

Strong Stability Preserving Multistage Integration Methods*

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Abstract. In this paper we systematically investigate explicit strong stability preserving (SSP) multistage integration methods, a subclass of general linear methods (GLMs), of order p and stage order $q \leq p$. Characterization of this class of SSP GLMs is given and examples of SSP methods of order $p \leq 4$ and stage order $q = 1, 2, \dots, p$ are provided. Numerical tests are reported which confirm that the constructed methods achieve the expected order of accuracy and preserve monotonicity.

Keywords: multistage integration methods, general linear methods, strong stability preserving, monotonicity, two-step Runge–Kutta methods.

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1 Introduction

Many practical problems in sciences and engineering are modeled by systems of ordinary differential equations (ODEs) which arise from semidiscretization of partial differential equations (PDEs) of mathematical physics. Such systems take the form

$$\begin{cases} y'(t) = f(t, y(t)), & t \in [t_0, t_{end}], \\ y(t_0) = y_0, \end{cases} \quad (1.1)$$

where the function $f : \mathbb{R} \times \mathbb{R}^m \rightarrow \mathbb{R}^m$ is assumed to have some degree of smoothness.

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We assume that the discretization of (1.1) by the forward Euler method

$$y_n = y_{n-1} + hf(t_{n-1}, y_{n-1}),$$

$n = 1, 2, \dots, N$, $Nh = t_{end} - t_0$, $t_n = t_0 + nh$, is monotone or contractive. This means that the following inequality holds

$$\|y_n\| \leq \|y_{n-1}\|, \quad (1.2)$$

$n = 1, 2, \dots, N$, in some norm or semi-norm $\|\cdot\|$, for a suitably restricted time step determined by the condition $h \leq h_{FE}$.

In the class of multistage integration methods we want to determine higher order numerical methods for (1.1), which preserve the monotonicity property (1.2), under the restriction

$$h \leq \mathcal{C} h_{FE}. \quad (1.3)$$

Numerical schemes for (1.1) that preserve the monotonicity condition (1.2) under the modified restriction (1.3) are called strong stability preserving (SSP) methods and the constant $\mathcal{C} \geq 0$ in (1.3) is called SSP coefficient.

SSP Runge–Kutta (RK) and linear multistep methods (LMMs) have been first studied, using the terminology total variation diminishing (TVD) time discretizations, by Shu and Osher [50]. Then, they were further investigated by Gottlieb et al. [22, 23, 24, 25, 27, 43], Spiteri and Ruuth [53], Hundsdorfer and Ruuth [32], Hundsdorfer, Ruuth and Spiteri [33], Higueras [28, 29, 30, 31] and Ferracina and Spijker [18, 19, 20, 21]. SSP two-step Runge–Kutta (TSRK) methods, introduced by Jackiewicz and Tracogna [40], were investigated by Ketcheson, Gottlieb and Macdonald in [42]. Constantinescu and Sandu [8] generalized Shu–Osher representation to a class of multistep multistage schemes, which form a special subclass of GLMs. SSP GLMs were investigated by Spijker [52] and by Izzo and Jackiewicz [36, 37].

In this paper we systematically investigate a subclass of explicit GLMs in order to derive methods with optimal SSP coefficient \mathcal{C} .

It is known that irreducible strong stability preserving Runge–Kutta methods have positive stage coefficients, $a_{ij} \geq 0$, and strictly positive weights, $b_j > 0$. A similar property holds for SSP two-step Runge–Kutta methods [23]. Gottlieb and Shu [26] proved that no four-stage, fourth-order SSPRK method exists having positive coefficients, while Ruuth and Spiteri [47] proved that an SSPRK method with positive coefficients and order $p > 4$ cannot exist (for general nonlinear problems). The class of general linear methods allows to break these two barriers and it also permits to construct methods with high stage order.

The paper is organized as follows: in Section 2 we report the formulation of general linear methods (GLMs), the related order conditions and a criterion to determine the SSP coefficient \mathcal{C} . In Sections 3 and 4 we characterize some classes of explicit SSP multistage integration methods of order p and stage order $q \leq p$ and investigate them to construct methods with a large SSP coefficient. In Section 5 we describe the starting and finishing procedures, while in Section 6 we present the results of numerical experiments to validate order and monotonicity preservation of the new SSP schemes. Finally, in Section 7 some concluding remarks are given and plans for future research are briefly outlined.

2 SSP Conditions for GLMs

2.1 General linear methods

General linear methods [1,2,3,39] for the numerical solution of ODEs (1.1) are defined by

$$\begin{cases} Y_i^{[n]} = h \sum_{j=1}^s a_{ij} f(t_{n-1} + c_j h, Y_j^{[n]}) + \sum_{j=1}^r u_{ij} y_j^{[n-1]}, & i = 1, 2, \dots, s, \\ y_i^{[n]} = h \sum_{j=1}^s b_{ij} f(t_{n-1} + c_j h, Y_j^{[n]}) + \sum_{j=1}^r v_{ij} y_j^{[n-1]}, & i = 1, 2, \dots, r, \end{cases} \quad (2.1)$$

$n = 1, 2, \dots, N$, where $Nh = t_{end} - t_0$. In (2.1) the internal approximations or stages approximate the solution y to (1.1) at the points $t_{n-1} + c_i h$ to the stage order q , i.e.,

$$Y_i^{[n]} = y(t_{n-1} + c_i h) + O(h^{q+1}), \quad i = 1, 2, \dots, s,$$

and the external approximations $y_i^{[n]}$ approximate the linear combinations of the scaled derivatives of the solution at the grid point t_n to the order p , i.e.,

$$y_i^{[n]} = \sum_{k=0}^p q_{ik} h^k y^{(k)}(t_n) + O(h^{p+1}), \quad i = 1, 2, \dots, r. \quad (2.2)$$

These methods are specified by the abscissa vector $\mathbf{c} = [c_1, \dots, c_s]^T \in \mathbb{R}^s$, four coefficient matrices

$$\mathbf{A} = [a_{ij}] \in \mathbb{R}^{s \times s}, \quad \mathbf{U} = [u_{ij}] \in \mathbb{R}^{s \times r}, \quad \mathbf{B} = [b_{ij}] \in \mathbb{R}^{r \times s}, \quad \mathbf{V} = [v_{ij}] \in \mathbb{R}^{r \times r},$$

the vectors $\mathbf{q}_i = [q_{1,i}, \dots, q_{r,i}]^T \in \mathbb{R}^r$, $i = 0, 1, \dots, p$, and four integers: the order of the method p , the stage order q , the number of external approximations r , and the number of internal approximations or stages s .

The framework of general linear methods have been used recently to analyze the numerical stability of several class of methods [4, 5, 9, 10, 11, 13, 14, 15]. General linear methods for second order equations were considered in [12,16,17] and for VIEs and VIDEs in [38,54].

2.2 Order conditions for GLMs

The order conditions for GLMs (2.1) of order $p \leq 4$ are reported in Table 1 (compare Butcher [3], Jackiewicz and Vermiglio [41], Cardone et. al. [6]), where

$$\begin{aligned} \gamma_0 &= \mathbf{e} - \mathbf{U}\mathbf{q}_0, & \gamma_k &= \frac{\mathbf{c}^k}{k!} - \frac{\mathbf{A}\mathbf{c}^{k-1}}{(k-1)!} - \mathbf{U}\mathbf{q}_k, & k &= 1, 2, \dots, p, \\ \widehat{\gamma}_0 &= \mathbf{q}_0 - \mathbf{V}\mathbf{q}_0, & \widehat{\gamma}_k &= \sum_{l=0}^k \frac{\mathbf{q}_l}{(k-l)!} - \frac{\mathbf{B}\mathbf{c}^{k-1}}{(k-1)!} - \mathbf{V}\mathbf{q}_k, & k &= 1, 2, \dots, p, \end{aligned}$$

Table 1. Order conditions for GLMs (2.1) of order $p \leq 4$.

Order	Corresponding order conditions
$p = 1$	$\hat{\gamma}_1 = 0$
$p = 2$	$\hat{\gamma}_2 = 0$
$p = 3$	$\hat{\gamma}_3 = 0$ $\mathbf{VB}\gamma_2 = 0$ or $\mathbf{B}\gamma_2 = 0$
$p = 4$	$\hat{\gamma}_4 = 0, \mathbf{VB}\gamma_3 = 0$ $\mathbf{VBA}\gamma_2 = 0, \mathbf{VB}\Gamma_{\mathbf{c}}\gamma_2 = 0$

and $\Gamma_{\mathbf{c}} = \text{diag}(c_1, \dots, c_s)$, $\mathbf{e} = [1, 1, \dots, 1]^T \in \mathbb{R}^s$. Let us remark that stage order q can be achieved by forcing $\gamma_k = 0$ for $k = 0, 1, \dots, q$.

It will be always assumed that

$$\sum_{j=1}^r v_{ij} = 1, \quad i = 1, 2, \dots, r \tag{2.3}$$

and $\mathbf{q}_0 = [1, 1, \dots, 1]^T \in \mathbb{R}^r$, so that the stage preconsistency condition $\gamma_0 = 0$, or $\mathbf{U}\mathbf{q}_0 = \mathbf{e}$, and the preconsistency condition $\tilde{\gamma}_0 = 0$, or $\mathbf{V}\mathbf{q}_0 = \mathbf{q}_0$, are automatically satisfied (compare [39]). When in Table 1 there is a couple of conditions separated by ‘or’, the first condition refer to order p methods, while the second condition refers to methods with order greater than p .

2.3 Characterization of SSP coefficient for GLMs

Following [37] we consider the componentwise inequalities

$$\begin{aligned} (\mathbf{I} + \gamma\mathbf{A})^{-1}\mathbf{U} &\geq 0, & \mathbf{I} - (\mathbf{I} + \gamma\mathbf{A})^{-1} &\geq 0, \\ \mathbf{V} - \gamma\mathbf{B}(\mathbf{I} + \gamma\mathbf{A})^{-1}\mathbf{U} &\geq 0, & \gamma\mathbf{B}(\mathbf{I} + \gamma\mathbf{A})^{-1} &\geq 0. \end{aligned} \tag{2.4}$$

It was demonstrated in [37] using the results of Spijker [52] that the SSP coefficient \mathcal{C} of GLMs (2.1) can be characterized as

$$\mathcal{C} = \mathcal{C}(\mathbf{c}, \mathbf{A}, \mathbf{U}, \mathbf{B}, \mathbf{V}) = \sup \{ \gamma \in \mathbb{R} : \gamma \text{ satisfies (2.3)} \}.$$

Similarly as in [42] this coefficient \mathcal{C} can be computed, by the solution to the constrained minimization problem

$$\min_{\gamma, \mathbf{c}, \mathbf{A}, \mathbf{U}, \mathbf{B}, \mathbf{V}, \mathbf{q}_1, \dots, \mathbf{q}_p} -\gamma, \tag{2.5}$$

subject to inequality constraints (2.3) and equality constraints

$$\Phi_{p,q}(\mathbf{c}, \mathbf{A}, \mathbf{U}, \mathbf{B}, \mathbf{V}, \mathbf{q}_1, \dots, \mathbf{q}_p) = 0,$$

where $\Phi_{p,q}$ represents the order conditions up to the order p and stage order conditions up to the stage order $q \leq p$.

In order to compare methods with different number of stages s we also define, as in [8] and [42], the effective SSP coefficient by the normalization $C_{\text{eff}} = C/s$.

Izzo and Jackiewicz [37] investigated the strong stability preserving property for a subclass of explicit general linear methods of order $p = 2, 3, 4$, stage order $q = 1, 2, \dots, p$, with $r = 2, 3$ external stages and $s = 2, 3, \dots, 10$ internal stages. Methods investigated in [37] contain the class of diagonally implicit multistage integration methods (DIMSIMS), the class of methods of order p and stage order $q = p$ or $q = p - 1$, with s internal stages and $r = s$ or $r = s + 1$ external stages, and rank one matrix \mathbf{V} .

In this paper we systematically investigate the SSP property for a subclass of explicit GLMs of order p and stage order $q = 1, 2, \dots, p$, characterized by having the number of external stages r and the number of internal stages s , which equal the order of the method p (i.e. $p = r = s$), and no restriction on the rank of \mathbf{V} is forced. Hereafter we will generally refer to this subclass as multistage integration methods.

3 Methods with $p = r = s$ and $\mathbf{U} = \mathbf{I}$

In this section we systematically investigate explicit multistage integration methods of order $p \leq 4$ and such that

$$\mathbf{U} = \mathbf{I}, \quad \text{and} \quad p = r = s, \quad q = 1, 2, \dots, p. \tag{3.1}$$

To characterize this class of methods we will need the following lemma.

Lemma 1. *For an explicit SSP GLM satisfying (3.1) the matrix \mathbf{A} must be identically equal to the zero matrix.*

Proof. Let $\mathbf{L} = [l_{ij}]_{i,j=1}^s$ be the matrix given by $\mathbf{L} = (\mathbf{I} + \gamma\mathbf{A})^{-1}$. Since \mathbf{A} is strictly lower triangular, \mathbf{L} is a lower triangular matrix such that $l_{ii} = 1$, $i = 1, 2, \dots, s$. Furthermore,

$$\mathbf{L} = (\mathbf{I} + \gamma\mathbf{A})^{-1} = \mathbf{I} - \gamma\mathbf{A} + \gamma^2\mathbf{A}^2 + \dots + (-\gamma\mathbf{A})^{s-1} = \sum_{i=0}^{s-1} (-\gamma\mathbf{A})^i,$$

and we have $\text{tril}(\mathbf{L}) = \sum_{i=1}^{s-1} (-\gamma\mathbf{A})^i$, where $\text{tril}(\mathbf{L})$ stands for the strictly lower triangular part of \mathbf{L} . Let us consider the two SSP conditions

$$\mathbf{L}\mathbf{U} \geq 0, \quad \mathbf{I} - \mathbf{L} \geq 0. \tag{3.2}$$

If $\mathbf{U} = \mathbf{I} \in \mathbb{R}^{s \times s}$, from (3.2) we have $0 \leq \mathbf{L} \leq \mathbf{I}$, hence $\text{tril}(\mathbf{L}) \equiv 0$, so that

$$\sum_{i=1}^{s-1} (-\gamma\mathbf{A})^i \equiv 0. \tag{3.3}$$

Since matrix \mathbf{A} is strictly lower triangular, from (3.3) we have $\gamma a_{i+1,i} = 0$, for $i = 1, 2, \dots, s - 1$. Hence for SSP methods with $\gamma > 0$ we have

$$a_{i+1,i} = 0, \quad i = 1, 2, \dots, s - 1. \tag{3.4}$$

From (3.3) and (3.4) we also obtain

$$a_{i+2,i} = 0, \quad i = 1, 2, \dots, s - 2.$$

Using induction it can be easily proved that

$$a_{ij} = 0, \quad \text{for } i, j = 1, 2, \dots, s. \quad \square$$

Remark. As consequence of Lemma 1, for GLMs satisfying (3.1), the stage order conditions $\gamma_k = 0, k = 0, \dots, q$, lead to

$$\mathbf{q}_k = \frac{\mathbf{c}^k}{k!}, \quad k = 0, \dots, q,$$

and the SSP constraints (2.3) reduce to

$$\mathbf{0} \leq \gamma \mathbf{B} \leq \mathbf{V}. \tag{3.5}$$

Equations (2.3) and (3.5) imply that $0 \leq v_{ij} \leq 1$ for all $i, j = 1, 2, \dots, s$, and, when γ is positive, $0 \leq b_{ij} \leq 1$ for all $i, j = 1, 2, \dots, s$. This information is helpful to set sharper (lower and upper) bounds on the parameters in the minimization process to solve the problem (2.5).

For SSP methods, from (3.5) we obtain $b_{ij} \geq 0$ for all $i, j = 1, 2, \dots, s$ and

$$0 \leq \gamma \leq \frac{v_{ij}}{b_{ij}}, \quad \text{for } i, j = 1, 2, \dots, s, \text{ and } b_{ij} \neq 0.$$

Since (3.5) are the only constraints, we obtain

$$\mathcal{C} = \min \left\{ \frac{v_{ij}}{b_{ij}} : i, j = 1, 2, \dots, r, \text{ and } b_{ij} \neq 0 \right\}. \tag{3.6}$$

In addition, (3.5) implies

$$\mathbf{0} \leq \gamma \mathbf{B} \mathbf{e} \leq \mathbf{V} \mathbf{e} = \mathbf{e}$$

and hence, for an SSP GLM satisfying (3.1) with SSP coefficient \mathcal{C} , the following necessary condition must hold

$$\mathcal{C} \leq 1 / \sum_{j=1}^s b_{ij} \quad \text{and} \quad \sum_{j=1}^s b_{ij} > 0, \quad i = 1, 2, \dots, s. \tag{3.7}$$

Furthermore, from order condition for $p = 1$

$$\mathbf{q}_0 + \mathbf{q}_1 - \mathbf{B} \mathbf{e} - \mathbf{V} \mathbf{c} = \mathbf{0},$$

we obtain

$$\mathbf{B} \mathbf{e} = \mathbf{e} + \mathbf{c} - \mathbf{V} \mathbf{c}.$$

This leads to

$$0 \leq \sum_{j=1}^s b_{ij} = 1 + c_i - \sum_{j=1}^s v_{ij} c_j, \quad i = 1, 2, \dots, s.$$

Hence the necessary condition (3.7) can be also written as

$$\mathcal{C} \leq \frac{1}{1 + c_i - \sum_{j=1}^s v_{ij} c_j} \quad \text{and} \quad 1 + c_i - \sum_{j=1}^s v_{ij} c_j > 0, \quad i = 1, 2, \dots, s.$$

3.1 Methods with $p = r = s = 2$

Consider the multistage integration method with coefficients

$$\left[\begin{array}{c|c} \mathbf{A} & \mathbf{U} \\ \mathbf{B} & \mathbf{V} \end{array} \right] = \left[\begin{array}{cc|cc} 0 & 0 & 1 & 0 \\ a_{21} & 0 & 0 & 1 \\ \hline b_{11} & b_{12} & v_1 & 1 - v_1 \\ b_{21} & b_{22} & v_2 & 1 - v_2 \end{array} \right], \quad \mathbf{c} = [c_1 \quad c_2]^T,$$

$$\mathbf{q}_0 = [1 \quad 1]^T, \quad \mathbf{q}_1 = [q_{11} \quad q_{21}]^T, \quad \mathbf{q}_2 = [q_{12} \quad q_{22}]^T.$$

3.1.1 Methods with $p = r = s = 2, q = 2$

Solving the order conditions for order $p = 2$ and stage order $q = 2$ we obtain a 5-parameter family depending on c_1, c_2, v_1, v_2 and a_{21} under the restriction $|v_1 - v_2| < 1$, which is equivalent to the power boundedness of the matrix \mathbf{V} , and hence it ensure the zero-stability of the method (compare [39]). Furthermore, from Lemma 1 we obtain $a_{21} = 0$.

Case $v_1 = v_2$ ($rank(\mathbf{V}) = 1$).

Maximizing the SSP coefficient \mathcal{C} , adding the restriction $c_1 < c_2$, we obtain:

$$\mathcal{C} = 1 - \frac{1}{\sqrt{2}} \quad \text{for } c_1 = 0, \quad c_2 = \sqrt{2} \text{ and } v_1 = \frac{1}{2}. \tag{3.8}$$

Case $v_1 \neq v_2$ ($rank(\mathbf{V}) = 2$).

Maximizing the SSP coefficient \mathcal{C} , adding the restriction $-1 \leq c_1 < c_2 \leq 1$, we obtain:

$$\mathcal{C} = \frac{1}{2} \quad \text{for } c_1 = -1, \quad c_2 = 1, \quad v_1 = \frac{53}{64} \text{ and } v_2 = \frac{1}{4}, \tag{3.9}$$

while, adding the restriction $-2 \leq c_1 < c_2 \leq 2$, we obtain:

$$\mathcal{C} = \frac{3}{4} \quad \text{for } c_1 = -2, \quad c_2 = 2, \quad v_1 = \frac{243}{256} \text{ and } v_2 = \frac{1}{16}. \tag{3.10}$$

Choosing larger bounds for c_1 and c_2 , the value of \mathcal{C} increases (up to 1) but unfortunately also the magnitude of the q 's increases. Our numerical search points out that in this case the best attainable value for \mathcal{C} seems to be

$$\mathcal{C} = 1 - \frac{1}{c_2 - c_1}.$$

For the values given by (3.9) the method has the coefficients:

$$\mathbf{B} = \left[\begin{array}{cc} \frac{37}{64} & \frac{5}{64} \\ 0 & \frac{3}{2} \end{array} \right], \quad \mathbf{V} = \left[\begin{array}{cc} \frac{53}{64} & \frac{11}{64} \\ \frac{1}{4} & \frac{3}{4} \end{array} \right],$$

$$\mathbf{c} = [-1, 1]^T, \quad \mathbf{W} = [\mathbf{q}_0, \mathbf{q}_1, \mathbf{q}_2] = \left[\begin{array}{cc} 1 & -1 & \frac{1}{2} \\ 1 & 1 & \frac{1}{2} \end{array} \right],$$

while, for the values given by (3.10) the method has the coefficients:

$$\mathbf{B} = \begin{bmatrix} \frac{99}{128} & \frac{3}{128} \\ 0 & \frac{5}{4} \end{bmatrix}, \quad \mathbf{V} = \begin{bmatrix} \frac{243}{256} & \frac{13}{256} \\ \frac{1}{16} & \frac{15}{16} \end{bmatrix},$$

$$\mathbf{c} = [-2, 2]^T, \quad \mathbf{W} = [\mathbf{q}_0, \mathbf{q}_1, \mathbf{q}_2] = \begin{bmatrix} 1 & -2 & 2 \\ 1 & 2 & 2 \end{bmatrix}.$$

In order to reach higher values for SSP coefficient \mathcal{C} , in the following subsection we consider methods of stage order $q = 1$.

3.1.2 Methods with $p = r = s = 2, q = 1$

Solving the order conditions for order $p = 2$ and stage order $q = 1$ we obtain a 7-parameter family depending on $c_1, c_2, v_1, v_2, q_{12}, q_{22}$ and a_{21} under the restriction $|v_1 - v_2| < 1$. Since we are looking for SSP methods, Lemma 1 implies $a_{21} = 0$. Maximizing the SSP coefficient \mathcal{C} , adding the restriction $-1 \leq c_1 < c_2 \leq 1$, we obtain:

$$\mathcal{C} = \frac{3}{4} \quad \text{for } c_1 = -1, c_2 = 1, v_1 = \frac{7}{10}, v_2 = \frac{1}{10} \text{ and } q_{12} = q_{22} + 3,$$

where q_{22} is still a free parameter. If we consider the restriction $-2 \leq c_1 < c_2 \leq 2$, the value for \mathcal{C} increases to $\frac{7}{8}$. In this case we have

$$\mathcal{C} = \frac{7}{8} \quad \text{for } c_1 = -2, c_2 = 2, v_1 = \frac{29}{36}, v_2 = \frac{1}{36} \text{ and } q_{12} = q_{22} + 10,$$

where q_{22} is still a free parameter. In this case, it seems that the maximal values of the coefficient \mathcal{C} the following relation holds:

$$\mathcal{C} = 1 - \frac{1}{2(c_2 - c_1)}.$$

3.2 Methods with $p = r = s = 3$

In this section we investigate methods with $p = r = s = 3$ and $q = 3, 2, 1$. In this and in the following section we assume that $c_s = 1$. Relaxing this condition allows abscissas shifting, but seems not to lead to larger values for the SSP coefficient.

3.2.1 Methods with $p = r = s = 3, q = 3$

Forcing strictly increasing abscissas, and $c_3 = 1$, the optimal SSP method has $\mathcal{C} = \sqrt{2} - 1$ and the following coefficients:

$$\mathbf{c} = [-1 - \sqrt{2} \quad -\sqrt{2} \quad 1]^T, \quad \mathbf{B} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 4 - 2\sqrt{2} & 0 \\ \frac{5}{2} - \frac{3}{\sqrt{2}} & 0 & \frac{9}{2} - 2\sqrt{2} \end{bmatrix},$$

$$\mathbf{V} = \begin{bmatrix} 0 & 1 & 0 \\ -1 + \sqrt{2} & -8 + 6\sqrt{2} & 10 - 7\sqrt{2} \\ \frac{19}{2} - \frac{13}{\sqrt{2}} & 0 & \frac{13}{\sqrt{2}} - \frac{17}{2} \end{bmatrix}.$$

For this method $C_{\text{eff}} = \frac{\sqrt{2}-1}{3} \approx 0.138$.

3.2.2 Methods with $p = r = s = 3, q = 2$

In this case, forcing the restriction $-5 \leq c_1 < c_2 < c_3 = 1$, we obtain that the optimal SSP method has $C = \frac{5}{6}$, while under the restriction $-3 \leq c_1 < c_2 < c_3 = 1$, we obtain that the optimal SSP method has $C = \frac{3}{4}$. The coefficients of this last method are:

$$\mathbf{B} = \begin{bmatrix} \frac{1317487}{1769472} & \frac{7973}{110592} & \frac{1075}{589824} \\ \frac{4955}{36864} & \frac{2089}{2304} & \frac{2543}{12288} \\ 0 & 0 & \frac{5}{4} \end{bmatrix}, \quad \mathbf{V} = \begin{bmatrix} \frac{3851}{4096} & \frac{473}{8192} & \frac{17}{8192} \\ \frac{35}{256} & \frac{359}{512} & \frac{83}{512} \\ \frac{1}{16} & 0 & \frac{15}{16} \end{bmatrix}, \quad (3.11)$$

$$\mathbf{c} = [-3 \quad 0 \quad 1]^T, \quad \mathbf{W} = [\mathbf{q}_0, \mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3] = \begin{bmatrix} 1 & -3 & \frac{9}{2} & 0 \\ 1 & 0 & 0 & -\frac{26}{9} \\ 1 & 1 & \frac{1}{2} & -\frac{26}{3} \end{bmatrix}. \quad (3.12)$$

Let us remark that for this method the value of C can be obtained as $C = v_{33}/b_{33} = 3/4$ (compare (3.6)) and so $C_{\text{eff}} = 1/4$. In this case, our numerical search points out that the best attainable value for C seems to be

$$C = 1 - \frac{1}{c_3 - c_1}.$$

3.2.3 Methods with $p = r = s = 3, q = 1$

In this case the higher SSP coefficient C is given by

$$C = \frac{v_{12}}{b_{12}} = -z \approx 0.782286,$$

where $z \approx -0.782286$ is a root of the polynomial

$$p(x) = -290965200 + 1284558760x + 2860364411x^2 - 7981097947x^3 + 19201804817x^4 - 9167715999x^5 + 1003129920x^6,$$

and $v_{11} = 1 - v_{12} \approx 0.795767$ is a root of the polynomial

$$p(x) = -120168990605590227 + 175319907436584132x + 41426367452248895x^2 - 77002533780794860x^3 - 16999999144346705x^4 + 47246885203112x^5 + 105800506695653x^6.$$

The coefficients of this methods are:

$$\mathbf{c} = \left[-3 \quad -\frac{29}{10} \quad 1 \right]^T,$$

$$\mathbf{B} = \begin{bmatrix} 0.7185038451423001 & 0.26107280720903675 & 0 \\ 0 & 0 & 0.2657061947964307 \\ 0 & 0 & 1.2096037031663531 \end{bmatrix},$$

$$\mathbf{V} = \begin{bmatrix} 0.7957665235133686 & 0.20423347648663137 & 0 \\ 0.7635281794723168 & 0.028613712027478297 & 0.20785810850020528 \\ 0 & 0.05374453927342392 & 0.9462554607265761 \end{bmatrix},$$

and

$$\mathbf{W} = [\mathbf{q}_0, \mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3] = \begin{bmatrix} 1 & -3 & 3.8829228414636545 & 9.177166775938929 \\ 1 & -2.9 & 5.903270746377843 & 0.4543609951704569 \\ 1 & 1 & 0.5 & -10 \end{bmatrix}.$$

This method has $C_{\text{eff}} \approx 0.261$, which represents just a slight improvement with respect to the value $C_{\text{eff}} = 1/4$ obtained for method (3.11)–(3.12) having same order $p = 3$, but a higher stage order $q = 2$.

3.3 Methods with $p = r = s = 4$

In this section we investigate methods with $p = r = s = 4$ and $q = 1, 2, 3, 4$.

3.3.1 Methods with $p = r = s = 4, q = 1$

Forcing strictly increasing abscissas, and $c_4 = 1$, the optimal SSP method has $C \approx 0.450$ and the following coefficients:

$$\mathbf{c} = [-1.2541132795031640 \quad -1.2110167921401000 \quad -1.1051947914593280 \quad 1],$$

$$\mathbf{B} = \begin{bmatrix} 0.2216307397474322 & 0.2885008731278295 & 0.4247750415788341 & 0.0043199970428693 \\ 0.1165966501056636 & 0.1517760370136278 & 0.2234678589848447 & 0.2460743776223290 \\ 0.2533513573132226 & 0.3297921934307524 & 0.4855704288106428 & 0.0028216788557943 \\ 0 & 0 & 0 & 1.6163180017841770 \end{bmatrix},$$

$$\mathbf{V} = \begin{bmatrix} 0.5233434195205922 & 0.1482774935168031 & 0.3257753410935703 & 0.0026037458690343 \\ 0.0524219998842081 & 0.6508084969235142 & 0.1861196295058758 & 0.1106498736864019 \\ 0.1138926593620751 & 0.6605498625171727 & 0.2182774999048495 & 0.0072799782159028 \\ 0.2733912307975496 & 0.0000285832038595 & 0 & 0.7265801859985909 \end{bmatrix},$$

and

$$\mathbf{W} = [\mathbf{q}_0, \mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3, \mathbf{q}_4] = \begin{bmatrix} 1 & -1.2541132795031640 & 0.0744315953870818 & 1.4781869068894780 & -1.0811488822422830 \\ 1 & -1.2110167921401000 & 1.5029715926335450 & -1.5989477159135420 & 2.8089651773117870 \\ 1 & -1.1051947914593280 & 0.4594421371313254 & -0.2828371135694487 & 2.0735645377692490 \\ 1 & 1 & 0.5 & 0.1666666666666664 & -2.3813563150667030 \end{bmatrix}.$$

For this method $C_{\text{eff}} \approx 0.112$.

3.3.2 Methods with $p = r = s = 4, q = 2$

In this case, forcing the restriction $-3 \leq c_1 < c_2 < c_3 < c_4 = 1$, we obtain that the optimal SSP method has $C \approx 0.507$, whose coefficients are

$$\mathbf{c} = [-3 \quad -1.5307929996603450 \quad -1.5207929996603450 \quad 1]^T,$$

$$\mathbf{B} = \begin{bmatrix} 0.3446530252761958 & 0 & 0 & 0.0026299108009584 \\ 0 & 0.5387417049219302 & 0.3156134630119571 & 0.1027295988157450 \\ 0 & 0.2900023222017333 & 1.0524245809100090 & 0.0430876450117072 \\ 0.3009115537533498 & 0 & 0 & 1.5509115537533500 \end{bmatrix},$$

$$\mathbf{V} = \begin{bmatrix} 0.5610128954739848 & 0 & 0.4376524983724827 & 0.0013346061535325 \\ 0.0647413008868319 & 0.2733963426787711 & 0.6097299591380859 & 0.0521323972963111 \\ 0.2968901298627457 & 0.1471680650188273 & 0.5340760307534204 & 0.0218657743650067 \\ 0.2129557768766749 & 0 & 0 & 0.7870442231233251 \end{bmatrix},$$

Table 2. C_{eff} for GLMp qrs (2.1) with order $p = 2$, stage order $q = 1, 2$, $r = 2$ external stages and $s = 2$ internal stages.

GLM2122	GLM2222
0.847	0.822

Table 3. C_{eff} for GLMp qrs (2.1) with order $p = 3$, stage order $q = 1, 2, 3$, $r = 3$ external stages and $s = 3$ internal stages.

GLM3133	GLM3233	GLM3333
0.667	0.578	0.554

Table 4. C_{eff} for GLMp qrs (2.1) with order $p = 4$, stage order $q = 1, 2, \dots, 4$, $r = 4$ external stages and $s = 4$ internal stages.

GLM4144	GLM4244	GLM4344	GLM4444
0.532	0.529	0.518	0.504

the sequential quadratic programming ('sqp') algorithm. Since `fmincon` is a local minimization routine, we ran an extensively numerical search using at least ten thousands random starting points, generated by means of the `rand` Matlab function. To the aim of speeding up this search for SSP methods when the number of free parameters and constraints increases the necessary condition provided by the following lemma can be useful (for example to provide sharper bounds for parameters and to obtain a better list of starting points).

Lemma 2. *If a general linear method (2.1) has a positive SSP coefficient, $C > 0$, then*

$$0 \leq \mathbf{L}\mathbf{e} \leq \mathbf{e}, \quad 0 \leq \gamma\mathbf{B}\mathbf{L}\mathbf{e} \leq \mathbf{e}, \tag{4.1}$$

where $\mathbf{L} = (\mathbf{I} + \gamma\mathbf{A})^{-1}$ and $0 < \gamma \leq C$.

Proof. Let us recall we are assuming that $\mathbf{U}\mathbf{e} = \mathbf{e}$ and $\mathbf{V}\mathbf{e} = \mathbf{e}$. From (2.3), $\mathbf{L}\mathbf{U} \geq 0$ implies $\mathbf{L}\mathbf{e} = \mathbf{L}\mathbf{U}\mathbf{e} \geq 0$, and $\mathbf{I} - \mathbf{L} \geq 0$ implies $\mathbf{L}\mathbf{e} \leq \mathbf{I}\mathbf{e} = \mathbf{e}$, hence the first part of inequalities (4.1) holds. Again, from (2.3), $\gamma\mathbf{B}\mathbf{L} \geq 0$ implies $\gamma\mathbf{B}\mathbf{L}\mathbf{e} \geq 0$, and $\mathbf{V} - \gamma\mathbf{B}\mathbf{L}\mathbf{U} \geq 0$ implies $\gamma\mathbf{B}\mathbf{L}\mathbf{U}\mathbf{e} \leq \mathbf{V}\mathbf{e}$, that is $\gamma\mathbf{B}\mathbf{L}\mathbf{e} \leq \mathbf{e}$, and so the second part of inequalities (4.1) holds, too. \square

The C_{eff} coefficients for methods with two, three and four external stages are respectively listed in Tables 2, 3 and 4, using the notation GLMp qrs , where p is the order of the method, q is the stage order, r is the number of external stages and s is the number of internal stages.

Here we report the coefficient matrices of optimal SSP GLMs of order $p = 2$, $p = 3$ and $p = 4$ and $p = q = r = s$. It is worth remarking that the coefficients listed here are computed using double precision accuracy and they are reported with 16 digits. A technique similar to the one used in [35] can be used when

more accurate coefficients are needed, for example for implementation in an extended precision environment.

Coefficients of GLM2222:

$$\begin{aligned}
 \mathbf{c} &= [0.5022655558767691 \quad 1]^T, \\
 \mathbf{A} &= \begin{bmatrix} 0 & 0 \\ 0.5708860675842338 & 0 \end{bmatrix}, \quad \mathbf{U} = \begin{bmatrix} 0.9184891352423395 & 0.0815108647576605 \\ 0.8621853383442499 & 0.1378146616557501 \end{bmatrix}, \\
 \mathbf{B} &= \begin{bmatrix} 0.5708860675842338 & 0.6081669766552923 \\ 0.2482943789611213 & 0.2645088930130668 \end{bmatrix}, \\
 \mathbf{V} &= \begin{bmatrix} 0.8621853383442499 & 0.1378146616557501 \\ 0.3749886103184382 & 0.6250113896815619 \end{bmatrix}, \\
 \mathbf{W} &= \begin{bmatrix} 1 & 0.6081669766552924 & -0.0000000000000001 \\ 1 & -0.6910637589451494 & 1.5474666436813336 \end{bmatrix}.
 \end{aligned}$$

This method has $\mathcal{C}_{\text{eff}} \approx 0.822$.

Coefficients of GLM3333:

$$\begin{aligned}
 \mathbf{c} &= [0.3295839783544315 \quad 0.6806617112619909 \quad 1]^T, \\
 \mathbf{A} &= \begin{bmatrix} 0 & 0 & 0 \\ 0.5124026992885452 & 0 & 0 \\ 0.4084203656103463 & 0.4796606306581744 & 0 \end{bmatrix}, \\
 \mathbf{U} &= \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0.8514777730453410 & 0.1485222269546588 \\ 0.1313458703216458 & 0.6786866342802576 & 0.1899674953980965 \end{bmatrix}, \\
 \mathbf{B} &= \begin{bmatrix} 0.5223463949514766 & 0.5348295830910508 & 0 \\ 0.3347759349512645 & 0.3931704919952592 & 0.4932702635381821 \\ 0 & 0 & 0 \end{bmatrix}, \\
 \mathbf{V} &= \begin{bmatrix} 0 & 0.8680015654661640 & 0.1319984345338356 \\ 0.2607207697861334 & 0.5563090669843533 & 0.1829701632295133 \\ 1 & 0 & 0 \end{bmatrix}, \\
 \mathbf{W} &= \begin{bmatrix} 1 & 0.2433831470792890 & -0.1453586170258652 & 0.0319049749709932 \\ 1 & 0.3295839783544315 & 0.0543127993939672 & 0.0059668761666100 \\ 1 & -0.7566168529207110 & 0.1112582358948458 & 0.1322884988698362 \end{bmatrix}.
 \end{aligned}$$

This method has $\mathcal{C}_{\text{eff}} \approx 0.554$.

Coefficients of GLM4444:

$$\begin{aligned}
 \mathbf{c} &= [0.2389332461541251 \quad 0.4860573286209339 \quad 0.7359123877762289 \quad 1], \\
 \mathbf{A} &= \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0.3876590107850190 & 0 & 0 & 0 \\ 0.3052895098296686 & 0.3907983774045524 & 0 & 0 \\ 0.2489878897536953 & 0.3187271759302078 & 0.4047222644510253 & 0 \end{bmatrix}, \\
 \mathbf{U} &= \begin{bmatrix} 0.0912599380251995 & 0 & 0.9077024591751040 & 0.0010376027996967 \\ 0.2893536053383063 & 0 & 0.7090920916129786 & 0.0015543030487151 \\ 0.3134061212806464 & 0.1269451063377834 & 0.5584247264993190 & 0.0012240458822511 \\ 0.2556076322999006 & 0.2876226025113369 & 0.4554398030738938 & 0.0013299621148688 \end{bmatrix}, \\
 \mathbf{B} &= \begin{bmatrix} 0.4084337666596042 & 0 & 0 & 0 \\ 0.3828018917763514 & 0.4900212858838719 & 0.0105574651913504 & 0 \\ 0.2475481687517574 & 0.2657257201220867 & 0.3374206007279392 & 0.4137187953380616 \\ 0.1081881397565976 & 0.1384906723289790 & 0.1758565404620620 & 0.2156215593100244 \end{bmatrix}, \\
 \mathbf{V} &= \begin{bmatrix} 0.0751122991274016 & 0.1721149858574717 & 0.7470925370715471 & 0.0056801779435796 \\ 0.2875479264730055 & 0.0027007530079466 & 0.7002076220630648 & 0.0095436984559831 \\ 0.2204520296708872 & 0.3255492887593254 & 0.4528063165607442 & 0.0011923650090433 \\ 0.1110644950381738 & 0.2259735764529201 & 0.1978939020464726 & 0.4650680264624335 \end{bmatrix},
 \end{aligned}$$

and

$$\mathbf{w} = \begin{bmatrix} 1 & -0.4024799023418847 & 0.0109880388418833 & 0.0335886630738861 & 0 \\ 1 & -0.0255262786434428 & -0.1034566363144243 & 0.0182430084929503 & 0.0229216637127512 \\ 1 & 0.3044460558739243 & 0.0291029904711275 & 0.0007065225928177 & -0.0019072286304098 \\ 1 & -0.6581482865003410 & 1.0841569582135440 & -1.3812585734008830 & 1.7993346354617410 \end{bmatrix}.$$

This method has $C_{\text{eff}} \approx 0.504$.

5 Starting and Finishing Procedures

It is the worth remarking that the multistage integration methods considered in this paper require a starting vector $y^{[0]}$ which satisfies the relation (2.2). In other words, these methods need a suitable starting procedure to attain the expected order of convergence [2, 3, 39]. In our implementation, we used starting procedures in the form of a generalized explicit RK method

$$\frac{\mathbf{c}^{(i)} \mid \mathbf{A}^{(i)}}{b_0^{(i)} \mid \mathbf{b}^{(i)T}} = \frac{\begin{array}{c|ccc} c_1^{(i)} = 0 & 0 & & \\ c_2^{(i)} & a_{2,1}^{(i)} & 0 & \\ \vdots & \vdots & \vdots & \ddots \\ c_{s_i}^{(i)} & a_{s_i,1}^{(i)} & a_{s_i,2}^{(i)} & \dots & 0 \end{array}}{\hline \begin{array}{c|ccc} b_0^{(i)} & b_1^{(i)} & b_2^{(i)} & \dots & b_{s_i}^{(i)} \end{array}} \tag{5.1}$$

with s_i stages, $i = 1, \dots, r$. Order conditions and a complete description of the construction of starting procedures of the form (5.1) can be found in [37].

Furthermore, from (2.2), the external stages of the GLMs (2.1) approximate a linear combination of the solution and its derivatives at grid points. So, usually, a finishing procedure is needed to recover an approximation for $y(t_{\text{end}})$. This finishing procedure, which is a suitable linear combination of external stages, does not involve any additional evaluation of the function f and can be constructed by using information coming only from the previous integration step. A possible way to determine a finishing procedure is the following. From (2.2) we know that

$$y_i^{[n]} = \sum_{k=0}^p q_{ik} h^k y^{(k)}(t_n) + O(h^{p+1}), \quad i = 1, 2, \dots, r, \tag{5.2}$$

and so

$$y_i^{[n-1]} = \sum_{k=0}^p q_{ik} h^k y^{(k)}(t_{n-1}) + O(h^{p+1}), \quad i = 1, 2, \dots, r.$$

Expanding $y^{(k)}(t_{n-1})$ in Taylor series about t_n , up to the power $p - k$, we obtain

$$y^{(k)}(t_{n-1}) = \sum_{j=0}^{p-k} \frac{(-1)^j h^j}{j!} y^{(k+j)}(t_n) + O(h^{p-k+1}),$$

and hence, for $i = 1, 2, \dots, r$, we have

$$\begin{aligned}
 y_i^{[n-1]} &= \sum_{k=0}^p q_{ik} h^k \left(\sum_{j=0}^{p-k} \frac{(-1)^j h^j}{j!} y^{(k+j)}(t_n) + O(h^{p-k+1}) \right) + O(h^{p+1}) \\
 &= \sum_{k=0}^p q_{ik} \left(\sum_{j=0}^{p-k} \frac{(-1)^j h^{k+j}}{j!} y^{(k+j)}(t_n) \right) + O(h^{p+1}) \\
 &= \sum_{k=0}^p \sum_{m=k}^p q_{ik} \frac{(-1)^{m-k} h^m}{(m-k)!} y^{(m)}(t_n) + O(h^{p+1}) \\
 &= \sum_{m=0}^p \sum_{k=0}^m q_{ik} \frac{(-1)^{m-k} h^m}{(m-k)!} y^{(m)}(t_n) + O(h^{p+1}) \\
 &= \sum_{m=0}^p \left(\sum_{k=0}^m \frac{(-1)^{m-k} q_{ik}}{(m-k)!} \right) h^m y^{(m)}(t_n) + O(h^{p+1}).
 \end{aligned}$$

So we obtain

$$y_i^{[n-1]} = \sum_{k=0}^p \left(\sum_{m=0}^k \frac{(-1)^{k-m} q_{im}}{(k-m)!} \right) h^k y^{(k)}(t_n) + O(h^{p+1}), \quad i = 1, 2, \dots, r. \quad (5.3)$$

Let us now consider the case $r = p$. If we define the matrix $\mathbf{W} \in \mathbb{R}^{r \times (p+1)}$ as $\mathbf{W} = [\mathbf{q}_0, \mathbf{q}_1, \dots, \mathbf{q}_p]$, we can recover a numerical approximation of order p for the value $y(t_n)$ by considering a suitable linear system whose coefficient matrix can be obtained adding a row to the matrix \mathbf{W} . To this aim, let us define the row vector $\tilde{\mathbf{q}} \in \mathbb{R}^{1 \times (p+1)}$ as

$$\tilde{\mathbf{q}} = \left[\sum_{m=0}^k \frac{(-1)^{k-m} q_{1m}}{(k-m)!} \right]_{k=0, \dots, p}.$$

We can consider the equality

$$\tilde{y}^{[n]} = \mathbf{Q} \tilde{y}_n + O(h^{p+1}), \quad \mathbf{Q} = \begin{bmatrix} \mathbf{W} \\ \tilde{\mathbf{q}} \end{bmatrix} \in \mathbb{R}^{(p+1) \times (p+1)},$$

where

$$\tilde{y}^{[n]} = [y_1^{[n]}, y_2^{[n]}, \dots, y_r^{[n]}, y_1^{[n-1]}]^T, \quad \tilde{y}_n = [y(t_n), y'(t_n), \dots, y^{(p)}(t_n)]^T.$$

When the matrix \mathbf{Q} is invertible, then $\tilde{y}_n = \mathbf{Q}^{-1} \tilde{y}^{[n]} + O(h^{p+1})$, and hence an approximation for the value of $y(t_n)$ can be computed as a scalar product of the first row of \mathbf{Q}^{-1} by the vector $\tilde{y}^{[n]}$. If the matrix \mathbf{Q} is not invertible, as in case of GLM3333, then the linear system can be obtained by choosing in a different way the $p + 1$ equations between the $2r$ equations given by (2.1) and (5.3).

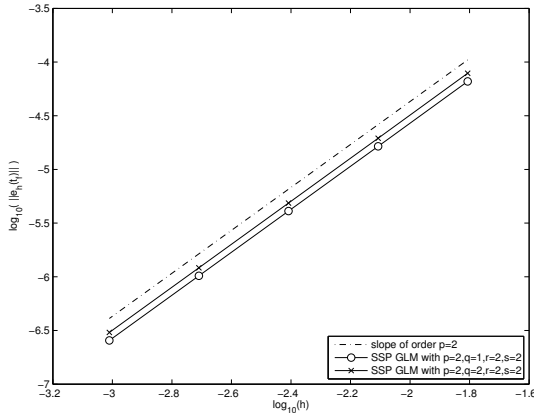


Figure 1. Order verification for SSP GLMs of order $p = 2$ and stage order $q = 1$ and 2 .

6 Numerical Experiments

6.1 Validation of convergence

To verify the order of convergence we apply the methods derived in this paper to the system of ODEs obtained by first order upwind discretization in space variable x of the test problem from [8, 49]

$$\frac{\partial y(x, t)}{\partial t} = -\frac{\partial y(x, t)}{\partial x} + \frac{t - x}{(1 + t)^2}, \quad 0 \leq x \leq 1, \quad 0 \leq t \leq 1, \quad (6.1)$$

with initial condition $y(x, 0) = 1 + x, 0 \leq x \leq 1$, and left boundary condition $y(0, t) = 1/(1 + t), 0 \leq t \leq 1$. The exact solution to this problem is

$$y(x, t) = \frac{1 + x}{1 + t}, \quad 0 \leq x \leq 1, \quad 0 \leq t \leq 1.$$

Since this solution is linear in space variable x , the resulting system of ODEs does not introduce any discretization error and have the solution

$$y_i(t) = y(x_i, t), \quad 0 \leq t \leq 1,$$

for any grid point $x_i, i = 0, \dots, N$, where $x_i = i\Delta x, i = 0, 1, \dots, N$, and $N\Delta x = 1$.

We have plotted on Figs. 1–3 in double logarithmic scale the norm of global error at the end point t_f of the interval of integration versus the temporal step-size h for methods of order $p = 2, p = 3, p = 4$, and stage order $q = 1, 2, \dots, p$. We can see that all methods achieve the expected order of convergence.

As already mentioned in the introduction the class of GLMs allows us to break the order four barrier for SSPRK methods. The work on the construction of SSP GLMs of high order and stage order will be reported elsewhere.

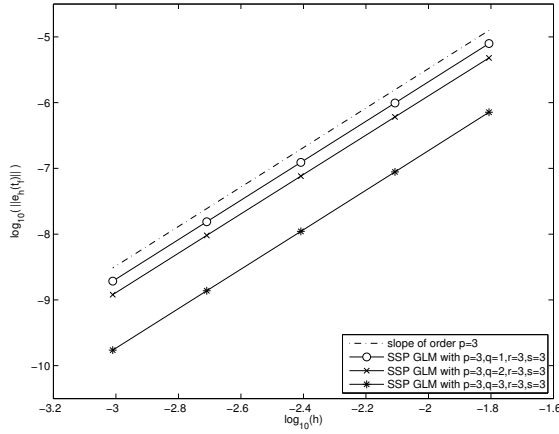


Figure 2. Order verification for GLMs of order $p = 3$ and stage order $q = 1, 2$ and 3 .

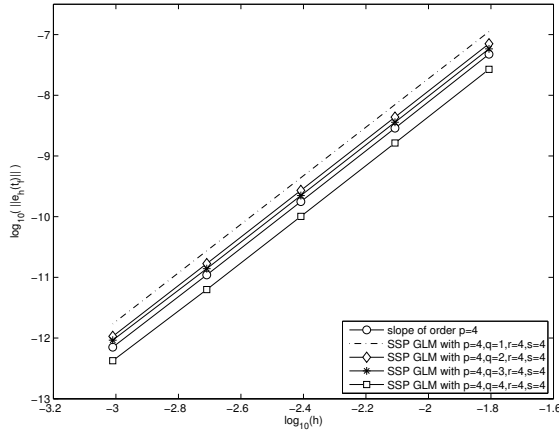


Figure 3. Order verification for GLMs of order $p = 4$ and stage order $q = 1, 2, 3$ and 4 .

6.2 Order preservation for high stage order methods

In order to further validate the order preservation for high stage order SSP multistage integration methods we report in Figs. 4 and 5 the results of numerical tests that point out that the constructed high order stages SSP multistage integration methods preserve the theoretical order of convergence p , while low stage order SSP Runge–Kutta methods suffer from the well known order reduction phenomenon. Specifically, following Constantinescu and Sandu [8], we considered problem (6.1) and pointed out that, when the spatial and temporal grids are refined simultaneously, SSPRK(3,3) method [22] and SSPRK(5,4) method [24, 44, 53] only achieve order $p = 2$, while GLM3333, of order $p = 3$ and stage order $q = 3$, preserves the expected order $p = 3$ (see Fig. 5).

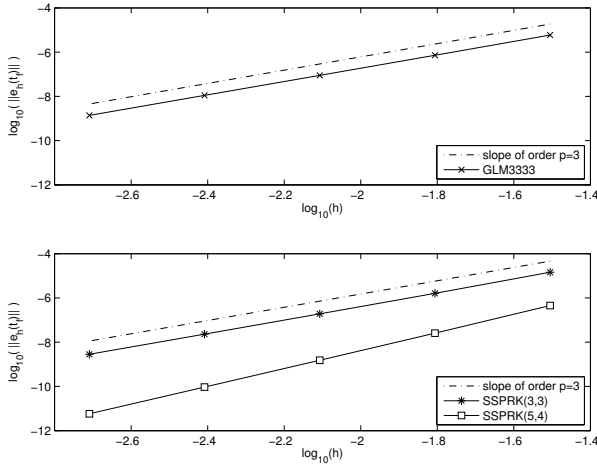


Figure 4. Order preservation for GLM3333, and for SSPRK(3,3) and SSPRK(5,4) on problem (6.1) when only the temporal grid is refined.

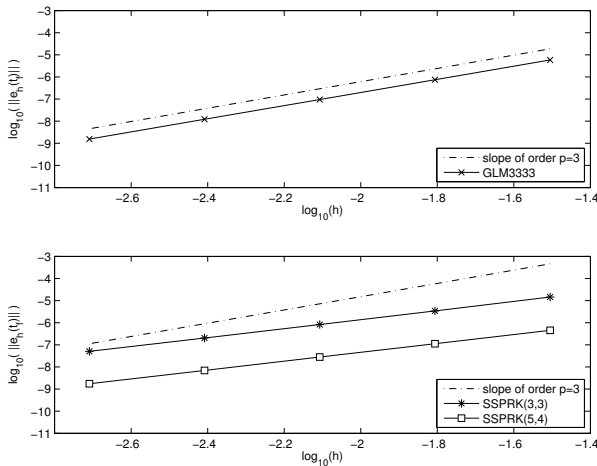


Figure 5. Order preservation for GLM3333 (top figure) and order reduction phenomenon for SSPRK(3,3) and SSPRK(5,4) (bottom figure) on problem (6.1) when spatial and temporal grids are refined simultaneously.

For the sake of completeness, it is worth to remark that when the space grid is maintained fixed, i.e. the ODE problem is fixed, then the expected order is preserved for all considered Runge–Kutta and multistage integration methods (see Fig. 4). The order reduction phenomenon for RK methods reported in Fig. 5 is due to naive implementation of a time-dependent Dirichlet boundary condition. This phenomenon has been analyzed in the literature and for linear hyperbolic equations it can be reduced or avoided by a suitable transformation or differentiation of the boundary conditions as shown in [7, 34, 48, 49].

6.3 Validation of monotonicity

To verify monotonicity properties of GLMs constructed in this paper we consider, following Ferracina and Spijker [21], Constantinescu and Sandu [8] and Ketcheson et. al. [42,43], the following problems (compare also with [34,45,53]).

Problem 1. The inviscid Burgers equation

$$\frac{\partial y(x, t)}{\partial t} + \frac{\partial}{\partial x} \left(\frac{1}{2} y^2(x, t) \right) = 0, \quad 0 \leq x \leq X, \quad 0 \leq t \leq t_f, \quad (6.2)$$

with $X = 2$, and with initial condition

$$y(x, 0) = \frac{1}{2} - \frac{1}{4} \sin(\pi x) \quad (6.3)$$

and periodic boundary conditions $y(0, t) = y(2, t)$, $0 \leq t \leq t_f$.

Problem 2. We consider again the Burgers equation (6.2). In this case with $X = 1$ and with discontinuous initial condition

$$y(x, 0) = \begin{cases} 1, & 0.18 \leq x \leq 0.44, \\ 0, & \text{otherwise,} \end{cases} \quad (6.4)$$

and periodic boundary conditions $y(0, t) = y(1, t)$, $0 \leq t \leq t_f$.

Problem 3. The Buckley–Leverett equation

$$\frac{\partial y(x, t)}{\partial t} + \frac{\partial}{\partial x} (\Phi(y(x, t))) = 0, \quad -1 \leq x \leq 1, \quad 0 \leq t \leq t_f, \quad (6.5)$$

where

$$\Phi(y) = \frac{y^2}{y^2 + a(1-y)^2}.$$

This equation models a two-phase flow through the porous media, see for example [46]. We take $a = 1/4$ and assume the discontinuous initial condition

$$y(x, 0) = \begin{cases} 1, & -0.5 \leq x \leq 0, \\ 0, & \text{otherwise,} \end{cases} \quad (6.6)$$

and periodic boundary conditions

$$y(-1, t) = y(1, t), \quad 0 \leq t \leq t_f.$$

For all these problems the space derivative was discretized by a fifth order finite difference weighted essentially non-oscillatory (WENO) scheme [51].

A numerical approximation obtained by the SSP multistage integration methods of order $p = 3$ and stage order $q = 3$ whose coefficients are listed in Section 4, is presented in Fig. 6, Fig. 7 and Fig. 8. For comparison purpose we have also also plotted the numerical approximation obtained by the SSPRK(3,3) method [22]. We can see that, using the same temporal stepsize

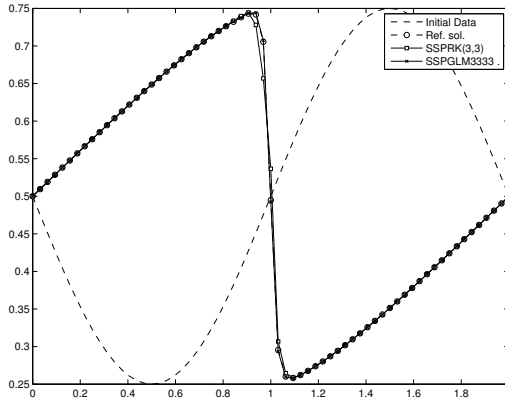


Figure 6. Numerical approximations at $t_f = 2$ to the discretization of Problem 1, with $N = 64$, $N_t = 44$ and $\nu = 1.091$, obtained by SSP GLM of order $p = 3$ and stage order $q = 3$, and by SSPRK(3,3).

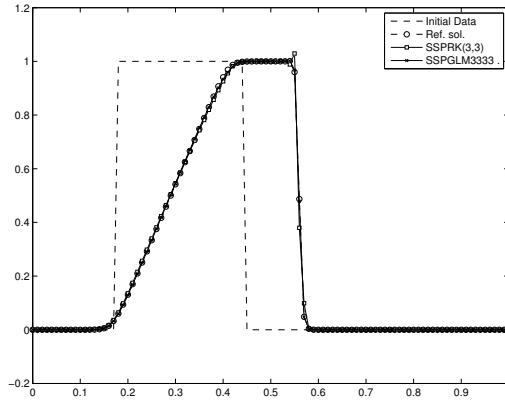


Figure 7. Numerical approximations at $t_f = 0.23$ to the discretization of Problem 2, with $N = 100$, $N_t = 19$ and $\nu = 1.211$, obtained by SSP GLM of order $p = 3$ and stage order $q = 3$, and by SSPRK(3,3).

Δt for both methods, the SSP multistage integration methods exhibits smooth behavior, while numerical solution obtained by SSPRK(3,3) method exhibits spurious oscillations.

In the caption of Figures 6–8 we denoted with ν the so-called Courant number (or CFL number) defined as $\nu = |a\Delta t/\Delta x|$, where $a = \max(y)$ for Problems 1 and 2, and $a = \max(\frac{d\Phi}{dy}(y))$ for Problem 3, $\Delta t = t_f/N_t$ and $\Delta x = X/N$.

As is well known, the solution of hyperbolic PDEs can develop discontinuities, even if the initial data is a smooth function. In Problem 1 a shock occurs at $t = 4/\pi$ as the characteristic lines cross. For Problems 2 and 3 the presence of shocks is due to the discontinuity in the initial data. Our numerical results confirm that the presented SSP multistage integration methods methods, combined with appropriate spatial discretization, perform well even if a shock

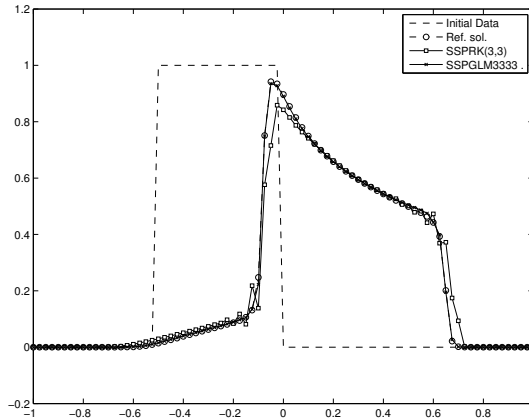


Figure 8. Numerical approximations at $t_f = 0.4$ to the discretization of Problem 3 with $N = 80$, $N_t = 28$ and $\nu = 1.493$, obtained by SSP of order $p = 3$ and stage order $q = 3$, and by SSPRK(3,3).

occurs.

Even if, for the sake of brevity, we are not reporting the results here, we verified that for sufficiently small values of CFL number ν the behavior of the methods derived in this paper is very similar to a SSPRK of the corresponding order (we used SSP(2,2), SSPRK(3,3) and SSPRK(5,4) from [22]) for several space discretization schemes (such as first, second and third order upwind, second order ENO, Lax-Wendroff, third-order upwind-biased flux limited [34, 45]).

Finally we report the results of the investigation of the SSP property by means of the total variation (TV) semi-norm:

$$TV(y(t, x)) = \sum_{i=1}^N |y(t, x_i) - y(t, x_{i-1})|,$$

(compare [8]). The preservation of the strong stability requires that the TV norm be nonincreasing from one step to the next. It follows that the maximum total variation change is nonpositive

$$\max_{i=1, \dots, N_t} (TV(y(t_i, x)) - TV(y(t_{i-1}, x))) \leq 0, \quad N_t = t_f / \Delta t.$$

In Figure 9 we plotted the maximum TV change for the numerical solution obtained by applying the Forward Euler method and the multistage integration methods listed in Section 4 to Problem 1 using the conservative first order upwind scheme for the spatial discretization, with $N = 100$ and $t_f = 2$. For comparison, we also reported in Figure 10 an analogous plot obtained by the Runge–Kutta methods SSP(2,2), SSPRK(3,3) and SSPRK(5,4) from [22]. Figures 9 and 10 show that, in this case, GLM2222 and GLM3333 preserve the monotonicity of the numerical solution for larger Courant numbers (and hence for larger temporal stepsize) than SSPRK(2,2) and SSPRK(3,3), respectively.

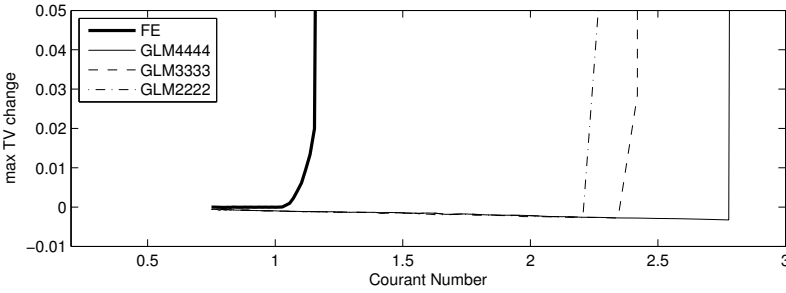


Figure 9. Maximum change of the Total Variation vs Courant Number, for the numerical solution to Problem 1, with $N = 100$ and $t_f = 2$, obtained by Forward Euler, GL2222, GL3333 and GL4444.

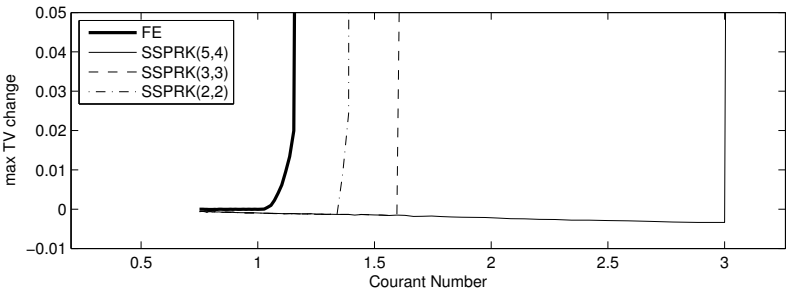


Figure 10. Maximum change of the Total Variation vs Courant Number, for the numerical solution to Problem 1, with $N = 100$ and $t_f = 2$, obtained by Forward Euler, SSPRK(2,2), SSPRK(3,3) and SSPRK(5,4).

A similar result holds for GLM4444 respect to SSPRK(5,4), if one take into account that SSPRK(5,4) has order four, but it has five stages, so the Courant number should be scaled by a factor of $4/5$. Hence SSPRK(5,4) would preserve the monotonicity of the numerical solution approximately up to an effective Courant number of 2.4 (compare [53]).

7 Concluding Remarks

We have used the monotonicity theory of general linear methods developed by Spijker [52] to construct methods which preserve the so-called strong stability property. To this aim, we systematically investigated the class of GLMs of order $p = 2, 3, 4$, stage order $q = 1, 2, \dots, p$ and such that the number of external stages r and the number of internal stages s both match the order of the method p . We also gave a characterization of methods for which $\mathbf{U} = \mathbf{I}$, and some useful necessary conditions to limit the search domain for the minimization problem (2.5) which is described in Section 2.3.

Numerical examples illustrate that the methods derived in this paper achieve the expected order of accuracy, and high stage order methods do not suffer

from the order reduction phenomenon. Moreover, under appropriate stepsize restrictions, these methods combined with appropriate spatial discretization, do not produce spurious oscillations when applied to semidiscretizations of hyperbolic conservation laws.

Future work will address the construction of implicit SSP GLMs and explicit SSP GLMs of high order, and the efficient implementation of these methods for semidiscretizations in space variables of partial differential equations.

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