

Strong stability preserving general linear methods

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Initial value problem for ODEs

Initial-value problem for ordinary differential equations (ODEs):

$$\begin{cases} y'(t) = f(y(t)), & t \in [t_0, T], \\ y(t_0) = y_0. \end{cases} \quad (1)$$

In many applications such systems arise from semidiscretization of spatial derivatives in PDEs of mathematical physics. Example: hyperbolic conservation law (in two dimensions):

$$\frac{\partial}{\partial t} u(x_1, x_2, t) + \frac{\partial}{\partial x_1} f_1(u(x_1, x_2, t)) + \frac{\partial}{\partial x_2} f_2(u(x_1, x_2, t)) = 0, \quad (2)$$

where $u : \mathbb{R}^2 \times \mathbb{R} \rightarrow \mathbb{R}^m$, and $f_1, f_2 : \mathbb{R}^m \rightarrow \mathbb{R}^m$, are given flux functions. Discretization of the equation (2) in space variables x_1 and x_2 leads to (1).

Strong stability preserving (SSP) property

We assume that the discretization of (1) by the forward Euler method

$$y_n = y_{n-1} + hf(t_{n-1}, y_{n-1}), \quad (3)$$

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

$$\|y_n\| \leq \|y_{n-1}\|, \quad (4)$$

$n = 1, 2, \dots, N$, in some norm or semi-norm $\|\cdot\|$, for a suitably restricted time step determined by the so-called Courant-Friedrichs-Levy (CFL) condition

$$h \leq h_{FE}. \quad (5)$$

It is then of interest to construct higher order numerical methods for (1), which preserve the monotonicity property (4), under the perhaps modified restriction on the time step of the form

$$h \leq \mathcal{C} \cdot h_{FE}, \quad (6)$$

measured by the CFL coefficient of the method $\mathcal{C} \geq 0$.

Terminology

Numerical schemes for (1), which preserve the monotonicity condition (4) under the modified restriction (6), are called strong stability preserving (SSP) methods with CFL coefficient $\mathcal{C} \geq 0$.

SSP time discretization methods were first developed by Shu (1988) and Shu and Osher (1988), and were called total variation diminishing (TVD) time discretizations.

Consider the explicit Runge-Kutta (RK) method with s stages for (1)

$$\begin{cases} Y_i^{[n]} = y_{n-1} + h \sum_{j=1}^{i-1} a_{ij} f(t_{n-1} + c_j h, Y_j^{[n]}), & i = 1, 2, \dots, s, \\ y_n = y_{n-1} + h \sum_{j=1}^s b_j f(t_{n-1} + c_j h, Y_j^{[n]}). \end{cases} \quad (7)$$

The search for SSP RK methods (7) is facilitated by a clever representation of these methods as convex combinations of Euler steps. This so-called Shu-Osher (1988) representation has the form

$$\begin{cases} Y_1^{[n]} = y_{n-1}, \\ Y_i^{[n]} = \sum_{j=1}^{i-1} (\alpha_{ij} Y_j^{[n]} + h \beta_{ij} f(t_{n-1} + c_j h, Y_j^{[n]})), & i = 2, 3, \dots, s, \\ y_n = \sum_{j=1}^s (\alpha_{s+1,j} Y_j^{[n]} + h \beta_{s+1,j} f(t_{n-1} + c_j h, Y_j^{[n]})). \end{cases} \quad (8)$$

Formulas for new coefficients

Here α_{ij} are scalars such that

$$\sum_{j=1}^{i-1} \alpha_{ij} = 1, \quad i = 2, 3, \dots, s+1,$$

and the coefficients β_{ij} are given by

$$\left\{ \begin{array}{l} \beta_{ij} = a_{ij} - \sum_{k=j+1}^{i-1} \alpha_{ik} a_{kj}, \quad i = 2, 3, \dots, s, j = 1, 2, \dots, i-1, \\ \beta_{s+1,j} = b_j - \sum_{k=j+1}^s \alpha_{s+1,k} a_{kj}, \quad j = 1, 2, \dots, s. \end{array} \right.$$

Characterization of SSP RK methods

The Shu-Osher representation (8) leads to the following characterization of SSP RK methods (7).

Theorem

(Shu, Osher (1988)). Assume that the forward Euler method (2) applied to (1) is strongly stable, i.e., the inequality $\|y_n\| \leq \|y_{n-1}\|$ holds under the time step restriction $h \leq h_{FE}$. Assume also that $\alpha_{ij} \geq 0$ and $\beta_{ij} \geq 0$. Then the solution $\{y_n\}$ obtained by the RK method (7) or (8) satisfies the strong stability bound

$$\|y_n\| \leq \|y_{n-1}\|,$$

$n = 1, 2, \dots, N$, under the time step restriction $h \leq C \cdot h_{FE}$, with CFL coefficient $C = C(\alpha, \beta)$ given by

$$C(\alpha, \beta) = \min \left\{ \frac{\alpha_{ij}}{\beta_{ij}} : i = 2, 3, \dots, s, j = 1, 2, \dots, i-1 \right\}.$$

Previous work on SSP methods

SSP RK and linear multistep methods (LMMs) have been studied by Shu and Osher (1988), Gottlieb, Shu, and Tadmor (2001), Spiteri and Ruuth (2002), Hundsdorfer, Ruuth, and Spiteri (2003), Gottlieb (2005), Gottlieb and Ruuth (2006), Gottlieb, Ketcheson, and Shu (2009), (2011), Higuera (2004), (2005), and Ferracina and Spijker (2004), (2005), (2008). SSP two-step Runge-Kutta (TSRK) methods introduced by Jackiewicz and Tracogna (1995) were investigated by Ketcheson, Gottlieb and Macdonald (2011). Constantinescu and Sandu (2010) generalized Shu-Osher representation to a class of multistep multistage schemes, which form a special subclass of GLMs. SSP general linear methods (GLMs) were investigated by Spijker in his seminal paper (2007). SSP GLMs were also investigated by Izzo and Jackiewicz (2015, 2018, 2020), Califano, Izzo and Jackiewicz (2018), and Braś, Izzo and Jackiewicz (2021).

In this talk we will employ Spijker's (2007) results to construct new classes of SSP GLMs up to the order $p = 4$ and stage order $1 \leq q \leq 4$.

Spijker formulation of GLMs

Following Spijker (2007) we consider the formulation of GLMs, for numerical solution of (1), of the form

$$\begin{cases} Y_i^{[n]} = h \sum_{j=1}^m t_{ij} f(t_{n-1} + c_j h, Y_j^{[n]}) + \sum_{j=1}^{\ell} s_{ij} y_j^{[n-1]}, & i = 1, 2, \dots, m, \\ y_i^{[n]} = Y_{m-\ell+i}^{[n]}, & i = 1, 2, \dots, \ell, \end{cases} \quad (9)$$

$n = 1, 2, \dots, N$, where $1 \leq \ell \leq m$. Here, $Y_i^{[n]}$, $i = 1, 2, \dots, m$, are internal approximations or stages, which are used to compute the external approximations $y_i^{[n]}$, $i = 1, 2, \dots, \ell$, which propagate from step to step. This method is specified by the abscissa vector $\mathbf{c} = [c_1, \dots, c_m]^T \in \mathbb{R}^m$, and the coefficient matrices $\mathbf{T} = [t_{ij}] \in \mathbb{R}^{m \times m}$ and $\mathbf{S} = [s_{ij}] \in \mathbb{R}^{m \times \ell}$. Different representations of (9) are discussed by Butcher (1987), (2003), (2008), Hairer, Nørsett, and Wanner (1993), Hairer and Wanner (1996), and Jackiewicz (2009).

Observe that the RK method (7) can be written as GLM (9) with $m = s + 1$, $\ell = 1$, and

$$\mathbf{T} = \left[\begin{array}{c|c} \mathbf{A} & \mathbf{0} \\ \hline \mathbf{b}^T & 0 \end{array} \right] \in \mathbb{R}^{(s+1) \times (s+1)}, \quad \mathbf{S} = \left[\begin{array}{c} \mathbf{e} \\ 1 \end{array} \right] \in \mathbb{R}^{s+1},$$

where $\mathbf{e} = [1, \dots, 1]^T \in \mathbb{R}^s$.

As in Spijker (2007) we shall assume that the parameters s_{ij} of the coefficient matrix \mathbf{S} satisfy the condition

$$\sum_{j=1}^{\ell} s_{ij} = 1, \quad i = 1, 2, \dots, m. \quad (10)$$

Observe that this assumption is automatically satisfied for the RK methods (7) and for the class of DIMSIMs. Moreover, as observed by Spijker (2007), this condition is no essential restriction on the method (9) since any preconsistent GLMs can be transformed into an equivalent GLM satisfying (10).

Transformations of GLMs are discussed by Butcher (2003), (2008) and Jackiewicz (2009).

Characterization of CFL coefficient

Denote by \mathbf{I} the identity matrix of dimension m , and let $[\mathbf{S} \mid \gamma\mathbf{T}]$, $\gamma \in \mathbb{R}$, stand for the $m \times (\ell + m)$ matrix whose first ℓ columns equal to those of \mathbf{S} and the last m columns equal to those of $\gamma\mathbf{T}$. Then following Spijker (2007), we consider the condition

$$\det(\mathbf{I} + \gamma\mathbf{T}) \neq 0 \quad \text{and} \quad (\mathbf{I} + \gamma\mathbf{T})^{-1}[\mathbf{S} \mid \gamma\mathbf{T}] \geq 0, \quad (11)$$

where the inequality in (11) should be interpreted componentwise. Then the essence of the fundamental result obtained by Spijker (2007) is that the CFL coefficient $\mathcal{C} = \mathcal{C}(\mathbf{S}, \mathbf{T})$ of the GLM (9) is given by

$$\mathcal{C} = \mathcal{C}(\mathbf{S}, \mathbf{T}) = \sup \left\{ \gamma \in \mathbb{R} : \gamma \text{ satisfies (11)} \right\}. \quad (12)$$

Computation of CFL coefficient

The CFL coefficient can be computed by the solution to the constrained minimization problem with the simple objective function F given by

$$F(\gamma, par) = -\gamma, \quad (13)$$

where par stands for the remaining unknown parameters of the GLM (9) (after satisfying the appropriate order, stage order, and perhaps some linear stability conditions), and the (in general nonlinear) constraints are given by

$$-(\mathbf{I} + \gamma\mathbf{T})^{-1}[\mathbf{S} | \gamma\mathbf{T}] \leq 0. \quad (14)$$

This process will be discussed in more detail later in this talk for specific examples of GLMs (9).

Minimization problem for Euler method

In particular, solving the minimization problem

$$F(\gamma) = -\gamma \longrightarrow \min,$$

for the forward Euler method (3), for which $m = 1$, $\ell = 1$, and

$$\mathbf{T} = \left[\begin{array}{c|c} 0 & 0 \\ \hline 1 & 0 \end{array} \right] \in \mathbb{R}^{2 \times 2}, \quad \mathbf{S} = \left[\begin{array}{c} 1 \\ 1 \end{array} \right] \in \mathbb{R}^2,$$

and the constrains (14) take the form

$$-(\mathbf{I} + \gamma\mathbf{T})^{-1}[\mathbf{S} \mid \gamma\mathbf{T}] = \begin{bmatrix} -1 & 0 & 0 \\ \gamma - 1 & -\gamma & 0 \end{bmatrix} \leq 0,$$

we obtain $\mathcal{C} = \mathcal{C}(\mathbf{S}, \mathbf{T}) = 1$, as should be the case.

Standard representation of GLMs

Consider the class of GLMs investigated by Burrage and Butcher (1980). On the grid $t_n = t_0 + nh$, $n = 0, 1, \dots, N$, $Nh = T - t_0$, these methods take the form

$$\begin{cases} Y_i^{[n]} = h \sum_{j=1}^s a_{ij} f(t_{n-1} + c_j h, Y_j^{[n]}) + \sum_{j=1}^r u_{ij} y_j^{[n-1]}, & i = 1, 2, \dots, s, \\ y_i^{[n]} = h \sum_{j=1}^s b_{ij} f(t_{n-1} + c_j h, Y_j^{[n]}) + \sum_{j=1}^r v_{ij} y_j^{[n-1]}, & i = 1, 2, \dots, r, \end{cases} \quad (15)$$

$n = 1, 2, \dots, N$. Here,

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

and

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

Coefficients matrices and vectors

These method 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

$$\mathbf{q}_i = [q_{1,i}, \dots, q_{r,i}]^T \in \mathbb{R}^r, \quad i = 0, 1, \dots, p,$$

and four integers:

p -the order of the method

q - the stage order of the method

r - the number of external approximations

s - the number of internal approximations or stages

GLMs with two external stages

In what follows we will restrict our attention to GLMs (15) with s internal stages and $r = 2$ external stages of order p and stage order $1 \leq q \leq p$. Moreover, we shall assume that the matrix \mathbf{A} is strictly lower triangular

$$\mathbf{A} = \begin{bmatrix} 0 & & & & \\ a_{2,1} & 0 & & & \\ \vdots & \ddots & \ddots & & \\ a_{s-1,1} & \ddots & \ddots & 0 & \\ a_{s,1} & a_{s,2} & \cdots & a_{s,s-1} & 0 \end{bmatrix} \in \mathbb{R}^{s \times s},$$

and the matrix \mathbf{U} has the form

$$\mathbf{U} = \begin{bmatrix} \mathbf{u}_1 \\ \vdots \\ \mathbf{u}_s \end{bmatrix} \in \mathbb{R}^{s \times 2}, \quad \mathbf{u}_i = \begin{bmatrix} u_{i,1} & u_{i,2} \end{bmatrix} \in \mathbb{R}^2, \quad u_{i,1} + u_{i,2} = 1.$$

Coefficient matrix \mathbf{V}

We shall also assume that the matrix \mathbf{V} is a rank one matrix of the following form

$$\mathbf{V} = \mathbf{e}\mathbf{v}^T, \quad \mathbf{e} = [1, 1]^T \in \mathbb{R}^2, \quad \mathbf{v} = [v_1, v_2]^T \in \mathbb{R}^r, \quad \mathbf{v}^T \mathbf{e} = 1.$$

Then it follows that \mathbf{V} is power bounded, and as a result the method (15) is zero-stable.

In order to get methods with higher \mathcal{C} coefficients we will also consider methods having $\text{rank}(\mathbf{V}) = 2$. In this case the matrix \mathbf{V} will assume the form

$$\mathbf{V} = \begin{bmatrix} v_1 & 1 - v_1 \\ v_2 & 1 - v_2 \end{bmatrix},$$

and its power boundedness will be ensured by the condition $|v_1 - v_2| < 1$.

Order conditions

Algebraic analysis of order of GLMs was developed in the monographs by Butcher (1987), (2003), (2008), Hairer, Nørsett, and Wanner (1993), and Jackiewicz (2009). Here, we discuss derivation of order conditions for GLMs using the approach by Albrecht (1985), (1987), (1989), (1996).

Put

$$\begin{cases} \gamma_0 = \mathbf{e} - \mathbf{U}\mathbf{q}_0, \\ \gamma_k = \frac{\mathbf{c}^k}{k!} - \frac{\mathbf{A}\mathbf{c}^{k-1}}{(k-1)!} - \mathbf{U}\mathbf{q}_k, \quad k = 1, 2, \dots, p, \end{cases} \quad (16)$$

$$\begin{cases} \hat{\gamma}_0 = \mathbf{q}_0 - \mathbf{V}\mathbf{q}_0, \\ \hat{\gamma}_k = \sum_{l=0}^k \frac{\mathbf{q}_l}{(k-l)!} - \frac{\mathbf{B}\mathbf{c}^{k-1}}{(k-1)!} - \mathbf{V}\mathbf{q}_k, \quad k = 1, 2, \dots, p, \end{cases} \quad (17)$$

where

$$\mathbf{e} = [1, \dots, 1]^T \in \mathbb{R}^s, \quad \mathbf{c}^i := [c_1^i, \dots, c_s^i]^T.$$

Preconsistency, consistency, stage consistency

It will be always assumed that

$$\mathbf{q}_0 = \mathbf{e} = [1, \dots, 1]^T \in \mathbb{R}^r,$$

so that the stage preconsistency condition

$$\gamma_0 = 0 \quad \text{or} \quad \mathbf{U}\mathbf{q}_0 = \mathbf{e},$$

and the preconsistency condition

$$\tilde{\gamma}_0 = 0 \quad \text{or} \quad \mathbf{V}\mathbf{q}_0 = \mathbf{q}_0,$$

are automatically satisfied. Moreover, we will always assume that the GLM (15) has stage order at least one, i.e.,

$$\gamma_1 = 0 \quad \text{or} \quad \mathbf{A}\mathbf{e} + \mathbf{U}\mathbf{q}_1 = \mathbf{c}.$$

Order conditions - continued

Assuming that the starting vector $y^{[0]}$ satisfies the condition

$$y^{[0]} = \mathbf{q}_0 y(t_0) + h\mathbf{q}_1 y'(t_0) + \cdots + h^p \mathbf{q}_p y^{(p)}(t_0) + O(h^{p+1}), \quad (18)$$

order conditions for GLMs (15) up to $p = 4$ are listed in Table 1, where

$$g_1(t) = \frac{\partial f}{\partial y} \left(t, y(t) \right), \quad \Gamma_{\mathbf{c}} = \text{diag}(c_1, \dots, c_s),$$

and when 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 . In this table we have also listed the recursive differentials used in Albrecht approach to the derivation of order conditions.

Order	Recursive differentials	Corresponding order conditions
$p = 1$	y'	$\hat{\gamma}_1 = 0$
$p = 2$	y''	$\hat{\gamma}_2 = 0$
$p = 3$	y'''	$\hat{\gamma}_3 = 0$
	$g_1 y''$	$\mathbf{VB}\gamma_2 = 0 \quad \text{or} \quad \mathbf{B}\gamma_2 = 0$
$p = 4$	$y^{(4)}$	$\hat{\gamma}_4 = 0$
	$g_1 y'''$	$\mathbf{VB}\gamma_3 = 0$
	$g_1^2 y''$	$\mathbf{VBA}\gamma_2 = 0$
	$g_1' y''$	$\mathbf{VB}\Gamma_{\mathbf{c}}\gamma_2 = 0$

Table: Recursive differentials and order conditions for $p \leq 4$

Spijker representation of GLMs

The methods (15) can be written as GLMs in Spijker form (9) with $m = s + r$, $\ell = r$, and the matrices \mathbf{T} and \mathbf{S} defined by

$$\mathbf{T} = \left[\begin{array}{c|c} \mathbf{A} & \mathbf{0} \\ \mathbf{B} & \mathbf{0} \end{array} \right] \in \mathbb{R}^{(s+r) \times (s+r)}, \quad \mathbf{S} = \left[\begin{array}{c} \mathbf{U} \\ \mathbf{V} \end{array} \right] \in \mathbb{R}^{(s+r) \times r}.$$

Observe that it follows from the assumptions on the form of \mathbf{U} and \mathbf{V} , that the condition

$$\sum_{j=1}^r s_{ij} = 1, \quad i = 1, 2, \dots, s + r,$$

on the coefficient matrix \mathbf{S} is automatically satisfied.

Reformulation of characterization of \mathcal{C} coefficient

We can reformulate the condition

$$\det(\mathbf{I} + \gamma\mathbf{T}) \neq 0 \quad \text{and} \quad (\mathbf{I} + \gamma\mathbf{T})^{-1}[\mathbf{S} \mid \gamma\mathbf{T}] \geq \mathbf{0}, \quad (19)$$

and the characterization of CFL coefficient $\mathcal{C} = \mathcal{C}(\mathbf{S}, \mathbf{T})$ of GLM in Spijker form (9) given by

$$\mathcal{C} = \mathcal{C}(\mathbf{S}, \mathbf{T}) = \sup \left\{ \gamma \in \mathbb{R} : \gamma \text{ satisfies (19)} \right\} \quad (20)$$

in terms of the abscissa vector \mathbf{c} , and the coefficient matrices \mathbf{A} , \mathbf{U} , \mathbf{B} , and \mathbf{V} of GLM (15). We have

$$\mathbf{I} + \gamma\mathbf{T} = \left[\begin{array}{c|c} \mathbf{I} + \gamma\mathbf{A} & \mathbf{0} \\ \hline \gamma\mathbf{B} & \mathbf{I} \end{array} \right].$$

Reformulation of \mathcal{C} - continued

It follows that

$$\det(\mathbf{I} + \gamma\mathbf{T}) \neq 0 \quad \text{if and only if} \quad \det(\mathbf{I} + \gamma\mathbf{A}) \neq 0.$$

Since \mathbf{A} is strictly lower triangular we have $\det(\mathbf{I} + \gamma\mathbf{A}) \neq 0$,

$$\left[\begin{array}{c|c} \mathbf{I} + \gamma\mathbf{A} & \mathbf{0} \\ \hline \gamma\mathbf{B} & \mathbf{I} \end{array} \right]^{-1} = \left[\begin{array}{c|c} (\mathbf{I} + \gamma\mathbf{A})^{-1} & \mathbf{0} \\ \hline -\gamma\mathbf{B}(\mathbf{I} + \gamma\mathbf{A})^{-1} & \mathbf{I} \end{array} \right],$$

and after some computations it follows that

$$(\mathbf{I} + \gamma\mathbf{T})^{-1}[\mathbf{S} | \gamma\mathbf{T}] = \left[\begin{array}{c|c|c} (\mathbf{I} + \gamma\mathbf{A})^{-1}\mathbf{U} & \mathbf{I} - (\mathbf{I} + \gamma\mathbf{A})^{-1} & \mathbf{0} \\ \hline \mathbf{V} - \gamma\mathbf{B}(\mathbf{I} + \gamma\mathbf{A})^{-1}\mathbf{U} & \gamma\mathbf{B}(\mathbf{I} + \gamma\mathbf{A})^{-1} & \mathbf{0} \end{array} \right].$$

Characterization of \mathcal{C} coefficient in terms of \mathbf{c} , \mathbf{A} , \mathbf{U} , \mathbf{B} , \mathbf{V}

Hence, it follows that the condition (19)

$$\det(\mathbf{I} + \gamma\mathbf{T}) \neq 0 \quad \text{and} \quad (\mathbf{I} + \gamma\mathbf{T})^{-1}[\mathbf{S} \mid \gamma\mathbf{T}] \geq 0,$$

is equivalent to

$$(\mathbf{I} + \gamma\mathbf{A})^{-1}\mathbf{U} \geq 0, \quad \mathbf{I} - (\mathbf{I} + \gamma\mathbf{A})^{-1} \geq 0, \tag{21}$$

$$\mathbf{V} - \gamma\mathbf{B}(\mathbf{I} + \gamma\mathbf{A})^{-1}\mathbf{U} \geq 0, \quad \gamma\mathbf{B}(\mathbf{I} + \gamma\mathbf{A})^{-1} \geq 0,$$

and the characterization of the CFL coefficient (20) for GLM (15) can be reformulated as

$$\mathcal{C} = \mathcal{C}(\mathbf{c}, \mathbf{A}, \mathbf{U}, \mathbf{B}, \mathbf{V}) = \sup \left\{ \gamma \in \mathbb{R} : \gamma \text{ satisfies (21)} \right\}. \tag{22}$$

Minimization problem

We will use characterization (22) of CFL coefficient \mathcal{C} to search for new methods, for which \mathcal{C} is as large as possible. We will systematically investigate GLMs with $2 \leq p \leq 4$, $1 \leq q \leq 4$, $r = 2$, and $2 \leq s \leq 10$. Consider the minimization problem

$$F(\gamma, \mathbf{c}, \mathbf{A}, \mathbf{U}, \mathbf{B}, \mathbf{V}) = -\gamma \longrightarrow \min \quad (23)$$

subject to the inequality constrains

$$(\mathbf{I} + \gamma\mathbf{A})^{-1}\mathbf{U} \geq 0, \quad \mathbf{I} - (\mathbf{I} + \gamma\mathbf{A})^{-1} \geq 0, \quad (24)$$

$$\mathbf{V} - \gamma\mathbf{B}(\mathbf{I} + \gamma\mathbf{A})^{-1}\mathbf{U} \geq 0, \quad \gamma\mathbf{B}(\mathbf{I} + \gamma\mathbf{A})^{-1} \geq 0,$$

and the equality constrains

$$\Phi_{p,q}(\mathbf{c}, \mathbf{A}, \mathbf{U}, \mathbf{B}, \mathbf{V}, \mathbf{q}_1, \dots, \mathbf{q}_p) = 0, \quad (25)$$

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

\mathcal{C}_{eff} coefficients for GLMs

The solution of this minimization problem (23), (24), and (25) leads to specific SSP GLMs (15) with CFL coefficient \mathcal{C} . To compare methods with different number of stages s we also define the effective CFL coefficient by the normalization

$$\mathcal{C}_{eff} = \frac{\mathcal{C}}{s}.$$

The \mathcal{C}_{eff} coefficients for methods with two external stages are listed in Tables 2–4, using the notation

GLM pqr ,

where p is the order, q is the stage order, and r now stands for the rank of the coefficient matrix \mathbf{V} . For comparison, in these tables we have also listed \mathcal{C}_{eff} coefficients for SSP TSRK methods investigated by Ketcheson Gottlieb and MacDonald (2011).

s	GLM 211	GLM 221	GLM 212	GLM 222	TSRK2
2					0.707
3					0.816
4					0.866
5					0.894
6					0.913
7					0.926
8					0.935
9					0.943
10					0.949

Table: \mathcal{C}_{eff} for GLMs (15) with $p = 2$, $q = 1, 2$ and $\text{rank}(\mathbf{V}) = 1, 2$, and \mathcal{C}_{eff} for TSRK methods of order $p = 2$, with s internal stages, $2 \leq s \leq 10$

s	GLM 211	GLM 221	GLM 212	GLM 222	TSRK2
2		0.691			0.707
3		0.787			0.816
4		0.837			0.866
5		0.868			0.894
6		0.889			0.913
7		0.905			0.926
8		0.916			0.935
9		0.925			0.943
10		0.936			0.949

Table: \mathcal{C}_{eff} for GLMs (15) with $p = 2$, $q = 1, 2$ and $\text{rank}(\mathbf{V}) = 1, 2$, and \mathcal{C}_{eff} for TSRK methods of order $p = 2$, with s internal stages, $2 \leq s \leq 10$

s	GLM 211	GLM 221	GLM 212	GLM 222	TSRK2
2	0.740	0.691			0.707
3	0.829	0.787			0.816
4	0.873	0.837			0.866
5	0.899	0.868			0.894
6	0.916	0.889			0.913
7	0.928	0.905			0.926
8	0.937	0.916			0.935
9	0.944	0.925			0.943
10	0.950	0.936			0.949

Table: \mathcal{C}_{eff} for GLMs (15) with $p = 2$, $q = 1, 2$ and $\text{rank}(\mathbf{V}) = 1, 2$, and \mathcal{C}_{eff} for TSRK methods of order $p = 2$, with s internal stages, $2 \leq s \leq 10$

s	GLM 211	GLM 221	GLM 212	GLM 222	TSRK2
2	0.740	0.691		0.822	0.707
3	0.829	0.787		0.881	0.816
4	0.873	0.837		0.910	0.866
5	0.899	0.868		0.928	0.894
6	0.916	0.889		0.940	0.913
7	0.928	0.905		0.948	0.926
8	0.937	0.916		0.955	0.935
9	0.944	0.925		0.960	0.943
10	0.950	0.936		0.964	0.949

Table: \mathcal{C}_{eff} for GLMs (15) with $p = 2$, $q = 1, 2$ and $\text{rank}(\mathbf{V}) = 1, 2$, and \mathcal{C}_{eff} for TSRK methods of order $p = 2$, with s internal stages, $2 \leq s \leq 10$

s	GLM 211	GLM 221	GLM 212	GLM 222	TSRK2
2	0.740	0.691	0.847	0.822	0.707
3	0.829	0.787	0.902	0.881	0.816
4	0.873	0.837	0.928	0.910	0.866
5	0.899	0.868	0.943	0.928	0.894
6	0.916	0.889	0.953	0.940	0.913
7	0.928	0.905	0.960	0.948	0.926
8	0.937	0.916	0.965	0.955	0.935
9	0.944	0.925	0.969	0.960	0.943
10	0.950	0.936	0.972	0.964	0.949

Table: \mathcal{C}_{eff} for GLMs (15) with $p = 2$, $q = 1, 2$ and $\text{rank}(\mathbf{V}) = 1, 2$, and \mathcal{C}_{eff} for TSRK methods of order $p = 2$, with s internal stages, $2 \leq s \leq 10$

s	GLM 311	GLM 321	GLM 331	GLM 312	GLM 322	GLM 332	TSRK
2	0.401	0.222		0.412	0.293		0.366
3	0.452	0.398	0.106	0.550	0.483	0.136	0.550
4	0.530	0.516	0.249	0.612	0.527	0.360	0.578
5	0.564	0.551	0.344	0.659	0.572	0.423	0.598
6	0.607	0.579	0.410	0.694	0.581	0.443	0.630
7	0.636	0.569	0.426	0.711	0.575	0.461	0.641
8	0.661	0.562	0.474	0.750	0.565	0.477	0.653
9	0.680	0.570	0.481	0.742	0.570	0.489	0.667
10	0.688	0.577	0.477	0.734	0.569	0.498	0.683

Table: C_{eff} for GLMs (15) with $p = 3$, $q = 1, 2, 3$ and $\text{rank}(\mathbf{V}) = 1, 2$, and C_{eff} for TSRK methods of order $p = 3$, with s internal stages, $2 \leq s \leq 10$

s	GLM 411	GLM 421	GLM 431	GLM 412	GLM 422	GLM 432	TSRK
3	0.277	0.239	0.017	0.318	0.293	0.030	0.286
4	0.393	0.368	0.114	0.409	0.444	0.156	0.398
5	0.471	0.455	0.219	0.485	0.477	0.260	0.472
6	0.507	0.479	0.302	0.541	0.495	0.395	0.506
7	0.543	0.500	0.415	0.569	0.513	0.422	0.534
8	0.575	0.515	0.434	0.583	0.520	0.434	0.562
9	0.609	0.516	0.444	0.609	0.516	0.447	0.586
10	0.629	0.518	0.451	0.619*	0.518	0.458	0.610

Table: C_{eff} for GLMs (15) with $p = 4$, $q = 1, 2, 3$ and $\text{rank}(\mathbf{V}) = 1, 2$, and C_{eff} for TSRK methods of order $p = 4$, with s internal stages, $3 \leq s \leq 10$

Stability regions of SSP GLMs with $p = 2$ and $q = 1$, $2 \leq s \leq 10$

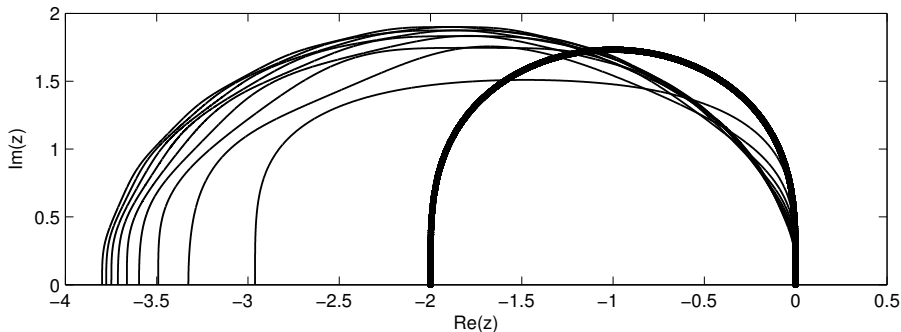


Figure: Stability region of RK method with $p = s = 2$ (thick line) and scaled stability regions of SSP GLMs of order $p = 2$ and stage order $q = 1$ with s stages (thin lines). These regions increase in size as s ranges from 2 to 10.

Stability regions of SSP GLMs with $p = 3$ and $q = 1$, $2 \leq s \leq 10$

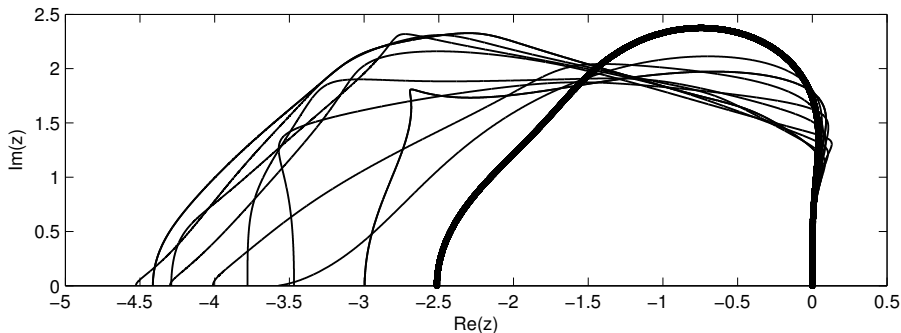


Figure: Stability region of RK method with $p = s = 3$ (thick line) and scaled stability regions of SSP GLMs of order $p = 3$ and stage order $q = 1$ with s stages (thin lines). These regions increase in size as s ranges from 2 to 10.

Stability regions of SSP GLMs with $p = 4$ and $q = 1$, $3 \leq s \leq 10$

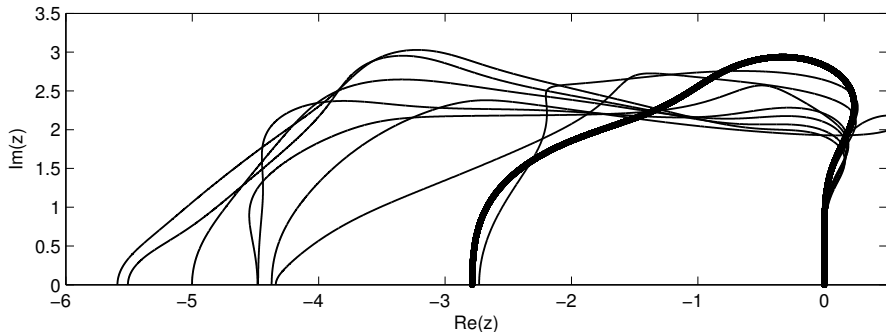


Figure: Stability region of RK method with $p = s = 4$ (thick line) and scaled stability regions of SSP GLMs of order $p = 4$ and stage order $q = 1$ with s stages (thin lines). These regions increase in size as s ranges from 3 to 10.

Test equation for order of convergence verification

To verify order of convergence of the methods discussed in this talk we will use the test problem from Sanz-Serna, Verwer, Hundsdorfer (1987) and Constantinescu and Sandu (2010)

$$\frac{\partial y(x, t)}{\partial t} = -\frac{\partial y(x, t)}{\partial x} + \frac{t - x}{(1 + t)^2}, \quad 0 \leq x \leq 1, \quad 0 \leq t \leq 1, \quad (26)$$

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

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

This solution is linear in space and, as observed by Constantinescu and Sandu (2010), we can use first-order upwind discretization in space variable x without introducing discretization errors.

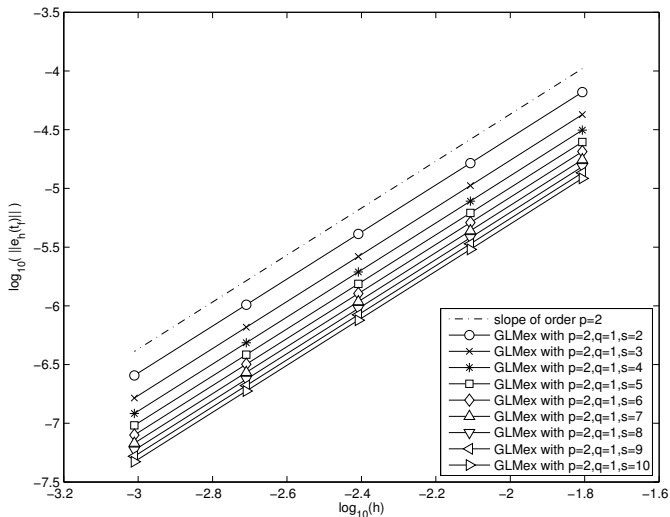


Figure: Order verification for GLMs of order $p = 2$ and stage order $q = 1$ with $2 \leq s \leq 10$ stages.

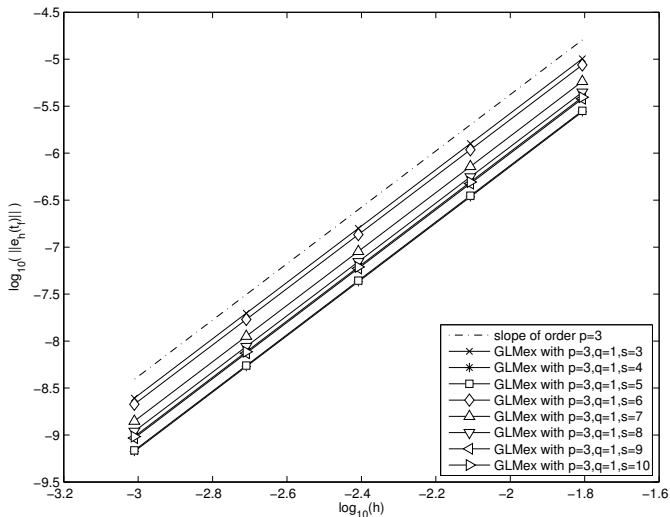


Figure: Order verification for GLMs of order $p = 3$ and stage order $q = 1$ with $2 \leq s \leq 10$ stages.

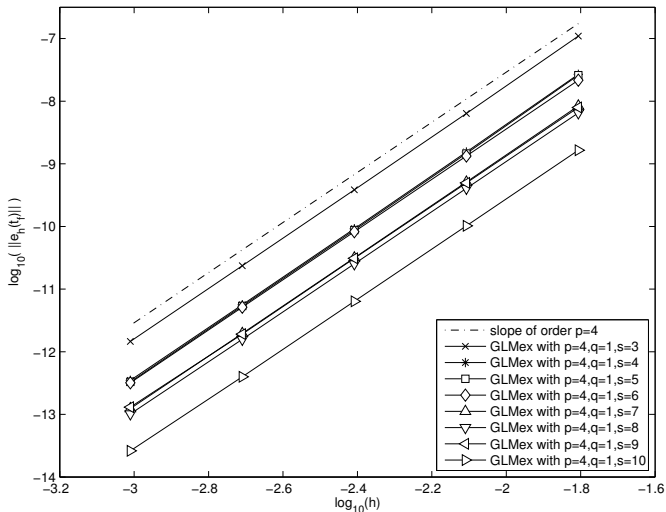


Figure: Order verification for GLMs of order $p = 4$ and stage order $q = 1$ with $2 \leq s \leq 10$ stages.

Order verification

N	SSP $p = s = 2, q = 1$		SSP $p = s = 3, q = 1$		SSP $p = s = 4, q = 1$	
	error	order	error	order	error	order
64	6.61e-05	–	1.01e-05	–	2.69e-08	–
128	1.64e-05	2.01	1.27e-06	3.00	1.54e-09	4.13
256	4.09e-06	2.00	1.58e-07	3.00	9.21e-11	4.06
512	1.02e-06	2.00	1.98e-08	3.00	5.63e-12	4.03
1024	2.55e-07	2.00	2.47e-09	3.00	3.49e-13	4.01

Table: Accuracy test for problem (26) for the SSP GLM methods with $p = s = 2$, $p = s = 3$, $p = s = 4$, and $q = 1$. The first columns displays the number of steps N .

Monotonicity verification

To verify monotonicity properties of GLMs discussed in this talk we consider, following Constantinescu and Sandu (2010) and Ketcheson, Gottlieb and MacDonald (2011), the inviscid Burgers equation

$$\frac{\partial y(x, t)}{\partial t} + \frac{\partial}{\partial x} \left(\frac{1}{2} y^2(x, t) \right) = 0, \quad 0 \leq x \leq 1, \quad 0 \leq t \leq t_{end}, \quad (27)$$

with discontinuous initial condition

$$y(x, 0) = \begin{cases} 0, & 0 \leq x < 0.5 \quad \text{or} \quad 1 < x \leq 2, \\ 1, & 0.5 \leq x \leq 2, \end{cases}$$

and periodic boundary conditions

$$y(0, t) = y(1, t), \quad 0 \leq t \leq t_{end}.$$

Space discretization

The space derivative in (27) was discretized by the conservative upwind approximation of the first order

$$y^2(x_i, t) \approx \frac{y^2(x_i, t) - y^2(x_{i-1}, t)}{\Delta x},$$

$i = 1, 2, \dots, N$, where $x_i = i\Delta x$, $i = 0, 1, \dots, N$, $N\Delta x = 2$.

The resulting system of ordinary differential equations corresponding to $N = 100$ spatial points was then solved on the time interval $[0, 0.5]$.

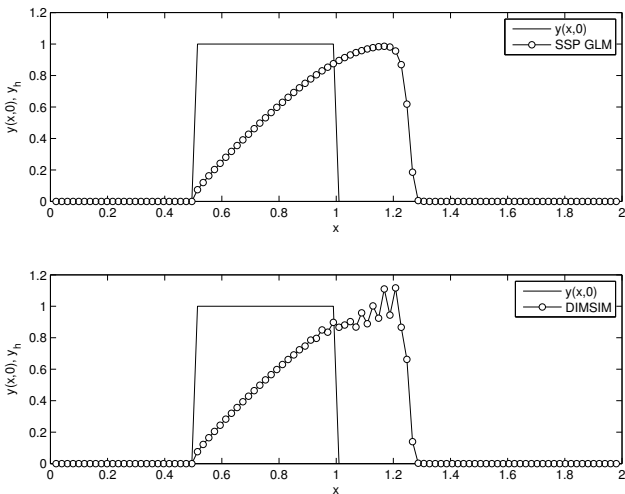


Figure: Numerical approximations at $t_{end} = 0.5$ to the discretization of Burgers equation with $N = 100$, obtained by SSP GLM of order $p = 2$ and stage order $q = 1$, and by DIMSIM of order $p = 2$ and stage order $q = 2$ which is not SSP

Buckley-Leverett equation

Following Ferracina and Spijker (2008) and Ketcheson, Gottlieb and MacDonald (2011) we consider also the Buckley-Leverett equation

$$\frac{\partial y(x, t)}{\partial t} + \frac{\partial}{\partial x} \left(\Phi(y(x, t)) \right) = 0, \quad 0 \leq x \leq 1, \quad 0 \leq t \leq t_{end}, \quad (28)$$

with

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

This equation models a two-phase flow through the porous media (LeVeque (2002)). We take $a = 1/3$ and assume the discontinuous initial condition

$$y(x, 0) = \begin{cases} 0, & 0 \leq x \leq 0.5, \\ 1, & 0.5 < x \leq 1, \end{cases}$$

and periodic boundary conditions

$$y(0, t) = y(1, t), \quad 0 \leq t \leq t_{end}.$$

Space discretization

As in Ferracina and Spijker (2008) the equation (28) was approximated by the system of ordinary differential equations of the form

$$y'_i(t) = \frac{\Phi(y_{i-\frac{1}{2}}(t)) - \Phi(y_{i+\frac{1}{2}}(t))}{\Delta x}, \quad (29)$$

where $y_i(t) \approx y(x_i, t)$, $x_i = i\Delta x$, $i = 0, 1, \dots, N$, $N\Delta x = 1$. We define

$$y_{j+\frac{1}{2}}(t) = y_j(t) + \frac{1}{2}\phi(\theta_j(t))(y_{j+1}(t) - y_j(t)),$$

where $\phi(\theta)$ is a limiter function, due to Koren (1993), which is defined by

$$\phi(\theta) = \max \left\{ 0, \min \left\{ 2, \frac{2}{3} + \frac{1}{3}\theta, 2\theta \right\} \right\},$$

and

$$\theta_j(t) = \begin{cases} 0, & j = 0, \\ \frac{y_j(t) - y_{j-1}(t)}{y_{j+1}(t) - y_j(t)}, & j = 1, 2, \dots, N. \end{cases}$$

Space discretization - continued

We semi-discretize the problem (28) using $N = 100$ spatial points and, as in Ferracina and Spijker (2008) and Ketcheson, Gottlieb and MacDonald (2011), we integrate the resulting system of ordinary differential equations (29) on the interval $[0, 1/8]$.

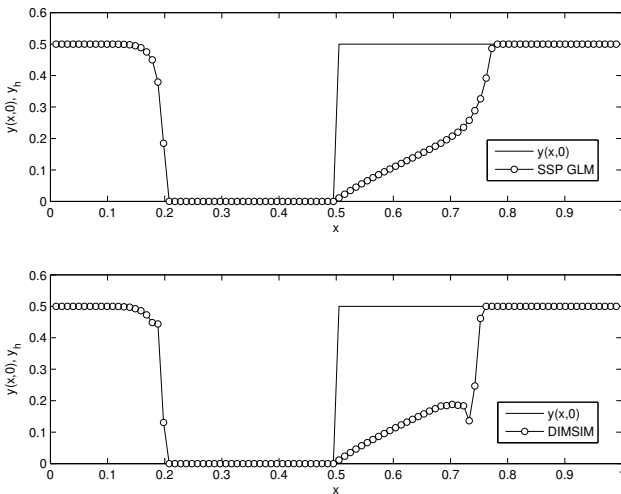


Figure: Numerical approximations at $t_{end} = 1/8$ to the discretization of the Buckley-Leverett equation with $N = 100$, obtained by SSP GLM of order $p = 2$ and stage order $q = 1$, and by DIMSIM with $p = q = 2$ which is not SSP

Concluding remarks

- We presented a systematic approach to the construction of SSP GLMs for ODEs.
- The search for SSP GLMs is based on the characterization of CFL coefficient, which was derived by Spijker (2007).
- SSP GLMs were computed by the solution of constrained optimization problem with inequality constrains which characterize CFL coefficient, and equality constrains corresponding to order and stage order conditions.
- SSP GLMs do not lead to spurious oscillations when applied to discretization of hyperbolic conservation laws with discontinuous initial conditions.
- SSP GLMs up to order $p = 4$ were analyzed. Future work will address the construction of SSP GLMs of higher order and the construction of implicit SSP GLMs.