Diagonally Implicit Runge-Kutta Methods for Stiff ODEs

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Abstract

Based principally on a recent review of diagonally implicit Runge-Kutta (DIRK) methods applied to stiff first-order ordinary differential equations (ODEs) by the present authors, several nearly optimal, general purpose, DIRK-type methods are presented. Methods given range from third- to sixth-order in four- to nine- stages. All are both stiffly-accurate and L-stable and many are internally L-stable on stages where this is possible. Focus is placed on stage-order two methods. To facilitate step-size control via error estimation, an embedded method is included with each method listed. Five new explicit first-stage, singly diagonally-implicit Runge-Kutta (ESDIRK) methods are presented based on lessons learned from the review.

1 Introduction

The diagonally implicit Runge-Kutta (DIRK) family of methods is possibly the most widely used implicit Runge-Kutta (IRK) method in practical applications involving stiff, first-order, ordinary differential equations (ODEs) for initial value problems (IVPs) due to their relative ease of implementation. They are characterized by a lower triangular **A**-matrix with at least one nonzero diagonal entry and are sometimes referred to as semi-implicit or semi-explicit Runge-Kutta methods. This structure permits solving for each stage individually rather than all stages simultaneously. They have been the subject of a recent review[7] by the present authors. This paper is based on that review. In the review, many aspects of DIRK-type methods are discussed which are relevant to proper design and application of such methods. These include the general structure, order conditions, simplifying assumptions, error, linear stability, nonlinear stability, internal stability, dense output, conservation, symplecticity, symmetry, dissipation and dispersion accuracy, memory economization[6], regularity, boundary and smoothness order reduction, efficiency[1], solvability, implementation, step-size control, iteration control, stage-value predictors, discontinuities and existing software. Several conclusions were reached in the review. Among them were that if general DIRK methods are intended to solve stiff equations, methods should possess a stage-order of two, L-stability, strong damping of stiff eigenvalues on the internal stages and minimized leading-order error. Such methods, along with error estimators, dense output and stage-value predictors form the basis of a robust and efficient integrator. The present paper focuses on methods which are at least fourth-order accurate and introduces four new ESDIRK methods based on leasons learned from [7]. Dense output and stage-value predictors are not included with these methods. Appendix A lists the method coefficients for five new ESDIRK methods.

2 Background

DIRK-type methods are used to solve ODEs of the form

$$\frac{dU}{dt} = F(t, U(t)), \qquad U(a) = U_0, \qquad t \in [a, b] \tag{1}$$

and are applied over s-stages as

$$\left.\begin{array}{lll} F_i = F(t_i, U_i), & U_i = U^{[n]} + (\Delta t)\sum_{j=1}^{s} a_{ij} F_j, & t_i = t^{[n]} + c_i \Delta t, \\[2ex] U^{[n+1]} = U^{[n]} + (\Delta t)\sum_{i=1}^{s} b_i F_i, & \hat{U}^{[n+1]} = U^{[n]} + (\Delta t)\sum_{i=1}^{s} \hat{b}_i F_i. & \end{array}\right\} \tag{2}$$

where $i = 1, 2, \cdots, s$, $F_i = F_i^{[n]} = F(U_i, t^{[n]} + c_i\Delta t)$. Also, $\Delta t > 0$ is the step-size, $U^{[n]} \simeq U(t^{[n]})$ is the value of the U-vector at time step n, $U_i = U_i^{[n]} \simeq U\left(t^{[n]} + c_i\Delta t\right)$ is the value of the U-vector on the ith-stage, and $U^{[n+1]} \simeq U(t^{[n]} + \Delta t)$. Both $U^{[n]}$ and $U^{[n+1]}$ are of classical order p. The U-vector associated with the embedded scheme, $\hat{U}^{[n+1]}$, is of order $\hat{p} = p - 1$. This constitutes a $(p, \hat{p})$ pair. Each of the respective Runge-Kutta coefficients a_{ij} (stage weights), b_i (scheme weights), $\hat{b}_i$ (embedded scheme weights), and c_i (abscissae or nodes), $i, j = 1, 2, \cdots, s$ are real and are constrained, at a minimum, by certain order of accuracy and stability considerations.

For the stiffly-accurate ($a_{sj} = b_j, j = 1, 2, \ldots, s$), stage-order two methods considered in this paper, ESDIRK methods are chosen. They are given by the general structure

$$\begin{array}{c|ccccccc}
0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\
2\gamma & \gamma & \gamma & 0 & \cdots & 0 & 0 & 0 \\
c_3 & a_{31} & a_{32} & \gamma & \ddots & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \ddots & \ddots & \vdots & \vdots \\
c_{s-2} & a_{s-2,1} & a_{s-2,2} & a_{s-2,3} & \ddots & \gamma & 0 & 0 \\
c_{s-1} & a_{s-1,1} & a_{s-1,2} & a_{s-1,3} & \cdots & a_{s-2,s-2} & \gamma & 0 \\
1 & b_1 & b_2 & b_3 & \cdots & b_{s-1} & b_s & \gamma \\
\hline
 & b_1 & b_2 & b_3 & \cdots & b_{s-2} & b_{s-1} & \gamma \\
\hline
 & \hat{b}_1 & \hat{b}_2 & \hat{b}_3 & \cdots & \hat{b}_{s-2} & \hat{b}_{s-1} & \hat{b}_s
\end{array}$$

Some authors prefer to decompose $\mathbf{A} = a_{ij}$, $\mathbf{b} = b_i$ and $\mathbf{c} = c_i$, into

$$\begin{array}{c|c} \mathbf{c} & \mathbf{A} \\ \hline & \mathbf{b}^T \end{array} = \begin{array}{c|cc} 0 & 0 & \mathbf{0}^T \\ \widehat{\mathbf{c}} & \mathsf{a} & \widehat{\mathbf{A}} \\ \hline & b_1 & \widehat{\mathbf{b}}^T \end{array} \qquad \text{with} \qquad \mathbf{A} = \begin{bmatrix} 0 & \mathbf{0}^T \\ \mathsf{a} & \widehat{\mathbf{A}} \end{bmatrix} \tag{3}$$

where $\mathbf{0}^T$ (composed of zeros), a^T, $\widehat{\mathbf{c}}^T$ and $\widehat{\mathbf{b}}^T$ are vectors of length (s-1), $\{0, \mathsf{a}^T\} = a_{.1}^T$, $\{0, \widehat{\mathbf{c}}^T\} = \mathbf{c}^T$, and $\{b_1, \widehat{\mathbf{b}}^T\} = \mathbf{b}^T$ and $\widehat{\mathbf{A}}$ is a square matrix of dimension $(s-1) \times (s-1)$. Hence, although $\mathbf{A}$ is not invertible, $\widehat{\mathbf{A}}$ is often invertible. The motivation for having an explicit first stage is primarily to allow stage-order two methods.

To identify certain schemes derived in this paper, they will be named ESDIRK$p(\hat{p})sS[q]X_x$, where p is the order of the main method, $\hat{p}$ is the order of the embedded method, s is the number of stages, S is some stability characterization of the method, q is the stage-order of the method, X is used for any other important characteristic of the method, and x distinguishes between family members of some type of method.

3 Order Conditions

Expressions for the equation of condition associated with the pth-order trees are of the form[2, 4, 5]

$$\tau_j^{(p)} = \frac{1}{\sigma}\Phi_j^{(p)} - \frac{\alpha}{p!} = \frac{1}{\sigma}\left(\Phi_j^{(p)} - \frac{1}{\gamma}\right), \quad \Phi_j^{(p)} = \sum_{i=1}^{s} b_i \Phi_{i,j}^{(p)}, \quad \alpha\sigma\gamma = p! \tag{4}$$

where α, ρ, γ are the cardinality, the order and the symmetry of the particular tree which represents the order condition. The elementary weights, $\Phi^{(p)}_{i,j}$ and $\Phi^{(p)}_{j}$, are Runge-Kutta coefficient products and their sums, and j represents the index of the order condition, i.e. each order may have more than one order condition. A Runge-Kutta method is said to be of order p if the local truncation error satisfies

$$U^{[n]} - U(t^{[n]}) = \mathcal{O}\left(\Delta t\right)^{p+1}. \tag{5}$$

3.1 Simplifying Assumptions

Simplifying assumptions are often made to facilitate the solution of Runge-Kutta order conditions and possibly to enforce higher stage-order. The three common ones are[2, 5]

$$B(p): \qquad \sum_{j=1}^{s} b_i c_i^{k-1} = \frac{1}{k}, \quad k = 1, ..., p, \tag{6}$$

$$C(\eta): \qquad \sum_{j=1}^{s} a_{ij} c_j^{k-1} = \frac{c_i^k}{k}, \quad k = 1, ..., \eta, \tag{7}$$

$$D(\zeta): \qquad \sum_{i=1}^{s} b_i c_i^{k-1} a_{ij} = \frac{b_j}{k}(1 - c_j^k), \quad k = 1, ..., \zeta. \tag{8}$$

A fourth simplifying assumption, $E(\eta, \zeta)$, is not needed for DIRK-type methods. The first is related to the quadrature conditions. Enforcing $B(p)$ forces $\tau_1^{(k)} = 0$, $k = 1, 2, \cdots, p$ for all orders up to and including p. Assumptions $C(\eta)$ and $D(\zeta)$ are sometimes referred to as the row and column simplifying assumptions, respectively. The stage-order of a Runge-Kutta method is the largest value of q such that $B(q)$ and $C(q)$ are both satisfied. As its name implies, stage-order is related to the order of accuracy of the intermediate stage values of the U-vector, U_i, and typically equals the lowest order amongst all stages.

Closely related to assumption $B(p)$, $p^{(k)}$ is defined as

$$p^{(k)} = \mathbf{b}^T \mathbf{C}^{k-1} \mathbf{e} - \frac{1}{k} = \tau_1^k (k-1)!, \tag{9}$$

where $\mathbf{C} = \text{diag}(\mathbf{c})$ and $\mathbf{Ce} = \mathbf{c}$. Writing $p_1^{(1,2,3,4)} = 0$ implies that $p_1^{(1)} = p_1^{(2)} = p_1^{(3)} = p_1^{(4)} = 0$. Powers of the vector $\mathbf{c}$ should be interpreted as componentwise multiplication. Hence $\mathbf{c}^3 = \mathbf{c} * \mathbf{c} * \mathbf{c} = \mathbf{C}^3 \mathbf{e}$ and $\mathbf{c}^0 = \mathbf{e}$. Powers of the $\mathbf{A}$-matrix are given by $\mathbf{A}^0 = \mathbf{I}$, $\mathbf{A}^1 = \mathbf{A}$, $\mathbf{A}^2 = \mathbf{AA}$ etcetera.

Similarly, $\mathbf{q}^{(k)}$ is closely related to assumption $C(\eta)$,

$$\mathbf{q}^{(k)} = \mathbf{AC}^{k-1}\mathbf{e} - \frac{1}{k}\mathbf{C}^k\mathbf{e}, \qquad \mathbf{q}^{(1)} = \mathbf{Ae} - \mathbf{c}, \qquad \text{Diag}\left(\mathbf{q}^{(k)}\right) = \mathbf{Q}^{(k)}, \tag{10}$$

where $\mathbf{q}^{(1)} = \mathbf{0}$ is simply the row-sum condition. Writing $q^{(k)}_{2,3,4,5,6} = 0$ implies that $q_2^{(k)} = q_3^{(k)} = q_4^{(k)} = q_5^{(k)} = q_6^{(k)} = 0$. Table 1 details the use of $\mathbf{q}^{(k)}$, and consequently $C(\eta)$, for order conditions up to order six. When $\mathbf{q}^{(3)} = 0$ is applied to a stage-order two ESDIRK, it is found that $q_2^{(3)} \neq 0$. To denote this case, a truncated version of $C(3)^*$ is defined as $q_i^{(3)} = 0, \quad i = 3, 4, \cdots, s$.

Lastly, closely related to assumption $D(\zeta)$, one may further define

$$\mathbf{r}^{(k)} \quad = \quad \mathbf{b}^T\mathbf{C}^{k-1}\mathbf{A} - \frac{1}{k}\mathbf{b}^T\left(\mathbf{I} - \mathbf{C}^k\right). \tag{11}$$

This assumption principally applies to subquadrature and extended subquadrature order conditions as most of the nonlinear order conditions cannot be reduced by using the column simplifying assumption. Because methods in this paper will enforce $C(2)$ to achieve stage-order two, the application of any $D(\zeta)$ assumptions is inappropriate.

Lastly, simplifying assumptions $B(p)$, $C(\eta)$ and $D(\zeta)$ may be related through $p^{(k)}$, $\mathbf{q}^{(k)}$ and $\mathbf{r}^{(k)}$ as

$$\mathbf{r}^{(k)}\mathbf{c}^{l-1} \quad = \quad \mathbf{b}^T\mathbf{C}^{k-1}\mathbf{q}^{(l)} + \frac{(k+l)}{kl}p^{(k+l)} - \frac{1}{k}p^{(l)}. \tag{12}$$

For orders up to six, order conditions are expressed in Table 1 where $\mathbf{r}^{(k)}$ is used. Table 2 shows the effect applying both $C(2)$ and $C(3)^*$ on all subquadrature, extended subquadrature and nonlinear order conditions up to sixth-order.

3.2 Error

Error in a *pth*-order Runge-Kutta scheme may be quantified in a general way by taking the L_2 principal error norm,

$$A^{(p+1)} = \|\tau^{(p+1)}\|_2 = \sqrt{\sum_{j=1}^{\mathsf{a}_{p+1}} \left(\tau_j^{(p+1)}\right)^2} \tag{13}$$

where $\tau_j^{(p+1)}$ are the a_{p+1} error coefficients associated with classical order of accuracy $p+1$ with $a_p = \{1, 1, 2, 4, 9, 20, 48, 115, 286, 719\}$ for $p = \{1, 2, 3, 4, 5, 6, 7, 8, 9, 10\}$, respectively. For single-step, embedded schemes where $\hat{p} = p - 1$, additional definitions are useful such as

$$\hat{\tau}_k^{(\hat{p})} \quad = \quad \frac{1}{\sigma}\sum_{i=1}^{s}\hat{b}_i\Phi_{i,k}^{(\hat{p})} - \frac{\alpha}{\hat{p}!}, \quad \hat{A}^{(\hat{p}+1)} = \|\hat{\tau}^{(\hat{p}+1)}\|_2, \tag{14}$$

$$B^{(\hat{p}+2)} = \frac{\hat{A}^{(\hat{p}+2)}}{\hat{A}^{(\hat{p}+1)}}, \quad C^{(\hat{p}+2)} = \frac{\|\hat{\tau}^{(\hat{p}+2)} - \tau^{(\hat{p}+2)}\|_2}{\hat{A}^{(\hat{p}+1)}}, \quad E^{(\hat{p}+2)} = \frac{A^{(\hat{p}+2)}}{\hat{A}^{(\hat{p}+1)}}, \tag{15}$$

and $D = \text{Max}\{|a_{ij}|, |b_i|, |\hat{b}_i|, |c_i|\}$ where the superscript circumflex denotes the values with respect to the embedded method. The order of the method, p, refers to the global order-of-accuracy while the local order-of-accuracy is given by $p+1$.

4 Stability

4.1 Linear Stability

Linear stability of DIRK-type methods applied to ODEs is studied based on the equation $U' = \lambda U$ by using the stabilty function

$$R(z) = \frac{P(z)}{Q(z)} \quad = \quad \frac{\sum_{i=1}^{s} p_i z^i}{\sum_{i=1}^{s} q_i z^i} \quad = \quad \frac{\text{Det}\left[\mathbf{I} - z\mathbf{A} + z\mathbf{e}\otimes\mathbf{b}^T\right]}{\text{Det}\left[\mathbf{I} - z\mathbf{A}\right]} = 1 + z\mathbf{b}^T\left[\mathbf{I} - z\mathbf{A}\right]^{-1}\mathbf{e}, \tag{16}$$

	$C(\eta)$	$D(\zeta)$
$\tau_2^{(3)}$	$\mathbf{b}^T\mathbf{q}^{(2)} + \tau_1^{(3)}$	$\mathbf{r}^{(1)}\mathbf{Ce} + \tau_1^{(2)} - 2\tau_1^{(3)}$
$\tau_2^{(4)}$	$\mathbf{b}^T\mathbf{Cq}^{(2)} + 3\tau_1^{(4)}$	$\mathbf{r}^{(2)}\mathbf{Ce} + \frac{1}{2}\tau_1^{(2)} - 3\tau_1^{(4)}$
$\tau_3^{(4)}$	$\frac{1}{2}\mathbf{b}^T\mathbf{q}^{(3)} + \tau_1^{(4)}$	$\frac{1}{2}\mathbf{r}^{(1)}\mathbf{C}^2\mathbf{e} + \tau_1^{(3)} - 3\tau_1^{(4)}$
$\tau_4^{(4)}$	$\mathbf{b}^T\mathbf{Aq}^{(2)} + \tau_3^{(4)}$	$\mathbf{r}^{(1)}\mathbf{ACe} + \tau_2^{(3)} - \tau_2^{(4)}$
$\tau_2^{(5)}$	$\frac{1}{2}\mathbf{b}^T\mathbf{C}^2\mathbf{q}^{(2)} + 6\tau_1^{(5)}$	$\frac{1}{2}\mathbf{r}^{(3)}\mathbf{Ce} + \frac{1}{6}\tau_1^{(2)} - 4\tau_1^{(5)}$
$\tau_3^{(5)}$	$\frac{1}{2}\mathbf{b}^T\left(\mathbf{q}^{(2)} + \mathbf{C}^2\right)\mathbf{q}^{(2)} + 3\tau_1^{(5)}$	No Simplification
$\tau_4^{(5)}$	$\frac{1}{2}\mathbf{b}^T\mathbf{Cq}^{(3)} + 4\tau_1^{(5)}$	$\frac{1}{2}\mathbf{r}^{(2)}\mathbf{C}^2\mathbf{e} + \frac{1}{2}\tau_1^{(3)} - 6\tau_1^{(5)}$
$\tau_5^{(5)}$	$\frac{1}{6}\mathbf{b}^T\mathbf{q}^{(4)} + \tau_1^{(5)}$	$\frac{1}{6}\mathbf{r}^{(1)}\mathbf{C}^3\mathbf{e} + \tau_1^{(4)} - 4\tau_1^{(5)}$
$\tau_6^{(5)}$	$\mathbf{b}^T\mathbf{CAq}^{(2)} + \tau_4^{(5)}$	$\mathbf{r}^{(2)}\mathbf{ACe} + \frac{1}{2}\tau_2^{(3)} - \tau_2^{(5)}$
$\tau_7^{(5)}$	$\mathbf{b}^T\mathbf{ACq}^{(2)} + 3\tau_5^{(5)}$	$\mathbf{r}^{(1)}\mathbf{CACe} + \tau_2^{(4)} - 2\tau_2^{(5)}$
$\tau_8^{(5)}$	$\frac{1}{2}\mathbf{b}^T\mathbf{Aq}^{(3)} + \tau_5^{(5)}$	$\frac{1}{2}\mathbf{r}^{(1)}\mathbf{AC}^2\mathbf{e} + \tau_3^{(4)} - \tau_4^{(5)}$
$\tau_9^{(5)}$	$\mathbf{b}^T\mathbf{AAq}^{(2)} + \tau_8^{(5)}$	$\mathbf{r}^{(1)}\mathbf{AACe} + \tau_4^{(4)} - \tau_6^{(5)}$
$\tau_2^{(6)}$	$\frac{1}{6}\mathbf{b}^T\mathbf{C}^3\mathbf{q}^{(2)} + 10\tau_1^{(6)}$	$\frac{1}{6}\mathbf{r}^{(4)}\mathbf{Ce} + (1/24)\tau_1^{(2)} - 5\tau_1^{(6)}$
$\tau_3^{(6)}$	$\frac{1}{2}\mathbf{b}^T\mathbf{C}\left(\mathbf{q}^{(2)} + \mathbf{C}^2\right)\mathbf{q}^{(2)} + 15\tau_1^{(6)}$	No Simplification
$\tau_4^{(6)}$	$\frac{1}{4}\mathbf{b}^T\mathbf{C}^2\mathbf{q}^{(3)} + 10\tau_1^{(6)}$	$\frac{1}{4}\mathbf{r}^{(3)}\mathbf{C}^2\mathbf{e} + (1/6)\tau_1^{(3)} - 10\tau_1^{(6)}$
$\tau_5^{(6)}$	$\frac{1}{2}\mathbf{b}^T\left(\mathbf{Q}^{(3)} + \frac{1}{3}\mathbf{C}^3\right)\mathbf{q}^{(2)} + \tau_4^{(6)}$	No Simplification
$\tau_6^{(6)}$	$\frac{1}{6}\mathbf{b}^T\mathbf{Cq}^{(4)} + 5\tau_1^{(6)}$	$\frac{1}{6}\mathbf{r}^{(2)}\mathbf{Ce} + (1/2)\tau_1^{(4)} - 10\tau_1^{(6)}$
$\tau_7^{(6)}$	$\frac{1}{24}\mathbf{b}^T\mathbf{q}^{(5)} + \tau_1^{(6)}$	$\frac{1}{24}\mathbf{r}^{(1)}\mathbf{C}^4\mathbf{e} + \tau_1^{(5)} - 5\tau_1^{(6)}$
$\tau_8^{(6)}$	$\frac{1}{2}\mathbf{b}^T\mathbf{C}^2\mathbf{Aq}^{(2)} + \tau_4^{(6)}$	$\frac{1}{2}\mathbf{r}^{(3)}\mathbf{ACe} + (1/6)\tau_2^{(3)} - \tau_2^{(6)}$
$\tau_9^{(6)}$	$\mathbf{b}^T\mathbf{Q}^{(2)}\mathbf{Aq}^{(2)} + \frac{1}{2}\mathbf{b}^T\mathbf{Q}^{(2)}\mathbf{q}^{(3)}$ $+\frac{1}{6}\mathbf{b}^T\mathbf{C}^3\mathbf{q}^{(2)} + \tau_8^{(6)}$	No Simplification
$\tau_{10}^{(6)}$	$\mathbf{b}^T\mathbf{CACq}^{(2)} + 3\tau_6^{(6)}$	$\mathbf{r}^{(2)}\mathbf{CACe} + (1/2)\tau_2^{(4)} - 3\tau_2^{(6)}$
$\tau_{11}^{(6)}$	$\frac{1}{2}\mathbf{b}^T\mathbf{AC}^2\mathbf{q}^{(2)} + 6\tau_7^{(6)}$	$\frac{1}{2}\mathbf{r}^{(1)}\mathbf{C}^2\mathbf{ACe} + \tau_2^{(5)} - 3\tau_2^{(6)}$
$\tau_{12}^{(6)}$	$\frac{1}{2}\mathbf{b}^T\mathbf{A}\left(\mathbf{q}^{(2)} + \mathbf{C}^2\right)\mathbf{q}^{(2)} + 3\tau_7^{(6)}$	$\frac{1}{2}\mathbf{r}^{(1)}\left(\mathbf{ACe}\right)^2 + \tau_3^{(5)} - \tau_3^{(6)}$
$\tau_{13}^{(6)}$	$\frac{1}{2}\mathbf{b}^T\mathbf{CAq}^{(3)} + \tau_6^{(6)}$	$\mathbf{r}^{(2)}\mathbf{AC}^2\mathbf{e} + (1/2)\tau_3^{(4)} - \tau_4^{(6)}$
$\tau_{14}^{(6)}$	$\frac{1}{2}\mathbf{b}^T\mathbf{ACq}^{(3)} + 4\tau_7^{(6)}$	$\frac{1}{2}\mathbf{r}^{(1)}\mathbf{CACe} + \tau_4^{(5)} - 2\tau_4^{(6)}$
$\tau_{15}^{(6)}$	$\frac{1}{6}\mathbf{b}^T\mathbf{Aq}^{(4)} + \tau_7^{(6)}$	$\frac{1}{6}\mathbf{r}^{(1)}\mathbf{AC}^3\mathbf{e} + \tau_5^{(5)} - \tau_6^{(6)}$
$\tau_{16}^{(6)}$	$\mathbf{b}^T\mathbf{CAAq}^{(2)} + \tau_{13}^{(6)}$	$\mathbf{r}^{(2)}\mathbf{AACe} + (1/2)\tau_4^{(4)} - \tau_8^{(6)}$
$\tau_{17}^{(6)}$	$\mathbf{b}^T\mathbf{ACAq}^{(2)} + \tau_{14}^{(6)}$	$\mathbf{r}^{(1)}\mathbf{CAACe} + \tau_6^{(5)} - 2\tau_8^{(6)}$
$\tau_{18}^{(6)}$	$\mathbf{b}^T\mathbf{AACq}^{(2)} + 3\tau_{15}^{(6)}$	$\mathbf{r}^{(1)}\mathbf{ACACe} + \tau_7^{(5)} - \tau_{10}^{(6)}$
$\tau_{19}^{(6)}$	$\frac{1}{2}\mathbf{b}^T\mathbf{AAq}^{(3)} + \tau_{15}^{(6)}$	$\frac{1}{2}\mathbf{r}^{(1)}\mathbf{AAC}^2\mathbf{e} + \tau_8^{(5)} - \tau_{13}^{(6)}$
$\tau_{20}^{(6)}$	$\mathbf{b}^T\mathbf{AAAq}^{(2)} + \tau_{19}^{(6)}$	$\mathbf{r}^{(1)}\mathbf{AAACe} + \tau_9^{(5)} - \tau_{16}^{(6)}$

Table 1: Order conditions expressed using $\mathbf{q}^{(k)}$ and $\mathbf{r}^{(k)}$ up to sixth-order for Runge-Kutta methods. Bushy tree order conditions, $\tau_1^{(l)}, l = 1, 2, \cdots, 6$, are not included.

	$C(\eta)$	$C(2)$	$C(3)^*$
$\tau_2^{(3)}$	$\mathbf{b}^T\mathbf{q}^{(2)} + \tau_1^{(3)}$	$\tau_1^{(3)}$	$\tau_1^{(3)}$
$\tau_2^{(4)}$	$\mathbf{b}^T\mathbf{C}\mathbf{q}^{(2)} + 3\tau_1^{(4)}$	$3\tau_1^{(4)}$	$3\tau_1^{(4)}$
$\tau_3^{(4)}$	$\frac{1}{2}\mathbf{b}^T\mathbf{q}^{(3)} + \tau_1^{(4)}$	$\frac{1}{2}\mathbf{b}^T\mathbf{q}^{(3)} + \tau_1^{(4)}$	$\frac{1}{2}b_2q_2^{(3)} + \tau_1^{(4)}$
$\tau_4^{(4)}$	$\mathbf{b}^T\mathbf{A}\mathbf{q}^{(2)} + \tau_3^{(4)}$	$\tau_3^{(4)}$	$\frac{1}{2}b_2q_2^{(3)} + \tau_1^{(4)}$
$\tau_2^{(5)}$	$\frac{1}{2}\mathbf{b}^T\mathbf{C}^2\mathbf{q}^{(2)} + 6\tau_1^{(5)}$	$6\tau_1^{(5)}$	$6\tau_1^{(5)}$
$\tau_3^{(5)}$	$\frac{1}{2}\mathbf{b}^T\left(\mathbf{q}^{(2)} + \mathbf{C}^2\right)\mathbf{q}^{(2)} + 3\tau_1^{(5)}$	$3\tau_1^{(5)}$	$3\tau_1^{(5)}$
$\tau_4^{(5)}$	$\frac{1}{2}\mathbf{b}^T\mathbf{C}\mathbf{q}^{(3)} + 4\tau_1^{(5)}$	$\frac{1}{2}\mathbf{b}^T\mathbf{C}\mathbf{q}^{(3)} + 4\tau_1^{(5)}$	$\frac{1}{2}b_2c_2q_2^{(3)} + 4\tau_1^{(5)}$
$\tau_5^{(5)}$	$\frac{1}{6}\mathbf{b}^T\mathbf{q}^{(4)} + \tau_1^{(5)}$	$\frac{1}{6}\mathbf{b}^T\mathbf{q}^{(4)} + \tau_1^{(5)}$	$\frac{1}{6}\mathbf{b}^T\mathbf{q}^{(4)} + \tau_1^{(5)}$
$\tau_6^{(5)}$	$\mathbf{b}^T\mathbf{C}\mathbf{A}\mathbf{q}^{(2)} + \tau_4^{(5)}$	$\tau_4^{(5)}$	$\frac{1}{2}b_2c_2q_2^{(3)} + 4\tau_1^{(5)}$
$\tau_7^{(5)}$	$\mathbf{b}^T\mathbf{A}\mathbf{C}\mathbf{q}^{(2)} + 3\tau_5^{(5)}$	$3\tau_5^{(5)}$	$3\tau_5^{(5)}$
$\tau_8^{(5)}$	$\frac{1}{2}\mathbf{b}^T\mathbf{A}\mathbf{q}^{(3)} + \tau_5^{(5)}$	$\frac{1}{2}\mathbf{b}^T\mathbf{A}\mathbf{q}^{(3)} + \tau_5^{(5)}$	$\frac{1}{2}b_ia_{i2}q_2^{(3)} + \tau_5^{(5)}$
$\tau_9^{(5)}$	$\mathbf{b}^T\mathbf{A}\mathbf{A}\mathbf{q}^{(2)} + \tau_8^{(5)}$	$\tau_8^{(5)}$	$\frac{1}{2}b_ia_{i2}q_2^{(3)} + \tau_5^{(5)}$
$\tau_2^{(6)}$	$\frac{1}{6}\mathbf{b}^T\mathbf{C}^3\mathbf{q}^{(2)} + 10\tau_1^{(6)}$	$10\tau_1^{(6)}$	$10\tau_1^{(6)}$
$\tau_3^{(6)}$	$\frac{1}{2}\mathbf{b}^T\mathbf{C}\left(\mathbf{q}^{(2)} + \mathbf{C}^2\right)\mathbf{q}^{(2)} + 15\tau_1^{(6)}$	$15\tau_1^{(6)}$	$15\tau_1^{(6)}$
$\tau_4^{(6)}$	$\frac{1}{4}\mathbf{b}^T\mathbf{C}^2\mathbf{q}^{(3)} + 10\tau_1^{(6)}$	$\frac{1}{4}\mathbf{b}^T\mathbf{C}^2\mathbf{q}^{(3)} + 10\tau_1^{(6)}$	$\frac{1}{4}b_2c_2^2q_2^{(3)} + 10\tau_1^{(6)}$
$\tau_5^{(6)}$	$\frac{1}{2}\mathbf{b}^T\left(\mathbf{Q}^{(3)} + \frac{1}{3}\mathbf{C}^3\right)\mathbf{q}^{(2)} + \tau_4^{(6)}$	$\tau_4^{(6)}$	$\frac{1}{4}b_2c_2^2q_2^{(3)} + 10\tau_1^{(6)}$
$\tau_6^{(6)}$	$\frac{1}{6}\mathbf{b}^T\mathbf{C}\mathbf{q}^{(4)} + 5\tau_1^{(6)}$	$\frac{1}{6}\mathbf{b}^T\mathbf{C}\mathbf{q}^{(4)} + 5\tau_1^{(6)}$	$\frac{1}{6}\mathbf{b}^T\mathbf{C}\mathbf{q}^{(4)} + 5\tau_1^{(6)}$
$\tau_7^{(6)}$	$\frac{1}{24}\mathbf{b}^T\mathbf{q}^{(5)} + \tau_1^{(6)}$	$\frac{1}{24}\mathbf{b}^T\mathbf{q}^{(5)} + \tau_1^{(6)}$	$\frac{1}{24}\mathbf{b}^T\mathbf{q}^{(5)} + \tau_1^{(6)}$
$\tau_8^{(6)}$	$\frac{1}{2}\mathbf{b}^T\mathbf{C}^2\mathbf{A}\mathbf{q}^{(2)} + \tau_4^{(6)}$	$\tau_4^{(6)}$	$\frac{1}{4}b_2c_2^2q_2^{(3)} + 10\tau_1^{(6)}$
$\tau_9^{(6)}$	$\mathbf{b}^T\mathbf{Q}^{(2)}\mathbf{A}\mathbf{q}^{(2)} + \frac{1}{2}\mathbf{b}^T\mathbf{Q}^{(2)}\mathbf{q}^{(3)}$ $+\frac{1}{6}\mathbf{b}^T\mathbf{C}^3\mathbf{q}^{(2)} + \tau_8^{(6)}$	$\tau_8^{(6)}$	$\frac{1}{4}b_2c_2^2q_2^{(3)} + 10\tau_1^{(6)}$
$\tau_{10}^{(6)}$	$\mathbf{b}^T\mathbf{C}\mathbf{A}\mathbf{C}\mathbf{q}^{(2)} + 3\tau_6^{(6)}$	$3\tau_6^{(6)}$	$3\tau_6^{(6)}$
$\tau_{11}^{(6)}$	$\frac{1}{2}\mathbf{b}^T\mathbf{A}\mathbf{C}^2\mathbf{q}^{(2)} + 6\tau_7^{(6)}$	$6\tau_7^{(6)}$	$6\tau_7^{(6)}$
$\tau_{12}^{(6)}$	$\frac{1}{2}\mathbf{b}^T\mathbf{A}\left(\mathbf{q}^{(2)} + \mathbf{C}^2\right)\mathbf{q}^{(2)} + 3\tau_7^{(6)}$	$3\tau_7^{(6)}$	$3\tau_7^{(6)}$
$\tau_{13}^{(6)}$	$\frac{1}{2}\mathbf{b}^T\mathbf{C}\mathbf{A}\mathbf{q}^{(3)} + \tau_6^{(6)}$	$\frac{1}{2}\mathbf{b}^T\mathbf{C}\mathbf{A}\mathbf{q}^{(3)} + \tau_6^{(6)}$	$\frac{1}{2}b_ic_ia_{i2}q_2^{(3)} + \tau_6^{(6)}$
$\tau_{14}^{(6)}$	$\frac{1}{2}\mathbf{b}^T\mathbf{A}\mathbf{C}\mathbf{q}^{(3)} + 4\tau_7^{(6)}$	$\frac{1}{2}\mathbf{b}^T\mathbf{A}\mathbf{C}\mathbf{q}^{(3)} + 4\tau_7^{(6)}$	$\frac{1}{2}b_ia_{i2}c_2q_2^{(3)} + 4\tau_7^{(6)}$
$\tau_{15}^{(6)}$	$\frac{1}{6}\mathbf{b}^T\mathbf{A}\mathbf{q}^{(4)} + \tau_7^{(6)}$	$\frac{1}{6}\mathbf{b}^T\mathbf{A}\mathbf{q}^{(4)} + \tau_7^{(6)}$	$\frac{1}{6}\mathbf{b}^T\mathbf{A}\mathbf{q}^{(4)} + \tau_7^{(6)}$
$\tau_{16}^{(6)}$	$\mathbf{b}^T\mathbf{C}\mathbf{A}\mathbf{A}\mathbf{q}^{(2)} + \tau_{13}^{(6)}$	$\tau_{13}^{(6)}$	$\frac{1}{2}b_ic_ia_{i2}q_2^{(3)} + \tau_6^{(6)}$
$\tau_{17}^{(6)}$	$\mathbf{b}^T\mathbf{A}\mathbf{C}\mathbf{A}\mathbf{q}^{(2)} + \tau_{14}^{(6)}$	$\tau_{14}^{(6)}$	$\frac{1}{2}b_ia_{i2}c_2q_2^{(3)} + 4\tau_7^{(6)}$
$\tau_{18}^{(6)}$	$\mathbf{b}^T\mathbf{A}\mathbf{A}\mathbf{C}\mathbf{q}^{(2)} + 3\tau_{15}^{(6)}$	$3\tau_{15}^{(6)}$	$3\tau_{15}^{(6)}$
$\tau_{19}^{(6)}$	$\frac{1}{2}\mathbf{b}^T\mathbf{A}\mathbf{A}\mathbf{q}^{(3)} + \tau_{15}^{(6)}$	$\frac{1}{2}\mathbf{b}^T\mathbf{A}\mathbf{A}\mathbf{q}^{(3)} + \tau_{15}^{(6)}$	$\frac{1}{2}b_ia_{ij}a_{j2}q_2^{(3)} + \tau_{15}^{(6)}$
$\tau_{20}^{(6)}$	$\mathbf{b}^T\mathbf{A}\mathbf{A}\mathbf{A}\mathbf{q}^{(2)} + \tau_{19}^{(6)}$	$\tau_{19}^{(6)}$	$\frac{1}{2}b_ia_{ij}a_{j2}q_2^{(3)} + \tau_{15}^{(6)}$

Table 2: Order conditions expressed using $\mathbf{q}^{(k)}$ up to sixth-order and their reduced from upon application of $C(2)$ or a truncated form of $C(3)^*$. Bushy tree order conditions, $\tau_1^{(l)}, l = 1, 2, \cdots, 6$, are not included.

$s_{\rm I}, p$	A-stable
$2,2$	$1/4 \leq \gamma \leq \infty$
$2,3$	$\gamma = (3+\sqrt{3})/6$
$3,3$	$1/3 \leq \gamma \leq 1.06857902130162880641883 4$
$3,4$	$\gamma = 1.068579021301628806418834$
$4,4$	$0.3943375672974064411272872 \leq \gamma \leq 1.2805797612753054573024841$
$4,5$	-
$5,5$	$0.2465051931428202746001423 \leq \gamma \leq 0.3618033988749894848204587$
	$0.4207825127659933063870173 \leq \gamma \leq 0.4732683912582953244555885$
$5,6$	$\gamma = 0.4732683912582953244555885$
$6,6$	$0.2840646380117982930387010 \leq \gamma \leq 0.5409068780733081049137798$
$6,7$	-
$7,7$	-
$7,8$	-
$8,8$	$0.2170497430943030918315779 \leq \gamma \leq 0.2647142465800596850440755$
$8,9$	-

Table 3: Bounds on γ for A-stable SDIRKs and ESDIRKs from orders two to nine where p is the order of accuracy and $s_{\rm I}$ is the number of implicit stages.

where $\mathbf{I}$ is the identity matrix and $z = \lambda \Delta t$. Similar expressions may be written for the embedded and dense output methods by simply replacing $\mathbf{b}$ with $\hat{\mathbf{b}}$ and $\mathbf{b}(\theta)$, respectively. A method is called A-stable and its stability function is called A-acceptable if $|R(z)| \leq 1$ for $\Re(z) \leq 0$. If, in addition to A-stability, $R(z)_{z \to -\infty} = 0$, then the method is called L-stable, and its stability function is called L-acceptable. L-acceptable stability functions have deg $Q(z) >$ deg $P(z)$. For SDIRKs and ESDIRKs, $Q(z) = s_I$ so that $p_i = 0$ for $i \geq s_I$ is necessary for an L-acceptable stability function.

A Runge-Kutta method is imaginary axis or I-stable if $|R(z)| \leq 1$ for $\Re(z) = 0$. To test for I-stability, the E-polynomial is used,

$$E(y) \;=\; Q(+iy)Q(-iy) - P(+iy)P(-iy) = \sum_{j=0}^{s} E_{2j} y^{2j}, \tag{17}$$

where $i = \sqrt{-1}$. I-stability requires that $E(y) \geq 0$ for all values of real y, which requires $E(y)$ to have only imaginary roots. With the E-polynomial, one may establish a priori the bounds on γ that will result in either A-stable or L-stable methods provided that $p \approx s$. These bounds are given in Tables 3 and 4. To build these tables, methods were tested up to order 25 for both A- and L-stable methods. When $p \ll s$, enforcing $E(y) \geq 0$ can be difficult although γ can typically be reduced considerably relative to methods with $s-1$ stages. Increasing the number of stages increases the number of right-hand-side evaluations as well as the required number of iterative solves but facilitates those iterative solves by reducing the condition number of the iteration matrix.

4.2 Nonlinear Stability

Defining the symmetric algebraic stability matrix as

$$\mathbf{M} = \mathbf{B}^T\mathbf{A} + \mathbf{A}^T\mathbf{B} - \mathbf{B}\mathbf{B}^T, \qquad M_{ij} = b_i a_{ij} + b_j a_{ji} - b_i b_j, \tag{18}$$

s_{I}, p	L-stable
$2,2$	$\gamma = (2 \pm \sqrt{2})/2$
$3,2$	$0.18042530642939856413458 31 \leq \gamma \leq 2.18560009735504008262914 00$
$3,3$	$\gamma = 0.43586652150845899941601945$
$4,3$	$0.22364780093417645106968 98 \leq \gamma \leq 0.57281606248213485540800 14$
$4,4$	$\gamma = 0.57281606248213485540800 14$
$5,4$	$0.24799463621274745516799 10 \leq \gamma \leq 0.67604239322628132887238 63$
$5,5$	$\gamma = 0.27805384113645232493158 62$
$6,5$	$0.18391465367517516323214 36 \leq \gamma \leq 0.33414236706805043595403 01$
$6,6$	$\gamma = 0.33414236706805043595403 01$
$7,6$	$0.20408345171588576337179 06 \leq \gamma \leq 0.37886489448532834402588 53$
$7,7$	-
$8,7$	$0.15665859939704394839245 06 \leq \gamma \leq 0.20293486084337767377793 49$
	$0.20519417194940071174606 14 \leq \gamma \leq 0.23437315960558355794755 89$
$8,8$	$\gamma = 0.23437315960558355794755 89$
$9,8$	$0.17089196255746353093322 23 \leq \gamma \leq 0.25942051048144255476694 95$
$9,9$	-
$10,9$	-
$10,10$	-
$11,10$	$0.14689893085911252606804 28 \leq \gamma \leq 0.16579261009805605710961 75$
	$0.19377336628009206357545 54 \leq \gamma \leq 0.19615242311088030031162 74$
$11,11$	-

Table 4: Bounds on γ for L-stable SDIRKs and ESDIRKs from orders two to eleven where p is the order of accuracy and s_{I} is the number of implicit stages.

where $\mathbf{B} = \mathrm{diag}(\mathbf{b})$ or $\mathbf{b} = \mathbf{Be}$. Algebraic-stability of irreducible methods requires that $a_{ii}, b_i > 0$ and $\mathbf{M} \geq O$. Consequently, SDIRKs may be algebraically stable but ESDIRKs may not.

4.3 Internal Stability

Beyond traditional stepwise stability, it may be useful to control the stability associated with each stage in addition to each step. This is particularly true for large scaled eigenvalues, z, associated with stiff problems. To determine the vector of internal stabilities of Runge-Kutta methods, one evaluates

$$\begin{aligned} R_{\text{int}}(z) &= (\mathbf{I} - z\mathbf{A})^{-1}\mathbf{e} = \{R_{\text{int}}^{(1)}(z), R_{\text{int}}^{(2)}(z), \cdots, R_{\text{int}}^{(s)}(z)\}^T \\ &= \left\{\frac{P_{\text{int}}^{(1)}(z)}{Q_{\text{int}}^{(1)}(z)}, \frac{P_{\text{int}}^{(2)}(z)}{Q_{\text{int}}^{(2)}(z)}, \cdots, \frac{P_{\text{int}}^{(s)}(z)}{Q_{\text{int}}^{(s)}(z)}\right\}^T. \end{aligned} \tag{19}$$

The primary concern will be the value of $R_{\text{int}}^{(i)}(-\infty)$. One may also consider the E-polynomial, (17), at internal stages to determine stagewise I-stability by using

$$E_{\text{int}}^{(i)}(y) = Q_{\text{int}}^{(i)}(iy)Q_{\text{int}}^{(i)}(-iy) - P_{\text{int}}^{(i)}(iy)P_{\text{int}}^{(i)}(-iy), \tag{20}$$

where $E_{\text{int}}^{(i)}(y) \geq 0$ implies stagewise I-stability. One could also consider a stagewise analog to the algebraic-stability matrix for irreducible methods where

$$M_{jk}^{(i)} = a_{ij}a_{jk} + a_{ik}a_{kj} - a_{ij}a_{ik} \geq 0, \quad a_{ij} \geq 0, \quad i, j, k = 1, 2, \ldots, s, \tag{21}$$

and $M_{jk}^{(i)}$ is the internal algebraic-stability matrix for stage i. Interestingly, the classic fully-implicit Runge-Kutta methods such as the Gauss, Radau (IA and IIA) and Lobatto (IIIA, IIIB and IIIC) methods are not internally algebraically stable on all stages. This suggests that internal algebraic stability is a rather severe requirement.

5 Implementation

For small systems of differential equations, one generally solves the implicit algebraic equations directly. In this case, using the definition $F_j = F\left(U_j, t^{[n]} + c_j\Delta t\right)$, one must solve

$$U_i = U^{[n]} + X_i + (\Delta t)\gamma F_i, \quad X_i = (\Delta t)\sum_{j=1}^{i-1} a_{ij}F_j, \quad 1 \leq i \leq s, \tag{22}$$

where X_i is explicitly computed from existing data. Combining (22) with an appropriate starting guess, a modified Newton iteration provides U_i and F_i. This is accomplished by solving

$$(\mathbf{I} - \gamma(\Delta t)\mathbf{J})(U_{i,k+1} - U_{i,k}) = -\left(U_{i,k} - U^{[n]}\right) + X_i + \gamma(\Delta t)F_i, \tag{23}$$

where the subscript k denotes the value on the kth iteration, $(\partial F/\partial U) = \mathbf{J}$ is the Jacobian, $\mathbf{I}$ is the identity matrix, $(\mathbf{I} - \gamma(\Delta t)\mathbf{J}) = \mathbf{N}$ is the (Newton) iteration matrix, and $(U_{i,k+1} - U_{i,k}) = \mathbf{d}_{i,k}$ is the displacement. The RHS of (23) is called the residual,

$\mathbf{r}_{i,k}$ where $\mathbf{N}\mathbf{d}_{i,k} = \mathbf{r}_{i,k}$. Solving for the displacement vector, $U_{i,k+1}$ is then updated. Ideally, this procedure is repeated until some convergence criterion has been met. The importance of reducing the value of γ can be seen by looking at the term $\gamma(\Delta t)$ within the iteration matrix. Keeping the condition number of iteration matrix the same, a reduction in γ then permits an increase in the step size.

6 Step-Size Control

Local integration error for Runge-Kutta methods is usually controlled by first creating a local error estimate via an embedded method. This error estimate is then fed to an error controller which adjusts the time step in order to maintain some user-specified relative error tolerance ϵ. Step-size controllers are considered of the form

$$\begin{aligned}(\Delta t)^{[n+1]} &= \kappa(\Delta t)^{[n]} \left\{ \frac{\epsilon}{||\delta^{[n+1]}||} \right\}^{\alpha} \left\{ \frac{||\delta^{[n]}||}{\epsilon} \right\}^{\beta} \left\{ \frac{\epsilon}{||\delta^{[n-1]}||} \right\}^{\gamma} \\ &\times \left\{ \frac{(\Delta t)^{[n]}}{(\Delta t)^{[n-1]}} \right\}^{\mathfrak{a}} \left\{ \frac{(\Delta t)^{[n-1]}}{(\Delta t)^{[n-2]}} \right\}^{\mathfrak{b}} \end{aligned} \tag{24}$$

for $p(\hat{p})$-pairs ($\hat{p} = p - 1$). In (24), $\kappa \approx 0.95$ is the safety factor, $(\Delta t)^{[n-i]} = t^{[n-i]} - t^{[n-i-1]}$ is the step size, and $\delta^{[n+1]}$ is the vector of most recent local error estimates of the integration from $t^{[n-1]}$ to $t^{[n]}$ associated with the computation of $U^{[n+1]}$. Many controllers exist and Table 5 lists coefficients for various controllers.

Controller	α	β	γ	$\mathfrak{a}$	$\mathfrak{b}$
I = H_0110	$\frac{1}{\hat{p}+1}$	0	0	0	0
H211	$\frac{1}{4\hat{p}}$	$\frac{-1}{4\hat{p}}$	0	$\frac{-1}{4}$	0
PC = H_0220	$\frac{2}{\hat{p}}$	$\frac{1}{\hat{p}}$	0	1	0
PID	$\frac{1}{18\hat{p}}$	$\frac{-1}{9\hat{p}}$	$\frac{1}{18\hat{p}}$	0	0
H312	$\frac{1}{8\hat{p}}$	$\frac{-1}{4\hat{p}}$	$\frac{1}{8\hat{p}}$	$\frac{-3}{8}$	$\frac{-1}{8}$
PPID	$\frac{6}{20\hat{p}}$	$\frac{-1}{20\hat{p}}$	$\frac{-5}{20\hat{p}}$	1	0
H321	$\frac{1}{3\hat{p}}$	$\frac{-1}{18\hat{p}}$	$\frac{-5}{18\hat{p}}$	$\frac{5}{6}$	$\frac{1}{6}$

Table 5: Error controller coefficients.

7 Third-Order Methods

7.1 Four Stages, $s_I = 3$

Stiffly-accurate, stage-order two ESDIRK methods in four stages appear as

$$\begin{array}{c|cccc} 0 & 0 & 0 & 0 & 0 \\ 2\gamma & \gamma & \gamma & 0 & 0 \\ c_3 & a_{31} & a_{32} & \gamma & 0 \\ 1 & b_1 & b_2 & b_3 & \gamma \\ \hline b_i & b_1 & b_2 & b_3 & \gamma \\ \hline \hat{b}_i & \hat{b}_1 & \hat{b}_2 & \hat{b}_3 & \hat{b}_4. \end{array} \tag{25}$$

To enforce third-order overall accuracy for ODEs, a stage-order of two, and L-stability, one must satisfy the following six equations: $\tau_1^{(1,2,3)} = p_3 = q_{2,3}^{(2)} = 0$, leaving a one-parameter family of methods in c_3. The general solution is

$$a_{32} = \frac{c_3(c_3 - 2\gamma)}{4\gamma}, \quad b_2 = \frac{-2 + 3c_3 + 6\gamma(1 - c_3)}{12\gamma(c_3 - 2\gamma)}, \quad b_3 = \frac{1 - 6\gamma + 6\gamma^2}{3c_3(c_3 - 2\gamma)} \tag{26}$$

where $c_3 - 2\gamma \neq 0$ and $c_3 \neq 0$. Demanding L-stability of the step requires that $\gamma = 0.43586652150845899941601945$. Selecting $c_3 = 3/5$, a method is found having $A^{(4)} = 0.03663$ and $R_{\text{int}}^{(3)}(-\infty) = -0.8057$. Stages 2 and 3 are both internally -I-stable. Second-order, A-stable, error-control is accomplished by solving $\hat{\tau}_1^{(1,2)} = \hat{p}_4 = 0$, $\hat{R}(-\infty) = -\hat{p}_3/\gamma^3 = \gamma/2$. ESDIRK3(2)4L[2]SA was given in [7] and its properties are listed in Table 6.

7.2 Five Stages, $s_I = 4$

To design a stiffly-accurate, stage-order two ESDIRK 3(2)-pair in five-stages, the following conditions are enforced

$$0 = \tau_1^{(1,2,3)} = q_{2,3,4,5}^{(1)} = q_{2,3,4}^{(2)} = p_4 = R_{\text{int}}^{(3,4)}(-\infty) = \hat{\tau}_1^{(1,2)} = \hat{p}_{4,5},\ \hat{\tau}_1^{(3)} = \frac{1}{600}. \tag{27}$$

leaving γ and c_4 in main method. L-stable methods may be found for

$$0.22364780093417645106968 98 \leq \gamma \leq 0.57281606248213485540800 14. \tag{28}$$

Setting $\gamma = 9/40 = 0.225$, $c_3 = 9(2 + \sqrt{2})/40$ and $c_4 = 3/5$ yields a method having $A^{(4)} = 0.0007769$. This represents over an order-of-magnitude reduction in both $A^{(4)}$ and $A^{(5)}$ relative to ESDIRK3(2)4L[2]SA as well as a reduction in γ by nearly 50%. The method is I-stable on all internal stages and, hence, A-stable on stage 2 and L-stable on stages 3, 4 and 5. Further, it has an L-stable embedded method. This scheme, ESDIRK3(2)5L[2]SA, was given in [7] while its properties are listed in Table 6. Minimum eigenvalues of the algebraic stability matrix, $\lambda_{\text{Min}}^{\mathbf{M}}$, and the internal algebraic stability matrix in stage i, $\lambda_{\text{Min}}^{\mathbf{M}^{(i)}}$, are similar between ESDIRK3(2)4L[2]SA and ESDIRK3(2)5L[2]SA.

8 Fourth-Order Methods

8.1 Five Stages, $s_I = 5$

Arguably, the most popular DIRK-type method is SDIRK4[5]. It is an SDIRK in five-stages which is fourth-order but has only stage-order one. Key properties for this reference method are given in Table 7, From this table, SDIRK4 can be seen to be strongly nonlinearly unstable with $\lambda_{\text{Min}}^{\mathbf{M}} = -112.1$.

Name	ESDIRK 3(2)4L[2]SA	ESDIRK 3(2)5L[2]SA
s	4	5
p	3	3
γ	0.4359	$\frac{9}{40}$
$A^{(4)}$	0.03663	0.000777
$A^{(5)}$	0.07870	0.005199
$A^{(6)}$	0.1192	0.007633
$\hat{A}^{(3)}$	0.02552	0.002357
$\hat{A}^{(4)}$	0.07418	0.002437
$\{B^{(5)}, C^{(5)}, E^{(5)}\}$	$\{2.90, 1.64, 1.44\}$	$\{1.03, 1.21, 0.330\}$
D	1.000	1.000
$\{\lambda^{\mathbf{M}}_{\text{Min}}, \lambda^{\hat{\mathbf{M}}}_{\text{Min}}\}$	$\{-1.133, -2.335\}$	$\{-0.484, -0.340\}$
$\{b_{i,\text{Min}}, a_{ij,\text{Min}}\}$	$\{-0.595, -0.595\}$	$\{-0.347, -0.347\}$
$\lambda^{\mathbf{M}^{(2)}}_{\text{Min}}$	-0.190	-0.051
$\lambda^{\mathbf{M}^{(3)}}_{\text{Min}}$	-0.099	-0.075
$\lambda^{\mathbf{M}^{(4)}}_{\text{Min}}$	-1.133	-0.051
$\lambda^{\mathbf{M}^{(5)}}_{\text{Min}}$	$-$	-0.484
$\{R(-\infty), \hat{R}(-\infty)\}$	$\{0.0, 0.2179\}$	$\{0.0, 0.0\}$

Table 6: Third-order methods.

8.2 Six Stages, $s_I = 5$

Six-stage, stage-order two, stiffly-accurate ESDIRK methods

$$\begin{array}{c|cccccc}
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
2\gamma & \gamma & \gamma & 0 & 0 & 0 & 0 \\
c_3 & a_{31} & a_{32} & \gamma & 0 & 0 & 0 \\
c_4 & a_{41} & a_{42} & a_{43} & \gamma & 0 & 0 \\
c_5 & a_{51} & a_{52} & a_{53} & a_{54} & \gamma & 0 \\
1 & b_1 & b_2 & b_3 & b_4 & b_5 & \gamma \\
\hline
b_i & b_1 & b_2 & b_3 & b_4 & b_5 & \gamma \\
\hline
\hat{b}_i & \hat{b}_1 & \hat{b}_2 & \hat{b}_3 & \hat{b}_4 & \hat{b}_5 & \hat{b}_6
\end{array} \tag{29}$$

provide $s(s+1)/2 - 4 = 17$ DOF, as shown, where $q_2^{(1,2)}$ and $\tau_1^{(1)}$ have already been applied. L-stable methods may be found for

$$0.247994636212747455167991 0 \leq \gamma \leq 0.676042393226281328872386 3. \tag{30}$$

Fourth-order methods are be obtained by solving

$$0 = \tau_1^{(1,2,3,4)} = q_{2,3,4,5}^{(1)} = q_{2,3,4,5}^{(2)} = \tau_3^{(4)} = p_5 = R_{\text{int}}^{(3,4,5)}(-\infty) \tag{31}$$

$$0 = \hat{\tau}_1^{(1,2,3)} = \hat{p}_{5,6},\ \hat{\tau}_1^{(4)} = \frac{1}{1000} \tag{32}$$

for the main method and the embedded methods. Selecting $c_3 = \gamma(2-\sqrt{2})$, three DOF remain, say c_4, c_5 and γ. Two solutions are given by

- ESDIRK4(3)6L[2]SA_1: $\gamma = \frac{1}{4},\ c_4 = \frac{5}{8},\ c_5 = \frac{26}{25}$
- ESDIRK4(3)6L[2]SA_2: $\gamma = \frac{248}{1000},\ c_4 = \frac{1043}{1706},\ c_5 = \frac{1361}{1300}$

Both methods are strictly internally A-stable on stage two but internally L-stable on stages three through six. Also, both embedded methods are L-stable. The first method, ESDIRK4(3)6L[2]SA_1, given in [7] while the second method, ESDIRK4(3)6L[2]SA_2, is a slight perturbation on ESDIRK4(3)6L[2]SA_1. Notice that one of abscissae, c_5, is just outside the integration step. This could be problematic when integrating across temporal discontinuities. Properties for both of these methods are given in Table 7.

8.3 Seven Stages, $s_I = 6$

Moving to seven stages, fourth-order methods are be obtained by solving

$$0 = \tau_1^{(1,2,3,4,5)} = q_{2,3,4,5,6}^{(1)} = q_{2,3,4,5,6}^{(2)} = \tau_3^{(4)} = \tau_{4,5}^{(5)} = p_6 = R_{\text{int}}^{(3,4,5,6)}(-\infty), \quad (33)$$

$$0 = \hat{\tau}_1^{(1,2,3)} = \hat{p}_{6,7} = \frac{\partial \hat{A}^{(4)}}{\partial \hat{b}_6}, \quad (34)$$

for the main method and for the embedded method. Four DOF remain, e.g. γ, c_4, c_5 and c_6 in the main method while one remains in the embedded method. The dominant motivation for creating a seven-stage, fourth-order ESDIRKs is that γ can be driven to quite small values while the leading order error can be driven quite low. Setting $\gamma = \frac{1}{8}$, $\hat{b}_6 = \frac{19}{140}$ and

$$c_2 = \frac{1}{4}, \quad c_3 = (2-\sqrt{2})/8, \quad c_4 = \frac{1}{2}, \quad c_5 = \frac{395}{567}, \quad c_6 = \frac{89}{126}, \quad c_7 = 1, \quad (35)$$

yields a method, ESDIRK4(3)7L[2]SA, which is L-stable, internally L-stable on stages three through seven and strictly A-stable on the second stage. Leading-order error has reduced six-fold from the similar six-stage method and a reduction in γ by nearly 50% relative to ESDIRK4(3)6L[2]SA_2. Key properties for ESDIRK4(3)7L[2]SA are given in Table 7.

9 Fifth-Order Methods

9.1 Seven Stages, $s_I = 6$

Seven-stage, stiffly-accurate ESDIRK methods take the form

$$\begin{array}{c|ccccccc}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
2\gamma & \gamma & \gamma & 0 & 0 & 0 & 0 & 0 \\
c_3 & a_{31} & a_{32} & \gamma & 0 & 0 & 0 & 0 \\
c_4 & a_{41} & a_{42} & a_{43} & \gamma & 0 & 0 & 0 \\
c_5 & a_{51} & a_{52} & a_{53} & a_{54} & \gamma & 0 & 0 \\
c_6 & a_{61} & a_{62} & a_{63} & a_{64} & a_{65} & \gamma & 0 \\
1 & b_1 & b_2 & b_3 & b_4 & b_5 & b_6 & \gamma \\
\hline
b_i & b_1 & b_2 & b_3 & b_4 & b_5 & b_6 & \gamma \\
\hline
\hat{b}_i & \hat{b}_1 & \hat{b}_2 & \hat{b}_3 & \hat{b}_4 & \hat{b}_5 & \hat{b}_6 & \hat{b}_7
\end{array} \quad (36)$$

provide 24 DOF, as shown, where $q_2^{(1,2)}$ and $\tau_1^{(1)}$ have already been applied. Row simplifying assumption $C(2)$ ensures a stage-order two method. L-stable methods may be found for a range γ values

$$0.18391465367517517516323214 36 \leq \gamma \leq 0.33414236706805043595403 01. \quad (37)$$

Name	SDIRK4	ESDIRK 4(3)6L[2]SA_1	ESDIRK 4(3)6L[2]SA_2	ESDIRK 4(3)7L[2]SA
s	5	6	6	7
p	4	4	4	4
γ	$\frac{1}{4}$	$\frac{1}{4}$	0.248	$\frac{1}{8}$
$A^{(5)}$	0.002504	0.001830	0.001686	0.000260
$A^{(6)}$	0.004511	0.003467	0.002893	0.001177
$\hat{A}^{(4)}$	0.01247	0.003187	0.003187	0.000301
$\hat{A}^{(5)}$	0.01638	0.004077	0.004319	0.000977
$\{B^{(5)}, C^{(5)}, E^{(5)}\}$	$\{1.31, 1.43, 0.201\}$	$\{1.28, 1.15, 0.574\}$	$\{1.36, 1.15, 0.529\}$	$\{3.24, 3.07, 0.861\}$
D	7.813	1.585	1.504	1.00
$\{\lambda^{\mathbf{M}}_{\mathrm{Min}}, \lambda^{\hat{\mathbf{M}}}_{\mathrm{Min}}\}$	$\{-112.1, -100.45\}$	$\{-0.197, -0.184\}$	$\{-0.174, -0.148\}$	$\{-1.990, -1.361\}$
$\{b_{i,\mathrm{Min}}, a_{ij,\mathrm{Min}}\}$	$\{-7.083, -7.083\}$	$\{-0.108, -0.727\}$	$\{-0.098, -0.690\}$	$\{-0.557, -0.557\}$
$\lambda^{\mathbf{M}^{(2)}}_{\mathrm{Min}}$	+0.063	−0.063	−0.062	−0.016
$\lambda^{\mathbf{M}^{(3)}}_{\mathrm{Min}}$	−0.022	−0.036	−0.035	−0.009
$\lambda^{\mathbf{M}^{(4)}}_{\mathrm{Min}}$	−0.029	−0.063	−0.075	−0.314
$\lambda^{\mathbf{M}^{(5)}}_{\mathrm{Min}}$	−112.1	−3.360	−3.033	−1.225
$\lambda^{\mathbf{M}^{(6)}}_{\mathrm{Min}}$	−	−0.197	−0.174	−0.204
$\lambda^{\mathbf{M}^{(7)}}_{\mathrm{Min}}$	−	−	−	−1.990
$\{R(-\infty), \hat{R}(-\infty)\}$	$\{0.0, 3.3\}$	$\{0.0, 0.0\}$	$\{0.0, 0.0\}$	$\{0.0, 0.0\}$

Table 7: Fourth-order methods.

Fifth-order methods are be obtained by solving

$$0 = \tau_1^{(1,2,3,4,5)} = q_{2,3,\ldots,6}^{(1)} = q_{2,3,4,5,6}^{(2)} = \tau_3^{(4)} = \tau_{4,5,8}^{(5)} = p_6 = R_{\mathrm{int}}^{(3,4,5,6)}(-\infty), \quad (38)$$

$$0 = \hat{\tau}_1^{(1,2,3,4)} = \hat{\tau}_3^{(4)} = \hat{p}_7, \quad (39)$$

for the main method and for the embedded methods. This leaves three remaining DOF in the main method e.g., c_4, c_6 and γ and $\hat{b}_7$ in the embedded method. As γ is probably best chosen as small as possible, $\gamma = 0.184 = 23/125$ is selected where $c_2 = 2\gamma$. The coefficient $\hat{b}_7$ has been used to enforce $\hat{p}_6/\gamma^6 = \hat{R}(-\infty)$. Two solutions to these conditions are shown in Table 8 and given by

- ESDIRK5(4)7L[2]SA_1: $c_3 = (2 - \sqrt{2})\gamma,\ c_4 = \frac{13}{25},\ c_5 = \frac{5906118540659}{9042400211275},\ c_6 = \frac{26}{25}$
- ESDIRK5(4)7L[2]SA_2: $c_3 = (2 + \sqrt{2})\gamma,\ c_4 = \frac{49}{353},\ c_5 = \frac{3706679970760}{5295570149437},\ c_6 = \frac{347}{382}$

The first method, ESDIRK5(4)7L[2]SA_1, was given in [7], as ESDIRK5(4)7L[2]SA. While ESDIRK5(4)7L[2]SA_1 is not I-stable and strongly nonlinearly unstable on the sixth-stage, ESDIRK5(4)7L[2]SA_2 is I-stable and only mildly nonlinearly unstable on the same stage.

9.2 Eight Stages, $s_I = 7$

If another stage is added, fifth-order methods are be obtained by solving

$$0 = \tau_1^{(1,2,3,4,5,6)} = q_{2,3,\ldots,7}^{(1)} = q_{2,3,\ldots,7}^{(2)} = \tau_3^{(4)} = \tau_{4,5,8}^{(5)} = \tau_{6,7}^{(6)} = p_7 = R_{\mathrm{int}}^{(3,4,5,6,7)}(-\infty) \quad (40)$$

$$0 = \hat{\tau}_1^{(1,2,3,4)} = \hat{\tau}_3^{(4)} = \hat{p}_{7,8} \quad (41)$$

for the main method and for the embedded method. As seen from Table 1, enforcement of $\tau_{1,6,7}^{(6)} = 0$ forces $\tau_{2,3,10,11,12}^{(6)} = 0$. Four abscissae, $c_{4,5,6,7}$, and γ remain to be specified.

Setting

$$\gamma = \frac{1}{7}, \quad c_2 = \frac{2}{7}, \quad c_3 = \frac{2+\sqrt{2}}{7}, \quad c_4 = \frac{150}{203}, \quad c_5 = \frac{27}{46}, \quad c_6 = \frac{473}{532}, \quad c_7 = \frac{30}{83}, \quad (42)$$

and $\hat{b}_8 = 36/233$, ESDIRK5(4)8L[2]SA is found. Its properties are shown in Table 8.

Though ESDIRKs and fully implicit Runge-Kutta methods are quite different, the latter serve as reference methods. In particular, the Radau IIA family of methods is both L- and algebraically-stable. The three-stage Radau IIA method is fifth-order accurate with a stage-order of three with leading-order errors of $A^{(6)} = 0.0009895$ and $A^{(7)} = 0.001714$. The minimum values of the internal algebraic stability matrix are $\{-0.05566, -0.01750, 0.0\}$ for stages $\{1,2,3\}$ so that only stage 3 is internally algebraically stable where the coefficients of $\mathbf{A}$ are all positive. All stages satisfy $R_{\text{int}}^{(i)}(-\infty) = 0$ but only stages 2 and 3 are internally I-stable.

10 Sixth-Order Methods

Assuming a nine-stage ($s = 9$), stiffly-accurate, 6(5)-pair, the main method is determined with $c_1 = 0$, $c_9 = 1$, $a_{9j} = b_j$ and

$$\begin{aligned} 0 &= \tau_1^{(1,2,3,4,5,6)} = q_{2,3,\ldots,8}^{(1)} = q_{2,3,\ldots,8}^{(2)} = q_{3,4,\ldots,8}^{(3)} = \tau_5^{(5)} = \tau_{6,7,15}^{(6)}, && (43)\\ &= \mathbf{b}^T\mathbf{e}_2 = \mathbf{b}^T\mathbf{A}\mathbf{e}_2 = \mathbf{b}^T\mathbf{C}\mathbf{A}\mathbf{e}_2 = \mathbf{b}^T\mathbf{A}\mathbf{A}\mathbf{e}_2 = p_8 = R_{\text{int}}^{(4,5,6,7,8)}(-\infty), && (44)\end{aligned}$$

where $\mathbf{e}_2 = \{0, 1, 0, 0, \cdots, 0\}$ is a vector of length s. As a consequence of $q_2^{(2)} = 0$, $c_2 = 2\gamma$, and since $q_3^{(3)} = 0$, $c_3 = (3 \pm \sqrt{3})\gamma$. The stiffly-accurate assumption along with $p_8 = 0$ ensures that $R(-\infty) = 0$. Expressions for the internal stability function and E-polynomial on stage three are found to be

$$R_{\text{int}}^{(3)}(-\infty) = \frac{c_3^2 - 4c_3\gamma + 2\gamma^2}{2\gamma^2}, \qquad E_{\text{int}}^{(3)} = \frac{c_3}{4}(4\gamma - c_3)(c_3 - 2\gamma)^2 y^4 \qquad (45)$$

To enforce $|R_{\text{int}}^{(3)}(-\infty)| < 1$, $c_3 = \left(3 - \sqrt{3}\right)\gamma$. In this case,

$$R_{\text{int}}^{(3)}(-\infty) = \left(1 - \sqrt{3}\right), \qquad E_{\text{int}}^{(3)} = \left(-3 + 2\sqrt{3}\right)\gamma^4 y^4 > 0. \qquad (46)$$

Hence, stage-three is I-stable and A-stable. Enforcing $R_{\text{int}}^{(4)}(-\infty) = 0$ where

$$R_{\text{int}}^{(4)}(-\infty) = \frac{-c_4^3 + 9c_4^2\gamma - 18c_4\gamma^2 + 6\gamma^3}{6\gamma^3}, \qquad (47)$$

gives $c_4 = \left\{3 + \sqrt{3}\sin(\theta) \pm 3\cos(\theta), 3 - 2\sqrt{3}\sin(\theta)\right\}\gamma$ where $\theta = \cot^{-1}\left(\sqrt{2}\right)/3$. Only one of these three solutions, $c_4 = \left[3 - 2\sqrt{3}\sin(\theta)\right]\gamma \approx \frac{803}{350}\gamma$, permits an I-stable fourth-stage where

$$\begin{aligned} E_{\text{int}}^{(4)} &= \left(\alpha_4 + \beta_4 y^2\right) y^4 && (48)\\ \alpha_4 &= \frac{c_4}{12}\left(c_4^3 - 12c_4^2\gamma + 36c_4\gamma^2 - 24\gamma^3\right) \\ \beta_4 &= \frac{c_4}{36}(6\gamma - c_4)(c_4 - 3\gamma)\left(c_4^3 - 9c_4^2\gamma + 18c_4\gamma^2 - 12\gamma^3\right), \end{aligned}$$

and $E_{\text{int}}^{(4)} \geq 0$ for $\alpha_4, \beta_4 \geq 0$. For stage five, enforcing $R_{\text{int}}^{(5)}(-\infty) = 0$ allows the internal E-polynomial for stage five to be written as

$$
\begin{aligned}
E_{\text{int}}^{(5)} &= \left(\alpha_5 + \beta_5 y^2 + \gamma^8 y^4\right) y^4 \\
\alpha_5 &= \frac{1}{12}\left(c_5^4 - 16c_5^3\gamma + 72c_5^2\gamma^2 - 96c_5\gamma^3 + 24\gamma^4\right) \\
\beta_5 &= \frac{1}{36}\left(c_5^3 - 12c_5^2\gamma + 36c_5\gamma^2 - 36\gamma^3\right)\left(c_5^3 - 12c_5^2\gamma + 36c_5\gamma^2 - 12\gamma^3\right).
\end{aligned} \tag{49}
$$

It may be determined that stage-five can be I-stable and L-stable if $E_{\text{int}}^{(5)} \geq 0$ for $y \geq 0$. This occurs if

$$
1.745761101158346575686816712518 \leq \frac{c_5}{\gamma} \leq 4.471316041664625579088042286147. \tag{50}
$$

There are five remaining DOF, say, γ and three abscissae from $c_{5,6,7,8}$. These DOF must be chosen so as to ensure I-stability of stages five through eight and the step. Satisfying those requirements, minimization of leading order error and nonlinear instability can be sought.

For the embedded method, there are more requirements than there are embedded scheme weights since, minimally, the embedded method must satisfy

$$
0 \;=\; = \hat{\tau}_1^{(1,2,3,4,5)} = \hat{b}_2 = \hat{\tau}_5^{(5)} = \hat{\mathbf{b}}^T \mathbf{A}\mathbf{e}_2 = \hat{p}_9. \tag{51}
$$

Since these conditions also apply to the main method, care must be taken to keep the main and embedded methods distinct. Further, $\left|\hat{R}(-\infty)\right| = |\hat{p}_8/q_8| < 1$ or, $|\hat{p}_8| < \gamma^8$, to enable an A-stable embedded method. Together, the complete method has four DOF, say, γ, one $\hat{b}$ and two abscissae from $c_{5,6,7,8}$.

To solve for the coefficients to the method, $\gamma = 2/9$ was selected and $\hat{b}_7$ was chosen as a proxy for $\hat{R}(-\infty)$. Lastly, c_5 as chosen to be with the range for I-stablity on stage five and c_8 was selected to be a number between 0 and 1. With these four coefficients selected, Two equations remained in two coefficients, c_6 and c_7. We were unable to find a good method that was I-stable on all stages. However, good methods were found with mild linear instability on stages six and seven. On each of the unstable stages, a small sliver of instability on the complex LHP exists, immediately adjacent to the imaginary axis, within $-0.025 < \Re(z) = 0$ and $-3 < \Im(z) < 3$. The maximum magnitude of the internal linear stability functions for these two stages are

$$
\begin{aligned}
\text{Max}\left(R_{\text{int}}^{(6)}\right) &= 1.00429, z = \{-0.00000036883, \pm 1.8198\} \\
\text{Max}\left(R_{\text{int}}^{(7)}\right) &= 1.00146, z = \{-0.00000088009, \pm 1.4273\}
\end{aligned}
$$

For ESDIRK6(5)9L[2]SA, with

$$
c_2 = 2\gamma, \quad c_3 = (3 - \sqrt{3})\gamma, \quad c_4 = \left[3 - 2\sqrt{3}\sin(\theta)\right]\gamma, \quad \theta = \cot^{-1}\left(\sqrt{2}\right)/3, \tag{52}
$$

the choices

$$
\gamma = \frac{2}{9}, \quad c_5 = \frac{183}{200}, \quad c_8 = \frac{97}{100}, \quad \hat{R}(-\infty) = \frac{\hat{p}_8}{\gamma^8} = \frac{1}{10}, \tag{53}
$$

Name	ESDIRK 5(4)7L[2]SA_1	ESDIRK 5(4)7L[2]SA_2	ESDIRK 5(4)8L[2]SA	ESDIRK 6(5)9L[2]SA
s	7	7	8	9
p	5	5	5	6
γ	$\frac{23}{125}$	$\frac{23}{125}$	$\frac{1}{7}$	$\frac{2}{9}$
$A^{(6)}$	0.001846	0.001272	0.0004459	–
$A^{(7)}$	0.003154	0.002184	0.0007294	0.0005388
$\hat{A}^{(5)}$	0.002171	0.002047	0.0003205	–
$\hat{A}^{(6)}$	0.001501	0.001882	0.0006473	0.003797
$\hat{A}^{(7)}$	0.000983	0.001215	0.0009153	0.0005831
$\{B^{(p+1)}, C^{(p+1)}, E^{(p+1)}\}$	$\{0.692, 1.31, 0.850\}$	$\{0.920, 1.26, 0.621\}$	$\{2.02, 1.77, 1.39\}$	$\{1.54, 1.60, 0.142\}$
D	8.971	1.634	1.000	0.9883
$\{\lambda^{\mathbf{M}}_{\text{Min}}, \lambda^{\hat{\mathbf{M}}}_{\text{Min}}\}$	$\{-0.800, -0.764\}$	$\{-0.405, -0.445\}$	$\{-1.256, -1.443\}$	$\{-1.254, -7.867\}$
$\{b_{i,\text{Min}}, a_{ij,\text{Min}}\}$	$\{-0.076, -5.036\}$	$\{-0.162, -0.539\}$	$\{-0.449, -0.847\}$	$\{-0.485, -0.922\}$
$\lambda^{\mathbf{M}(2)}_{\text{Min}}$	-0.034	-0.034	-0.020	-0.049
$\lambda^{\mathbf{M}(3)}_{\text{Min}}$	-0.019	-0.050	-0.030	-0.028
$\lambda^{\mathbf{M}(4)}_{\text{Min}}$	-0.012	-0.012	-0.033	-0.223
$\lambda^{\mathbf{M}(5)}_{\text{Min}}$	-4.290	-1.443	-0.033	-1.696
$\lambda^{\mathbf{M}(6)}_{\text{Min}}$	-131.4	-2.519	-0.711	-0.331
$\lambda^{\mathbf{M}(7)}_{\text{Min}}$	-0.800	-0.405	-1.259	-0.396
$\lambda^{\mathbf{M}(8)}_{\text{Min}}$	–	–	-1.256	-2.866
$\lambda^{\mathbf{M}(9)}_{\text{Min}}$	–	–	–	-1.254
$E^{(i)}_{\text{int}}(y) < 0$	$i = 6$	–	–	$i = 6, 7$
$\{R(-\infty), \hat{R}(-\infty)\}$	$\{0.0, 0.35\}$	$\{0.0, -0.25\}$	$\{0.0, 0.0\}$	$\{0.0, 0.1\}$

Table 8: Fifth- and sixth-order methods.

give a method with

$$c_6 = \frac{62409086037595}{296036819031271}, \quad c_7 = \frac{81796628710131}{911762868125288}. \tag{54}$$

Its properties are shown in Table 8. Stages 4, 5, 8 and 9 are L-stable while stage 2 is strictly A-stable and stage 3 is strongly A-stable. Stages 6 and 7 are not I-stable but satisfy $R^{(6,7)}_{\text{int}}(-\infty) = 0$.

11 Test Problems

Testing of schemes is conducted on two singular perturbation problems, van der Pol's (vdP) equation and Kaps' problem.

11.1 van der Pol's equation

In 1926, Balthasar van der Pol wrote the equations describing a linear oscillating circuit. The van der Pol's (vdP) equation may be written as

$$\dot{y}_1 = y_2, \qquad \dot{y}_2 = \varepsilon^{-1}\left[(1 - y_1^2)y_2 - y_1\right] \tag{55}$$

It may be seen that for $\varepsilon \to 0$, the second equations become an algebraic relation, $1 = y_1^2 y_2 + y_1$. This now constitutes an index-1 differential algebraic system. Unperturbed

ICs are given by[5]

$$y_1(0) = 2 \qquad y_2(0) = -\frac{2}{3} + \frac{10}{81}\varepsilon - \frac{292}{2187}\varepsilon^2 + \frac{15266}{59049}\varepsilon^3 + \mathcal{O}(\varepsilon^4). \tag{56}$$

11.2 Kaps' Problem

Dekker and Verwer[3] investigate a nonlinear problem (experiment 7.5.2) originally given by Peter Kaps,

$$\dot{y}_1 = -\left(\varepsilon^{-1} + 2\right) y_1 + \varepsilon^{-1} y_2^2, \qquad \dot{y}_2 = y_1 - y_2 - y_2^2, \tag{57}$$

where $0 \leq t \leq 1$ and whose exact solution is $y_1 = y_2^2, \quad y_2 = \exp(-t)$. As $\varepsilon \to 0$, the equations become

$$y_1 = y_2^2, \qquad \dot{y}_2 = y_1 - y_2 - y_2^2, \tag{58}$$

which is an index-1 DAE. Equilibrium (unperturbed) initial conditions are given by $y_1(0) = y_2(0) = 1$.

For the stiffly acurate methods considered here, it may be anticipated that the observed orders of accuracy for the differential and algebraic variables while integrating these test problems are $h^p + \varepsilon h^{q+1}$ for the differential variable and $h^p + \varepsilon h^q$ for the algebraic variable where $h = (\Delta t)$[5].

12 Discussion

The goal of the limited testing is to establish whether methods are appropriate for general purpose settings and are free of substantial shortcomings based on their convergence behavior on the two singular-pertubation test problems. Ten proposed and existing (E)SDIRK-type methods of third-, fourth-, fifth- and sixth-order accuracy are considered:

- Third-order: ESDIRK3(2)4L[2]SA and ESDIRK3(2)5L[2]SA,
- Fourth-order: SDIRK4, ESDIRK4(3)6L[2]SA_1 ESDIRK4(3)6L[2]SA_2 and ESDIRK4(3)7L[2]SA. Since ESDIRK4(3)6L[2]SA_1 and ESDIRK4(3)6L[2]SA_2 generate virtually identical test results, only the former will be shown.
- Fifth-order: ESDIRK5(4)7L[2]SA_1, ESDIRK5(4)7L[2]SA_2 and ESDIRK5(4)8L[2]SA
- Sixth-order: ESDIRK6(5)9L[2]SA

The two third-order methods, ESDIRK3(2)4L[2]SA and ESDIRK3(2)5L[2]SA, were previously tested[7]. ESDIRK3(2)5L[2]SA was found to be a better method. The methods ESDIRK4(3)6L[2]SA_1 and ESDIRK5(4)7L[2]SA_1 were also the subject of previous testing but are included here in the capacity of reference methods. SDIRK4 is included as it has, historically, been one of the most popular used DIRK methods.

12.1 Convergence

All convergence tests were done using the either the vdP or the Kaps' singular perturbation test problems, with the same ICs for each test problem, and integrating them over the same time interval. Step-sizes were held constant. Singular perturbation problems are very useful for detecting shortcomings of methods but may not be particularly illuminating at distinguishing which well designed method is more accurate in practical settings. They also fail to exercise many important implementation matters.

12.1.1 Third-Order Methods

Figure 1 shows differences in convergence rates between ESDIRK3(2)4L[2]SA$_2$ and ESDIRK3(2)5L[2]SA$_1$ on both Kaps' problem and van der Pol's equation. For Kaps'

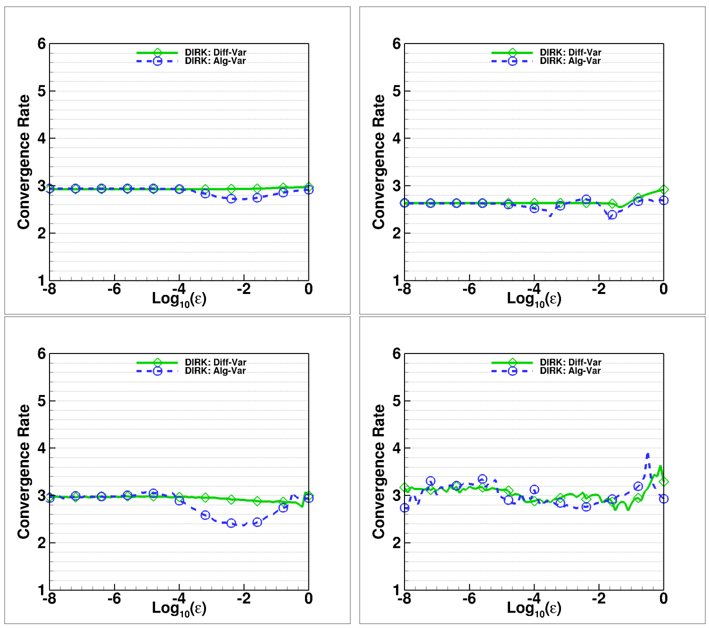

Figure 1: A convergence rate comparison between ESDIRK3(2)4L[2]SA (left) and ESDIRK3(2)5L[2]SA (right) on Kaps' problem (top) and van der Pol's equation (bottom).

problem, an error versus work comparison may be made between these same four methods at different values of the stiffness parameter. These are shown in Figure 2 for the differential variable and for the algebraic variables. Similarly, for van der Pol's equation, Figure 3 shows these same quantities.

12.1.2 Fourth-Order Methods

Four of the eight methods tested in this paper are L-stable, stiffly-accurate, fourth-order methods: SDIRK4, ESDIRK4(3)6L[2]SA_1, ESDIRK4(3)6L[2]SA_2 and ESDIRK4(3)7L[2]SA. In testing[7], ESDIRK4(3)6L[2]SA_1 showed markedly better convergence for the algebraic variable. From all of the fourth-order methods tested, it was recommended as a good general-purpose method. Based on this, ESDIRK4(3)6L[2]SA_2 was designed to eke out the last remaining performance out of ESDIRK4(3)6L[2]SA_1. Principally, this was done by simply reducing γ from 0.250 to 0.248. This resulted in a slight improvement in most method properties but there is likely to be little discernable difference between the methods. Hence results for ESDIRK4(3)6L[2]SA_2 will not be plotted below. By adding a seventh-stage, the important quantity γ can be cut in half. This can be expected to have a positive effect on the iterative convergence behavior of the

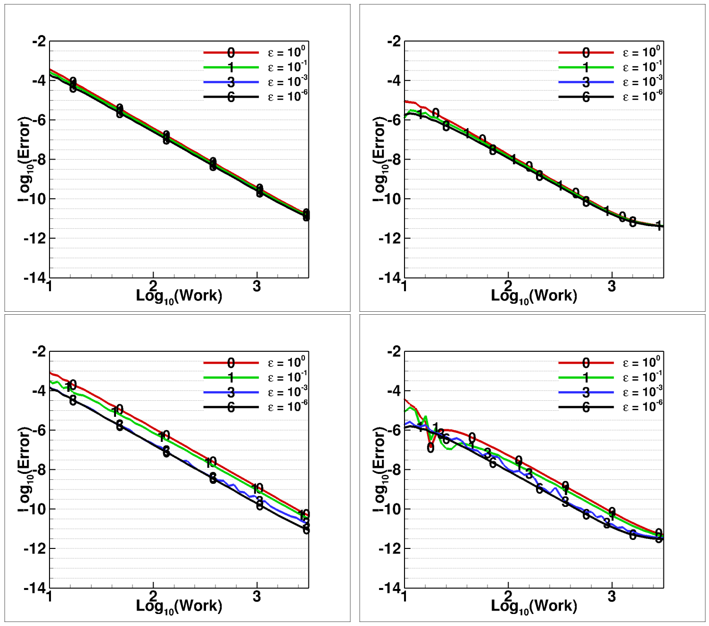

Figure 2: An error versus work comparison between ESDIRK3(2)4L[2]SA (left) and ESDIRK3(2)5L[2]SA (right) for the differential variable (top) and algebraic variable (bottom) on Kaps' problem

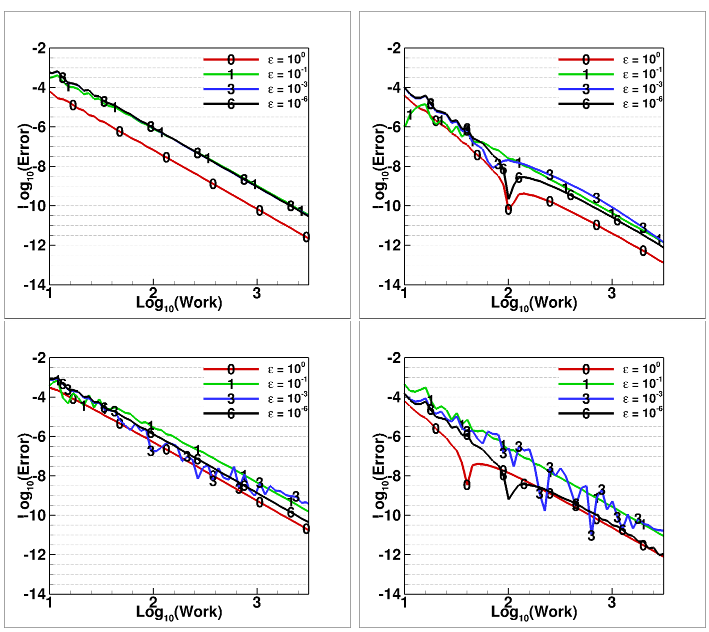

Figure 3: An error versus work comparison between ESDIRK3(2)4L[2]SA (left) and ESDIRK3(2)5L[2]SA (right) for the differential variable (top) and algebraic variable (bottom) on van der Pol's equation.

method. Besides improving iterative convergence, the method is substantially more accurate than ESDIRK4(3)6L[2]SA_2.

This and having only stage-order one likely explain the shortcomings of SDIRK4.

4 shows differences in convergence rates between SDIRK4, ESDIRK4(3)6L[2]SA$_1$ and ESDIRK4(3)7L[2]SA$_1$. Comparing the fourth-order methods using an error versus

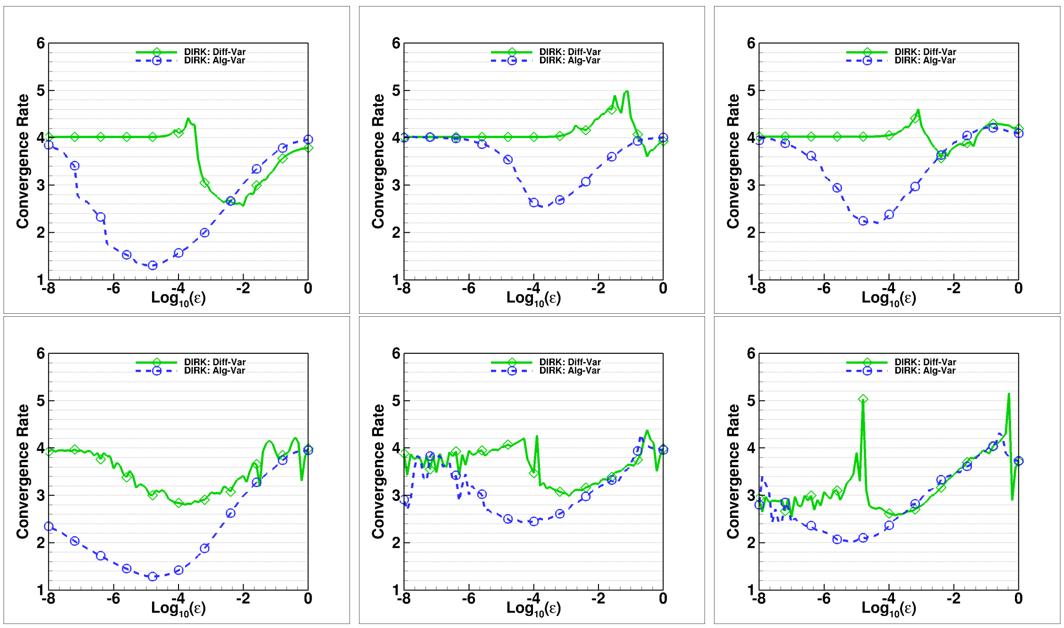

Figure 4: A convergence rate comparison between SDIRK4 (upper left), ESDIRK4(3)6L[2]SA$_1$ (upper right), ESDIRK4(3)6L[2]SA$_2$ (lower left) and ESDIRK4(3)7L[2]SA$_1$ (lower right) on Kaps' problem (top) and van der Pol's equation (bottom).

work comparison may be made at different values of the stiffness parameter with Kaps' problem. These are shown in for the differential and algebraic variables. Doing the same for the van der POl's equation, Figure 12.1.3 shows differences in convergence rates between the same three methods.

12.1.3 Fifth-Order Methods

Convergence rate testing of higher-order ESDIRKs involved three fifth-order methods: ESDIRK5(4)7L[2]SA_1, ESDIRK5(4)7L[2]SA_2 and ESDIRK5(4)8L[2]SA. Method ESDIRK5(4)7L[2]SA_1 was given in [7] but did not behave as well as had been hoped. This was likely caused by either the lack of I-stability or strong nonlinear instability on stage six. To address these issues, ESDIRK5(4)7L[2]SA_2 was created. Unlike its predecessor, it is internally I-stable on all stages and is not significantly nonlinearly unstable on any stage. Further, the leading order error was reduced by 30%. In attempt to see if adding an additional stage could improve this class of methods, ESDIRK5(4)8L[2]SA was created. It is potentially slightly more efficient than ESDIRK5(4)7L[2]SA_2 by virtue of having a reduced value of the product $\gamma(s-1)$. It also offers an L-stable embedded method and a reduced leading-order error relative to ESDIRK5(4)7L[2]SA_2. However, with strong order-reduction present, lower leading-order error is not significant.

7 shows differences in convergence rates between ESDIRK5(4)7L[2]SA$_1$, ESDIRK5(4)7L[2]SA$_2$ and ESDIRK5(4)8L[2]SA$_1$.

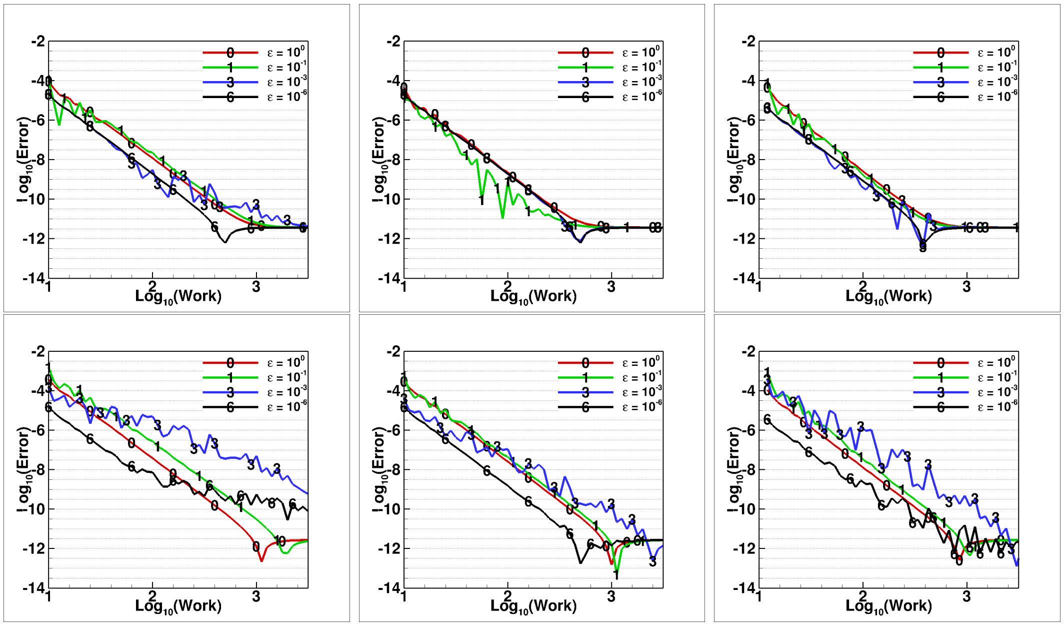

Figure 5: An error versus work comparison between SDIRK4 (left), ESDIRK4(3)6L[2]SA$_1$ (middle) and ESDIRK4(3)7L[2]SA$_1$ (right) for the differential (top) and algebraic (bottom) variable on Kaps' problem

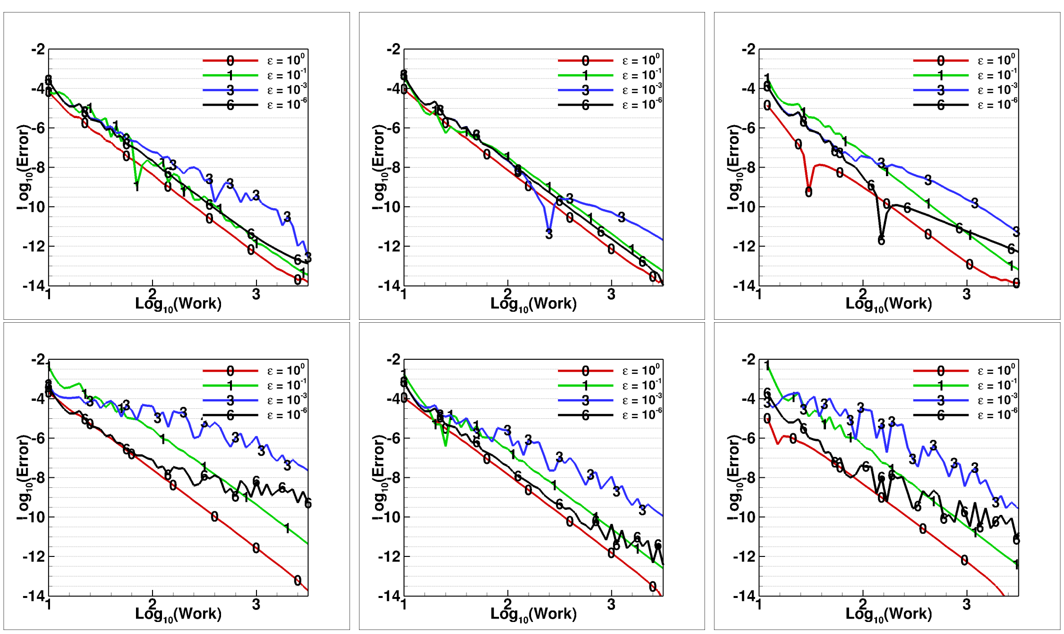

Figure 6: An error versus work comparison between SDIRK4 (upper left), ESDIRK4(3)6L[2]SA$_1$ (upper right), ESDIRK4(3)6L[2]SA$_2$ (lower left) and ESDIRK4(3)7L[2]SA$_1$ (lower right) for the differential (top) and algebraic (bottom) variable on van der Pol's equation.

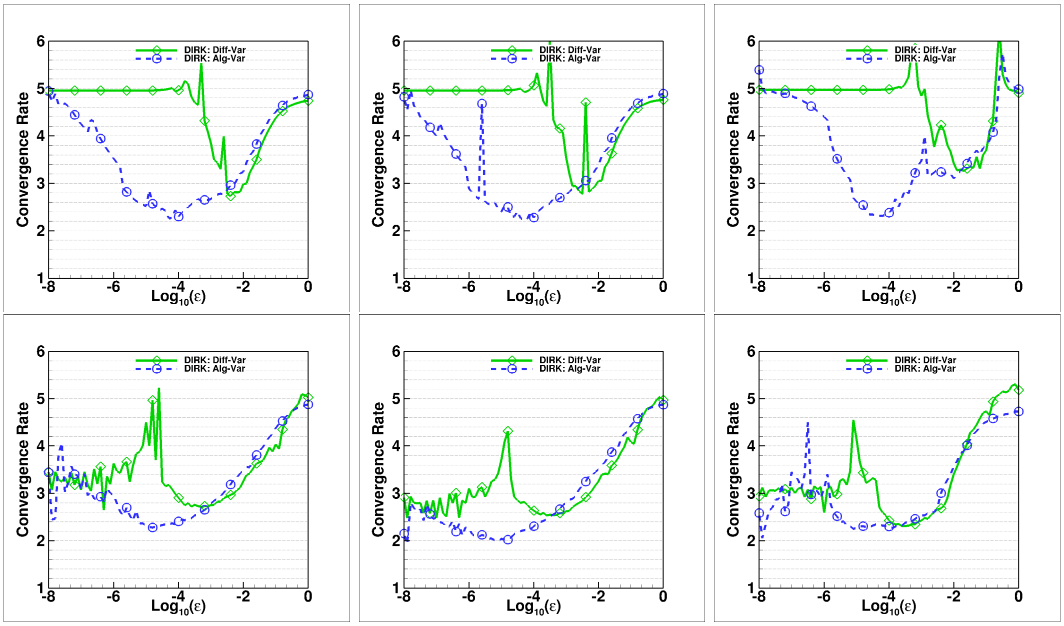

Figure 7: A convergence rate comparison between ESDIRK5(4)7L[2]SA$_1$ (left), ESDIRK5(4)7L[2]SA$_2$ (middle) and ESDIRK5(4)8L[2]SA$_1$ (right) on Kaps' problem (top) and van der Pol's equation (bottom).

Kaps' problem Alternatively, an error versus work comparison may be made between these same four methods at different values of the stiffness parameter. These are shown in for the differential and algebraic variables.

van der Pol's Equation **??** shows differences in convergence rates between ESDIRK5(4)7L[2]SA$_1$, ESDIRK5(4)7L[2]SA$_2$ and ESDIRK5(4)8L[2]SA$_1$. Alternatively, an error versus work comparison may be made between these same four methods at different values of the stiffness parameter. These are shown in for the differential and algebraic variables.

12.1.4 Sixth-Order Method

?? shows differences in convergence rates between ESDIRK6(5)9L[2]SA on Kaps' and van der Pol's Equation. Alternatively, an error versus work comparison may be made between this method at different values of the stiffness parameter. These are shown in **??** for the differential and algebraic variables, for both test equations.

13 Conclusions

This paper is based on a comprehensive review of DIRK-type methods applied to first-order ODEs but it extends the review with four new general-purpose ESDIRK methods based on lessons learned. Though it does not include a dense-output method nor stage-value predictors for these new methods, the methods were designed with these accoutrements in mind.

Based on the review of method characteristics, these methods focus on having a stage order of two, stiff accuracy, L-stability, internal L-stability, a high quality embedded

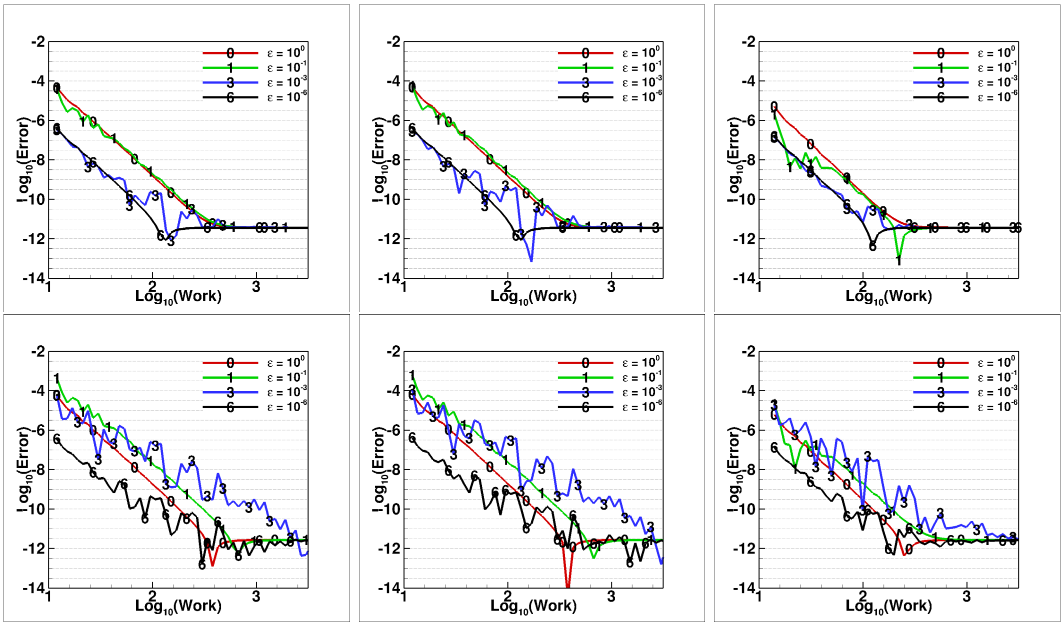

Figure 8: An error versus work comparison between ESDIRK5(4)7L[2]SA$_1$ (left), ESDIRK5(4)7L[2]SA$_2$ (middle) and ESDIRK5(4)8L[2]SA$_1$ (right) for the differential (top) and algebraic (bottom) variables on Kaps' problem.

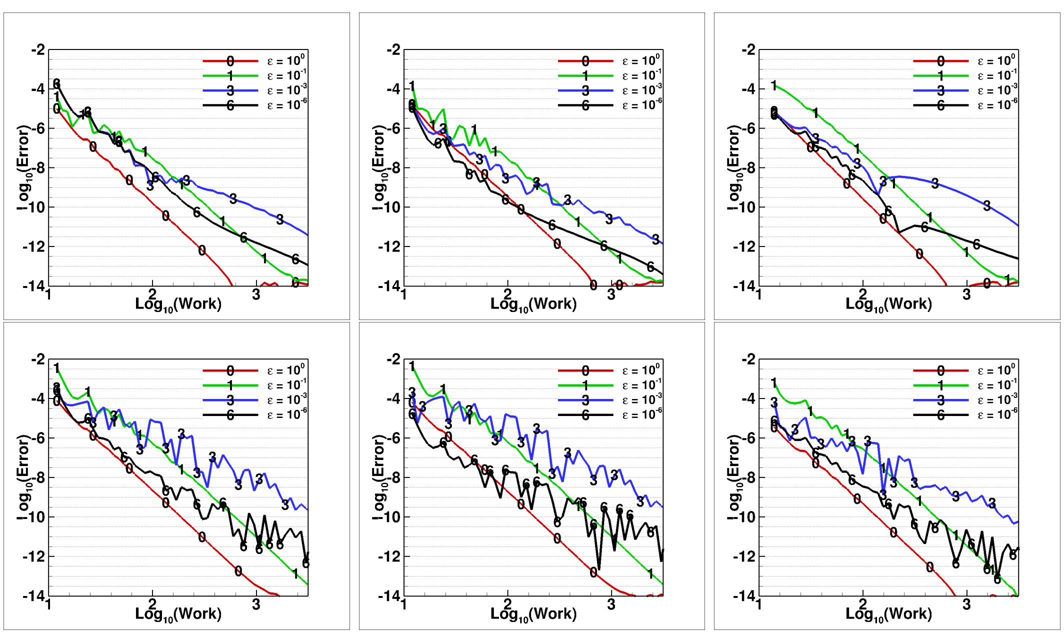

Figure 9: An error versus work comparison between ESDIRK5(4)7L[2]SA$_1$ (left), ESDIRK5(4)7L[2]SA$_2$ (middle) and ESDIRK5(4)8L[2]SA$_1$ (right) for the differential (top) and algebraic (bottom) variables on van der Pols Equation.

method, small magnitudes of the algebraic stability matrix eigenvalues, small values of a_{ii}, and small or vanishing values of the internal stability functions for large eigenvalues. These choices are also consistent with maximizing scheme efficiency. As stage-order governs the severity of order reduction, focusing on stage-order two methods facilitates accuracy.

Observed order reduction is very problem dependent. Methods exhibited little order reduction on the Pareschi and Russo problem, moderate order reduction on Kaps' problem, and severe order reduction on the vdP problem. Therefore, the choice of the optimal method is to some extent a function of the problem severity.

Users wishing to have a high quality, general purpose DIRK-type method might consider trying ESDIRK4(3)6L[2]SA, Table 7, in conjunction with the H321 or PPID error-controller, Table 5, If the problem at hand is not particularly stiff and error tolerances are sufficiently demanding then the higher-order methods could also be considered.

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A Methods

A.1 ESDIRK4(3)6L[2]SA_2

0	0	0	0	0	0	0
$\frac{62}{125}$	a_{21}	$\frac{31}{125}$	0	0	0	0
$\frac{486119545908}{3346201505189}$	a_{31}	$\frac{-360286518617}{7014585480527}$	$\frac{31}{125}$	0	0	0
$\frac{1043}{1706}$	a_{41}	$\frac{-506388693497}{5937754990171}$	$\frac{7149918333491}{13390931526268}$	$\frac{31}{125}$	0	0
$\frac{1361}{1300}$	a_{51}	$\frac{-7628305438933}{11061539393788}$	$\frac{21592626537567}{14352247503901}$	$\frac{11630056083252}{17263101053231}$	$\frac{31}{125}$	0
1	b_1	$\frac{-12917657251}{5222094901039}$	$\frac{5602338284630}{15643096342197}$	$\frac{9002339615474}{18125249312447}$	$\frac{-2420307481369}{24731958684496}$	$\frac{31}{125}$
b_i	b_1	$\frac{-12917657251}{5222094901039}$	$\frac{5602338284630}{15643096342197}$	$\frac{9002339615474}{18125249312447}$	$\frac{-2420307481369}{24731958684496}$	$\frac{31}{125}$
$\hat{b}_i$	$\hat{b}_1$	$\frac{-1007911106287}{12117826057527}$	$\frac{17694008993113}{35931961998873}$	$\frac{5816803040497}{11256217655929}$	$\frac{-538664890905}{7490061179786}$	$\frac{2032560730450}{8872919773257}$

Table 9: ESDIRK4(3)6L[2]SA_2 with $a_{i1} = a_{i2}$, $b_1 = b_2$ and $\hat{b}_1 = \hat{b}_2$.

A.2 ESDIRK4(3)7L[2]SA

0	0	0	0	0	0	0	0
$\frac{1}{4}$	a_{21}	$\frac{1}{8}$	0	0	0	0	0
$\frac{1200237871921}{16391473681546}$	a_{31}	$\frac{-39188347878}{1513744654945}$	$\frac{1}{8}$	0	0	0	0
$\frac{1}{2}$	a_{41}	$\frac{1748874742213}{5168247530883}$	$\frac{-1748874742213}{5795261096931}$	$\frac{1}{8}$	0	0	0
$\frac{395}{567}$	a_{51}	$\frac{-6429340993097}{17896796106705}$	$\frac{9711656375562}{10370074603625}$	$\frac{1137589605079}{3216875020685}$	$\frac{1}{8}$	0	0
$\frac{89}{126}$	a_{61}	$\frac{405169606099}{1734380148729}$	$\frac{-264468840649}{6105657584947}$	$\frac{118647369377}{6233854714037}$	$\frac{683008737625}{4934655825458}$	$\frac{1}{8}$	0
1	b_1	$\frac{-5649241495537}{14093099002237}$	$\frac{5718691255176}{6089204655961}$	$\frac{2199600963556}{4241893152925}$	$\frac{8860614275765}{11425531467341}$	$\frac{-3696041814078}{6641566663007}$	$\frac{1}{8}$
b_i	b_1	$\frac{-5649241495537}{14093099002237}$	$\frac{5718691255176}{6089204655961}$	$\frac{2199600963556}{4241893152925}$	$\frac{8860614275765}{11425531467341}$	$\frac{-3696041814078}{6641566663007}$	$\frac{1}{8}$
$\hat{b}_i$	$\hat{b}_1$	$\frac{-1517409284625}{6267517876163}$	$\frac{8291371032348}{12587291883523}$	$\frac{5328310281212}{10646448185159}$	$\frac{5405006853541}{7104492075037}$	$\frac{-4254786582061}{7445269677723}$	$\frac{19}{140}$

Table 10: ESDIRK4(3)7L[2]SA with $a_{i1} = a_{i2}$, $b_1 = b_2$ and $\hat{b}_1 = \hat{b}_2$.

A.3 ESDIRK5(4)7L[2]SA_2

0	0	0	0	0	0	0	0
$\frac{46}{125}$	a_{21}	$\frac{23}{125}$	0	0	0	0	0
$\frac{7121331996143}{11335814405378}$	a_{31}	$\frac{791020047304}{3561426431547}$	$\frac{23}{125}$	0	0	0	0
$\frac{49}{353}$	a_{41}	$\frac{-158159076358}{11257294102345}$	$\frac{-85517644447}{5003708988389}$	$\frac{23}{125}$	0	0	0
$\frac{3706679970760}{5295570149437}$	a_{51}	$\frac{-1653327111580}{4048416487981}$	$\frac{1514767744496}{9099671765375}$	$\frac{14283835447591}{12247432691556}$	$\frac{23}{125}$	0	0
$\frac{347}{382}$	a_{61}	$\frac{-4540011970825}{8418487046959}$	$\frac{-1790937573418}{7393406387169}$	$\frac{10819093665085}{7266595846747}$	$\frac{4109463131231}{7386972500302}$	$\frac{23}{125}$	0
1	b_1	$\frac{-188593204321}{4778616380481}$	$\frac{2809310203510}{10304234040467}$	$\frac{1021729336898}{2364210264653}$	$\frac{870612361811}{2470410392208}$	$\frac{-1307970675534}{8059683598661}$	$\frac{23}{125}$
b_i	b_1	$\frac{-188593204321}{4778616380481}$	$\frac{2809310203510}{10304234040467}$	$\frac{1021729336898}{2364210264653}$	$\frac{870612361811}{2470410392208}$	$\frac{-1307970675534}{8059683598661}$	$\frac{23}{125}$
$\hat{b}_i$	$\hat{b}_1$	$\frac{-582099335757}{7214068459310}$	$\frac{615023338567}{3362626566945}$	$\frac{3192122436311}{6174152374399}$	$\frac{6156034052041}{14430468657929}$	$\frac{-1011318518279}{9693750372484}$	$\frac{1914490192573}{13754262428401}$

Table 11: ESDIRK4(3)7L[2]SA_2 with $a_{i1} = a_{i2}$, $b_1 = b_2$ and $\hat{b}_1 = \hat{b}_2$.

A.4 ESDIRK5(4)8L[2]SA

0	0	0	0	0	0	0	0	0
$\frac{2}{7}$	a_{21}	$\frac{1}{7}$	0	0	0	0	0	0
c_3	a_{31}	$\frac{1521428834970}{8822750406821}$	$\frac{1}{7}$	0	0	0	0	0
$\frac{150}{203}$	a_{41}	$\frac{5338711108027}{29869763600956}$	$\frac{1483184435021}{6216373359362}$	$\frac{1}{7}$	0	0	0	0
$\frac{27}{46}$	a_{51}	$\frac{2264935805846}{12599242299355}$	$\frac{1330937762090}{13140498839569}$	$\frac{-287786842865}{17211061626069}$	$\frac{1}{7}$	0	0	0
$\frac{473}{532}$	a_{61}	$\frac{118352937080}{527276862197}$	$\frac{-2960446233093}{7419588050389}$	$\frac{-3064256220847}{46575910191280}$	$\frac{6010467311487}{7886573591137}$	$\frac{1}{7}$	0	0
$\frac{30}{83}$	a_{71}	$\frac{1134270183919}{9703695183946}$	$\frac{4862384331311}{10104465681802}$	$\frac{1127469817207}{2459314315538}$	$\frac{-9518066423555}{11243131997224}$	$\frac{-811155580665}{7490894181109}$	$\frac{1}{7}$	0
1	b_1	$\frac{2162042939093}{22873479087181}$	$\frac{-4222515349147}{9397994281350}$	$\frac{3431955516634}{4748630552535}$	$\frac{-374165068070}{9085231819471}$	$\frac{-1847934966618}{8254951855109}$	$\frac{5186241678079}{7861334770480}$	$\frac{1}{7}$
b_i	b_1	$\frac{2162042939093}{22873479087181}$	$\frac{-4222515349147}{9397994281350}$	$\frac{3431955516634}{4748630552535}$	$\frac{-374165068070}{9085231819471}$	$\frac{-1847934966618}{8254951855109}$	$\frac{5186241678079}{7861334770480}$	$\frac{1}{7}$
$\hat{b}_i$	$\hat{b}_1$	$\frac{701879993119}{7084679725724}$	$\frac{-8461269287478}{14654112271769}$	$\frac{6612459227430}{11388259134383}$	$\frac{2632441606103}{12598871370240}$	$\frac{-2147694411931}{10286892713802}$	$\frac{4103061625716}{6371697724583}$	$\frac{4103061625716}{6371697724583}$

Table 12: ESDIRK5(4)8[2]SA with $a_{i1} = a_{i2}$, $b_1 = b_2$, $\hat{b}_1 = \hat{b}_2$ and $c_3 = \frac{5779892736881}{11850239716711}$.

A.5 ESDIRK6(5)9L[2]SA

The remaining coefficients of the ESDIRK6(5)9[2]SA method are

$$
\begin{aligned}
a_{87} &= \frac{339987959782520}{552150039467091}, \qquad b_7 = \frac{127306093275639}{658941305589808}, \qquad b_8 = \frac{-319515475352107}{658842144391777} \\
\hat{b}_7 &= \frac{2013538191006793}{972919262949000}, \qquad \hat{b}_8 = \frac{352681731710820}{726444701718347}, \qquad \hat{b}_9 = \frac{-12107714797721}{746708658438760} \\
c_3 &= \frac{376327483029687}{1335600577485745}, \qquad c_4 = \frac{433625707911282}{850513180247701}, \qquad c_6 = \frac{62409086037595}{296036819031271}
\end{aligned}
$$

0	0	0	0	0	0	0	0	0	0
$\frac{4}{9}$	$\frac{2}{9}$	$\frac{2}{9}$	0	0	0	0	0	0	0
c_3	$\frac{1}{9}$	$\frac{-52295652026801}{1014133226193379}$	$\frac{2}{9}$	0	0	0	0	0	0
c_4	$\frac{37633260247889}{456511413219805}$	$\frac{-162541608159785}{642690962402252}$	$\frac{186915148640310}{408032288622937}$	$\frac{2}{9}$	0	0	0	0	0
$\frac{183}{200}$	$\frac{-37161579357179}{532208945751958}$	$\frac{-211140841282847}{266150973773621}$	$\frac{884359688045285}{894827558443789}$	$\frac{845261567597837}{1489150009616527}$	$\frac{2}{9}$	0	0	0	0
c_6	$\frac{32386175866773}{281337331200713}$	$\frac{498042629717897}{1553069719539220}$	$\frac{-73718535152787}{262520491717733}$	$\frac{-147656452213061}{931530156064788}$	$\frac{-16605385309793}{2106054502776008}$	$\frac{2}{9}$	0	0	0
c_7	$\frac{-38317091100349}{1495803980405525}$	$\frac{233542892858682}{880478953581929}$	$\frac{-281992829959331}{709729395317651}$	$\frac{-52133614094227}{895217507304839}$	$\frac{-9321507955616}{673810579175161}$	$\frac{79481371174259}{817241804646218}$	$\frac{2}{9}$	0	0
$\frac{97}{100}$	$\frac{-486324380411713}{1453057025607868}$	$\frac{-1085539098090580}{1176943702490991}$	$\frac{370161554881539}{461122320759884}$	$\frac{804017943088158}{886363045286999}$	$\frac{-15204170533868}{934878849212545}$	$\frac{-248215443403879}{815097869999138}$	a_{87}	$\frac{2}{9}$	0
1	0	0	0	$\frac{281246836687281}{672805784366875}$	$\frac{250674029546725}{464056298040646}$	$\frac{88917245119922}{798581755375683}$	b_7	b_8	$\frac{2}{9}$
b_i	0	0	0	$\frac{281246836687281}{672805784366875}$	$\frac{250674029546725}{464056298040646}$	$\frac{88917245119922}{798581755375683}$	b_7	b_8	$\frac{2}{9}$
$\hat{b}_i$	$\frac{-204006714482445}{253120897457864}$	0	$\frac{-818062434310719}{743038324242217}$	$\frac{1376520686137389}{1064235527052079}$	$\frac{-574817982095666}{1374329821545869}$	$\frac{-507643245828272}{1001056758847831}$	$\hat{b}_7$	$\hat{b}_8$	$\hat{b}_9$

Table 13: ESDIRK6(5)9[2]SA

$$c_7 = \frac{81796628710131}{911762868125288}$$