Mathematical Modelling and Analysis
Volume 19 Number 1, February 2014, 18–43
http://dx.doi.org/10.3846/13926292.2014.892903

Publisher: Taylor&Francis and VGTU
http://www.tandfonline.com/TMMA
Print ISSN: 1392-6292
Online ISSN: 1648-3510

Extrapolated Implicit–Explicit Runge–Kutta Methods

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Received August 1, 2013; revised February 2, 2014; published online February 20, 2014

Abstract. We investigate a new class of implicit–explicit singly diagonally implicit Runge–Kutta methods for ordinary differential equations with both non-stiff and stiff components. The approach is based on extrapolation of the stage values at the current step by stage values in the previous step. This approach was first proposed by the authors in context of implicit–explicit general linear methods.

Keywords: non-stiff and stiff processes, extrapolated IMEX methods, Runge–Kutta methods, error and stability analysis, construction of highly stable methods.

AMS Subject Classification: 65L05; 65L20.

1 Introduction

The discretization in space of time-dependent advection–diffusion–reaction differential equations leads to large systems of ordinary differential equations (ODEs) of the form

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

where $f(y)$ represents the non-stiff processes, obtained by discretization of advection terms, and $g(y)$ represents stiff processes, obtained by discretization of diffusion or chemical reaction terms. For such systems it is, in general, not practical to apply the same integration formula to the different parts of the system, and the better approach is to treat non-stiff parts by explicit method and stiff parts by implicit formula. To formulate this approach consider first the class of singly diagonally-implicit Runge–Kutta (SDIRK) methods defined on the uniform grid $t_n = t_0 + nh$, $n = 0, 1, \ldots, N$, $Nh = T - t_0$, by

$$\begin{cases} Y_i^{[n+1]} = y_n + h \sum_{j=1}^{i} a_{ij} \big(f\big(Y_j^{[n+1]}\big) + g\big(Y_j^{[n+1]}\big) \big), \quad i = 1, 2, \ldots, s, \\ y_{n+1} = y_n + h \sum_{j=1}^{s} b_j \big(f\big(Y_j^{[n+1]}\big) + g\big(Y_j^{[n+1]}\big) \big), \end{cases} \tag{1.2}$$

$n = 0, 1, \ldots, N-1$, $a_{ii} = \lambda$, $i = 1, 2, \ldots, s$. Here, $Y_i^{[n+1]}$ is an approximation to $y(t_n + c_i h)$ and y_n is an approximation of order p to $y(t_n)$. Similarly as in [11] we propose to handle the non-stiff terms $f(Y_j^{[n+1]})$ in (1.2) in an explicit manner by applying the extrapolation formula of the form

$$\begin{aligned} f(Y_j^{[n+1]}) \approx \alpha_{j,0} f(y_{n-1}) + \sum_{k=1}^{s} \alpha_{jk} f\big(Y_k^{[n]}\big) \\ + \beta_{j,0} f(y_n) + \sum_{k=1}^{j-1} \beta_{jk} f\big(Y_k^{[n+1]}\big), \quad j = 1, 2, \ldots, s. \end{aligned} \tag{1.3}$$

Substituting (1.3) into (1.2) and proceeding as in [11], i.e., changing the order of summation in the resulting double sums and interchanging the indices j and k, we obtain a class of so-called extrapolated implicit–explicit (IMEX) SDIRK schemes defined by the formulas

$$\begin{cases} Y_i^{[n+1]} = y_n + h\bar{a}_{i,0} f(y_{n-1}) + h \sum_{j=1}^{s} \bar{a}_{ij} f\big(Y_j^{[n]}\big) + h a_{i,0}^{*} f(y_n) \\ \qquad + h \sum_{j=1}^{i-1} a_{ij}^{*} f\big(Y_j^{[n+1]}\big) + h \sum_{j=1}^{i} a_{ij} g\big(Y_j^{[n+1]}\big), \quad i = 1, 2, \ldots, s, \\ y_{n+1} = y_n + h\bar{b}_0 f(y_{n-1}) + h \sum_{j=1}^{s} \bar{b}_j f\big(Y_j^{[n]}\big) \\ \qquad + h b_0^{*} f(y_n) + h \sum_{j=1}^{s-1} b_j^{*} f\big(Y_j^{[n+1]}\big) + h \sum_{j=1}^{s} b_j g\big(Y_j^{[n+1]}\big), \end{cases} \tag{1.4}$$

$n = 0, 1, \ldots, N-1$, where the coefficients $\bar{a}_{ij}$, a_{ij}^{*}, $\bar{b}_j$, and b_j^{*} are given by

$$\bar{a}_{ij} = \sum_{k=1}^{i} a_{ik} \alpha_{kj}, \quad a_{ij}^{*} = \sum_{k=j+1}^{i} a_{ik} \beta_{kj}, \quad i = 1, 2, \ldots, s, \ j = 0, 1, \ldots, s,$$

$$\bar{b}_j = \sum_{k=1}^{s} b_k \alpha_{kj}, \quad b_j^* = \sum_{k=j+1}^{s} b_k \beta_{kj}, \quad j = 0, 1, \ldots, s.$$

Observe that (1.4) is a two-step method which requires a starting procedure to compute $Y_i^{[0]}$ such that

$$Y_i^{[0]} = y\big(t_0 + (c_i - 1)h\big) + O\big(h^p\big), \quad i = 1, 2, \ldots, s, \tag{1.5}$$

where p is the order of the SDIRK formula (1.2), and it is assumed that the solution $y(t)$ to (1.1) is also defined on the initial interval $[t_0 - h, t_0]$. Putting

$$Y^{[n]} = \begin{bmatrix} Y_1^{[n]} \\ \vdots \\ Y_s^{[n]} \end{bmatrix}, \quad f\big(Y^{[n]}\big) = \begin{bmatrix} f\big(Y_1^{[n]}\big) \\ \vdots \\ f\big(Y_s^{[n]}\big) \end{bmatrix}, \quad g\big(Y^{[n]}\big) = \begin{bmatrix} g\big(Y_1^{[n]}\big) \\ \vdots \\ g\big(Y_s^{[n]}\big) \end{bmatrix},$$

the method (1.4) can be written in a more compact vector form

$$\begin{cases} Y^{[n+1]} = y_n \mathbf{e} + h\mathbf{a}_0 f(y_{n-1}) + h\bar{\mathbf{A}} f\big(Y^{[n]}\big) \\ \qquad\qquad + h\mathbf{a}_0^* f(y_n) + h\mathbf{A}^* f\big(Y^{[n+1]}\big) + h\mathbf{A} g\big(Y^{[n+1]}\big), \\ y_{n+1} = y_n + h\bar{b}_0 f(y_{n-1}) + h\bar{\mathbf{b}}^T f\big(Y^{[n]}\big) \\ \qquad\qquad + b_0^* f(y_n) + h\mathbf{b}^{*T} f\big(Y^{[n+1]}\big) + h\mathbf{b}^T g\big(Y^{[n+1]}\big), \end{cases} \tag{1.6}$$

$n = 0, 1, \ldots, N-1$. Here, $\mathbf{e} = [1, \ldots, 1]^T \in \mathbb{R}^s$,

$$\bar{\mathbf{a}}_0 = \begin{bmatrix} a_{1,0} & \cdots & a_{s,0} \end{bmatrix}^T, \quad \bar{\mathbf{A}} = [\bar{a}_{ij}]_{i,j=1}^s, \quad \mathbf{A}^* = \big[a_{ij}^*\big]_{i,j=1}^s, \quad \mathbf{A} = [a_{ij}]_{i,j=1}^s,$$
$$\bar{\mathbf{b}} = \begin{bmatrix} \bar{b}_1 & \cdots & \bar{b}_s \end{bmatrix}^T, \quad \mathbf{b}^* = \begin{bmatrix} b_1^* & \cdots & b_s^* \end{bmatrix}^T, \quad \mathbf{b} = \begin{bmatrix} b_1 & \cdots & b_s \end{bmatrix}^T.$$

Observe that

$$\bar{\mathbf{a}}_0 = \mathbf{A}\alpha_0, \quad \bar{\mathbf{A}} = \mathbf{A}\alpha, \quad \mathbf{a}_0^* = \mathbf{A}\beta_0, \quad \mathbf{A}^* = \mathbf{A}\beta,$$
$$\bar{b}_0 = \mathbf{b}^T\alpha_0, \quad \bar{\mathbf{b}}^T = \mathbf{b}^T\alpha, \quad b_0^* = \mathbf{b}^T\beta_0, \quad \mathbf{b}^{*T} = \mathbf{b}^T\beta,$$

where $\alpha_0 = \begin{bmatrix} \alpha_{1,0} & \cdots & \alpha_{s,0} \end{bmatrix}^T$, $\alpha = [\alpha_{i,j}]_{i,j=1}^s$, $\beta_0 = \begin{bmatrix} \beta_{1,0} & \cdots & \beta_{s,0} \end{bmatrix}^T$, $\beta = [\beta_{i,j}]_{i,j=1}^s$. Observe also that the coefficient matrix $\mathbf{A}^*$ is strictly lower triangular, and that $b_s^* = 0$.

The computational kernel of our method consists of the solution of s non linear systems of dimension d, which is simplified by the assumption $a_{ii} = \lambda$, for all $i = 1, \ldots, s$. This is the same computational cost as the IMEX RK methods proposed by Ascher et al. [1]. As a matter of fact our method, written as in (1.4) has the same form of the method proposed in [1]. We underline that our method has uncoupled order conditions, as we will show in the following, while the previous one has coupled order conditions, and this aspect reduces the degree of freedom in the search for optimal methods.

Assuming that $g(y) = 0$ in (1.1), the formula (1.6) reduces to the explicit two-step method

$$\begin{cases} Y^{[n+1]} = y_n\mathbf{e} + h\bar{\mathbf{a}}_0 f(y_{n-1}) + h\bar{\mathbf{A}} f\big(Y^{[n]}\big) \\ \qquad\qquad + h\mathbf{a}_0^* f(y_n) + h\mathbf{A}^* f\big(Y^{[n+1]}\big), \\ y_{n+1} = y_n + h\bar{b}_0 f(y_{n-1} + h\bar{\mathbf{b}}^T f\big(Y^{[n]}\big) \\ \qquad\qquad + hb_0^* f(y_n) + h\mathbf{b}^{*T} f\big(Y^{[n+1]}\big), \end{cases} \tag{1.7}$$

$n = 0, 1, \ldots, N-1$. These methods, which depend on stage values on two consecutive steps, are somewhat more general than two-step Runge–Kutta (TSRK) methods, which were introduced in [19] and further investigated in [2, 3, 20, 21, 23, 24, 25] and the monograph [18]. They can be represented as general linear methods (GLMs) of the form

$$\begin{bmatrix} y_{n-1} \\ Y^{[n]} \\ y_n \\ Y^{[n+1]} \\ \hline Y^{[n+1]} \\ y_{n+1} \\ y_n \end{bmatrix} = \left[\begin{array}{cccc|ccc} 0 & \mathbf{0}^T & 0 & \mathbf{0}^T & \mathbf{0}^T & 0 & 1 \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{I} & \mathbf{0} & \mathbf{0} \\ 0 & \mathbf{0}^T & 0 & \mathbf{0}^T & \mathbf{0}^T & 1 & 0 \\ \bar{\mathbf{a}}_0 & \bar{\mathbf{A}} & \mathbf{a}_0^* & \mathbf{A}^* & \mathbf{0} & \mathbf{e} & \mathbf{0} \\ \hline \bar{\mathbf{a}}_0 & \bar{\mathbf{A}} & \mathbf{a}_0^* & \mathbf{A}^* & \mathbf{0} & \mathbf{e} & \mathbf{0} \\ \bar{b}_0 & \bar{\mathbf{b}}^T & b_0^* & \mathbf{b}^{*T} & \mathbf{0}^T & 1 & 0 \\ 0 & \mathbf{0}^T & 0 & \mathbf{0}^T & \mathbf{0}^T & 1 & 0 \end{array}\right] \begin{bmatrix} hf(y_{n-1}) \\ hf\big(Y^{[n]}\big) \\ hf(y_n) \\ hf\big(Y^{[n+1]}\big) \\ \hline Y^{[n]} \\ y_n \\ y_{n-1} \end{bmatrix}, \tag{1.8}$$

$n = 0, 1, \ldots, N-1$, where $\mathbf{0}$ stands for zero matrix of dimension $s \times s$ or zero column vector of dimension s. Representations of TSRK methods are discussed in [18, 19, 26].

The paper is organized as follows. Section 2 is devoted to the convergence analysis of IMEX extrapolated methods. In Section 3 the study of the linear stability of the proposed methods is illustrated. In Section 4 we construct IMEX SDRK methods with optimal stability properties, up to order four. In Section 5 we present the results of numerical experiments which confirm the expected order of the IMEX schemes constructed in this paper. Last section contains some concluding remarks.

2 Order Conditions for Extrapolated IMEX SDIRK Methods

We will demonstrate in this section that the IMEX scheme (1.4) corresponding to SDIRK method (1.2) of order p and extrapolation formula (1.3) of order p is convergent with the same order p. We recall that the method (1.2) is said to have order p if for sufficiently smooth problems (1.1) we have

$$\big\|y(t_0 + h) - y_1\big\| = O\big(h^{p+1}\big)$$

as $h \to 0$, where $y(t)$ is the solution to (1.1) and y_1 is a numerical approximation to $y(t_0+h)$ computed by the formula (1.2) corresponding to $n = 0$, compare [15].

The extrapolation formula (1.3) is said to have order p if for sufficiently smooth functions $f(y(t))$ we have

$$\begin{aligned}\alpha_{j,0} f(y_{n-1}) + \sum_{k=1}^{s} \alpha_{jk} f\big(Y_k^{[n]}\big) + \beta_{j,0} f(y_n) + \sum_{k=1}^{j-1} \beta_{jk} f\big(Y_k^{[n+1]}\big) \\ = f\big(y(t_n + c_j h)\big) + \mathcal{O}\big(h^p\big), \quad j = 1, 2, \ldots, s. \end{aligned} \tag{2.1}$$

We first construct high order function extrapolation formulas.

2.1 Construction of high order function extrapolation formulas

We first build the explicit Runge–Kutta method with $s + j + 1$ stages

$$\begin{array}{c|c} \widehat{\mathbf{c}}^{(j)} & \widehat{\mathbf{A}}^{(j)} \\ \hline & \widehat{\mathbf{b}}^{(j)\,T} \\ \hline & \widehat{\mathbf{d}}^{(j)\,T} \end{array}, \tag{2.2}$$

where the weights $\widehat{\mathbf{b}}^{(j)}$ are used for solution extrapolation, and the weights $\widehat{\mathbf{d}}^{(j)}$ for function extrapolation. The extended Butcher tableau is defined by

$$\begin{array}{c|cccc} 0 & 0 & 0_{1\times s} & 0 & 0_{1\times(j-1)} \\ c & 0_{s\times 1} & A & 0_{s\times 1} & 0_{s\times(j-1)} \\ 1 & 0 & b^T & 0 & 0_{1\times(j-1)} \\ 1_{(j-1)\times 1} + c_{1:j-1} & 0_{(j-1)\times 1} & 1_{(j-1)\times 1}\cdot b^T & 0_{(j-1)\times 1} & A_{1:j-1,1:j-1} \\ \hline & \mu_{j,0} & \mu_{j,1:s} & \nu_{j,0} & \nu_{j,1:j-1} \\ \hline & \alpha_{j,0} & \alpha_{j,1:s} & \beta_{j,0} & \beta_{j,1:j-1} \end{array}.$$

Note that if the first stage of the SDIRK method is explicit then we fix $\mu_{j,0} = \alpha_{j,0} = 0$. Similarly, if the SDIRK method is stiffly accurate we fix $\nu_{j,0} = \beta_{j,0} = 0$.

To construct high order function extrapolation formulas we make use of S-series [14]. Let ϕ be a smooth scalar function. An S-series is a formal expansion of the form

$$S\,(a, h\phi, hf, y) = \sum_{t\in T} \frac{h^{|t|}}{\sigma(t)}\, a(t)\, \varPhi(t)(y),$$

where the elementary differentials $\varPhi$ are defined as

$$\varPhi(\bullet)(y) = \phi(y), \quad \varPhi(t) = \phi^{(m)}(y)\big(F(t_1)(y), \ldots, F(t_m)(y)\big), \quad t = [t_1, \ldots, t_m].$$

Here $F(t)(y)$ are the elementary differentials associated with the solution of the original ODE. Here $t \in T$ and T is the set of labelled Butcher trees [15]. The tree densities are denoted by $\gamma(t)$.

The essential property of S-series is that they allow to expand the function ϕ applied to a regular B-series [14]

$$h\,\phi\big(B(a, hf, y)\big) = S(a', h\phi, hf, y),$$

where $a'(t) = a(t_1) \cdot a(t_2) \cdots a(t_m)$, $t = [t_1, \ldots, t_m]$.

We seek to build extrapolation formulas for the smooth scalar function ϕ using its values at the stage vectors $\phi(Y_j^{[n]})$ and $\phi(Y_j^{[n+1]})$. The ϕ function applied to the exact solution is represented as the following S-series

$$h\,\phi\big(y(t_{n+1} + c_j h)\big) = S\big(e_j', h\phi, h(f+g), y\big), \tag{2.3}$$

where e represents the B-series of the exact solution

$$y(t_{n+1} + c_j h) \sim e_j, \quad \text{where } e_j(t) = \frac{(1+c_j)^{\rho(t)}}{\gamma(t)} \text{ for } t \in T.$$

The coefficients of the B-series e_j and its derivative e_j' are given in Table 1 for trees up to order 4.

Table 1. The B-series of the exact solution together with its derivative. The tree notation follows the one in [15, Table 2.2, page 148].

Tree	Children	e_j	e_j'
τ		$1+c_j$	
$t_{2,1}$	τ	$(1+c_j)^2/2$	$1+c_j$
$t_{3,1}$	$\tau;\tau$	$(1+c_j)^3/3$	$(1+c_j)^2$
$t_{3,2}$	$t_{2,1}$	$(1+c_j)^3/6$	$(1+c_j)^2/2$
$t_{4,1}$	$\tau;\tau;\tau$	$(1+c_j)^4/4$	$(1+c_j)^3$
$t_{4,2}$	$\tau;t_{2,1}$	$(1+c_j)^4/8$	$(1+c_j)^3/2$
$t_{4,3}$	$t_{3,1}$	$(1+c_j)^4/12$	$(1+c_j)^3/3$
$t_{4,4}$	$t_{3,2}$	$(1+c_j)^4/24$	$(1+c_j)^3/6$

Recall the extended Runge–Kutta method (2.2). We have the following B-series for the stage vectors $\widehat{Y}_\ell^{(j)} \sim \widehat{\Psi}_\ell^{(j)}$. We have that

$$\widehat{\Psi}_\ell^{(j)}(\emptyset) = 1, \quad \widehat{\Psi}_\ell^{(j)}(t) = \sum_k \widehat{a}_{\ell,k}\big(\widehat{\Psi}_k^{(j)}\big)'(t).$$

We notice that $\big(\widehat{\Psi}_\ell^{(j)}\big)' = \widehat{\Phi}_\ell^{(j)}$, where $\widehat{\Phi}$ are the B-series used in the traditional analysis of Runge–Kutta schemes [15, Table 2.2, page 148].

The smooth function ϕ applied to the stage vectors has the following S-series representation:

$$h\,\phi\big(\widehat{Y}_\ell^{(j)}\big) = S\big(\big(\widehat{\Psi}_\ell^{(j)}\big)', h\phi, h(f+g), y\big) = S\big(\widehat{\Phi}_\ell^{(j)}, h\phi, h(f+g), y\big). \tag{2.4}$$

The coefficients of the series $\widehat{\Psi}_\ell^{(j)}$ and their derivatives $\widehat{\Phi}_\ell^{(j)}$ are given in Table 2 for trees up to order 4.

We are now ready to state the extrapolation order conditions result.

Table 2. The B-series of the numerical solutions together with their derivatives. The tree notation follows the one in [15, Table 2.2, page 148].

Tree	Children	$\widehat{\Psi}_\ell^{(j)}$	$\left(\widehat{\Psi}_\ell^{(j)}\right)' \equiv \widehat{\Phi}_\ell^{(j)}$
$\emptyset$		1	
τ	$\emptyset$	$\widehat{\mathbf{c}}_\ell^{(j)}$	1
$t_{2,1}$	τ	$\widehat{\mathbf{A}}_{\ell,:}^{(j)} \cdot \widehat{\mathbf{c}}_:^{(j)}$	$\widehat{\mathbf{c}}_\ell^{(j)}$
$t_{3,1}$	$\tau;\tau$	$\widehat{\mathbf{A}}_{\ell,:}^{(j)} \left(\widehat{\mathbf{c}}_:^{(j)}\right)^2$	$\left(\widehat{\mathbf{c}}_\ell^{(j)}\right)^2$
$t_{3,2}$	$t_{2,1}$	$\widehat{\mathbf{A}}_{\ell,:}^{(j)} \cdot \widehat{\mathbf{A}}_{:,:}^{(j)} \cdot \widehat{\mathbf{c}}_:^{(j)}$	$\widehat{\mathbf{A}}_{\ell,:}^{(j)} \cdot \widehat{\mathbf{c}}_:^{(j)}$
$t_{4,1}$	$\tau;\tau;\tau$	$\widehat{\mathbf{A}}_{\ell,:}^{(j)} \left(\widehat{\mathbf{c}}_:^{(j)}\right)^3$	$\left(\widehat{\mathbf{c}}_\ell^{(j)}\right)^3$
$t_{4,2}$	$\tau;t_{2,1}$	$\widehat{\mathbf{c}}_\ell^{(j)}\, \widehat{\mathbf{A}}_{\ell,:}^{(j)} \cdot \widehat{\mathbf{c}}_:^{(j)}$	$\widehat{\mathbf{c}}_\ell^{(j)}\, \widehat{\mathbf{A}}_{\ell,:}^{(j)} \cdot \widehat{\mathbf{c}}_:^{(j)}$
$t_{4,3}$	$t_{3,1}$	$\widehat{\mathbf{A}}_{\ell,:}^{(j)} \cdot \widehat{\mathbf{A}}_{:,:}^{(j)} \cdot \left(\widehat{\mathbf{c}}_:^{(j)}\right)^2$	$\widehat{\mathbf{A}}_{\ell,:}^{(j)} \left(\widehat{\mathbf{c}}_:^{(j)}\right)^2$
$t_{4,4}$	$t_{3,2}$	$\widehat{\mathbf{A}}_{\ell,:}^{(j)} \cdot \widehat{\mathbf{A}}_{:,:}^{(j)} \cdot \widehat{\mathbf{A}}_{:,:}^{(j)} \cdot \widehat{\mathbf{c}}_:^{(j)}$	$\widehat{\mathbf{A}}_{\ell,:}^{(j)} \cdot \widehat{\mathbf{A}}_{:,:}^{(j)} \cdot \widehat{\mathbf{c}}_:^{(j)}$

Theorem 1 [Order conditions for function extrapolation]. *The extrapolation formula*

$$\sum_{\ell=1}^{s+j+1} \widehat{\mathbf{d}}_\ell^{(j)}\, h\phi\big(\widehat{Y}_\ell^{(j)}\big) = \alpha_{j,0}\, h\phi(y_{n-1}) + \sum_{k=1}^{s} \alpha_{jk}\, h\phi\big(Y_k^{[n]}\big) + \beta_{j,0}\, h\phi(y_n) + \sum_{k=1}^{j-1} \beta_{jk}\, h\phi\big(Y_k^{[n+1]}\big) \tag{2.5}$$

(for any $j = 1, 2, \ldots, s$) has order p

$$\sum_{\ell=1}^{s+j+1} \widehat{\mathbf{d}}_\ell^{(j)}\, h\phi\big(\widehat{Y}_\ell^{(j)}\big) = h\phi\big(y(t_n + c_j h)\big) + \mathcal{O}\big(h^{p+1}\big)$$

if and only if the following order conditions are fulfilled:

$$\sum_{\ell=1}^{s+j+1} \widehat{\mathbf{d}}_\ell^{(j)}\, \widehat{\Phi}_\ell^{(j)}(t) = e_j'(t), \quad \forall t \in T\colon\ \rho(t) \le p. \tag{2.6}$$

Proof. From (2.4) the extrapolation (2.5) has the following S-series:

$$\sum_{\ell=1}^{s+j+1} \widehat{\mathbf{d}}_\ell^{(j)}\, h\phi\big(\widehat{Y}_\ell^{(j)}\big) = S\left(\sum_{\ell=1}^{s+j+1} \widehat{\mathbf{d}}_\ell^{(j)} \big(\widehat{\Phi}_\ell^{(j)}\big)', h\phi, hf, y\right).$$

The proof is based on matching the S-series coefficients of the extrapolation formula to those of the exact solution (2.3) for all trees of order up to p. □

Using the series coefficients given in Tables 1 and 2 we obtain the following function extrapolation order conditions (2.6) for up to order 4:

1.	$1 = \widehat{\mathbf{d}}^{(j)\,T} \cdot \mathbf{1}_{(s+j+1)\times 1}$
2.	$1 + c_j = \widehat{\mathbf{d}}^{(j)\,T} \cdot \widehat{\mathbf{c}}^{(j)}$
3.	$(1 + c_j)^2 = \widehat{\mathbf{d}}^{(j)\,T} \cdot \big(\widehat{\mathbf{c}}^{(j)}\big)^2$
	$(1 + c_j)^2/2 = \widehat{\mathbf{d}}^{(j)\,T} \cdot \widehat{\mathbf{A}}^{(j)} \cdot \widehat{\mathbf{c}}^{(j)}$
4.	$(1 + c_j)^3 = \widehat{\mathbf{d}}^{(j)\,T} \cdot \big(\widehat{\mathbf{c}}^{(j)}\big)^3$
	$(1 + c_j)^3/2 = \Big(\widehat{\mathbf{d}}^{(j)} \odot \widehat{\mathbf{c}}^{(j)}\Big)^T \cdot \widehat{\mathbf{A}}^{(j)} \cdot \widehat{\mathbf{c}}^{(j)}$
	$(1 + c_j)^3/3 = \widehat{\mathbf{d}}^{(j)\ T} \cdot \widehat{\mathbf{A}}^{(j)} \cdot \big(\widehat{\mathbf{c}}^{(j)}\big)^2$
	$(1 + c_j)^3/6 = \widehat{\mathbf{d}}^{(j)\ T} \cdot \widehat{\mathbf{A}}^{(j)} \cdot \widehat{\mathbf{A}}^{(j)} \cdot \widehat{\mathbf{c}}^{(j)}$

Here $(\cdot)$ represents matricial multiplication, and $(\odot)$ component-wise multiplication. Vector powers are taken component-wise.

2.2 Construction of high order solution extrapolation formulas

We now consider the solution extrapolation formula:

$$\begin{aligned}
\widehat{Y}_j^{[n+1]} &= y_{n-1} + \sum_{\ell=1}^{s+j+1} \widehat{\mathbf{n}}_\ell^{(j)}\, h(f+g)\big(\widehat{Y}_\ell^{(j)}\big) \\
&= y_{n-1} + h\mu_{j,0}(f+g)(y_{n-1}) + h\sum_{k=1}^{s} \mu_{j,k}(f+g)\big(Y_k^{[n]}\big) \\
&\quad + h\nu_{j,0}(f+g)(y_n) + h\sum_{k=1}^{j-1} \nu_{j,k}(f+g)\big(Y_k^{[n+1]}\big), \quad j = 1, 2, \ldots, s. \qquad (2.7)
\end{aligned}$$

We have the following.

Theorem 2 [Order conditions for solution extrapolation]. *The solution extrapolation* (2.7) *has order* p

$$\widehat{Y}_j^{[n+1]} = y(t_n + c_j h) + \mathcal{O}\big(h^p\big)$$

if and only if the following order conditions hold:

$$\sum_{\ell=1}^{s+j+1} \widehat{\mathbf{b}}_\ell^{(j)}\, \widehat{\Phi}_\ell^{(j)}(t) = \frac{(1+c_j)^{\rho(t)}}{\gamma(t)}, \quad \forall t \in T\colon\, \rho(t) \le p-1. \qquad (2.8)$$

Proof. The result follows directly from the Runge–Kutta order conditions theory. □

Using the series coefficients from Table 1 one obtains the following order conditions for solution extrapolation (2.8), for up to order 4:

1.	$1+c_j = \widehat{\mathbf{b}}^{(j)\,T}\cdot \mathbf{1}_{(s+j+1)\times 1}$
2.	$(1+c_j)^2/2 = \widehat{\mathbf{b}}^{(j)\,T}\cdot \widehat{\mathbf{c}}^{(j)}$
3.	$(1+c_j)^3/3 = \widehat{\mathbf{b}}^{(j)\,T}\cdot \big(\widehat{\mathbf{c}}^{(j)}\big)^2$
	$(1+c_j)^3/6 = \widehat{\mathbf{b}}^{(j)\,T}\cdot \widehat{\mathbf{A}}^{(j)}\cdot \widehat{\mathbf{c}}^{(j)}$
4.	$(1+c_j)^4/4 = \widehat{\mathbf{b}}^{(j)\,T}\cdot \big(\widehat{\mathbf{c}}^{(j)}\big)^3$
	$(1+c_j)^4/8 = \big(\widehat{\mathbf{b}}^{(j)}\odot \widehat{\mathbf{c}}^{(j)}\big)^T\cdot \widehat{\mathbf{A}}^{(j)}\cdot \widehat{\mathbf{c}}^{(j)}$
	$(1+c_j)^4/12 = \widehat{\mathbf{b}}^{(j)\,T}\cdot \widehat{\mathbf{A}}^{(j)}\cdot \big(\widehat{\mathbf{c}}^{(j)}\big)^2$
	$(1+c_j)^4/24 = \widehat{\mathbf{b}}^{(j)\,T}\cdot \widehat{\mathbf{A}}^{(j)}\cdot \widehat{\mathbf{A}}^{(j)}\cdot \widehat{\mathbf{c}}^{(j)}$

Here $(\cdot)$ represents matricial multiplication, and $(\odot)$ component-wise multiplication. Vector powers are taken component-wise.

Consider the SDIRK method (1.2) together with the solution extrapolation formula (2.7) where the previous step solution approximations (2.7) are used

$$\begin{cases} \widehat{Y}_i^{[n+1]} = y_{n-1} + h\mu_{i,0}(f+g)(y_{n-1}) + h\displaystyle\sum_{k=1}^{s}\mu_{i,k}\big(f\big(Y_k^{[n]}\big)+g\big(Y_k^{[n]}\big)\big) \\ \qquad\qquad + h\nu_{i,0}(f+g)(y_n) + h\displaystyle\sum_{k=1}^{i-1}\nu_{i,k}\big(f\big(Y_k^{[n+1]}\big)+g\big(Y_k^{[n+1]}\big)\big), \\ Y_i^{[n+1]} = y_n + h\displaystyle\sum_{j=1}^{i}a_{ij}\big(f\big(Y_j^{[n+1]}\big)+g\big(Y_j^{[n+1]}\big)\big), \\ \qquad\qquad + ha_{ii}\big(f\big(\widehat{Y}_i^{[n+1]}\big)+g\big(Y_i^{[n+1]}\big)\big), \quad i=1,2,\ldots,s, \\ y_{n+1} = y_n + h\displaystyle\sum_{j=1}^{s}b_j\big(f\big(Y_j^{[n+1]}\big)+g\big(Y_j^{[n+1]}\big)\big), \end{cases} \tag{2.9}$$

$n=0,1,\ldots,N-1$, $a_{ii}=\lambda$, $i=1,2,\ldots,s$.

2.3 Convergence of IMEX SDIRK schemes

Theorem 3. *Assume that the SDIRK method* (1.2) *has order p and that the extrapolation formula* (1.3) *has order p. Then the IMEX SDIRK scheme* (1.4) *is convergent with the same order p, i.e., $\big\|y(t_0+h)-y_1\big\| = O\big(h^{p+1}\big)$ as $h\to 0$, where y_1 is a numerical approximation to $y(t_0+h)$ computed by the formula* (1.4) *corresponding to $n=0$.*

Proof. Substituting $y(t_0+c_ih)$ for $Y_i^{[1]}$, $y(t_0+(c_j-1)h)$ for $Y_j^{[0]}$, $y(t_0)$ for y_0, and $y(t_0+h)$ for y_1 in the formula (1.4) corresponding to $n=0$ we obtain

$$
\begin{aligned}
y(t_0+c_ih) &= y(t_0) + h\bar{a}_{i,0} f\big(y(t_0-h)\big) + h\sum_{j=1}^{s} \bar{a}_{ij} f\big(y\big(t_0+(c_j-1)h\big)\big) \\
&\quad + ha^*_{i,0} f\big(y(t_0)\big) + h\sum_{j=1}^{i-1} a^*_{ij} f\big(y(t_0+c_jh)\big) + h\sum_{j=1}^{i} a_{ij} g\big(y(t_0+c_jh)\big) \\
&\quad + hd(t_0+c_ih), \quad i=1,2,\ldots,s, \\
y(t_1) &= y(t_0) + h\bar{b}_0 f\big(y(t_0-h)\big) + h\sum_{j=1}^{s} \bar{b}_j f\big(y\big(t_0+(c_j-1)h\big)\big) + hb^*_0 f\big(y(t_0)\big) \\
&\quad + h\sum_{j=1}^{s-1} b^*_j f\big(y(t_0+c_jh)\big) + h\sum_{j=1}^{i} b_j f\big(y(t_0+c_jh)\big) + h\widehat{d}(t_1),
\end{aligned}
$$

where $hd(t_0+c_ih)$ are local discretization errors of the stage values $Y_i^{[1]}$, and $h\widehat{d}(t_1)$ is local discretization error of the approximation y_1 to $y(t_1)$ which propagates to the next step. Using the formulas for $\bar{a}_{ij}$, a^*_{ij}, $\bar{b}_j$, and b^*_j, and then interchanging the indices j and k, and changing the order of summation in the resulting double sums we obtain

$$
\begin{aligned}
y(t_0+c_ih) &= y(t_0) + h\sum_{j=1}^{i} a_{ij}\Big(\alpha_{j,0} f\big(y(t_0-h)\big) \\
&\quad + \sum_{k=1}^{s} \alpha_{jk} f\big(y\big(t_0+(c_k-1)h\big)\big) + \beta_{j,0} f\big(y(t_0)\big) + \sum_{k=1}^{j-1} \beta_{jk} f\big(y(t_0+c_kh)\big)\Big) \\
&\quad + h\sum_{j=1}^{i} a_{ij} g\big(y(t_0+c_jh)\big) + hd(t_0+c_ih), \quad i=1,2,\ldots,s, \\
y(t_1) &= y(t_0) + h\sum_{j=1}^{s} b_j\Big(\alpha_{j,0} f\big(y(t_0-h)\big) + \sum_{k=1}^{s} \alpha_{jk} f\big(y\big(t_0+(c_k-1)h\big)\big) \\
&\quad + \beta_{j,0} f\big(y(t_0)\big) + \sum_{k=1}^{j-1} \beta_{jk} f\big(y(t_0+c_kh)\big)\Big) + h\sum_{j=1}^{s} b_j g\big(y(t_0+c_jh)\big) + h\widehat{d}(t_1).
\end{aligned}
$$

Using the relation (2.1) this leads to

$$
\begin{aligned}
y(t_0+c_ih) &= y(t_0) + h\sum_{j=1}^{i} a_{ij}\Big(f\big(y(t_0+c_jh)\big) + g\big(y(t_0+c_jh)\big)\Big) \\
&\quad + hd(t_0+c_ih) + h\sum_{j=1}^{i} a_{ij}\eta(t_0+c_jh), \quad i=1,2,\ldots,s,
\end{aligned}
$$

$$y(t_1) = y(t_0) + h\sum_{j=1}^{s} b_j\big(f\big(y(t_0+c_jh)\big) + g\big(y(t_0+c_jh)\big)\big)$$
$$+ h\widehat{d}(t_1) + h\sum_{j=1}^{s} b_j\eta(t_0+c_jh). \qquad (2.10)$$

Substituting $y(t_0+c_ih)$ for $Y_i^{[1]}$, $y(t_0)$ for y_0, and $y(t_1)$ for y_1 in (1.2) with $n=0$ we have also

$$y(t_0+c_ih) = y(t_0) + h\sum_{j=1}^{s} a_{ij}\big(f\big(y(t_0+c_jh)\big) + g\big(y(t_0+c_jh)\big)\big)$$
$$+ hd_{RK}(t_0+c_ih), \quad i=1,2,\ldots,s,$$
$$y(t_1) = y(t_0) + h\sum_{j=1}^{s} b_j\big(f\big(y(t_0+c_jh)\big) + g\big(y(t_0+c_jh)\big)\big) + h\widehat{d}_{RK}(t_1), \quad (2.11)$$

where $hd_{RK}(t_0+c_ih)$ are local discretization errors of the stage values $Y_i^{[1]}$, and $h\widehat{d}_{RK}(t_1)$ is local discretization error of the approximation y_1 to $y(t_1)$ computed by the method (1.2). Comparing (2.10) and (2.11) it follows that

$$d(t_0+c_ih) = d_{RK}(t_0+c_ih) + O\big(h^{p+1}\big), \qquad \widehat{d}(t_1) = \widehat{d}_{RK}(t_1) + O\big(h^{p+1}\big).$$

These relations imply that the Taylor series for the exact solution $y(t_0+h)$ and numerical solution y_1 defined by IMEX scheme (1.4) coincide up to the terms of order p as they do for the underlying Runge–Kutta method (1.2), i.e.,

$$\big\|y(t_0+h) - y_1\big\| = O\big(h^{p+1}\big)$$

as $h \to 0$. This completes the proof. □

3 Linear Stability Analysis

In this section we will investigate the stability properties of IMEX SDIRK methods (1.4) with respect to the scalar complex test equation

$$y'(t) = \lambda_0 y(t) + \lambda_1 y(t), \quad t \geq 0, \qquad (3.1)$$

where $\lambda_0, \lambda_1 \in \mathbb{C}$. Stability with respect to this test equation generalizes the concept of absolute stability to systems of equations which are the sum of non-stiff $\lambda_0 y(t)$ and stiff $\lambda_1 y(t)$ parts. Stability properties of some classes of IMEX methods with respect to (3.1) were examined in [11, 17, 22, 27, 28].

Applying (1.6) to (3.1) and putting $z_i = h\lambda_i$, $i=0,1$, we obtain the vector recurrence relations

$$Y^{[n+1]} = y_n\mathbf{e} + z_0\bar{\mathbf{a}}_0 y_{n-1} + z_0\bar{\mathbf{A}}Y^{[n]} + z_0\mathbf{a}_0^* y_n + z_0\mathbf{A}^*Y^{[n+1]} + z_1\mathbf{A}Y^{[n+1]},$$
$$y_{n+1} = y_n + z_0\bar{b}_0 y_{n-1} + z_0\bar{\mathbf{b}}^TY^{[n]} + z_0 b_0^* y_n + z_0{\mathbf{b}^*}^TY^{[n+1]} + z_1\mathbf{b}^TY^{[n+1]},$$

$n = 0, 1, \ldots, N-1$. This is equivalent to the implicit matrix recurrence relation

$$\begin{bmatrix} \mathbf{I}-z_0\mathbf{A}^*-z_1\mathbf{A} & \mathbf{0} & \mathbf{0} \\ -z_0\mathbf{b}^{*T}-z_1\mathbf{b}^T & 1 & 0 \\ \mathbf{0}^T & 0 & 1 \end{bmatrix} \begin{bmatrix} Y^{[n+1]} \\ y_{n+1} \\ y_n \end{bmatrix} = \begin{bmatrix} z_0\bar{\mathbf{A}} & \mathbf{e}+z_0\mathbf{a}_0^* & z_0\bar{\mathbf{a}}_0 \\ z_0\bar{\mathbf{b}}^T & 1+z_0 b_0^* & z_0\bar{b}_0 \\ \mathbf{0}^T & 1 & 0 \end{bmatrix} \begin{bmatrix} Y^{[n]} \\ y_n \\ y_{n-1} \end{bmatrix}. \quad (3.2)$$

Since

$$\begin{bmatrix} \mathbf{I}-z_0\mathbf{A}^*-z_1\mathbf{A} & \mathbf{0} & \mathbf{0} \\ -z_0\mathbf{b}^{*T}-z_1\mathbf{b}^T & 1 & 0 \\ \mathbf{0}^T & 0 & 1 \end{bmatrix}^{-1} = \begin{bmatrix} (\mathbf{I}-z_0\mathbf{A}^*-z_1\mathbf{A})^{-1} & \mathbf{0} & \mathbf{0} \\ (z_0\mathbf{b}^{*T}+z_1\mathbf{b}^T)(\mathbf{I}-z_0\mathbf{A}^*-z_1\mathbf{A})^{-1} & 1 & 0 \\ \mathbf{0}^T & 0 & 1 \end{bmatrix},$$

the recurrence relation (3.2) can be written in the explicit form

$$\begin{bmatrix} Y^{[n+1]} \\ y_{n+1} \\ y_n \end{bmatrix} = \mathbf{M}(z_0, z_1) \begin{bmatrix} Y^{[n]} \\ y_n \\ y_{n-1} \end{bmatrix}, \quad (3.3)$$

where the stability matrix $\mathbf{M}(z_0, z_1)$ is defined by

$$\mathbf{M}(z_0, z_1) = \begin{bmatrix} m_{11}(z_0,z_1) & m_{12}(z_0,z_1) & m_{13}(z_0,z_1) \\ m_{21}(z_0,z_1) & m_{22}(z_0,z_1) & m_{23}(z_0,z_1) \\ \mathbf{0}^T & 1 & 0 \end{bmatrix}$$

with

$$\begin{aligned} m_{11}(z_0,z_1) &= z_0(\mathbf{I}-z_0\mathbf{A}^*-z_1\mathbf{A})^{-1}\bar{\mathbf{A}}, \\ m_{12}(z_0,z_1) &= (\mathbf{I}-z_0\mathbf{A}^*-z_1\mathbf{A})^{-1}(\mathbf{e}+z_0\mathbf{a}_0^*), \\ m_{13}(z_0,z_1) &= z_0(\mathbf{I}-z_0\mathbf{A}^*-z_1\mathbf{A})^{-1}\bar{\mathbf{a}}_0, \\ m_{21}(z_0,z_1) &= z_0\big(\bar{\mathbf{b}}^T+(z_0\mathbf{b}^{*T}+z_1\mathbf{b}^T)(\mathbf{I}-z_0\mathbf{A}^*-z_1\mathbf{A})^{-1}\bar{\mathbf{A}}\big), \\ m_{22}(z_0,z_1) &= 1+z_0\mathbf{b}_0^*+\big(z_0\mathbf{b}^{*T}+z_1\mathbf{b}^T\big)(\mathbf{I}-z_0\mathbf{A}^*-z_1\mathbf{A})^{-1}(\mathbf{e}+z_0\mathbf{a}_0^*), \\ m_{23}(z_0,z_1) &= z_0\big(\bar{\mathbf{b}}_0+\big(z_0\mathbf{b}^{*T}+z_1\mathbf{b}^T\big)(\mathbf{I}-z_0\mathbf{A}^*-z_1\mathbf{A})^{-1}\bar{\mathbf{a}}_0\big). \end{aligned}$$

We define also the stability function of the IMEX SDIRK method (1.4) as a characteristic polynomial of the stability matrix $\mathbf{M}(z_0, z_1)$, i.e.,

$$p(w, z_0, z_1) = \det\big(w\mathbf{I} - \mathbf{M}(z_0, z_1)\big).$$

Putting $z_0 = 0$ the stability matrix reduces to

$$\mathbf{M}(0, z_1) = \begin{bmatrix} \mathbf{0} & (\mathbf{I}-z_1\mathbf{A})^{-1}\mathbf{e} & \mathbf{0} \\ \mathbf{0}^T & 1+z_1\mathbf{b}^T(\mathbf{I}-z_1\mathbf{A})^{-1}\mathbf{e} & 0 \\ \mathbf{0}^T & 1 & 0 \end{bmatrix},$$

and it follows that the stability function takes the form

$$p(0, z_1) = w^{s+1}\big(w - R(z_1)\big),$$

where $R(z) = 1 + z\mathbf{b}^T(\mathbf{I} - z\mathbf{A})^{-1}\mathbf{e}$ is the stability function of the underlying SDIRK method (1.2). Putting $z_1 = 0$ the stability matrix takes the form

$$\mathbf{M}(z_0,0) = \begin{bmatrix} z_0(\mathbf{I} - z_0\mathbf{A}^*)^{-1}\bar{\mathbf{A}} & (\mathbf{I} - z_0\mathbf{A}^*)^{-1}(\mathbf{e} + z_0\mathbf{a}_0^*) & z_0(\mathbf{I} - z_0\mathbf{A}^*)^{-1}\bar{\mathbf{a}}_0 \\ m_{21}(z_0,0) & m_{22}(z_0,0) & m_{23}(z_0,0) \\ \mathbf{0}^T & 1 & 0 \end{bmatrix}$$

with

$$\begin{aligned} m_{21}(z_0,z_1) &= z_0\big(\bar{\mathbf{b}}^T + z_0\mathbf{b}^{*T}(\mathbf{I} - z_0\mathbf{A}^*)^{-1}\bar{\mathbf{A}}\big), \\ m_{22}(z_0,z_1) &= 1 + z_0\mathbf{b}_0^* + z_0\mathbf{b}^{*T}(\mathbf{I} - z_0\mathbf{A}^*)^{-1}(\mathbf{e} + z_0\mathbf{a}_0^*), \\ m_{23}(z_0,z_1) &= z_0\big(\bar{\mathbf{b}}_0 + z_0\mathbf{b}^{*T}(\mathbf{I} - z_0\mathbf{A}^*)^{-1}\bar{\mathbf{a}}_0\big). \end{aligned}$$

It can be verified that this corresponds to the stability matrix

$$\mathbf{V} + z_0\mathbf{G}(\mathbf{I} - z_0\mathbf{Q})^{-1}\mathbf{U}$$

of the explicit method (1.8) with

$$\mathbf{Q} = \begin{bmatrix} 0 & \mathbf{0}^T & 0 & \mathbf{0}^T \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ 0 & \mathbf{0}^T & 0 & \mathbf{0}^T \\ \bar{\mathbf{a}}_0 & \bar{\mathbf{A}} & \mathbf{a}_0^* & \mathbf{A}^* \end{bmatrix}, \qquad \mathbf{U} = \begin{bmatrix} \mathbf{0}^T & 0 & 1 \\ \mathbf{I} & \mathbf{0} & \mathbf{0} \\ \mathbf{0}^T & 1 & 0 \\ \mathbf{0} & \mathbf{e} & \mathbf{0} \end{bmatrix},$$

$$\mathbf{G} = \begin{bmatrix} \bar{\mathbf{a}}_0 & \bar{\mathbf{A}} & \mathbf{a}_0^* & \mathbf{A}^* \\ \bar{b}_0 & \bar{\mathbf{b}}^T & b_0^* & \mathbf{b}^{*T} \\ 0 & \mathbf{0}^T & 0 & \mathbf{0}^T \end{bmatrix}, \qquad \mathbf{V} = \begin{bmatrix} \mathbf{0} & \mathbf{e} & \mathbf{0} \\ \mathbf{0}^T & 1 & 0 \\ \mathbf{0}^T & 1 & 0 \end{bmatrix}.$$

We say that the IMEX GLM (2.1) is stable for given $z_0, z_1 \in \mathbb{C}$ if all the roots $w_i(z_0,z_1)$, $i = 1,2,\ldots,s+2$, of the stability function $p(w,z_0,z_1)$ are inside of the unit circle. In this paper we will be mainly interested in IMEX SDIRK schemes which are $A(\alpha)$- or A-stable with respect to the implicit part $z_1 \in \mathbb{C}$. To investigate such methods we consider, similarly as in [11, 17, 27], the sets

$$\mathcal{S}_\alpha = \big\{z_0 \in \mathbb{C}\colon \text{the IMEX SDIRK method is stable for any } z_1 \in \mathcal{A}_\alpha\big\},$$

where the set $\mathcal{A}_\alpha \subset \mathbb{C}$ is defined by

$$\mathcal{A}_\alpha = \big\{z \in \mathbb{C}\colon \mathrm{Re}(z) < 0 \text{ and } \big|\mathrm{Im}(z)\big| \le \tan(\alpha)\big|\mathrm{Re}(z)\big|\big\}.$$

It follows from the maximum principle that $\mathcal{S}_\alpha$ has a simpler representation given by

$$\mathcal{S}_\alpha = \left\{\begin{matrix} z_0 \in \mathbb{C}\colon \text{the IMEX SDIRK method is stable for any} \\ z_1 = -|y|/\tan(\alpha) + iy,\ y \in \mathbb{R} \end{matrix}\right\}. \tag{3.4}$$

As in [11], for fixed values of $y \in \mathbb{R}$ we define also the sets

$$\mathcal{S}_{\alpha,y} = \left\{\begin{matrix} z_0 \in \mathbb{C}\colon \text{the IMEX SDIRK method is stable for fixed} \\ z_1 = -|y|/\tan(\alpha) + iy \end{matrix}\right\}. \tag{3.5}$$

Observe that $\mathcal{S}_\alpha = \bigcap_{y\in\mathbb{R}} \mathcal{S}_{\alpha,y}$. Observe also that the region $\mathcal{S}_{\alpha,0}$ is independent of α, and corresponds to the region of absolute stability of the explicit method (1.8). This region will be denoted by $\mathcal{S}_E$. We have $\mathcal{S}_\alpha \subset \mathcal{S}_E$, and we will look for IMEX SDIRK schemes for which the stability region $\mathcal{S}_\alpha$ contains a large part of the stability region $\mathcal{S}_E$ of the explicit method (1.8). We will start our search for such IMEX SDIRK schemes with the explicit formulas (1.8) with sufficiently large regions of absolute stability $\mathcal{S}_E$.

The boundary $\partial\mathcal{S}_{\alpha,y}$ of the region $\mathcal{S}_{\alpha,y}$ can be determined by the boundary locus method which computes the locus of the curve

$$\partial\mathcal{S}_{\alpha,y} = \big\{z_0 \in \mathbb{C}\colon p\big(e^{i\theta}, z_0, -|y|/\tan(\alpha) + iy\big) = 0,\ \theta \in [0, 2k\pi]\big\},$$

where k is a positive integer. In [11] we have also developed an algorithm to compute the boundary $\partial\mathcal{S}_\alpha$ of the stability region $\mathcal{S}_\alpha$ of the IMEX GLMs. This algorithm, which is applicable to the methods considered in this paper, will be used in Section 4 to determine stability regions $\mathcal{S}_\alpha$ for IMEX SDIRK schemes (1.4) up to the order $p = 4$.

4 Construction of Highly Stable IMEX Schemes

In this section we will describe a search for IMEX SDIRK schemes with large regions of absolute stability of the explicit part of the method, assuming that the implicit part of the scheme, corresponding to $z_1 \in \mathbb{C}$, is $A(\alpha)$- or A-stable. We would like to find methods which are A-stable with respect to the implicit part, but especially for higher order methods, we relax this condition to the $A(\alpha)$-stability in order to find larger stability regions for the explicit part. This search is based on maximizing the area of the region of absolute stability $\mathcal{S}_\alpha$ for fixed $\alpha \in (0, \pi/2]$. This area $A(\mathcal{S}_\alpha)$ can be computed by integration in polar coordinates and is given by

$$A(\mathcal{S}_\alpha) = \int_0^{\pi/2} r(\theta)\, ds = \int_0^{\pi/2} r^2(\theta)\, d\theta,$$

where $r(\theta)$ is the ray from the point $z_0 = 0$ to the boundary $\partial\mathcal{S}_\alpha$ of $\mathcal{S}_\alpha$, and θ is the angle between this ray and the negative real axis. This integral can be approximate by composite trapezoidal rule, and the ray $r(\theta)$ can be computed by the bisection method applied to the function

$$p\big(w, -r(\theta)\cos(\theta) + ir(\theta)\sin(\theta), -|y|/\tan(\alpha) + iy\big) = 0$$

with $|w| = 1$ and appropriate value of y, which corresponds to the point on the boundary $\partial\mathcal{S}_\alpha$. We refer the reader to [11] for a more detailed description of this process. Some techniques have been suitably adapted from the techniques used for the construction of Nordsieck methods with quadratic stability [4, 5, 8, 9]. Using this procedure, we found methods with relatively large stability regions $\mathcal{S}_{\pi/2}$ as compared to other IMEX methods from the literature. These methods are suitable to efficiently solve ODEs with a stiff and a non-stiff part, since they have no restrictions on the stepsize as regards the stiff part and have acceptable restrictions on the stepsize as regards the non-stiff part.

4.1 IMEX SDIRK methods with $p = s = 1$

The SDIRK method with $p = s = 1$ is the implicit θ-method

$$\begin{cases} Y^{[n+1]} = h\theta\big(f\big(Y^{[n+1]}\big) + g\big(Y^{[n+1]}\big)\big) + y_n, \\ y_{n+1} = h\big(f\big(Y^{[n+1]}\big) + g\big(Y^{[n+1]}\big)\big) + y_n, \end{cases} \tag{4.1}$$

$n = 0, 1, \ldots, N-1$, which is A-stable for $\theta \in [1/2, 1]$ and L-stable for $\theta \in (1/2, 1]$. We consider the extrapolation procedure of the form

$$f\big(Y^{[n+1]}\big) = f\big(Y^{[n]}\big), \tag{4.2}$$

$n = 1, 2, \ldots, N-1$, which does not depend on $f(y_{n-1})$ and $f(y_n)$. Substituting (4.3) into (4.2) we obtain IMEX θ-method

$$\begin{cases} Y^{[n+1]} = h\theta\big(f\big(Y^{[n]}\big) + g\big(Y^{[n+1]}\big)\big) + y_n, \\ y_{n+1} = h\big(f\big(Y^{[n]}\big) + g\big(Y^{[n+1]}\big)\big) + y_n, \end{cases} \tag{4.3}$$

$n = 1, 2, \ldots, N-1$. These methods were already analyzed in [11] and in what follows we summarize briefly the results from this paper. Let $\mathcal{S}_E = \mathcal{S}_E(\theta)$ be the stability region of the explicit method corresponding to $g(y) = 0$ in (4.3), and $\mathcal{S}_\alpha = \mathcal{S}_\alpha(\theta)$ be the stability region of the IMEX scheme (4.3), assuming that the implicit part of the method is $A(\alpha)$-stable. Then

$$\mathcal{S}_{\pi/2}(1) = \mathcal{S}_E(1) = \big\{z_0 \in \mathbb{C}\colon |z_0 + 1| < 1\big\},$$
$$\mathcal{S}_{\pi/2}(\theta) \subset \mathcal{S}_E(\theta) \quad \text{and} \quad \mathcal{S}_{\pi/2}(\theta) \neq \mathcal{S}_E(\theta), \quad \theta \in (1/2, 1)$$

and $\mathcal{S}_{\pi/2}(1/2)$ is empty. These relations are illustrated on Fig 1, where we have plotted stability regions $\mathcal{S}_E(\theta)$ of explicit methods (dashed lines), and stability regions $\mathcal{S}_{\pi/2}(\theta)$ of IMEX schemes (solid lines) for $\theta = 1/2$, $2/3$, $3/4$, and 1.

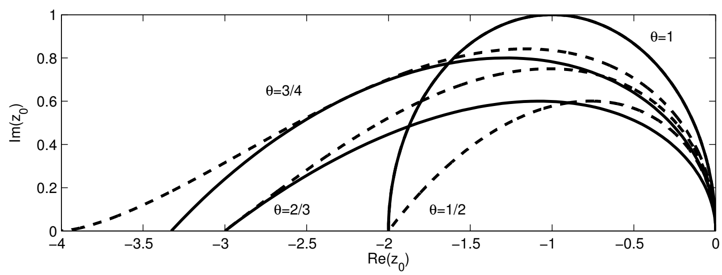

Figure 1. Stability regions $\mathcal{S}_E(\theta)$ of explicit methods (dashed lines), and stability regions $\mathcal{S}_{\pi/2}(\theta)$ of IMEX schemes (solid lines) for $\theta = 1/2$, $2/3$, $3/4$, and 1.

4.2 IMEX SDIRK methods with $p = s = 2$

SDIRK methods with $s = p = 2$ have the coefficients

$$\begin{array}{c|c} \mathbf{c} & \mathbf{A} \\ \hline & \mathbf{b}^T \end{array} = \begin{array}{c|cc} \lambda & \lambda & \\ c_2 & c_2 - \lambda & \lambda \\ \hline & \frac{2c_2-1}{2(c_2-\lambda)} & \frac{1-2\lambda}{2(c_2-\lambda)} \end{array}. \tag{4.4}$$

The stability function of the methods (4.4) does not depend on c_2 and has the form $R(z) = P(z)/Q(z)$, with

$$P(z) = 1 + (1-2\lambda)z + \big(1/2 - 2\lambda + \lambda^2\big)z^2, \quad Q(z) = (1-\lambda z)^2.$$

It can be verified that this method is A-stable for $\lambda \geq 1/4$ and L-stable for $\lambda = (2 \pm \sqrt{2})/2$, see [6]. We consider the extrapolation procedure (1.3) with $\alpha_0 = [0,0]^T$ and $\beta_0 = [0,0]^T$:

$$f\big(Y_j^{[n+1]}\big) = \sum_{k=1}^{2} \alpha_{jk} f\big(Y_k^{[n]}\big) + \sum_{k=1}^{j-1} \beta_{jk} f\big(Y_k^{[n+1]}\big), \quad j = 1,2,$$

$n = 1, 2, \ldots, N-1$, which as in Section 4.1 does not depend on $f(y_{n-1})$ and $f(y_n)$. It can be verified that the order conditions take the form

$$\begin{aligned} &\alpha_{11} + \alpha_{12} = 1, \quad \lambda\alpha_{11} + c_2\alpha_{12} = 1 + \lambda, \\ &\alpha_{21} + \alpha_{22} + \beta_{21} = 1, \quad \lambda\alpha_{21} + c_2\alpha_{22} + (1+\lambda)\beta_{21} = 1 + c_2. \end{aligned} \tag{4.5}$$

Solving the system (4.5) with respect to α_{11}, α_{12}, α_{21} and α_{22} leads to the coefficient matrices α and β of the form

$$\alpha = \begin{bmatrix} \frac{c_2-\lambda-1}{c_2-\lambda} & \frac{1}{c_2-\lambda} \\ \frac{\beta_{21}(1-c_2+\lambda)-1}{c_2-\lambda} & \frac{1+c_2-\beta_{21}-\lambda}{c_2-\lambda} \end{bmatrix}, \qquad \beta = \begin{bmatrix} 0 & 0 \\ \beta_{21} & 0 \end{bmatrix},$$

where β_{21} is a free parameter. The stability polynomial $p(w, z_0, z_1)$ of the corresponding IMEX SDIRK method takes the form

$$p(w, z_0, z_1) = (1-\lambda z_1)^2\big(w^3 - p_2(z_0,z_1)w^2 + p_1(z_0,z_1)w - p_0(z_0,z_1)\big)$$

with the coefficients $p_2(z_0, z_1)$, $p_1(z_0, z_1)$, and $p_0(z_0, z_1)$ which are polynomials of degree less than or equal to two with respect to z_0 and z_1. These coefficients depend also on c_2, λ, and β_{21}.

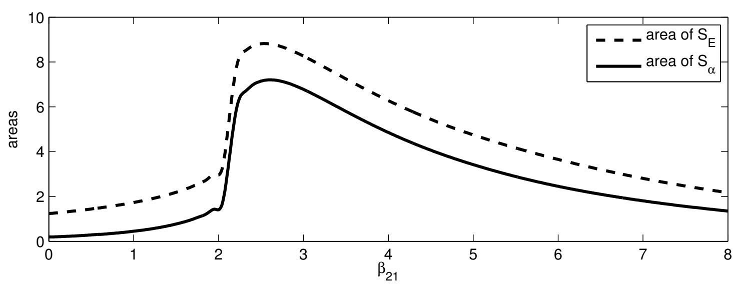

Figure 2. Areas of the stability regions $\mathcal{S}_E = \mathcal{S}_E(\beta_{21})$ (dashed line) and $\mathcal{S}_\alpha = \mathcal{S}_\alpha(\beta_{21})$ (solid line) for $\alpha = \pi/2$, $c_2 = 1$, $\lambda = (2-\sqrt{2})/2$, and $\beta_{21} \in [0, 8]$.

We will investigate first stability properties of IMEX schemes corresponding to $c_2 = 1$, where the underlying SDIRK method is L-stable. We will choose

$\lambda = (2-\sqrt{2})/2$ since this leads to larger regions of $\mathcal{S}_E$ and $\mathcal{S}_{\pi/2}$ than those corresponding to $\lambda = (2+\sqrt{2})/2$. We have plotted in Fig. 2 the area of the stability region $\mathcal{S}_E = \mathcal{S}_E(\beta_{21})$ of the explicit method (corresponding to $z_1 = 0$) and the area of the stability region $\mathcal{S}_{\pi/2} = \mathcal{S}_{\pi/2}(\beta_{21})$ of the IMEX scheme for $\beta_{21} \in [0, 8]$. It can be verified that the explicit formula attains the maximal area of $\mathcal{S}_E$, approximately equal to 8.83, for $\beta_{21} \approx 2.54$, and the IMEX scheme attains the maximal area of $\mathcal{S}_{\pi/2}$, approximately equal to 7.20, for $\beta_{21} \approx 2.61$.

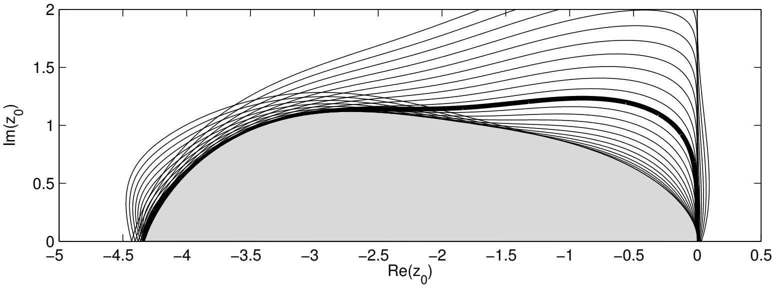

Figure 3. Stability regions $\mathcal{S}_{\pi/2,y}$, $y = -2.0, 1.8, \ldots, 2.0$ (thin lines), $\mathcal{S}_{\pi/2}$ (shaded region), and $\mathcal{S}_E$ (thick line) for $\lambda = (2-\sqrt{2})/2$, $c_2 = 1$ and $\beta_{21} \approx 2.61$.

On Fig. 3 we have plotted stability regions $\mathcal{S}_{\pi/2,y}$ for $y = -2.0, -1.8, \ldots, 2.0$ (thin lines), stability region $\mathcal{S}_{\pi/2}$ (shaded region), and stability region $\mathcal{S}_E$ (thick line), corresponding to $c_2 = 1$, $\lambda = (2-\sqrt{2})/2$, and $\beta_{21} \approx 2.61$. We can see that $\mathcal{S}_{\pi/2}$ contains a significant part of $\mathcal{S}_E$.

We have also displayed on Fig. 4 the contour plots of the area of the stability region $\mathcal{S}_{\pi/2}$ of the IMEX SDIRK schemes corresponding to $c_2 = 1$, $\lambda \in [0.25, 0.35]$, and $\beta_{21} \in [1, 5]$. This area attains its maximum value approximately equal to 7.55 for $\lambda \approx 0.30$ and $\beta_{21} \approx 2.48$. This point is marked by the symbol '$\times$' on Fig. 4. On Fig. 5 we have plotted stability regions $\mathcal{S}_{\pi/2,y}$ for $y = -2.0, -1.8, \ldots, 2.0$ (think lines), stability region $\mathcal{S}_{\pi/2}$ (shaded region), and stability region $\mathcal{S}_E$ (thick line), corresponding to $c_2 = 1$, $\lambda \approx 0.30$, and $\beta_{21} \approx 2.48$. We can see again that $\mathcal{S}_{\pi/2}$ contains a significant part of $\mathcal{S}_E$. We can see also that the interval of absolute stability is somewhat smaller than the interval of absolute stability corresponding to $c_2 = 1$, $\lambda = (2-\sqrt{2})/2$, and $\beta_{21} \approx 2.61$.

4.3 IMEX SDIRK methods with $p = s = 3$

SDIRK methods with $s = p = 3$ have the following coefficients

$$\begin{array}{c|c} \mathbf{c} & \mathbf{A} \\ \hline & \mathbf{b}^T \end{array} = \begin{array}{c|ccc} \lambda & \lambda & & \\ c_2 & c_2-\lambda & \lambda & \\ c_3 & a_{31} & a_{32} & \lambda \\ \hline & \frac{-3c_3+c_2(6c_3-3)+2}{6(c_2-\lambda)(c_3-\lambda)} & \frac{-3\lambda+c_3(6\lambda-3)+2}{6(c_2-c_3)(c_2-\lambda)} & \frac{c_2(3-6\lambda)+3\lambda-2}{6(c_2-c_3)(c_3-\lambda)} \end{array} \tag{4.6}$$

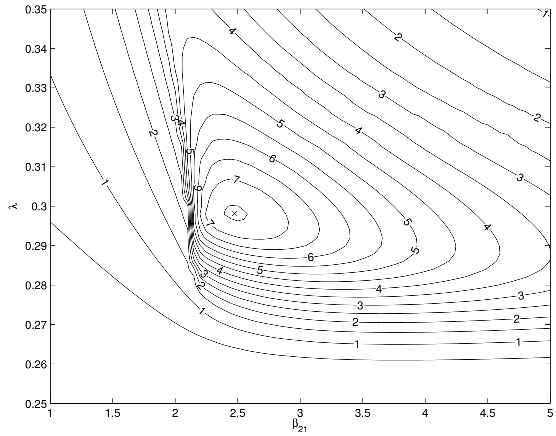

Figure 4. Contour plots of the area of stability region $\mathcal{S}_{\pi/2}$ of IMEX SDIRK methods for $s = p = 2$ corresponding to $c_2 = 1$, $\lambda \in [0.25, 0.35]$, and $\beta_{21} \in [1, 5]$.

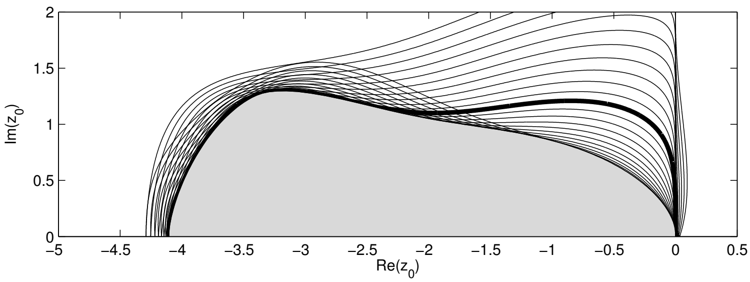

Figure 5. Stability regions $\mathcal{S}_{\pi/2,y}$, $y = -2.0, 1.8, \ldots, 2.0$ (thin lines), $\mathcal{S}_{\pi/2}$ (shaded region), and $\mathcal{S}_E$ (thick line) for $\lambda \approx 0.30$, , $c_2 = 1$ and $\beta_{21} \approx 2.48$.

with

$$a_{31} = \frac{(c_3 - \lambda)((3 - 6\lambda)c_2^2 + (6\lambda - 3)c_2 + (2 - 3\lambda)\lambda + c_3(6\lambda^2 - 6\lambda + 1))}{(3 - 6\lambda)c_2^2 + (6\lambda^2 - 2)c_2 + (2 - 3\lambda)\lambda},$$

$$a_{32} = \frac{(c_2 - c_3)(c_3 - \lambda)(6\lambda^2 - 6\lambda + 1)}{(3 - 6\lambda)c_2^2 + (6\lambda^2 - 2)c_2 + (2 - 3\lambda)\lambda}.$$

The stability function of methods (4.6) does not depend on the abscissas c_2 and c_3, and takes the form $R(z) = P(z)/Q(z)$, with

$$P(z) = 1 + (1 - 3\lambda)z + \left(\frac{1}{2} - 3\lambda + 3\lambda^2\right)z^2 + \left(\frac{1}{6} - \frac{3}{2}\lambda + 3\lambda^2 - \lambda^3\right)z^3,$$

$Q(z) = (1 - \lambda z)^3$. These methods are A-stable for $\lambda \in [\frac{1}{3}, 1.06790213]$, and L-stable for $\lambda \approx 0.4358665215$, which is one of the roots of the polynomial $\varphi(\lambda) = 6\lambda^3 - 18\lambda^2 + 9\lambda - 1$ [16].

The stability function of IMEX SDIRK methods takes the form

$$p(w, z_0, z_1) = (1-\lambda z_1)^3 w^4 - p_3(z_0, z_1)w^3 + p_2(z_0, z_1)w^2 - p_1(z_0, z_1)w + p_0(z_0, z_1),$$

where $p_i(z_0,z_1)$, $i=0,1,2,3$, are polynomials of degree less than or equal to three with respect to z_0 and z_1. These coefficients depend also on λ, c_2, c_3, β_{21}, β_{31}, and β_{32}.

Putting $\lambda=1/2$, $c_2=3/4$ and $c_3=1$, the SDIRK method takes the form

$$\begin{array}{c|c} \mathbf{c} & \mathbf{A} \\ \hline & \mathbf{b}^T \end{array} = \begin{array}{c|ccc} \frac{1}{2} & \frac{1}{2} & & \\ \frac{3}{4} & \frac{1}{4} & \frac{1}{2} & \\ 1 & 1 & -\frac{1}{2} & \frac{1}{2} \\ \hline & \frac{5}{3} & -\frac{4}{3} & \frac{2}{3} \end{array}.$$

It can be verified that the conditions for the IMEX SDIRK methods of order $p=3$ take the form:
$p=3$, $j=1$:

$$\alpha_{10}+\alpha_{11}+\alpha_{12}+\alpha_{13}+\beta_{10}=1, \qquad \frac{\alpha_{11}}{2}+\frac{3\alpha_{12}}{4}+\alpha_{13}+\beta_{10}=\frac{3}{2},$$
$$\frac{\alpha_{11}}{4}+\frac{9\alpha_{12}}{16}+\alpha_{13}+\beta_{10}=\frac{9}{4}, \qquad \frac{\alpha_{11}}{4}+\frac{\alpha_{12}}{2}+\frac{5\alpha_{13}}{8}+\frac{\beta_{10}}{2}=\frac{9}{8},$$

$p=3$, $j=2$:

$$\begin{aligned} &\alpha_{20}+\alpha_{21}+\alpha_{22}+\alpha_{23}+\beta_{20}+\beta_{21}=1, \\ &\frac{\alpha_{21}}{2}+\frac{3\alpha_{22}}{4}+\alpha_{23}+\beta_{20}+\frac{3\beta_{21}}{2}=\frac{7}{4}, \\ &\frac{\alpha_{21}}{4}+\frac{9\alpha_{22}}{16}+\alpha_{23}+\beta_{20}+\frac{9\beta_{21}}{4}=\frac{49}{16}, \\ &\frac{\alpha_{21}}{4}+\frac{\alpha_{22}}{2}+\frac{5\alpha_{23}}{8}+\frac{\beta_{20}}{2}+\frac{5\beta_{21}}{4}=\frac{49}{32}, \end{aligned}$$

$p=3$, $j=3$:

$$\begin{aligned} &\alpha_{30}+\alpha_{31}+\alpha_{32}+\alpha_{33}+\beta_{30}+\beta_{31}+\beta_{32}=1, \\ &\frac{\alpha_{31}}{2}+\frac{3\alpha_{32}}{4}+\alpha_{33}+\beta_{30}+\frac{3\beta_{31}}{2}+\frac{7\beta_{32}}{4}=2, \\ &\frac{\alpha_{31}}{4}+\frac{9\alpha_{32}}{16}+\alpha_{33}+\beta_{30}+\frac{9\beta_{31}}{4}+\frac{49\beta_{32}}{16}=4, \\ &\frac{\alpha_{31}}{4}+\frac{\alpha_{32}}{2}+\frac{5\alpha_{33}}{8}+\frac{\beta_{30}}{2}+\frac{5\beta_{31}}{4}+\frac{7\beta_{32}}{4}=2. \end{aligned}$$

Solving these order conditions with respect to $\alpha_{i,0}$, $i=1,2,3$, and α_{ij}, $i,j=1,2,3$, leads to a six parameter family of IMEX SDIRK methods with respect to the parameters β_{10}, β_{20}, β_{30}, β_{21}, β_{31}, and β_{32}, for which the vector α_0 and the matrix α are given by

$$\alpha_0=\left[\frac{\beta_{10}+5}{5} \quad \frac{4\beta_{20}-24\beta_{21}+41}{20} \quad \frac{\beta_{30}-6\beta_{31}-12\beta_{32}+17}{5}\right]^T,$$

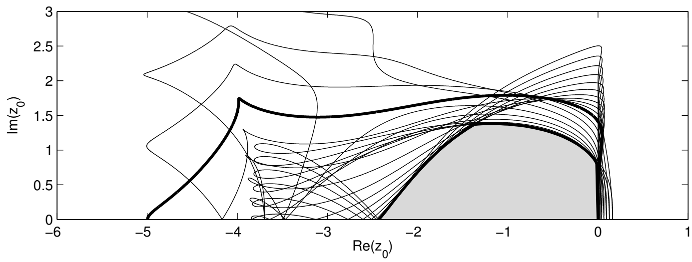

Figure 6. Stability regions $\mathcal{S}_{\pi/2,y}$, $y = -2.0, 1.8, \ldots, 2.0$ (thin lines), $\mathcal{S}_{\pi/2}$ (shaded region), and $\mathcal{S}_E$ (thick line) for $\beta_{10} = 3.088176567590889$, $\beta_{20} = 3.144648727948133$, $\beta_{30} = 4.411911013354342$, $\beta_{21} = 0.727840859205079$, $\beta_{31} = 0.837957009491469$ and $\beta_{32} = 0.443641071336429$.

$$\alpha = \begin{bmatrix} -\dfrac{5+2\beta_{10}}{5} & \dfrac{8\beta_{10}}{5} & \dfrac{15-8\beta_{10}}{5} \\ -\dfrac{3(21+4\beta_{20}-14\beta_{21})}{10} & \dfrac{7+8\beta_{20}-8\beta_{21}}{5} & \dfrac{77-32\beta_{20}-48\beta_{21}}{20} \\ \alpha_{31} & \alpha_{32} & \alpha_{33} \end{bmatrix}$$

with

$$\alpha_{31} = -\frac{52+6\beta_{30}-21\beta_{31}-42\beta_{32}}{5}, \quad \alpha_{32} = \frac{16+8\beta_{30}-8\beta_{31}-21\beta_{32}}{5},$$
$$\alpha_{33} = \frac{2(12-4\beta_{30}-6\beta_{31}-7\beta_{32}}{5}.$$

We performed a numerical search in the parameter space β_{10}, β_{20}, β_{30}, β_{21}, β_{31}, and β_{32}, trying to maximize the area of the stability region $\mathcal{S}_E$ of the explicit method. This corresponds to

$$\beta_0 = \begin{bmatrix} 3.088176567590889 & 3.144648727948133 & 4.411911013354342 \end{bmatrix}^T,$$
$$\beta = \begin{bmatrix} 0 & 0 & 0 \\ 0.727840859205079 & 0 & 0 \\ 0.837957009491469 & 0.443641071336429 & 0 \end{bmatrix},$$
$$\alpha_0 = \begin{bmatrix} 1.617635313518178 & 1.805520714543532 & 2.212095220073677 \end{bmatrix}^T,$$
$$\alpha = \begin{bmatrix} -6.705811881109066 & 4.941082508145422 & -1.941082508145423 \\ -7.016646864876432 & 5.266892589988879 & -2.928256026809203 \\ -8.448288776935042 & 7.055033906567607 & -5.512349443888470 \end{bmatrix},$$

for which the area of $\mathcal{S}_E$ is approximately equal to 14.19. The area of the corresponding IMEX SDIRK scheme is approximately equal to 5.00. We have plotted in Fig. 6 regions $\mathcal{S}_{\pi/2,y}$ for $y = -2.0, -1.8, \ldots, 2.0$ (thin lines), the stability region $\mathcal{S}_{\pi/2}$ (shaded region) and $\mathcal{S}_E$ (thick line).

We have also performed a similar search trying to maximize directly the area of the stability region $\mathcal{S}_{\pi/2}$ of the IMEX scheme assuming that the implicit part

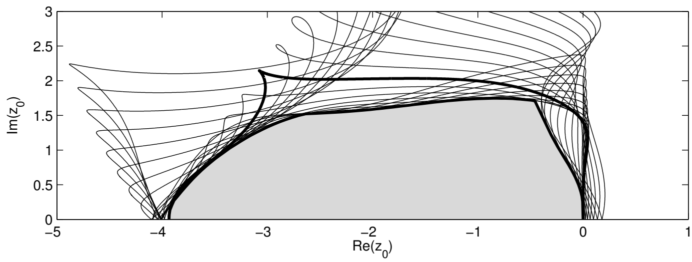

Figure 7. Stability regions $\mathcal{S}_{\pi/2,y}$, $y=-2.0,1.8,\ldots,2.0$ (thin lines), $\mathcal{S}_{\pi/2}$ (shaded region), and $\mathcal{S}_E$ (thick line) for $\beta_{10}=6.679846861853708$, $\beta_{20}=6.776533083751429$, $\beta_{30}=8.549694721430665$, $\beta_{21}=0.726731199717484$, $\beta_{31}=0.052947612675072$, and $\beta_{32}=0.934356862537509$.

of the method is A-stable. This corresponds to

$$\beta_0=\begin{bmatrix}6.679846861853708\\6.776533083751429\\8.549694721430665\end{bmatrix}^T,\quad \alpha_0=\begin{bmatrix}2.335969372370742\\2.533229177089304\\2.803945338986028\end{bmatrix}^T,$$

$$\beta=\begin{bmatrix}0&0&0\\0.726731199717484&0&0\\0.052947612675072&0.934356862537509&0\end{bmatrix},$$

$$\alpha=\begin{bmatrix}-11.015816234224447&10.687754978965932&-7.687754978965934\\-11.379568661688278&11.079683014454300&-8.736607813324252\\-12.588656047166431&12.870496551351414&-11.622785039814261\end{bmatrix},$$

for which the area of $\mathcal{S}_{\pi/2}$ is approximately equal to 10.65. The area of the corresponding explicit method is approximately equal to 13.42. As before we have plotted in Fig. 7 regions $\mathcal{S}_{\pi/2,y}$ for $y=-2.0,-1.8,\ldots,2.0$ (thin lines), the stability region $\mathcal{S}_{\pi/2}$ (shaded region) and $\mathcal{S}_E$ (thick line).

4.4 IMEX SDIRK methods with $s=5$ and $p=4$

It can be verified that the IMEX schemes of order $p=4$ with four stages do not exist and we examine methods with $s=5$.
Consider SDIRK method with $s=5$ with coefficients

$$\begin{array}{c|ccccc}
\frac{1}{2} & \frac{1}{2} \\
\frac{5}{8} & \frac{1}{8} & \frac{1}{2} \\
\frac{3}{4} & \frac{17}{388} & \frac{20}{97} & \frac{1}{2} \\
\frac{7}{8} & \frac{12347}{4850} & -\frac{27313}{9700} & \frac{129}{200} & \frac{1}{2} \\
1 & \frac{71131}{59752} & -\frac{56193}{59752} & \frac{1}{8} & \frac{1}{8} & \frac{1}{2} \\
\hline
 & \frac{139}{26} & -\frac{122}{13} & \frac{185}{39} & \frac{50}{39} & -\frac{77}{78}
\end{array}.$$

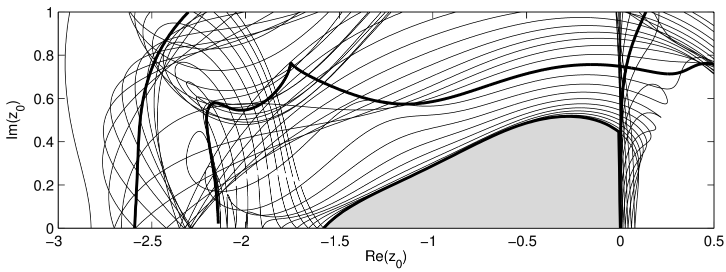

Figure 8. Stability regions $\mathcal{S}_{\pi/2,y}$, $y = -2.0, 1.8, \ldots, 2.0$ (thin lines), $\mathcal{S}_{\pi/2}$ (shaded region), and $\mathcal{S}_E$ (thick line) for $\beta_{32} = -0.187138232278862$, $\beta_{42} = -0.949874624336551$, $\beta_{43} = 0.143116001991357$, $\beta_{52} = 1.048854330707973$, $\beta_{53} = 1.729639735631708$, and $\beta_{54} = 0.785190812828783$.

This method has order $p = 4$. The stability polynomial of this method takes the form $R(z) = P(z)/Q(z)$ with

$$P(z) = 1 - \frac{3}{2}\,z + \frac{1}{2}\,z^2 + \frac{1}{6}\,z^3 - \frac{1}{16}\,z^4 - \frac{60373}{4842240}\,z^5, \quad Q(z) = \left(1 - \frac{1}{2}\,z\right)^5,$$

and it can be verified that this method is A-stable.

The stability function of IMEX SDIRK methods takes the form

$$\begin{aligned} p(w, z_0, z_1) &= (1 - \lambda z_1)^5 w^7 - p_6(z_0, z_1) w^6 + p_5(z_0, z_1) w^5 - p_4(z_0, z_1) w^4 \\ &\quad + p_3(z_0, z_1) w^3 - p_2(z_0, z_1) w^2 + p_1(z_0, z_1) w - p_0(z_0, z_1), \end{aligned}$$

where $p_i(z_0, z_1)$, $i = 0, 1, 2, 3, 4, 5, 6$, are polynomials of degree less than or equal to three with respect to z_0 and less than or equal to five with respect to z_1. These coefficients depend on the free parameters of the method.

Solving the conditions for IMEX SDIRK methods of order $p = 4$ with respect to α_0, α, β_0, and the first column of β we obtain a six parameter family of IMEX SDIRK methods depending on β_{32}, β_{42}, β_{43}, β_{52}, β_{53}, and β_{54}.

We performed next a numerical search in this six dimensional parameter space trying to maximize first the area of the stability region $\mathcal{S}_E$ of the underlying explicit method. This leads to IMEX scheme with coefficients given in [10], for which the area of $\mathcal{S}_E$ is approximately equal to 2.82. The area of the corresponding IMEX SDIRK method is approximately equal 1.06. We have plotted in Fig. 8 regions $\mathcal{S}_{\pi/2,y}$ for $y = -2.0, -1.8, \ldots, 2.0$ (thin lines), the stability region $\mathcal{S}_{\pi/2}$ (shaded region) and $\mathcal{S}_E$ (thick line).

We performed a similar numerical search trying to maximize the area of the stability region $\mathcal{S}_{\pi/2}$ of the IMEX SDIRK method. This leads to the IMEX scheme with coefficients given in [10], for which the area of $\mathcal{S}_{\pi/2}$ is approximately equal to 1.50. The area of the stability region $\mathcal{S}_E$ of the corresponding explicit method is approximately equal to 2.47. We have plotted in Fig. 9 regions $\mathcal{S}_{\pi/2,y}$ for $y = -2.0, -1.8, \ldots, 2.0$ (thin lines), the stability region $\mathcal{S}_{\pi/2}$ (shaded region) and $\mathcal{S}_E$ (thick line).

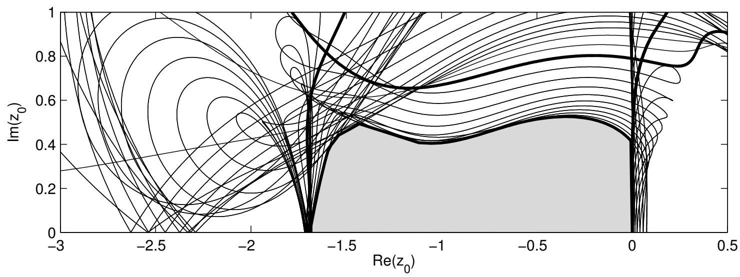

Figure 9. Stability regions $\mathcal{S}_{\pi/2,y}$, $y = -2.0, 1.8, \ldots, 2.0$ (thin lines), $\mathcal{S}_{\pi/2}$ (shaded region), and $\mathcal{S}_E$ (thick line) for $\beta_{32} = -0.103241056324758$, $\beta_{42} = -1.642317211614867$, $\beta_{43} = 0.371951766360894$, $\beta_{52} = -2.912021006631820$, $\beta_{53} = 3.197905476549485$, and $\beta_{54} = 0.896467288791007$.

5 Numerical Experiments

To verify the order of convergence, we have applied the IMEX SDIRK schemes to a standard nonlinear oscillatory test problem, van der Pol equation [15] (in a vector form)

$$\begin{bmatrix} y' \\ z' \end{bmatrix} = f(y,z) + g(y,z) = \begin{bmatrix} z \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ \big((1-y^2)z - y\big)/\varepsilon \end{bmatrix} \tag{5.1}$$

over the integration interval $[0, 0.55139]$. Initial conditions are chosen to be

$$y(0) = 2, \qquad z(0) = -\frac{2}{3} + \frac{10}{81}\varepsilon - \frac{292}{2187}\varepsilon^2 - \frac{1814}{19683}\varepsilon^3 + O(\varepsilon^4) \tag{5.2}$$

and $\varepsilon = 0.1$. Since our objective here is the verification of order, all methods are implemented with fixed step sizes. $f(y,z)$ is treated explicitly while $g(y,z)$ is handled implicitly. We compare the results at the final step against a reference solution, obtained using MATLAB's ode15s routine with very small tolerances $rtol = 2.22045 \times 10^{-14}$ and $atol = 1 \times 10^{-14}$. Starting values are also obtained using ode15s with the same tolerance settings.

In Figure 10 we have plotted the absolute error for the algebraic variable z, against step size h. For notational convenience, we use '(a)' or '(b)' to indicate that the corresponding IMEX SDIRK method has maximal stability region of the explicit part or maximal stability region of the IMEX method respectively. The observed orders match with the theoretical orders of accuracy. Furthermore, methods with maximal stability region of $\mathcal{S}_E$ give almost the same results with methods with maximal stability region of $\mathcal{S}_{\pi/2}$. Table 3 gives the errors and order of accuracy for each IMEX SDIRK(a) method computed by $\log_2(e_{N/2}/e_N)$ where e_N denotes the error in solution when N number of steps is used.

6 Conclusions

We have proposed a new family of IMEX methods, based on SDIRK methods and on an explicit extrapolation formula. We proved that the order of the

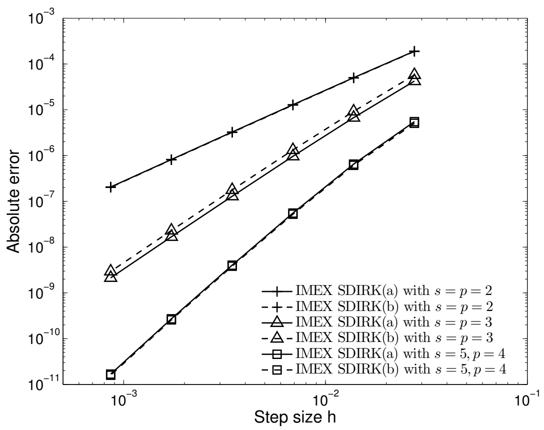

Figure 10. Absolute error vs. step size for the van der Pol equation with $\varepsilon = 10^{-1}$ using IMEX SDIRK methods. 'a' or 'b' indicate that the corresponding IMEX SDIRK method has maximal stability region of the explicit part or maximal stability region of the IMEX method respectively.

Table 3. Accuracy test with the van der Pol equation for the IMEX SDIRK(a) methods. The first column displays the number of steps (N).

N	2nd-order IMEX SDRIK		3rd-order IMEX SDRIK		4th-order IMEX SDRIK	
	error	order	error	order	error	order
20	1.90×10^{-4}		4.23×10^{-5}		5.50×10^{-6}	
40	5.02×10^{-5}	1.92	6.73×10^{-6}	2.65	6.49×10^{-7}	3.08
80	1.29×10^{-5}	1.96	9.62×10^{-7}	2.81	5.53×10^{-8}	3.55
160	3.26×10^{-6}	1.98	1.29×10^{-7}	2.90	4.04×10^{-9}	3.78
320	8.20×10^{-7}	1.99	1.68×10^{-8}	2.95	2.72×10^{-10}	3.89
640	2.06×10^{-7}	2.00	2.14×10^{-9}	2.97	1.68×10^{-11}	4.02

SDIRK method is preserved, if the extrapolation formula has the same order. We examined the linear stability properties of these methods. We carried out an extensive search for IMEX SDIRK methods with strong stability properties and gave examples of optimal methods of order $p = 1, 2, 3$ and 4.

Future developments of this work include the implementation of these methods in a variable stepsize environment and a comparison with other IMEX schemes. Another issue is the development of parallel IMEX methods to solve large dimension problems, and some algorithmic strategies used in [7,12,13] for integral equations, can be suitably adapted for an efficient implementation on a distributed-memory architecture.

Acknowledgement

This work was supported by National Group of Computing Science (GNCS-INDAM): GNCS 2014 Projects "Stabilità nella modellistica numerica di equazioni differenziali ed integrali".

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