac{1}{6} \Delta t F(u^{(4)}) \right) \\
  u^{(6)} &= \frac{1}{4} \left( u^n + \frac{1}{6} \Delta t F(u^n) \right) + \frac{3}{4} \left( u^{(5)} + \frac{1}{6} \Delta t F(u^{(5)}) \right) \\
  u^{(7)} &= \frac{1}{3} \left( u^{(1)} + \frac{1}{6} \Delta t F(u^{(1)}) \right) + \frac{2}{3} \left( u^{(6)} + \frac{1}{6} \Delta t F(u^{(6)}) \right) \\
  u^{(8)} &= y^{(7)} + \frac{1}{6} \Delta t F(u^{(7)}) \\
  u^{n+1} &= y^{(8)} + \frac{1}{6} \Delta t F(u^{(8)}).
\end{align*}
\]

The abscissas are \(c_1 = 0, c_2 = \frac{1}{6}, c_3 = \frac{2}{6}, c_4 = \frac{3}{6}, c_5 = c_6 = c_7 = c_8 = \frac{4}{6}, c_9 = \frac{5}{6}\), which simplifies the computation of the matrix exponential, as only one needs to be computed.

For fourth order methods, we no longer have rational coefficients.
eSSPRK\(^+(5,4)\) This method has SSP coefficient \(C = r = 1.346586417284006\), and non-decreasing abscissas \(c_1 = 0,\ c_2 \approx 0.4549,\ c_3 = c_4 \approx 0.5165,\ c_5 \approx 0.9903:\

\[
\begin{align*}
\dot{u}^{(1)} &= 0.387392167970373 \ u^n + 0.612607832092627 \left( u^n + \frac{\Delta t}{r} F(u^n) \right) \\
\dot{u}^{(2)} &= 0.568702484115635 \ u^n + 0.431297515884365 \left( u^{(1)} + \frac{\Delta t}{r} \Delta t F(u^{(1)}) \right) \\
\dot{u}^{(3)} &= 0.589791736452092 \ u^n + 0.410208263547908 \left( u^{(2)} + \frac{\Delta t}{r} F(u^{(2)}) \right) \\
\dot{u}^{(4)} &= 0.213474206786187 \ u^n + 0.786525793213812 \left( u^{(3)} + \frac{\Delta t}{r} F(u^{(3)}) \right) \\
\dot{u}^{n+1} &= 0.270147144537063 \ u^n + 0.029337521506634 \left( u^n + \frac{\Delta t}{r} F(u^n) \right) \\
&\quad + 0.234095162611706 \left( u^{(4)} + \frac{\Delta t}{r} F(u^{(4)}) \right).
\end{align*}
\]

eSSPRK\(^+(6,4)\) This method has SSP coefficient \(C = r = 2.273802749301517\), and non-decreasing abscissas \(c_1 = 0,\ c_2 \approx 0.4398,\ c_3 \approx 0.4515,\ c_4 = c_5 \approx 0.5461,\ c_6 \approx 0.9859:\

\[
\begin{align*}
\dot{u}^{(1)} &= u^n + \frac{\Delta t}{r} F(u^n) \\
\dot{u}^{(2)} &= 0.486695314011133u^n + 0.513304685988867 \left( u^{(1)} + \frac{\Delta t}{r} \Delta t F(u^{(1)}) \right) \\
\dot{u}^{(3)} &= 0.387273961537322 \ u^n + 0.612726038462678 \left( u^{(2)} + \frac{\Delta t}{r} F(u^{(2)}) \right) \\
\dot{u}^{(4)} &= 0.419340376206589 \ u^n + 0.048271190433595 \left( u^n + \frac{\Delta t}{r} F(u^n) \right) + 0.53238843359815 \left( u^{(3)} + \frac{\Delta t}{r} F(u^{(3)}) \right) \\
\dot{u}^{(5)} &= \left( u^{(4)} + \frac{\Delta t}{r} F(u^{(4)}) \right) \\
\dot{u}^{n+1} &= 0.122021674306995 \ u^n + 0.104714614292281 \left( u^{(1)} + \frac{\Delta t}{r} \Delta t F(u^{(1)}) \right) + 0.316675962670361 \left( u^{(2)} + \frac{\Delta t}{r} \Delta t F(u^{(2)}) \right) + 0.057551178672633 \left( u^{(4)} + \frac{\Delta t}{r} \Delta t F(u^{(4)}) \right) + 0.399036570057729 \left( u^{(5)} + \frac{\Delta t}{r} \Delta t F(u^{(5)}) \right).
\end{align*}
\]
6 Numerical Results

In this section, we test the explicit SSP integrating factor Runge–Kutta (eSSPIFRK) methods based on eSSPRK+ methods presented in Section 5 for convergence and SSP properties. First, we test these methods for convergence on a nonlinear system of ODEs to confirm that the new methods exhibit the desired orders. Next, we study the behavior of these methods in terms of their allowable time-step on linear and nonlinear problems with spatial discretizations that are provably total variation diminishing (TVD). While the utility of SSP methods goes well beyond its initial purpose of preserving the TVD properties of the spatial discretization coupled with forward Euler, the simple TVD test in this section has been used extensively because it tends to demonstrate the sharpness of the SSP time-step.

Example 1: Convergence study. To verify the order of convergence of these methods we test their performance on a nonlinear system of ODEs

\[
\begin{align*}
    u'_1 &= u_2 \\
    u'_2 &= (-u_1 + (1 - u_1^2)u_2)
\end{align*}
\]

known as the van der Pol problem. We split the problem in two different ways into a linear part \(L\) and a nonlinear part \(N(u)\) given by:

(a) \(L = \begin{pmatrix} 0 & 1 \\ -1 & 1 \end{pmatrix}\), \(N(u) = \begin{pmatrix} 0 \\ -u_1^2u_2 \end{pmatrix}\)

and

(b) \(L = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\), \(N(u) = \begin{pmatrix} 0 \\ (1 - u_1^2)u_2 \end{pmatrix}\)

We use initial conditions \(u_0 = (2; 0)\), and run the problem to final time \(T_{final} = 0.50\), with \(\Delta t = 0.02, 0.04, 0.06, 0.08, 0.10\). The exact solution (for error calculation) was calculated by MATLAB’s ODE45 routine with tolerances set to \(\text{AbsTol}=10^{-15}\) and \(\text{RelTol}=10^{-15}\). For each splitting, we tested all the methods represented in Table 3 above and calculated the slopes of the orders by MATLAB’s \text{polyfit} function; we found that they all exhibit the expected order of convergence. Due to space constraints, we show only a representative selection in Figure 3. While the splitting affects the magnitude of the errors, we see that the order of the errors is not affected by the different splittings. As expected, the error constants are smaller for methods with more stages.

Note that we used a van der Pol problem that is not highly oscillatory or stiff. This is because it is well known that integrating factor methods suffer from order reduction when applied to stiff problems. This convergence study purposely avoids this issue in order to test the formal convergence of the generated methods. However, we explore this issue in the next example.
Figure 3: Example 1. The x-axis is $\log_{10}$ of the time-step, while the y-axis is $\log_{10}$ of the errors. The second order methods are in red, third order in blue, and fourth order in green. The eSSPIFRK methods with $(s, p) = (2, 2), (3, 3), (5, 4)$ have a dashed line, those with $(s, p) = (4, 2), (4, 3), (7, 4)$ have a solid line, and those with $s = 9$ have a dot-dash line. On the left is splitting (a) while on the right is splitting (b).

Example 2: Accuracy study. Consider the

$$u_t + 10u_x + \left(\frac{1}{2}u^2\right)_x = 0 \quad u(0, x) = e^{\sin(2\pi x)}$$

on the domain $0 \leq x \leq 1$. We use a first order upwind finite difference to spatially discretize the linear advection term and the fifth order WENO for the nonlinear term. We use $N = 64$ points in space and the globalorder.m script in the package EXPINT [2, 1] with its built-in exponential time-differencing (ETD) Runge–Kutta methods of orders $p = 2, 3, 4$ (the schemes by Cox and Matthews called ETDRK2, ETDRK3, and ETDRK4 in EXPINT) and our eSSPIFRK methods with $(s, p) = (2, 2), (3, 3), (5, 4)$. The globalorder.m script uses MATLAB’s embedded ODE15s with $AbsTol = 10^{-15}$ and $RelTol = 5 \times 10^{-14}$ to compute the highly accurate reference solution. In Figure 4 (left) we observe that the eSSPIFRK methods are competitive with the ETD methods in terms of accuracy. Despite the fact that we see order reduction in the third and fourth order eSSPIFRK methods, the accuracy of these methods is comparable to that of the corresponding ETD method. A comparison of the CPU times needed for a given level of accuracy in Figure 4 (right) reveals that the ETD methods are generally somewhat more efficient on this smooth problem. However, we will see below that the ETD methods in fact require inefficiently small time-steps for nonlinear stability in problems with discontinuities that are of interest to us.

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Figure 4: Example 2. The second order methods are in red, third order in blue, and fourth order in green, dashed lines represent the ETD methods while solid lines are the eSSPIFRK methods. Left: on x-axis is the step-size while on the y-axis is the error. Right: on x-axis is the CPU time while on the y-axis is the error.

Example 3: Sharpness of SSP time-step for a linear problem. We consider the linear advection equation with a step function initial condition:

\[ u_t + au_x + u_x = 0 \]
\[ u(0, x) = \begin{cases} 
1, & \text{if } \frac{1}{4} \leq x \leq \frac{3}{4} \\
0, & \text{else}
\end{cases} \]

on the domain \([0, 1]\) with periodic boundary conditions. We used a first-order forward difference for each of the spatial derivatives to semi-discretize this problem on a grid of \(0 \leq x \leq 1\) with \(N = 1000\) points and evolved it ten time-steps forward. It is known that this spatial discretization

| \(a\) | \(C\) | \(C_{\text{obs}}\) for \(a = 0\) | \(C_{\text{obs}}\) for \(a = 1.0\) | \(C_{\text{obs}}\) for \(a = 10\) | \(C_{\text{obs}}\) for \(a = 20\) |
|---|---|---|---|---|---|
| \(2, 2\) | \(9, 2\) | \(3, 3\) | \(4, 3\) | \(9, 3\) | \(5, 4\) | \(6, 4\) | \(9, 4\) |
| \(C\) | \(1, 8\) | \(3/4\) | \(20/11\) | \(6\) | \(1.346\) | \(2.273\) | \(4.306\) |
| \(C_{\text{obs}}\) for \(a = 0\) | \(1, 8\) | \(3/2\) | \(20/11\) | \(6\) | \(2.158\) | \(2.273\) | \(4.306\) |
| \(C_{\text{obs}}\) for \(a = 1.0\) | \(1, 8\) | \(3/2\) | \(20/11\) | \(6\) | \(2.158\) | \(2.273\) | \(4.306\) |
| \(C_{\text{obs}}\) for \(a = 10\) | \(1, 8\) | \(3/2\) | \(20/11\) | \(6\) | \(2.158\) | \(2.273\) | \(4.306\) |
| \(C_{\text{obs}}\) for \(a = 20\) | \(1, 8\) | \(3/2\) | \(20/11\) | \(6\) | \(2.158\) | \(2.273\) | \(4.306\) |

Table 5: The observed SSP coefficient compared to the predicted SSP coefficient for Example 3.
when coupled with forward Euler is TVD, under the time-step restriction \( \tilde{\Delta}t_{FE} = \frac{1}{a} \Delta x \) for the term \( Lu \approx au_x \), and the restriction \( \Delta t_{FE} = \Delta x \) for the term \( N(u) \approx u_x \).

We measure the total variation of the numerical solution at each stage, and compare it to the total variation at the previous stage. We are interested in the size of time-step \( \Delta t \) at which the total variation begins to rise. We refer to this value as the observed TVD time-step. We are interested in comparing this value with the expected TVD time-step dictated by the theory. We call the SSP coefficient corresponding to the value of the observed TVD time-step the observed SSP coefficient \( C_{obs} \).

Using \( a = 0 \), we verify the expected TVD time-step for most of the methods considered (Table 5). However, we observed that for the methods eSSPIFRK(3,3) and eSSPIFRK(5,4), \( C_{obs} > C \). For the eSSPIFRK(3,3) method, \( C = \frac{3}{4} \) but the observed value is \( C_{obs} = 1 \). This is easy to understand because for this linear problem with no exponential component \((a = 0)\), all methods with the same number of stages as order \((s = p)\) are equivalent. Thus, for this special case, our eSSPIFRK(3,3) method can be re-arranged into the eSSPRK(3,3) Shu-Osher method, and we observe the expected TVD time-step for that method.

A similar phenomenon occurs for the eSSPIFRK(5,4) method. In this case, we can write the stability polynomial of each stage recursively. If we look at the stability polynomial \( P(z) \) of the fourth stage, we observe that its third derivative becomes negative at \( z = 1.5594 \), which is precisely the observed TVD time-step for this method. When we look into the stages to see where the rise in TV occurs, we see that it first happens in the fourth stage of the first time-step.

Next, we consider various values of \( a > 0 \). The results in Table 5 confirm that value of \( a \) does not impact the observed SSP coefficient for this linear example.\(^1\) In these cases too, we observe that for most methods \( C_{obs} = C \) for all values of \( a \). The observed TVD time-step for eSSPIFRK(3,3) and eSSPIFRK(5,4) are, once again, larger than expected. For the eSSPIFRK(3,3) method \( C_{obs} = \frac{3}{2} \) is a result of the rise in TV from the first stage, which has a step-size \( \frac{3}{2} \Delta t \).

**Example 4: Sharpness of SSP time-step for a nonlinear problem.** Consider the equation:

\[
    u_t + au_x + \left( \frac{1}{2} u^2 \right)_x = 0
\]

\[
    u(0, x) = \begin{cases} 
        1, & \text{if } 0 \leq x \leq 1/2 \\
        0, & \text{if } x > 1/2 
    \end{cases}
\]

on the domain \([0, 1]\) with periodic boundary conditions. We used a first-order upwind difference to semi-discretize this linear term, and a fifth order WENO finite difference for the nonlinear terms. We solved this problem on a spatial grid with \( N = 400 \) points and evolved it forward 25 time steps using \( \Delta t = \lambda \Delta x \). We measured the total variation at each stage, and calculated the maximal rise in total variation over each stage for these 25 time steps.

\(^1\)We note that for values larger than \( a = 20 \), the significant damping that occurs due to the exponential masks the oscillation and its associated rise in total variation.
Figure 5: Example 4 with $a = 5$. On the x-axis is the value of $\lambda = \frac{\Delta t}{\Delta x}$, on the y axis is $\log_{10}$ of the maximal rise in TV. The red solid line is the eSSPIFRK(3,3) method, the blue dotted line is the IFRK method based on the eSSPRK(3,3) Shu-Osher method, the black dash-dot line is the ETDRK3 method, and the green dashed line is the third order explicit eSSPRK(3,3) Shu-Osher method.

Figure 6: Example 4 with $a = 10$. On the x-axis is the value of $\lambda = \frac{\Delta t}{\Delta x}$, on the y axis is $\log_{10}$ of the maximal rise in TV. The dashed magenta line with x markers is the SSP IMEX (5,4) method. The dash-dot red line with filled circle markers is the ETDRK4 method. The dotted cyan line with + markers is the SSPRK(10,4) method by Ketcheson. The solid lines are the SSPIFRK methods: the black line with star markers for (5,4), green line with square markers for (6,4) and blue line with circle markers for (9,4).
In Figure 5 we use the value of \( a = 5 \) and graph the \( \log_{10} \) of the maximal rise in total variation versus the ratio \( \lambda = \frac{\Delta t}{\Delta x} \). We observe that our eSSPIFRK(3,3) method (18) maintains a very small maximal rise in total variation until close to \( \lambda = 0.8 \), while the fully explicit third order Shu-Osher method begins to feature a large rise in total variation for a much smaller value of \( \lambda = 0.15 \approx \frac{1}{1+a} \). In contrast, the three-stage third order ETD Runge–Kutta [3] and the integrating factor method based on Shu-Osher method (17) both have a maximal rise in total variation that increases rapidly with \( \lambda \).

In Figure 6 we show a similar study using wavespeed \( a = 10 \) and fourth order methods, versus the ratio \( \lambda = \frac{\Delta t}{\Delta x} \). We observe that our eSSPIFRK(5,4), eSSPIFRK(6,4), and eSSPIFRK(9,4) methods maintain a very small maximal rise in total variation until close to \( \lambda = 1.06, 1.21, 2.41 \), respectively. In comparison, the SSP IMEX (5,4) method features an observed \( \lambda \) value of \( \lambda_{\text{obs}} = 0.25 \), the fully explicit SSPRK(10,4) has \( \lambda_{\text{obs}} = 0.58 \), and the maximal total variation from the simulation using the ETDRK4 method starts rising rapidly from the smallest value of \( \lambda \).

7 Conclusions

This is the first work to consider strong stability integrating factor Runge–Kutta methods. In this work we presented sufficient conditions for preservation of strong stability for integrating factor Runge–Kutta methods. These eSSPIFRK methods are based on eSSPRK methods with non-decreasing abscissas. We used these conditions to develop an optimization problem which we used to find such eSSPRK\(^+\) methods. We then showed that these eSSPIFRK methods perform in practice as expected, significantly out-performing the implicit-explicit (IMEX) SSP Runge–Kutta methods and the ETD methods of Cox and Matthews on problems that require the SSP property.

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