

A Class of Explicit Second Derivative General Linear Methods for Non-Stiff ODEs

Mohammad Sharifi^a, Ali Abdi^{a,b}, Michal Brašc^c and Gholamreza Hojjati^{a,b}

^a*Faculty of Mathematics, Statistics and Computer Science, University of Tabriz, Tabriz, Iran*

^b*Research Department of Computational Algorithms and Mathematical Models, University of Tabriz, Tabriz, Iran*

^c*AGH University of Science and Technology, Faculty of Applied Mathematics al. Mickiewicza 30, 30059 Kraków, Poland*

E-mail: moh.sharifi@tabrizu.ac.ir

E-mail(*corresp.*): a.abdi@tabrizu.ac.ir

E-mail: bras@agh.edu.pl

E-mail: ghojjati@tabrizu.ac.ir

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Abstract. In this paper, we construct explicit second derivative general linear methods (SGLMs) with quadratic stability and a large region of absolute stability for the numerical solution of non-stiff ODEs. The methods are constructed in two different cases: SGLMs with $p = q = r = s$ and SGLMs with $p = q$ and $r = s = 2$ in which p , q , r and s are respectively the order, stage order, the number of external stages and the number of internal stages. Examples of the methods up to order five are given. The efficiency of the constructed methods is illustrated by applying them to some well-known non-stiff problems and comparing the obtained results with those of general linear methods of the same order and stage order.

Keywords: non-stiff ODEs, general linear methods, second derivative methods, order conditions, quadratic stability.

AMS Subject Classification: 65L05.

1 Introduction

Explicit numerical integrators are usually utilized in dealing with non-stiff or mildly stiff systems of ordinary differential equations (ODEs) such as Hamil-

tonian problems and the systems resulting from discretization of the equations coming from systems of hyperbolic conservation laws. These integrators are straightforward to implement and sufficiently accurate if the stepsizes are small enough.

One of the directions to construct methods with high order and extensive absolute stability region is using the higher derivatives of the solution into the integration formulas. Many efficient methods incorporating the second derivative and even higher derivatives terms of the solution have been already introduced in different classes; for instance, second derivative of extended backward differentiation formulas (SDEBDFs) by Cash [9], second derivative of multistep methods (SDMMs) by Chakravarti and Kamel [10], Enright [12] and Gupta [16], two-derivative Runge-Kutta (TDRK) methods by Chan and Tsai [11, 26] and Fang et al. [14], three-derivative Runge-Kutta (ThDRK) methods by Turaci and Öziş [27] and high order multiderivative methods by Gottlieb et al. [15], Schütz et al. [23] and Seal et al. [24].

In this paper, we are going to construct the explicit second derivative general linear methods (SGLMs) up to order five with a large region of absolute stability. The class of SGLMs for the numerical solution of the autonomous system of ODEs with initial values

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

in which $f : \mathbb{R}^m \rightarrow \mathbb{R}^m$, $y : \mathbb{R} \rightarrow \mathbb{R}^m$, with m as the dimension of the system, is an extension of the class of general linear methods (GLMs) [5, 6, 19] incorporating the second derivative of the solution $g(y(t)) := y''(t) = f_y(y)f(y)$ into the formula. SGLMs which have been first introduced by Butcher and Hojjati in [7] and studied more by Abdi and Hojjati, for instance, in [1, 2, 25], are characterized by four integers (p, q, r, s) where p is the order, q is the stage order, r is the number of external stages, and s is the number of internal stages. Let $c = [c_1 \ c_2 \ \dots \ c_s]^T$ be the abscissa vector and $[Y_i^{[n]}]_{i=1}^s$ be an approximation of order q to the vector $y(x_{n-1} + ch) := [y(x_{n-1} + c_i h)]_{i=1}^s$, and the vectors $F(Y^{[n]}) := [f(Y_i^{[n]})]_{i=1}^s$ and $G(Y^{[n]}) := [g(Y_i^{[n]})]_{i=1}^s$ indicate the stage first and second derivative values. An s -stage/ r -value SGLM, with the stepsize h and the rm -dimensional vectors $y^{[n-1]}$ and $y^{[n]}$ as the input and output vectors, for the numerical solution of (1.1) is given by

$$\begin{aligned} Y^{[n]} &= h(A \otimes I_m)F(Y^{[n]}) + h^2(\bar{A} \otimes I_m)G(Y^{[n]}) + (U \otimes I_m)y^{[n-1]}, \\ y^{[n]} &= h(B \otimes I_m)F(Y^{[n]}) + h^2(\bar{B} \otimes I_m)G(Y^{[n]}) + (V \otimes I_m)y^{[n-1]}, \end{aligned} \tag{1.2}$$

where $n = 1, 2, \dots, N$, $Nh = \bar{t} - t_0$, I_m is the identity matrix of dimension m , and \otimes is the Kronecker product of two matrices. The coefficients matrices of the method (1.2) given by

$$A, \bar{A} \in \mathbb{R}^{s \times s}, \quad U \in \mathbb{R}^{s \times r}, \quad B, \bar{B} \in \mathbb{R}^{r \times s}, \quad V \in \mathbb{R}^{r \times r},$$

are usually represented as a partitioned $(s + r) \times (2s + r)$ matrix

$$\left[\begin{array}{c|c|c} A & \bar{A} & U \\ \hline B & \bar{B} & V \end{array} \right].$$

An SGLM with the input vector satisfying

$$y^{[n-1]} = (W \otimes I_m) z(x_{n-1}, h) + \mathcal{O}(h^{p+1}),$$

where $z(t, h)$ is the Nordsieck vector given by

$$z(t, h) := \begin{bmatrix} y(t) \\ hy'(t) \\ \vdots \\ h^p y^{(p)}(t) \end{bmatrix},$$

and $W := [\alpha_{ij}] \in \mathbb{R}^{r \times (p+1)}$ is a real matrix containing the parameters of the method, has order p and stage order q when its internal and external stage values satisfy

$$Y^{[n]} = y(x_{n-1} + ch) + \mathcal{O}(h^{q+1}),$$

and

$$y^{[n]} = (W \otimes I_m) z(x_n, h) + \mathcal{O}(h^{p+1}).$$

The paper is organized as follows. A brief review of SGLMs is presented in Section 2. Construction of quadratically stable explicit SGLMs are discussed in Sections 3 and 4 in two different classes: methods with $p = q = r = s$ and two-stage/two-value methods with $p = q$. Examples of such methods are given up to order five with small error constants and a large absolute stability region resulted from minimizing the objective function for the negative area of the intersection of the absolute stability region with the negative half plane. By giving a suitable starting procedures for the proposed methods, some numerical experiments are given in Section 5 illustrating the efficiency of the methods and verifying the theoretical order of convergence. Moreover, the results are compared with those of quadratically stable explicit GLMs presented in [4]. Finally, the paper is closed in Section 6 by concluding remarks and giving ideas for future work.

2 A brief review of SGLMs

In this section, we review some results on SGLMs that have been already studied and developed in previous works.

Abdi and Hojjati investigated the main features of these methods, such as consistency, stability, and convergency. For more details, we refer the reader to review the references in the papers [1, 2, 25]. Some types of these methods depending on the problems to be solved have been successfully constructed and implemented in a variety of ways. The order and stage order conditions for SGLMs with the input and output vectors approximating the Nordsieck

vector, methods with the matrix $W = I_r$, and RKS property were obtained by Butcher and Hojjati [7] for the case $p = q$. The order and stage order conditions of SGLMs of order p and stage order q in general form, rather than Nordsieck form, for the case $q = p$ are given by (cf. [2, 25])

$$\exp(cz) = zA \exp(cz) + z^2\bar{A} \exp(cz) + UWZ + \mathcal{O}(z^{p+1}), \tag{2.1}$$

$$\exp(z)WZ = zB \exp(cz) + z^2\bar{B} \exp(cz) + VWZ + \mathcal{O}(z^{p+1}), \tag{2.2}$$

in which $\exp(cz) = [\exp(c_1z) \exp(c_2z) \cdots \exp(c_s z)]$ and $Z = [1 \ z \ \cdots \ z^p]$. In the case of $r = s$ and $U = I_s$, the matrix W is uniquely determined by (2.1) in terms of the coefficients of the method as (cf. [2, 25])

$$W = C - ACK - \bar{A}CK^2, \tag{2.3}$$

where $C = (C_{ij}) \in \mathbb{R}^{s \times (p+1)}$ is the scaled Vandermonde matrix with components

$$C_{ij} = c_i^{j-1} / (j-1)!, \quad 1 \leq i \leq s, \quad 1 \leq j \leq p+1,$$

and $K \in \mathbb{R}^{(p+1) \times (p+1)}$ is the shifting matrix defined by $K = [0 \ e_1 \ \cdots \ e_p]$ with e_j as the j th unit vector.

The stability behavior of SGLMs with respect to Dahlquist linear test problem $y' = \xi y$, with $\xi \in \mathbb{C}$, is governed by the stability matrix [7]

$$M(z) = V + z(B + z\bar{B})(I_s - zA - z^2\bar{A})^{-1}U, \tag{2.4}$$

with $z = h\xi$, and therefore the stability function $p(w, z)$ defined by

$$p(w, z) / \det(I_s - zA - z^2\bar{A}) = \det(wI_r - M(z)),$$

which is a polynomial of degree r with respect to w whose coefficients are polynomials of degree at most $2s$ with respect to z . Moreover, the region \mathcal{A} of absolute stability (1.2) is defined by

$$\mathcal{A} = \{z \in \mathbb{C} : |w_i(z)| < 1, i = 1, 2, \dots, r\},$$

where $w_i(z)$, $i = 1, 2, \dots, r$ are the roots of $p(w, z)$. As the complexity of the stability function $p(w, z)$ dramatically increases as the order is increased, it would be desirable to construct methods with the stability function in the form

$$p(w, z) = w^{r-1}(p_r(z)w - p_{r-1}(z)), \tag{2.5}$$

or in the form

$$p(w, z) = w^{r-2}(p_r(z)w^2 - p_{r-1}(z)w + p_{r-2}(z)), \tag{2.6}$$

with $p_r(z) := \det(I_s - zA - z^2\bar{A})$. An SGLM is said to possess Runge–Kutta stability (RKS) or quadratic stability (QS) property if its stability function is respectively in the form (2.5) or (2.6). Indeed, the conditions for methods to have RKS or QS property respectively are

$$p_0(z) \equiv p_1(z) \equiv \cdots \equiv p_{r-2}(z) \equiv 0, \quad p_0(z) \equiv p_1(z) \equiv \cdots \equiv p_{r-3}(z) \equiv 0. \tag{2.7}$$

Abdi and Hojjati introduced second derivative diagonally implicit multi-stage integration methods (SDIMSIMs) as a new subclass of SGLMs and divided them into four types together with two order barriers for two types of parallel methods with RKS property. For more details, the reader can track the references in the papers [2,25]. Also, the order barriers for two types of sequential SGLMs with RKS properties were studied and obtained by these authors; more details can be found by reviewing the references in the papers [1, 2, 25]. The order conditions for SDIMSIMs were obtained for the case of $p = q = r = s$, $U = I_s$ and $Ve = e$ with e as the all-ones s -dimensional vector, as [2]

$$B = B_0 - AB_1 - \bar{A}B_2 - VB_3 - (\bar{B} - V\bar{A})B_4 + VA, \tag{2.8}$$

where the (i, j) elements of B_0, B_1, B_2, B_3 , and B_4 are respectively given by

$$\frac{\int_0^{1+c_i} \Phi_j(x)dx}{\Phi_j(c_j)}, \quad \frac{\Phi_j(1+c_i)dx}{\Phi_j(c_j)}, \quad \frac{\Phi'_j(1+c_i)dx}{\Phi_j(c_j)}, \quad \frac{\int_0^{c_i} \Phi_j(x)dx}{\Phi_j(c_j)}, \quad \frac{\Phi'_j(c_i)dx}{\Phi_j(c_j)},$$

with

$$\Phi_i(x) = \prod_{j=1, j \neq i}^s (x - c_j), \quad i = 1, 2, \dots, s.$$

Some examples of such methods with RKS property for all four types with $p = q = r = s \leq 4$ were constructed in [2]. Due to impossibility of solving RKS property conditions in the construction of SDIMSIMs of high orders by symbolic manipulation packages, some variants of the Fourier series approach were used to construct SDIMSIMs with RKS property with $p = q = r = s \geq 5$ [25].

Although, it is desirable to construct SGLMs with RKS property, due to requiring to solve large systems of polynomial-equations of high degree for large values of r and s parameters, it is complicated task. To made easier to achieve RKS property, in [13], the authors introduced a special case of SGLMs as $A - \bar{A} - V$ methods. One approach to construct the methods with high order is to relax the concept of RKS property to the concept of QS property. Such implicit methods have been discussed by Abdi [1] and Movahedinejad et al. [21].

The implementation issues of SGLMs including the starting procedures, stage predictors, local error estimation, and changing stepsize are studied in [22]. Moreover, practical implementation of SGLMs in a VS environment were studied (see reference no. 5 in the paper [25]) by developing the MATLAB code, SGLM4, which outperforms the code ode15s from MATLAB ODE suite on systems whose Jacobian has eigenvalues which are close to the imaginary axis.

3 Construction of explicit SGLMs with $p = q = r = s$ and QS property

In this section, we construct explicit SGLMs with $p = q = r = s$ up to order five with QS property. In these methods $A = [a_{ij}]_{i,j=1}^s$ and $\bar{A} = [\bar{a}_{ij}]_{i,j=1}^s$ are strictly lower triangular matrices. Here, we consider $U = I_r, \bar{B} = V\bar{A}$, and $V = ev^T$, with $v^T = [1 - \nu \quad v_1 \quad v_2 \quad \dots \quad v_{r-1}]$ and $\nu = \sum_{i=1}^{r-1} v_i$. This form

for the matrix V guarantees the zero-stability of the methods. The matrix B is computed by (2.8) as an equivalence relation for the order conditions. In the construction of the methods, we use “ C -condition” meaning that the error constant of the proposed methods are less than or equal to a specific value. To do this, we need to derive a formula for the error constant of the methods. Following is a theorem and a remark that can lead to such a formula. To state the theorem, let us introduce the vector $\hat{y}^{[n]} := (W \otimes I_m) z(x_n, h)$.

Theorem 1. *For the SGLM (1.2) of order p and stage order $q = p$ with $V = ev^T$, we have*

$$\hat{y}^{[n]} = M(z)\hat{y}^{[n-1]} + \varphi_p z^{p+1} + \mathcal{O}(z^{p+2}), \tag{3.1}$$

where $M(z)$ is defined by (2.4) and φ_p is given by

$$\varphi_p = \frac{Bc^p}{p!} + \frac{\overline{B}c^{p-1}}{(p-1)!} - WE_{p+1},$$

with $E_{p+1} = [1/(p+1)! \ 1/p! \ \dots \ 1/1!]^T$.

Proof. For the method (1.2) of order p and stage order $q = p$ applied to the test problem $y' = \xi y$, with $\xi \in \mathbb{C}$, we have

$$y(x_{n-1} + ch) = (I_s - zA - z^2\overline{A})^{-1}U\hat{y}^{[n-1]} + \mathcal{O}(z^{p+1}),$$

and also using of Taylor series we get

$$\begin{aligned} \hat{y}^{[n]} &= (zB + z^2\overline{B})y(x_{n-1} + ch) + V\hat{y}^{[n-1]} \\ &+ \left(\frac{Bc^p}{p!} + \frac{\overline{B}c^{p-1}}{(p-1)!} - WE_{p+1} \right) z^{p+1} + \mathcal{O}(z^{p+2}), \end{aligned}$$

with c^j as the component-wise powers of abscissa vector c . Substituting the relation for $y(x_{n-1} + ch)$ into the last one, we find

$$\hat{y}^{[n]} = M(z)\hat{y}^{[n-1]} + \left(\frac{Bc^p}{p!} + \frac{\overline{B}c^{p-1}}{(p-1)!} - WE_{p+1} \right) z^{p+1} + \mathcal{O}(z^{p+2}),$$

which completes the proof. \square

Remark 1. The error in the performing the steps of the method (1.2) with a rank-one matrix V in the form $V = ev^T$ is principally propagated through the quantity $(v^T \otimes I_m)y^{[n-1]}$. Therefore, it is more important to find a relation for $(v^T \otimes I_m)\hat{y}^{[n]}$ instead of $\hat{y}^{[n]}$. Multiplying (3.1) on the left by v^T gives

$$v^T\hat{y}^{[n]} = v^T M(z)\hat{y}^{[n-1]} + v^T\varphi_p z^{p+1} + \mathcal{O}(z^{p+2}).$$

Here, the quantity $v^T\varphi_p$ is called the *error constant* of the method.

After solving the C -condition and the conditions for QS property for some parameters in the matrices A, \overline{A} , and V , a number of coefficients of the method remain as the free parameters which are used to construct methods with large

absolute stability regions. To do this, defining an objective function for the negative area of the intersection of the absolute stability region with \mathbb{C}^- denoted by $-\mathbf{area}$, we solve the minimization problem

$$\min \quad -\mathbf{area}, \tag{3.2}$$

using the subroutines `fminsearch` or `fmincon` in MATLAB. Since every method has a symmetric region of absolute stability with respect to the real axis, the integral in polar coordinates can be used to calculate the area of its intersection with the negative half plane, as

$$\mathbf{area} := \int_0^{\pi/2} r^2(\theta)d\theta,$$

where $r = r(\theta)$ stands for the ray that extends from the coordinate origin to the boundary $\partial\mathcal{A}$ of the region of absolute stability \mathcal{A} , and θ denotes the angle formed by the ray and the negative real axis. Following [3], here we use the composite trapezoidal rule to compute an approximation of this area in the form

$$\mathbf{area} \approx \Delta\theta \left(\frac{1}{2}r^2(\theta_0) + \sum_{k=1}^{N-1} r^2(\theta_k) + \frac{1}{2}r^2(\theta_N) \right),$$

where N is a large enough positive integer and $\theta_k = k\Delta\theta$, $k = 0, 1, \dots, N$, $N\Delta\theta = \frac{\pi}{2}$. Also, to compute the rays $r_k := r(\theta_k)$ corresponds to the point on the boundary of absolute stability region \mathcal{A} , we use the bisection method applied to the equation

$$p(w, -r_k e^{i\theta_k}) = 0,$$

where $|w| = 1$ and i is the imaginary unit. In the case of using `fmincon` command, we use the nonlinear inequality constraint $C_{p+1} \leq C_{p+1}^*$ in which C_{p+1}^* is the error constant of GLM with inherent QS (IQS) property of order $p = q = s = r - 1$, denoted by GLM_p , constructed in [4]. The constructed methods of order p in this section are denoted by SGLM_p .

3.1 Construction of order two methods

In this subsection, we construct methods of order $p = q = 2$ and the abscissa vector $c = [0 \ 1]^T$ with the error constant $C_3 = 10^{-2}$. Imposing the C -condition for the parameter v_1 , yields $v_1 = \frac{14}{75(1-\bar{a}_{21})}$ and we obtain a two-parameter family of the methods with QS property depending on a_{21} and \bar{a}_{21} . By (2.8) and $\bar{B} = V\bar{A}$, we get

$$B = \begin{bmatrix} \frac{7-14a_{21}}{75(\bar{a}_{21}-1)} + \frac{1}{2} & \frac{7}{75(\bar{a}_{21}-1)} + \frac{1}{2} \\ \frac{7-14a_{21}}{75(\bar{a}_{21}-1)} + \bar{a}_{21} & \frac{7}{75(\bar{a}_{21}-1)} - a_{21} - \bar{a}_{21} + 2 \end{bmatrix}, \bar{B} = \begin{bmatrix} -\frac{14\bar{a}_{21}}{75(\bar{a}_{21}-1)} & 0 \\ -\frac{14\bar{a}_{21}}{75(\bar{a}_{21}-1)} & 0 \end{bmatrix}.$$

To derive a method with a large absolute stability region, solving the minimization problem (3.2) by using `fminsearch` command for two free parameters leads

to $a_{21} = 0.30322602$ and $\bar{a}_{21} = 0.73766292$. The coefficients matrices of this method are given by

$$\left[\begin{array}{cc|cc|cc} 0 & 0 & 0 & 0 & 1 & 0 \\ 0.30322602 & 0 & 0.73766292 & 0 & 0 & 1 \\ \hline 0.35998493 & 0.14422363 & 0.52488608 & 0 & 0.28844725 & 0.71155275 \\ 0.59764786 & 0.60333469 & 0.52488608 & 0 & 0.28844725 & 0.71155275 \end{array} \right],$$

where the coefficients are rounded to eight decimal places. The area of the absolute stability region for the constructed SGLM₂ is larger than that for GLM₂ (12.39 vs. 9.10) with smaller error constant (0.01 vs. 0.0159). The absolute stability regions for SGLM₂ and GLM₂ have been plotted in Figure 1.

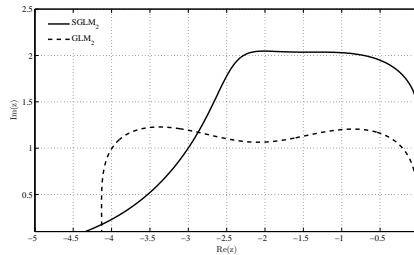


Figure 1. The absolute stability regions for SGLM₂ and GLM₂.

3.2 Construction of order three methods

In this subsection, we construct methods of order $p = q = 3$ and the abscissa vector $c = [0 \ \frac{1}{2} \ 1]^T$. Imposing stage order and order conditions (2.3) and (2.8) and solving the QS conditions (2.7), we obtain a six-parameter family of the methods of order and stage order three depending on $a_{31}, a_{32}, \bar{a}_{31}, \bar{a}_{32}, v_1,$ and v_2 . Now, solving the minimization problem (3.2) for these free parameters by using `fmincon` command with the nonlinear inequality constraint $C_4 \leq C_4^*$, we get

$$\begin{aligned} a_{31} &= -0.16271773, & a_{32} &= 0.96977667, & \bar{a}_{31} &= -0.11707611, \\ a_{32} &= 0.14104315, & v_1 &= 0.39504596, & v_2 &= 0.63733893. \end{aligned}$$

The coefficients matrices of this method are

$$A = \begin{bmatrix} 0 & 0 & 0 \\ 0.66029057 & 0 & 0 \\ -0.162718 & 0.96977667 & 0 \end{bmatrix}, \bar{A} = \begin{bmatrix} 0 & 0 & 0 \\ 0.117643 & 0 & 0 \\ -0.117076 & 0.141043 & 0 \end{bmatrix},$$

$$V = e \cdot [-0.03238489 \ 0.39504596 \ 0.63733893],$$

where these coefficients are rounded to eight decimal places. The matrix B is computed by the formula (2.8) and $\bar{B} = V\bar{A}$. The area of the absolute stability region for the constructed SGLM₃ is larger than that for GLM₃ (34.02 vs. 14.61) with smaller error constant (0.00166 vs. -0.016). The absolute stability regions for SGLM₃ and GLM₃ have been plotted in Figure 2.

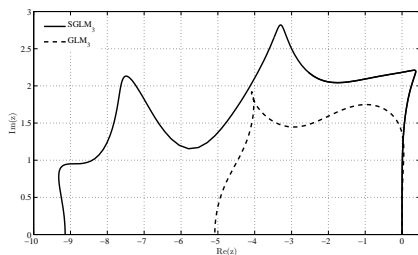


Figure 2. The absolute stability regions for SGLM₃ and GLM₃.

3.3 Construction of order four methods

In this subsection, we derive methods of order $p = q = 4$ and the abscissa vector $c = [0 \quad \frac{1}{3} \quad \frac{2}{3} \quad 1]^T$. We first impose stage order and order conditions (2.3) and (2.8) and solve the QS conditions (2.7) which results a five-parameter family of the methods of order and stage order four depending on a_{32} , \bar{a}_{21} , \bar{a}_{41} , \bar{a}_{42} , and \bar{a}_{43} . Then, solving the minimization problem (3.2) for these free parameters by using `fmincon` command with the nonlinear inequality constraint $C_5 \leq C_5^*$, gives

$$\begin{aligned} a_{32} &= 0.22767727, & \bar{a}_{21} &= 0.08769797, & \bar{a}_{41} &= 0.21933010, \\ \bar{a}_{42} &= 0.05744625, & \bar{a}_{43} &= 0.05563617. \end{aligned}$$

The coefficients matrices of the derived method take the form

$$\begin{aligned} A &= \begin{bmatrix} 0 & 0 & 0 & 0 \\ 1.53703704 & 0 & 0 & 0 \\ 3.06662395 & 0.22767727 & 0 & 0 \\ 3.59736627 & -0.07066786 & 0.46830189 & 0 \end{bmatrix}, \\ \bar{A} &= \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0.08769797 & 0 & 0 & 0 \\ 0.16252472 & 0.07907716 & 0 & 0 \\ 0.21933100 & 0.05744625 & 0.05563617 & 0 \end{bmatrix}, \\ V &= e \cdot \begin{bmatrix} -0.02564103 & 0.15576923 & -0.48461538 & 1.35448718 \end{bmatrix}. \end{aligned}$$

The coefficient matrices B and \bar{B} are respectively computed by (2.8) and the formula $\bar{B} = V\bar{A}$. The area of the absolute stability region for the derived SGLM₄ is larger than that for GLM₄ (32.91 vs. 18.36) with smaller error constant (0.0034 vs. -0.011). The absolute stability regions for SGLM₄ and GLM₄ have been plotted in Figure 3.

3.4 Construction of order five methods

In this subsection, we are going to construct methods of order $p = q = 5$ and the abscissa vector $c = [0 \quad \frac{1}{4} \quad \frac{1}{2} \quad \frac{3}{4} \quad 1]^T$. We were not able to produce the QS conditions by using symbolic manipulation tools (MATHEMATICA or MAPLE) for these methods that is generally the case for the methods of orders

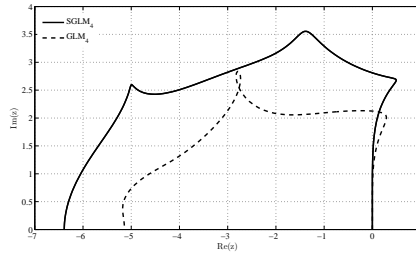


Figure 3. The absolute stability regions for SGLM₄ and GLM₄.

$p \geq 5$. Therefore, another approach to construct such methods is required. Here, we use the Fourier series approach which has been already introduced in [8] (see also [19,25]). By using this approach, the coefficients matrices of the derived method with QS property are

$$A = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0.44285749 & 0 & 0 & 0 & 0 \\ 0.25502163 & 0.31699667 & 0 & 0 & 0 \\ 0.95070766 & -0.02870187 & 0.38693336 & 0 & 0 \\ -0.17734588 & -0.00192383 & -0.08825992 & 0.86107843 & 0 \end{bmatrix},$$

$$\bar{A} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0.03843793 & 0 & 0 & 0 & 0 \\ 0.04868241 & 0.03247894 & 0 & 0 & 0 \\ 0.06281438 & -0.04443033 & 0.05682884 & 0 & 0 \\ 0.02091070 & 0.33735117 & -0.38762185 & 0.05996707 & 0 \end{bmatrix},$$

$$V = e \cdot \begin{bmatrix} -0.13481821 & 0.37627890 & -0.16849319 & 0.55340489 & 0.37362761 \end{bmatrix},$$

and the matrices B and \bar{B} are respectively computed by (2.8) and the formula $\bar{B} = V\bar{A}$. The area of the absolute stability region for the derived SGLM₅ is larger than that for GLM₅ (34.56 vs. 24.84) with smaller error constant (9.54×10^{-4} vs. -0.0031). The absolute stability regions for SGLM₅ and GLM₅ have been plotted in Figure 4.

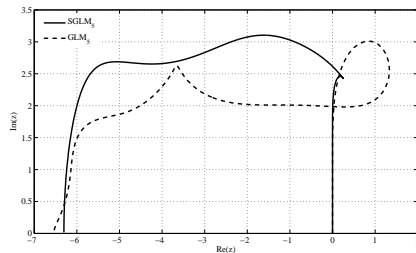


Figure 4. The absolute stability regions for SGLM₅ and GLM₅.

4 Construction of explicit two-stage SGLMs with $p = q$

In this section, we construct explicit two-value/two-stage SGLMs with $p = q$ up to order five. These coefficients matrices of the methods are

$$\left[\begin{array}{c|c|c} A & \bar{A} & U \\ \hline B & \bar{B} & V \end{array} \right] = \left[\begin{array}{cc|cc|cc} 0 & 0 & 0 & 0 & 1 & 0 \\ a_{21} & 0 & \bar{a}_{21} & 0 & 0 & 1 \\ \hline b_{11} & b_{12} & \bar{b}_{11} & \bar{b}_{12} & 1 - v_1 & v_1 \\ b_{21} & b_{22} & \bar{b}_{21} & \bar{b}_{22} & 1 - v_1 & v_1 \end{array} \right].$$

The stability function of such methods has the form

$$p(w, z) = w^2 - p_1(z)w + p_0(z),$$

where p_1 and p_0 are polynomials of degree at most 4. Indeed, the methods are automatically quadratically stable. To derive methods, we use the same approach proposed in Section 3. The constructed methods of order p in this section are denoted by SGLM $_p^2$.

4.1 Construction of two-stage order two methods

In this subsection, we construct method of order $p = q = 2$ and the abscissa vector $c = [0 \ 1]^T$ with the error constant $C_3 = 10^{-2}$. Solving stage order and order conditions (2.1) and (2.2) together with C -condition (3.1), we obtain a six-parameter family of the methods of order $p = q = 2$ depending on $a_{21}, \bar{a}_{21}, \bar{b}_{11}, \bar{b}_{12}, \bar{b}_{21}$, and \bar{b}_{22} . Now, we use these parameters to obtain a method with a large region of absolute stability which leads to

$$\begin{aligned} a_{21} &= 2.16694043, & \bar{a}_{21} &= 0.11179872, & \bar{b}_{11} &= 0.04659473, \\ \bar{b}_{12} &= 0.01885751, & \bar{b}_{21} &= -0.34896561, & \bar{b}_{22} &= -0.23192573. \end{aligned}$$

The coefficients of the derived SGLM $_2^2$ are

$$\left[\begin{array}{cc|cc|cc} 0 & 0 & 0 & 0 & 1 & 0 \\ 2.16694043 & 0 & 0.11179872 & 0 & 0 & 1 \\ \hline 0.95675662 & 0.33686864 & 0.04659473 & 0.0188575 & 0.748380 & 0.251620 \\ -0.07778824 & 0.20447307 & -0.34896561 & -0.231926 & 0.748380 & 0.251620 \end{array} \right].$$

The area of the absolute stability region of this method is ≈ 19.05 which is larger than that of SGLM $_2$ and GLM $_2$. The absolute stability regions for these three methods have been plotted in Figure 5.

4.2 Construction of two-stage order three methods

In this subsection, we construct method of order $p = q = 3$ and abscissa vector $c = [0 \ 1]^T$. Solving stage order and order conditions (2.1) and (2.2), we obtain a five-parameter family of the methods of order $p = q = 3$ depending on $a_{21}, \bar{a}_{21}, \bar{b}_{12}, \bar{b}_{22}$, and v_1 . Now, solving the minimization problem (3.2) for

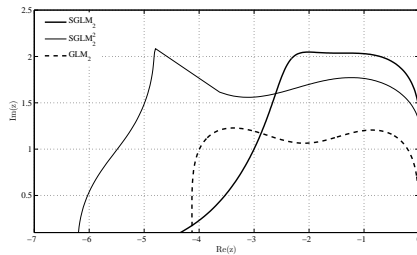


Figure 5. The absolute stability regions for $SGLM_2$, $SGLM_2^2$ and GLM_2 .

these free parameters by using `fmincon` command with the nonlinear inequality constraint $C_4 \leq C_4^*$, we obtain

$$a_{21} = 2.10393975, \quad \bar{a}_{21} = 0.37764397, \quad \bar{b}_{12} = 0.04637007, \\ \bar{b}_{22} = -0.07649131, \quad v_1 = 0.15227298.$$

The coefficients of the constructed $SGLM_3^2$ are

$$\left[\begin{array}{cc|cc|cc} 0 & 0 & 0 & 0 & 1 & 0 \\ 2.1039397 & 0 & 0.37764397 & 0 & 0 & 1 \\ \hline 0.9782647 & 0.18983554 & 0.24516288 & 0.0463701 & 0.847727 & 0.152273 \\ 0.1544965 & -0.090336 & -0.333388 & -0.076491 & 0.847727 & 0.152273 \end{array} \right],$$

The area of the absolute stability region of this method is ≈ 20.68 and its error constant is $C_4 = 0.00998$. These properties are better than those of GLM_3 . The absolute stability regions of the order three methods have been plotted in Figure 6.

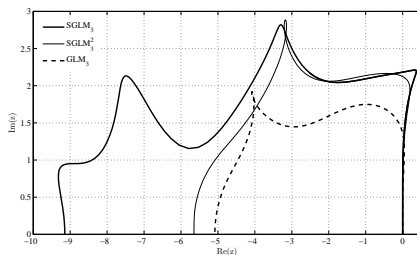


Figure 6. The absolute stability regions for $SGLM_3$, $SGLM_3^2$ and GLM_3 .

4.3 Construction of two-stage order four methods

In this subsection, we construct methods of order $p = q = 4$ and the abscissa vector $c = [0 \ 1]^T$. Solving stage order and order conditions (2.1) and (2.2), we obtain a three-parameter family of the methods of order $p = q = 4$ depending on a_{21} , \bar{a}_{21} , and v_1 . Now, solving the minimization problem (3.2) for these free parameters by using `fmincon` command with the nonlinear inequality constraint $C_5 \leq C_5^*$, leads to a method with very small absolute stability region; therefore, we ignore the constraint $C_5 \leq C_5^*$ and try to construct method with

an error constant close to that of GLM₄, a large absolute stability region, and ‘nice’ coefficient. By this approach, we get

$$a_{21} = -4.65867033, \quad \bar{a}_{21} = -0.05147224, \quad v_1 = 0.66210402.$$

The coefficients matrices of the derived SGLM₄² are

$$\left[\begin{array}{cc|cc|cc} 0 & 0 & 0 & 0 & 1 & 0 \\ -4.65867033 & 0 & -0.05147224 & 0 & 0 & 1 \\ \hline -2.9155764 & 0.168948 & -0.005922 & -0.028157 & 0.337896 & 0.6621040 \\ -1.4155764 & 4.327618 & 0.5774113 & 1.4399809 & 0.337896 & 0.6621040 \end{array} \right].$$

The area of the absolute stability region of this method is ≈ 10.77 and its error constant is $C_5 = 0.0290$. Although the area of the absolute stability region for this method is smaller than that for GLM₄, considering the fact that this method has only two stages, the scaled-area—computed by dividing the area by s —corresponding to this method is larger than that of GLM₄. The absolute stability regions of the order four methods have been plotted in Figure 7.

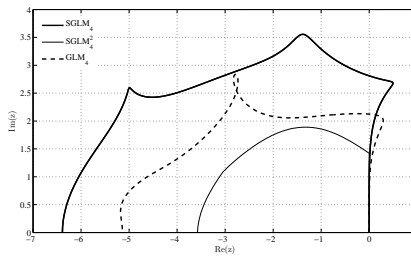


Figure 7. The absolute stability regions for SGLM₄, SGLM₄² and GLM₄.

4.4 Construction of two-stage order five methods

In this subsection, we construct method of order $p = q = 5$ and the abscissa vector $c = [c_1 \ 1]^T$. Solving stage order and order conditions (2.1) and (2.2), we obtain a two-parameter family of the methods of order $p = q = 5$ depending on c_1 and a_{21} . Similar to what has been done in the construction of two-stage order four methods in the previous subsection, we ignore the constraint $C_6 \leq C_6^*$ and try to construct method with an error constant close to that of GLM_p, a large absolute stability region, and ‘nice’ coefficient. This approach gives

$$c_1 = 0.17410748, \quad a_{21} = -7.00000000.$$

The coefficients matrices of the derived SGLM₅² are

$$\left[\begin{array}{cc|cc|cc} 0 & 0 & 0 & 0 & 1 & 0 \\ -7.00000000 & 0 & 2.57041942 & 0 & 0 & 1 \\ \hline -7.9240789 & 0.1136010 & 2.8891227 & 0.0269051 & -0.125811 & 1.125811 \\ -9.2810997 & 9.2965144 & 2.5414193 & -1.612969 & -0.125811 & 1.125811 \end{array} \right].$$

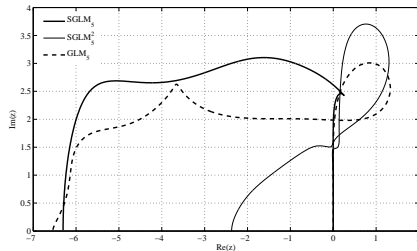


Figure 8. The absolute stability regions for $SGLM_5$, $SGLM_5^2$ and GLM_5 .

The area of the absolute stability region of this method is ≈ 5.09 and its error constant is $C_6 = 0.00417$. The absolute stability regions of the order five methods have been plotted in Figure 8.

In Table 1, the error constants and the area of the absolute stability regions of the methods discussed in the previous and the present section have been compared.

Table 1. Comparison of the error constants and the area of the absolute stability regions of the methods.

Order	Method	Error constant	Area
2	$SGLM_2$	1.00×10^{-2}	12.39
	GLM_2	1.59×10^{-2}	9.10
	$SGLM_2^2$	1.00×10^{-2}	19.05
3	$SGLM_3$	1.66×10^{-3}	34.02
	GLM_3	-1.60×10^{-2}	14.61
	$SGLM_3^2$	9.98×10^{-3}	20.68
4	$SGLM_4$	3.40×10^{-3}	32.91
	GLM_4	-1.10×10^{-2}	18.36
	$SGLM_4^2$	2.90×10^{-2}	10.77
5	$SGLM_5$	9.54×10^{-4}	34.56
	GLM_5	-3.10×10^{-3}	24.84
	$SGLM_5^2$	4.17×10^{-3}	5.09

5 Numerical experiment

In this section, we present the results of some numerical experiments to confirm the theoretical order, accuracy and efficiency of constructed methods in Sections 3 and 4. Also, we give the number of function evaluations, nfe , in terms of the global error of these methods and compare them with those of GLM_p . To implement the constructed methods in Sections 3 and 4 of order $p \geq 3$, a suitable starting procedure is required to approximate the initial vector $y^{[0]}$. We carry out one step of explicit Runge–Kutta methods of orders $p^* = 3, 4, 5$ [6] which give sufficient output information to obtain a reliable approximation to

the vector $y^{[0]}$ as the starting procedure. For more details see the references in the paper [25].

Computational experiments are done by applying the proposed methods to the following problems:

P1. The nonlinear system of ODEs [20]

$$\begin{cases} y_1'(t) = -(4 + \varepsilon^{-1})y_1(t) + \varepsilon^{-1}y_2^4(t), & y_1(0) = 1, \\ y_2'(t) = y_1(t) - y_2(t)(1 + y_2^3(t)), & y_2(0) = 1, \end{cases}$$

with $\varepsilon = 10^{-1}$ and the exact solution is

$$[y_1(t) \quad y_2(t)]^T = [\exp(-4t) \quad \exp(-t)]^T, \text{ and } t \in [0, 2].$$

P2. The system of equations describing the motion of a rigid body without external forces [17]

$$\begin{cases} y_1'(t) = y_2(t)y_3(t), & y_1(0) = 0, \\ y_2'(t) = -y_1(t)y_3(t), & y_2(0) = 1, \\ y_3'(t) = -0.51y_1(t)y_2(t), & y_3(0) = 1, \end{cases}$$

and $t \in [0, 10]$. To compute the global error of the methods, we use the reference solution obtained by solving the problem using the `ode45` code from MATLAB with the tolerances $Atol = Rtol = 2.22045 \times 10^{-14}$.

P3. The BRUSS problem [18]

$$\begin{cases} \frac{\partial u}{\partial t} = A + u^2v - (B + 1)u + \alpha \frac{\partial^2 u}{\partial x^2}, \\ \frac{\partial v}{\partial t} = Bu - u^2v + \alpha \frac{\partial^2 v}{\partial x^2}, \end{cases}$$

with $0 \leq x \leq 1$ which using the method of lines for the diffusion terms, the solution u can be approximated as the solution of the system of ODEs

$$\begin{cases} u_i' = A + u_i^2v_i - (B + 1)u_i + \frac{\alpha}{(\Delta x)^2} (u_{i-1} - 2u_i + u_{i+1}), \\ v_i' = Bu_i - u_i^2v_i + \frac{\alpha}{(\Delta x)^2} (v_{i-1} - 2v_i + v_{i+1}), \end{cases}$$

for $i = 1, 2, \dots, \bar{N}$. We consider $\bar{N} = 50$ which leads to a mildly stiff problem in a higher dimension $2\bar{N} = 100$. Following [18], we take $A = 1$, $B = 3$, $\alpha = 1/50$, $x_i = i/(\bar{N} + 1)$ ($1 \leq i \leq \bar{N}$), $\Delta x = 1/(\bar{N} + 1)$, the initial values

$$u_i(0) = 1 + \sin(2\pi x_i), \quad v_i(0) = 3, \quad i = 1, 2, \dots, \bar{N},$$

and periodic boundary conditions

$$u_0 = u_{\bar{N}+1} = 1, \quad v_0 = v_{\bar{N}+1} = 3, \quad \bar{t} = 10.$$

Table 2. Numerical results of the orders two and three methods for the problem P1.

h		2^{-5}	2^{-6}	2^{-7}	2^{-8}	2^{-9}
SGLM ₂	$\ e_h(\bar{t})\ $	4.74e-6	1.15e-6	2.82e-7	7.00e-8	1.74e-8
	p		2.05	2.02	2.01	2.01
SGLM ₂ ²	$\ e_h(\bar{t})\ $	4.30e-6	1.09e-6	2.76e-7	6.92e-8	1.73e-8
	p		2.05	2.02	2.01	2.01
SGLM ₃	$\ e_h(\bar{t})\ $	3.46e-8	3.95e-9	4.67e-10	5.66e-11	6.86e-12
	p		3.14	3.08	3.04	3.05
SGLM ₃ ²	$\ e_h(\bar{t})\ $	2.32e-7	2.93e-8	3.68e-9	4.62e-10	5.78e-11
	p		2.98	2.99	2.99	3.00

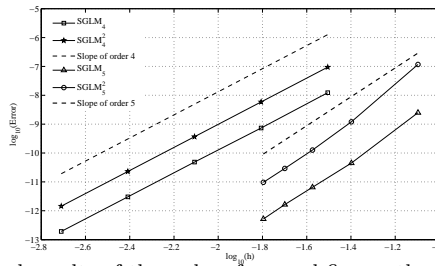


Figure 9. Numerical results of the orders four and five methods for the problem P1.

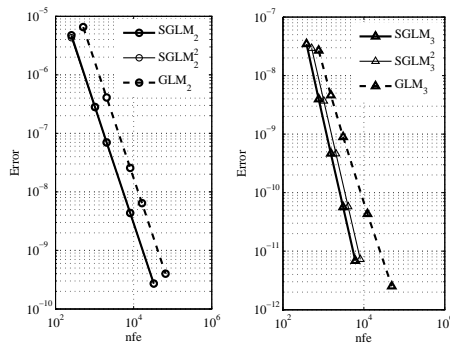


Figure 10. The global error versus the number of function evaluation of the methods of order 2 (left) and 3 (right) for the problem P1.

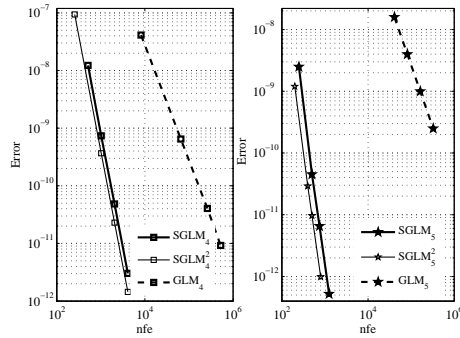


Figure 11. The global error versus the number of function evaluation of the methods of order 4 (left) and 5 (right) for the problem P1.

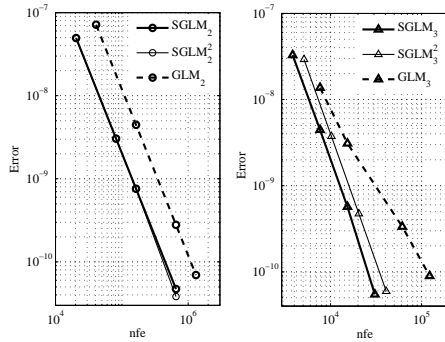


Figure 12. The global error versus the number of function evaluation of the methods of order 2 (left) and 3 (right) for the problem P2.

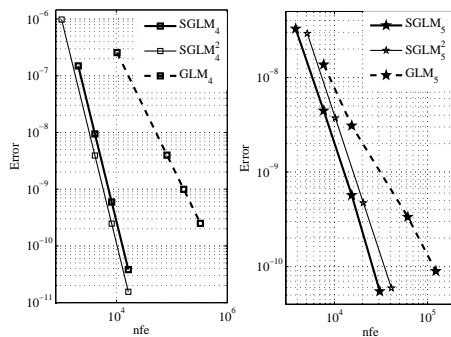


Figure 13. The global error versus the number of function evaluation of the methods of order 4 (left) and 5 (right) for the problem P2.

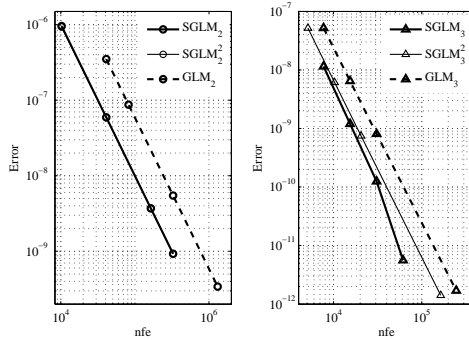


Figure 14. The global error versus the number of function evaluation of the methods of order 2 (left) and 3 (right) for the problem P3.

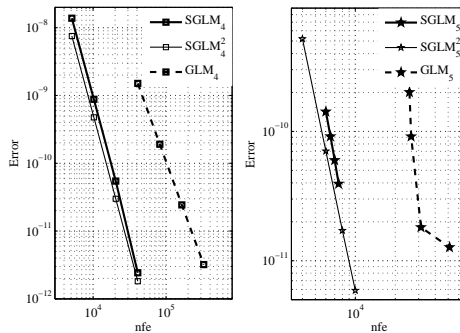


Figure 15. The global error versus the number of function evaluation of the methods of order 4 (left) and 5 (right) for the problem P3.

The results of the numerical experiments for the problems P1, P2, and P3 have been represented in Table 2 and Figures 9–15. These figures together with Table 2 demonstrate the efficiency of the methods and beautifully verify that the global error decreases with the theoretical order of the proposed methods. In Table 2, the numerical estimate to the order of convergence, p , is computed by the formula

$$p = \log_2 \left(\frac{\|e_h(\bar{t})\|}{\|e_{h/2}(\bar{t})\|} \right),$$

in which $e_h(\bar{t})$ stands for the global error of the method with the stepsize h . Moreover, in Figures 10–15, the global errors of the $SGLM_p$ and $SGLM_p^2$, $p = 2, 3, 4, 5$, have been plotted in terms of the required number of function evaluation, nfe . These results have been compared with those for GLM_p which illustrate the constructed methods are more cost-effective.

6 Conclusions

We described the construction of the quadratically stable explicit SGLMs of order p and stage order $q = p$ in two classes: methods with $r = s = p$, and with $r = s = 2$. We derived the methods up to order five with a large stability regions

and small error constants. As it was illustrated by the numerical experiments, the proposed methods are capable in solving non-stiff and mildly stiff ODEs; moreover they are more efficient and cost-effective than the quadratically stable GLMs of the same order. It is natural to extend the research for variable-stepsize implementation that it could be future work.

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