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Abstract We study explicit strong stability preserving (SSP) multiderivative general linear methods (MDGLMs) for the numerical solution of hyperbolic conservation laws. Sufficient conditions for MDGLMs up to four derivatives to be SSP are determined. In this work we describe the construction of two external stages explicit SSP MDGLMs based on Taylor series conditions, and present examples of constructed methods up to order nine and three internal stages along with their SSP coefficients. It is difficult to apply these methods to the discretization of partial differential equations, as higher-order flux derivatives must be calculated analytically, but a Jacobian-free approach based on the recent development of explicit Jacobian-free multistage multiderivative solvers (Chouchoulis et al. in J Sci Comput 90:96, 2022) provides a practical application of MDGLMs. To show the capability of our novel methods in achieving the predicted order of convergence and preserving required stability properties, several numerical test cases for scalar and systems of equations are provided.

Keywords Hyperbolic conservation laws · Strong stability preserving · Multiderivative methods · General linear methods · Lax–Wendroff · Finite differences

Mathematics Subject Classification (2010) 65M06 · 65M08 · 65M12 · 35L65

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1 Introduction

In this work, we construct a novel class of high-order time integration schemes to solve one-dimensional hyperbolic conservation laws of form

$$Y_t + f(Y)_x = 0, \tag{1}$$

where Y is a conserved physical quantity and f is a flux function. The numerical approximation of such systems faces challenges when the exact solution becomes discontinuous, which can happen even if the initial profile is smooth. There exist a variety of successful approaches for developing high resolution spatial discretizations capable of handling the presence of a discontinuity and shocks, see e.g. [13,42, 45,47] and references therein for an overview. One of the most commonly used approaches in developing these schemes is the methods of lines (MOL) technique which decouples the spatial and temporal discretizations and reduces the partial differential equation (PDE) (1) to the semi-discrete form

$$y'(t) = \Phi(y). \tag{2}$$

The term $\Phi(y)$ is typically computed using a conservative spatial discretization D_x applied to the flux

$$\Phi(y) = D_x(-f(y)).$$

Commonly, used spatial discretizations have special nonlinear stability properties (e.g., total variation stability or positivity preservation) if combined with the forward Euler method. Mathematically, this means that when the semi-discretized equation (2) is advanced using a first order forward Euler method, the resulting numerical solution satisfies the following strong stability property if only the time step Δt is sufficiently small:

$$\|y^n + \Delta t \Phi(y^n)\| \leq \|y^n\|, \quad 0 \leq \Delta t \leq \Delta t_{\text{FE}}, \tag{3}$$

where $\|\cdot\|$ is a norm or semi-norm. Rather than using first-order time-stepping methods, we are interested in using higher-order time-stepping integration while still satisfying the strong stability property, i.e.,

$$\|y^{n+1}\| \leq \|y^n\|, \tag{4}$$

under a modified time-step limit, $\Delta t \leq \mathscr{C} \Delta t_{\text{FE}}$. Methods that achieve (4) under the assumption that (3) holds, are called strong stability preserving (SSP) methods [41]; the coefficient $\mathscr{C}$ is referred to as the SSP coefficient [21]. Significant effort has been put into developing different classes of SSP methods with large enough SSP coefficients, such as SSP linear multistep methods (LMMs), Runge–Kutta (RK) methods, two derivative RK methods, general linear methods (GLMs), and second derivative GLMs to maximize the SSP coefficient, see e.g. [8,14,19,20,21,24,25,26,28,31]. In this paper, we aim to explore a novel class of SSP methods with higher derivatives: explicit multiderivative general linear methods (MDGLMs) up to four derivatives. Indeed, higher derivatives of the unknown solutions y are used in the method's formulation. While GLMs rely on only evaluating Φ, for multiderivative GLMs, we also make use of the quantities[1] $\dot{\Phi}(y) := y''(t) \equiv \Phi'(y)\Phi(y)$, $\ddot{\Phi}(y) := y'''(t) \equiv \cdots$ and so on. In the case of two derivative methods, preserving just the forward Euler condition (3) is not enough, and another condition involving the second derivative is required. Considering a second derivative condition in the form

$$\|y^n + \Delta t^2 \dot{\Phi}(y^n)\| \leq \|y^n\|, \quad \Delta t \leq \widehat{\alpha} \Delta t_{\mathrm{FE}}, \tag{5}$$

Christlieb et al. [14] obtained SSP two-derivative RK methods up to order six preserving the strong stability properties of the forward Euler condition (3) along with the second derivative condition (5). Here, the constant $\widehat{\alpha} > 0$ is associated with the stability condition of the second derivative and forward Euler terms. Building upon that work, Moradi et al. [31] developed the SSP approach to construct SSP second derivative GLMs (SGLMs) as a class of multistep multistage second derivative time-stepping methods, further studied in [32, 33, 34, 35, 36]. To accomplish the present work, we use, as before, the forward Euler and second derivative conditions, but add to them Taylor series conditions for both third and fourth derivatives, and derive sufficient conditions for multiderivative GLMs to be SSP. By using multiple derivatives, the order of convergence can be increased without adding more stages. We focus on the construction of two and three stages methods up to four derivatives.

For such schemes, the calculation of temporal derivatives directly from their definition tends to be computationally prohibitive. A commonly used approach to compute these time derivatives is a Lax–Wendroff (LW) type of approach [29], which expresses temporal derivatives of the unknown function y in terms of the fluxes through the Cauchy–Kowalevskaya procedure. The main drawback of this procedure comes from the fact that it results in highly complex symbolic calculations which increase computational costs and make a modular implementation more difficult. Nevertheless, LW-methods have a great deal of potential that is well-known among researchers, and there have been considerable efforts on developing high-order variants of LW-methods for nonlinear systems. For example the ADER (Arbitrary order using Derivatives) methods attracted a lot of attention, see e.g., [16, 17, 18, 40, 43, 44] and references therein. To get rid of complex symbolic calculations of flux derivatives, Carrillo and Parés in [9] have developed the *compact approximate Taylor* (CAT) procedure based on Taylor series methods and Chouchoulis et al. in [11] extended this approach to the class of multiderivative Runge–Kutta (MDRK) methods and presented a novel collection of explicit Jacobian-free MDRK solvers for hyperbolic conservation laws. In this paper, after introducing SSP multiderivative GLMs, to avoid the necessary cumbersome calculation of flux derivatives, we extend the idea of the Jacobian-free technique to SSP multiderivative GLMs and present a new class of explicit Jacobian-free SSP multiderivative GLMs for hyperbolic conservation laws.

The structure of the paper is as follows. In Sect. 2, we introduce multiderivative GLMs for ODEs along with the necessary and sufficient conditions for such methods to be of order p and stage order q. Thereafter, in Sect. 3, sufficient conditions for multiderivative GLMs up to four derivatives to be SSP are derived and examples of constructed SSP third derivative GLMs up to order seven and SSP fourth

[1] The dot $(\cdot)$ stands for the time derivative d/dt, whereas the prime $(')$ stands for the Jacobian of the vector valued Φ w.r.t. y.

derivative GLMs up to order nine are given. After a short review of the Jacobian-free approach of the CAT method and MDRK solvers, we introduce the explicit Jacobian-free MDGLMs for hyperbolic conservation laws, referred to as CAMDGLM, in Sect. 4. To verify our theoretical results we present several numerical cases in Sect. 5. At last, we close this work with conclusions and a spotlight for future work in Sect. 6.

2 Explicit Multiderivative General Linear Methods

The class of general linear methods (GLMs) was first introduced by Butcher [5] for the numerical solution of ODEs defined by Eq. (2) in which Φ is a function of the solution variable $y \in \mathbb{R}^d$. GLMs are a large family of schemes, containing traditional methods including RK methods and LMMs. The introduction of GLMs opened the possibility of developing new methods that were neither RK methods, nor LMMs, nor minor alterations of these methods, see, for instance, [6,27].

There has been a great deal of research on numerical methods for solving systems of ODEs which use the second derivative of the solution, $y''(t) \equiv \Phi'(y)\Phi(y)$, as part of their integration formula, see, e.g., [10,12,23]. The family of second derivative general linear methods (SGLMs) was first introduced by Butcher and Hojjati in [7] and was later investigated by Abdi et al. in [1,2,3,4], just to name a few. In recent years, there has been some progress on developing a multiderivative RK framework for temporal integration, for instance see [12,14,11,37,39] and references therein. By following this direction, the main class of time-stepping methods in this work are explicit multiderivative general linear methods (MDGLMs) as a generalization of GLMs by adding extra temporal derivatives of $\Phi(y)$ up to, at most, four derivatives. It is crucial to note that these temporal derivatives can be recursively calculated via the chain rule, so that

$$\frac{\mathrm{d}^k}{\mathrm{d}t^k}\Phi(y) = \frac{\mathrm{d}^{k-1}}{\mathrm{d}t^{k-1}}\left(\Phi'(y)\Phi(y)\right).$$

Consider $0 \le t^0 < t^1 < \cdots < t^N = T_f$ to be uniform partition of the temporal domain with a fixed timestep $\Delta t = \frac{T_f - t^0}{N}$. We define MDGLMs as follows:

Definition 1 Explicit m-derivative general linear methods of order p and stage order q are r-value and s-stage methods of the form

$$Y_l^{[n]} = \sum_{\nu=1}^{r} u_{l\nu} y_\nu^{[n-1]} + \sum_{k=1}^{m} \Delta t^k \sum_{\nu=1}^{l-1} a_{l\nu}^{\{k\}} \frac{\mathrm{d}^{k-1}}{\mathrm{d}t^{k-1}} \Phi(Y_\nu^{[n]}), \quad l = 1,2,\ldots,s, \tag{6a}$$

$$y_l^{[n]} = \sum_{\nu=1}^{r} v_{l\nu} y_\nu^{[n-1]} + \sum_{k=1}^{m} \Delta t^k \sum_{\nu=1}^{s} b_{l\nu}^{\{k\}} \frac{\mathrm{d}^{k-1}}{\mathrm{d}t^{k-1}} \Phi(Y_\nu^{[n]}), \quad l = 1,2,\ldots,r. \tag{6b}$$

Here, $Y_l^{[n]}$ is an approximation of stage order q to the solution y of (2) at time $t^{n-1} + c_l \Delta t$, i.e.,

$$Y_l^{[n]} = y(t^{n-1} + c_l \Delta t) + O(\Delta t^{q+1}), \quad l = 1,2,\ldots,s. \tag{7}$$

$y_\nu^{[n-1]}$ is an approximation of order p to some linear combination of the solution y and its derivatives at time t^{n-1}, i.e.,

$$y_\nu^{[n-1]} = \sum_{\kappa=0}^{p} w_{\nu\kappa} y^{(\kappa)}(t^{n-1})\Delta t^\kappa + O(\Delta t^{p+1}), \quad \nu = 1,2,\ldots,r \tag{8}$$

for real parameters $w_{\nu\kappa}$. As the method is of order p, this implies that the output values $y_\nu^{[n]}$ fulfill

$$y_\nu^{[n]} = \sum_{\kappa=0}^{p} w_{\nu\kappa} y^{(\kappa)}(t^{n})\Delta t^\kappa + O(\Delta t^{p+1}), \quad \nu = 1,2,\ldots,r. \tag{9}$$

For the sake of convenience, we represent MDGLMs through a partitioned $(s+r)\times(ms+r)$ Butcher tableau:

$$\left[\begin{array}{c|c|c|c|c} A^{\{1\}} & A^{\{2\}} & \cdots & A^{\{m\}} & U \\ \hline B^{\{1\}} & B^{\{2\}} & \cdots & B^{\{m\}} & V \end{array}\right],$$

where $A^{\{k\}} := [a_{l\nu}^{\{k\}}]_{s\times s}$ and similarly for $B^{\{k\}}$, U and V.

2.1 Order and stage Order Conditions

To derive order conditions for the stages and the output values using a straightforward application of Taylor's theorem, let us denote the vectors

$$Z := [1\ z\ \cdots\ z^p]^T, \quad e^{cz} = [e^{c_1 z}\ e^{c_2 z}\ \cdots\ e^{c_s z}],$$

and introduce the matrix W as

$$W := [w_0\ w_1\ \cdots\ w_p],$$

with $w_\kappa := [w_{1\kappa}\ w_{2\kappa}\ \cdots\ w_{r\kappa}]^T$ for $\kappa = 0,1,\ldots,p$. The necessary and sufficient conditions for MDGLMs to be of order p and stage order $q = p$, and $q = p-1$, respectively, are given in the following theorem:

Theorem 1 *Suppose that $y_l^{[n-1]}$ satisfies* (8). *Then the m-derivative GLM* (6) *of order p and stage order $q = p$ satisfies* (7) *and* (9) *iff*

$$\begin{aligned} e^{cz} &= \sum_{k=1}^{m} z^k A^{\{k\}} e^{cz} + UWZ + O(z^{p+1}), \\ e^z WZ &= \sum_{k=1}^{m} z^k B^{\{k\}} e^{cz} + VWZ + O(z^{p+1}), \end{aligned} \tag{10}$$

and of order p and stage order $q = p-1$ satisfies (7) *and* (9) *iff*

$$\begin{aligned} e^{cz} &= \sum_{k=1}^{m} z^k A^{\{k\}} e^{cz} + UWZ \\ &\quad + \left(\frac{c^p}{p!} - \sum_{k=1}^{m} A^{\{k\}} \frac{c^{p-k}}{(p-k)!} - Uw_p \right) z^p + O(z^{p+1}), \\ e^z WZ &= \sum_{k=1}^{m} z^k B^{\{k\}} e^{cz} + VWZ + O(z^{p+1}). \end{aligned} \tag{11}$$

Here, the exponential is applied component-wise to a vector.

It should be noted that the proofs are simple generalizations of those given for SGLMs [7] and [2], and are hence neglected here. In line with what has been done for GLMs and SGLMs, it can be clarified that (10) and (11) are equivalents

$$\frac{c^\kappa}{\kappa!} - A^{\{1\}} \frac{c^{\kappa-1}}{(\kappa-1)!} - A^{\{2\}} \frac{c^{\kappa-2}}{(\kappa-2)!} - \cdots - A^{\{m\}} \frac{c^{\kappa-m}}{(\kappa-m)!} - Uw_\kappa = 0, \quad \kappa = 0,1,\ldots,q,$$

and

$$\sum_{j=0}^{\kappa} \frac{w_{\kappa-j}}{j!} - B^{\{1\}} \frac{c^{\kappa-1}}{(\kappa-1)!} - B^{\{2\}} \frac{c^{\kappa-2}}{(\kappa-2)!} - \cdots - B^{\{m\}} \frac{c^{\kappa-m}}{(\kappa-m)!} - Vw_\kappa = 0, \quad \kappa = 0,1,\ldots,p,$$

for $q = p$ or $q = p-1$, respectively.

3 SSP conditions for Multiderivative GLMs

3.1 Monotonicity theory for Multiderivative GLMs

Following the formulation of SGLMs introduced in [31], to determine sufficient conditions for multiderivative GLMs (6) to be SSP, we reformulate (6) as

$$\begin{aligned} Y_l^{[n]} &= \sum_{\nu=1}^{r} s_{l\nu} y_\nu^{[n-1]} + \sum_{k=1}^{m} \Delta t^k \sum_{\nu=1}^{s+r} t_{l\nu}^{\{k\}} \frac{\mathrm{d}^{k-1}}{\mathrm{d}t^{k-1}} \Phi(Y_\nu^{[n]}), \quad l = 1,2,\ldots,s+r, \\ y_l^{[n]} &= Y_{s+l}^{[n]}, \quad l = 1,2,\ldots,r, \end{aligned} \tag{12}$$

where $n = 1,2,\ldots,N$. This method is characterized by the matrices $T^{\{k\}} = [t_{l\nu}^{\{k\}}] \in \mathbb{R}^{(s+r)\times(s+r)}$, $k = 1,2,\ldots,m$, and $S = [s_{l\nu}] \in \mathbb{R}^{(s+r)\times r}$ defined by

$$T^{\{k\}} = \begin{pmatrix} A^{\{k\}} & \mathbf{0} \\ B^{\{k\}} & \mathbf{0} \end{pmatrix}, \quad \text{and} \quad S = \begin{pmatrix} U \\ V \end{pmatrix}.$$

In a similar manner to [26,31], we assume that the components of the matrix S fulfill the condition

$$\sum_{\nu=1}^{r} s_{l\nu} = 1, \quad l = 1,2,\ldots,s+r.$$

We will say that an explicit m-derivative GLM (12) is monotonic if

$$\left\|Y_l^{[n]}\right\| \leq \max_{1\leq \nu \leq r} \left\|y_\nu^{[n-1]}\right\|, \quad \text{for} \quad l = 1,2,\ldots,s+r. \tag{13}$$

To obtain the strong stability conditions for multiderivative GLMs up to four derivatives, let us to introduce the vector

$$\Phi(Y^{[n]}) := \left[\Phi(Y_1^{[n]})^T \quad \Phi(Y_2^{[n]})^T \quad \cdots \quad \Phi(Y_{s+r}^{[n]})^T\right]^T, \quad k = 1,2,\ldots,m,$$

and similarly for $\frac{\mathrm{d}^{k-1}}{\mathrm{d}t^{k-1}}\Phi(Y^{[n]})$. To preserve (13), the forward Euler condition (3) and the second derivative condition (5) are needed together with two further conditions that include third- and fourth-order temporal derivatives. These are given as Taylor series conditions, i.e.,

$$\left\|Y^{[n]} + \Delta t \Phi(Y^{[n]}) + \frac{\Delta t^2}{2}\dot{\Phi}(Y^{[n]}) + \frac{\Delta t^3}{6}\ddot{\Phi}(Y^{[n]})\right\| \leq \left\|Y^{[n]}\right\|, \quad \forall \Delta t \leq \overline{\alpha}\Delta t_{\mathrm{FE}} \tag{14}$$

and

$$\left\|Y^{[n]} + \Delta t \Phi(Y^{[n]}) + \frac{\Delta t^2}{2}\dot{\Phi}(Y^{[n]}) + \frac{\Delta t^3}{6}\ddot{\Phi}(Y^{[n]}) + \frac{\Delta t^4}{24}\dddot{\Phi}(Y^{[n]})\right\| \leq \left\|Y^{[n]}\right\|, \quad \forall \Delta t \leq \widetilde{\alpha}\Delta t_{\mathrm{FE}}. \tag{15}$$

Here, $\overline{\alpha}$, and $\widetilde{\alpha}$ are scaling factors that compare the stability condition of the m-derivative method, for $m = 3$ and $m = 4$ respectively, to that of the forward Euler method. Using these conditions, we are able to formulate sufficient conditions so that a fourth-derivative GLM satisfies the desired monotonicity condition under a given timestep.

Theorem 2 *Given spatial discretizations Φ, $\dot{\Phi}$, $\ddot{\Phi}$ and $\dddot{\Phi}$ that satisfy the forward Euler condition* (3)*, the second derivative condition* (5) *and Taylor series conditions* (14) *and* (15)*, respectively, a multiderivative GLM of the form* (12) *with $m = 4$ preserves the strong stability property $\left\|Y^{[n+1]}\right\| \leq \left\|Y^{[n]}\right\|$ under the timestep restriction $\Delta t \leq \beta \Delta t_{\mathrm{FE}}$ if it satisfies the conditions*

$$\begin{aligned}
&\mathbf{R}S \geq 0,\\
&\beta\mathbf{R}\left(T^{\{1\}} - 6\tfrac{\beta^2}{\overline{\alpha}^2}T^{\{3\}} + 24\tfrac{\beta}{\widetilde{\alpha}}\left(\tfrac{\beta^2}{\overline{\alpha}^2} - \tfrac{\beta^2}{\widetilde{\alpha}^2}\right)T^{\{4\}}\right) \geq 0,\\
&\tfrac{\beta^2}{\widehat{\alpha}^2}\mathbf{R}\left(T^{\{2\}} - 3\tfrac{\beta}{\overline{\alpha}}T^{\{3\}} + 12\tfrac{\beta}{\widetilde{\alpha}}\left(\tfrac{\beta}{\overline{\alpha}} - \tfrac{\beta}{\widetilde{\alpha}}\right)T^{\{4\}}\right) \geq 0,\\
&6\tfrac{\beta^3}{\overline{\alpha}^3}\mathbf{R}\left(T^{\{3\}} - 4\tfrac{\beta}{\widetilde{\alpha}}T^{\{4\}}\right) \geq 0,\\
&24\tfrac{\beta}{\widetilde{\alpha}^4}\mathbf{R}T^{\{4\}} \geq 0,
\end{aligned} \tag{16}$$

where

$$\mathbf{R} = \left(I + \beta T^{\{1\}} + \frac{\beta^2}{\widehat{\alpha}}T^{\{2\}} + 3\frac{\beta^3}{\overline{\alpha}^3\widehat{\alpha}^2}\left(2\widehat{\alpha}^2 - 2\overline{\alpha}\widehat{\alpha}^2 - \overline{\alpha}^2\right)T^{\{3\}} + \left(24\frac{\beta^4(1-\widetilde{\alpha})}{\widetilde{\alpha}^4} + 12\frac{\beta^4(\widetilde{\alpha}-\overline{\alpha})}{\overline{\alpha}\widehat{\alpha}^2\widetilde{\alpha}^2} + 24\frac{\beta^4(\overline{\alpha}-1)}{\widetilde{\alpha}\overline{\alpha}^3}\right)T^{\{4\}}\right)^{-1},$$

for some $\beta > 0$. In the above conditions, the inequalities are to be understood component-wise.

Proof. Considering the method (12) with $m = 4$ and adding $\beta T^{\{1\}}Y^{[n]}$, $\widehat{\beta}^2 T^{\{2\}}Y^{[n]}$, $\left(6\overline{\beta}^3 - 6\beta\overline{\beta}^2 - 3\widehat{\beta}^2\overline{\beta}\right) T^{\{3\}}Y^{[n]}$, and $\left(24\widetilde{\beta}^3(\widetilde{\beta}-\beta) + 12\widetilde{\beta}\widehat{\beta}^2(\overline{\beta}-\widetilde{\beta}) + 24\widetilde{\beta}\overline{\beta}^2(\beta-\overline{\beta})\right) T^{\{4\}}Y^{[n]}$ to both sides, results in

$$
\begin{aligned}
&\Big(I + \beta T^{\{1\}} + \widehat{\beta}^2 T^{\{2\}} + \left(6\overline{\beta}^3 - 6\beta\overline{\beta}^2 - 3\widehat{\beta}^2\overline{\beta}\right) T^{\{3\}} \\
&+ \left(24\widetilde{\beta}^3(\widetilde{\beta}-\beta) + 12\widetilde{\beta}\widehat{\beta}^2(\overline{\beta}-\widetilde{\beta}) + 24\widetilde{\beta}\overline{\beta}^2(\beta-\overline{\beta})\right) T^{\{4\}}\Big) Y^{[n]} \\
=&Sy^{[n-1]} + \beta\left(T^{\{1\}} - 6\overline{\beta}^2 T^{\{3\}} + 24\widetilde{\beta}(\overline{\beta}^2 - \widetilde{\beta}^2)T^{\{4\}}\right)\left(Y^{[n]} + \frac{\Delta t}{\beta}\Phi(Y^{[n]})\right) \\
&+ \widehat{\beta}^2\left(T^{\{2\}} - 3\overline{\beta}T^{\{3\}} + 12\widetilde{\beta}(\overline{\beta}-\widetilde{\beta})T^{\{4\}}\right)\left(Y^{[n]} + \frac{\Delta t^2}{\widehat{\beta}^2}\dot{\Phi}(Y^{[n]})\right) \\
&+ 6\overline{\beta}^3\left(T^{\{3\}} - 4\widetilde{\beta}T^{\{4\}}\right)\left(Y^{[n]} + \frac{\Delta t}{\overline{\beta}}\Phi(Y^{[n]}) + \frac{\Delta t^2}{2\overline{\beta}^2}\dot{\Phi}(Y^{[n]}) + \frac{\Delta t^3}{6\overline{\beta}^3}\ddot{\Phi}(Y^{[n]})\right) \\
&+ 24\widetilde{\beta}^4 T^{\{4\}}\left(Y^{[n]} + \frac{\Delta t}{\widetilde{\beta}}\Phi(Y^{[n]}) + \frac{\Delta t^2}{2\widetilde{\beta}^2}\dot{\Phi}(Y^{[n]}) + \frac{\Delta t^3}{6\widetilde{\beta}^3}\ddot{\Phi}(Y^{[n]}) + \frac{\Delta t^4}{24\widetilde{\beta}^4}\dddot{\Phi}(Y^{[n]})\right).
\end{aligned}
$$

Supposing that the matrix in front of $Y^{[n]}$ on the left-hand side is invertible and setting

$$
\begin{aligned}
\mathbf{R} =& \Big(I + \beta T^{\{1\}} + \widehat{\beta}^2 T^{\{2\}} + \left(6\overline{\beta}^3 - 6\beta\overline{\beta}^2 - 3\widehat{\beta}^2\overline{\beta}\right) T^{\{3\}} \\
&+ \left(24\widetilde{\beta}^3(\widetilde{\beta}-\beta) + 12\widetilde{\beta}\widehat{\beta}^2(\overline{\beta}-\widetilde{\beta}) + 24\widetilde{\beta}\overline{\beta}^2(\beta-\overline{\beta})\right) T^{\{4\}}\Big)^{-1}, \\
\mathbf{G} =& \beta\mathbf{R}\left(T^{\{1\}} - 6\overline{\beta}^2 T^{\{3\}} + 24\widetilde{\beta}(\overline{\beta}^2 - \widetilde{\beta}^2)T^{\{4\}}\right), \\
\mathbf{H} =& \widehat{\beta}^2\mathbf{R}\left(T^{\{2\}} - 3\overline{\beta}T^{\{3\}} + 12\widetilde{\beta}(\overline{\beta}-\widetilde{\beta})T^{\{4\}}\right), \\
\mathbf{J} =& 6\overline{\beta}^3\mathbf{R}\left(T^{\{3\}} - 4\widetilde{\beta}T^{\{4\}}\right), \quad \mathbf{L} = 24\widetilde{\beta}^4\mathbf{R}T^{\{4\}},
\end{aligned}
$$

we obtain

$$
\begin{aligned}
Y^{[n]} =& \mathbf{R}Sy^{[n-1]} + \mathbf{G}\left(Y^{[n]} + \frac{\Delta t}{\beta}\Phi(Y^{[n]})\right) + \mathbf{H}\left(Y^{[n]} + \frac{\Delta t^2}{\widehat{\beta}^2}\dot{\Phi}(Y^{[n]})\right)\\
&+\mathbf{J}\left(Y^{[n]} + \frac{\Delta t}{\overline{\beta}}\Phi(Y^{[n]}) + \frac{\Delta t^2}{2\overline{\beta}^2}\dot{\Phi}(Y^{[n]}) + \frac{\Delta t^3}{6\overline{\beta}^3}\ddot{\Phi}(Y^{[n]})\right)\\
&+\mathbf{L}\left(Y^{[n]} + \frac{\Delta t}{\widetilde{\beta}}\Phi(Y^{[n]}) + \frac{\Delta t^2}{2\widetilde{\beta}^2}\dot{\Phi}(Y^{[n]}) + \frac{\Delta t^3}{6\widetilde{\beta}^3}\ddot{\Phi}(Y^{[n]}) + \frac{\Delta t^4}{24\widetilde{\beta}^4}\dddot{\Phi}(Y^{[n]})\right).
\end{aligned}
$$

An easy computation shows that $\mathbf{R}+\mathbf{G}+\mathbf{H}+\mathbf{J}+\mathbf{L}=I$. In combination with the fact that the elements of $\mathbf{G}$, $\mathbf{H}$, $\mathbf{J}$, $\mathbf{L}$ and $\mathbf{R}S$ are all non-negative, and using

$$
\|Sy^{n-1}\| \le \sum_{\nu=1}^{r} s_{l\nu} \max_j \|y_j^{[n-1]}\| \le \max_j \|y_j^{[n-1]}\|, \quad l = 1,2,\ldots,s+r,
$$

these five terms describe a convex combination of terms which are SSP, and the resulting value is SSP as well:

$$
\begin{aligned}
\left\|Y^{[n]}\right\| \le& \mathbf{R}S\left\|y^{[n-1]}\right\| + \mathbf{G}\left\|Y^{[n]} + \frac{\Delta t}{\beta}\Phi(Y^{[n]})\right\| + \mathbf{H}\left\|Y^{[n]} + \frac{\Delta t^2}{\widehat{\beta}^2}\dot{\Phi}(Y^{[n]})\right\|\\
&+\mathbf{J}\left\|Y^{[n]} + \frac{\Delta t}{\overline{\beta}}\Phi(Y^{[n]}) + \frac{\Delta t^2}{2\overline{\beta}^2}\dot{\Phi}(Y^{[n]}) + \frac{\Delta t^3}{6\overline{\beta}^3}\ddot{\Phi}(Y^{[n]})\right\|\\
&+\mathbf{L}\left\|Y^{[n]} + \frac{\Delta t}{\widetilde{\beta}}\Phi(Y^{[n]}) + \frac{\Delta t^2}{2\widetilde{\beta}^2}\dot{\Phi}(Y^{[n]}) + \frac{\Delta t^3}{6\widetilde{\beta}^3}\ddot{\Phi}(Y^{[n]}) + \frac{\Delta t^4}{24\widetilde{\beta}^4}\dddot{\Phi}(Y^{[n]})\right\|,
\end{aligned}
$$

under the time-step restrictions $\Delta t \le \beta\Delta t_{\mathrm{FE}}$, $\Delta t \le \widehat{\alpha}\widehat{\beta}\Delta t_{\mathrm{FE}}$, $\Delta t \le \overline{\alpha}\overline{\beta}\Delta t_{\mathrm{FE}}$ and $\Delta t \le \widetilde{\alpha}\widetilde{\beta}\Delta t_{\mathrm{FE}}$. Equating these four timestep restrictions leads to the optimal timestep, i.e., we require $\beta = \widehat{\alpha}\widehat{\beta} = \overline{\alpha}\overline{\beta} = \widetilde{\alpha}\widetilde{\beta}$. Therefore, for $\widehat{\beta} = \frac{\beta}{\widehat{\alpha}}$, $\overline{\beta} = \frac{\beta}{\overline{\alpha}}$, and $\widetilde{\beta} = \frac{\beta}{\widetilde{\alpha}}$, the SSP conditions (16) ensure that $\mathbf{G}\ge 0$, $\mathbf{H}\ge 0$, $\mathbf{J}\ge 0$, $\mathbf{L}\ge 0$ and $\mathbf{R}S \ge 0$ component-wise and the method (12) with $m=4$ preserves the strong stability condition $\left\|Y^{[n+1]}\right\| \le \left\|Y^{[n]}\right\|$ under the timestep restriction $\Delta t \le \beta\Delta t_{\mathrm{FE}}$. □

This theorem provides sufficient conditions for fourth-derivative GLMs to be SSP for any $\Delta t \le \beta\Delta t_{\mathrm{FE}}$. It should be noted that SSP conditions for third-derivative GLMs can be derived by setting $T^{\{4\}} = 0$ in (16). Similar to [14,31], the search for optimal SSP MDGLMs can be cast into an optimization problem with the aim of maximizing the SSP coefficient $\mathscr{C} = \max\beta$ subject to the SSP conditions (16) and order conditions (10) (for methods of order $p=q$) or (11) (for methods of order $p=q+1$) as inequality and equality constraints, respectively.

3.2 **Optimal SSP Multiderivative GLMs**

In this section, we develop optimal SSP third- and fourth-derivative GLMs and their corresponding SSP coefficients. The value of the SSP coefficient $\mathscr{C}$ is a function of the parameters $\widehat{\alpha}$, $\overline{\alpha}$ and $\widetilde{\alpha}$, which depend on the spatial discretizations for the first, second, third and fourth derivatives. Following the existing publications on SSP second derivative methods, e.g. in [14], we consider the convection equation $Y_t = Y_x$. Φ is defined to be the original first-order upwind method

$$\Phi(y^n)_i := \frac{y^n_{i+1} - y^n_i}{\Delta x} \approx Y_x(x_i),$$

and $\dot{\Phi}$ is defined via the second order centered discretization to Y_{xx} as

$$\dot{\Phi}(y^n)_i := \frac{y^n_{i+1} - 2y^n_i + y^n_{i-1}}{\Delta x^2} \approx Y_{xx}(x_i).$$

Both approaches were proved to be total variation diminishing (TVD) [14] in the following sense:

$$y^{n+1} = y^n + \Delta t \Phi(y^n), \qquad \text{is TVD for} \qquad \Delta t \leq \Delta x \tag{17}$$

$$y^{n+1} = y^n + \Delta t^2 \dot{\Phi}(y^n), \qquad \text{is TVD for} \qquad \Delta t \leq \frac{\sqrt{2}}{2}\Delta x. \tag{18}$$

To determine the values of $\overline{\alpha}$ and $\widetilde{\alpha}$ for the same problem, we consider the following discretization schemes to approximate third- and fourth-order temporal derivatives

$$\ddot{\Phi}(y^n)_i = \frac{y^n_{i+2} - 3y^n_{i+1} + 3y^n_i - y^n_{i-1}}{\Delta x^3} \approx Y_{xxx}(x_i),$$

$$\dddot{\Phi}(y^n)_i = \frac{y^n_{i+2} - 4y^n_{i+1} + 6y^n_i - 4y^n_{i-1} + y^n_{i-2}}{\Delta x^4} \approx Y_{xxxx}(x_i).$$

Using these discretizations, we can directly compute the values of $\overline{\alpha}$ and $\widetilde{\alpha}$ for which the Taylor series conditions (14) and (15) are TVD. That is, with $\widetilde{\alpha} := \frac{\Delta t}{\Delta x} \geq 0$, for the fourth-derivative Taylor series condition, we observe that

$$\begin{aligned}\|y^{n+1}\|_{TV} =& \Bigg\| \left(\frac{\widetilde{\alpha}^3}{6} + \frac{\widetilde{\alpha}^4}{24}\right) y^n_{i+2} + \left(\widetilde{\alpha} + \frac{\widetilde{\alpha}^2}{2} - \frac{\widetilde{\alpha}^3}{2} - \frac{\widetilde{\alpha}^4}{6}\right) y^n_{i+1} \\ &+ \left(1 - \widetilde{\alpha} - \widetilde{\alpha}^2 + \frac{\widetilde{\alpha}^3}{2} + \frac{\widetilde{\alpha}^4}{4}\right) y^n_i + \left(\frac{\widetilde{\alpha}^2}{2} - \frac{\widetilde{\alpha}^3}{6} - \frac{\widetilde{\alpha}^4}{6}\right) y^n_{i-1} + \frac{\widetilde{\alpha}^4}{24} y^n_{i-2} \Bigg\|_{TV} \\ \leq& \|y^n\|_{TV}\end{aligned}$$

provided that

$$\left.\begin{aligned} &\widetilde{\alpha} + \tfrac{\widetilde{\alpha}^2}{2} - \tfrac{\widetilde{\alpha}^3}{2} - \tfrac{\widetilde{\alpha}^4}{6} \geq 0, \\ &1 - \widetilde{\alpha} - \widetilde{\alpha}^2 + \tfrac{\widetilde{\alpha}^3}{2} + \tfrac{\widetilde{\alpha}^4}{4} \geq 0, \\ &\tfrac{\widetilde{\alpha}^2}{2} - \tfrac{\widetilde{\alpha}^3}{6} - \tfrac{\widetilde{\alpha}^4}{6} \geq 0, \end{aligned}\right\} \Longleftrightarrow \widetilde{\alpha} \leq 0.73205....$$

In a similar way, setting $\overline{\alpha} := \frac{\Delta t}{\Delta x}$ and plugging the above definitions of Φ, $\dot{\Phi}$ and $\ddot{\Phi}$ into the third-order Taylor condition (14), we have

$$\left.\begin{aligned} &\overline{\alpha} + \frac{\overline{\alpha}^2}{2} - \frac{\overline{\alpha}^3}{2} \geq 0, \\ &1 - \overline{\alpha} - \overline{\alpha}^2 + \frac{\overline{\alpha}^3}{2} \geq 0, \\ &\frac{\overline{\alpha}^2}{2} - \frac{\overline{\alpha}^3}{6} \geq 0, \end{aligned}\right\} \Longleftrightarrow \overline{\alpha} \leq 0.68889....$$

Considering the values of $\widehat{\alpha} = \frac{\sqrt{2}}{2}$, $\overline{\alpha} = 0.68889$ and $\widetilde{\alpha} = 0.73205$ we are able to derive SSP third-derivative GLMs (when $T^{\{4\}} = 0$) and fourth-derivative GLMs by solving an optimization problem with objective function of the form

$$\min \ -\beta, \tag{19}$$

subject to inequality constraints corresponding to the SSP conditions (16), depending on the value of β and the coefficients matrices of the methods, and equality constraints corresponding to the order and stage order conditions (10) (for methods of order $p = q$) or (11) (for methods of order $p = q+1$). In this work, we restrict our attention to MDGLMs (12) with $s = 2$ and $s = 3$ internal stages and $r = 2$ external stages of order p, with stage order $q = p$ and $q = p-1$. We assume that the matrices $A^{\{k\}} \in \mathbb{R}^{s\times s}$, $k = 1,2,\ldots,m$, are strictly lower triangular, i.e.,

$$A^{\{k\}} = \begin{bmatrix} 0 & & & & \\ a_{21}^{\{k\}} & 0 & & & \\ \vdots & \ddots & \ddots & & \\ a_{s-1,1}^{\{k\}} & \ddots & \ddots & 0 & \\ a_{s,1}^{\{k\}} & a_{s,2}^{\{k\}} & \cdots & a_{s,s-1}^{\{k\}} & 0 \end{bmatrix}.$$

To ensure zero-stability, we also assume that the matrix V is a rank one matrix of the form $V = ev^T$ with $e = [1\ 1]^T$, $v = [v_1\ v_2]^T$ and $v^T e = 1$. Solving the optimization problem (19) using the MATLAB function `fmincon` choosing the sequential programming ("sqp") algorithm, we derive two external stages SSP third-derivative GLMs of order $p = q = 4,5$ with $s = 2$ and of order $p = q+1 = 6,7$ with $s = 3$, and fourth-derivative GLMs of order $p = q = 4,5,6$, $p = q+1 = 7$ with $s = 2$, and of order $p = q+1 = 6,7,8,9$ with $s = 3$. In Table 1, we report the obtained values of SSP coefficients for the constructed SSP third-derivative and fourth-derivative GLMs referred to as SSP 3DGLM and SSP 4DGLM, respectively, together with those for second derivative GLMs obtained in [31] referred to by SSP 2DGLM. In this table, dashes indicate that such methods cannot be constructed due to the lack of free parameters for solving order and stage order conditions. The coefficients can be found in MATLAB code at https://www.uhasselt.be/nl/wie-is-wie/jochen-schuetz under "Codes developed in my group"; they are also available upon request mailto: afsaneh.moradi@univaq.it.

Table 1: SSP coefficients of the two and three stages SSP second, third and fourth derivative GLMs of order p and stage order $q=p$ and $q=p-1$.

$p=$	$q=$	SSP 2DGLM	SSP 3DGLM	SSP 4DGLM
$s=2$				
4	4	0.738	1.116	1.436
5	5	–	0.755	1.223
6	6	–	–	1.013
7	6	–	–	0.775
$s=3$				
6	5	–	0.589	1.819
7	6	–	0.282	1.344
8	7	–	–	0.826
9	8	–	–	0.328

4 Multiderivative GLMs for Hyperbolic Conservation Laws

On the uniform partition of the domain Ω with M cells of the size Δx, i.e., $\{x_1,\dots,x_M\}$, multiderivative GLMs (6) applied to Eq. (1) can be expressed as

$$Y_{i,l}^{[n]} = \sum_{\nu=1}^{r} u_{l\nu} y_{i,\nu}^{[n-1]} - \sum_{k=1}^{m} \Delta t^k \sum_{\nu=1}^{l-1} a_{l\nu}^{\{k\}} D_x D_t^{k-1} f(Y_{i,\nu}^{[n]}), \qquad l=1,2,\dots,s, \tag{20a}$$

$$y_{i,l}^{[n]} = \sum_{\nu=1}^{r} v_{l\nu} y_{i,\nu}^{[n-1]} - \sum_{k=1}^{m} \Delta t^k \sum_{\nu=1}^{s} b_{l\nu}^{\{k\}} D_x D_t^{k-1} f(Y_{i,\nu}^{[n]}), \qquad l=1,2,\dots,r, \tag{20b}$$

where $n=1,2,\dots,N$, and $i=1,2,\dots,M$. Here, D_x and D_t stand for suitable approximations of ∂_x and ∂_t. This section aims to avoid using Jacobians of the flux function f that occur as a result of higher temporal derivatives used in the formulation of our methods. To do this, we follow the Jacobian-free technique outlined in [11]. This technique is based on the compact approximate Taylor (CAT) approach proposed in [9] as an extension to the work in [48]. These techniques heavily rely on discrete differentiation. In what follows, we introduce the required notations and describe the Jacobian-free technique when applied to MDGLMs (20) in the sequel.

4.1 Discrete Differentiation

The aim of this part is to fix some notation on using finite differences similar as in [9, 11]. We will use two families of interpolatory formulas: the numerical approximations for the k-th derivative based on $(2\overline{p}+1)$-point stencils and $2\overline{p}$-point stencils.

Assuming that $\{x_i\}$ are the points of a uniform mesh of step Δx, the first family based on a $(2\overline{p}+1)$-point stencil is given by

$$(\mathscr{P}_i \varphi)^{(k)}(x_i) := \frac{1}{\Delta x^k} \sum_{j=-\overline{p}}^{\overline{p}} \delta_{\overline{p},j}^{k} \varphi(x_{i+j}), \tag{21}$$

where $\mathscr{P}_i\varphi$ are the Lagrangian interpolation polynomials of degree $2\overline{p}$ interpolating $\varphi:\mathbb{R}\to\mathbb{R}$ at the $2\overline{p}+1$ points $x_{i-\overline{p}},\dots,x_{i+\overline{p}}$; and $\delta_{\overline{p},j}^{k}$ are related to the Lagrange polynomials

$$L_{\overline{p},j}(\omega) := \prod_{\substack{r=-\overline{p}\\ r\neq j}}^{\overline{p}} \frac{\omega - r}{j - r}, \quad j = -\overline{p}, \ldots, \overline{p}. \tag{22}$$

through

$$\delta^k_{\overline{p},j} := L^{(k)}_{\overline{p},j}(0), \quad j = -\overline{p}, \ldots, \overline{p}.$$

We will also use the following numerical differentiation formulas based on a $2\overline{p}$-point stencil,

$$(\mathscr{Q}_i \varphi)^{(k)}(x_{i+\mathbf{m}}) := \frac{1}{\Delta x^k} \sum_{j=-\overline{p}+1}^{\overline{p}} \gamma^{k,\mathbf{m}}_{\overline{p},j} \varphi(x_{i+j}), \tag{23}$$

that approximate the k-th derivative at the points $x_i + \mathbf{m}\Delta x$, $\mathbf{m} = -\overline{p}+1, \ldots, \overline{p}$. Here, $\mathscr{Q}_i\varphi$ are the Lagrangian interpolation polynomials of degree $2\overline{p}-1$ interpolating φ at the $2\overline{p}$ points $x_{i-\overline{p}+1}, \ldots, x_{i+\overline{p}}$, and $\gamma^{k,\mathbf{m}}_{\overline{p},j}$ are related to the Lagrange polynomials

$$\ell_{\overline{p},j}(\omega) := \prod_{\substack{r=-\overline{p}+1\\ r\neq j}}^{\overline{p}} \frac{\omega - r}{j - r}, \quad j = -\overline{p}+1, \ldots, \overline{p} \tag{24}$$

through

$$\gamma^{k,\mathbf{m}}_{\overline{p},j} := \ell^{(k)}_{\overline{p},j}(\mathbf{m}), \quad j, \mathbf{m} = -\overline{p}+1, \ldots, \overline{p}.$$

The corresponding linear operators to Eqs. (21) and (23) are defined by

$$P^{(k)} : \mathbb{R}^{2\overline{p}+1} \to \mathbb{R}, \quad \mathbf{v} \mapsto \frac{1}{\Delta x^k} \sum_{j=-\overline{p}}^{\overline{p}} \delta^k_{\overline{p},j} v_j,$$

$$Q^{(k)}_{\mathbf{m}} : \mathbb{R}^{2\overline{p}} \to \mathbb{R}, \quad \mathbf{w} \mapsto \frac{1}{\Delta x^k} \sum_{j=-\overline{p}+1}^{\overline{p}} \gamma^{k,\mathbf{m}}_{\overline{p},j} w_j.$$

In order to have the method in conservation form, auxiliary centered coefficients $\lambda^{k-1}_{\overline{p},j}$ have been introduced in [48] via the relations

$$\begin{aligned}
\delta^k_{\overline{p},\overline{p}} &=: \lambda^{k-1}_{\overline{p},\overline{p}}, \\
\delta^k_{\overline{p},j} &=: \lambda^{k-1}_{\overline{p},j} - \lambda^{k-1}_{\overline{p},j+1}, \quad j = -\overline{p}+1, \ldots, \overline{p}-1, \\
\delta^k_{\overline{p},-\overline{p}} &=: -\lambda^{k-1}_{\overline{p},-\overline{p}+1}.
\end{aligned}$$

Considering these auxiliary centered coefficients allows for an alternative form for (21) as differences of new 'half-way point' interpolation operators:

$$(\mathscr{P}_i \varphi)^{(k)}(x_i) = \frac{\left(\Lambda^{(k-1)}\varphi\right)(x_{i+1/2}) - \left(\Lambda^{(k-1)}\varphi\right)(x_{i-1/2})}{\Delta x}, \tag{25}$$

with $\Lambda^{(k-1)}$ as an operator mapping to $\mathbb{P}_{2\overline{p}-1}$ given by

$$\left(\Lambda^{(k-1)}\varphi\right)(x_{i+1/2}) := \frac{1}{\Delta x^{k-1}} \sum_{j=-\overline{p}+1}^{\overline{p}} \lambda^{k-1}_{\overline{p},j} \varphi(x_{i+j}). \tag{26}$$

For a detailed description of interpolation operators we refer to [9, 11] and the references therein.

4.2 Jacobian-free MDGLMs

With the aim of assembling the class of compact approximate MDGLMs (CAMDGLMs), we define the conservative form of the solution via

$$Y_{i,l}^{[n]} := \sum_{\nu=1}^{r} u_{l\nu} y_{i,\nu}^{[n-1]} - \frac{\Delta t}{\Delta x}\left(\widetilde{F}_{i+1/2,l}^{[n]} - \widetilde{F}_{i-1/2,l}^{[n]}\right), \quad l = 1,2,\ldots,s, \tag{27a}$$

$$y_{i,l}^{[n]} := \sum_{\nu=1}^{r} v_{l\nu} y_{i,\nu}^{[n-1]} - \frac{\Delta t}{\Delta x}\left(F_{i+1/2,l}^{[n]} - F_{i-1/2,l}^{[n]}\right), \quad l = 1,2,\ldots,r, \tag{27b}$$

where the numerical fluxes are given by

$$\widetilde{F}_{i+1/2,l}^{[n]} = \sum_{k=1}^{m} \Delta t^{k-1} \sum_{\nu=1}^{l-1} a_{l\nu}^{\{k\}} \Lambda^{(0)} (\widetilde{\mathbf{f}}^{\nu})_{i,\langle 0\rangle}^{(k-1)}, \quad l = 1,2,\ldots,s \tag{28a}$$

$$F_{i+1/2,l}^{[n]} = \sum_{k=1}^{m} \Delta t^{k-1} \sum_{\nu=1}^{s} b_{l\nu}^{\{k\}} \Lambda^{(0)} (\widetilde{\mathbf{f}}^{\nu})_{i,\langle 0\rangle}^{(k-1)}, \quad l = 1,2,\ldots,r. \tag{28b}$$

Here, the angled brackets stand for the local stencil function

$$\langle\cdot\rangle : \mathbb{Z} \to \mathbb{Z}^{2\overline{p}} : w \mapsto (w - \overline{p} + 1, \ldots, w + \overline{p})^T,$$

and will be used for both the spatial index i and temporal index n. As in [11], to compute $\widetilde{\mathbf{f}}_{i,\langle 0\rangle}^{(k-1)}$ we use the compact approximate Taylor (CAT) procedure [9] and hence, the flux derivatives are computed by the linear operator alternative of (25) determined by

$$\Lambda^{(0)} \widetilde{\mathbf{f}}_{i,\langle 0\rangle}^{(k-1)} := \sum_{j=-\overline{p}+1}^{\overline{p}} \lambda_{\overline{p},j}^{0} \widetilde{\mathbf{f}}_{i,j}^{(k-1)},$$

in which

$$\widetilde{\mathbf{f}}_{i,j}^{(k-1)} := Q_0^{(k-1)} (\mathfrak{f}_T)_{i,j}^{k-1,\langle n\rangle}, \quad j = -\overline{p}+1, \ldots, \overline{p}$$

are local approximations for the temporal derivatives of the flux and depend on the approximate flux values $(\mathfrak{f}_T)_{i,j}^{k-1,n+r} \approx f(Y_{i+j}^{[n+r]})$. Indeed, the following approximate flux is taken to approximately evaluate the $(k-1)$-st discrete temporal derivative in x_{i+j}:

$$(\mathfrak{f}_T)_{i,j}^{k-1,n+r} := f\left(Y_{i+j}^{[n]} + \sum_{\ell=1}^{k-1} \frac{(r\Delta t)^{\ell}}{\ell!} \widetilde{Y}_{i,j}^{(\ell)}\right), \qquad j, r = -\overline{p}+1, \ldots, \overline{p}.$$

All that remains to be defined are the quantities $\widetilde{Y}_{i,j}^{(\ell)} \approx \frac{\partial^{\ell}}{\partial t^{\ell}} Y_{i+j}^{[n]}$. To do this, we make use of the CauchyKovalevskaya identity

$$\partial_t^{\ell} y = -\partial_x \partial_t^{\ell-1} f(y),$$

so we have

$$\widetilde{Y}_{i,j}^{(\ell)} := -Q_j^{(1)} \widetilde{\mathbf{f}}_{i,\langle 0\rangle}^{(\ell-1)}, \quad j = -\overline{p}+1, \ldots, \overline{p}.$$

A summary of the compact approximate mDGLMp-s procedure to obtain the stage values is provided in Alg. 1. It should be noted that the flux at the left half-way point is determined by a shift of the index, i.e. $\widetilde{F}^{[n]}_{i-1/2,l} = \widetilde{F}^{[n]}_{i-1+1/2,l}$ or is given by the boundary condition.

Algorithm 1 Stages of compact approximate mDGLMp-s, an m-derivative, p-th order, s-stage CAMDGLM

Stage solution ($l = 2,\dots,s$):

for $j = -\overline{p}+1$ **to** $\overline{p}$ **do**

$\quad (\widetilde{f}^{l-1})^{(0)}_{i,j} = f(Y^{[n]}_{i+j,l})$

end

$\widetilde{F}^{[n]}_{i+1/2,l} = \sum_{\nu=1}^{l-1} a^{\{1\}}_{l\nu} \Lambda^{(0)} (\widetilde{\mathbf{f}}^{\nu})^{(0)}_{i,\langle 0\rangle}$

for $k = 2$ **to** $\mathtt{r}$ **do**

$\quad$ Get $(\widetilde{\mathbf{f}}^{l-1})^{(k-1)}_{i,j}$ via CAT procedure.

$\quad \widetilde{F}^{[n]}_{i+1/2,l} \mathrel{+}= \Delta t^{k-1} \sum_{\nu=1}^{l-1} a^{\{k\}}_{l\nu} \Lambda^{(0)} (\widetilde{\mathbf{f}}^{\nu})^{(k-1)}_{i,\langle 0\rangle}$

end

$Y^{[n]}_{i,l} = \sum_{\nu=1}^{2} u_{l\nu} y^{[n-1]}_{i,\nu} - \frac{\Delta t}{\Delta x}\left(\widetilde{F}^{[n]}_{i+1/2,l} - \widetilde{F}^{[n]}_{i-1/2,l}\right)$

CAT procedure [9] ($k = 2,\dots,m$):

for $j = -\overline{p}+1$ **to** $\overline{p}$ **do**

$\quad \widetilde{Y}^{(k-1)}_{i,j} = -Q^{(1)}_j \widetilde{\mathbf{f}}^{(k-2)}_{i,\langle 0\rangle} = -\frac{1}{\Delta x} \sum_{r=-\overline{p}+1}^{\overline{p}} \gamma^{1,j}_{\overline{p},r} \widetilde{\mathbf{f}}^{(k-2)}_{i,r}$

$\quad$ **for** $r = -\overline{p}+1$ **to** $\overline{p}$ **do**

$\quad\quad (\mathfrak{f}_T)^{k-1,n+r}_{i,j} = f\left(Y^{[n]}_{i+j} + \sum_{\ell=1}^{k-1} \frac{(r\Delta t)^\ell}{\ell!} \widetilde{Y}^{(\ell)}_{i,j}\right)$

$\quad$ **end**

$\quad \widetilde{\mathbf{f}}^{(k-1)}_{i,j} = Q^{(k-1)}_0 (\mathfrak{f}_T)^{k-1,\langle n\rangle}_{i,j} = \frac{1}{\Delta t^{k-1}} \sum_{r=-\overline{p}+1}^{\overline{p}} \gamma^{k-1,0}_{\overline{p},r} (\mathfrak{f}_T)^{k-1,n+r}_{i,j}$

end

Following [11], the expected order is the minimum of the underlying multiderivative GLMs and the order of the interpolation ($2\overline{p}$). Assuming that both f and y are smooth functions in C^∞, and $\mathcal{O}(\Delta t) = \mathcal{O}(\Delta x)$, we have the following theorem stating the order of Jacobian-free MDGLMs.

Theorem 3 *The order of an explicit compact approximate mDGLMp-s is given by* $\min(2\overline{p}, p)$ *where* p *is the order of the underlying MDGLM, while the stencil to update* $y(x_i,t^n)$ *in the CAT procedure is given by* $\{i-\overline{p}, i-\overline{p}+1, \dots, i+\overline{p}\}$.

The proof is similar to [11, Theorem 1], and is hence left out.

4.3 A Jacobian-free Starting Procedure

Due to the structure of the input vector of a multiderivative GLM, a starting procedure is needed to approximate the initial vector $y^{[0]}$ using sufficient output information. As mentioned in Sect. 2, see. Eq. (8), the components of the input vector $y^{[0]}_{i,\nu}$, $i = 1,2,\dots,M$, are approximations of order p to the linear combinations of the solution y and its derivatives at the point (x_i,t^0), i.e.,

$$y^{[0]}_{i,\nu} = \sum_{\kappa=0}^{p} w_{\nu\kappa} \partial_t^\kappa y(x_i,t^0) + O(\Delta t^{p+1}). \tag{29}$$

To calculate higher derivatives $\partial_t^\kappa y(x_i,t^0)$ directly, we use the CauchyKovalevskaya identity

$$\partial_t^\kappa y(x_i,t^0) = -\partial_x \partial_t^{\kappa-1} f(y(x_i,t^0)),$$

once again, and the approximate Taylor procedure [9] to derive the expression of the initial vector $y^{[0]}$. The flux derivatives can be computed by

$$\partial_t^\kappa y(x_i,t^0) \approx \widetilde{y}_i^{(\kappa)} := -P^{(1)} \widetilde{f}_{\langle i \rangle}^{(\kappa-1)},$$

in which the approximations $\widetilde{f}_{i+j}^{(\kappa-1)} \approx \partial_t^{\kappa-1} f(y(x_{i+j},t^0))$ are given by

$$\widetilde{f}_{i+j}^{(\kappa-1)} := P^{(\kappa-1)} (\mathfrak{f}_T)_{i+j}^{\kappa-1,\langle 0 \rangle}, \quad j = -\overline{p},\dots,\overline{p},$$

with

$$(\mathfrak{f}_T)_{i+j}^{\kappa-1,r} := f\left(y(x_{i+j},t^0) + \sum_{\ell=1}^{\kappa-1} \frac{(r\Delta t)^\ell}{\ell!} \widetilde{y}_{i+j}^{(\ell)} \right),$$

for $r = -\overline{p},\dots,\overline{p}$. Via the described steps, the values $\widetilde{f}_{i+j}^{(\kappa-1)}$ are recursively obtained.

A summary of the approximate Taylor (AT) procedure to obtain time-derivatives $\partial_t^{(\kappa)} y(x_i,t^0)$ is provided in Alg. 2.

Algorithm 2 Values of initial vector $y^{[0]}$ obtained via an approximate Taylor procedure

Time derivatives:

for $j = -\overline{p}$ **to** $\overline{p}$ **do**
  $\widetilde{f}_{i+j}^{(0)} = f(y(x_{i+j},t^0))$
end

$$\partial_t y(x_i,t^0) = -\frac{1}{\Delta x} \sum_{j=-\overline{p}}^{\overline{p}} \delta_{\overline{p},j}^1 \widetilde{f}_{i+j}^{(0)}$$

for $\kappa = 2$ **to** p **do**
  Get $\widetilde{f}_{i+j}^{(\kappa-1)}$ via AT procedure.
  $\partial_t^\kappa y(x_i,t^0) = -\frac{1}{\Delta x} \sum_{j=-\overline{p}}^{\overline{p}} \delta_{\overline{p},j}^1 \widetilde{f}_{i+j}^{(\kappa-1)}$
end

AT procedure [9] ($\kappa = 2,\dots,p$):

$$\widetilde{y}_{i+j}^{(\kappa-1)} = -P^{(1)} \widetilde{\mathbf{f}}_{\langle i \rangle}^{(\kappa-2)} = -\frac{1}{\Delta x} \sum_{r=-\overline{p}}^{\overline{p}} \delta_{\overline{p},r}^1 \widetilde{f}_{i+r}^{(\kappa-2)}$$

for $r = -\overline{p}$ **to** $\overline{p}$ **do**
  $(\mathfrak{f}_T)_{i+j}^{\kappa-1,r} = f\left(y(x_{i+j},t^0) + \sum_{\ell=1}^{\kappa-1} \frac{(r\Delta t)^\ell}{\ell!} \widetilde{y}_{i+j}^{(\ell)} \right)$
end

$$\widetilde{f}_{i+j}^{(\kappa-1)} = P^{(\kappa-1)} (\mathfrak{f}_{\boldsymbol{T}})_{i+j}^{\kappa-1,\langle 0 \rangle} = \frac{1}{\Delta t^{\kappa-1}} \sum_{r=-\overline{p}}^{\overline{p}} \delta_{\overline{p},r}^{\kappa-1} (\mathfrak{f}_T)_{i+j}^{\kappa-1,r}$$

5 Numerical results

In this section, we show numerical experiments verifying the accuracy and monotonicity properties of the constructed methods. To accomplish this, we consider several linear and nonlinear test cases with smooth and discontinuous initial data. It should be noted that to obtain the expected order of convergence, we avoid setups where shock formation occurs. Hence, we do not need to apply flux limiting techniques in convergence studies. To measure the accuracy we use the scaled L_1-error at the final time $t^N \equiv T_f$ given by

$$\|\mathbf{y}(T_f) - \mathbf{y}^{]}\| := \Delta x \sum_{i=1}^{M} |y(x_i, T_f) - y_i^N|,$$

where $\mathbf{y}(T_f)$ represents a vector of reference solution values in the spatial grids $x_1, x_2, \ldots, x_M$ at time T_f; and $\mathbf{y}^N$ stands for the vector of approximations y_i^N at time t^N. For monotonicity study, it is vital to check the behaviour of the numerical solutions close to a discontinuity or shock, which may produce strong oscillations. To avoid possible oscillations, we shall include flux limiting techniques to this work which can be involved in a straightforward way as in [9]. In all the following test cases we will use the van Albada flux limiter function.

In what follows, we perform several numerical experiments on a variety of 1d scalar conservation laws and systems: transport, Burgers, Buckley–Leverett equations, and system of Euler equations. In these test cases both spatial and temporal grids are refined simultaneously by means of the relation

$$\Delta t := \frac{\sigma \Delta x}{\max_i |\lambda_{\text{eig,i}}|},$$

where σ and $\lambda_{\text{eig,i}}$ stand for the obtained SSP coefficient, and the local eigenvalues of the Jacobian w.r.t initial value, respectively. In all the test cases with smooth initial data the expected order of convergence is preserved for the proposed Jacobian-free SSP multiderivative GLMs.

5.1 **Linear Transport Equation**

We consider first a linear advection problem $\partial_t Y + \partial_x Y = 0$ with periodic boundary conditions and smooth sine-wave initial condition

$$Y(x,0) = \frac{1}{4}\sin(\pi x), \qquad x \in [0,2]. \tag{30}$$

Adopting the Jacobian-free technique described in Alg. 1, we apply the explicit SSP 3DGLMs and 4DGLMs constructed in this work together with the SSP 2DGLMs obtained in [31] to this problem. In order to calculate the L_1-error for the CAMDGLMs, we run the simulation up to $T_f = 0.8$ with co-refinement of the spatial and temporal grids. The results with different values of CFL corresponding to each method are visualized in Figs.1 and 2, indicating that all expected convergence orders, $\min(2\overline{p}, p)$, are achieved. The compact approximate 3DGLM5-2 and 3DGLM6-3 behave in a very alike manner.

To show the capability of the constructed methods in preserving the stability properties near the appearance of shocks, we apply two stages compact approximate

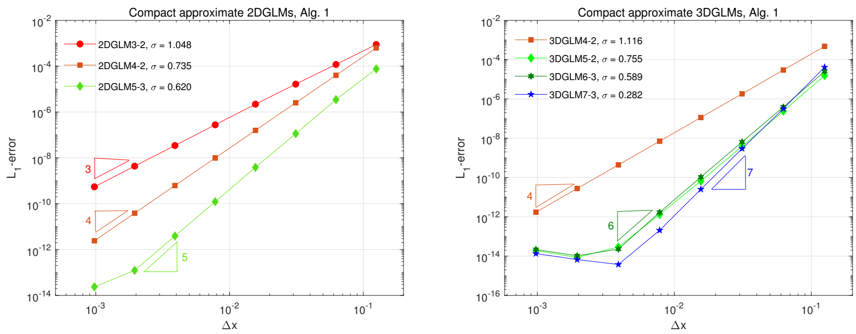

Fig. 1: Convergence order of explicit compact approximate SSP 2DGLMs (left) and 3DGLMs (right) applied to the linear transport equation on the sine-wave $Y_0(x) = \frac{1}{4}\sin(\pi x)$ up to $T_f = 0.8$

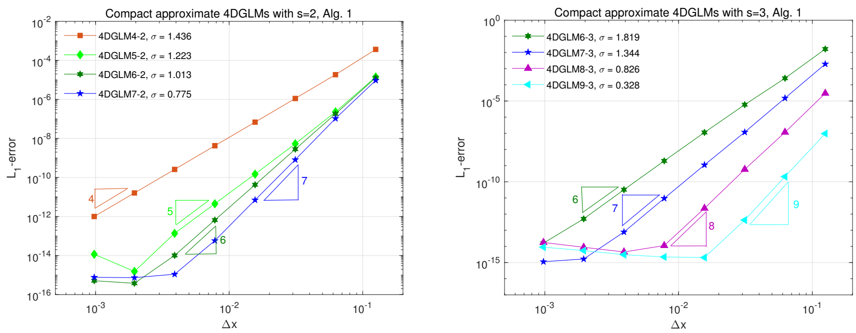

Fig. 2: Convergence order of explicit compact approximate SSP 4DGLMs applied to the linear transport equation on the sine-wave $Y_0(x) = \frac{1}{4}\sin(\pi x)$ up to $T_f = 0.8$

MDGLMs of order four with flux limiter technique: FL-2DGLM4-2, FL-3DGLM4-2 and FL-4DGLM4-2, to the above-mentioned transport equation with initial condition

$$Y(x,0) = \begin{cases} 1, & 0 \leq x < 0.2 \\ 2, & 0.2 \leq x < 0.7 \\ 1, & 0.7 \leq x \leq 1 \end{cases} \tag{31}$$

and run the simulation up to $T_f = 1.0$ with $M = 100$ points and CFL values $\sigma = 0.8$ and $\sigma = 0.5$. The numerical simulation are shown in Fig.3 where the van Albada flux limiter function is used. As it is clear, for $\sigma = 0.8$ the results given by FL-3DGLM4-2 and FL-4DGLM4-2 maintain stable near the discontinuities while FL-2DGLM4-2 with the same CFL value show strong oscillations. However, it can be seen from Fig. 3 (right) that for $\sigma = 0.5$, the FL-2DGLM4-2 behaves way better, yet, some slight oscillations still occur.

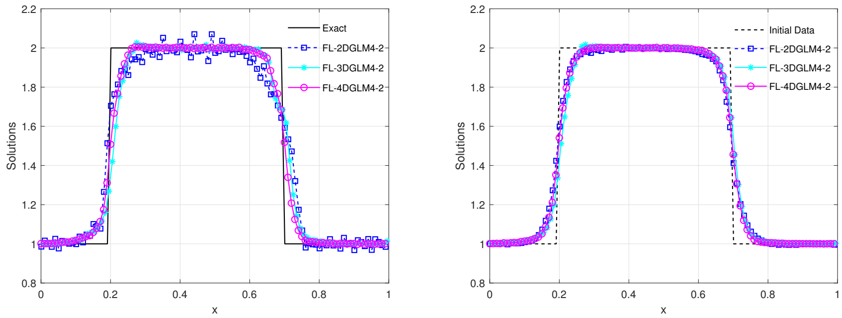

Fig. 3: Comparison of the performance of compact approximate MDGLMs of the same order for linear transport equation with initial condition (31), $\sigma = 0.8$ (left), $\sigma = 0.5$ (right) and $T_f = 1$

5.2 **Burgers Equation**

We consider Burgers equation

$$\partial_t Y + \partial_x \left(\frac{Y^2}{2}\right) = 0,$$

with the sine-wave initial condition (30) and periodic boundary conditions on the spatial domain $x \in [0,2]$. As observed in [30,46], a shock is formed at $t^* = \frac{4}{\pi} \approx 1.27$. To certify the theoretical accuracy of $\min(2\overline{p}, p)$ we set the final time to $T_f = 0.8$, before shock formation. As in the previous test case, we apply CAMDGLMs to this problem and run the simulations up to $T_f = 0.8$ to obtain L_1-errors when both the temporal and spatial grids are refined simultaneously. The obtained results are shown in Figs. 4 and 5. The orders coincide in all cases with the expected one, $\min(2\overline{p}, p)$. For the methods 3DGLM5-2 and 4DGLM5-2, the convergence order is slightly better than expected. Here the spatial order of accuracy is higher than the temporal one, and the spatial error dominate the overall behaviour.

Next, the same problem with all the same parameters but different initial condition

$$Y(x,0) = \frac{1}{4}\exp(\cos(\pi x) + \sin(\pi x)),$$

is solved using FL-2DGLM4-2, FL-3DGLM4-2 and FL-4DGLM4-2. Using $\sigma = 0.8$ and $\sigma = 0.5$, a resolution of $M = 100$ points and $T_f = 1.0$, after shock formation –the breaking time is $t^* = \frac{4}{\pi e}$ [11]– the numerical results are depicted in Fig. 6 revealing that for $\sigma = 0.8$ (left side) the third-derivative and fourth-derivative GLMs with flux limiter function exhibit smooth behaviour close to the shock while second-derivative GLM of the same order shows oscillations. It can also be seen from this figure (right side) that for $\sigma = 0.5$ all the methods behave correctly.

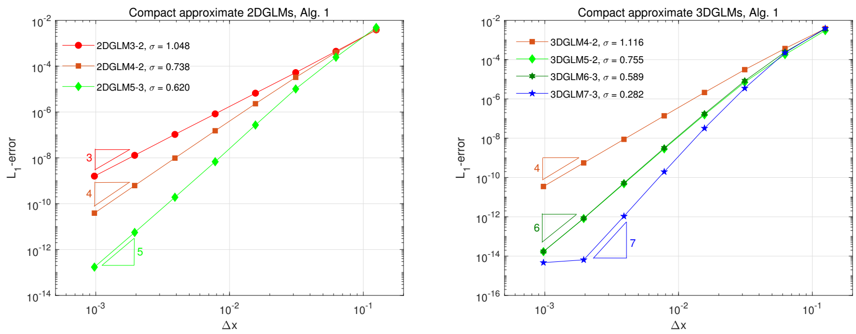

Fig. 4: Convergence order of explicit compact approximate SSP 2DGLMs and 3DGLMs applied to Burgers equation on the sine wave $Y_0(x) = \frac{1}{4}\sin(\pi x)$ up to $T_f = 0.8$

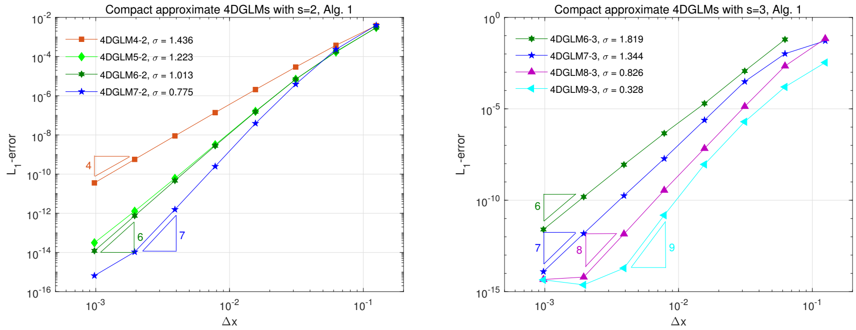

Fig. 5: Convergence order of explicit compact approximate SSP 4DGLMs applied to Burgers equation on the sine wave $Y_0(x) = \frac{1}{4}\sin(\pi x)$ up to $T_f = 0.8$.

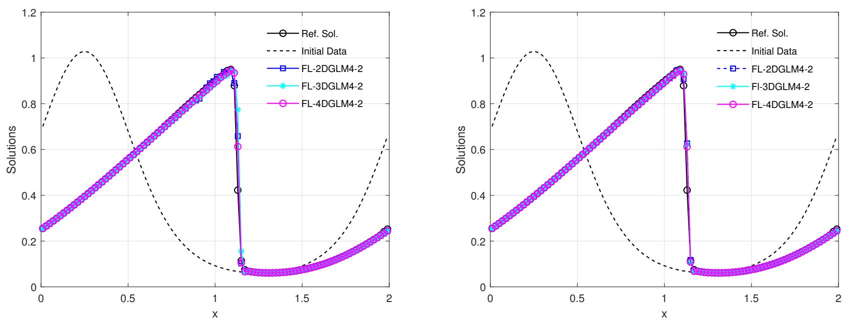

Fig. 6: Comparison of the performance of compact approximate MDGLMs of the same order for Burgers equation with initial condition $Y_0(x) = \frac{1}{4}\exp(\cos(\pi x) + \sin(\pi x))$, $\sigma = 0.8$ (left), $\sigma = 0.5$ (right) and $T_f = 1.0$

5.3 **Buckley–Leverett Equation**

Next, we consider the Buckley–Leverett flux [30]

$$\partial_t Y + \partial_x \left(\frac{Y^2}{Y^2 + a(1-Y)^2} \right) = 0,$$

with $a = 1/4$. This equation models a two-phase flow through a porous medium and contains more nonlinearities compared to Burgers flux. For this problem, we consider the following initial condition

$$Y(x,0) = 1 - \frac{3}{4}\cos^2\left(\frac{\pi}{2}x\right),$$

with periodic boundary conditions on the domain $x \in [-1,1]$. As a first test in this subsection, we set $T_f = 0.1$, so that we have a continuous solution which enables us to compute the exact solution via its characteristics. As in previous test cases, we refine both temporal and spatial grids concurrently, and calculate the L_1-errors for CAMDGLMs. The convergence results are plotted in Figs. 7 and 8; the expected order of convergence are attained. Better performance than expected is observed for methods 2DGLM5-3, 3DGLM5-2, 4DGLM5-2, and 4DGLM7-3, as a result of the spatial order of accuracy is higher than the temporal one. Indeed, bearing in mind that the compact approximate approach has been investigated as a natural extension of Lax–Wendroff methods with an even-order accuracy, in most of the test cases when $2\overline{p} > p$, the odd-order MDGLMs take advantage and behave similar to the methods of order $2\overline{p}$.

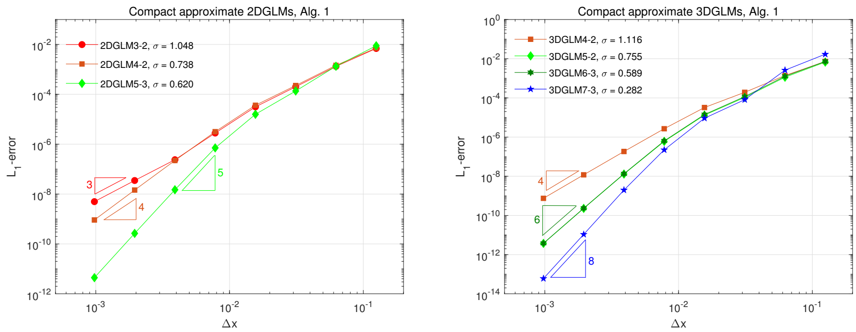

Fig. 7: Convergence order of explicit compact approximate SSP 2DGLMs and 3DGLMs applied to Buckley–Leverett equation with initial condition $Y_0(x) = 1 - \frac{3}{4}\cos^2(\frac{\pi}{2}x)$ up to $T_f = 0.1$

In a similar way as for the previous examples, we conclude this test case by solving the same problem with all the same parameters except for the final time, which we set to $T_f = 0.4$, after shock appearance, and CFL numbers $\sigma = 0.8$ and $\sigma = 0.5$.

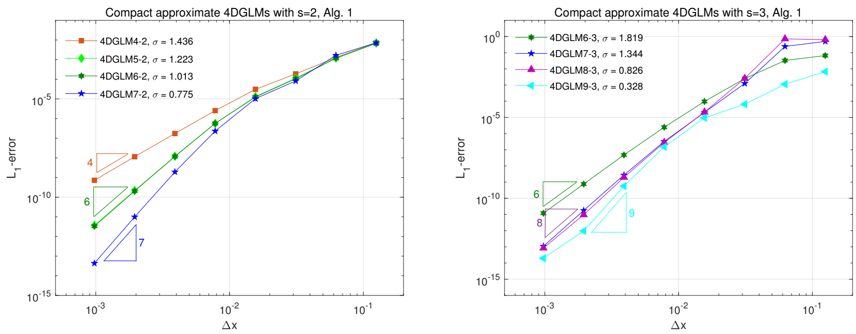

Fig. 8: Convergence order of explicit compact approximate SSP 4DGLMs applied to Buckley–Leverett equation with initial condition $Y_0(x) = 1 - \frac{3}{4}\cos^2(\frac{\pi}{2}x)$ up to $T_f = 0.1$

Using two stages multiderivative GLMs of order four with the van Albada flux limiter function, we obtain numerical solutions with a quite similar behaviour to those for the Burgers equation, as can be seen in the left-side of Fig. 9: FL-3DGLM4-2 and FL-4DGLM4-2 indicate smooth behaviour while 2DGLM4-2 shows numerical instability. The right side of this figure presents the behaviour of the numerical solutions for $\sigma = 0.5$ indicating that all of the methods preserve the required stability property near shock.

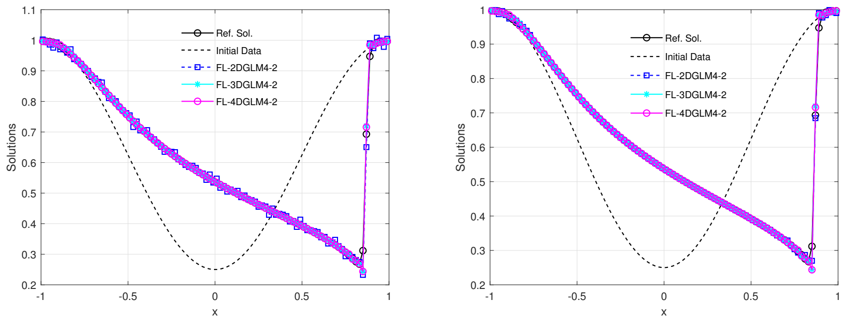

Fig. 9: Comparison of the performance of compact approximate MDGLMs of the same order for Buckley–Leverett equation with initial condition $Y_0(x) = 1 - \frac{3}{4}\cos^2(\frac{\pi}{2}x)$, $M = 100$, $\sigma = 0.8$ (left), $\sigma = 0.5$ (right) and $T_f = 0.4$

5.4 **One-Dimensional Euler Equations**

Finally, we consider the nonlinear system of Euler equations defined by

$$\partial_t Y + \partial_x f(Y) = 0,$$

with

$$Y = \begin{pmatrix} \rho \\ \rho v \\ E \end{pmatrix}, \quad f(Y) = \begin{pmatrix} \rho v \\ \rho v^2 + P \\ v(E+P) \end{pmatrix},$$

where ρ stands for the density, E is the total energy, v is the velocity, and P is the pressure given by

$$P = (\gamma - 1)\left(E - \frac{1}{2}\rho v^2\right),$$

with $\gamma = 1.4$, for ideal gas [30,46]. We consider the following initial condition

$$Y(x,0) = \frac{1}{4}\begin{pmatrix} 3 \\ 1 \\ 3 \end{pmatrix} + \frac{\sin(\pi x)}{2}\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix},$$

on $x \in [0,2]$ with periodic boundary conditions and $T_f = 0.2$. To examine the accuracy of constructed methods for this test problem, a reference solution has been computed via a third-order discontinuous Galerkin (DG) method in space and a third-order SSP RK method in time [21] using $M = 10240$ cells and a CFL number of $\sigma = 0.15$. The L_1-errors for CAMDGLMs are calculated at final time $T_f = 0.2$. The convergence results are visualized in Figs. 10 and 11. It is clear from these figures that all expected orders were obtained. Very similar behaviour can be seen between the methods that use the same $\overline{p}$.

As in the previous test cases, running the simulations for each methods with their corresponding CFL values, we observed that not all simulations were stable. Indeed, 3DGLMs and 4DGLMs with $s = 2$ diverged for $M = 16, 32$ and 64, and with $s = 3$ diverged for $M = 16, 32, 64$ and 128. In the case of 3DGLM7-3 and 4DGLM9-3, we also observed divergenc for $M = 16, 32$ and 64 (when the case is 4DGLM9-3) for CFL value $\sigma = 0.15$.

6 Conclusions

In this paper, following an introduction to multiderivative GLMs, we studied the monotonicity theory of multiderivative GLMs and derived sufficient conditions for multiderivative GLMs to be SSP. Solving an optimization problem with the aim of maximizing SSP coefficients and subject to the order and SSP conditions as equality and inequality constraints, respectively, we obtained high-order explicit SSP multiderivative GLMs with two external stages and $s = 2$ and $s = 3$ internal stages up to four derivatives and order nine for hyperbolic conservation laws. Such methods involve cumbersome calculation of the flux derivatives. To conquer this flaw, based on recent developments of explicit Jacobian-free multistage multiderivative solvers in

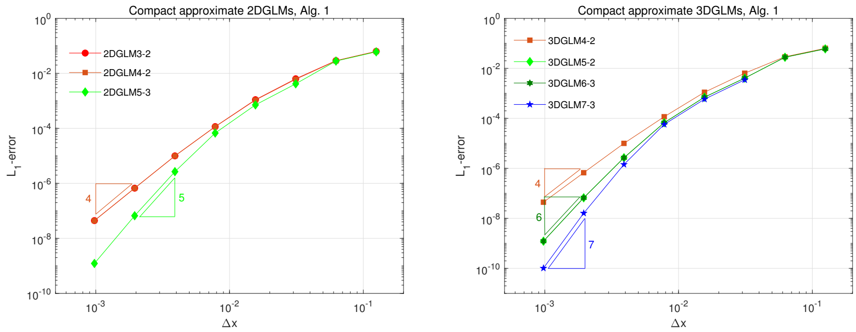

Fig. 10: Convergence order of explicit compact approximate SSP 2DGLMs and 3DGLMs applied to Euler equations with $\rho_0(x) = 0.75 + 0.5\sin(\pi x)$, $(\rho v)_0(x) = 0.25 + 0.5\sin(\pi x)$ and $E_0(x) = 0.75 + 0.5\sin(\pi x)$ on $x \in [0,2]$ up to $T_f = 0.2$ with $\sigma = 0.15$

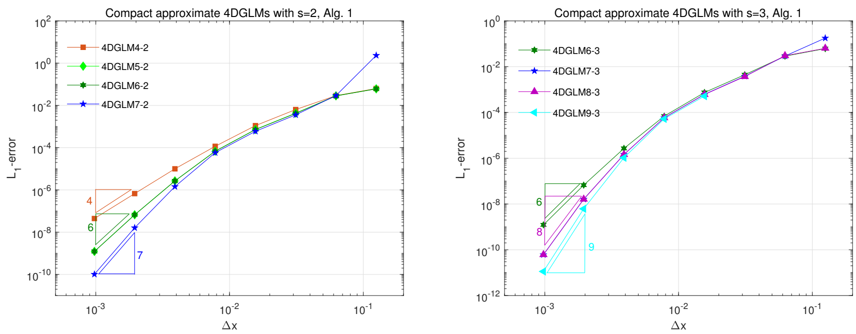

Fig. 11: Convergence order of explicit compact approximate SSP 4DGLMs applied to Euler equations with $\rho_0(x) = 0.75 + 0.5\sin(\pi x)$, $(\rho v)_0(x) = 0.25 + 0.5\sin(\pi x)$, and $E_0(x) = 0.75 + 0.5\sin(\pi x)$ on $x \in [0,2]$ up to $T_f = 0.2$ with $\sigma = 0.15$

[11], we adopted a Jacobian-free technique for multiderivative GLMs in which time derivatives of fluxes use local approximations based on discrete differentiations recursively. Aside from not requiring costly symbolic computations, by this Jacobian-free approach, higher order multiderivative GLMs can be of more practical use in solving PDEs. Through a variety of numerical test cases, it is shown that the desired convergence order $\min(2\overline{p}, p)$ is attained, where $2\overline{p}$ stands for the spatial order and p for temporal order.

In future works, the novel scheme will be extended and applied to more challenging settings, for instance a combination of MDGLMs and discontinues Galerkin techniques [38] is of high interest. In the case of problems with diffusion, very small local mesh sizes are often needed and hence, acceptable time-steps become very small. In order to take care of these diffusive effects, or other ‘stiff’ effects such as the singular perturbance that comes from low-Mach equations, the class of implicit and IMEX SSP MDGLMs with *A*- and *L*-stability properties will be considered.

Declarations

Data availability

The datasets generated and/or analyzed during the current study are available from the corresponding author on reasonable request mailto: afsaneh.moradi@univaq.it.

Conflict of Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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