Mathematical Modelling and Analysis
Volume 28, Issue 1, 53–70, 2023
https://doi.org/10.3846/mma.2023.16102

VILNIUS TECH
Vilnius Gediminas Technical University

High Order Second Derivative Diagonally Implicit Multistage Integration Methods for ODEs

Mohammad Sharifi[a], Ali Abdi[a,b], Michal Braś[c] and Gholamreza Hojjati[a,b]

[a] *Faculty of Mathematical Sciences, University of Tabriz*
Tabriz, Iran
[b] *Research Department of Computational Algorithms and Mathematical Models, University of Tabriz*
Tabriz, Iran
[c] *Faculty of Applied Mathematics, AGH University of Science and Technology*
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

Received December 8, 2021; revised November 17, 2022; accepted November 17, 2022

Abstract. Construction of second derivative diagonally implicit multistage integration methods (SDIMSIMs) as a subclass of second derivative general linear methods with Runge–Kutta stability property requires to generate the corresponding conditions depending of the parameters of the methods. These conditions which are a system of polynomial equations can not be produced by symbolic manipulation packages for the methods of order $p \geq 5$. In this paper, we describe an approach to construct SDIMSIMs with Runge–Kutta stability property by using some variant of the Fourier series method which has been already used for the construction of high order general linear methods. Examples of explicit and implicit SDIMSIMs of order five and six are given which respectively are appropriate for both non-stiff and stiff differential systems in a sequential computing environment. Finally, the efficiency of the constructed methods is verified by providing some numerical experiments.

Keywords: general linear methods, second derivative methods, order conditions, $A-$ and $L-$stability, Fourier series.

AMS Subject Classification: 65L05.

1 Introduction

One efficient technique to construct numerical methods for the system of ordinary differential equations (ODEs)

$$\begin{cases} y'(x) = f\big(y(x)\big), & x \in [x_0, \bar{x}], \\ y(x_0) = y_0, \end{cases} \tag{1.1}$$

where $f : \mathbb{R}^m \to \mathbb{R}^m$ and $y : \mathbb{R} \to \mathbb{R}^m$, with desirable convergence and stability properties is incorporating the higher derivatives of the solution into the formula. This idea has been applied in designing, for instance, methods based on:

- Taylor series [9, 19]; such methods are based on differentiating the ODEs to obtain the high-order derivatives of the solution incorporating in Taylor series expansions of the solution. In [9], by giving an approximation to the high-order derivatives, an scheme is proposed which its implementation only depends on the function f. Although the number of function evaluations for these methods in comparison with the Runge–Kutta methods is higher, however it is much easier to produce arbitrary high-order schemes.

- Runge–Kutta approach [18, 20, 28]; it has been shown that two-derivative Runge–Kutta (TDRK) methods can be more efficient than the standard Runge–Kutta methods. This is because the higher order TDRK methods require fewer stages and have a higher stage order with favorable stability properties compared to the Runge–Kutta methods.

- Multistep approach [15, 17, 22, 23, 24, 25]; by Dahlquist's second barrier [21], the order of A–stable implicit linear multistep method cannot exceed two. To circumvent this barrier, one of the most popular and successful approaches is including the second derivative of the solution into the formula.

For the methods using higher derivatives of the solution into the formula, the computational costs can become very severe. In the case of second derivative methods, however, it can be nearly ineffective; indeed, in solving stiff problems, we need to compute the Jacobian matrix $\partial f/\partial y$, so in the case of autonomous problem (1.1), without any additional cost, the second derivative function g can be computed by $g := (\partial f/\partial y)f$ and the Jacobian matrix of the function g can be approximated by $(\partial f/\partial y)^2$. Although the number of the Jacobian evaluations in the practical codes based on the second derivative methods, due to the presence of the Jacobian matrix into the formula, is usually more than that for the codes based on the fist derivative methods, the former are totally more cost-effective than the latter, particularly in solving ODEs resulting from the discretization of the spatial derivatives in the partial differential equations. This feature has been experimentally illustrated in [5].

Second derivative general linear methods (SGLMs) for the numerical solution of (1.1) as a general framework for the traditional second derivative methods are an extension of general linear methods (GLMs) [11,12,26]. These methods incorporating the second derivative of the solution into the formula have been studied, for instance, in [2,3,4,6,7,8,10,13]. SGLMs for solving (1.1) can be represented by abscissa vector $c = [c_1 \quad c_2 \quad \cdots \quad c_s]^T$, and six coefficients matrices $A = \big[a_{ij}\big] \in \mathbb{R}^{s\times s}$, $\overline{A} = \big[\overline{a}_{ij}\big] \in \mathbb{R}^{s\times s}$, $U = \big[u_{ij}\big] \in \mathbb{R}^{s\times r}$, $B = \big[b_{ij}\big] \in \mathbb{R}^{r\times s}$, $\overline{B} = \big[\overline{b}_{ij}\big] \in \mathbb{R}^{r\times s}$, and $V = \big[v_{ij}\big] \in \mathbb{R}^{r\times r}$. On the uniform grid $x_n = x_0 + nh$, $n = 1, 2, \ldots, N$, $Nh = \overline{x} - x_0$, these methods take the form

$$Y_i^{[n]} = h\sum_{j=1}^{s} a_{ij} f\big(Y_j^{[n]}\big) + h^2\sum_{j=1}^{s}\overline{a}_{ij} g\big(Y_j^{[n]}\big) + \sum_{j=1}^{r} u_{ij} y_j^{[n-1]},\ i = 1, 2, \ldots, s,$$

$$y_i^{[n]}=h\sum_{j=1}^{s} b_{ij} f\big(Y_j^{[n]}\big)+h^2\sum_{j=1}^{s}\overline{b}_{ij} g\big(Y_j^{[n]}\big) + \sum_{j=1}^{r} v_{ij} y_j^{[n-1]},\ i = 1, 2, \ldots, r, \quad (1.2)$$

where s is the number of internal stages, r is the number of external stages, and h is the stepsize. Here, the vector of stage values $Y^{[n]} := \big[Y_i^{[n]}\big]_{i=1}^{s}$ is an approximation of stage order q to the vector $\big[y(x_{n-1} + c_i h)\big]_{i=1}^{s}$, and the function g stands for the second derivative of the solution, $g(\cdot) = f'(\cdot)f(\cdot)$. Moreover, the input and output vectors $y^{[n-1]} = \big[y_i^{[n-1]}\big]_{i=1}^{r}$ and $y^{[n]} = \big[y_i^{[n]}\big]_{i=1}^{r}$ are approximation of order p to the linear combinations of scaled derivatives of the solution at the points x_{n-1} and x_n. These methods are usually represented conveniently by their coefficients matrices as a partitioned $(s + r) \times (2s + r)$ matrix

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

According to a standard linear stability analysis, the stability matrix of these methods takes the form $M(z) = V + z(B + z\overline{B})(I_s - zA - z^2\overline{A})^{-1}U$ in which z is a complex number and I_ℓ stands for the identity matrix of dimension ℓ. Then the stability function is defined as the characteristic polynomial of the stability matrix $M(z)$, i.e.,

$$p(w, z) = \det\big(wI_r - M(z)\big). \quad (1.3)$$

The stability region of SGLM (1.2) are all the points $z \in \mathbb{C}$ for which the all roots of $p(w, z)$ defined by (1.3) lie within the unit circle except for the roots on the unit circle which are distinct. One of the most popular approach to derive a desirable method is that its stability region be similar to that of a Runge–Kutta method. The reasons for this are that Runge–Kutta methods not only have convenient stability properties from the analysis point of view but also that their stability properties are usually superior to those of alternative methods [12]. The method is said to possess Runge–Kutta stability (RKS) property, if its stability function has the form

$$p(w, z) = w^{r-1}\big(w - R(z)\big).$$

As with Runge–Kutta formulas, the coefficients matrices A and $\overline{A}$ play an important role in SGLMs. They determine how much each method costs to implement. Therefore, we always assume that the matrices A and $\overline{A}$ have the lower triangular form with the same parameters λ and μ on the diagonal, respectively. SGLMs have been divided into four types [6]: For the methods of types 1 (with $\lambda = \mu = 0$) and 2 (with $\lambda > 0$ and $\mu < 0$), not all the entries a_{ij} and $\overline{a}_{ij}$, for $i > j$, of matrices A and $\overline{A}$ are zero which means that the internal stages of these types of the methods must be computed sequentially. Therefore, these methods are suitable for nonstiff (type 1) and stiff (type 2) problems in a sequential computing environment. Also, for the methods of types 3 (with $\lambda = \mu = 0$) and 4 (with $\lambda > 0$ and $\mu < 0$), we have $a_{ij} = \overline{a}_{ij} = 0$, for $i > j$, which means that the internal stages of these types of the methods are independent and computed in parallel. Therefore, these methods are suitable for nonstiff (type 3) and stiff (type 4) problems in a parallel computing environment.

Second derivative diagonally implicit multistage integration methods (SDIMSIMs) as a subclass of SGLMs have been introduced in [6]. In these methods V is a rank-one matrix, all the numbers p, q, r, and s are approximately equal, and moreover the matrices A and $\overline{A}$ have lower triangular form with the same diagonal elements in each matrix.

SDIMSIMs of orders up to four in various types with RKS property have been derived in [4] by solving the generated nonlinear equations related to RKS conditions by symbolic manipulation packages such as MATHEMATICA or MAPLE. Symbolic manipulation tools could no longer produce the corresponding systems of nonlinear equations in a reasonable form for higher orders ($p \geq 5$); therefore another approach to construct such methods is required. In this paper, we describe the construction of high order SDIMSIMs of type 1 and 2 using the Fourier series approach which has been already used in the context of diagonally implicit multistage integration methods in [14] (see also [16, 26]).

The organization of the paper is as follows: In Section 2, we review the order conditions for SGLMs and present the key result of the construction of SDIMSIMs. Section 3 is devoted to description of the Fourier series approach and the construction of examples of (p, q, r, s) SDIMSIMs with $p = q = r = s = 5$ and 6 in two types 1 and 2. Numerical experiments are given in Section 4 to verify the theoretical results. The paper is closed in Section 5, by concluding remarks and giving ideas for future work.

2 The structure of order conditions

This section reviews the structure of the order conditions for SGLMs in their general form, as detailed in [7]. The fundamental concept is to use input vector of the form

$$y_i^{[n-1]} = \sum_{k=0}^{p} h^k \alpha_{ik} y^{(k)}(x_{n-1}) + \mathcal{O}(h^{p+1}), \quad i = 1, 2 \ldots, r, \tag{2.1}$$

for some real parameters α_{ik}, $i = 1, 2, \ldots, r$, $k = 0, 1, \ldots, p$, where $y_i^{[n]}$ denotes approximation number i at integration point number n. We then request that the stage values $Y_i^{[n]}$ within the current step with stepsize h be approximations of order q to the solution at the points $x_{n-1}+c_ih$, that is,

$$Y_i^{[n-1]}=\sum_{k=0}^{p}\frac{c_i^k}{k!}h^k y^{(k)}(x_{n-1})+\mathcal{O}(h^{q+1}),\qquad i=1,2\dots,s, \tag{2.2}$$

and the output values computed at the end of current step satisfy

$$y_i^{[n]}=\sum_{k=0}^{p}h^k\alpha_{ik}y^{(k)}(x_n)+\mathcal{O}(h^{p+1}),\qquad i=1,2\dots,r, \tag{2.3}$$

for the same numbers α_{ik}. Let us denote $\alpha_k:=\begin{bmatrix}\alpha_{1k} & \alpha_{2k} & \dots & \alpha_{rk}\end{bmatrix}^T$ for $k=0,1,\dots,p$. Pre-consistency and consistency vectors are denoted by α_0 and α_1, respectively (see [6]). Also let us denote $Z:=\begin{bmatrix}1 & z & \dots & z^p\end{bmatrix}^T\in\mathbb{C}^{p+1}$ and collect the vectors α_k in the matrix W as $W=[\alpha_0\ \ \alpha_1\ \ \cdots\ \ \alpha_p]$.

Theorem 1. *[7] Assume that $y^{[n-1]}$ satisfies* (2.1)*. Then the SGLM* (1.2) *of order p and stage order $q=p$ satisfies* (2.2) *and* (2.3) *if and only if*

$$\begin{aligned}\exp(cz)&=zA\exp(cz)+z^2\overline{A}\exp(cz)+UWZ+\mathcal{O}(z^{p+1}),\\ \exp(z)WZ&=zB\exp(cz)+z^2\overline{B}\exp(cz)+VWZ+\mathcal{O}(z^{p+1}).\end{aligned} \tag{2.4}$$

Here, the exp *function is applied component-wise to a vector.*

Second derivative diagonally implicit multistage integration methods (SDIMSIMs) as a subclass of SGLMs were introduced in [6] in which the matrix V is a rank-one matrix and usually p=q=r=s. By choosing $r=s$ and $U=I_s$, the stage order condition (2.4) in Theorem 1 will be satisfied if and only if

$$W=C-ACK-\overline{A}CK^2,$$

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

$$C_{ij}=\frac{c_i^{j-1}}{(j-1)!},\qquad 1\le i\le s,\ \ 1\le j\le p+1,$$

and $K\in\mathbb{R}^{(p+1)\times(p+1)}$ is the shifting matrix defined by $K=\begin{bmatrix}0 & e_1 & \cdots & e_p\end{bmatrix}$ with e_j as the jth unit vector (cf. [7]). In this case, an equivalent formula for the order conditions of SDIMSIMs is given by the following theorem.

Theorem 2. *[4] Let $r=s$ and $U=I_s$. Then the SDIMSIM*

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

with $Ve=e$, has order p and stage order q equal to $p=q=r=s$ if and only if

$$B=B_0-AB_1-\overline{A}B_2-VB_3-(\overline{B}-V\overline{A})B_4+VA, \tag{2.5}$$

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

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

with

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

3 High order SDIMSIMs with RKS

Construction of SDIMSIMs with $p = q = r = s$ and RKS property have been already studied in [4]. In this section, we are going to construct such methods in types 1 and 2 of high orders $p = 5$ and 6 which completes the set for orders 1–6. To do this, we consider $U = I_s$, and assume that V is a rank-one matrix of the form $V = ev^T$, where $e = \begin{bmatrix}1 & 1 & \dots & 1\end{bmatrix}^T \in \mathbb{R}^r$ and $v^T e = 1$. The latter guarantees the zero-stability of the methods [6, 7].

In what follows, we will consider $\overline{B} = V\overline{A}$ for both types, and the abscissa vector c to be values uniformly in the interval $[0, 1]$ so that

$$c = \begin{bmatrix}0 & \frac{1}{s-1} & \cdots & \frac{s-2}{s-1} & 1\end{bmatrix}^T .$$

For type 1 SDIMSIMs (1.2), the stability function $p(w, z)$ has the form

$$p(w, z) = w^s - p_{s-1}(z)w^{s-1} + \cdots + (-1)^{s-1}p_1(z)w + (-1)^s p_0(z),$$

where $p_i(z)$, $i = 0, 1, \dots, s-1$, are polynomials of degree less than or equal to $2s-1$ with respect to z and given by

$$\begin{aligned}
p_{s-1}(z) =& 1 + p_{s-1,1}z + p_{s-1,2}z^2 + \cdots + p_{s-1,2s-1}z^{2s-1},\\
p_{s-2}(z) =& p_{s-2,1}z + p_{s-2,2}z^2 + \cdots + p_{s-2,2s-2}z^{2s-2},\\
&\vdots\\
p_1(z) =& p_{1,s-2}z^{s-2} + p_{1,s-1}z^{s-1} + p_{1,s}z^s + p_{1,s+1}z^{s+1},\\
p_0(z) =& p_{0,s-1}z^{s-1} + p_{0,s}z^s.
\end{aligned} \tag{3.1}$$

Also, for type 2 methods, the stability function $p(w, z)$ takes the form

$$p(w, z) = (1-\lambda z-\mu z^2)^s w^s - p_{s-1}(z)w^{s-1} + \cdots + (-1)^{s-1}p_1(z)w + (-1)^s p_0(z),$$

where again, $p_i(z)$, $i = 0, 1, \dots, s-1$, are polynomial of degree less than or equal to $2s-1$ with respect to z in the form (3.1). Then, the method (1.2) has RKS property if we impose the conditions

$$p_i(z) \equiv 0, \quad i = 0, 1, \dots, s-2,$$

or equivalently,

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

For the case $p = q = r = s$ and $U = I_s$, it follows from Theorem 2 that the coefficient matrix B can be computed from the formula (2.5), and also considering $\overline{B} = V\overline{A}$, the coefficients p_{ij} of the polynomials $p_i(z)$ are in terms of a_{ij}, $\overline{a}_{ij}$, $i = 2, 3, \dots, s$, $j = 1, 2, \dots, i-1$, and v_i, $i = 1, 2, \dots, s-1$. Therefore, the RKS conditions lead to the system of $\sum_{i=0}^{s-2}(2i+2) = s(s-1)$ nonlinear equations. Moreover, for the RKS methods, we have

$$p(w, z) = w^{s-1}(D(z)w - p_{s-1}(z)),$$

in which $D(z) \equiv 1$ or $D(z) = (1 - \lambda z - \mu z^2)^s$ respectively for the type 1 or 2 methods. Indeed, we must have

$$p_{s-1}(z) = D(z)\exp(z) - \sum_{i=1}^{s-1} C_{p+i} z^{p+i} + \mathcal{O}(z^{2s}),$$

where C_{p+i}, $i = 1, 2, \ldots, s-1$, are constant numbers and define different methods. So, to construct a specified method, we must set these constants and impose their related conditions which give other $s-1$ nonlinear conditions. Then, in the case of type 2 methods, the A–stable (and so L–stable) choices of the pair (λ, μ) are obtained for the specified stability function $R(z) = p_{s-1}(z)/D(z)$ and for the parameters λ and μ, a single pair is selected from these values. By this discussion, we must solve $s(s-1) + s - 1 = (s-1)(s+1)$ nonlinear equations with respect to the $(s-1)(s+1)$ unknown coefficients a_{ij}, $\overline{a}_{ij}$, and v_i, for $i = 2, 3, \ldots, s$ and $j = 1, 2, \ldots, i-1$.

To construct high order methods for $p \geq 5$, symbolic manipulation tools could not produce $p_{j,k}$; therefore another approach to construct such methods is required. Here we use Fourier series approach which has been already presented in [14] (see also [16, 26]). Let

$$w_\zeta = \exp\left(-2\pi\zeta\,\mathrm{i}/N_1\right), \quad \zeta = 0, 1, \ldots, N_1 - 1,$$
$$z_\eta = \exp\left(-2\pi\eta\,\mathrm{i}/N_2\right), \quad \eta = 0, 1, \ldots, N_2 - 1,$$

with i as the imaginary unit, are complex numbers uniformly distributed on the unit circle, and N_1 and N_2 are sufficiently large integers. Multiplying $p(w_\zeta, z)$ by w_ζ^{-j} and summing on ζ we obtain

$$p_j(z) = (-1)^{s-j}\frac{1}{N_1}\sum_{\zeta=0}^{N_1-1} w_\zeta^{-j} p\left(w_\zeta, z\right), \qquad j = 0, 1, \ldots, s-1. \tag{3.2}$$

Similarly, multiplying

$$p_j\left(z_\eta\right) = p_{j,0} + p_{j,1} z_\eta + \cdots + p_{j,s} z_\eta^s,$$

by z_η^{-k} and summing on η, we get

$$p_{j,k} = \frac{1}{N_2}\sum_{\eta=0}^{N_2-1} z_\eta^{-k} p_j\left(z_\eta\right), \qquad k = s-1-j, s-j, \ldots, s+j.$$

Then, substituting (3.2) into the last relation, we obtain

$$p_{j,k} = (-1)^{s-j}\frac{1}{N_1 N_2}\sum_{\zeta=0}^{N_1-1}\sum_{\eta=0}^{N_2-1} w_\zeta^{-j} z_\eta^{-k} p\left(w_\zeta, z_\eta\right), \tag{3.3}$$

for $j = 0, 1, \ldots, s-1$, $k = s-1-j, s-j, \ldots, s+j$. Finally, we numerically solve the system

$$\sum_{\zeta=0}^{N_1-1}\sum_{\eta=0}^{N_2-1} w_\zeta^{-j} z_\eta^{-k} p\left(w_\zeta, z_\eta\right) = 0, \quad j = 0, 1, \ldots, s-1, \quad k = s-1-j, s-j, \ldots, s+j, \tag{3.4}$$

using subroutine `fsolve.m` utilizing the algorithm 'levenberg–marquardt' in MATLAB.

3.1 Construction of type 1 SDIMSIM with $p = q = r = s = 5$

In this subsection, we investigate methods of order $p = q = 5$ with RKS property. The stability function of such methods has the form

$$R(z) = \sum_{i=0}^{5} \frac{z^i}{i!} + \gamma_6 z^6 + \gamma_7 z^7 + \gamma_8 z^8 + \gamma_9 z^9,$$

in which γ_{5+i}, $i = 1, 2, 3, 4$ are complicated expressions in terms of the coefficients of the method. Therefore,

$$\exp(z) - R(z) = C_6 z^6 + C_7 z^7 + C_8 z^8 + C_9 z^9 + \mathcal{O}(z^{10}),$$

with $C_6 := \frac{1}{6!} - \gamma_6$ as the error constant of the methods and $C_{5+i} := \frac{1}{(5+i)!} - \gamma_{5+i}$, $i = 2, 3, 4$. We solve the system (3.4) for the constants $C_6 = 10^{-5}$, $C_7 = 0.32 \times 10^{-4}$, $C_8 = 0.13 \times 10^{-4}$, $C_9 = 0.2 \times 10^{-5}$, which gives a method with a good balance between accuracy (small error constant) and the stability (the interval of absolute stability is $\approx (-6.26, 0)$). The region of absolute stability for the resulting SDIMSIM has been plotted in Figure 1. The coefficients

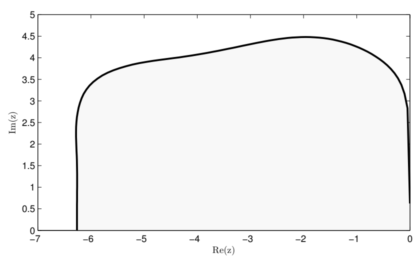

Figure 1. Region of absolute stability for type 1 SDIMSIM with $p = q = r = s = 5$.

matrices of the derived method are

$$c = \begin{bmatrix} 0 & 0.25 & 0.5 & 0.75 & 1 \end{bmatrix}^T, \qquad U = I_s, \qquad \overline{B} = V\overline{A},$$

$$A = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0.13051305 & 0 & 0 & 0 & 0 \\ 0.12988322 & 0.15199878 & 0 & 0 & 0 \\ 0.16415410 & -0.13973596 & 0.46377291 & 0 & 0 \\ -0.00252378 & 0.58118300 & -0.29967459 & 0.62233751 & 0 \end{bmatrix},$$

$$v^T = [-1.02175258 \; 2.16234499 \; 1.86504402 \; -1.53823102 \; -0.46740541],$$

$$\overline{A} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0.05620319 & 0 & 0 & 0 & 0 \\ 0.07199361 & 0.05449118 & 0 & 0 & 0 \\ 0.10984392 & -0.00560975 & 0.02924933 & 0 & 0 \\ 0.05414928 & 0.03637955 & -0.05081925 & 0.02828469 & 0 \end{bmatrix},$$

with the matrix B computed by formula (2.5). Here, the coefficients are rounded to eight decimal places.

3.2 Construction of type 1 SDIMSIM with $p = q = r = s = 6$

In this subsection, we investigate methods of order $p = q = 6$ with RKS property. The stability function of such methods has the form

$$R(z) = \sum_{i=0}^{6} \frac{z^i}{i!} + \sum_{i=7}^{11} \gamma_i z^i,$$

in which γ_{6+i}, $i = 1, 2, 3, 4, 5$ are complicated expressions in terms of the coefficients of the method. Therefore,

$$\exp(z) - R(z) = \sum_{i=7}^{11} C_i z^i + \mathcal{O}(z^{12}),$$

with $C_7 := \frac{1}{7!} - \gamma_7$ as the error constant of the methods and $C_{6+i} := \frac{1}{(6+i)!} - \gamma_{6+i}$, $i = 2, 3, 4, 5, 6$. We solve the system (3.4) for the constants $C_7 = 10^{-5}$, $C_8 = 0.57 \times 10^{-5}$, $C_9 = 0.15 \times 10^{-5}$, $C_{10} = 0.02 \times 10^{-5}$, $C_{11} = 0.002 \times 10^{-5}$, which gives a method with a good balance between accuracy and the stability. The interval of absolute stability is $\approx (-5.16, 0)$. The region of absolute stability for the resulting SDIMSIM has been plotted in Figure 2. The coefficients matrices

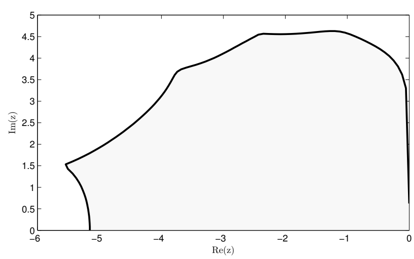

Figure 2. Region of absolute stability for SDIMSIM with $p = q = r = s = 6$.

of the derived method are

$$c = \begin{bmatrix} 0 & 0.2 & 0.4 & 0.6 & 0.8 & 1 \end{bmatrix}^T, \quad U = I_s, \quad \overline{B} = V\overline{A},$$

$$A = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0.28612857 & 0 & 0 & 0 & 0 & 0 \\ 0.32513987 & 0.27700572 & 0 & 0 & 0 & 0 \\ 0.26790873 & 0.76617243 & -0.03578032 & 0 & 0 & 0 \\ 0.18932349 & 1.39200756 & -0.33433966 & 0.18913924 & 0 & 0 \\ 6.56624562 & 26.68190641 & 0.82954569 & -5.25257936 & 0.60419836 & 0 \end{bmatrix},$$

$$\overline{A} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0.02693906 & 0 & 0 & 0 & 0 & 0 \\ 0.03777414 & 0.01465161 & 0 & 0 & 0 & 0 \\ 0.03171482 & -0.01591904 & 0.05690168 & 0 & 0 & 0 \\ -0.00348899 & -0.06838026 & 0.10279461 & 0.0277815 & 0 & 0 \\ -10.84358337 & -8.48729062 & -3.17980076 & 8.4337437 & -2.410013 & 0 \end{bmatrix},$$

$$v^T = \begin{bmatrix} -1.28802668 & 8.13831641 & -19.4135010 & 21.2038727 & -7.65481983 & 0.01415825 \end{bmatrix},$$

with the matrix B computed by formula (2.5).

3.3 Construction of type 2 SDIMSIM with $p = q = r = s = 5$

In this subsection, we investigate type 2 methods of order $p = q = 5$ with RKS property. At first, we consider how to choose λ and μ to ensure the $L-$stability property. Therefore, we look for methods for which the stability function has the form

$$R(z) = \frac{N(z)}{D(z)} = \frac{1 + \sum_{i=1}^{9} \gamma_i z^i}{(1 - \lambda z - \mu z^2)^5},$$

where, because of the order conditions,

$$\exp(z)(1 - \lambda z - \mu z^2)^5 - 1 - \sum_{i=1}^{9} \gamma_i z^i = C_6 z^6 + C_7 z^7 + C_8 z^8 + C_9 z^9 + \mathcal{O}(z^{10}),$$

with C_6 as the error constant of the methods and C_{5+i}, $i = 2, 3, 4$ as constants depending on the coefficients of the methods.

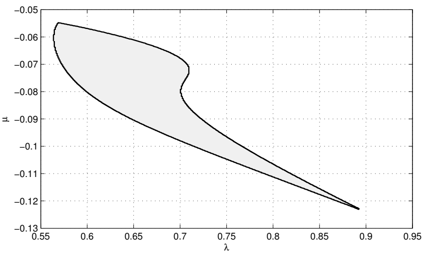

Figure 3. A–stable choices of (λ, μ) in domain $[0, 2] \times [-2, 0]$ for $p = q = r = s = 5$.

The necessary and sufficient conditions for these methods to be A–stable are that $\lambda > 0$ and $\mu < 0$, and the $E-$polynomial $E(y)$ defined by

$$\begin{aligned} E(y) &= |D(iy)|^2 - |N(iy)|^2 \\ &= y^6 \left(E_0 + E_1 y^2 + E_2 y^4 + E_3 y^6 + E_4 y^8 + E_5 y^{10} + E_6 y^{12} + E_7 y^{14}\right), \end{aligned}$$

is non-negative for all real y, where the coefficients E_0, E_1, E_2, E_3, E_4, E_5, E_6, and E_7 are complicated expressions in λ and μ. By choosing $C_6 = -C_7 = C_8 = -C_9 = -10^{-5}$, we have searched for the acceptable pairs of (λ, μ) in domain $[0, 2] \times [-2, 0]$. These pairs have been plotted in Figure 3.

We select single example, characterized by $(\lambda,\mu) = (0.65, -0.08)$ which the coefficients matrices for the resulting $L-$stable method are

$$c = \begin{bmatrix} 0 & 0.25 & 0.5 & 0.75 & 1 \end{bmatrix}^T, \qquad U = I_s, \qquad \overline{B} = V\overline{A},$$

$$A = \begin{bmatrix} 0.65 & 0 & 0 & 0 & 0 \\ 0.03827227 & 0.65 & 0 & 0 & 0 \\ -2.76554295 & -1.71123707 & 0.65 & 0 & 0 \\ -4.65198201 & -2.99689614 & 0.16864806 & 0.65 & 0 \\ -4.48956349 & -3.56719862 & 1.08564364 & -0.31350211 & 0.65 \end{bmatrix},$$

$$\overline{A} = \begin{bmatrix} -0.08 & 0 & 0 & 0 & 0 \\ 0.27949936 & -0.08 & 0 & 0 & 0 \\ -0.13264894 & 0.19729592 & -0.08 & 0 & 0 \\ -0.48175946 & 0.34142387 & -0.08340842 & -0.08 & 0 \\ -0.55184507 & 0.38519816 & -0.13389264 & -0.02449703 & -0.08 \end{bmatrix},$$

$$v^T = \begin{bmatrix} 0.08266754 & -0.52241582 & 1.43462986 & -2.16317788 & 2.16829631 \end{bmatrix},$$

with the matrix B computed by formula (2.5).

3.4 Construction of type 2 SDIMSIM with $p = q = r = s = 6$

In this subsection, we investigate type 2 methods of order $p = q = 6$ with RKS property. Again, we first investigate how to choose λ and μ to ensure the $L-$stability property. The stability function of these methods has the form

$$R(z) = \frac{N(z)}{D(z)} = \frac{1 + \sum_{i=1}^{11} \gamma_i z^i}{(1 - \lambda z - \mu z^2)^6},$$

where, because of the order conditions,

$$\exp(z)(1 - \lambda z - \mu z^2)^6 - 1 - \sum_{i=1}^{11} \gamma_i z^i = \sum_{i=1}^{5} C_{6+i} z^{6+i} + \mathcal{O}(z^{12}),$$

with C_7 as the error constant of the methods and C_{6+i}, $i = 2, 3, 4, 5$ as constants depending on the coefficients of the methods.

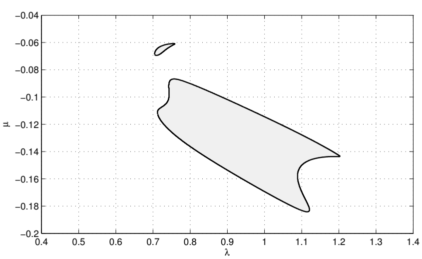

Figure 4. A–stable choices of (λ,μ) in domain $[0, 2] \times [-2, 0]$ for $p = q = r = s = 6$.

In a similar way in the construction of the methods of order $p = 5$, the acceptable pairs of (λ,μ) in domain $[0, 2] \times [-2, 0]$ have been plotted in Figure

4 for $C_7 = -C_8 = C_9 = C_{10} = -C_{11} = 10^{-5}$. We select single example, characterized by $(\lambda, \mu) = (0.8, -0.1)$ which the coefficients matrices for the resulting $L-$stable method are

$$c = \begin{bmatrix} 0 & 0.2 & 0.4 & 0.6 & 0.8 & 1 \end{bmatrix}^T, \qquad U = I_s, \qquad \overline{B} = V\overline{A},$$

$$A = \begin{bmatrix} 0.8 & 0 & 0 & 0 & 0 & 0 \\ 0.33517682 & 0.8 & 0 & 0 & 0 & 0 \\ 1.40254199 & -0.01580809 & 0.8 & 0 & 0 & 0 \\ 3.40104965 & 0.27900818 & -0.5555559 & 0.8 & 0 & 0 \\ 1.73702717 & -0.82196142 & 0.96759266 & -0.2816882 & 0.8 & 0 \\ -2.44140745 & -2.31392254 & 3.21296914 & -0.6879719 & 0.105985 & 0.8 \end{bmatrix}$$

$$\overline{A} = \begin{bmatrix} -0.1 & 0 & 0 & 0 & 0 & 0 \\ 3.21737272 & -0.1 & 0 & 0 & 0 & 0 \\ 1.29995749 & 0.00944788 & -0.1 & 0 & 0 & 0 \\ -3.8305285 & -0.0028237 & 0.03113729 & -0.1 & 0 & 0 \\ -3.3852781 & 0.28254378 & -0.4122369 & 0.056437 & -0.1 & 0 \\ 1.21243552 & 0.64912059 & -1.0306730 & 0.179521 & -0.070936 & -0.1 \end{bmatrix},$$

$$v^T = \begin{bmatrix} 0.26339203 & -1.66314188 & 4.53409895 & -6.87461831 & 7.31986767 & -2.57959846 \end{bmatrix},$$

with the matrix B computed by formula (2.5).

4 Numerical experiment

The proposed types 1 and 2 SDIMSIMs in the previous section, are implemented on some nonstiff, mildly stiff and stiff problems. To compare, the results of DIMSIMs of the same orders are also reported.

To compute the starting vector $y^{[0]}$, we carry out one step of the A–stable Gauss Runge–Kutta method of order six, with coefficients given in [12], which gives sufficient output information as components of a linear combination approximating the elements of the vector $y^{[0]}$. For more details see [5] where the implementation issues including starting procedure have been discussed.

Computational experiments for the proposed methods are done by applying these methods on the following problems:

P1. The nonlinear system of ODEs [27]

$$\begin{cases} y_1'(x) = -\left(4 + \epsilon^{-1}\right) y_1(x) + \epsilon^{-1} y_2(x)^4, & y_1(0) = 1, \\ y_2'(x) = y_1(x) - y_2(x)\left(1 + y_2(x)^3\right), & y_2(0) = 1, \end{cases}$$

where the exact solution is $[y_1(x), y_2(x)]^T = [\exp(-4x), \exp(-x)]^T$ and $x \in [0, 2]$.

P2. The famous nonlinear van der Pol system

$$\begin{cases} y_1'(x) = y_2(x), \\ y_2'(x) = \left((1 - y_1(x)^2) y_2(x) - y_1(x)\right)/\epsilon, \end{cases}$$

with the initial value

$$[y_1(0), y_2(0)]^T = \left[2, -\frac{2}{3} + \frac{10}{81}\epsilon - \frac{292}{2187}\epsilon^2 - \frac{1814}{19683}\epsilon^3\right]^T,$$

and $x \in [0, 0.55139]$. To compute the global error of the methods, we use the reference solution obtained by solving the problem using the `ode15s` code from MATLAB with tolerances $Atol = Rtol = 2.22045 \times 10^{-14}$.

P3. The BRUSS problem [24]

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

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

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

for $i = 1, 2, \ldots, N$. We consider $N = 500$ which leads to a stiff problem in a higher dimension $2 \cdot N = 1000$. Following [24], we take $A = 1$, $B = 3$, $\alpha = 1/50$, $x_i = i/(N+1)$ $(1 \leq i \leq N)$, $\Delta x = 1/(N+1)$, the initial values

$$u_i(0) = 1 + \sin(2\pi x_i), \quad v_i(0) = 3, \quad i = 1, 2, \ldots, N,$$

and periodic boundary conditions

$$u_0 = u_{N+1} = 1, \qquad v_0 = v_{N+1} = 3.$$

with $t_{out} = 10$.

We solve the problem P1 with two different values for ϵ as $\epsilon = 10^{-1}$ and $\epsilon = 10^{-4}$ which respectively make the problem to be nonstiff and stiff problem. The numerical results for this problem with these values of ϵ, have been reported in Tables 1–3.

In the tables, $\|e_h(\overline{x})\|$ stands for the norm of error at the endpoint of integration $\overline{x}$ with the stepsize h. Also, p denotes a numerical estimation to the order of convergence of the methods, computed by the formula

$$p = \frac{\log\left(\|e_{h_1}(\overline{x})\| / \|e_{h_2}(\overline{x})\|\right)}{\log\left(h_1/h_2\right)}.$$

Moreover, the numerical results of the proposed methods for the problems P2 with $\epsilon = 10^{-1}$ and $\epsilon = 10^{-6}$ and P3 have been represented in Table 4 and Figures 7, 8, and 9.

Table 1. Numerical results of type 1 SDIMSIM of orders $p = q = r = s = 5$ and 6 for the problem P1 with $\epsilon = 10^{-1}$.

h	Type 1 SDIMSIM of order 5		Type 1 SDIMSIM of order 6	
	$\|e_h(\overline{x})\|$	p	$\|e_h(\overline{x})\|$	p
$\frac{1}{8}$	1.80e-9		1.56e-8	
$\frac{1}{16}$	5.37e-11	5.07	7.74e-11	7.90
$\frac{1}{32}$	2.78e-12	4.27	9.11e-13	6.41
$\frac{1}{64}$	1.04e-13	4.74	1.49e-14	5.93
$\frac{1}{128}$	4.75e-15	4.46	2.75e-14	-0.88

Table 2. Numerical results of type 2 methods of orders $p = q = r = s = 5$ for the problem P1 with $\epsilon = 10^{-4}$.

h	Type 2 SDIMSIM of order 5		Type 2 DIMSIM of order 5	
	$\|e_h(\overline{x})\|$	p	$\|e_h(\overline{x})\|$	p
$\frac{1}{5}$	1.47e-9		9.94e-8	
$\frac{1}{10}$	7.97e-11	4.21	2.24e-9	5.47
$\frac{1}{15}$	1.19e-11	4.69	2.61e-10	5.30
$\frac{1}{20}$	3.00e-12	4.79	5.83e-11	5.21
$\frac{1}{25}$	1.01e-12	4.86	1.84e-11	5.17

Table 3. Numerical results of type 2 methods of orders $p = q = r = s = 6$ for the problem P1 with $\epsilon = 10^{-4}$.

h	Type 2 SDIMSIM of order 6		Type 2 DIMSIM of order 6	
	$\|e_h(\overline{x})\|$	p	$\|e_h(\overline{x})\|$	p
$\frac{1}{4}$	3.06e-9		2.74e-7	
$\frac{1}{8}$	5.66e-11	5.75	5.98e-10	8.84
$\frac{1}{16}$	7.69e-13	6.21	5.68e-12	6.71
$\frac{1}{32}$	1.88e-13	2.03	1.52e-13	5.22

Table 4. Numerical results of type 1 SDIMSIM of orders $p = q = r = s = 5$ and 6 for the problem P2 with $\epsilon = 10^{-1}$.

h	Type 1 SDIMSIM of order 5		Type 1 SDIMSIM of order 6	
	$\|e_h(\overline{x})\|$	p	$\|e_h(\overline{x})\|$	p
$\frac{1}{8}$	1.27e-6		3.48e-4	
$\frac{1}{16}$	3.04e-8	5.39	1.57e-7	11.11
$\frac{1}{32}$	7.96e-10	5.26	3.51e-9	5.49
$\frac{1}{64}$	1.44e-11	5.79	4.67e-11	6.23
$\frac{1}{128}$	1.50e-13	6.58	5.34e-13	6.45

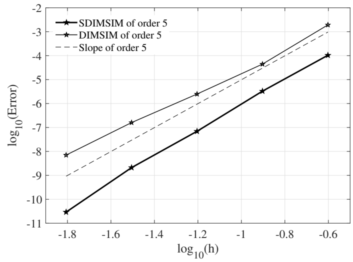

Figure 5. Numerical results of type 2 methods of orders $p = 5$ for the problem P2 with $\epsilon = 10^{-3}$.

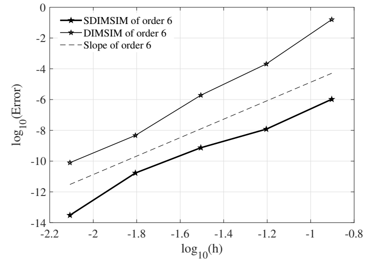

Figure 6. Numerical results of type 2 methods of orders $p = 6$ for the problem P2 with $\epsilon = 10^{-3}$.

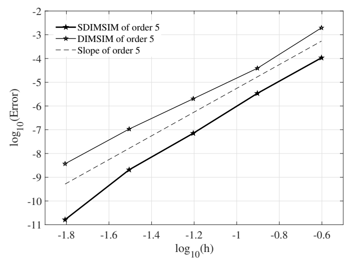

Figure 7. Numerical results of type 2 methods of orders $p = 5$ for the problem P2 with $\epsilon = 10^{-6}$.

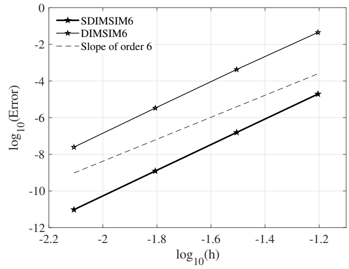

Figure 8. Numerical results of type 2 methods of orders $p = 6$ for the problem P2 with $\epsilon = 10^{-6}$.

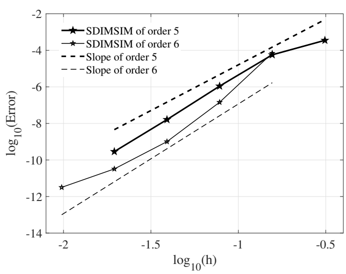

Figure 9. Numerical results of type 2 SDIMSIMs of orders $p = 5$ and $p = 6$ for the problem P3.

The results show capability and high efficiency of the proposed methods in solving stiff and nonstiff problems. These results illustrate that the errors of the methods decay with the expected theoretical order of convergence. In Tables 1 and 3, the results reach machine precision respectively for stepsizes $h = \frac{1}{128}$ and $h = \frac{1}{32}$ which explain some smaller experimental orders in the last row of these tables for SDIMSIM of order 6. Furthermore, the tables and Figures 5–8 confirm that results of the constructed SDIMSIMs are more accurate than those of DIMSIMs of the same order constructed in [14].

As it can be seen in Figure 9, the behavior of error for SDIMSIM of order 6 is not as regular for SDIMSIM of order 5, but the average observed orders of convergence for this method is 6.10; indeed the errors for the stepsizes $h = 10/2^6$ and $h = 10/2^{10}$ are respectively 7.00×10^{-5} and 3.18×10^{-12}. The Matlab programs which implement the proposed methods are given in [1].

5 Conclusions

In this paper, we described the construction of SDIMSIMs of high order and stage order, with $p = q = r = s$, using a variant of Fourier series approach [14]. Examples of the constructed explicit and implicit methods in types 1 and 2 of orders five and six were given. The numerical results demonstrated that the proposed methods are efficient in solving nonstiff and stiff problems and do not suffer from order reduction phenomenon.

Acknowledgements

The work of the third author (M. Braś) was partially supported by the Faculty of Applied Mathematics AGH UST statutory tasks within subsidy of Ministry of Education and Science.

References

[1] A. Abdi. Personal page of Ali Abdi. `https://asatid.tabrizu.ac.ir/en/pages/download.aspx?aa.abdi`.

[2] A. Abdi. Construction of high-order quadratically stable second-derivative general linear methods for the numerical integration of stiff ODEs. *Journal of Computational and Applied Mathematics*, **303**:218–228, 2016. https://doi.org/10.1016/j.cam.2016.02.054.

[3] A. Abdi and B. Behzad. Efficient Nordsieck second derivative general linear methods: construction and implementation. *Calcolo*, **55**(28):1–16, 2018. https://doi.org/10.1007/s10092-018-0270-7.

[4] A. Abdi, M. Braś and G. Hojjati. On the construction of second derivative diagonally implicit multistage integration methods for ODEs. *Applied Numerical Mathematics*, **76**:1–18, 2014. https://doi.org/10.1016/j.apnum.2013.08.006.

[5] A. Abdi and D. Conte. Implementation of second derivative general linear methods. *Calcolo*, **57**(20):1–29, 2020. https://doi.org/10.1007/s10092-020-00370-w.

[6] A. Abdi and G. Hojjati. An extension of general linear methods. *Numerical Algorithms*, **57**(2):149–167, 2011. https://doi.org/10.1007/s11075-010-9420-y.

[7] A. Abdi and G. Hojjati. Maximal order for second derivative general linear methods with Runge–Kutta stability. *Applied Numerical Mathematics*, **61**(10):1046–1058, 2011. https://doi.org/10.1016/j.apnum.2011.06.004.

[8] A. Abdi and G. Hojjati. Implementation of Nordsieck second derivative methods for stiff ODEs. *Applied Numerical Mathematics*, **94**:241–253, 2015. https://doi.org/10.1016/j.apnum.2015.04.002.

[9] A. Baeza, S. Boscarino, P. Mulet, G. Russo and D. Zorío. Reprint of: Approximate Taylor methods for ODEs. *Computers & Fluids*, **169**:87–97, 2018. https://doi.org/10.1016/j.compfluid.2018.03.058.

[10] B. Behzad, B. Ghazanfari and A. Abdi. Construction of the Nordsieck second derivative methods with RK stability for stiff ODEs. *Computational and Applied Mathematics*, **37**(4):5098–5112, 2018. https://doi.org/10.1007/s40314-018-0619-1.

[11] J.C. Butcher. On the convergence of numerical solutions to ordinary differential equations. *Mathematics of Computation*, **20**(93):1–10, 1966. https://doi.org/10.1090/S0025-5718-1966-0189251-X.

[12] J.C. Butcher. *Numerical methods for ordinary differential equations*. John Wiley & Sons, 2016. https://doi.org/10.1002/9781119121534.

[13] J.C. Butcher and G. Hojjati. Second derivative methods with RK stability. *Numerical Algorithms*, **40**(4):415–429, 2005. https://doi.org/10.1007/s11075-005-0413-1.

[14] J.C. Butcher and Z. Jackiewicz. Construction of high order diagonally implicit multistage integration methods for ordinary differential equations. *Applied Numerical Mathematics*, **27**(1):1–12, 1998. https://doi.org/10.1016/S0168-9274(97)00109-8.

[15] J.C. Butcher and P. Sehnalová. Predictor–corrector Obreshkov pairs. *Computing*, **95**(5):355–371, 2013. https://doi.org/10.1007/s00607-012-0258-0.

[16] A. Cardone and Z. Jackiewicz. Explicit Nordsieck methods with quadratic stability. *Numerical Algorithms*, **60**(1):1–25, 2012. https://doi.org/10.1007/s11075-011-9509-y.

[17] J.R. Cash. Second derivative extended backward differentiation formulas for the numerical integration of stiff systems. *SIAM Journal on Numerical Analysis*, **18**(1):21–36, 1981. https://doi.org/10.1137/0718003.

[18] R.P.K. Chan and A.Y.J. Tsai. On explicit two-derivative Runge-Kutta methods. *Numerical Algorithms*, **53**(2):171–194, 2010. https://doi.org/10.1007/s11075-009-9349-1.

[19] Y.F. Chang and G. Corliss. ATOMFT: solving ODEs and DAEs using Taylor series. *Computers & Mathematics with Applications*, **28**(10):209–233, 1994. https://doi.org/10.1016/0898-1221(94)00193-6.

[20] A.J. Christlieb, S. Gottlieb, Z. Grant and D.C. Seal. Explicit strong stability preserving multistage two-derivative time-stepping schemes. *Journal of Scientific Computing*, **68**(3):914–942, 2016. https://doi.org/10.1007/s10915-016-0164-2.

[21] G. Dahlquist. A special stability problem for linear multistep methods. *BIT Numerical Mathematics*, **3**(1):27–43, 1963. https://doi.org/10.1007/BF01963532.

[22] W.H. Enright. Second derivative multistep methods for stiff ordinary differential equations. *SIAM Journal on Numerical Analysis*, **11**(2):321–331, 1974. https://doi.org/10.1137/0711029.

[23] G.K. Gupta. Implementing second-derivative multistep methods using the Nordsieck polynomial representation. *Mathematics of Computation*, **32**(141):13–18, 1978. https://doi.org/10.1090/S0025-5718-1978-0478630-7.

[24] E. Hairer and G. Wanner. *Solving ordinary differential equations II: Stiff and Differential-Algebraic Problems*. Springer Berlin Heidelberg, 2010.

[25] G. Hojjati, M.Y. Rahimi Ardabili and S.M. Hosseini. New second derivative multistep methods for stiff systems. *Applied Mathematical Modelling*, **30**(5):466–476, 2006. https://doi.org/10.1016/j.apm.2005.06.007.

[26] Z. Jackiewicz. *General Linear Methods for Ordinary Differential Equations*. John Wiley & Sons, 2009. https://doi.org/10.1002/9780470522165.

[27] P. Kaps. *Rosenbrock-type methods. In: Numerical Methods for Solving Stiff Initial Value Problems. Proceeding, Oberwolfach 28.6.4.7.1981 (Dahlquist, G., Jeltsch, R., eds.). Bericht Nr. 9, Institut für Geometrie und Praktische Mathematik, RWTH Aachen, Templergraben 55, D-5100 Aachen.* Templergraben 55, D-5100 Aachen, 1981.

[28] A.Y.J. Tsai, R.P.K. Chan and S. Wang. Two-derivative Runge–Kutta methods for PDEs using a novel discretization approach. *Numerical Algorithms*, **65**(3):687–703, 2014. https://doi.org/10.1007/s11075-014-9823-2.