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Singly-Implicit Runge–Kutta Methods for Stiff, Ordinary Differential-Equations

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Abstract

Singly-Implicit Runge–Kutta (SIRK) methods are designed for integrating systems of stiff, first-order ordinary differential equations (ODEs). The accuracy and stability properties of the new SIRKs are similar to those of the Radau IIA methods, at potentially reduced implementation costs. Nine stiffly-accurate, L-stable and internally L-stable SIRK methods, having stage-orders three or four, with step-orders three through six are given, each with an embedded method. A stage-order five method is included as well. The accuracies of the new SIRKs and Radau IIA methods, are compared on three singular perturbation problems. Order reduction of the SIRKs is generally minimal and they perform nearly as well as Radau IIA methods. There is evidence that SIRKs can be implemented at costs commensurate with diagonally implicit methods (i.e, DIRK/SDIRK/ESDIRK), making them highly competitive integrators. Efficient implementation of SIRKs at scale however, will not be reported herein.

Keywords

Singly-Implicit Runge–Kutta (SIRK), Multiply-Implicit Runge–Kutta (MIRK), Fully-Implicit Runge–Kutta (FIRK), Radau, Gauss and Lobatto Methods, Stiffness, Stage-Order, Algebraic-, Internal- and L-Stability, van der Pol's equation, Kaps' equation. Kreiss' problem

Contents

1 Introduction

It is generally accepted that a Runge–Kutta method intended for the integration of stiff, first-order, ordinary differential equations (ODEs) should be at least A-stable and have the highest stage-order possible. Even better, the method should be L-stable, stiffly-accurate and algebraically stable. Properties of the stages matter as well as those of the step. Hence, we would like internal L-stability and internal algebraic-stability. Such a method would then be well-suited to not only stiff ODEs but also to differential-algebraic equations (DAEs).

Among the many choices of implicit Runge–Kutta methods suited to solving stiff ODEs, two disparate classes of methods are commonly employed: Diagonally implicit Runge–Kutta (DIRK) [3, 15, 55, 100, 117–119] and fully implicit Runge–Kutta (FIRK) methods [51, 74, 102] such as the Gauss, Radau and Lobatto families of methods. While both classes include members which are both L-stable and stiffly-accurate, they differ substantially in their ability to attain high stage-order and their cost of implementation. DIRK methods can have a stage-order no greater than two but have relatively low implementation costs. Within the FIRK class, the s-stage Radau IIA offers stage-order s members with, additionally, algebraic stability but does so with relatively high implementation costs. Our goal is in the paper is simple. We wish to find high stage-order, implicit Runge–Kutta methods, for application to stiff ODEs, with properties approaching certain FIRKs but with the implementation costs approaching that of DIRKs. While such a goal is neither original nor completely realistic, it may be possible to nearly reach the goal. To keep the scope of this discussion manageable, no recourse will be made to the broader class of methods which also include a multistep or multiderivative character. There are three principal steps required to reach our goal. First, method classes need to be identified and then actual methods need to be designed which reasonably match those of FIRK methods in terms of stage-order, linear-, internal and nonlinear stability, leading-order error and coefficient magnitudes. The new methods must also include high-quality embedded methods and readily permit the construction of high-quality dense-output and stage-prediction methods. Next, these methods should be tested on severe test problems to confirm that they do indeed resemble FIRKs in terms of accuracy and stability. Succeeding at the first two steps, the third step is to demonstrate that these new methods are, in fact, less expensive to implement than FIRK methods of similar stage-order. In this paper, we will address the first two goals as well as develop high-quality embedded methods for all new SIRKs. Developing dense-output, stage-value predictors as well as demonstrating the efficacy of the new methods on large scale problems are all large undertakings and will be forsaken herein.

The challenge to making implicit Runge–Kutta methods with a stage-order of greater than two is that the $\mathbf{A}$-matrix, using real coefficients, must necessarily have nonzero coefficients in the upper-triangular region of the matrix. This immediately drives up implementation costs relative to DIRKs. Hence, we seek a class of methods which, effectively, mask the fullness of the $\mathbf{A}$-matrix while simultaneously permitting high stage-order and good stability properties. There have been two general approaches to this challenge of which we are aware.

The first approach is to create methods which are akin to DIRKs with positive and real eigenvalues to the $\mathbf{A}$-matrix. Eigenvalues can be identical (singly implicit) or different (multiply implicit). Whereas the $\mathbf{A}$-matrix with DIRK and SDIRK methods are lower triangular so that the eigenvalues reside on the diagonal, this related class of methods recasts the $\mathbf{A}$-matrix using a Jordan similarity transformation as [29]

$$\mathbf{A} = \mathbf{S}\mathcal{J}\mathbf{S}^{-1}, \qquad \mathcal{J} = \mathbf{S}^{-1}\mathbf{A}\mathbf{S}, \qquad (\lambda\mathbf{I} - \mathbf{A}) = \mathbf{S}\left(\lambda\mathbf{I} - \mathcal{J}\right)\mathbf{S}^{-1}, \tag{1}$$

where $\mathcal{J}$ is the upper bidiagonal Jordan canonical form of the $\mathbf{A}$-matrix,

$$\mathcal{J} \;=\; \begin{bmatrix} \lambda_1 & 1 & \cdots & 0 & 0 \\ 0 & \lambda_2 & \ddots & 0 & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & \ddots & \lambda_{s-1} & 1 \\ 0 & 0 & \cdots & 0 & \lambda_s \end{bmatrix}, \tag{2}$$

and the diagonal entries to $\mathcal{J}$ are the eigenvalues of the $\mathbf{A}$-matrix. Alternatively, it may be preferable to recast the $\mathbf{A}$-matrix using a Schur decomposition rather than using the Jordan canonical form. To do this, one writes [7]

$$\mathbf{A} = \mathcal{Q}\mathcal{U}\mathcal{Q}^T \tag{3}$$

where $\mathcal{Q}$ is an orthogonal matrix (i.e., $\mathcal{Q}\mathcal{Q}^T = \mathbf{I}$) and $\mathcal{U}$ is an upper triangular matrix with the diagonal entries being the eigenvalues of the $\mathbf{A}$-matrix. If all eigenvalues are the same, the method is referred to as a singly-implicit Runge–Kutta (SIRK) method, akin to an SDIRK method [17, 18, 22, 29, 31, 36, 48, 51, 67, 74, 94, 102, 142, 147]. If not, the method is referred to as a multiply-implicit Runge–Kutta (MIRK) method [6, 9–11, 13, 115, 116, 143–145, 149–151], akin to a DIRK method. As pointed out by Bendtsen [9], a key challenge with SIRK (and MIRK) methods is the potential for $\mathbf{A}$-matrices having large condition numbers. He states that methods with more than nine stages are effectively infeasible.

SIRK methods are a natural generalization of SDIRK methods. The methods first appeared in the works of Butcher [29, 31] and Nørsett [142] and were followed by Burrage [17, 18, 22, 147]. Many of the early SIRK methods were considered as collocation methods where the stage-order of the method was at least equal to the number of stages and the abscissae were distinct. Additional discussions of SIRK methods are found elsewhere [36, 48, 51, 67, 74, 102]. From an applications perspective, SIRKs have been used in Finite-Element Analysis (FEA) [2, 86, 132, 133]. They have also been studied in the context of other partial differential equations [134, 177]. An approximate matrix factorization technique applied to FIRK, DIRK and SIRK methods appears in the work of González-Pinto [94].

Besides ODEs, SIRK methods have been applied to DAEs [40,141] and Delay-Differential Equations (DDEs) [5,35,69,121,122], as well as for second-order ODEs in [188]. The creation of symplectic methods has been considered [108,188]. Early comparisons between the performance of SIRK methods with other classes of methods appear in Addison [1] and Gaffney [87]. Both studies used SIRK methods from the STRIDE code, discussed in Appendix E.

Within the SIRK and MIRK classes of methods are the following generalizations; diagonally extended SIRK (DESI) methods [34, 37, 45, 67, 77, 78, 163], diagonally extended, effective-order SIRK (DESIRE) methods [39, 42, 47, 67, 77], SIRK methods satisfying effective (E) order-conditions [41, 43, 44, 46, 47, 49, 65–67] and those SIRKs with an explicit (e) first-stage [45]. Many of these generalizations have been created, in part, to deal with abscissae which might otherwise extend outside of the present step when high-stage order methods are generated. It should be mentioned that SIRK methods have been extended into the broader class of general linear methods [23, 24, 32, 70, 160]. Not all implicit Runge–Kutta methods with only real eigenvalues are intended for stiff systems. Liu and Sun [125] derive symplectic methods and partitioned symmetric methods.

A second approach to producing high stage-order IRKs with potentially reduced implementation costs is to consider the class of parameterized implicit Runge–Kutta (PIRK) methods described by Muir and Enright [135]. They may be written as

$$\mathbf{U}^{[n+1]} = \mathbf{U}^{[n]} + (\Delta t)\sum_{i=1}^{s} b_i \mathbf{F}_i(\mathbf{U}), \qquad \mathbf{U}_i = (1-\gamma_i)\mathbf{U}^{[n]} + \gamma_i \mathbf{U}^{[n+1]} + (\Delta t)\sum_{j=1}^{s} x_{ij}\mathbf{F}_j(\mathbf{U}), \tag{4}$$

where the parameter, γ_i, should not be confused with the diagonal coefficient (DIRKs and SDIRKs) or eigenvalues seen in SIRKs or MIRKs. If the $\mathbf{X}$-matrix, x_{ij}, is taken to be strictly lower triangular, then one has mono-implicit Runge–Kutta methods [14, 25, 54, 56–62, 76, 79, 81, 84, 96, 135–138, 158, 169–174, 181, 182, 187]. This class of methods readily supports a stage-order of three and has found most of its applications in boundary value ODE's. Relatively less work has been done of mono-implicit Runge–Kutta methods for initial value problems. For better properties, $\mathbf{X}$-matrix may be considered as lower-triangular rather than strictly lower-triangular. However, the implementation costs rise considerably. Taking mono-implicit Runge–Kutta methods further, Dow [81] considers a generalized class of mono-implicit Runge–Kutta methods where the $\mathbf{X}$-matrix is no longer lower triangular. In this paper, we reserve the acronym MIRK exclusively for multiply-implicit Runge–Kutta methods and not mono-implicit Runge–Kutta methods. In general, besides making such a (mono-implicit Runge–Kutta) method with stiff-accuracy, L-stability and high stage-order, one must create an iteration matrix that keeps the implementation costs competitive. The difficulty in doing this suggests that SIRK methods are likely the better candidates to compete with FIRK methods, not mono-implicit Runge–Kutta methods.

To facilitate an informed comparison of the new SIRK methods to the broad class of FIRK methods, Appendix D gives a comprehensive listing of the properties to 15 distinct FIRK methods: one Gauss method, six Radau methods and eight Lobatto methods. From this, we infer that the Radau IIA class of methods is arguably the gold-standard for stiff integrators using FIRKs. Other choices exist for high stage-order implicit Runge–Kutta (IRK) methods. In Appendix E, the properties of SIRK methods from the STRIDE code [17, 18, 31], DESI methods [34, 37, 45, 67, 77, 78, 163] and MIRK methods [9, 10, 12, 13] are reviewed. However, none of these methods are included in our testing.

In contrast to older studies of SIRKs methods, we do not consider SIRKs as collocation methods. Further, an important distinction between this work and many recent efforts studying SIRK methods is that we do not set any coefficients in the $\mathbf{A}$-matrix to zero. We forsake algebraic stability in favor of near algebraic-stability but we require internal L-stability to, among other things, facilitate better performance of future stage-value predictors.

Embracing SIRK methods as a competitive alternative to DIRKs and FIRKs, Appendix F provides a high-level overview of their implementation on realistic systems of ODEs derived from an aeronautical engineering setting. (Large-Eddy Simulations of the equations of fluid mechanics, routinely require linear- and nonlinear solver mechanics on systems of dimension in excess of 10^{10}.) Although sophisticated solvers are not necessary for the small canonical test cases studied herein, they are essential in large-scale applications when dealing with Newton, quasi-Newton, or Newton-Krylov iterative methods. Of particular importance is the construction of the preconditioner needed to efficiently solve the linear systems. Appendix F provides a terse derivation of a typical preconditioner used for SIRK methods and motivates our assertion that the implementation cost of SIRKs will exceed that of DIRK methods of similar step-order by only a small factor. The similarity in implementation cost derives from the fact that both approaches require only one preconditioner per timestep, used effectively on all stages. As compared with FIRKs, SIRKs don't suffer the complications of contending with complex eigenvalues in the $\mathbf{A}$-matrix. Among the many different approaches used to implement FIRKs, most rely on building a distinct preconditioner for each stage of the method, or building one preconditioner and hoping that it will effectively precondition all stages. Although superconvergent FIRKs typically require substantially fewer stages as DIRKs or SIRKs of comparable order or stage-order, they must contend with the complications arising for complex conjugate eigen-pairs. Often a locally coupled iteration for each eigen-pair is required, which effectively increases the cost of that stage by more than a factor two.

Sections 1 and 2 will provide an introduction and background to implicit Runge–Kutta methods. Methods ranging from third-order to sixth-order and stage-orders three to five will be designed in Section 3. Three singular-perturbation test problems are described in section 4. They are Kaps' problem, van der Pol's (vdP) equation and Kreiss's problem. The latter problem is included because it has proven to be very challenging [179] as well as to get a sense of how the new SIRK methods might perform, relative to Radau IIA methods, on index-2 DAEs where the differential variable is stiff. Such a situation occurs when solving the Navier-Stokes equations for an incompressible fluid where stiffness is caused by the grid and turbulence models. However, to properly test methods for index-2 equations, one might consider the modified Kaps' problem [38, 154] instead as Kreiss' problem which is only an index-2 DAE at $\varepsilon = 0$.

Merits of the implicit schemes are discussed in Section 5 and comparisons are made with existing implicit Runge–Kutta (IRK) methods. We do not focus on optimal implementations nor do we seek to determine which error-controller is best for these SIRK methods. In Section 6, conclusions are drawn as to the utility of the various schemes. Appropriate appendices are also included. All new methods presented in this study were solved completely using Mathematica™, Version 13 [186]. Coefficients of the new SIRK schemes, including the $\mathbf{S}$, $\mathbf{S}^{-1}$, $\mathcal{Q}$ and $\mathcal{U}$ matrices are provided to at least 25 digits of accuracy in Appendix A. A derivation as well as scheme coefficients for the only ESDIRK created in this paper are shown in Appendix B. Appendix C contains the simplified order conditions to order eight and Appendix D presents a review of FIRK method properties. Lastly, Appendix E gives the gross properties of several SIRK (from the STRIDE code), DESI and MIRK methods from the literature.

Several supplementary files are included with this paper. Fifteen files are included which contain the coefficients to the 15 Gauss, Radau and Lobatto methods discussed in Appendix D up to 30 stages.

2 Background

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

$$\frac{d\mathbf{U}}{dt} = \mathbf{F}(t, \mathbf{U}(t)), \qquad \mathbf{U}(a) = \mathbf{U}_0, \qquad t \in [a, b], \tag{5}$$

and are applied over s-stages as

$$\left.\begin{array}{lll} \mathbf{F}_i = \mathbf{F}(t_i, \mathbf{U}_i), & \mathbf{U}_i = \mathbf{U}^{[n]} + (\Delta t)\sum_{j=1}^{s} a_{ij}\mathbf{F}_j, & t_i = t^{[n]} + c_i\Delta t, \\ \mathbf{U}^{[n+1]} = \mathbf{U}^{[n]} + (\Delta t)\sum_{i=1}^{s} b_i\mathbf{F}_i, & \hat{\mathbf{U}}^{[n+1]} = \mathbf{U}^{[n]} + (\Delta t)\sum_{i=1}^{s} \hat{b}_i\mathbf{F}_i. & \end{array}\right\} \tag{6}$$

where $i = 1, 2, \cdots, s$, $\mathbf{F}_i = \mathbf{F}_i^{[n]} = \mathbf{F}(\mathbf{U}_i, t^{[n]} + c_i\Delta t)$. Also, $\Delta t > 0$ is the step-size, $\mathbf{U}^{[n]} \simeq \mathbf{U}(t^{[n]})$ is the value of the $\mathbf{U}$-vector at time step n, $\mathbf{U}_i = \mathbf{U}_i^{[n]} \simeq \mathbf{U}\left(t^{[n]} + c_i\Delta t\right)$ is the value of the $\mathbf{U}$-vector on the ith-stage, and $\mathbf{U}^{[n+1]} \simeq \mathbf{U}(t^{[n]} + \Delta t)$. Both $\mathbf{U}^{[n]}$ and $\mathbf{U}^{[n+1]}$ are of classical order p. The $\mathbf{U}$-vector associated with the embedded scheme, $\hat{\mathbf{U}}^{[n+1]}$, 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.

The stiffly-accurate, ($a_{sj} = b_j, j = 1, 2, \ldots, s$), SIRK methods considered in this paper are given by the general structure

$$
\begin{array}{c|c}
\mathbf{c}^T & \mathbf{A} \\
\hline
 & \mathbf{b}^T \\
\hline
 & \hat{\mathbf{b}}^T
\end{array}
=
\begin{array}{c|ccccc}
c_1 & a_{11} & a_{12} & \cdots & a_{1,s-1} & a_{1,s} \\
c_2 & a_{21} & a_{22} & \cdots & a_{2,s-1} & a_{2,s} \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
c_{s-1} & a_{s-1,1} & a_{s-1,2} & \cdots & a_{s-1,s-1} & a_{s-1,s} \\
1 & b_1 & b_2 & \cdots & b_{s-1} & b_s \\
\hline
 & b_1 & b_2 & \cdots & b_{s-1} & b_s \\
\hline
 & \hat{b}_1 & \hat{b}_2 & \cdots & \hat{b}_{s-1} & \hat{b}_s,
\end{array}
\tag{7}
$$

To identify certain schemes derived in this paper, they will be named

$$
\mathrm{SIRK}p(\hat{p})sS[\mathsf{q}]X\_x, \tag{8}
$$

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.

2.1 Order Conditions

Expressions for the equations of condition or truncation error coefficients for ODEs, $\tau_j^{(p)}$, associated with the order-p trees are of the form [51, 100, 102]

$$
\begin{aligned}
\tau_j^{(p)} &= \frac{1}{\sigma}\Phi_j^{(p)} - \frac{\alpha}{p!} = \frac{1}{\sigma}\left(\Phi_j^{(p)} - \frac{1}{\gamma}\right), \ p = 1, 2, \cdots, \ j = 1, 2, \cdots, \mathsf{a}_p, && (9) \\
\Phi_j^{(p)} &= \sum_{i=1}^{s} b_i \Phi_{i,j}^{(p)}, \quad \alpha\sigma\gamma = p! && (10)
\end{aligned}
$$

where $\mathsf{a}_p = \{1, 1, 2, 4, 9, 20, 48, 115, 286, 719\}$ for $p = \{1, 2, 3, 4, 5, 6, 7, 8, 9, 10\}$. Also, $\alpha = \alpha(t)$, $\rho = \rho(t)$ and $\gamma = \gamma(t)$ are, respectively, the cardinality, the order and the symmetry of the particular tree, $t = t_j^{(p)}$, which represents the order condition. The elementary weights, $\Phi_{i,j}^{(p)}$ and $\Phi_j^{(p)}$, 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. Simplified order conditions are given in Appendix C where they are couched in the terminology of section 2.1.2.

The local truncation error of a Runge–Kutta method is given by [30, 155],

$$
\mathbf{U}\left(t^{[n]} + (\Delta t)\right) - \mathbf{U}^{[n+1]} = \sum_{i=1}^{\infty} (\Delta t)^i \sum_{j=1}^{\mathsf{a}_i} \tau_j^{(i)} \mathcal{F}_j^{(i)}\left(U^{[n]}\right). \tag{11}
$$

where $\mathcal{F}_j^{(i)}(\mathbf{U}) = \mathcal{F}_j^{(i)}$ are elementary differentials associated with $\mathbf{F}(\mathbf{U}(t))$. A Runge–Kutta method is said to be of order p if the local truncation error satisfies

$$
\mathbf{U}^{[n]} - \mathbf{U}(t^{[n]}) = \mathcal{O}\left((\Delta t)^{p+1}\right), \tag{12}
$$

A phase-lag analysis [117, 120] of SIRK methods is not considered in this paper.

2.1.1 Error

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

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

For single-step, embedded schemes where $\hat{p} = p - 1$, additional definitions are useful such as

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

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

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 $p + 1$. In explicit Runge–Kutta methods, where order reduction is not a concern, $B^{(\hat{p}+2)}$, $C^{(\hat{p}+2)}$ and $D^{(\hat{p}+2)}$ should each be close to 1.0. For SIRK methods where the order of the method, p, is no greater than the stage-order plus two, we expect these criteria to also be sensible.

2.1.2 Simplifying Assumptions

Simplifying assumptions are often made to facilitate the solution of Runge–Kutta order conditions, $\tau_j^{(p)}$, and possibly to enforce other desirable method characteristics such as higher stage-order. The two used in this study are [51, 102]

$$B(p): \qquad \sum_{j=1}^{s} b_i c_i^{k-1} = \frac{1}{k}, \quad k = 1, ..., p, \tag{16}$$

$$C(\eta): \qquad \sum_{j=1}^{s} a_{ij} c_j^{k-1} = \frac{c_i^k}{k}. \quad k = 1, ..., \eta. \tag{17}$$

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. The stage-order of a Runge–Kutta method, which we denote with the symbol $\mathfrak{q}$ 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 $\mathbf{U}$-vector, $\mathbf{U}_i$, and equals the lowest order amongst all stages. Closely related to assumption $B(p)$, $p^{(k)}$ is defined as

$$p^{(k)} = \mathbf{b}^T \mathbf{C}^{k-1}\mathbf{e} - \frac{1}{k} = \tau_1^k (k-1)!, \tag{18}$$

where $\mathbf{C} = \text{diag}(\mathbf{c})$, $\mathbf{e} = \{1, 1, \cdots, 1\}^T$ and $\mathbf{Ce} = \mathbf{c}$. Powers of the vector $\mathbf{c}$ or the matrix $\mathbf{A}$ should be interpreted as componentwise multiplication. Similarly, $\mathbf{q}^{(k)}$ is closely related to assumption $C(\eta)$,

$$\mathbf{q}^{(k)} = \mathbf{AC}^{k-1}\mathbf{e} - \frac{1}{k}\mathbf{C}^k\mathbf{e}, \qquad \mathbf{q}^{(1)} = \mathbf{Ae} - \mathbf{c}, \qquad \text{Diag}\left(\mathbf{q}^{(k)}\right) = \mathbf{Q}^{(k)}, \tag{19}$$

where $\mathbf{q}^{(1)} = \mathbf{0}$ is simply the row-sum condition. Further discussion on the application of the row-simplifying assumption, in the form of $\mathbf{q}^{(k)}$, is provided in Appendix C.

2.2 Stability

2.2.1 Linear Stability

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

$$R(z) = \frac{P(z)}{Q(z)} = \frac{\sum_{i=1}^{s} p_i z^i}{\sum_{i=1}^{s} q_i z^i} = \frac{\mathrm{Det}\left[\mathbf{I} - z\mathbf{A} + z\mathbf{e} \otimes \mathbf{b}^T\right]}{\mathrm{Det}\left[\mathbf{I} - z\mathbf{A}\right]} = 1 + z\mathbf{b}^T \left[\mathbf{I} - z\mathbf{A}\right]^{-1} \mathbf{e}, \tag{20}$$

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 $\mathbf{b}$ in (20) with $\hat{\mathbf{b}}$ and $\mathbf{b}(\theta)$, respectively. For SIRK and MIRK methods, respectively

$$Q(z)_{\mathrm{SIRK}} = (1 - \gamma z)^s, \qquad Q(z)_{\mathrm{MIRK}} = \prod_{i=1}^{s} (1 - \gamma_i z). \tag{21}$$

The relationship between SIRKs and MIRKs is analogous to the relationship between SDIRKs and DIRKs, respectively.

During the design of various SIRK methods, we will often impose $p_k = 0$ for a particular value of k where, again,

$$P(z) = \sum_{i=1}^{s} p_i z^i = \mathrm{Det}\left[\mathbf{I} - z\mathbf{A} + z\mathbf{e} \otimes \mathbf{b}^T\right], \qquad \hat{P}(z) = \sum_{i=1}^{s} \hat{p}_i z^i = \mathrm{Det}\left[\mathbf{I} - z\mathbf{A} + z\mathbf{e} \otimes \hat{\mathbf{b}}^T\right]. \tag{22}$$

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 $P(z)$. 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,

$$E(y) = Q(+iy)Q(-iy) - P(+iy)P(-iy) = \sum_{j=0}^{s} E_{2j} y^{2j}, \tag{23}$$

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. Any L-acceptable stability function to an implicit Runge–Kutta method having an $\mathbf{A}$-matrix with only a single, real, s-fold eigenvalue, will have bounds on the value of this eigenvalue, γ. These bounds [102, 117, 184] are given in Table 1 for specific values the number of implicit stages, s_I, and the order, p, of the method. However, for many SIRK methods in this paper, $p + 1 < s_I$. This implies that finding an L-stable method is much more challenging.

2.2.2 Nonlinear Stability

The symmetric algebraic stability matrix is defined as [21, 26, 51, 74, 101, 102, 140]

$$\mathbf{M} = \mathbf{B}^T\mathbf{A} + \mathbf{A}^T\mathbf{B} - \mathbf{b}\mathbf{b}^T, \qquad M_{ij} = b_i a_{ij} + b_j a_{ji} - b_i b_j, \tag{24}$$

where $\mathbf{B} = \mathrm{diag}(\mathbf{b})$ or $\mathbf{b} = \mathbf{B}\mathbf{e}$. Algebraic-stability of irreducible methods requires that $a_{ii}, b_i > 0$ and $\mathbf{M} \geq O$.

Table 1: Bounds on γ for L-stable SIRKs and ESDIRKs from orders three to six

s_I, p	L-stable
$3, 3$	$\gamma = 0.43586652150845899941601945$
$4, 3$	$0.22364780093417645106968 98 \leq \gamma \leq 0.57281606248213485540800 14$
$4, 4$	$\gamma = 0.5728160624821348554080014$
$5, 4$	$0.2479946362127474551679910 \leq \gamma \leq 0.6760423932262813288723863$
$5, 5$	$\gamma = 0.2780538411364523249315862$
$6, 5$	$0.1839146536751751632321436 \leq \gamma \leq 0.3341423670680504359540301$
$6, 6$	$\gamma = 0.3341423670680504359540301$
$7, 6$	$0.2040834517158857633717906 \leq \gamma \leq 0.3788648944853283440258853$
$7, 7$	-
$8, 7$	$0.1566585993970439483924506 \leq \gamma \leq 0.2029348608433776737779349$
	$0.2051941719494007117460614 \leq \gamma \leq 0.2343731596055835579475589$
$8, 8$	$\gamma = 0.2343731596055835579475589$

2.2.3 Internal Stability

Beyond traditional stepwise stability, it may be useful to control the linear and nonlinear stability associated with each stage in addition to each step. This is particularly true for large scaled eigenvalues, z, associated with stiff problems. The vector of internal stabilities of Runge–Kutta methods are determined by evaluating

$$\begin{aligned} R_{\text{int}}(z) &= (\mathbf{I} - z\mathbf{A})^{-1}\mathbf{e} = \{R_{\text{int}}^{(1)}(z), R_{\text{int}}^{(2)}(z), \cdots, R_{\text{int}}^{(s)}(z)\}^T \\ &= \left\{ \frac{P_{\text{int}}^{(1)}(z)}{Q_{\text{int}}^{(1)}(z)}, \frac{P_{\text{int}}^{(2)}(z)}{Q_{\text{int}}^{(2)}(z)}, \cdots, \frac{P_{\text{int}}^{(s)}(z)}{Q_{\text{int}}^{(s)}(z)} \right\}^T. \end{aligned} \tag{25}$$

The primary concern will be the value of $R_{\text{int}}^{(i)}(-\infty)$. One may also consider the E-polynomial, (23), at internal stages to determine stagewise I-stability by using

$$E_{\text{int}}^{(i)}(y) = Q_{\text{int}}^{(i)}(iy)Q_{\text{int}}^{(i)}(-iy) - P_{\text{int}}^{(i)}(iy)P_{\text{int}}^{(i)}(-iy), \tag{26}$$

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

$$M_{jk}^{(i)} = a_{ij}a_{jk} + a_{ik}a_{kj} - a_{ij}a_{ik} \geq 0, \quad a_{ij} \geq 0, \quad i, j, k = 1, 2, \ldots, s, \tag{27}$$

and $M_{jk}^{(i)}$ is the internal algebraic-stability matrix for stage i. Interestingly, none of the classic fully-implicit Runge–Kutta methods, i.e. the Gauss, Radau and Lobatto methods, are internally algebraically stable on all stages. This suggests that internal algebraic stability is a rather severe requirement. Even internal A-stability on all stages occurs only with Lobatto IIIA. No attempt is made to consider partitioned FIRK methods such as a Lobatto IIIA - Lobatto IIIB pair [167].

2.3 Implementation

Various discussions on the implementation of SIRK methods may be found in the literature [19,29,33,65, 67,71,72,141,153,161,180]. Jackson [110] considers implementing SIRKs on large systems of stiff ODEs while Nørsett [148], and later, Cooper and Vignesvaran [73] devise algorithms for SIRK methods on parallel computers. Bendtsen considers parallel computation with MIRKs [9–11,13]. Lastly, Chartier [64] considers parallel, iterated SIRK methods.

Although the optimal implementation of SIRK methods is not the focus herein, an explicit derivation of a SIRK Newton iteration is included to, hopefully, offer some clarity on the implementation of the methods in the context of directly solving the linear systems. Indices are specifically included so that misinterpretations are less likely to occur.

To solve for the s stage-values, for all m equations, at a given time step, we must iteratively solve

$$\mathbf{U}_{i,m} = U_m^{[n]}\mathbf{e}_{i,m} + (\Delta t)\sum_{j=1}^{s}\mathbf{A}_{ij}\mathbf{F}_{j,m}. \tag{28}$$

To set up this iteration, we expand $\mathbf{U}$ and $\mathbf{F}$ in a Taylor-series,

$$\mathbf{U}_{i,m} + d\mathbf{U}_{i,m} + \cdots = U_m^{[n]}\mathbf{e}_{i,m} + (\Delta t)\sum_{j=1}^{s}\mathbf{A}_{ij}\left(\mathbf{F}_{j,m} + \sum_{k=1}^{s}\frac{\partial \mathbf{F}_{j,m}}{\partial \mathbf{U}_{k,m}}d\mathbf{U}_{k,m} + \cdots\right). \tag{29}$$

Subtracting (28) from (29), linearizing and replacing $\frac{\partial \mathbf{F}}{\partial \mathbf{U}}$ with $\mathbf{J}$, we find

$$d\mathbf{U}_{i,m} = -\left(\mathbf{U}_{i,m} - U_m^{[n]}\mathbf{e}_{i,m}\right) + (\Delta t)\sum_{j=1}^{s}\mathbf{A}_{ij}\mathbf{F}_{j,m} + (\Delta t)\sum_{j,k=1}^{s}\mathbf{A}_{ij}\mathbf{J}_{jk,m}d\mathbf{U}_{k,m}. \tag{30}$$

Collecting $d\mathbf{U}_{k,m}$ in (30), we have

$$\left[\sum_{k=1}^{s}\left(\mathbf{I}_{ik,m} - (\Delta t)\sum_{j=1}^{s}\mathbf{A}_{ij}\mathbf{J}_{jk,m}\right)\right]d\mathbf{U}_{k,m} = -\left(\mathbf{U}_{i,m} - U_m^{[n]}\mathbf{e}_{i,m}\right) + (\Delta t)\sum_{j=1}^{s}\mathbf{A}_{ij}\mathbf{F}_{j,m}. \tag{31}$$

Left multiplying both sides of (31) by $\mathbf{S}_{pi}^{-1}$ gives

$$\begin{aligned}&\left[\sum_{i,k=1}^{s}\left(\mathbf{S}_{pi}^{-1}\mathbf{I}_{ik,m} - (\Delta t)\sum_{j=1}^{s}\mathbf{S}_{pi}^{-1}\mathbf{A}_{ij}\mathbf{J}_{jk,m}\right)\right]d\mathbf{U}_{k,m} = \\ &-\sum_{i=1}^{s}\mathbf{S}_{pi}^{-1}\left(\mathbf{U}_{i,m} - U_m^{[n]}\mathbf{e}_{i,m}\right) + (\Delta t)\sum_{i,j=1}^{s}\mathbf{S}_{pi}^{-1}\mathbf{A}_{ij}\mathbf{F}_{j,m},\end{aligned} \tag{32}$$

Using the Jordan canonical form of $\mathbf{A}$,

$$\mathbf{A}_{ij} = \sum_{p,q=1}^{s}\mathbf{S}_{ip}\mathcal{J}_{pq}\mathbf{S}_{qj}^{-1}, \qquad \sum_{i=1}^{s}\mathbf{S}_{pi}^{-1}\mathbf{A}_{ij} = \sum_{q=1}^{s}\mathcal{J}_{pq}\mathbf{S}_{qj}^{-1}, \qquad \mathcal{J}_{pq} = \sum_{i,j=1}^{s}\mathbf{S}_{pi}^{-1}\mathbf{A}_{ij}\mathbf{S}_{jq}, \tag{33}$$

allows us to write the LHS of (32) as

$$\left[\sum_{i,k=1}^{s}\left(\mathbf{S}_{pi}^{-1}\mathbf{I}_{ik,m}-(\Delta t)\sum_{j,q=1}^{s}\mathcal{J}_{pq}\mathbf{S}_{qj}^{-1}\mathbf{J}_{jk,m}\right)d\mathbf{U}_{k,m}\right]=$$
$$\left[\sum_{i,k,r,t=1}^{s}\left(\mathbf{S}_{pi}^{-1}\mathbf{I}_{ik,m}-(\Delta t)\sum_{j,q=1}^{s}\mathcal{J}_{pq}\mathbf{S}_{qj}^{-1}\mathbf{J}_{jk,m}\right)\mathbf{S}_{kr}\mathbf{S}_{rt}^{-1}d\mathbf{U}_{t,m}\right]=$$
$$\left[\sum_{t,r=1}^{s}\left(\mathbf{I}_{pr,m}-(\Delta t)\sum_{j,k,q=1}^{s}\mathcal{J}_{pq}\mathbf{S}_{qj}^{-1}\mathbf{J}_{jk,m}\mathbf{S}_{kr}\right)\mathbf{S}_{rt}^{-1}d\mathbf{U}_{t,m}\right]. \tag{34}$$

Hence, the iteration, (32), is

$$\left[\sum_{t,r=1}^{s}\left(\mathbf{I}_{pr,m}-(\Delta t)\sum_{j,k,q=1}^{s}\mathcal{J}_{pq}\mathbf{S}_{qj}^{-1}\mathbf{J}_{jk,m}\mathbf{S}_{kr}\right)\mathbf{S}_{rt}^{-1}d\mathbf{U}_{t,m}\right]=$$
$$-\sum_{i=1}^{s}\mathbf{S}_{pi}^{-1}\left(\mathbf{U}_{i,m}-U_m^{[n]}\mathbf{e}_{i,m}\right)+(\Delta t)\sum_{j,q=1}^{s}\mathcal{J}_{pq}\mathbf{S}_{qj}^{-1}\mathbf{F}_{j,m}. \tag{35}$$

If we define the new variables

$$\sum_{t=1}^{s}\mathbf{S}_{rt}^{-1}\mathbf{U}_{t,m}=\mathbb{U}_{r,m},\quad \sum_{j=1}^{s}\mathbf{S}_{qj}^{-1}\mathbf{F}_{j,m}=\mathbb{F}_{q,m},\quad \sum_{i=1}^{s}\mathbf{S}_{pi}^{-1}\mathbf{e}_{i,m}=\mathbb{E}_{p,m},\quad \sum_{j,k=1}^{s}\mathbf{S}_{qj}^{-1}\mathbf{J}_{jk,m}\mathbf{S}_{kr}=\mathbb{J}_{qr,m}, \tag{36}$$

then

$$\left[\sum_{r=1}^{s}\left(\mathbf{I}_{pr,m}-(\Delta t)\sum_{q=1}^{s}\mathcal{J}_{pq}\mathbb{J}_{qr,m}\right)d\mathbb{U}_{r,m}\right]=-\left(\mathbb{U}_{p,m}-U_m^{[n]}\mathbb{E}_{p,m}\right)+(\Delta t)\sum_{q=1}^{s}\mathcal{J}_{pq}\mathbb{F}_{q,m}. \tag{37}$$

To perform a direct solve, the iteration matrix, $\mathbf{N}$, and the residual, $\mathbf{r}$, are defined as

$$\mathbf{N}=\left[\mathbf{I}-(\Delta t)\mathcal{J}\mathbb{J}\right],\qquad \mathbf{r}=-\left(\mathbb{U}-U^{[n]}\mathbb{E}\right)+(\Delta t)\mathcal{J}\mathbb{F}, \tag{38}$$

where indices have been suppressed. The Newton displacement is then solved recursively

$$\mathbf{N}\mathbf{d}_{(k)}=\mathbf{r}_{(k)},\qquad \mathbf{d}_{(k)}=\left(\mathbb{U}_{(k+1)}-\mathbb{U}_{(k)}\right), \tag{39}$$

where k is the iteration number, and direct (or indirect) methods are used to find

$$\mathbf{U}_{(k+1)}=\mathbf{U}_{(k)}+\mathbf{S}\mathbf{d}_{(k)}. \tag{40}$$

Iteration is continued by computing an updated residual, $\mathbf{r}_{(k+1)}$, so that $\mathbf{d}_{(k+1)}$ may be computed. This is repeated until the scaled displacement vector is sufficiently small (displacement test) or the residual vector is sufficiently small (residual test).

Very large systems of equations are beyond the scope of direct solver techniques and require an iterative procedure with an effective preconditioner. This situation is discussed in Appendix F where a preconditioner design in included to motivate the assertion that the iterative costs of SIRKs and SDIRKs are approximately equivalent. The stopping threshold when using the orthogonal Schur-rotation depends only on the displacement vector.

2.4 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 [105, 164]

$$(\Delta t)^{[n+1]} = \kappa(\Delta t)^{[n]} \left\{\frac{\epsilon}{||\delta^{[n]}||}\right\}^{\alpha} \left\{\frac{||\delta^{[n-1]}||}{\epsilon}\right\}^{\beta} \left\{\frac{\epsilon}{||\delta^{[n-2]}||}\right\}^{\gamma} \left\{\frac{(\Delta t)^{[n]}}{(\Delta t)^{[n-1]}}\right\}^{\mathfrak{a}} \left\{\frac{(\Delta t)^{[n-1]}}{(\Delta t)^{[n-2]}}\right\}^{\mathfrak{b}} \tag{41}$$

for $p(\hat{p})$-pairs ($\hat{p} = p - 1$) (local extrapolation mode). In (41), $\kappa \approx 0.95$ is the safety factor, $(\Delta t)^{[n-i]} = t^{[n-i]} - t^{[n-i-1]}$ is the step size, and $\delta^{[n]}$ is the vector of most recent local error estimates of the integration from $t^{[n-1]}$ to $t^{[n]}$ associated with the computation of $\mathbf{U}^{[n]}$. Many controllers exist and Table 2 [164] lists

Table 2: Error controller coefficients.

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

coefficients for various controllers. The I-controller is used for the first step and the $H211$ or PC-controllers are for the second step. After the second step, the PPID or H321 controllers could be employed [117]. The value of k depends on whether one is interested in the error-per-step (EPS) or the error-per-unit step (EPUS). For EPS, in local extrapolation mode, it is typically quoted as equal to $\hat{p} + 1$. See the Note in [97]

3 New SIRK Methods

All SIRK methods discussed below are designed to be stiffly-accurate, L-stable and internally L-stable. They have a stage-order of three, four or five, occurring in three- to eight-stages. Of the methods investigated, nine produced methods with properties not unlike Radau-IIA methods and one that does not resemble Radau IIA methods. Four of the methods have a stage-order of three, five possess a stage-order of four and one has stage-order five. Many other SIRK methods were considered but are not discussed below because they did not resemble Radau IIA methods. If a high-quality SIRK method is needed to integrate stiff systems of equations, stage-order three requires four or more stages while a high quality method having a stage-order of four requires at least six-stages. At stage-order five, high-quality SIRK methods are probably not possible but methods that are potentially usable are possible.

With this, it appears that the methods given below are most competitive when a stage-order of three or four is needed. Below a stage-order of three, DIRK methods are likely more useful. If a stage-order of at least five or six is needed, Radau IIA methods might be best within the class of Runge–Kutta methods. In such cases, general linear methods or multiderivative Runge–Kutta methods could also be considered.

Lastly, though it is quite straightforward to generate the $\mathbf{S}$ and $\mathbf{S}^{-1}$ from the $\mathbf{A}$-matrix and γ which are provided, precision would be lost. For this reason, the $\mathbf{S}$ and $\mathbf{S}^{-1}$ are included in Appendix A to the same precision as that contained in the $\mathbf{A}$-matrix. The orthogonal and upper triangular matrices for a Schur-decomposition of the $\mathbf{A}$ matrix are also included to the same precision.

3.1 Three-Stage Methods

Only one SIRK method is considered in three implicit stages. With $C(s)$ and distinct abscissae, it is an example of a collocation method [17].

3.1.1 Order Three, Stage-Order Three Methods

At third-order, a stage-order of three with singly-implicitness in s stages requires that

$$0 = \tau_1^{(1,2,3)} = \mathbf{q}^{(1,2,3)} = 0, \qquad Q(z) = \mathrm{Det}\left[\mathbf{I} - z\mathbf{A}\right] = (1-\gamma z)^3 \tag{42}$$

be imposed. With this, a third-order, L-stable method is produced for $\gamma \cong 0.43587$. (See Table 1). There are two real solutions to these requirements where $c_1 \neq c_2$ may take the approximate values of $\{0.1812222097969362934440 3416, 2.7415764837791947013001 4089\}$. Because of the one large abscissae, neither of these methods is of practical use. This method offers an interesting comparison to the three-stage Radau-IIA method. By forcing the $\mathbf{A}$-matrix to have only real eigenvalues for a SIRK method, it is completely uncompetitive with the similar size Radau IIA method. Hence, requiring real eigenvalues is a severe constraint. This same behavior with very large abscissae is also seen from other similarly-designed collocation-SIRK methods having $\mathfrak{q} = s$, at least for $3 \leq s \leq 6$.

3.2 Four-Stage Methods

Increasing s to four, three method-types are investigated but only one is found useful. That is SIRK3(2)4L[3]SA. With only four stages, it appears that the maximum practical stage-order of the SIRKs designed here is three.

3.2.1 Order Three, Stage-Order Three Methods

For third-order, a stage-order of three and singly implicitness in 4 stages,

$$0 = \tau_1^{(1,2,3)} = \hat{\tau}_1^{(1,2)} = \mathbf{q}^{(1,2,3)} = \hat{p}_4, \quad Q(z) = \mathrm{Det}\left[\mathbf{I} - z\mathbf{A}\right] = (1-\gamma z)^4 \tag{43}$$

is imposed. With this, a third-order, L-stable method is built with $0.22365 \lesssim \gamma \lesssim 0.57282$. (See Table 1). Internal I-stability is achieved for

$$1.7457611011583465756868167 \lesssim \frac{c_i}{\gamma} \lesssim 4.4713160416646255790880423, \quad i = 1,2,3. \tag{44}$$

To achieve stage-order three, $R(-\infty) = R_{\text{int}}^{(i)}(-\infty) = 0$ on all stages, $\gamma = 0.224 = 28/125$ is enforced. For the embedded method, the fourth condition applied is

$$\hat{\tau}_1^{(3)} = \frac{2468369}{1171875000}. \tag{45}$$

The three parameters which define this family of solutions are taken to be the unspecified abscissae, $c_i,\ i = 1, 2, 3$. The method, SIRK3(2)4L[3]SA, is derived by optimizing the above method using the three degrees of freedom (DoF) where we impose

$$\{c_1, c_2, c_3\} = \left\{\frac{31}{79}, \frac{29}{56}, \frac{83}{94}\right\}. \tag{46}$$

The term optimizing is meant to imply the subjective balancing between important properties such as nonlinear stability of the step and stages, method truncation error, scheme coefficient magnitudes, abscissae locations, the magnitude of γ and the condition number of the $\mathbf{A}$-matrix. This constitutes the derivation of SIRK3(2)4L[3]SA. Coefficients to the method are shown in Appendix A.1.1 and method properties are given in Table 6.

3.2.2 Order Four, Stage-Order Three Methods

Increasing the order to four, a stage-order of three SIRK requires the following conditions be enforced,

$$0 = \tau_1^{(1,2,3,4)} = \mathbf{q}^{(1,2,3)} = 0, \qquad Q(z) = \text{Det}\left[\mathbf{I} - z\mathbf{A}\right] = (1 - \gamma z)^4. \tag{47}$$

With this, a fourth-order, L-stable method is constructed using $\gamma \approx 0.57282$. (See Table 1). Additionally, $R(-\infty) = 0$ and $R_{\text{int}}^{(i)}(-\infty) = 0$ are enforced on all stages. Internal I-stability is impossible for the first three stages if $0 < c_i < 1,\ i = 1, 2, 3$. Hence, the method is no longer considered.

3.2.3 Order Four, Stage-Order Four Methods

Requesting the stage-order to be four, based on the previous stiffly-accurate method, is not expected to produce anything useful as it represents an additional constraint on an already inviable method. Imposing

$$0 = \tau_1^{(1,2,3,4)} = \mathbf{q}^{(1,2,3,4)} = 0, c_4 = 1, \tag{48}$$

creates a method with only three DoF for all other considerations; $\{c_2, c_3, \gamma\}$. However, enforcing

$$Q(z) = \text{Det}\left[\mathbf{I} - z\mathbf{A}\right] = (1 - \gamma z)^s, \tag{49}$$

produces 24 solutions and, for the solutions with $\gamma \approx 0.57281606248213485540800014$, they always have at least one abscissa greater than one. As was anticipated, the method is no longer considered. Again, stiffly-accurate, collocation SIRKs with $q = s$ do not produce good stiff integrators.

3.3 Five-Stage Methods

Of seven methods considered in five stages, four useful methods were derived using five stages, SIRK3(2)5L[3]SA, SIRK4(3)5L[3]SA, SIRK4(3)5L[3]SA_DAE and SIRK5(4)5L[3]SA, each having a stage-order of three. All methods enforce

$$Q(z) = \text{Det}\left[\mathbf{I} - z\mathbf{A}\right] = (1 - \gamma z)^5. \tag{50}$$

Attempts to increase the stage-order to four or five produced low-quality stiff-integrators.

3.3.1 Order Three, Stage-Order Three Methods

To produce a third-order method with stage-order three and singly implicitness in five stages, we enforce

$$0 = \tau_1^{(1,2,3)} = \hat{\tau}_1^{(1,2)} = \mathbf{q}^{(1,2,3)} = \hat{p}_5, \quad \gamma = \frac{81}{500} = 0.162. \tag{51}$$

To optimize the method, we set

$$\mathbf{q}_{1,2,3,4}^{(4)} = \left\{ \frac{-7}{200000}, \frac{-236}{200000}, \frac{-17}{200000}, \frac{-249}{200000} \right\}, \quad \mathbf{c} = \left\{ \frac{21}{82}, \frac{32}{83}, \frac{94}{143}, \frac{155}{182}, 1 \right\}. \tag{52}$$

For the embedded method, we enforce

$$\hat{\tau}_1^{(3,4)} = \left\{ \frac{1}{400}, \frac{1}{800} \right\}. \tag{53}$$

This constitutes the derivation of SIRK3(2)5L[3]SA. Coefficients to the method are shown in Appendix A.1.2 and method properties are given in Table 6.

3.3.2 Order Four, Stage-Order Three Methods

Increasing the order to four but retaining a stage-order of three, an L-stable method is achieved for

$$0.2479946362127474551679910 \lesssim \gamma \lesssim 0.6760423932262813288723863. \tag{54}$$

The method, SIRK4(3)5L[3]SA, is derived by enforcing the following conditions

$$0 = \tau_1^{(1,2,3,4)} = \hat{\tau}_1^{(1,2,3)} = \mathbf{q}^{(1,2,3)} = \hat{p}_5, \quad \gamma = \frac{31}{125} = 0.248. \tag{55}$$

Additionally, we set

$$\mathbf{q}_{1,2,3,4}^{(4)} = \left\{ \frac{-135}{100000}, \frac{-954}{100000}, \frac{-333}{100000}, \frac{-1440}{100000} \right\}, \quad \mathbf{c} = \left\{ \frac{17}{49}, \frac{55}{107}, \frac{62}{71}, \frac{41}{46}, 1 \right\}. \tag{56}$$

For the embedded method, we also enforce

$$\hat{\tau}_1^{(4)} = \frac{-6692373546271}{974131537318413}. \tag{57}$$

This constitutes the derivation of SIRK4(3)5L[3]SA. Coefficients to the method are shown in Appendix A.1.3 and method properties are given in Table 6.

For a slightly different version of this method, potentially better suited to index-2 DAE problems, we instead set

$$\mathbf{q}_{2,3,4}^{(4)} = \left\{ \frac{-260}{100000}, \frac{-900}{100000}, \frac{-459}{100000} \right\}, \quad \mathbf{c} = \left\{ \frac{9}{26}, \frac{53}{107}, \frac{52}{99}, \frac{148}{169}, 1 \right\}, \quad \hat{\tau}_1^{(4)} = \frac{-261}{100000}, \tag{58}$$

but replace the specification of $\mathbf{q}_1^{(4)}$ with (111). The overall properties of this method, SIRK4(3)5L[3]SA_DAE, are very similar to those of SIRK4(3)5L[3]SA. We consider this method more of a curiosity than a useful method.

3.3.3 Order Five, Stage-Order Three Methods

Retaining a stage-order of three but increasing the order to five, an L-stable method is designed with one of the roots to

$$0 = 1 - 25\gamma + 200\gamma^2 - 600\gamma^3 + 600\gamma^4 - 120\gamma^5, \qquad \gamma \approx 0.27805384113645232493158618511 9. \tag{59}$$

The method, SIRK5(4)5L[3]SA, is derived by enforcing the following conditions

$$0 = \tau_1^{(1,2,3,4,5)} = \hat{\tau}_1^{(1,2,3,4)} = \tau_5^{(5)} = \mathbf{q}^{(1,2,3)}. \tag{60}$$

Additionally, we set

$$\mathbf{q}_{2,3,4}^{(4)} = \left\{-\frac{821}{100000}, -\frac{2094}{100000}, -\frac{1610}{100000}\right\}, \qquad \hat{\tau}_1^{(5)} = +\frac{222}{1000000}, \tag{61}$$

$$\mathbf{c} = \left\{\frac{500}{1283}, \frac{438}{929}, \frac{1826}{2635}, \frac{586}{651}, 1\right\}. \tag{62}$$

This constitutes the derivation of SIRK5(4)5L[3]SA. Coefficients to the method are shown in Appendix A.1.4 and method properties are given in Table 6.

3.3.4 Order Four, Stage-Order Four Methods

If one wishes each stage and the step to be fourth-order in a five-stages, then a stiffly-accurate SIRK method requires, minimally, the satisfaction of

$$0 = \tau_1^{(1,2,3,4)} = \hat{\tau}_1^{(1,2,3)} = \mathbf{q}^{(1,2,3,4)} = 0, c_5 = 1, Q(z) = \mathrm{Det}\left[\mathbf{I} - z\mathbf{A}\right] = (1 - \gamma z)^5. \tag{63}$$

For L-stability, $0.24799463621274745516799 10 \leq \gamma \leq 0.67604239322628132887238 63$, so that four DoF remain, $\{c_1, c_2, c_3, c_4\}$. Selecting $\gamma = 0.248$, a search was performed for acceptable methods. In all schemes investigated, the algebraic and internal algebraic stability matrices had both large negative and positive eigenvalues. Further, the coefficients to the method were too large. This method is unlikely to produce a useful SIRK method for the contexts envisioned in this work.

3.3.5 Order Five, Stage-Order Four Methods

Increasing the order to five from the previous method, we seek a 5(4)-pair which is stiffly-accurate. To do this, the method must satisfy

$$0 = \tau_1^{(1,2,3,4,5)} = \hat{\tau}_1^{(1,2,3,4)} = \mathbf{q}^{(1,2,3,4)} = 0, c_5 = 1, Q(z) = \mathrm{Det}\left[\mathbf{I} - z\mathbf{A}\right] = (1 - \gamma z)^5, \tag{64}$$

Apart from the embedded method, the difference between this method and the proceeding is the value of γ. Here, $\gamma \approx 0.27805384113645232493158 62$ while in the previous there was a range of acceptable values for γ. As with the previous method the algebraic and internal algebraic stability matrices had both large negative and positive eigenvalues. This method is unlikely to produce a useful SIRK method.

3.3.6 Order Five, Stage-Order Five Methods

For a stage-order five method, with $q = s$, a stiffly-accurate collocation method, we initially impose only

$$0 = \tau_1^{(1,2,3,4,5)} = \mathbf{q}^{(1,2,3,4,5)} = 0, c_5 = 1, \tag{65}$$

to find a method with four DoF for all other considerations; $\{c_2, c_3, c_4, \gamma\}$. However, L-stability requires $\gamma \approx 0.27805384113645232493 15862$. Upon enforcing,

$$Q(z) = \text{Det}\left[\mathbf{I} - z\mathbf{A}\right] = (1 - \gamma z)^5, \tag{66}$$

we find 120 solutions. All 120 solution produce poor solutions because either one abscissae is outside of the step or γ is not the required value, i.e. $0 \nleq c_i \nleq 1$ or $\gamma \not\approx 0.278053841136452324931 5862$. Hence, this class of methods is no longer considered.

3.4 Six-Stage Methods

Having six-stages or more, we no longer discuss SIRK methods that have been derived but are not of use as stiff integrators. Also, moving forward, we only consider methods having stage-order four or greater. Two useful methods are given with six stages: SIRK4(3)6L[4]SA and SIRK5(4)6L[4]SA.

3.4.1 Order Four, Stage-Order Four Methods

With a sixth-stage, we now wish to design a stiffly-accurate SIRK method whose order and stage-order are both four. To begin, we enforce

$$0 = \tau_1^{(1,2,3,4)} = \hat{\tau}_1^{(1,2,3)} = \mathbf{q}^{(1,2,3,4)} = \hat{p}_6, \quad \gamma = \frac{19}{100} = 0.19 \tag{67}$$

$$Q(z) = \text{Det}\left[\mathbf{I} - z\mathbf{A}\right] = (1 - \gamma z)^6 \tag{68}$$

Additionally, we set $\tau_1^{(5)} = 2/10^4$ and

$$\mathbf{q}^{(5)}_{1,2,3,4,5} = \frac{1}{78125}\left\{92, 87, 138, 123, 332\right\}, \quad \mathbf{c} = \left\{\frac{24}{109}, \frac{20}{33}, \frac{17}{52}, \frac{6}{7}, \frac{35}{48}, 1\right\}. \tag{69}$$

To make a useful embedded method, we impose

$$\hat{\tau}_1^{(4,5)} = \frac{4}{10^8}\left\{-15150, -9999\right\}. \tag{70}$$

This constitutes the derivation of SIRK4(3)6L[4]SA. Coefficients to the method are shown in Appendix A.2.1 and method properties are given in Table 7.

We remark that if one is singularly interested in reducing the value of γ, then a different method can be made. The above recipe is followed with the following alterations

$$\gamma = \frac{179}{1000} = 0.179, \qquad \tau_1^{(5)} = -213/10^6, \qquad \hat{\tau}_1^{(4,5)} = \frac{1}{10^6}\left\{-365, -479\right\}, \tag{71}$$

$$\mathbf{q}^{(5)}_{1,2,3,4,5} = \frac{1}{10^5}\left\{55, 208, 141, -421, -279\right\}, \quad \mathbf{c} = \left\{\frac{13}{62}, \frac{43}{111}, \frac{44}{63}, \frac{82}{107}, \frac{44}{49}, 1\right\}. \tag{72}$$

The properties of this method are close to those of SIRK4(3)6L[4]SA. Below, it will be seen that picking an intermediate value of γ leads to a fifth-order method.

3.4.2 Order Five, Stage-Order Four Methods

To generate an order five, stage-order four method, we enforce

$$0 = \tau_1^{(1,2,3,4,5)} = \hat{\tau}_1^{(1,2,3,4)} = \mathbf{q}^{(1,2,3,4)}, \qquad Q(z) = \mathrm{Det}\,[\mathbf{I} - z\mathbf{A}] = (1-\gamma z)^6. \tag{73}$$

For this method, L-stability occurs for

$$0.18391465367517516323214364197 2 \lesssim \gamma \lesssim 0.33414236706805043595403009293 4. \tag{74}$$

With the remaining DoF, we set $\gamma = 23/125 = 0.184$ and

$$\mathbf{q}^{(5)}_{1,2,3,4,5} = \frac{5}{10^7}\{1725, 10850, 3725, 1, 5600\}, \quad \mathbf{c} = \left\{\frac{386}{1809}, \frac{242}{425}, \frac{105}{337}, \frac{519}{793}, \frac{802}{961}, 1\right\}. \tag{75}$$

For the embedded method, we also enforce

$$\left\{\hat{\tau}_1^{(5)}, \hat{\tau}_1^{(6)}\right\} = \frac{1}{10^6}\{111, 87\} \tag{76}$$

This constitutes the derivation of SIRK5(4)6L[4]SA. Coefficients to the method are shown in Appendix A.2.2 and method properties are given in Table 7.

3.5 Seven-Stage Methods

At seven-stages, six method-types were investigated and three were found useful: SIRK5(4)7L[4]SA, SIRK5(4)7L[5]SA and SIRK6(5)8L[4]SA. The only stage-order five method presented in this paper, SIRK5(4)7L[5]SA, is somewhat inconsistent with the goal of producing Radau-IIA-like methods.

3.5.1 Order Five, Stage-Order Four Methods

Extending the SIRK5(4)6L[4]SA method to seven stages, we set

$$0 = \tau_1^{(1,2,3,4,5)} = \hat{\tau}_1^{(1,2,3,4)} = \mathbf{q}^{(1,2,3,4)} = \hat{p}_7, \quad \gamma = \frac{1}{7}, \qquad Q(z) = \mathrm{Det}\,[\mathbf{I} - z\mathbf{A}] = (1-\gamma z)^7. \tag{77}$$

Additionally, we set $\tau_1^{(6)} = 21 \times 10^{-6}$ and

$$\mathbf{q}^{(5)}_{1,2,3,4,5,6} = \frac{8}{10^9}\{62937, 106596, 55566, 28917, 57834, 17010\}, \tag{78}$$

$$\mathbf{q}^{(6)}_{1,2,3,4,5,6} = \frac{1}{10^9}\{2895312, 3929352, 2429994, 2791908, 3231375, 2636802, 2520000\}, \tag{79}$$

$$\mathbf{c} = \left\{\frac{11}{67}, \frac{47}{180}, \frac{55}{119}, \frac{85}{127}, \frac{41}{43}, \frac{161}{193}, 1\right\}. \tag{80}$$

For the remaining two embedded-method DoF, we enforce

$$\hat{\tau}_1^{(5,6)} = \frac{4}{10^{11}}\{-2331000, -1624707\}. \tag{81}$$

This constitutes the derivation of SIRK5(4)7L[4]SA. Coefficients to the method are shown in Appendix A.2.3 and method properties are given in Table 7.

3.5.2 Order Six, Stage-Order Four Methods

To construct an order six, stage-order four method, we enforce

$$0 = \tau_1^{(1,2,3,4,5,6)} = \hat{\tau}_1^{(1,2,3,4,5)} = \mathbf{q}^{(1,2,3,4)} = \tau_7^{(6)} = \hat{p}_7, \qquad Q(z) = \text{Det}\left[\mathbf{I} - z\mathbf{A}\right] = (1-\gamma z)^7. \tag{82}$$

An L-stable method requires that $0.2040834517158857633717906 \leq \gamma \leq 0.3788648944853283440258853$, so we select $\gamma = \frac{2041}{10000}$. With the remaining DoF, we set

$$\mathbf{q}^{(5)}_{1,2,3,4,5} = \frac{1}{10^6}\left\{420, 754, 666, 521, 388\right\}, \tag{83}$$

$$\mathbf{q}^{(6)}_{1,2,3,4,5,6} = \frac{1}{10^5}\left\{359, 385, 463, 516, 217, 276\right\}, \tag{84}$$

$$\mathbf{c} = \left\{\frac{315}{1478}, \frac{160}{563}, \frac{901}{2075}, \frac{312}{457}, \frac{220}{427}, \frac{1071}{1142}, 1\right\}. \tag{85}$$

For the last embedded-method DoF, we enforce $\hat{b}_6 = -1/5$. This constitutes the derivation of SIRK6(5)7L[4]SA. Coefficients to the method are shown in Appendix A.2.4 and method properties are given in Table 7.

3.5.3 Order Five, Stage-Order Five Methods

Extending the SIRK5(4)7L[4]SA method to stage-order five, we set

$$0 = \tau_1^{(1,2,3,4,5)} = \hat{\tau}_1^{(1,2,3,4)} = \mathbf{q}^{(1,2,3,4,5)} = \hat{p}_7, \quad \gamma = \frac{1}{7}, \qquad Q(z) = \text{Det}\left[\mathbf{I} - z\mathbf{A}\right] = (1-\gamma z)^7. \tag{86}$$

Additionally, we set $\tau_1^{(6)} = 162 \times 10^{-7}$ and

$$\mathbf{q}^{(6)}_{1,2,3,4,5,6} = \frac{1}{62,500,000}\left\{37179, 7290, 4617, 20898, 101331, 91125, 121500\right\}, \tag{87}$$

$$\mathbf{c} = \left\{\frac{167}{382}, \frac{133}{365}, \frac{161}{264}, \frac{257}{359}, \frac{109}{169}, \frac{379}{405}, 1\right\}. \tag{88}$$

For the remaining two embedded-method DoF, we enforce

$$\hat{\tau}_1^{(5,6)} = \left\{\frac{-40257}{5\times 10^8}, \frac{-24274971}{5\times 10^{11}}\right\}. \tag{89}$$

This constitutes the derivation of SIRK5(4)7L[5]SA. Coefficients to the method are shown in Appendix A.3.1 and method properties are given in Tables 8 and 9.

3.6 Eight-Stage Methods

At eight-stages, only one method is considered, SIRK6(5)8L[4]SA. Relative to SIRK6(5)7L[4]SA, the goal would be to reduce γ as much as possible so as to compensate for the work incurred by adding another stage. The new method reduces γ by ∼21% while increasing the number of stages by ∼14%. In moving to eight-stages with a stage-order of four, the condition number of the **A**-matrix must be managed during the design of the method.

3.6.1 Order Six, Stage-Order Four Methods

To generate an order five, stage-order four method, we enforce

$$0 = \tau_1^{(1,2,3,4,5,6)} = \hat{\tau}_1^{(1,2,3,4,5)} = \tau_7^{(6)} = \mathbf{q}^{(1,2,3,4)} = \hat{p}_8, \quad \gamma = \frac{16}{100}, \quad Q(z) = \mathrm{Det}\left[\mathbf{I} - z\mathbf{A}\right] = (1-\gamma z)^8. \tag{90}$$

Additionally, we set $\tau_1^{(7)} = 22 \times 10^{-7}$ and

$$\mathbf{q}^{(5)}_{1,2,3,4,5,6} = \frac{4}{10^8}\left\{2970, 3234, 2574, 1749, 2079, 1452\right\}, \tag{91}$$

$$\mathbf{q}^{(6)}_{1,2,3,4,5,6,7} = \frac{8}{10^9}\left\{34848, 41019, 59169, 68970, 64977, 49368, 38841\right\}, \tag{92}$$

$$\mathbf{q}^{(7)}_{1,2,3,4,5,6,7} = \frac{4}{10^9}\left\{52569, 55814, 72688, 41536, 74635, 39589, 75933\right\}, \tag{93}$$

$$\mathbf{c} = \left\{\frac{17}{112}, \frac{89}{421}, \frac{99}{272}, \frac{201}{355}, \frac{323}{415}, \frac{521}{567}, \frac{197}{200}, 1\right\}. \tag{94}$$

An embedded method is created with the following additional order conditions

$$\left\{\hat{\tau}_1^{(6)}, \hat{\tau}_1^{(7)}\right\} = \frac{1}{10^7}\{98, 46\}. \tag{95}$$

This constitutes the derivation of SIRK6(5)8L[4]SA. Coefficients to the method are shown in Appendix A.2.5 and method properties are given in Table 7.

3.7 Comparison to Radau IIA methods

In spite of their exceptional properties as stiff integrators, Radau IIA methods are rarely used in engineering contexts on problems where as many as one billion coupled ODEs are being solved. This is, in part, due to their high implementation costs [16, 92, 113]. Since many large engineering codes cannot employ direct solvers in the iterative solution of the stage- and step equations, they will typically employ Newton-Krylov techniques [75]. Hence, understanding the true implementation costs of Radau IIA methods is difficult to determine. A multitude of things will influence the implementation costs of Radau IIA methods in these contexts and this broad subject is beyond the scope of this paper [107,112,152,157,165]. Therefore, this paper focuses on finding SIRK methods which nearly match Radau IIA methods of the same stage-order in terms of properties. Because of the structure of the **A**-matrix of SIRK methods with a single, real eigenvalue, there is good reason to hope that SIRKs of stage-orders three, four and five can be implemented at less cost than the corresponding Radau IIA methods.

Though Radau IIA methods are of order $2s-1$ and have stage-order s, the stage order is the more relevant quantity for very stiff problems. SIRK methods are competitive with Radau IIA methods when the stiffness is strong enough for significant order reduction. A second consideration in comparing SIRK methods with Radau IIA methods is algebraic stability. SIRK methods may be designed to be algebraically stable but the methods presented in this paper have forsaken this attribute and settle for "almost" algebraically stable methods. This capitulation has allowed the design of internally L-stable methods, one of the few desirable properties that Radau IIA methods do not possess. In terms of implementation, SIRK methods are known to sometimes suffer from **A**-matrices with large condition numbers. It is for this reason that we include not only the coefficients to the **A**-, but also the **S**- and $\mathbf{S}^{-1}$-matrices. This particular issue does not afflict Radau IIA methods.

A significant distinction between SIRK and Radau IIA methods is in the eigenvalues of their **A**-matrices. All SIRK methods considered herein have a real, s-fold eigenvalue, namely γ. In the case of Radau IIA methods, s-eigenvalues come in complex conjugate pairs. When the number of stages is odd, one of the eigenvalues is real. If we write these eigenvalue pairs as $\{r, \theta\}$ to represent $r \exp(i\theta)$ where $i = \sqrt{-1}$ and θ is an angle in radians, then the first six Gauss, Radau IIA and Lobatto IIIC methods have Eig. $(\mathbf{A}) = \lambda$ which are given, approximately, in Tables 3, 4 and 5, respectively

s	λ
1	$\{0.50000, 0\}$
2	$\{0.28868, \pm 0.52360\}$
3	$\{\{0.21531, 0\}, \{0.19673, \pm 0.76188\}\}$
4	$\{\{0.16538, \pm 0.29094\}, \{0.14752, \pm 0.90116\}\}$
5	$\{\{0.13711, 0\}, \{0.13235, \pm 0.47944\}, \{0.11734, \pm 0.99373\}\}$
6	$\{\{0.11531, \pm 0.20143\}, \{0.10949, \pm 0.61275\}, \{0.097103, \pm 1.0603\}\}$

Table 3: Eigenvalue to the **A**-matrices of Gauss methods

s	λ
1	$\{1.0000, 0\}$
2	$\{0.40825, \pm 0.61548\}$
3	$\{\{0.27489, 0\}, \{0.24623, \pm 0.84975\}\}$
4	$\{\{0.19852, \pm 0.31643\}, \{0.17380, \pm 0.97835\}\}$
5	$\{\{0.15907, 0\}, \{0.15284, \pm 0.51285\}, \{0.13341, \pm 1.0613\}\}$
6	$\{\{0.13048, \pm 0.21318\}, \{0.12320, \pm 0.64816\}, \{0.10786, \pm 1.1201\}\}$

Table 4: Eigenvalue to the **A**-matrices of Radau IIA methods

s	λ
2	$\{0.70711, \pm 0.78540\}$
3	$\{\{0.38083, 0\}, \{0.33077, \pm 0.97877\}\}$
4	$\{\{0.24856, \pm 0.35017\}, \{0.21204, \pm 1.0804\}\}$
5	$\{\{0.18950, 0\}, \{0.18101, \pm 0.55454\}, \{0.15482, \pm 1.1456\}\}$
6	$\{\{0.15029, \pm 0.22729\}, \{0.14094, \pm 0.69065\}, \{0.12141, \pm 1.1917\}\}$

Table 5: Eigenvalue to the **A**-matrices of Lobatto IIIC methods

Other parts of a good integrator are the embedded error estimator, stage-value predictors and a dense-output method. Because Radau IIA methods are such optimal methods, they achieve stage-order $\mathfrak{q}$ in $\mathfrak{q} = s$ stages. This is problematic for the design of the embedded error estimators [91, 95], stage-value predictors [89, 90, 126] and dense-output methods. Constructing these ancillary methods with desirable properties requires using information from both the current and one or more previous timesteps. The relative inefficiency of SIRK methods implies that $s > \mathfrak{q}$ and hence only information from the current and one previous timestep is needed. Thus, constructing the ancillary methods is less problematic.

3.7.1 Stage-Order Three Methods

Four principal methods created in this paper have a stage-order of three. They are SIRK 3(2)4L[3]SA, SIRK 3(2)5L[3]SA, SIRK 4(3)5L[3]SA and SIRK 5(4)5L[3]SA. In Table 6, these methods are compared to the three-stage Radau IIA method. In this table, s is the number of stages in the method, p is the order of the method, $\hat{p}$ is the order of the embedded method, γ is the s-fold eigenvalue of the **A**-matrix, γs is a potential indicator of relative iteration costs, $A^{(p+1)}$ and $A^{(p+2)}$ are the leading and next-to-leading order error of the method, $A^{(\mathfrak{q}+1)}_{(\mathrm{int})}$ and $A^{(\mathfrak{q}+2)}_{(\mathrm{int})}$ are the leading and next-to-leading stage-order error of the method, $A^{(\hat{p}+1)}$ is the leading order error of the embedded method, $(B, C, E)^{(\hat{p}+1)}$ are the embedded-method quality metrics from (15), $\{R(-\infty), \hat{R}(-\infty)\}$ are the values of the linear stability functions to the main and embedded methods for $z \to -\infty$ and λ_{M} and $\lambda_{\mathrm{M}_{(\mathrm{int})}}$ are the eigenvalues to the algebraic and internal algebraic stability matrices. To understand the uniformity of the abscissae placement and the degree to which they are monotonically increasing, we create a quantity

$$\mathcal{C} = \sqrt{(\mathbf{c} - \mathfrak{c}) \cdot (\mathbf{c} - \mathfrak{c})}, \qquad \mathfrak{c}_i = i/s, \quad i = 1, 2, \ldots, s. \tag{96}$$

It is a crude measure of the departure in the abscissae values relative to a uniform spacing, $\mathfrak{c}_i$. Lastly, C(**A**) is the condition number of the **A** matrices in a 2-norm. In Mathematica™, we compute this as

$$C(\mathbf{A}) = \mathrm{Norm}[\mathbf{A}, 2] \times \mathrm{Norm}[\mathbf{A}^{-1}, 2]. \tag{97}$$

From Table 6, the SIRK methods appear to be comparable to the Radau IIA method in terms of the fourth-order, internal errors. Coefficient magnitudes of SIRK 3(2)5L[3]SA resemble Radau IIA but the other three methods have slightly larger coefficient magnitudes. The same is true for the eigenvalues of the internal algebraic stability and algebraic stability matrices. However, Radau IIA methods always have nonnegative eigenvalues to the algebraic stability matrix, i.e. they are algebraically stable with their nonnegative step weights.

Collectively, we liken the magnitude of the method coefficients, the eigenvalues of the algebraic stability matrix and the condition number of the **A**-matrix to a measure of *strain* within a method. As order and stage-order are increased, while the stage number is fixed, *strain* increases. To attain an order of five and a stage-order of three, as does the three-stage Radau IIA, SIRK 5(4)5L[3]SA is relatively much more *strained*. Of the SIRK methods, SIRK 5(4)5L[3]SA is the most *strained* while SIRK 3(2)5L[3]SA is the least. Only SIRK 3(2)5L[3]SA appears to be so *unstrained* as to resemble Radau IIA.

3.7.2 Stage-Order Four Methods

Five methods created in this paper have a stage-order of four but as 4(3), 5(4) and 6(5) pairs. They are SIRK 4(3)6L[4]SA, SIRK 5(4)6L[4]SA, SIRK 5(4)7L[4]SA, SIRK 6(5)7L[4]SA and SIRK 6(5)8L[4]SA. In Table 7, these methods are compared to the four-stage Radau IIA method. As with the stage-order three SIRK methods from the previous section, appear to be loosely comparable to the analogous Radau IIA method. The 6(5) pair in eight stages appears to be the most *strained* of the methods but not severely so. This may be seen in the eigenvalues to the algebraic-stability matrix. In both the 5(4)- and 6(5)-pairs, addition of a stage reduces the *strain* in the method as well as γs. In comparing the two six-stage methods here, SIRK 4(3)6L[4]SA and SIRK 5(4)6L[4]SA, it is unclear why one would ever prefer SIRK 4(3)6L[4]SA over SIRK 5(4)6L[4]SA.

Name	SIRK 3(2)4L[3]SA	SIRK 3(2)5L[3]SA	SIRK 4(3)5L[3]SA	SIRK 5(4)5L[3]SA	Radau IIA 5()3L[3]SA
$(s, p, \hat{p}, \mathfrak{q})$	$(4, 3, 2, 3)$	$(5, 3, 2, 3)$	$(5, 4, 3, 3)$	$(5, 5, 3, 3)$	$(3, 5, -, 3)$
γ	$\frac{28}{125} = 0.224$	$\frac{81}{500} = 0.162$	$\frac{31}{125} = 0.248$	~ 0.27805	–
γs	0.896	0.810	1.24	1.39	–
$A^{(p+1)}$	$1.46(-3)$	$1.73(-3)$	$7.14(-3)$	$3.59(-3)$,	$9.90(-4)$
$A^{(p+2)}$	$1.18(-2)$	$6.30(-3)$	$1.86(-2)$	$9.74(-3)$,	$1.71(-3)$
Min. $A^{(\mathfrak{q}+1)}_{(\mathrm{int})}$	$6.69(-5)$	$1.01(-4)$	$7.79(-4)$	$1.00(-3)$	$2.87(-3)$
Max. $A^{(\mathfrak{q}+1)}_{(\mathrm{int})}$	$1.46(-3)$	$3.59(-3)$	$8.31(-3)$	$1.21(-2)$	$2.87(-3)$
$\hat{A}^{(\hat{p}+1)}$	$2.98(-3)$	$3.54(-3)$	$2.38(-2)$	$2.87(-3)$	–
$\hat{A}^{(\hat{p}+2)}$	$5.08(-3)$	$4.33(-3)$	$5.83(-2)$	$1.06(-2)$	–
$(B, C, E)^{(\hat{p}+2)}$	$(1.71, 2.20, 0.49)$	$(1.22, 1.71, 0.49)$	$(2.45, 2.15, 0.30)$	$(3.68, 2.84, 1.25)$	$(-, -, -)$
$\{R(-\infty), \hat{R}(-\infty)\}$	$\{0, 0\}$	$\{0, 0\}$	$\{0, 0\}$	$\{0, -0.365\}$	$\{0, -\}$
Min., Max. $\mathbf{A}$	$(-2.74, 2.53)$	$(-0.633, 0.898)$	$(-1.60, 1.57)$	$(-7.85, 5.71)$	$(-0.066, 0.512)$
Min., Max. $\mathbf{b}$	$(-2.11, 2.17)$	$(-0.397, 0.819)$	$(-1.06, 1.33)$	$(-7.15, 5.17)$	$(0.111, 0.512)$
Min., Max. $\hat{\mathbf{b}}$	$(-2.03, 2.13)$	$(-0.431, 0.846)$	$(-2.38, 3.00)$	$(-8.45, 5.86)$	–
Min., Max. λ_{M}	$(-0.259, 15.7)$	$(-0.070, 1.44)$	$(-0.144, 5.13)$	$(-0.562, 39.4)$	$(0.0, 0.031)$
Min., Max. $\lambda_{\hat{\mathrm{M}}}$	$(-0.240, 15.4)$	$(-0.071, 1.14)$	$(-6.15, 4.37)$	$(-2.14, 25.6)$	
Min., Max. $\lambda_{\mathrm{M}_{(\mathrm{int})}}$	$(-0.391, -0.221)$	$(-0.085, -0.060)$	$(-0.254, -0.126)$	$(-2.11, -0.985)$	$(-0.056, 0.097)$
$\mathcal{C}$	0.196	0.096	0.343	0.244	0.189
C($\mathbf{A}$)	2503	544	1129	8500	8.69

Table 6: Stage-order three methods.

3.7.3 Stage-Order Five Methods

One newly created seven stage method is a 5(4) pair having a stage-order of five: SIRK 5(4)7L[5]SA. The algebraic stability properties of the method are shown in Table 8, and a comparison with the five-stage Radau IIA method is shown in Table 9. The coefficients for this SIRK method are large, as is the condition number of the **A**-matrix. One algebraic stability eigenvalue for each of the internal stages, the step and the embedded method is large and positive (see Table 8) It is clear from these tables that SIRK 5(4)7L[5]SA does not resemble the five-stage Radau IIA method in terms of its properties. These large positive eigenvalues, large coefficients and a large condition number are very undesirable. This method should be employed with caution.

4 Test Problems

A demanding set of test problems is used to identify promising new SIRK methods and to compare them with the Radau IIA methods of the same stage-order. Testing is conducted on three singular perturbation problems, in increasing order of difficulty: Kaps' problem, van der Pol's (vdP) equation and Kreiss' problem. The first two tend to index-1 Differential-Algebraic Equations (DAEs) in the limit as $\varepsilon \to 0$ while Kreiss' problem tends to an index-2 DAE in the limit as $\varepsilon \to 0$ (see Section VII.7, Exercises in [102]). A broad test suite of problems is also available elsewhere [128].

Name	SIRK 4(3)6L[4]SA	SIRK 5(4)6L[4]SA	SIRK 5(4)7L[4]SA	SIRK 6(5)7L[4]SA	SIRK 6(5)8L[4]SA	Radau IIA 7()4L[4]SA
$(s, p, \hat{p}, \mathfrak{q})$	$(6, 4, 3, 4)$	$(6, 5, 4, 4)$	$(7, 5, 4, 4)$	$(7, 6, 5, 4)$	$(8, 6, 5, 4)$	$(4, 7, -, 4)$
γ	$\frac{19}{100}$	$\frac{23}{125} = 0.184$	$\frac{1}{7} \sim 0.14286$	$\frac{2041}{10000}$	$\frac{16}{100}$	$-$
γs	1.140	1.104	1.000	1.429	1.280	$-$
$A^{(p+1)}$	$1.89(-3)$	$7.97(-4)$	$7.18(-4)$	$3.59(-4)$	$3.17(-4)$	$3.47(-5)$
$A^{(p+2)}$	$5.53(-3)$	$2.22(-3)$	$1.94(-3)$	$7.64(-4)$	$8.96(-4)$	$7.77(-5)$
Min. $A^{(\mathfrak{q}+1)}_{(\mathrm{int})}$	$4.40(-4)$	$1.98(-7)$	$5.38(-5)$	$1.53(-4)$	$2.30(-5)$	$2.47(-4)$
Max. $A^{(\mathfrak{q}+1)}_{(\mathrm{int})}$	$1.90(-3)$	$2.14(-3)$	$3.37(-4)$	$2.98(-4)$	$5.11(-5)$	$4.57(-4)$
$\hat{A}^{(\hat{p}+1)}$	$2.10(-3)$	$1.05(-3)$	$8.85(-4)$	$7.15(-4)$	$3.17(-4)$	$-$
$\hat{A}^{(\hat{p}+2)}$	$3.79(-3)$	$2.92(-3)$	$2.16(-3)$	$2.18(-3)$	$6.35(-4)$	$-$
$(B, C, E)^{(\hat{p}+1)}$	$(1.81, 2.71, 0.90)$	$(2.77, 2.06, 0.76)$	$(2.44, 3.25, 0.81)$	$(3.04, 3.02, 0.503)$	$(2.00, 2.97, 0.998)$	$-$
$\{R(-\infty), \hat{R}(-\infty)\}$	$\{0, 0\}$	$\{0, 0\}$	$\{0, 0\}$	$\{0, 0\}$	$\{0, 0\}$	$\{0, -\}$
Min., Max. $\mathbf{A}$	$(-1.05, 1.04)$	$(-1.26, 1.18)$	$(-0.48, 0.54)$	$(-1.51, 1.38)$	$(-1.35, 1.67)$	$(-0.048, 0.406)$
Min., Max. $\mathbf{b}$	$(-0.98, 1.04)$	$(-0.57, 0.82)$	$(-0.48, 0.53)$	$(-1.51, 1.38)$	$(-1.35, 1.67)$	$(0.063, 0.388)$
Min., Max. $\hat{\mathbf{b}}$	$(-0.659, 0.883)$	$(-0.82, 0.96)$	$(-1.00, 1.29)$	$(-0.818, 0.992)$	$(-2.52, 1.77)$	$-$
Min., Max. λ_{M}	$(-0.243, 2.25)$	$(-0.093, 1.97)$	$(-0.154, 0.490)$	$(-1.77, 2.43)$	$(-2.75, 2.76)$	$(0.0, 0.031)$
Min., Max. $\lambda_{\hat{\mathrm{M}}}$	$(-0.202, 2.21)$	$(-0.173, 2.22)$	$(-4.85, 0.65)$	$(-0.854, 2.35)$	$(-7.07, 5.32)$	$-$
Min., Max. $\lambda_{\mathrm{M}_{(\mathrm{int})}}$	$(-0.298, -0.159)$	$(-0.275, -0.142)$	$(-0.111, -0.054)$	$(-1.65, -0.529)$	$(-1.74, -0.839)$	$(-0.029, 0.051)$
$\mathcal{C}$	0.393	0.306	0.264	0.252	0.266	0.189
C($\mathbf{A}$)	1381	1205	739	2168	4857	13.97

Table 7: Stage-order four methods.

$$
\begin{aligned}
\lambda_{\mathrm{M}^{(1)}_{(\mathrm{int})}} &= \{-5.915, \; -0.9817, \; -0.3104, \; -0.1063, \; 1.485, \; 15.09, \; 692.4\} \\
\lambda_{\mathrm{M}^{(2)}_{(\mathrm{int})}} &= \{-6.320, \; -1.087, \; -0.3640, \; -0.1220, \; 1.574, \; 15.87, \; 691.9\} \\
\lambda_{\mathrm{M}^{(3)}_{(\mathrm{int})}} &= \{-6.348, \; -1.124, \; -0.3841, \; -0.1285, \; 1.599, \; 15.78, \; 692.3\} \\
\lambda_{\mathrm{M}^{(4)}_{(\mathrm{int})}} &= \{-6.114, \; -1.034, \; -0.3399, \; -0.1159, \; 1.519, \; 15.59, \; 692.7\} \\
\lambda_{\mathrm{M}^{(5)}_{(\mathrm{int})}} &= \{-5.610, \; -0.7753, \; -0.1914, \; -0.05982, \; 1.264, \; 13.27, \; 683.4\} \\
\lambda_{\mathrm{M}^{(6)}_{(\mathrm{int})}} &= \{-5.642, \; -0.8702, \; -0.1649, \; -0.03704, \; 1.223, \; 12.84, \; 683.7\} \\
\lambda_{\mathrm{M}^{(7)}_{(\mathrm{int})}} &= \{-5.631, \; -0.8009, \; -0.1331, \; 0.01270, \; 1.155, \; 11.40, \; 675.4\} \\
\lambda_{\mathrm{M}} &= \{-5.631, \; -0.8009, \; -0.1331, \; 0.01270, \; 1.155, \; 11.40, \; 675.4\} \\
\lambda_{\hat{\mathrm{M}}} &= \{-6.453, \; -1.126, \; -0.2944, \; -0.1273, \; 1.214, \; 15.02, \; 690.2\}.
\end{aligned}
$$

Table 8: Algebraic stability eigenvalues for SIRK 5(4)7L[5]SA

Name	SIRK 5(4)7L[5]SA	Radau IIA 9()5L[5]SA
$(s, p, \hat{p}, \mathfrak{q})$	$(7, 5, 4, 5)$	$(5, 9, -, 5)$
γ	$\frac{1}{7} \sim 0.14286$	$-$
γs	1	$-$
$A^{(p+1)}$	$5.41(-4)$	$1.16(-6)$
$A^{(p+2)}$	$9.29(-4)$	$3.28(-6)$
Min. $A^{(\mathfrak{q}+1)}_{(\text{int})}$	$2.06(-5)$	$1.16(-5)$
Max. $A^{(\mathfrak{q}+1)}_{(\text{int})}$	$5.41(-4)$	$3.28(-5)$
$\hat{A}^{(\hat{p}+1)}$	$2.10(-3)$	$-$
$\hat{A}^{(\hat{p}+2)}$	$3.79(-3)$	$-$
$(B, C, E)^{(\hat{p}+1)}$	$(2.12, 2.83, 0.709)$	$-$
$\{R(-\infty), \hat{R}(-\infty)\}$	$\{0, 0\}$	$\{0, -\}$
Min., Max. $\mathbf{A}$	$(-14.8, 13.0)$	$(-0.036, 0.326)$
Min., Max. $\mathbf{b}$	$(-12.8, 9.60)$	$(0.040, 0.312)$
Min., Max. $\hat{\mathbf{b}}$	$(-13.7, 11.6)$	$-$
Min., Max. λ_{M}	$(-5.63, 675)$	$(0.0, 0.020)$
Min., Max. $\lambda_{\hat{\mathrm{M}}}$	$(-6.45, 690))$	$-$
Min., Max. $\lambda_{\mathrm{M}_{(\text{int})}}$	$(-6.35, 693)$	$(-0.021, 0.036)$
$\mathcal{C}$	0.397	0.199
C($\mathbf{A}$)	668565	20.43

Table 9: Stage-order five methods.

4.1 Kaps' Problem

Dekker and Verwer [74] investigate a nonlinear problem (experiment 7.5.2) originally given by Peter Kaps,

$$\dot{y}_1 = -\left(\varepsilon^{-1} + 2\right) y_1 + \varepsilon^{-1} y_2^2, \qquad \dot{y}_2 = y_1 - y_2 - y_2^2, \tag{98}$$

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

$$y_1 = y_2^2, \qquad \dot{y}_2 = y_1 - y_2 - y_2^2, \tag{99}$$

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

4.2 van der Pol's equation

The van der Pol's (vdP) equation may be written as [102]

$$\dot{y}_1 = y_2, \qquad \dot{y}_2 = \varepsilon^{-1}\left[(1 - y_1^2) y_2 - y_1\right]. \tag{100}$$

As $\varepsilon \to 0$, the second equation becomes an algebraic relation, $y_2 = y_1 / \left(1 - y_1^2\right)$ (this corrects an error in [119]). This now constitutes an index-1 differential algebraic system where y_2 has emerged as the algebraic variable as $\varepsilon \to 0$. Unperturbed initial conditions are given by [93, 102]

$$y_1(0) = 2 \qquad y_2(0) = -\frac{2}{3} + \frac{10}{81}\varepsilon - \frac{292}{2187}\varepsilon^2 + \frac{15266}{59049}\varepsilon^3 + \mathcal{O}(\varepsilon^4). \tag{101}$$

4.3 Kreiss' Problem

In 1978, Kreiss [123] gave a particularly difficult singularly-perturbed differential equations problem. A special case of this problem is discussed in §7.5 of [74] for $\mathbf{y}(t) = \{y_1(t), y_2(t)\}^T$ and given by

$$\begin{bmatrix} \dot{y}_1 \\ \dot{y}_2 \end{bmatrix} = E(t) \begin{bmatrix} -\varepsilon^{-1} & 0 \\ 0 & -1 \end{bmatrix} E(t)^{-1} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}, \qquad E(t) = \begin{bmatrix} \cos(t) & -\sin(t) \\ \sin(t) & \cos(t) \end{bmatrix}. \tag{102}$$

Expanding, one finds

$$\begin{aligned} \dot{y}_1 &= -y_1 \sin(t)^2 + y_2 \cos(t)\sin(t) - \frac{1}{\varepsilon}\left[y_1 \cos(t)^2 + y_2 \cos(t)\sin(t)\right] && (103) \\ \dot{y}_2 &= -y_2 \cos(t)^2 + y_1 \cos(t)\sin(t) - \frac{1}{\varepsilon}\left[y_2 \sin(t)^2 + y_1 \cos(t)\sin(t)\right]. && (104) \end{aligned}$$

The solution to this equation is

$$\begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = E(t) \begin{bmatrix} \varepsilon & \varepsilon \\ 1+\varepsilon\lambda_+ & 1+\varepsilon\lambda_- \end{bmatrix} \begin{bmatrix} C_+ \exp(\lambda_+ t) \\ C_- \exp(\lambda_- t) \end{bmatrix}, \qquad 0 \le t \le 2\pi, \tag{105}$$

where

$$\lambda_\pm = -\left(\frac{1+\varepsilon^{-1}}{2}\right) \pm \frac{1}{2}\sqrt{(1-\varepsilon^{-1})^2 - 4}. \tag{106}$$

and consistent initial conditions (ICs) given by

$$\begin{bmatrix} y_1(0) \\ y_2(0) \end{bmatrix} = \begin{bmatrix} \varepsilon & \varepsilon \\ 1+\varepsilon\lambda_+ & 1+\varepsilon\lambda_- \end{bmatrix} \begin{bmatrix} C_+ \\ C_- \end{bmatrix}, \qquad 0 \le t \le 2\pi. \tag{107}$$

Dekker and Verwer note that the solution to this problem exhibits both a smooth and a nonsmooth solution. The amplitude of the two solution components is initiated by the choice of the initial condition parameters C_+ and C_-. This becomes evident by expanding the solutions for small values of the parameter ε. As $\varepsilon \to 0$,

$$\lambda_+ \to -1 - \varepsilon - \varepsilon^2 - 2\varepsilon^3 - 4\varepsilon^4 - 9\varepsilon^5 + \ldots \qquad \lambda_- \to -\varepsilon^{-1} + \varepsilon + \varepsilon^2 + 2\varepsilon^3 + 4\varepsilon^4 + 9\varepsilon^5 \ldots \tag{108}$$

Hence, for small ε, the solution becomes

$$\begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = E(t) \begin{bmatrix} \varepsilon & \varepsilon \\ 1-\varepsilon-\varepsilon^2 & \varepsilon^2 \end{bmatrix} \begin{bmatrix} C_+ \exp(-t) \\ C_- \exp\left(-\varepsilon^{-1} t\right) \end{bmatrix}, \qquad 0 \le t \le 2\pi. \tag{109}$$

Note that for $C_- \neq 0$ and small values of ε, a steep transition layer exists in the $t \to 0$ limit. Dekker and Verwer select the smooth solution by setting $C_+ = 1$ and $C_- = 0$. Thus, as $\varepsilon \to 0$, the equations become

$$\begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = E(t) \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \exp(-t) \\ 0 \end{bmatrix} = \begin{bmatrix} -\exp(-t)\sin(t) \\ +\exp(-t)\cos(t) \end{bmatrix}, \qquad 0 \le t \le 2\pi. \tag{110}$$

which is an index-2 DAE system with y_1 being the algebraic variable [102].

Two sets of initial conditions are studied to establish the performance of the new methods on equations that behave asymptotically as index-2 DAE systems in the limit $\varepsilon \to 0$. The first ICs $\{C_+, C_-\} = \{1, 0\}$ [74], constrain the solution to the smooth manifold, while the second ICs $\{C_+, C_-\} = \{1, 1\}$ [20] excite both the smooth and nonsmooth solution components. A literature survey on this problem reveals various authors [20, 74, 99, 129, 175, 176] have selected a great variety of ICs, $\mathbf{y}_0$. Ultimately, solutions that exist on the nonsmooth manifold result from *inconsistent initial conditions*, and are studied extensively in the DAE literature [85, 139].

4.4 Anticipated Convergence Rates

The global convergence rates on index-2 DAE problems for the stiffly-accurate and stage-order s Radau IIA methods are $\{2s-1, s\}$ for the $\{y, z\}$ variables, respectively (see Hairer and Wanner [102]). Similarly, for index-1 problems, the global convergence rates are expected to be $\{2s-1, s\}$ for the z-variable. From Table 3 in [117], we might expect the present SIRK methods to behave similarly to DIRK-type methods on Kaps' problem and the van der Pol equation where the differential variable order behaves as $\mathcal{O}\left((\Delta t)^p\right) + \mathcal{O}\left(\varepsilon(\Delta t)^{q+1}\right)$ while the algebraic variable behaves as $\mathcal{O}\left((\Delta t)^p\right) + \mathcal{O}\left(\varepsilon(\Delta t)^{q}\right)$. Convergence of Kreiss' problem would be expected to be no better than this.

We remark that it is possible to increase the order of convergence for the index-2, z-variable ($DAE2_z$) for the SIRK methods considered here as well as other stiffly-accurate implicit Runge–Kutta (IRK) methods such as ESDIRK methods. The context here is one in which all ODE order-conditions have been satisfied to at least the order that we wish to obtain. For stage-order $\mathfrak{q}$, stiffly accurate IRKs, the first unsatisfied $DAE2_z$ order conditions are at order $\mathfrak{q}$ [52, 53]. To attain order $\mathfrak{q}$ and order $\mathfrak{q}+1$ for the $DAE2_z$-variable using stiffly-accurate IRKs, we must enforce the following order conditions [52, 53]

$$\tau_a^{[DAE2_z],\mathfrak{q}} \propto \frac{1}{\mathfrak{q}+1}\mathbf{b}^T\mathbf{W}^2\mathbf{c}^{\mathfrak{q}+1} - 1, \tag{111}$$

$$\tau_a^{[DAE2_z],\mathfrak{q}+1} \propto \frac{1}{\mathfrak{q}+2}\mathbf{b}^T\mathbf{W}^2\mathbf{c}^{\mathfrak{q}+2} - 1, \qquad \tau_b^{[DAE2_z],\mathfrak{q}+1} \propto \frac{(\mathfrak{q}+1)!}{\mathfrak{q}+2}\mathbf{b}^T\mathbf{W}^2\mathbf{C}\mathbf{A}^{\mathfrak{q}}\mathbf{c} - 1, \tag{112}$$

which are valid for $\mathfrak{q} = 2, 3$. Possibly, these relations also apply for $\mathfrak{q} > 3$. In cases where the $\mathbf{A}$-matrix is singular, as in the cases of ESDIRK and Lobatto IIIA methods, we define

$$\begin{array}{c|c} \mathbf{c} & \mathbf{A} \\ \hline & \mathbf{b}^T \end{array} = \begin{array}{c|cc} 0 & 0 & \mathbf{0}^T \\ \tilde{\mathbf{c}} & \mathsf{a} & \tilde{\mathbf{A}} \\ \hline & b_1 & \tilde{\mathbf{b}}^T \end{array} \quad \text{with} \quad \mathbf{A} = \begin{bmatrix} 0 & \mathbf{0}^T \\ \mathsf{a} & \tilde{\mathbf{A}} \end{bmatrix}, \quad \mathbf{b}^T = \begin{bmatrix} b_1 \\ \tilde{\mathbf{b}}^T \end{bmatrix}, \quad \mathbf{c} = \begin{bmatrix} 0 \\ \tilde{\mathbf{c}} \end{bmatrix}. \tag{113}$$

where $\mathbf{0}^T$ (composed of zeros), a^T, $\tilde{\mathbf{c}}^T$ and $\tilde{\mathbf{b}}^T$ are vectors of length (s-1), $\{0, \mathsf{a}_i^T\} = a_{i1}$, $\{0, \tilde{\mathbf{c}}^T\} = \mathbf{c}^T$, and $\{b_1, \tilde{\mathbf{b}}^T\} = \mathbf{b}^T$, $\tilde{\mathbf{A}}$ is a square, invertible matrix of dimension $(s-1) \times (s-1)$ and $\tilde{\mathbf{W}} = \tilde{\mathbf{A}}^{-1}$.

For an ESDIRK or a Lobatto IIIA method, we reinterpret these order conditions as

$$\tau_a^{[DAE2_z],\mathfrak{q}} \propto \frac{1}{\mathfrak{q}+1}\tilde{\mathbf{b}}^T\tilde{\mathbf{W}}^2\tilde{\mathbf{c}}^{\mathfrak{q}+1} - 1, \tag{114}$$

$$\tau_a^{[DAE2_z],\mathfrak{q}+1} \propto \frac{1}{\mathfrak{q}+2}\tilde{\mathbf{b}}^T\tilde{\mathbf{W}}^2\tilde{\mathbf{c}}^{\mathfrak{q}+2} - 1, \qquad \tau_b^{[DAE2_z],\mathfrak{q}+1} \propto \frac{(\mathfrak{q}+1)!}{\mathfrak{q}+2}\tilde{\mathbf{b}}^T\tilde{\mathbf{W}}^2\tilde{\mathbf{C}}\tilde{\mathbf{A}}^{\mathfrak{q}}\tilde{\mathbf{c}} - 1. \tag{115}$$

Appendix B contains a seven-stage, stage-order 2 ESDIRK made in attempt to improve the performance of this class of methods on Kreiss' problem by imposing these three order conditions. Note that the order conditions given by Cameron [52, 53] do not permit the evaluation of truncation errors but do permit the satisfaction of particular order conditions.

5 Discussion

In Section 3, ten new SIRK methods were designed as well as two test methods targeted at index-2 DAE order conditions, one SIRK and one ESDIRK. The ten methods have stage-order three, four or five, from four to eight stages, formal orders-of-accuracy, $p = \{3, 4, 5, 6\}$ and include an embedded method with order $p - 1$. Compared to the stage-order three and four Radau IIA methods, the new SIRK methods have similar stability properties and small coefficient magnitudes. However, the stage-order five SIRK does not share the exemplary properties of the stage-order five Radau IIA method. Some important differences between the SIRKs and the Radau IIA methods should be mentioned. The SIRK methods are internally L-stable while the Radau IIA methods are not but the Radau IIA methods are algebraically stable while the SIRKs are not. During implementation, the SIRK methods with $\mathbf{A}$ matrices having larger condition numbers, may cause challenges that Radau IIA methods, with their smaller condition numbers, do not. Next, Radau IIA methods exhibit an order of $p = 2\mathfrak{q} - 1$ while the SIRKs considered here have $p = \{\mathfrak{q}, \mathfrak{q} + 1, \mathfrak{q} + 2\}$. Alternatively, $p - \mathfrak{q}$ equals $\mathfrak{q} - 1$ for Radau IIA methods and $\{0, 1, 2\}$ for the SIRK methods. This quantity is often related to a worst-case order reduction of the method. For very stiff problems, the stage-order may be at least as important as the formal order, p, of the method. Lastly, the new SIRK methods have an embedded method while embedded methods for Radau IIA schemes generally require a more complicated two-step embedded method. All together, we believe that at stage-orders three and four, the SIRK methods are competitive with the Radau IIA methods in terms of their properties or, at least, not uncompetitive.

The goal of the limited testing discussed below is to establish whether methods are appropriate for general purpose settings and are free of substantial shortcomings based on their convergence behavior on the three singular-perturbation test problems. However, the behavior of any of these methods on these singular perturbation problems do not necessarily reflect the precise performance that will be seen when integrating very large systems of couple ODEs. The methods being tested include:

- Stage-order two methods: ESDIRK4(3)7L[2]SA [119], ESDIRK4(3)7L[2]SA_DAE, ESDIRK4(3)8L[2]SA [55], ESDIRK5(4)8L[2]SA [119], ESDIRK6(5)9L[2]SA [119],
- FIRK methods:

  Gauss methods - $\mathfrak{q} = \{1, 2, 3, 4\}$ where $p = 2s$ and $\mathfrak{q} = s$

  Lobatto IIIC methods - $\mathfrak{q} = \{1, 2, 3, 4, 5\}$ where $p = 2s - 2$ and $\mathfrak{q} = s - 1$

  Radau IIA methods - $\mathfrak{q} = \{2, 3, 4, 5\}$ where $p = 2s - 1$ and $\mathfrak{q} = s$
- Stage-order three SIRK methods: SIRK 3(2)4L[3]SA, SIRK 3(2)5L[3]SA, SIRK 4(3)5L[3]SA, SIRK 4(3)5L[3]SA_DAE, SIRK 5(4)5L[3]SA and
- Stage-order four SIRK methods: SIRK 4(3)6L[4]SA, SIRK 5(4)6L[4]SA, SIRK 5(4)7L[4]SA, SIRK 6(5)7L[4]SA, SIRK 6(5)8L[4]SA
- Stage-order five SIRK methods: SIRK 5(4)7L[5]SA.

The two methods, ESDIRK4(3)7L[2]SA_DAE and SIRK 4(3)5L[3]SA_DAE are included to see the effect of increasing the order of accuracy of the $DAE2_z$ variable. While the benefit is subject to testing, the loss in $A^{(5)}$ in ESDIRK4(3)7L[2]SA_DAE was a full order of magnitude relative to ESDIRK4(3)7L[2]SA as three new order conditions were imposed. As only one new order condition was imposed with SIRK 4(3)5L[3]SA_DAE, it is much more similar to SIRK 4(3)5L[3]SA.

Absent from the list of methods above are any of the methods described in Appendix E. From those methods, the DESI methods appear to be a substantial improvement upon the SIRKs from the STRIDE code. The six- and seven-stage methods, with stage-order three and four seem the most promising. Implementation concerns given the multiple values of γ_i keep us from delving deeply into MIRKs.

5.1 Solver Mechanics

There is a potential for excessive ill-conditioning in the **A**-matrices of SIRK methods. This ill-conditioning combined with exceedingly small values of the parameter ε, rendered the Newton iteration matrices of dimension $(2s, 2s)$ extremely ill-conditioned. Condition numbers as high as 10^{14} were encountered when solving the SIRK matrices. As a consequence of this ill-conditioning, Newton's method occasionally failed to converge to the specified target threshold.

Two modifications of the iterative solver mechanics were necessary to ensure reliable iterative convergence. First, 128-bit arithmetic was used for all test simulations, with a target convergence threshold set at 10^{-23}. This provided a working precision of approximately 26 digits and allowed much deeper convergence studies to be performed. A second necessity was the use of orthogonal inversion techniques. Specifically, orthogonal Householder reflectors were used to invert all matrices. Despite these solver augmentations, an attempt to design a nine-stage SIRKs with a condition number of 386208 resulted in a method where we were unable to simulate parameter values in the range $10^{-8} \leq \varepsilon \leq 10^{-5}$ for van der Pol's equation. This method was abandoned. This experience reinforces Bendtsen's assertion [9] that high-quality SIRKs with more than nine stages are infeasible.

5.2 Convergence

A convergence test was performed using each method on each of the three singular perturbation problems (SPPs) discussed above. Each method used the same initial conditions, time interval and sweep of stiffness parameters, ε from the interval $10^{-8} \leq \varepsilon \leq 10^{0}$. The solution error was tabulated as a function of timestep Δt over a range of timesteps. The largest timestep was chosen so that all methods achieve an order property at the coarsest timestep. The smallest timestep was adjusted to ensure that design order solution accuracy was observed well above the specified convergence threshold. (Typically three to four orders of magnitude variation in timestep was sufficient.) Convergence rates were determined by measuring the slope of a least-squares fit to the logarithm of the solution and timestep data. Convergence plots are provided for both the differential and algebraic variables.

Ultimately, we wish to understand the degree to which the new SIRK methods perform as well as the Radau IIA methods on these three test problems. The convergence-rate plots can be a bit deceiving when FIRK methods are compared to non-FIRK methods because Gauss, Lobatto IIIC, Radau IIA plots contain a range of stage-orders while the ESDIRK and SIRKs all have the same stage-order but different formal order. Severe order-reduction presents another complication when measuring the convergence rate of a method. Typically two distinct orders of accuracy are observed, 1) the step order is observed for large timesteps, while the stage order dominates for small timesteps. No attempt was made to untangle these two rates. The reported convergence rate is therefore an average of the two rates observed over the specified Δt range.

The order of presentation will be Kaps' problem, vdP' equation and then Kreiss's problem in the smooth and nonsmooth cases. For methods, we show ESDIRKs first as they represent ideal low-cost performance for problems requiring only stage-order two methods. Next, we show Gauss, Lobatto IIIC and Radau IIA to see what performance is available at high implementation costs. Lastly, we show the new SIRK methods.

We reiterate the disclaimer about the generality of our SPP tests. Although these tests effectively identify undesirable integration behavior and are a necessary condition for further investigation of a new SIRK, they are not sufficient to predict the efficacy/performance that will be encountered when integrating very large systems of couple ODEs.

5.2.1 Kaps' Problem

Kaps' problem is a challenging test for a stiff integrators although it is the least difficult of the three test problems considered. The first integrators tested are those that presently exist in the open literature. This paper seeks to find methods which have implementation costs close to that of ESDIRKs yet the accuracy and stability of the best FIRK methods.

- **ESDIRK**, Figure 1: At the extreme values of ε, the differential variable converges at design order. For intermediate stiffness, $\varepsilon \sim 10^{-3} - 10^{-4}$, the fifth- and sixth-order method exhibit reduced convergence rates of ~ 3.5. In the case of the algebraic variable, methods exhibit their formal order only with no stiffness. All methods order reduce but the fortified method, ESDIRK4(3)7L[2]SA_DAE, recovers its convergence rate better at $\varepsilon \sim 10^{-4} - 10^{-8}$ than the other ESDIRKs.

- **Gauss** $p(\mathfrak{q})$, Figure 2: In spite of not being L-stable, the four Gauss methods retain convergence rate of at least their stage-order ($\mathfrak{q} = s$) as stiffness increased (ε is reduced). Interestingly, methods with an odd number of stages seem to behave better than those with an even number of stages. This may be related to the fact that Gauss methods with an odd number of stages have one real eigenvalue to their **A**-matrices (see Table 3). This is apparent in both the differential and algebraic variables. At $\varepsilon = 1$, each Gauss method exhibits its design order; $p = 2s$.

- **Lobatto IIIC** $p(\mathfrak{q})$, Figure 3: These methods have order $p = 2s - 2$ and stage-order $\mathfrak{q} = s - 1$. Alternatively, the difference between formal order and stage-order is $s-1$. Relative to Gauss methods of the same p and $\mathfrak{q}$, the convergence rate recovers from order reduction better at $\varepsilon \sim 10^{-4} - 10^{-8}$. It is possible that the $s = 6$, Lobatto IIIC is manifesting reduced convergence rates at $\varepsilon = 1$ due to loss of numerical precision. Unsurprisingly, order reduction is manifested in the algebraic variable more than the differential variable.

- **Radau IIA** $p(\mathfrak{q})$, Figure 4: These methods have order $p = 2s - 1$ and stage-order $\mathfrak{q} = s$. Like the Lobatto IIIC methods, $p - \mathfrak{q} = s - 1$. Qualitatively, the Lobatto IIIC and Radau IIA methods have the same stage-order and behave similarly. However, the Radau IIA methods appear to show less variation in convergence rates with changes in the stiffness parameter, ε. It is possible that the $s = 5$ Radau IIA is manifesting reduced convergence rates at $\varepsilon = 1$ due to loss of numerical precision.

- **SIRK** Stage-order 3, Figure 5: All stage-order three SIRKs appear to be remarkably insensitive to all values of the stiffness parameter. There is virtually no order reduction for the differential variable. Only the fifth-order method displays nontrivial order reduction on the algebraic variable where the observed convergence rate drops to $\mathfrak{q} + 1$.

- **SIRK** Stage-orders 4 and 5, Figure 6: As with the $\mathfrak{q} = 3$ SIRK methods, the $\mathfrak{q} = 4$ SIRK methods show modest sensitivity to stiffness though a bit more. Order reduction is most apparent in the 6(5)-pairs where $p = \mathfrak{q} + 2$. All stage-order three and four methods recover their design order, p at the extreme values of the stiffness parameter. In spite of less than ideal properties, the stage-order five SIRK shows virtually no order reductions.

All methods tested on Kaps' problem behaved well with convergence rates that never dropped below the stage-order. ESDIRK and SIRK methods showed increased order reduction as $p - \mathfrak{q}$ was increased. Both stage-order three and four SIRK methods were only modestly sensitive to the stiffness parameter, unlike the ESDIRKs. The stage-order five SIRK performed quite well, exhibiting virtually no order reduction. Of the three classes of FIRK methods, Gauss methods seemed least suited to solving stiff problems. Both Lobatto IIIC and Radau IIA methods performed well although the Radau IIA methods appeared less sensitive to the stiffness parameter.

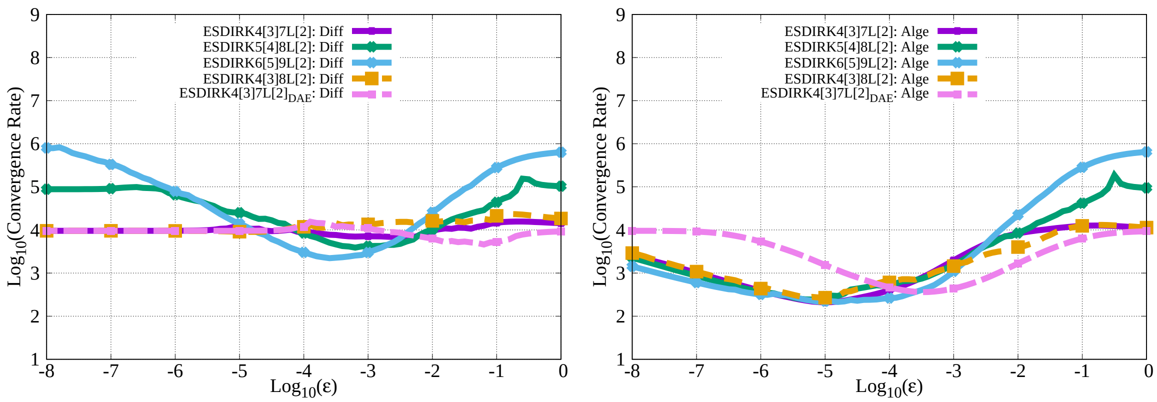

Figure 1: A convergence-rate comparison on Kaps' problem between ESDIRK methods; differential variable (left) and algebraic variable (right)

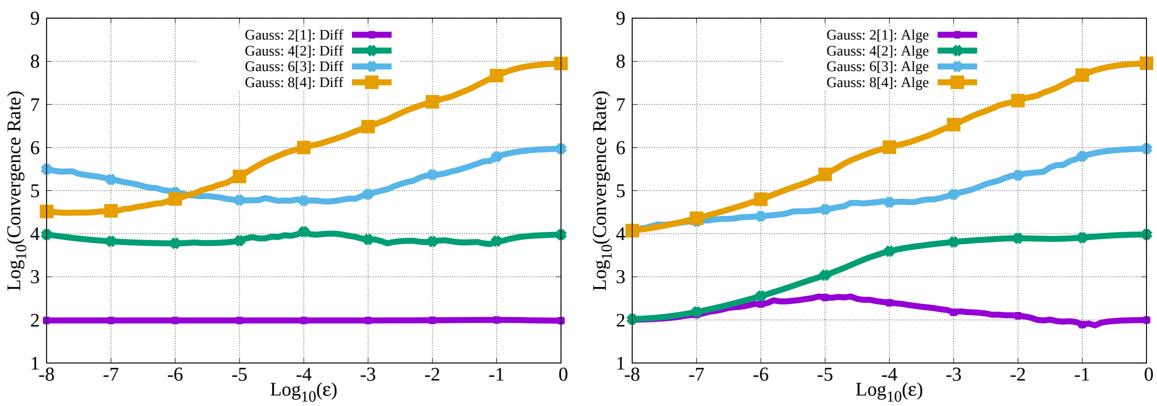

Figure 2: A convergence-rate comparison on Kaps' problem between Gauss methods; differential variable (left) and algebraic variable (right)

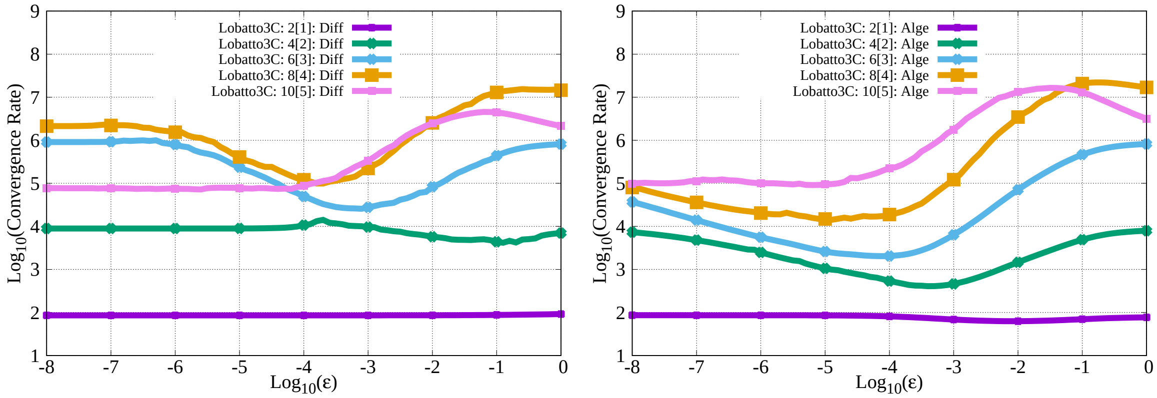

Figure 3: A convergence-rate comparison on Kaps' problem between Lobatto IIIC methods; differential variable (left) and algebraic variable (right)

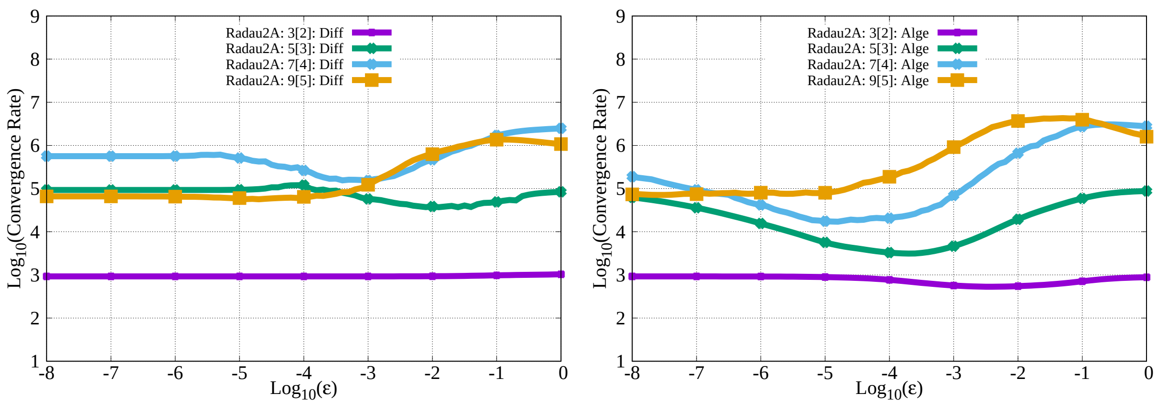

Figure 4: A convergence-rate comparison on Kaps' problem between Radau IIA methods; differential variable (left) and algebraic variable (right)

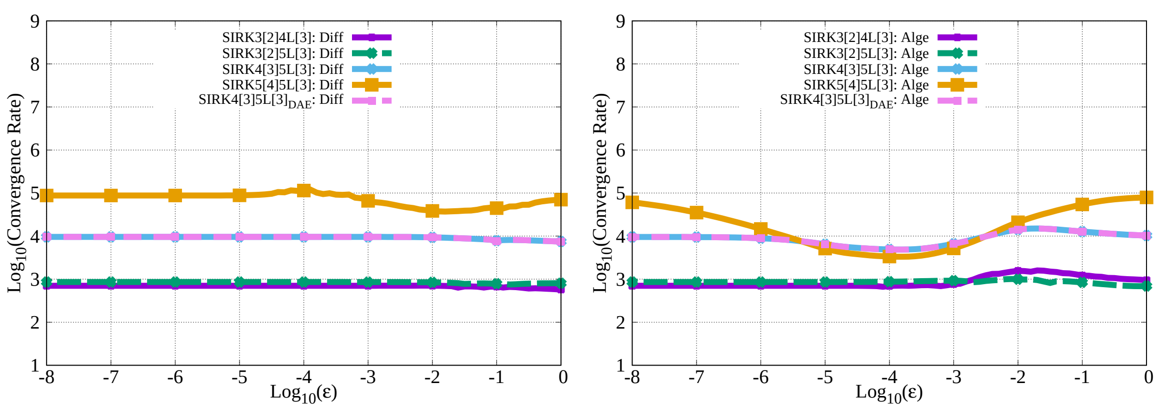

Figure 5: A convergence-rate comparison on Kaps' problem between stage-order three SIRK methods; differential variable (left) and algebraic variable (right)

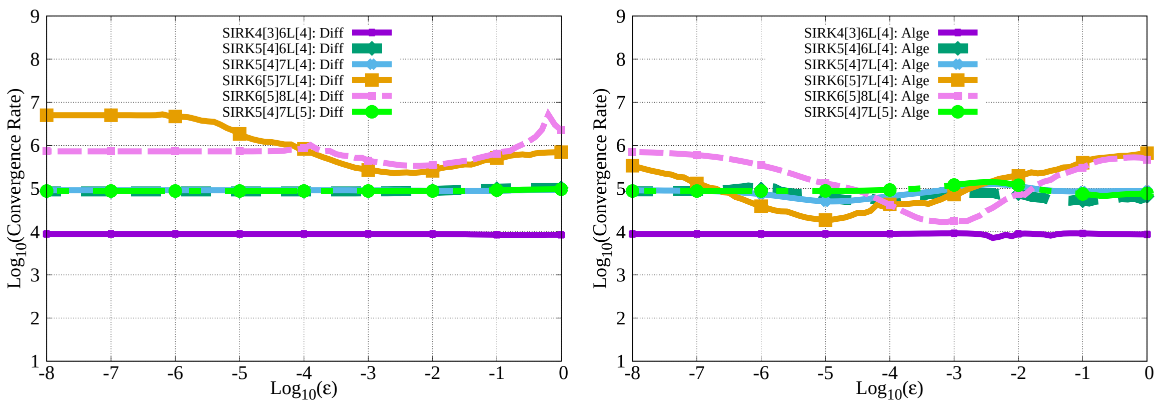

Figure 6: A convergence-rate comparison on Kaps' problem between stage-orders four and five SIRK methods; differential variable (left) and algebraic variable (right)

5.2.2 van der Pol's Equation

The van der Pol equation is probably the most challenging singular-perturbation test problem commonly used to test stiff integrators with the caveat that it tends to an index-1 DAE as the stiffness parameter tends to zero. Performance of all methods on the vdP equation will be no better than on Kaps' problem and often noticeably worse.

- **ESDIRK**, Figure 7: Relative to Kaps' problem, ESDIRK methods display slightly lower convergence rates for both the differential and algebraic variables on the vdP equation. The ESDIRK4(3)7L[2]SA_DAE method loses a full order in its convergence rate on the differential variable. On the algebraic variable, it is unable to recover fourth-order at $\varepsilon = 10^{-8}$ as it did on Kaps' problem.

- **Gauss** $p(\mathfrak{q})$, Figure 8: Gauss methods perform similarly on the vdP equation as they do on Kaps' problem. That is, they retain convergence rate of at least their stage-order ($\mathfrak{q} = s$) as stiffness increased (ε is reduced).

- **Lobatto IIIC** $p(\mathfrak{q})$, Figure 9: Lobatto IIIC methods perform similarly on the vdP equation as they do on Kaps' problem. Again, unlike the Gauss methods, the Lobatto IIIC methods tend to display a recovery in their convergence rates from $\varepsilon \sim 10^{-4} - 10^{-8}$. However, the tenth-order method behaves differently, a likely artifact of insufficient numerical precision during testing.

- **Radau IIA** $p(\mathfrak{q})$, Figure 10: Radau IIA methods perform similarly on the vdP equation as they do on Kaps' problem. They perform similarly to the Lobatto IIIC methods, that is to say they perform very well. The ninth-order method here is likely displaying insufficient numerical precision during testing.

- **SIRK** Stage-order 3, Figure 11: All stage-order three SIRK methods perform similarly on the vdP equation as they do on Kaps' problem. There is no obvious order reduction in the differential variable and a modest amount in the algebraic variable.

- **SIRK** Stage-orders 4 and 5, Figure 12: All stage-order four and five SIRK methods perform similarly on the vdP equation as they do on Kaps' problem. Order reduction seen in the differential variable is highest for the sixth-order methods where $p - \mathfrak{q} = 2$. For the algebraic variable, order reduction reduces the worst convergence rate by approximately one.

All methods tested on vdP's equation behaved much as they did on Kaps' problem, with the exception of the ESDIRK methods, which seemed to struggle more on vdP's equation. This is an encouraging result for the newly designed SIRK methods. Methods of orders nine and ten appeared to suffer from inadequate precision used during testing.

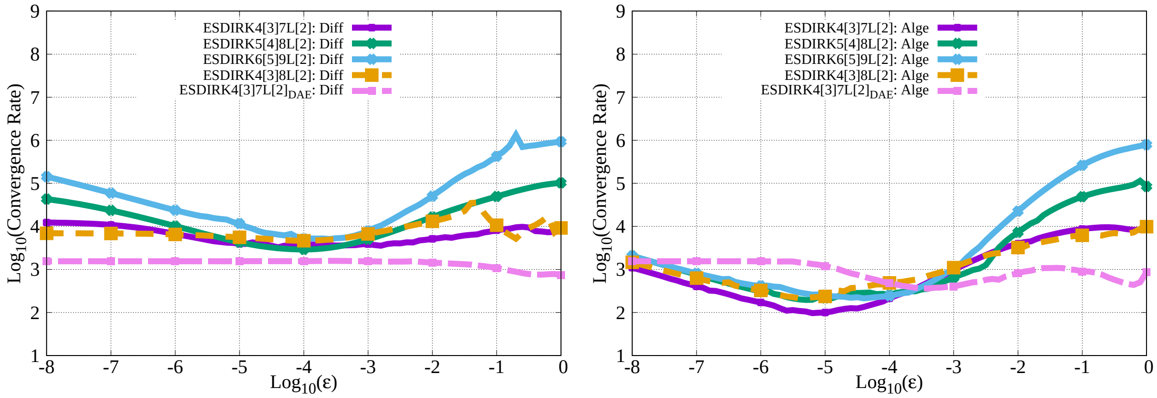

Figure 7: A convergence-rate comparison on van der Pol's equation between ESDIRK methods; differential variable (left) and algebraic variable (right)

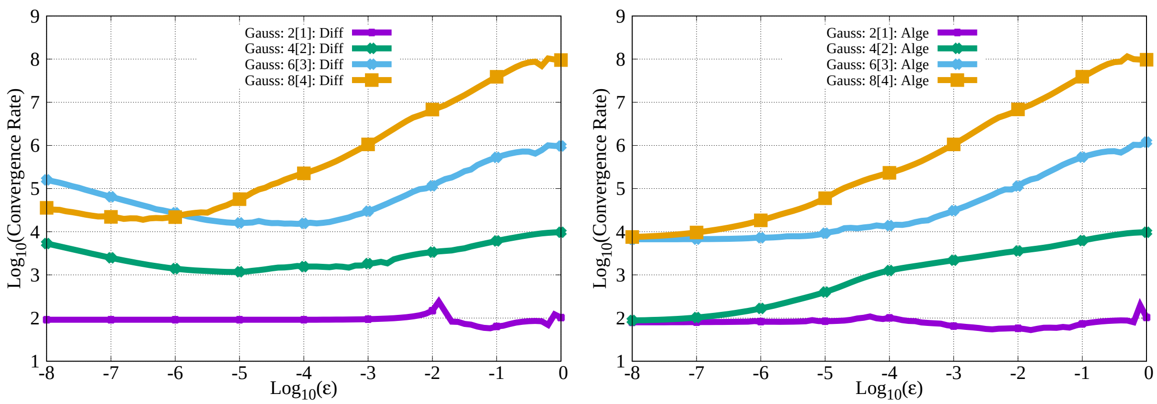

Figure 8: A convergence-rate comparison on van der Pol's equation between Gauss methods; differential variable (left) and algebraic variable (right)

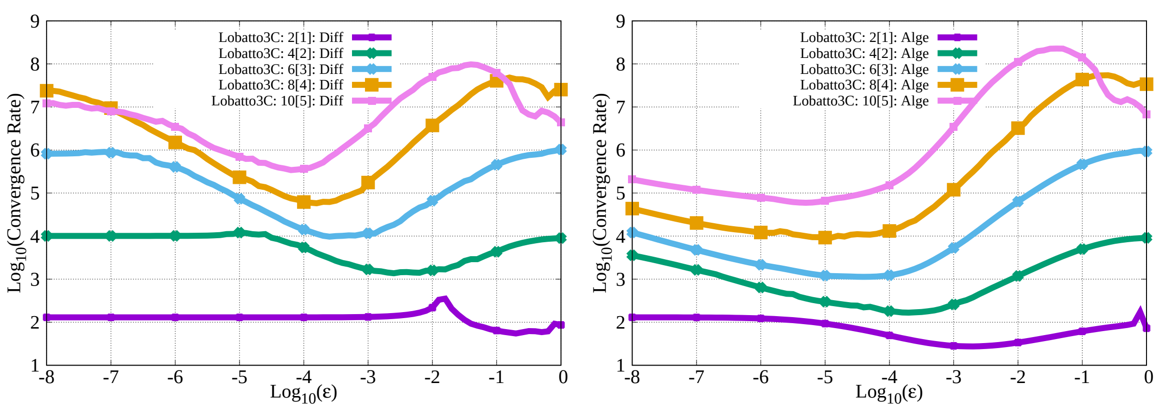

Figure 9: A convergence-rate comparison on van der Pol's equation between Lobatto IIIC methods; differential variable (left) and algebraic variable (right)

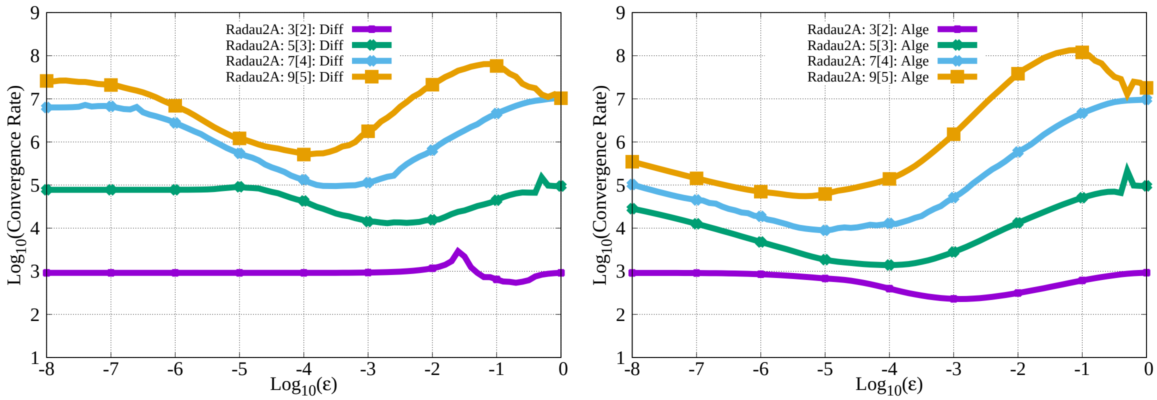

Figure 10: A convergence-rate comparison on van der Pol's equation between Radau IIA methods; differential variable (left) and algebraic variable (right)

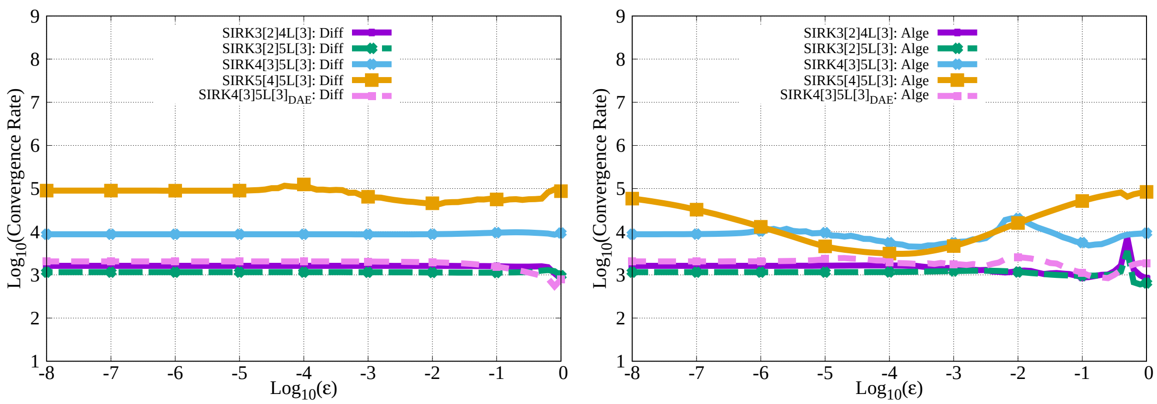

Figure 11: A convergence-rate comparison on van der Pol's equation between stage-order three SIRK methods; differential variable (left) and algebraic variable (right)

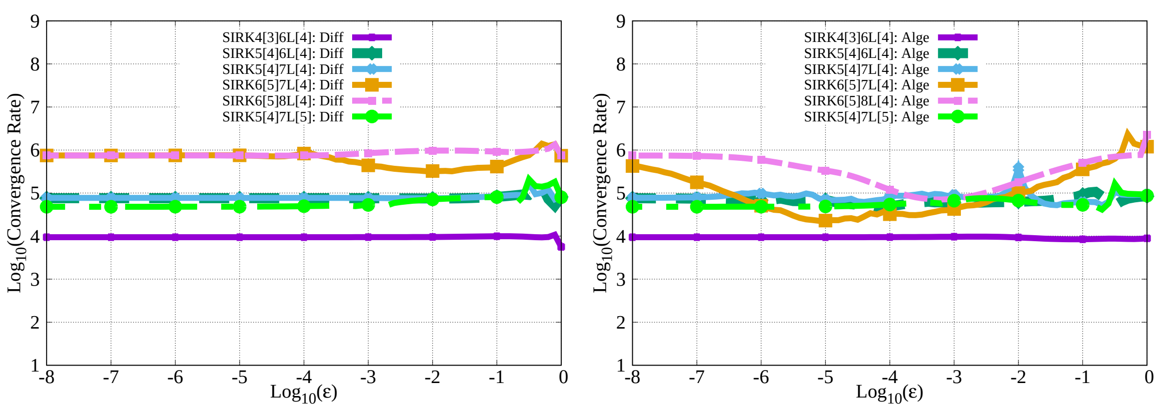

Figure 12: A convergence-rate comparison on van der Pol's' equation between stage-orders four and five SIRK methods; differential variable (left) and algebraic variable (right)

5.2.3 Kreiss' Problem

Kreiss' problem is different from the preceding two test equations in that it tends to an index-2 DAE set of equations as the stiffness parameter tends to zero while the other two tend to index-1 equations. Depending on the choice of initial conditions to Kreiss' problem, one encounters a smooth or nonsmooth solution, the latter being more challenging for the integration method.

- **ESDIRK**, Figures 13,14: On Kreiss's problem, ESDIRK methods generally display a monotonic decline in convergence rates as the stiffness parameter is reduced and stiffness is increased, for both the smooth and nonsmooth solutions. For the smooth solution, the differential variable order reduces to third-order for all ESDIRKs by $\varepsilon = 10^{-8}$ but between second- and third-order in the nonsmooth case. For the algebraic variable, the behavior of the solution was less sensitive to the initial conditions. However, the ESDIRK4(3)7L[2]SA_DAE method behaved differently on the smooth and nonsmooth solutions at $\varepsilon = 10^{-8}$. Convergence rates on the smooth solution are higher than those for the nonsmooth solution.

- **Gauss** $p(\mathfrak{q})$, Figures 15,16: Gauss methods appear to be quite sensitive to whether the stiff component is present. This may be cause by the lack of stiff-accuracy and the lack of L-stability. On the smooth solution, the methods perform very well for the differential variable but less so on the algebraic variable. The behavior of the eighth-order method is confusing. On the nonsmooth solution, Gauss methods behave very poorly.

- **Lobatto IIIC** $p(\mathfrak{q})$, Figures 17,18: Lobatto IIIC methods appear to solve the smooth and nonsmooth solutions with similar rates of convergence. For the $\mathfrak{q} = \{1, 2, 3\}$ methods, the differential variable exhibits no order reduction. At higher stage-order, numerical precision may be influencing the results whereby there seems to be noticeable order reduction. For the algebraic variable, the methods appear to manifest their formal order of accuracy with no stiffness and then degrade to convergence rates near their stage-order.

- **Radau IIA** $p(\mathfrak{q})$, Figures 19,20: The performance of the Radau IIA methods is strong and is similar to that of the Lobatto IIIC methods. Though the convergence rates for the nonsmooth solution degrade for the differential variable, they are still quite good.

- **SIRK** Stage-order 3, Figures 21,22: For the smooth solution, the differential variable seems largely unaffected by stiffness and the algebraic variable is only modestly impacted by the stiffness. However, when inconsistent initial conditions are chosen, the convergence rates of these SIRKs suffer greatly. Ultimately, at $\varepsilon = 10^{-8}$, both differential and algebraic variables return to a convergence rate equal to their stage-order. At intermediate stiffness values, the order reduction is severe enough for a convergence rate well below the stage-order. It is unclear what is causing such a severe order reduction. Note that the 4(3) pair which satisfies one $DAE2_z$ order condition fares no better than the other SIRKs. In order of severity of order reduction, it appears that SIRK 3(2)4L[3]SA $<$ SIRK 5(4)5L[3]SA $<$ SIRK 4(3)5L[3]SA $<$ SIRK 4(3)5L[3]SA_DAE $<$ SIRK 3(2)5L[3]SA. This order does not correlate with properties such as the condition number of **A**-matrix, γ, s, the eigenvalues of either the step or internal algebraic stability matrices or the maximum coefficient magnitudes. Although there is high confidence that all FIRKs and SIRKs were identically implemented, one should never discount implementation issues as a possible cause of inconsistent results.

- **SIRK** Stage-orders 4 and 5, Figures 23,24: Convergence rates for the stage-order four SIRKs, on the smooth solution resemble the third-order SIRKs except with a bit more order reduction. A similar story may be told for the nonsmooth solution. Both differential and algebraic variables suffer massive order reduction here. One can ask what is the difference between the stage-order three and stage-order four methods. In order of severity of order reduction, it appears that SIRK 4(3)6L[4]SA < SIRK 6(5)7L[4]SA < SIRK 5(4)6L[4]SA < SIRK 5(4)7L[4]SA < SIRK 6(5)8L[4]SA. As with the stage-order three methods, the cause for the underperformance is unclear.

All methods considered exhibit convergence behaviors on the smooth solutions to Kreiss' problem that are reminiscent of their behaviors on Kaps' problem and the vdP equation. However, when solving Kreiss's problem with the nonsmooth solution, Radau IIA and Lobatto IIIC were relatively unchanged while ESDIRK, Gauss and SIRK methods collapsed. This behavior appears to be caused by what is called *inconsistent initial conditions* in the DAE literature [85, 139]. What is demonstrated here is that there are certain order conditions, which are satisfied by Radau IIA and Lobatto IIIC methods but not by the ESDIRK and SIRK methods, which dramatically influence the performance of the methods in cases with inconsistent initial conditions.

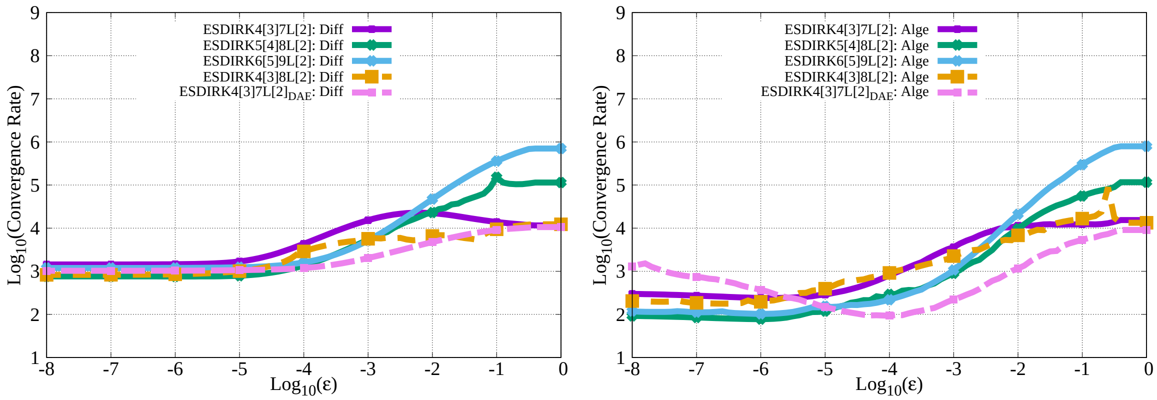

Figure 13: A convergence-rate comparison on Kreiss' problem between ESDIRK methods - smooth solution; differential variable (left) and algebraic variable (right)

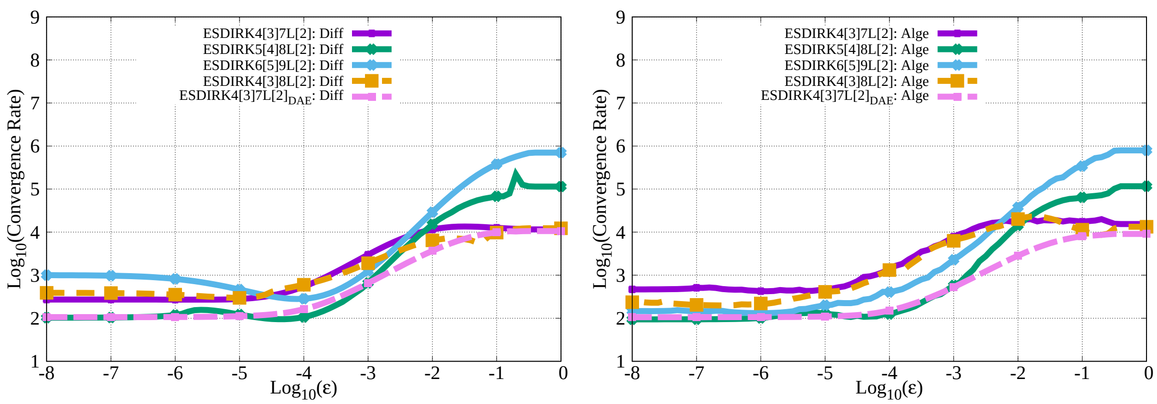

Figure 14: A convergence-rate comparison on Kreiss' problem between ESDIRK methods - nonsmooth solution; differential variable (left) and algebraic variable (right)

It should be noted that a new method considered, SIRK7(6)9L[4]SA, exhibited the negative effects of $\mathbf{A}_s$ matrix ill-conditioning. This is consistent with Bendtsen's remark that methods with more than nine stages are not practical.

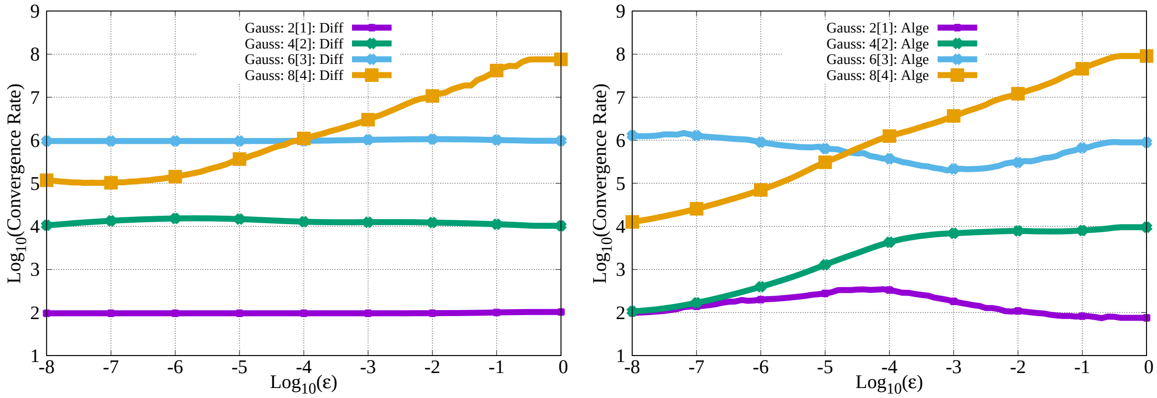

Figure 15: A convergence-rate comparison on Kreiss' problem between Gauss methods - smooth solution; differential variable (left) and algebraic variable (right)

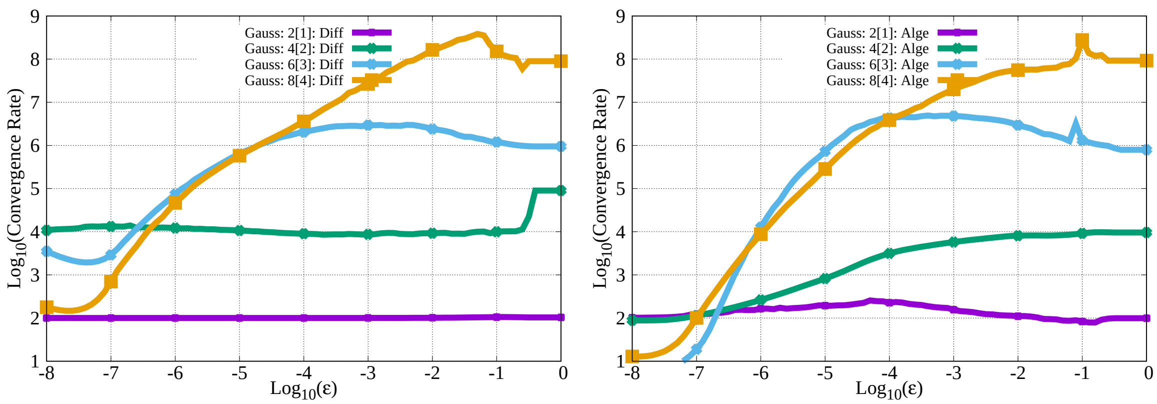

Figure 16: A convergence-rate comparison on Kreiss' problem between Gauss methods - nonsmooth solution; differential variable (left) and algebraic variable (right)

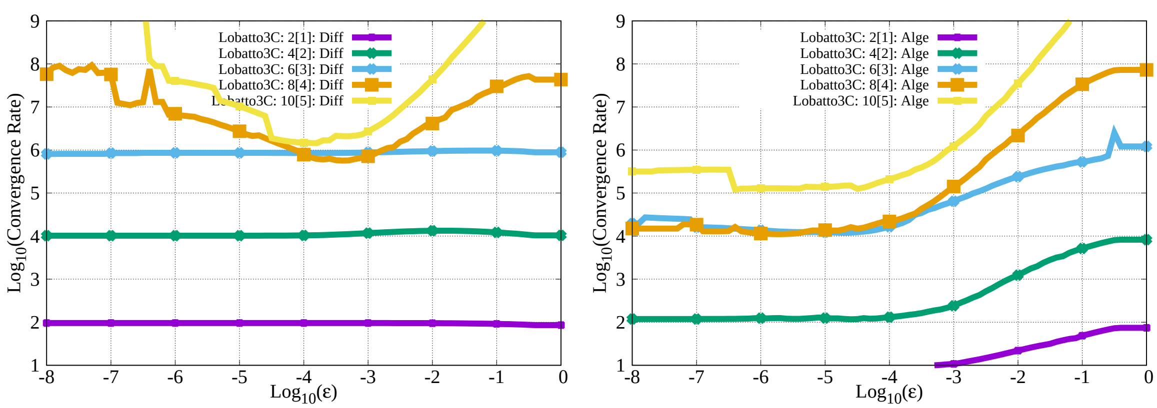

Figure 17: A convergence-rate comparison on Kreiss' problem between Lobatto IIIC methods - smooth solution; differential variable (left) and algebraic variable (right)

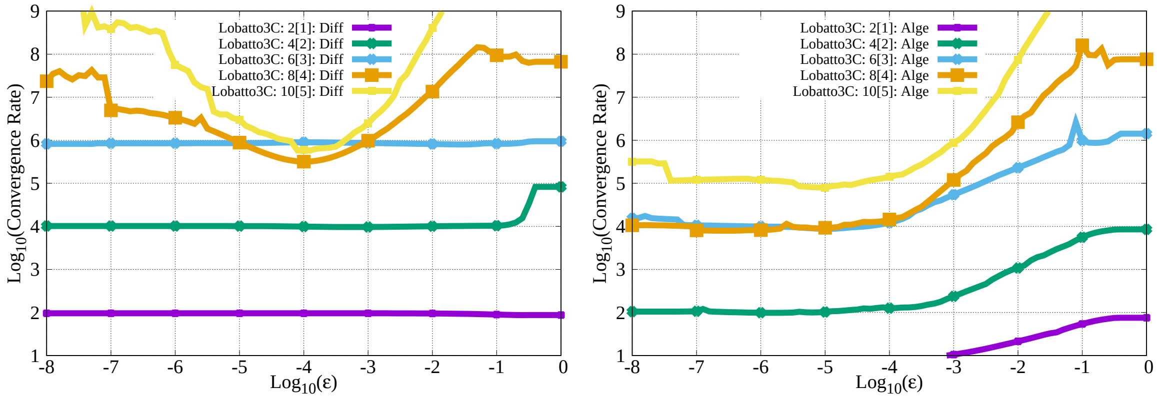

Figure 18: A convergence-rate comparison on Kreiss' problem between Lobatto IIIC methods - nonsmooth solution; differential variable (left) and algebraic variable (right)

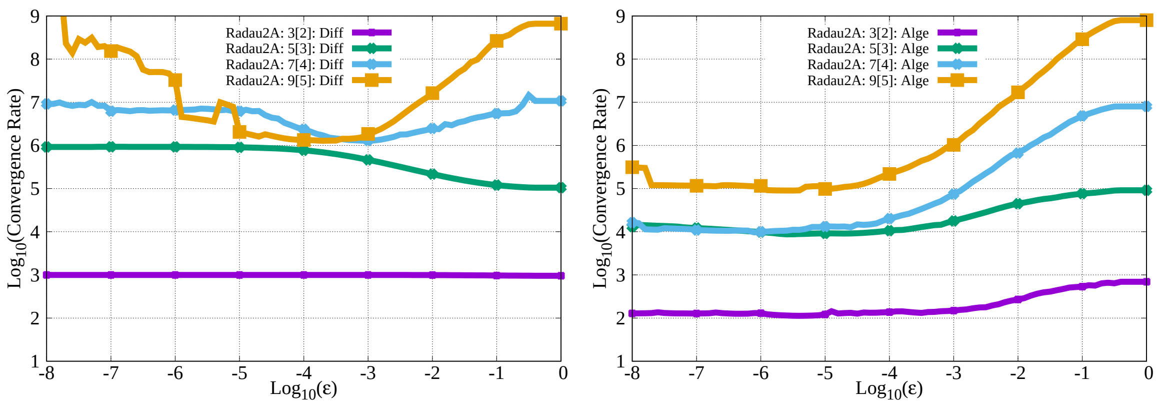

Figure 19: A convergence-rate comparison on Kreiss' problem between Radau IIA methods - smooth solution; differential variable (left) and algebraic variable (right)

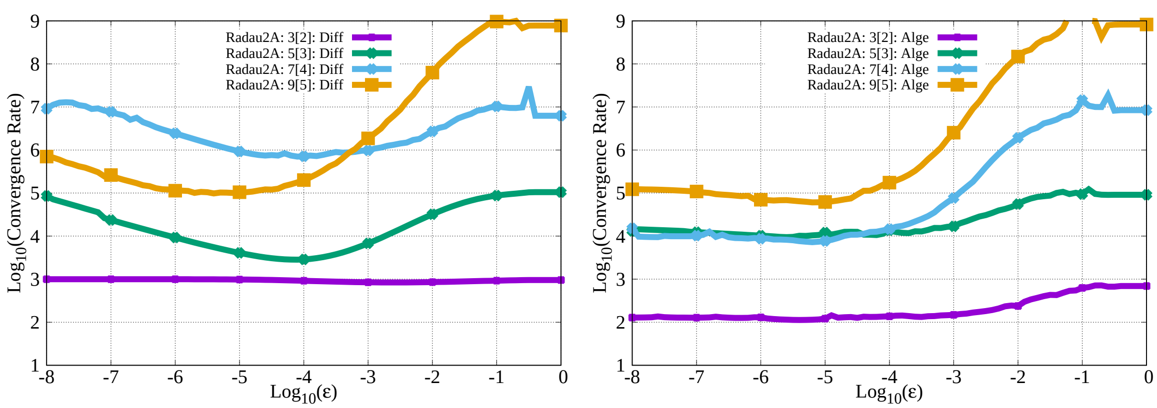

Figure 20: A convergence-rate comparison on Kreiss' problem between Radau IIA methods - nonsmooth solution; differential variable (left) and algebraic variable (right)

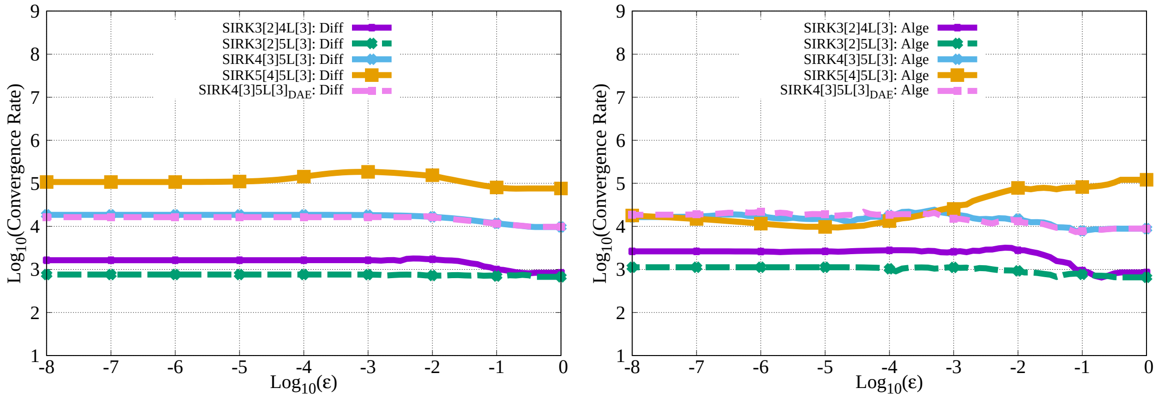

Figure 21: A convergence-rate comparison on Kreiss' problem between stage-order three SIRK methods - smooth solution; differential variable (left) and algebraic variable (right)

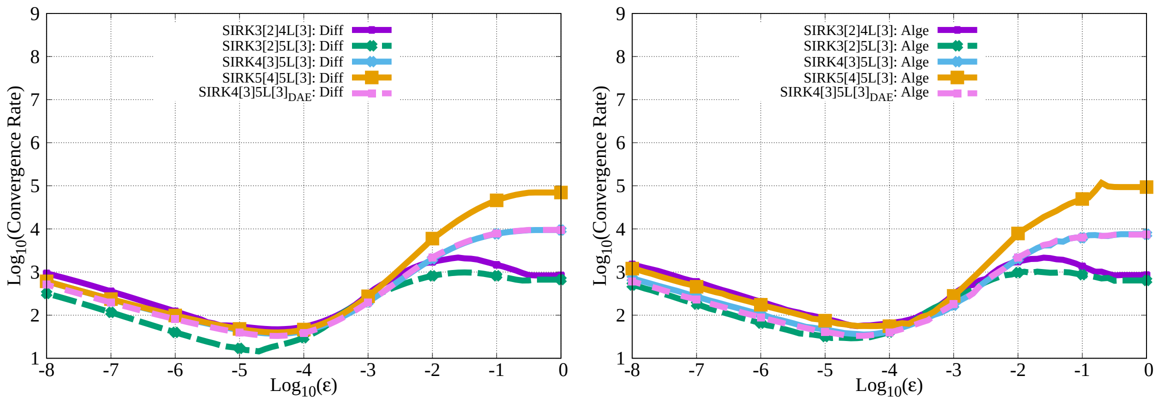

Figure 22: A convergence-rate comparison on Kreiss' problem between stage-order three SIRK methods - nonsmooth solution; differential variable (left) and algebraic variable (right)

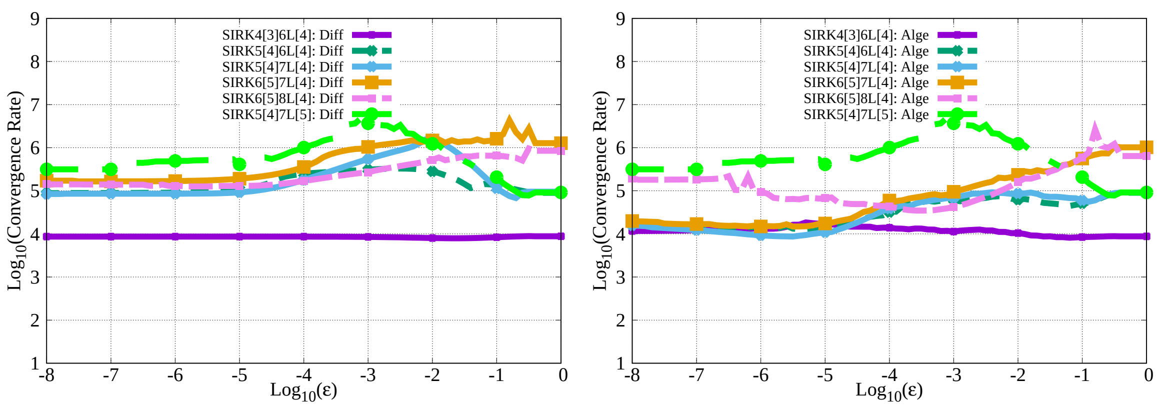

Figure 23: A convergence-rate comparison on Kreiss' problem between stage-order four SIRK and five methods - smooth solution; differential variable (left) and algebraic variable (right)

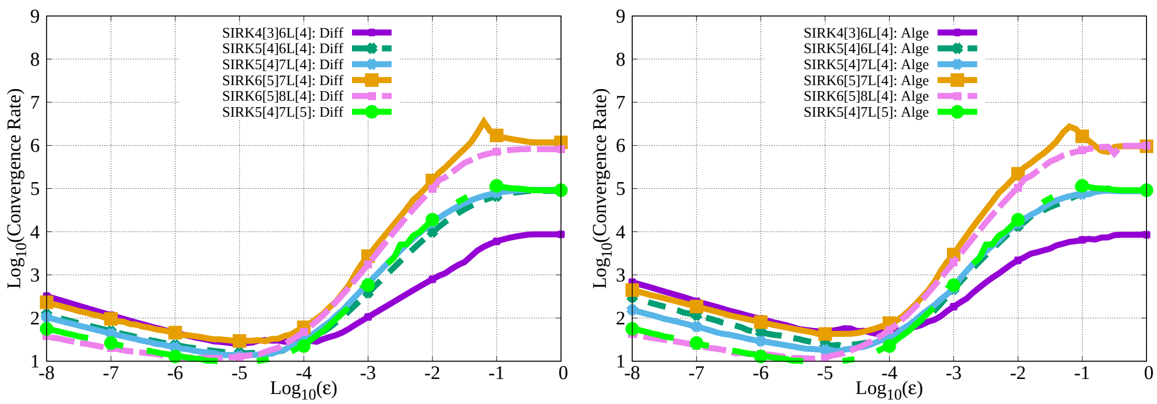

Figure 24: A convergence-rate comparison on Kreiss' problem between stage-orders four and five SIRK methods - nonsmooth solution; differential variable (left) and algebraic variable (right)

6 Conclusions

This paper asks the question of whether there is a class of implicit Runge–Kutta methods that can be made to nearly match the stability and accuracy properties of FIRK methods with respect to the integration of stiff ODEs, while doing so at a lower implementation cost. More specifically, can SIRK methods be made to nearly match the properties of Radau IIA methods but incur a smaller implementation cost similar to that seen with DIRK/SDIRK/ESDIRK methods. As a first step towards this, one must have a strong understanding of the properties possessed by FIRK methods in order to understand the properties required for the new SIRKs. This is the motivation for the contents of Appendix D. The specific properties manifested by Radau IIA methods are then used as the target properties for new SIRK methods. In Section 3, nine primary SIRK methods, having either a stage order of three or four, are identified as having properties not unlike the the Radau IIA methods with the same stage order. In addition, a single stage-order five method is given though it is not similar to a Radau IIA method. This fulfills the first step in our goal.

As a second step towards viable alternatives to Radau IIA methods, a range of methods are tested using three challenging singular-perturbation problems: Kaps' and van der Pol's equations and Kreiss's problem (with consistent or inconsistent initial conditions). In these tests, order reduction of the new SIRKs was minimal except on Kreiss' problem when inconsistent initial conditions are used. However, the relevance of this particular case in the context of stiff ODEs is unclear. Given the minimal order reduction seen in the stage-order three and four SIRKs, and the typically modest increase in matrix condition numbers, this constitutes satisfaction of the second step in our goal.

The last step towards our goal is to show that the new SIRK methods, while offering nearly similar performance to Radau IIA methods, can do so at a reduced implementation cost. We do not demonstrate this but merely suggest that it is plausible. This is a broad and future topic that will require a large investment of time and energy, an investment that will not be made here. Appendix F provides a high-level overview for constructing an efficient/effective preconditioner for SIRK methods, recognizing that a good preconditioner is only one component contributing to the overall efficacy of a method.

Other components of a high-quality, stiff integrator include accurate/reliable error estimators, stepsize controllers like the H321 or PPID controllers shown in Table 2, good stage-value predictors and dense-output methods for all competitive SIRKs. The latter two, dense-output methods and stage-value predictors are not included in this study. A significant advantage of SIRKs over most FIRKs is the availability of $p(p-1)$-pairs of intrastep embedded error estimators. Most FIRKs require previous timestep data to construct $p(p-1)$-pairs. Lastly, all these attributes must be woven into a fully integrated method including iteration control. Note that controlling error while maximizing efficiency [98], is an extremely difficult task and frequently involves both design heuristics and rigorous mathematics.

7 Acknowledgements

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Appendix A

New SIRK Methods

A.1 Stage-Order Three Methods

A.1.1 SIRK3(2)4L[3]SA

$$
\begin{array}{c|c}
\mathbf{c}^T & \mathbf{A} \\
\hline
 & \mathbf{b}^T \\
\hline
 & \hat{\mathbf{b}}^T
\end{array}
=
\begin{array}{c|cccc}
\frac{31}{79} & \frac{4783396728397957}{2266523577527685} & \frac{-2647563713972094}{1144006995361037} & \frac{3210684183084084}{2522776014286931} & \frac{-789724215472725}{1167472046181577} \\
\frac{29}{56} & \frac{2326913609352083}{946022760872741} & \frac{-2464293013905623}{899859900855167} & \frac{1524146046600233}{850770634443326} & \frac{-2234328056230635}{2246047124919004} \\
\frac{83}{94} & \frac{1967360629700260}{777646236567989} & \frac{-2785931316081475}{1023888125223952} & \frac{2406242809268325}{1051139311357133} & \frac{-996035411241107}{819677381399927} \\
1 & \frac{2826975679162216}{1304799141207799} & \frac{-9752127902772385}{4627724292068513} & \frac{1704164157419377}{999023358192832} & \frac{-15977473228921}{20882812500000} \\
\hline
b_i & \frac{2826975679162216}{1304799141207799} & \frac{-9752127902772385}{4627724292068513} & \frac{1704164157419377}{999023358192832} & \frac{-15977473228921}{20882812500000} \\
\hline
\hat{b}_i & \frac{2324884253982426}{1089322965426587} & \frac{-1323224273690905}{652278104980391} & \frac{3590104309545367}{2316912895809890} & \frac{-171016611865999}{261035156250000}
\end{array}
$$

with

$$
\mathbf{S} = \begin{bmatrix}
\frac{-35598175607}{2042266145800} & \frac{70855127022640}{1087087628163049} & \frac{-92185180154961}{177847922536282} & \frac{-3124397266328984}{796156768283083} \\
\frac{511252967}{727436595200} & \frac{120168964844177}{870980255059440} & \frac{-66985075062343}{272674503484474} & \frac{-1340288763559144}{978014920087505} \\
\frac{248721088433}{3440445044800} & \frac{156565323871747}{896721818711178} & \frac{118091608156036}{749539294240793} & \frac{1687072721229563}{1189534600423563} \\
\frac{17}{200} & \frac{8}{125} & \frac{-81}{200} & \frac{-2821}{1000}
\end{bmatrix}
$$

$$
\mathbf{S}^{-1} = \begin{bmatrix}
\frac{-3067444867310023}{861419580928628} & \frac{-4343734214828539}{770355157169917} & \frac{1512263785963235}{603996172071797} & \frac{16234248857669836}{1813553120654515} \\
\frac{4053770465519419}{788344492691004} & \frac{-608334847647063}{832169836655027} & \frac{3060635043003533}{527037027939790} & \frac{-4182338088230930}{1078313650659509} \\
\frac{21442163515680088}{1511003508673003} & \frac{-19996099358799781}{1151691072091846} & \frac{17674610565079579}{1665619203859673} & \frac{-5177758573166287}{867075370575309} \\
\frac{-2583773197838327}{1274090412055651} & \frac{2642973502228511}{1146046058467671} & \frac{-1524486238141067}{1158202221796308} & \frac{372275876746261}{543823242187500}
\end{bmatrix}
$$

and $\mathcal{J}$ is given by (2) with $\gamma = 28/125$. For the Schur decomposition of the **A**-matrix, we have

$$
\mathcal{Q} = \begin{bmatrix}
\frac{181360744760415}{1175111503405571} & \frac{-142924022700197}{302962827868093} & \frac{-517696269002069}{818469907343958} & \frac{-1284231596709874}{2159819943522249} \\
\frac{-6357283204524}{1021602748837585} & \frac{-3138500576575331}{4293770114851474} & \frac{-220039088991413}{2391691877105876} & \frac{57619995479959}{85213974172446} \\
\frac{-553865195896066}{865281226454275} & \frac{-430566631682640}{1033298936865391} & \frac{225971083087147}{436746693251866} & \frac{-349046968300405}{904426113430298} \\
\frac{-425928260770080}{565937824788991} & \frac{233321695056405}{884792657642507} & \frac{-267385592005726}{469923456785049} & \frac{227813881539195}{1135014450643228}
\end{bmatrix}
$$

and

$$
\mathcal{U} = \begin{bmatrix}
\frac{28}{125} & \frac{223051071052461}{370246718881346} & \frac{-549942416813210}{1204974715247227} & \frac{3452275249687981}{689156386452076} \\
\frac{0}{1} & \frac{28}{125} & \frac{-277027125905443}{978852412808415} & \frac{7703590815907195}{1367460729487784} \\
\frac{0}{1} & \frac{0}{1} & \frac{28}{125} & \frac{3167849117778602}{1402177958317911} \\
\frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{28}{125}
\end{bmatrix}
$$

A.1.2 SIRK3(2)5L[3]SA

The SIRK method, SIRK3(2)5L[3]SA, is given by

$$
\begin{array}{c|ccccc}
\frac{21}{82} & \frac{1474281924932186}{1952371688995909} & \frac{-412958667332915}{705587397971974} & \frac{-17485462680611}{295612208184605} & \frac{102948180578905}{368387366634381} & \frac{-83309893875091}{621423359608146} \\
\frac{32}{83} & \frac{1022908247984596}{1138684981116423} & \frac{-547865828466157}{864965008334574} & \frac{-48277366024589}{476358302807563} & \frac{813542730710541}{1804638009268678} & \frac{-282861578962254}{1236038197633837} \\
\frac{94}{143} & \frac{2912697333550337}{3648586350671507} & \frac{-932594326245055}{2453898662595723} & \frac{81734072021249}{565326449230152} & \frac{323646391361143}{1528570816618639} & \frac{-137290418070859}{1171122932455868} \\
\frac{155}{182} & \frac{222462025861571}{269023580306671} & \frac{-66152309156827}{176528479801661} & \frac{1780051060589}{175648863700746} & \frac{575403547004867}{848237090663332} & \frac{-644978865476729}{2231592498092281} \\
1 & \frac{1050379369822896}{1282248443840773} & \frac{-282547194442154}{712449891784871} & \frac{107797719578987}{730701170197158} & \frac{434143421085421}{769012162557214} & \frac{-23231966998411}{172525877589063} \\
\hline
b_i & \frac{1050379369822896}{1282248443840773} & \frac{-282547194442154}{712449891784871} & \frac{107797719578987}{730701170197158} & \frac{434143421085421}{769012162557214} & \frac{-23231966998411}{172525877589063} \\
\hline
\hat{b}_i & \frac{629351645271055}{744047090183874} & \frac{-470917768418927}{1092008561637032} & \frac{195791933442169}{1008363386912982} & \frac{447483981783011}{959093320967504} & \frac{-105421987243244}{1399152155249621}
\end{array}
$$

where $\mathbf{S}$ and $\mathbf{S}^{-1}$ are, respectively.

$$
\begin{bmatrix}
\frac{940957925477}{804523927664814} & \frac{-22266146259683}{1162333382699060} & \frac{370843840514142}{1774618814358539} & \frac{-859605518404753}{719901593213822} & \frac{-821456310150992}{506844155480523} \\
\frac{18299043825104}{6256834044094745} & \frac{850371311002}{211365442547193} & \frac{232620128022729}{811019840519960} & \frac{-703624283060523}{762091566625342} & \frac{6697723188630053}{1320554123102447} \\
\frac{-4388111091513}{1111634013250549} & \frac{35759122997986}{509044251317659} & \frac{-435947238018613}{1272154158660078} & \frac{-4814299926247993}{3540577707478966} & \frac{-17527530328384663}{1514501773982167} \\
\frac{29690606221130}{1679443591659741} & \frac{39858422486127}{509620081523605} & \frac{-43326741639218}{559395044720119} & \frac{1495822732341038}{2102689734150139} & \frac{5567979038450009}{1360735729618720} \\
\frac{31}{1000} & \frac{21}{1000} & \frac{-39}{200} & \frac{-91}{125} & \frac{-677}{100}
\end{bmatrix}
$$

$$
\begin{bmatrix}
\frac{8574152217505918}{1408645669017997} & \frac{-476529033340579}{274279697298505} & \frac{-12662657942920967}{885725004300208} & \frac{7971266665251999}{1077372024825869} & \frac{29234681099829495}{1117856486225722} \\
\frac{8900049737362229}{489602241899391} & \frac{-5988908565348519}{605457763865578} & \frac{709689617488758}{177499423198213} & \frac{23976186100985422}{1455267181997881} & \frac{-8877485556045407}{1027580926787281} \\
\frac{9680239717006527}{832001672159987} & \frac{-3725452351751203}{529276987556900} & \frac{-403100449275749}{322489880857581} & \frac{5825944057729860}{1142951978276809} & \frac{-1074706761179651}{378288265877143} \\
\frac{1748793142003951}{1191437392724954} & \frac{-1031322729207064}{678788343974297} & \frac{-283990338999410}{885991878853821} & \frac{1005805065921484}{1194834161327753} & \frac{-81143826602588}{187435940917295} \\
\frac{-354791932213224}{868089181393541} & \frac{227393710580177}{694365016604106} & \frac{35596023081347}{2044545783065189} & \frac{-131593919016863}{863728081793869} & \frac{43671781121094}{593149588095857}
\end{bmatrix}
$$

and $\mathcal{J}$ is created using (2) and $\gamma = \frac{81}{500}$. For the Schur decomposition of the $\mathbf{A}$-matrix, we have

$$
\mathcal{Q} = \begin{bmatrix}
\frac{58996444619195}{1818053669131507} & \frac{257667362574373}{1213506489053108} & \frac{391906679010757}{1101145230479827} & \frac{-129959203618871}{247234713373779} & \frac{-129726922309611}{174783669444784} \\
\frac{17986809694499}{221662627737099} & \frac{-1209910883141}{1272087693795296} & \frac{821449782300429}{1140098821610971} & \frac{-1170342154359093}{3370142486610709} & \frac{145361029450285}{244420429773343} \\
\frac{-96108943234752}{877526244101327} & \frac{-722317584455991}{933305545723805} & \frac{-215359600448925}{762621487786253} & \frac{-404029055113205}{727674537057372} & \frac{26977838814835}{853262473235316} \\
\frac{160773161249767}{327772117426808} & \frac{-886814598098661}{1589823652237292} & \frac{587118028422419}{1483086341212028} & \frac{513070839261098}{1106546348572213} & \frac{-142780424518803}{516047902827005} \\
\frac{1024049504035917}{1190615019085042} & \frac{101228853452082}{478313077676327} & \frac{-332553195684478}{969191661826049} & \frac{-93800103224574}{332000019662357} & \frac{184964671986740}{1383350542885147}
\end{bmatrix}
$$

and

$$
\mathcal{U} = \begin{bmatrix}
\frac{81}{500} & \frac{-821468972980167}{2224965834444953} & \frac{221118084821687}{560477703542195} & \frac{10863362173142}{1071271522134629} & \frac{-1653126362612113}{1159492216630822} \\
\frac{0}{1} & \frac{81}{500} & \frac{-215454124843346}{913832121515455} & \frac{54785093288519}{454210658532458} & \frac{1769398064220510}{2073579293259967} \\
\frac{0}{1} & \frac{0}{1} & \frac{81}{500} & \frac{315456619398913}{1705679753787811} & \frac{-1275686337862817}{1219503721825754} \\
\frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{81}{500} & \frac{1561715024994547}{1266799612689913} \\
\frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{81}{500}
\end{bmatrix}
$$

A.1.3 SIRK4(3)5L[3]SA

The SIRK method, SIRK4(3)5L[3]SA, is given by

$$
\begin{array}{c|ccccc}
\frac{17}{49} & \frac{2561764438911047}{1939789253777994} & \frac{-1632682096348781}{1145312109265568} & \frac{235429318632550}{446580178534171} & \frac{753193691149766}{1629115422698627} & \frac{-932937740852569}{1735108233142127} \\
\frac{55}{107} & \frac{583764573708861}{381129116922874} & \frac{-835098527363259}{522851745095743} & \frac{645805423011557}{778711094908326} & \frac{3858731724206175}{7955887253791259} & \frac{-941823920383309}{1281750181102200} \\
\frac{62}{71} & \frac{697014030698718}{502721655507907} & \frac{-1772772827174231}{1502834578192291} & \frac{904466620498489}{806555106243156} & \frac{12714387171186}{78374591819131} & \frac{-531194532852658}{860592577411115} \\
\frac{41}{46} & \frac{31197241638190267}{19873208737963304} & \frac{-647383974885653}{422479248163463} & \frac{578642772887107}{635344161767978} & \frac{692734315342246}{767155189738535} & \frac{-1501956758189227}{1564684009360966} \\
1 & \frac{513361653177515}{386823049866276} & \frac{-691676781603508}{651711025093649} & \frac{782479806459993}{1003344489740524} & \frac{553664976816304}{1198001794678177} & \frac{-207922402463867}{409435549695520} \\
\hline
b_i & \frac{513361653177515}{386823049866276} & \frac{-691676781603508}{651711025093649} & \frac{782479806459993}{1003344489740524} & \frac{553664976816304}{1198001794678177} & \frac{-207922402463867}{409435549695520} \\
\hline
\hat{b}_i & \frac{2135761529758181}{1061388085349794} & \frac{-1335550384883183}{560757396067403} & \frac{189667883158228}{1357459306710033} & \frac{916505133693061}{305927250903775} & \frac{-536210124226979}{303613600464194}
\end{array}
$$

where $\mathbf{S}$ and $\mathbf{S}^{-1}$ are, respectively.

$$
\begin{bmatrix}
\frac{459714210720243}{4248533817298400} & \frac{836581187098014}{2073113513869903} & \frac{22685929536080832}{4923441466363193} & \frac{8409671183154463}{567257646244341} & \frac{-134362631025134609}{1464996806146358} \\
\frac{-21248758488421}{9056844646330223} & \frac{-217049106063053}{791448429780142} & \frac{1861661633699858}{1587111873649275} & \frac{725258377970191}{332668887083636} & \frac{-2270846552427277}{73419319789734} \\
\frac{-120748850361625}{396843549408491} & \frac{-1224926305504686}{883349002551967} & \frac{-2807715612829827}{394458608480474} & \frac{-26664044665433248}{795315513016861} & \frac{-6536359006338247}{604712173631931} \\
\frac{-73754167270449}{412473544868800} & \frac{-16411479508440}{988791509682109} & \frac{4982962276928847}{1541148389690456} & \frac{14898168895943721}{818073047793701} & \frac{40617657503407867}{776017626915776} \\
\frac{-23}{100} & \frac{-43}{1000} & \frac{1133}{1000} & \frac{-1987}{1000} & \frac{-94127}{1000}
\end{bmatrix}
$$

$$
\begin{bmatrix}
\frac{1479657908173445}{1192939750132769} & \frac{3284287457374613}{1574016116773814} & \frac{53116994710997}{1063045274489419} & \frac{-774768328248143}{529350877723054} & \frac{-3844810258357645}{1416753815641769} \\
\frac{-1355115954958214}{1039579969335293} & \frac{-110994548223088}{200272711014879} & \frac{-1094873402561725}{1071876856059757} & \frac{-3090433845903283}{4990274073492262} & \frac{1505212802774341}{1228577337360420} \\
\frac{-1901244572373845}{631738880896751} & \frac{2237564711886825}{599167950151337} & \frac{-1611199145776513}{977963981270317} & \frac{-666029438414573}{759802374924066} & \frac{844813927196231}{600413763309813} \\
\frac{4356837846164835}{6234504815312224} & \frac{-356842354406251}{442024655401526} & \frac{346700741738141}{935640226690647} & \frac{375344401311986}{1641087295556381} & \frac{-230776513087673}{697172434252717} \\
\frac{-108026741033017}{2022479523713178} & \frac{82451487525737}{1442778286491687} & \frac{-12321719196554}{451203582797337} & \frac{-9434693987465}{818966230049229} & \frac{16427291560479}{847995789391712}
\end{bmatrix}
$$

and $\mathcal{J}$ is created using (2) and $\gamma = \frac{31}{125}$. For the Schur decomposition of the $\mathbf{A}$-matrix, we have

$$
\mathcal{Q} = \begin{bmatrix}
\frac{289524601441849}{1163754812599436} & \frac{-546821194740631}{4115188022723108} & \frac{557532964956161}{947600216511289} & \frac{373164661075327}{862225623560992} & \frac{274956941376109}{442004411938755} \\
\frac{-2897034983911}{537058957530267} & \frac{166276355970087}{603947313506824} & \frac{826067144943691}{1207278160319848} & \frac{126172704185050}{1106049290674793} & \frac{-693404599172407}{1041830044755591} \\
\frac{-371662360502437}{531263242495828} & \frac{843906991674039}{1334921484168332} & \frac{29272408607167}{861040915283391} & \frac{68345747963574}{735810691041119} & \frac{276282699480821}{868688316169016} \\
\frac{-1068512218225985}{2599045573160872} & \frac{-642318160325479}{1434804383669820} & \frac{395217551228836}{946086781884035} & \frac{-713006032435108}{1077265606922719} & \frac{125775600196465}{937440325355191} \\
\frac{-354826832681789}{670986041300006} & \frac{-553669413225971}{1000100396693679} & \frac{-54978426456385}{550233142143992} & \frac{572256519914321}{963194541676965} & \frac{-203709275719987}{902916506461602}
\end{bmatrix}
$$

and

$$
\mathcal{U} = \begin{bmatrix}
\frac{31}{125} & \frac{-218161015330634}{488813283049989} & \frac{-310236932935181}{713056372909934} & \frac{79053222139850}{454921202677941} & \frac{-2065476230425378}{663304906588651} \\
\frac{0}{1} & \frac{31}{125} & \frac{-183627552950816}{849644506746337} & \frac{313461285599657}{943957943401370} & \frac{-2899873397162253}{6045987949750568} \\
\frac{0}{1} & \frac{0}{1} & \frac{31}{125} & \frac{-4385105261628083}{9416881624874393} & \frac{1133581789376847}{287708408915756} \\
\frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{31}{125} & \frac{4782502237767455}{5752132869594289} \\
\frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{31}{125}
\end{bmatrix}
$$

A.1.4 SIRK5(4)5L[3]SA

The SIRK method, SIRK5(4)5L[3]SA, is given by

$$
\begin{array}{c|ccccc}
\frac{500}{1283} & \frac{2957049942028058}{876045806633349} & \frac{-7367890837823199}{1876855807279201} & \frac{1199044101003599}{1188831840677425} & \frac{1248115473413211}{6584668783623740} & \frac{-399029564166168}{1545295130760569} \\
\frac{438}{929} & \frac{5782601018059159}{1420606742941844} & \frac{-3780135671512331}{757609492392709} & \frac{2937161236252365}{1689468692888797} & \frac{-205751551717192}{1001641746157963} & \frac{-104674590900190}{734142050582233} \\
\frac{1826}{2635} & \frac{7394083672781104}{1319945803780631} & \frac{-8950380810148821}{1187320031645512} & \frac{3375736202914051}{889671208768069} & \frac{-3002156479453317}{2044522098300845} & \frac{91322401030988}{300895169052357} \\
\frac{586}{651} & \frac{1708518008575793}{299075407615103} & \frac{-5400512213871233}{688012371705711} & \frac{2641426696311999}{594917923091426} & \frac{-1125611165168923}{545842097353498} & \frac{562046211519962}{852750518279525} \\
\frac{1}{1} & \frac{22282049043593853}{4308368588372464} & \frac{-9770202945607981}{1366223293570423} & \frac{4032747790297437}{876818153986988} & \frac{-3904193967064637}{1349987776494300} & \frac{17145800759}{13477640670} \\
\hline
b_i & \frac{22282049043593853}{4308368588372464} & \frac{-9770202945607981}{1366223293570423} & \frac{4032747790297437}{876818153986988} & \frac{-3904193967064637}{1349987776494300} & \frac{17145800759}{13477640670} \\
\hline
\hat{b}_i & \frac{6683572101201647}{1140236019835067} & \frac{-6965102855558180}{824301485227613} & \frac{5142000300260830}{879537376700627} & \frac{-4453112745386595}{1094364347301302} & \frac{152550917183879}{84235254187500}
\end{array}
$$

where $\mathbf{S}$ and $\mathbf{S}^{-1}$ are, respectively. For the Schur decomposition of the $\mathbf{A}$-matrix, we have

$$
\begin{bmatrix}
\frac{201393105359643}{1194403708609630} & \frac{-20516684842087}{109379704906302} & \frac{2409847596174989}{1441170238751822} & \frac{4522438509842500}{1087150260297723} & \frac{-16149976387338469}{757137551540145} \\
\frac{81426915156082}{689016400804627} & \frac{-225150213476501}{663476887173847} & \frac{1693647520602978}{767300732552357} & \frac{5098882303450060}{1482754123611527} & \frac{8715555438263851}{1081235957976694} \\
\frac{-288864418051340}{2332417360495537} & \frac{-377952213803336}{623788391278757} & \frac{4586727003849041}{1434163008195675} & \frac{1828586631631551}{625942414237586} & \frac{119984144825656187}{1546038544875504} \\
\frac{-131676336521081}{358251747621084} & \frac{-703834316636314}{1572025984026703} & \frac{2542664007336841}{681164540295387} & \frac{26269121089209281}{5987920192290019} & \frac{52409918001374421}{1027074246053590} \\
\frac{-127}{250} & \frac{-461}{1000} & \frac{1327}{500} & \frac{6259}{1000} & \frac{-56411}{1000}
\end{bmatrix}
$$

$$
\begin{bmatrix}
\frac{-89957481715103}{498994245222560} & \frac{2655716331477634}{927374983593481} & \frac{-498171810395274}{1045565683014773} & \frac{-947675191154187}{1444865177521733} & \frac{-1318995440158681}{1709802407854398} \\
\frac{2225358352662202}{1492362073478237} & \frac{-744280564626399}{808902814065898} & \frac{-4154324942676507}{1354331551569367} & \frac{1121778019888789}{307260795063127} & \frac{-708338921339936}{439194995959531} \\
\frac{-2347847329437913}{1134746643200454} & \frac{5434701740106448}{1746002253851229} & \frac{-1144241020488351}{722193231997478} & \frac{724654505890237}{857282386306285} & \frac{-306641701623361}{1631356539549147} \\
\frac{1819820042809130}{1322170936522801} & \frac{-14254238908577967}{8176212184474735} & \frac{1031481726999560}{1553662247656101} & \frac{-91549980136523}{585936870270971} & \frac{1319867142414}{534777269031733} \\
\frac{22608084060361}{504545995924246} & \frac{-60874880583971}{932798226649535} & \frac{32303907556580}{1134318496967719} & \frac{-1779069892820}{1189019684499431} & \frac{-5483024354153}{888739839024187}
\end{bmatrix}
$$

and $\mathcal{J}$ is created using (2) and $\gamma = \frac{588179516983801}{2115343972878826}$. For the Schur decomposition of the $\mathbf{A}$-matrix, we have

$$
\mathcal{Q} = \begin{bmatrix}
\frac{-158421375028944}{660494135853625} & \frac{-135662191692539}{361483225546080} & \frac{191740524886703}{430237920399382} & \frac{256677060523021}{523213641501330} & \frac{350847946071506}{582851597367183} \\
\frac{-124819389415603}{778157397500910} & \frac{-2604034378518969}{4531811458828265} & \frac{69235042660345}{543266928285804} & \frac{213481722920267}{770436179724267} & \frac{-526152259290423}{708774500504581} \\
\frac{217653958337663}{1073997884058408} & \frac{-2059476955089430}{2835482370303217} & \frac{-190562380699463}{567725872950681} & \frac{-163443058066217}{332340199020697} & \frac{269967866159701}{973811004977446} \\
\frac{1048493143056392}{1905670925005897} & \frac{-15579948010040}{895282992111053} & \frac{813569626792337}{1064575519239127} & \frac{-696911782823636}{2161016421739333} & \frac{-26977595856449}{285195807667627} \\
\frac{723096924940391}{955292167314234} & \frac{-38116519686868}{1135210118426779} & \frac{-379336635479412}{1275519796535263} & \frac{1738528953824046}{2996172173963285} & \frac{10257972467219}{366815589029066}
\end{bmatrix}
$$

and

$$
\mathcal{U} = \begin{bmatrix}
\frac{462534531056787}{1663471107488864} & \frac{-1367995668196441}{896233813350642} & \frac{-8277242252878787}{2364952501061068} & \frac{-342630589823929}{993073805297501} & \frac{18295767145179029}{1384701755305125} \\
\frac{0}{1} & \frac{462534531056787}{1663471107488864} & \frac{163248020801414}{803286658425581} & \frac{334091934707342}{543667918766043} & \frac{-13485733648205469}{985734587366036} \\
\frac{0}{1} & \frac{0}{1} & \frac{462534531056787}{1663471107488864} & \frac{-310400074820811}{1086120415763042} & \frac{3634376055852039}{732486316263583} \\
\frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{462534531056787}{1663471107488864} & \frac{7510414847390378}{4300981426270077} \\
\frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{462534531056787}{1663471107488864}
\end{bmatrix}
$$

A.2 Stage-Order Four Methods

A.2.1 SIRK4(3)6L[4]SA

The SIRK method, SIRK4(3)6L[4]SA, is given by

$$
\begin{array}{c|cccccc}
\frac{24}{109} & \frac{2336787847068001}{2577597209547077} & \frac{184181518573427}{367545806244361} & \frac{-1176370393322581}{1183614399998885} & \frac{-388820208129589}{995235974449893} & \frac{68918101404262}{1142193133663625} & \frac{79942680880535}{584724670267658} \\
\frac{20}{33} & \frac{1303373347362601}{1421071765691043} & \frac{638122698474866}{891131705234247} & \frac{-1814595755870581}{2373646754872588} & \frac{-103071312929787}{278696656719829} & \frac{-21448090630146}{771271351384927} & \frac{162583302861941}{1205025499674641} \\
\frac{17}{52} & \frac{1550390398362573}{1558870192991855} & \frac{805813171551199}{1203788602791491} & \frac{-608814087551129}{597908835631392} & \frac{-302205448115847}{908106608262061} & \frac{-77979084958639}{641948067716429} & \frac{180815339552081}{1334794232419763} \\
\frac{6}{7} & \frac{441921432010484}{490393908566383} & \frac{254027129987149}{512176380576381} & \frac{-427524720938786}{598658636359573} & \frac{-191226066685539}{308818705345568} & \frac{746979177137745}{1258092448220744} & \frac{114066996283037}{571400458575477} \\
\frac{35}{48} & \frac{1266214116743344}{1253783462082657} & \frac{664889167992880}{1141998771500451} & \frac{-1225448219131643}{1342971467831446} & \frac{-672738007412623}{640850097512132} & \frac{342183731841472}{440133265132407} & \frac{217413543090059}{675552070935089} \\
1 & \frac{1385663128040700}{1327077573237439} & \frac{1003869408750454}{1435056349422203} & \frac{-1284915601194427}{1307725860796871} & \frac{-3952719904197168}{4639929430019699} & \frac{2126364384743569}{2980500007713724} & \frac{316967309207526}{839993898697303} \\
\hline
b_i & \frac{1385663128040700}{1327077573237439} & \frac{1003869408750454}{1435056349422203} & \frac{-1284915601194427}{1307725860796871} & \frac{-3952719904197168}{4639929430019699} & \frac{2126364384743569}{2980500007713724} & \frac{316967309207526}{839993898697303} \\
\hline
\hat{b}_i & \frac{763634524559279}{865195452834827} & \frac{1385893896792718}{2580895821446749} & \frac{-715438867383588}{1085711292766657} & \frac{2546219819722}{1171257634643167} & \frac{110197627399649}{687625425311110} & \frac{62385229158339}{810937590128560}
\end{array}
$$

where $\mathbf{S}$ and $\mathbf{S}^{-1}$ are, respectively.

$$
\begin{bmatrix}
\frac{-145107398043603}{834340554625670} & \frac{240929708951899}{530951508007574} & \frac{-13210433683121503}{1674906236570338} & \frac{20460504276585799}{482928353468497} & \frac{12134027588534683}{2735900365779328} & \frac{29216687068978538 6}{836024636541157} \\
\frac{1269350622344086}{8121378803393613} & \frac{-1464455248227451}{708331325777664} & \frac{5119529427748831}{665181785805360} & \frac{-19509473236338886}{1109881643925867} & \frac{-104466084405725784}{406181934792793} & \frac{-827465355617565357}{323981268844769} \\
\frac{31047057144246}{812478254215157} & \frac{146976752686477}{818055440034983} & \frac{-1950590842960369}{463832453523160} & \frac{16301453670115735}{540294592025926} & \frac{-78962223020375197}{385301437239550} & \frac{-1525082309310069751}{1544534682449428} \\
\frac{-110115373040733}{137410683205250} & \frac{-2188173253832560}{812926588047509} & \frac{1773909529809306}{376776021398363} & \frac{4249531676987155}{1308786050826526} & \frac{70548846440135788}{796711676915165} & \frac{-197800884898984691}{1290139734416414} \\
\frac{-555636259497901}{1351322005031590} & \frac{-2165651241670921}{627880515677163} & \frac{2823169491880915}{927619487130236} & \frac{-4697571025501327}{734834975327147} & \frac{128507829468165230}{1212322746443211} & \frac{319276167573508044}{727397653992985} \\
\frac{-373}{250} & \frac{-117}{125} & \frac{-503}{250} & \frac{16111}{1000} & \frac{-54217}{1000} & \frac{-247713}{1000}
\end{bmatrix}
$$

$$
\begin{bmatrix}
\frac{76285684442416}{494294700254463} & \frac{37965098694607}{946093196729638} & \frac{1164766503754258}{4718810836136203} & \frac{-92472053336745}{1831139498651219} & \frac{167918458767825}{690282505683737} & \frac{-574608923817962}{800712216908445} \\
\frac{-139075419368485}{890077962313663} & \frac{-71634919258327}{588434662122987} & \frac{36597403398723}{991916254389053} & \frac{202918934098453}{847053762860185} & \frac{-251875686882492}{598511990933935} & \frac{-8780844949441}{1397353407369260} \\
\frac{-468845624594513}{1164496638440623} & \frac{-497889453549438}{2005650277170187} & \frac{510754698397021}{1207779725956645} & \frac{287218950405214}{827568355949221} & \frac{-61811266989973}{515117351216822} & \frac{-49269092405426}{405231765470661} \\
\frac{-17431548172177}{562725371498321} & \frac{-18568666797089}{579351827481696} & \frac{69261040947523}{1152737966694229} & \frac{56981880437729}{998583146550763} & \frac{-26587011198641}{1334348777443565} & \frac{-2904419974435}{124305037914956} \\
\frac{18779735119861}{1246451215524655} & \frac{1769849229736}{216044140633427} & \frac{-10253037806359}{606050251618499} & \frac{-4189502802272}{3004313517592493} & \frac{-3998098833601}{1443135572431971} & \frac{98020275235}{541247022927131} \\
\frac{-1303649573629}{547449115251392} & \frac{-1764349471066}{1073896093906655} & \frac{2398378424869}{940666160560230} & \frac{381922053349}{640233291913319} & \frac{510489416693}{1244898917149661} & \frac{-144083053737}{548603772391807}
\end{bmatrix}
$$

and $\mathcal{J}$ is created using (2) and $\gamma = \frac{19}{100}$. For the Schur decomposition of the $\mathbf{A}$-matrix, we have

$$
\mathcal{Q} = \begin{bmatrix}
\frac{-57966413132662}{586207749955279} & \frac{352057708646224}{2086510963393257} & \frac{-571857584421476}{799854626179871} & \frac{283076480295193}{1129566760298442} & \frac{153089439156025}{1054323995810236} & \frac{-902204898588125}{1489856570070767} \\
\frac{157987417458904}{1777837228629795} & \frac{-484524752509064}{888286933878045} & \frac{160035248186266}{621394761850497} & \frac{208514649197963}{486538576211518} & \frac{-289531442198925}{557178943340651} & \frac{-464061628275629}{1110733061483550} \\
\frac{22188420841393}{1021266363906106} & \frac{26143816147109}{894781846277366} & \frac{-2001533569676298}{4414915204850063} & \frac{399276353166871}{830969158606508} & \frac{-657296499982162}{1745039554018299} & \frac{93240759126112}{143806991707523} \\
\frac{-404083653462232}{886880601092043} & \frac{-137507253328409}{384747330782248} & \frac{96198597157231}{671528750165870} & \frac{770873377029683}{1642949191074967} & \frac{669434039615170}{1057158347774751} & \frac{54695071619813}{360552159189267} \\
\frac{-230710230655238}{986862058648855} & \frac{-612226935261785}{908213414591054} & \frac{-348257041186489}{826711871006912} & \frac{-547387049924383}{1004333317737870} & \frac{-93757604887025}{1258295855286277} & \frac{169864933909004}{1628948931675769} \\
\frac{-155736850076463}{183587831567999} & \frac{451612229494340}{1497024344481031} & \frac{125997754350593}{913954442321314} & \frac{-43892636866549}{594611800774485} & \frac{-871536553433881}{2175635418930201} & \frac{-79621653696938}{1192157037806237}
\end{bmatrix}
$$

and

$$\mathcal{U} = \begin{bmatrix} \frac{19}{100} & \frac{541612464959981}{1297740562774416} & \frac{1020573445252863}{1302372457536010} & \frac{1050875675766104}{964563697304705} & \frac{1877996302499711}{2330793925562261} & \frac{3815096741193031}{1649774300229087} \\ \frac{0}{1} & \frac{19}{100} & \frac{285223740406765}{584945537372783} & \frac{186799839264170}{362379195243379} & \frac{364652677802843}{699384593799095} & \frac{1633178268362047}{1105700192257792} \\ \frac{0}{1} & \frac{0}{1} & \frac{19}{100} & \frac{461266320773551}{1142118708204274} & \frac{194323258852757}{1197611677570857} & \frac{1130557593216792}{681788337143461} \\ \frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{19}{100} & \frac{28100770323423}{369484032261041} & \frac{-152370522143235}{110528887699756} \\ \frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{19}{100} & \frac{612877213228136}{553898027906807} \\ \frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{19}{100} \end{bmatrix}$$

A.2.2 SIRK5(4)6L[4]SA

The SIRK method, SIRK5(4)6L[4]SA, is given by

$$\begin{array}{c|cccccc} \frac{386}{1809} & \frac{276962354096155}{310042368383017} & \frac{487922857655662}{1417528413635365} & \frac{-1275518769180729}{1333097314890362} & \frac{96036017665733}{725134278339489} & \frac{-547747175261128}{1913554197835981} & \frac{81994499371270}{948117029494929} \\ \frac{242}{425} & \frac{829435706824353}{705647422294547} & \frac{1188779244889388}{1165055284845815} & \frac{-3346166099863205}{2660227656848502} & \frac{5184261417995}{236313322494113} & \frac{-600422899632515}{1010417486336011} & \frac{241540214047847}{1185370876464130} \\ \frac{105}{337} & \frac{1155048223015395}{1173332741338939} & \frac{407347413874943}{1118021450334608} & \frac{-449018487193627}{455939791559625} & \frac{207511817161525}{991988059685181} & \frac{-298767041617331}{790704276770661} & \frac{116120241232955}{998535280258039} \\ \frac{519}{793} & \frac{583997751728484}{702125335017143} & \frac{277568820680765}{864344466785424} & \frac{-206515848429042}{344159971307021} & \frac{332702663616837}{1051209857378648} & \frac{-185855598979876}{633921816372771} & \frac{77298443819223}{986781812931221} \\ \frac{802}{961} & \frac{944505387630485}{908449391984093} & \frac{804517633531877}{876139915036949} & \frac{-284717749297916}{281325738061557} & \frac{48294411671209}{1042694629153382} & \frac{-199870997724822}{715861967753219} & \frac{97241005810263}{800015806449134} \\ 1 & \frac{624473784440231}{761596737518277} & \frac{171873571350442}{755141847561719} & \frac{-452297413754756}{790038882788739} & \frac{315838954947561}{653089604402989} & \frac{-108196917644231}{1120920833102201} & \frac{147494140982767}{1069882318456709} \\ \hline b_i & \frac{624473784440231}{761596737518277} & \frac{171873571350442}{755141847561719} & \frac{-452297413754756}{790038882788739} & \frac{315838954947561}{653089604402989} & \frac{-108196917644231}{1120920833102201} & \frac{147494140982767}{1069882318456709} \\ \hline \hat{b}_i & \frac{2406303879626438}{2513932861617879} & \frac{381935975066630}{1180159275804439} & \frac{-769378513179247}{938678136827297} & \frac{385731786567940}{584666589430579} & \frac{-1117420603294271}{3301936476765577} & \frac{258578331636886}{1188922524452835} \end{array}$$

where $\mathbf{S}$ and $\mathbf{S}^{-1}$ are, respectively.

$$\begin{bmatrix} \frac{361546174681847}{772070215576993} & \frac{-682478202019348}{847041653148777} & \frac{5427925424030651}{229669944237809} & \frac{-9074852168663363}{908096435993956} & \frac{-3552195954492762 18}{1540425438362759} & \frac{-2278166524415233239}{861741434728967} \\ \frac{342555838412822}{1130844917755401} & \frac{8601371834074601}{972463225435366} & \frac{1981009495899103}{152627855429126} & \frac{77249743051555532}{1225587782054795} & \frac{162841163816888433}{1234423801868107} & \frac{-2108360746291803983}{451696204104997} \\ \frac{-3372854965521}{516928401842377} & \frac{-158223817187048}{422135316836495} & \frac{8463252433420206}{566110132227301} & \frac{-58591493595427532}{711935548175669} & \frac{1532210089736347319}{3051691843463469} & \frac{2157014831561386597}{734595399311860} \\ \frac{-43186925485747}{600901128847053} & \frac{6387090508471499}{912716868403381} & \frac{-9996733622555059}{499134320394571} & \frac{46170134078336023}{823640532656768} & \frac{1000724194489031909}{1378148235731517} & \frac{4953910884295763548}{718283008597231} \\ \frac{1855380962155227}{708195557310580} & \frac{8100592089426067}{663352800281648} & \frac{27914616744492453}{1572896232131815} & \frac{28298758009456272}{512874789863989} & \frac{-1062590983218389318}{782767342636349} & \frac{-1817528601902200 8150}{1010620299736207} \\ \frac{3663}{1000} & \frac{19}{8} & \frac{0}{1} & \frac{2829}{100} & \frac{16053}{100} & \frac{-29}{4} \end{bmatrix}$$

$$\begin{bmatrix} \frac{20371628100689}{624298878188762} & \frac{-27685221599546}{345551679521617} & \frac{-3735963187232}{624705392592429} & \frac{-794610141803}{112452149464025} & \frac{9050033849975}{741587386564071} & \frac{1138999864279795}{4272691537121674} \\ \frac{146970549939537}{989863648610711} & \frac{8556307836541}{734114124000444} & \frac{-81891101493179}{972807965487394} & \frac{41837586708522}{322173531590039} & \frac{8790910126359}{783782433709409} & \frac{-32570001308399}{1273803105537900} \\ \frac{146909365802959}{1089395347351870} & \frac{84050113738479}{1100630446073971} & \frac{-119061991219693}{895414839393800} & \frac{9947215870560}{1296878557506473} & \frac{-52240648718504}{894236531513507} & \frac{17601819351627}{970251307428124} \\ \frac{6481220981131}{431075584400260} & \frac{10609678821947}{717412606818225} & \frac{-23271806684228}{911392093896947} & \frac{-1012069570153}{845971271536057} & \frac{-3160855276954}{296014328997497} & \frac{2000770951048}{452338500628909} \\ \frac{-4723017606545}{849611971032582} & \frac{-556206983954}{590459631210263} & \frac{3577680887113}{611596106809592} & \frac{-1419626529764}{921941510385717} & \frac{1056859935878}{740956828789799} & \frac{-165067580105}{656648932240079} \\ \frac{410243334790}{582418388665129} & \frac{212045147395}{1127435903195831} & \frac{-1318080106603}{1858716095712388} & \frac{547117366269}{2639580603088984} & \frac{-295028843770}{1207732658693779} & \frac{164357624253}{2285306684327143} \end{bmatrix}$$

and $\mathcal{J}$ is created using (2) and $\gamma = \frac{23}{125}$. For the Schur decomposition of the **A**-matrix, we have

$$\mathcal{Q} = \begin{bmatrix} \frac{93085057377297}{902154188653397} & \frac{-110447692322226}{870674182003949} & \frac{442846915017740}{752671681658499} & \frac{75392307281987}{173598924861978} & \frac{-80684109040097}{1260156056429965} & \frac{245425289515553}{372378643891501} \\ \frac{49896595153633}{747567407989385} & \frac{539635605507040}{916950195212273} & \frac{670090752612866}{2446783278066307} & \frac{-248001809806737}{636173295787714} & \frac{392445758246698}{627405564351831} & \frac{141355756928693}{803246667603136} \\ \frac{-457274197401}{318065961766304} & \frac{-32078644101685}{1239927644444734} & \frac{745028921922049}{1898069598424479} & \frac{507247767583448}{972303064691563} & \frac{532512995563031}{1461136152222872} & \frac{-86075207376872}{129724271783755} \\ \frac{-11455592695513}{723395940836827} & \frac{1751020667785910}{3422433254783819} & \frac{-144028280243683}{260687842460082} & \frac{183152481794465}{294751578588417} & \frac{36708742708681}{386751569881852} & \frac{194107556966138}{1000849510621723} \\ \frac{440952433816431}{763870286799206} & \frac{441210737907239}{905376938602781} & \frac{80441833197995}{364256796685076} & \frac{-37016301765272}{1176748438604211} & \frac{-930613023350343}{1626700836501239} & \frac{-192781561265165}{843419690017493} \\ \frac{348221841608208}{431446410793255} & \frac{-116531309005183}{314096758674760} & \frac{-182567114576284}{686457231521017} & \frac{22442368419909}{1819010042397988} & \frac{432126518626593}{1173811164741013} & \frac{62854521705062}{934034827640527} \end{bmatrix}$$

and

$$\mathcal{U} = \begin{bmatrix} \frac{23}{125} & \frac{280153706118370}{862194180039583} & \frac{244789826831938}{1103321436894925} & \frac{-28249166893712}{480378508780797} & \frac{21356760420602}{81657294340119} & \frac{2252737661337764}{1098185455283739} \\ \frac{0}{1} & \frac{23}{125} & \frac{364546497241940}{999949674675921} & \frac{-540359343901279}{1068701797803337} & \frac{698579841456329}{1295223148546519} & \frac{1927633429322669}{1021316712593729} \\ \frac{0}{1} & \frac{0}{1} & \frac{23}{125} & \frac{-470535341922090}{951334059221587} & \frac{140200076057965}{831816669645383} & \frac{1557911376361741}{1136788267111079} \\ \frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{23}{125} & \frac{-81057255552664}{1239891286409623} & \frac{904833979884418}{698752979682603} \\ \frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{23}{125} & \frac{3423862561732266}{2703772862913223} \\ \frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{23}{125} \end{bmatrix}$$

A.2.3 SIRK5(4)7L[4]SA

The SIRK method, SIRK5(4)7L[4]SA, is given by

$$\begin{array}{c|ccccccc} \frac{11}{67} & \frac{582245450361074}{1208758455789599} & \frac{-243429299008671}{602266063145477} & \frac{24402457342270}{746294201193267} & \frac{43571412442966}{325537679839697} & \frac{-168848407513680}{737157299180749} & \frac{-20916883459178}{779593068240793} & \frac{66135590161502}{375726509921817} \\ \frac{47}{180} & \frac{206221629094637}{385225919113430} & \frac{-209432948387219}{570939085468559} & \frac{18157175144536}{458426028171763} & \frac{100535424915499}{764945899663129} & \frac{-184531833740884}{612329994724739} & \frac{-695306758769}{928979827129520} & \frac{138316838063853}{618371196048044} \\ \frac{55}{119} & \frac{799974631724624}{1502890033042705} & \frac{-255637748505395}{856190148599299} & \frac{866968324675276}{3557567952575069} & \frac{41607173131916}{1791079395339627} & \frac{-36137249733531}{229632872524766} & \frac{-1759572345831}{871489428601909} & \frac{113588619802143}{939280713455987} \\ \frac{85}{127} & \frac{297285246922069}{720102109519750} & \frac{-11509730061167}{549009586327029} & \frac{-59123198851172}{2628167462108675} & \frac{534332011655153}{1021753668537666} & \frac{-242134056652609}{1215274077324624} & \frac{-376348967826533}{1741444920758171} & \frac{270537571749202}{1406750621289951} \\ \frac{41}{43} & \frac{682966354392994}{1483657888287899} & \frac{-196053728397509}{1479287288391776} & \frac{223359485336592}{1826000494224475} & \frac{514913264507261}{1239406634480537} & \frac{-285150266115772}{889667685750017} & \frac{141885744633556}{987503761583197} & \frac{415831337143299}{1570634228061452} \\ \frac{161}{193} & \frac{537424291980239}{1324745321882355} & \frac{-12178239934966}{1242512696334751} & \frac{-9237481276157}{570249798578157} & \frac{850898184028364}{1597254697458717} & \frac{-388372610642494}{919814860853569} & \frac{21519123483768}{541119409166693} & \frac{326502310783548}{1073131607505529} \\ 1 & \frac{297743072816555}{789845569649653} & \frac{56609825977467}{1084573844009858} & \frac{-87555961211227}{1214612266615875} & \frac{221980066313075}{417537501414289} & \frac{-322657284369505}{674663436187378} & \frac{229561562374607}{1206257839104655} & \frac{237114614160652}{593936141003489} \\ \hline b_i & \frac{297743072816555}{789845569649653} & \frac{56609825977467}{1084573844009858} & \frac{-87555961211227}{1214612266615875} & \frac{221980066313075}{417537501414289} & \frac{-322657284369505}{674663436187378} & \frac{229561562374607}{1206257839104655} & \frac{237114614160652}{593936141003489} \\ \hline \hat{b}_i & \frac{341628971014197}{470298835699016} & \frac{-992264775188544}{1167778517259859} & \frac{1244030178759544}{966426844377631} & \frac{-1731380430865750}{1740391974739577} & \frac{-27775117826363}{1060856862895032} & \frac{878885009166788}{918790350111783} & \frac{-92867194051835}{933187118757357} \end{array}$$

where **S** and $\mathbf{S}^{-1}$ are, respectively.

$$\begin{bmatrix} \frac{-7386913556697}{1080545206029881} & \frac{250505299660641}{1138463054669896} & \frac{-3377925459783851}{2081597276650265} & \frac{38671823912228415}{1764481688921672} & \frac{-60723416256446891}{394554413601518} & \frac{141851370633461855}{188780841453448} & \frac{-1096282392159381170}{600377164835169} \\ \frac{19202055507455}{1186292473690239} & \frac{12570119045143}{844790060635986} & \frac{955700329434024}{1034268290483753} & \frac{5840925980773111}{964359410556181} & \frac{-1668839052226545449}{1420730883417881} & \frac{518464093022872424}{877566740892151} & \frac{-1248107857172620331}{371447915065773} \\ \frac{18737662033183}{1211011245079164} & \frac{-271806642868439}{2939170276385936} & \frac{2645448441934294}{670110585920487} & \frac{-24221359533612536}{864630927342875} & \frac{18776290236293123}{162191617088354} & \frac{113692614488234382}{1224021803699335} & \frac{945250873778975536}{238827601944277} \\ \frac{15425625405169}{1052566852635539} & \frac{1585035329459834}{1844515942824589} & \frac{-103057058229668}{288195032659079} & \frac{-6215544748634022}{723912251270713} & \frac{64514472371808343}{544526053523746} & \frac{1522674397505811}{387624829781371} & \frac{2639281195638665952}{683795772112561} \\ \frac{755856214679284}{2444078672407739} & \frac{948112286240371}{1279137401908106} & \frac{-4854317712371753}{1178179333856568} & \frac{34015414975287081}{1858305467970128} & \frac{-21112091178390255}{660611392427777} & \frac{699960882101656651}{1156460540520664} & \frac{274493713300193233}{143100521027229} \\ \frac{593207359727552}{4464551030344145} & \frac{1384910967465031}{1088443227959867} & \frac{-4079085830903074}{925745436657039} & \frac{15472376947296853}{1101584796514761} & \frac{-48237966148755243}{2196053250385318} & \frac{155202518845436821}{1427270865843711} & \frac{420270860757081638}{818972739265353} \\ \frac{459}{1000} & \frac{47}{500} & \frac{1}{1000} & \frac{193}{1000} & \frac{-2743}{500} & \frac{-901}{5} & \frac{-10277}{10} \end{bmatrix}$$

$$
\begin{bmatrix}
\frac{-32953996534802}{2233295882121187} & \frac{-71611627134175}{676988725195649} & \frac{247817019297921}{775028493339737} & \frac{-489425018254259}{2099223305391088} & \frac{2953067952991882}{4352941112929477} & \frac{-165735347787679}{479983045158265} & \frac{1744266834072496}{957499272546893} \\
\frac{1435169551070977}{1647265474059310} & \frac{-19221598861755}{867889449232624} & \frac{-2360018092788}{237816640418387} & \frac{843828429935891}{870540399581040} & \frac{-1045173900220391}{1036476079906562} & \frac{503627281530631}{950294566266378} & \frac{465607736399935}{914477555612898} \\
\frac{577433993636700}{929878478662661} & \frac{-127925996227780}{629583495245697} & \frac{-123758289655294}{755401334902227} & \frac{304287281469141}{493987468048951} & \frac{-266189712083189}{692363701835279} & \frac{-78843980693621}{235042124400807} & \frac{125951420455751}{351412439789306} \\
\frac{15864164952181}{174766150657850} & \frac{-22497815021791}{584690846339245} & \frac{-93056919002563}{1087724025258082} & \frac{151950093733837}{1094283257317116} & \frac{-75406014659918}{2549427510289903} & \frac{-113220824434421}{1112735684735181} & \frac{19506811348712}{385951038619551} \\
\frac{-5113659351185}{368024718258543} & \frac{11924052509887}{909552977787820} & \frac{-15175442479388}{953244432100775} & \frac{25721392860178}{1408444669132453} & \frac{5314812962443}{584298627918394} & \frac{-2516859286136}{153609374746755} & \frac{-1716124889787}{816695661124727} \\
\frac{-2265434067712}{1207215012496231} & \frac{1921816710075}{893800257307817} & \frac{-417099594515}{989025984622126} & \frac{218498048358}{593556894537713} & \frac{4146465334989}{2294898059913077} & \frac{-1216433752670}{1273162833297759} & \frac{-840404513974}{806443839929143} \\
\frac{525236991003}{1063301247299218} & \frac{-370708424337}{735982743884794} & \frac{200884162116}{705833217623515} & \frac{-831036238879}{5509895484894193} & \frac{-205473767017}{1279926300534732} & \frac{163299037129}{1257928997318661} & \frac{91641976303}{1007867499556073}
\end{bmatrix}
$$

and $\mathcal{J}$ is created using (2) and $\gamma = \frac{1}{7}$. For the Schur decomposition of the **A**-matrix, we have

$$
\mathcal{Q} = \begin{bmatrix}
\frac{-79143949497776}{6597293135409327} & \frac{130474984521081}{870542514918359} & \frac{267025038027697}{1361974588178466} & \frac{1170929551857110}{1658108925886573} & \frac{-129199838789612}{546494613826139} & \frac{-159721625263033}{1571700259888291} & \frac{528250927255038}{863737415045845} \\
\frac{7547932476305}{265729762280578} & \frac{-5240571286113}{1053683383589483} & \frac{-706840518482951}{3480518293339432} & \frac{393071402973184}{568373764588179} & \frac{149286616990684}{500788156860261} & \frac{-36891274494257}{851325400019717} & \frac{-336531025976605}{539635773026214} \\
\frac{34216761424778}{1260200984511017} & \frac{-64696098384827}{869285572904310} & \frac{-381442463581589}{504577711338565} & \frac{-44821907137739}{828751794890150} & \frac{779595632126698}{2827201270264505} & \frac{-204029600223707}{435871703810206} & \frac{355698684514851}{1009436722738922} \\
\frac{30792661232424}{1197353176899713} & \frac{171361318093583}{312819785993411} & \frac{-1039219411381357}{2200877468886369} & \frac{-19171316230040}{1183978315761351} & \frac{-580253645348047}{899512827202925} & \frac{73007186478851}{461327325580023} & \frac{-431467544576877}{2310531946489091} \\
\frac{443831303947880}{817828162569233} & \frac{228965748723617}{1126113060495414} & \frac{313691103982307}{1038779267568573} & \frac{-6210595927521}{65320989738448} & \frac{-364910989347736}{2586665850095593} & \frac{-658259644666149}{926757151235177} & \frac{-131223878100139}{660209690424814} \\
\frac{176083781153963}{755194389326418} & \frac{233228241507455}{328388534812423} & \frac{76563144710980}{1105130940920959} & \frac{-81743081765592}{1115688433359613} & \frac{349533447459320}{601723583661521} & \frac{186222587546069}{715229570865447} & \frac{143315040522270}{891671162058119} \\
\frac{224239632938026}{278399099831381} & \frac{-157954323145409}{444740338453272} & \frac{-111414451406504}{644465258655767} & \frac{80414184038887}{1090515495522176} & \frac{-105016831841324}{1384794416492543} & \frac{334537056916499}{808183176981348} & \frac{112930784218109}{1003140545550144}
\end{bmatrix}
$$

and

$$
\mathcal{U} = \begin{bmatrix}
\frac{1}{7} & \frac{963946462417486}{2590626469443051} & \frac{-512156633358663}{981126097102370} & \frac{972362431224769}{1856937309001882} & \frac{-1196682213820347}{2420586583462757} & \frac{717018205382478}{875203451358017} & \frac{225637017238526}{421472734821205} \\
\frac{0}{1} & \frac{1}{7} & \frac{-532004394065746}{1692047695522713} & \frac{238203628183601}{710307072667110} & \frac{-743223735871375}{1307759656689984} & \frac{398132915401151}{1176066988559196} & \frac{328894735130031}{970054225003862} \\
\frac{0}{1} & \frac{0}{1} & \frac{1}{7} & \frac{-153295848299271}{584259457704656} & \frac{466215056312072}{1476243362138865} & \frac{-127117094588299}{1308918691558469} & \frac{-568442752110098}{1208852034471801} \\
\frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{1}{7} & \frac{-319921294274913}{878364926223776} & \frac{428978097006155}{1408611357947947} & \frac{831918562133317}{1075284463521852} \\
\frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{1}{7} & \frac{102714425623415}{1251416674878962} & \frac{457577927646037}{2534561755234119} \\
\frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{1}{7} & \frac{-329034683043261}{656003470182002} \\
\frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{1}{7}
\end{bmatrix}
$$

A.2.4 SIRK6(5)7L[4]SA

The SIRK method, SIRK6(5)7L[4]SA, is given by

$$
\begin{array}{c|ccccccc}
\frac{315}{1478} & \frac{1393106712015778}{1445042073773939} & \frac{-829745190667821}{978492644573104} & \frac{-181494282254396}{648021299404851} & \frac{136876985590598}{1199760291836705} & \frac{430601419500463}{1150785430053135} & \frac{-72659588954263}{222344814508863} & \frac{83804707700673}{388624687446694} \\
\frac{160}{563} & \frac{657279807271213}{563144535926102} & \frac{-871492134525669}{764687277038030} & \frac{-126413258322727}{873236653864028} & \frac{-32845967863247}{257134833027264} & \frac{550995289209196}{980198786220721} & \frac{-88653640579347}{620404970520319} & \frac{112077896806234}{1019114741691147} \\
\frac{901}{2075} & \frac{633625582266259}{622344297574402} & \frac{-861367584263665}{1013402605528803} & \frac{290889396023063}{953355173438137} & \frac{102009195350375}{264592829995152} & \frac{-116613582929960}{485377633468273} & \frac{-741015642556489}{1473710148590233} & \frac{303265399366288}{952204994665799} \\
\frac{312}{457} & \frac{79322745815537}{115270876430830} & \frac{-118981346613409}{1227289904602060} & \frac{-768105323264493}{1085437422005587} & \frac{363861002133521}{684403406951518} & \frac{320325834313071}{617501905928725} & \frac{-351847077835969}{518267159089510} & \frac{15356355927452}{35907594911337} \\
\frac{220}{427} & \frac{1152798092030275}{937374120436764} & \frac{-588913599387299}{486931553494149} & \frac{4115892676536}{1169448456997793} & \frac{-500859026911441}{1367313200818842} & \frac{298131089873929}{370635840689801} & \frac{73303710171213}{949479256707403} & \frac{-27839028985592}{1162483488747029} \\
\frac{1071}{1142} & \frac{998900237373849}{920242077096968} & \frac{-580617012750148}{684312903316221} & \frac{-494142487075212}{764205231261569} & \frac{-311519184031744}{1775473955788955} & \frac{1293589847415290}{950841728087699} & \frac{228857372167489}{1072948703211830} & \frac{-44139863014863}{867543818735444} \\
\frac{1}{1} & \frac{342058879474588}{247719565460375} & \frac{-1242156892003476}{821956816784831} & \frac{47996106307509}{613169560650038} & \frac{-513370256818603}{1083398076347323} & \frac{461378680164967}{397240231852477} & \frac{785047896003256}{1277255591155965} & \frac{-93564869305313}{374061922633495} \\
\hline
b_i & \frac{342058879474588}{247719565460375} & \frac{-1242156892003476}{821956816784831} & \frac{47996106307509}{613169560650038} & \frac{-513370256818603}{1083398076347323} & \frac{461378680164967}{397240231852477} & \frac{785047896003256}{1277255591155965} & \frac{-93564869305313}{374061922633495} \\
\hline
\hat{b}_i & \frac{991417089953590}{999909103080897} & \frac{-532827012667917}{651724446129560} & \frac{358809077318909}{997779313389769} & \frac{750730560172731}{1275392967392356} & \frac{-223531138026967}{1489301836546267} & \frac{-1}{5} & \frac{1728909943061667}{7585787459483518}
\end{array}
$$

where $\mathbf{S}$ and $\mathbf{S}^{-1}$ are, respectively.

$$\begin{bmatrix}
\frac{13884668392930}{234640369937491} & \frac{-111924915847013}{1243578048073566} & \frac{1199343886032593}{654921782933786} & \frac{-6401941315505151}{515912413620623} & \frac{28727638579444078}{813414156902871} & \frac{170374990866475687}{1132419499428970} & \frac{275980426853477268\,1}{2553917080411984} \\
\frac{10030900316005}{2086651180696992} & \frac{-62673149138093}{761465978621715} & \frac{1182964664526971}{899335587864597} & \frac{-11479209389157228}{1368511250198383} & \frac{78238937606712389}{1736600738523312} & \frac{-92826333827584669}{795003401369665} & \frac{-871676801219517295}{518190491703074} \\
\frac{-118926908001586}{741556480234705} & \frac{-1457717872423556}{5505358634971407} & \frac{-3684513303517213}{1388292422159759} & \frac{4071172898461189}{842352222047766} & \frac{82092391266613375}{1403579858338522} & \frac{-607951097504380238\,3}{879850815377234\,3} & \frac{-7535154066810288087}{656055885585335} \\
\frac{163389078737796}{1676938597354207} & \frac{771859583982829}{793560781909564} & \frac{-5807497627726841}{3646133147584209} & \frac{1411297603653727}{677061483401999} & \frac{-23310318193897411}{1331440923797542} & \frac{64181179682972813}{2709856686863621} & \frac{-975868075615430859}{981717577311134} \\
\frac{-81409724936607}{858304079330089} & \frac{322889295503924}{899799578278057} & \frac{-1148507005194423}{721499965982111} & \frac{15852417762707122}{1975560909115597} & \frac{17943613659692992}{814401710950203} & \frac{-464159630914273131}{868997965155074} & \frac{-8631519879070296515}{1130568142313476} \\
\frac{319728859087345}{673977848232406} & \frac{690850749542290}{972787271713013} & \frac{591543083950045}{574731519529754} & \frac{-9688805162168654}{1343665809655477} & \frac{5133417605418287}{861982502393729} & \frac{78767728338978230}{395150135553529} & \frac{3100450007869423784}{1251320947580945} \\
\frac{217}{500} & \frac{-137}{1000} & \frac{19}{1000} & \frac{-219}{500} & \frac{2047}{40} & \frac{-506647}{1000} & \frac{-142287}{20}
\end{bmatrix}$$

$$\begin{bmatrix}
\frac{-224583810743497}{835658459684364} & \frac{-266340219889795}{194128712471624} & \frac{194083424557917}{596015596186465} & \frac{-151323120320761}{420802701537120} & \frac{-986431919640355}{1094629525967692} & \frac{997552819096673}{907177951296954} & \frac{316685334255365}{273441938015053} \\
\frac{-34272205822221}{928263910684753} & \frac{451331801192905}{1910078891311353} & \frac{-59813143004998}{960228521504825} & \frac{-34887964106540}{134559320735893} & \frac{1648310699035691}{1416522406493986} & \frac{753567172972702}{741225315122187} & \frac{-547726721442317}{668487843817165} \\
\frac{1668832798627285}{1184318715197992} & \frac{-1517438867816515}{1223893929609999} & \frac{-221106274845421}{391963754980713} & \frac{-508219926509968}{1412855673360475} & \frac{270055782607000}{239102658130867} & \frac{-232448852793691}{1062506123984403} & \frac{208172959453409}{1157249607735424} \\
\frac{193932798991100}{960768572079533} & \frac{-3191974337205863}{6839173715927833} & \frac{174094560410129}{1226805748548574} & \frac{-804925454081409}{1688367508630018} & \frac{308741974894477}{837785740241172} & \frac{39055111701635}{88703625360441} & \frac{-341607478795681}{1295894870517333} \\
\frac{-4422333570519}{567830984102087} & \frac{-38611815516196}{982293300916963} & \frac{69106153326872}{1177198877332049} & \frac{-15437501840549}{145453568799292} & \frac{71839747386566}{1568130372042529} & \frac{250931436067465}{2031620944171006} & \frac{-67245837211427}{862361284163790} \\
\frac{24436899127039}{1382845012238094} & \frac{-23925701496773}{1061307446938191} & \frac{2697357776123}{870195461216581} & \frac{-8128634146325}{855541573587084} & \frac{20795725555026}{1926207924580201} & \frac{4350256034075}{584568766938861} & \frac{-18702670696353}{4016706188656877} \\
\frac{-2105531783949}{1572654837832550} & \frac{869275205439}{689974113077162} & \frac{302800293331}{1425983567760854} & \frac{-90208029193}{1196846626638976} & \frac{-1290469871861}{2405955585539766} & \frac{382805575637}{1011913444644642} & \frac{-225718789055}{846187954928258}
\end{bmatrix}$$

and $\mathcal{J}$ is created using (2) and $\gamma = \frac{2041}{10000}$. For the Schur decomposition of the $\mathbf{A}$-matrix, we have

$$\mathcal{Q} = \begin{bmatrix}
\frac{-74173778003186}{851201897099829} & \frac{-161442752974919}{1372228782161028} & \frac{588811710819229}{1429733279531747} & \frac{-474800425140695}{818344979923196} & \frac{145622171562358}{1135737590055179} & \frac{-7254104644621}{842788727260764} & \frac{954361711909219}{1413571149514804} \\
\frac{-6497095689585}{917791780616324} & \frac{-324788217499153}{4422448798635346} & \frac{413208724118165}{1278019410394237} & \frac{-491213389965485}{1307258458110309} & \frac{1017311321000757}{1974017135173955} & \frac{-261988062705647}{928531239224153} & \frac{-551951573627673}{868779434993566} \\
\frac{435759042681284}{1845123647330127} & \frac{-40090987585129}{350198681824630} & \frac{-351732038840582}{524820331942975} & \frac{-3452259233801737}{5560415114143492} & \frac{-23601870903605}{1313680413993738} & \frac{171538583253559}{589424581900771} & \frac{-67338926156191}{628865062563894} \\
\frac{-101954732278433}{710585735951213} & \frac{644542846739388}{846894697029131} & \frac{-147808601864945}{847785603828173} & \frac{-21545003732369}{86485786849853} & \frac{-170463277554779}{847275894814603} & \frac{-613449696111293}{1189843172459221} & \frac{32532052531628}{855929159266327} \\
\frac{258221907768775}{1848727641548511} & \frac{87636439958686}{235981840721183} & \frac{-343569955262871}{1564827531144430} & \frac{167741348227875}{711204716523316} & \frac{283955502617206}{356742719317177} & \frac{169906268661721}{949482977156046} & \frac{360364484256404}{1332339091199197} \\
\frac{-762082157259048}{1090888939158431} & \frac{341649847192803}{1236037000265683} & \frac{99711217406954}{939517105474451} & \frac{-60617900078028}{547717963654571} & \frac{-13333861963703}{774268701406449} & \frac{525642698932173}{857944624585067} & \frac{-121197542488657}{635319194869354} \\
\frac{-450391957640419}{704718800067350} & \frac{-703377571416843}{1685631967348262} & \frac{-262529551485247}{607371712278048} & \frac{223749340697995}{2719056680051122} & \frac{115379268767451}{554393028947246} & \frac{-319396516450588}{792545204629257} & \frac{140362222982231}{1043475884822326}
\end{bmatrix}$$

and

$$\mathcal{U} = \begin{bmatrix}
\frac{2041}{10000} & \frac{-354987662412033}{613677340227106} & \frac{-794905360908234}{2034864564909977} & \frac{-370968900444055}{795820872868964} & \frac{-415728041276675}{437235120639133} & \frac{-422766734376738}{391629122144561} & \frac{-1971736436481569}{907549586276435} \\
\frac{0}{1} & \frac{2041}{10000} & \frac{329801813959259}{1035645072871735} & \frac{423129320141057}{1409495646403855} & \frac{423188213011404}{745391137697999} & \frac{-895474171701779}{1054812162549264} & \frac{1040778288299717}{1871189336267854} \\
\frac{0}{1} & \frac{0}{1} & \frac{2041}{10000} & \frac{334525126426769}{860831074456571} & \frac{147472145197341}{877737194743208} & \frac{-284188687836854}{1175119922863599} & \frac{-548117705086703}{559172391092150} \\
\frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{2041}{10000} & \frac{157035215668981}{965163862739829} & \frac{110221183712507}{170783166311616} & \frac{-2069271269244413}{987459624630215} \\
\frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{2041}{10000} & \frac{1095221105986178}{921862932646443} & \frac{720883378319623}{270388168528247} \\
\frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{2041}{10000} & \frac{-70180812148470}{721153820238977} \\
\frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{2041}{10000}
\end{bmatrix}$$

A.2.5 SIRK6(5)8L[4]SA

The SIRK method, SIRK6(5)8L[4]SA, is given by

$$
\begin{array}{c|ccccccc|c}
\frac{17}{112} & \frac{269570883029939665}{331674831632514566} & \frac{-173322143057470473}{179576108495039885} & \frac{99072516173208544}{229185445114180855} & \frac{-419066228173826 85}{248218958849173348} & \frac{270273573279353 73}{604228893033957446} & \frac{4381286009657193}{275959614801729965} & \frac{-19662097071745592}{327775905639499873} & a_{81} \\
\frac{89}{421} & \frac{125772670721920401}{162124613931352459} & \frac{-132455900399448 0199}{166019106936203911} & \frac{88296910359008141}{306214410359484152} & \frac{-4841864449348973}{224011777440909296} & \frac{-67694824553608269}{524415933166540007} & \frac{77787484297820103}{293999474758558858} & \frac{-138423315825207143}{311333436827460069} & a_{82} \\
\frac{99}{272} & \frac{145489418645116010}{325050419411792461} & \frac{-28930880033942773}{411999129751770637} & \frac{-52422095821503152}{196440840846136329} & \frac{171281518034106832}{301582460149749357} & \frac{-363154579557993199}{509164709427898108} & \frac{378291433996723806}{449557450604062019} & \frac{-349808295645643243}{393316213466493268} & a_{83} \\
\frac{201}{355} & \frac{25958993343828703}{145908421991461677} & \frac{167749822601331812}{353051398750817281} & \frac{-327998973207757798}{451195596516977579} & \frac{350458907169523611}{289087168334277634} & \frac{-1766454865067936273}{1487162097924792433} & \frac{3509467466787442895}{3275076884904867496} & \frac{-232078632841350901}{508601156194794077} & a_{84} \\
\frac{323}{415} & \frac{78548552968909917}{247607769560731381} & \frac{116993862909154743}{610268924991071812} & \frac{-870967951174658289}{1924577658653388581} & \frac{712633044962863127}{670057157095801960} & \frac{-1335396221658967827}{1594283336588292130} & \frac{248212107748603971}{249928418398614800} & \frac{-163043833799419567}{184610729332786038} & a_{85} \\
\frac{521}{567} & \frac{245210646202916096}{608599774113529763} & \frac{4031129601108493}{271848926804696600} & \frac{-34947361708837022}{128482296179088327} & \frac{414728180227585387}{462041881004981920} & \frac{-340233730811266888}{527120452665821801} & \frac{189729413780828741}{174178764973180221} & \frac{-67535674634968870}{55053627005495087} & a_{86} \\
\frac{197}{200} & \frac{204279693383710993}{278377281019193493} & \frac{-163250621434689603}{244108637768655476} & \frac{165184564209613761}{379367093580901519} & \frac{46834154278272820}{223414421557675273} & \frac{20556731936445664}{262684672987882261} & \frac{152459421547044922}{533290129208452727} & \frac{-100356199389490559}{419637584019074502} & a_{87} \\
1 & \frac{42844233904725781}{306608537187267181} & \frac{148523771785943774}{257794743174373335} & \frac{-694451210057151527}{771547093439640555} & \frac{817551006934380097}{523319762469009434} & \frac{-108032879312695765}{80300679078296808} & \frac{743582462931690623}{445996296431698441} & \frac{-399055158805306170}{396263628853972487} & a_{88} \\
\hline
b_i & \frac{42844233904725781}{306608537187267181} & \frac{148523771785943774}{257794743174373335} & \frac{-694451210057151527}{771547093439640555} & \frac{817551006934380097}{523319762469009434} & \frac{-108032879312695765}{80300679078296808} & \frac{743582462931690623}{445996296431698441} & \frac{-399055158805306170}{396263628853972487} & b_8 \\
\hline
\hat{b}_i & \frac{74468595368519393}{257641559138640021} & \frac{92645841224556447}{464219760140501777} & \frac{-57215570907920219}{174176478573724129} & \frac{121498013809149781}{153663135633702134} & \frac{-208140412092392936}{457582338437486163} & \frac{401896472833013005}{319415345717249896} & \frac{-1421379013638106027}{563176251137575190} & \hat{b}_8
\end{array}
$$

where $\mathbf{S}$ and $\mathbf{S}^{-1}$ are, respectively.

$$
\begin{bmatrix}
\frac{-3548212425365339}{1444596204994236 44} & \frac{86032132488932754}{535275672314464651} & \frac{-109520610329179301}{59099519604282678} & \frac{459851891567490 8404}{262011935582939705} & \frac{-3870122452188873 2599}{337371463043162990} & \frac{1737793589119585 2575}{308693883833338877} & \frac{-1400649795725155794845}{332525066304956357} \\
\frac{15647034169518927}{370424420296800511} & \frac{123693163762025126}{770891541512061191} & \frac{367549870310265911}{392276758411642475} & \frac{4708882852838111837}{1053083781936548369} & \frac{-39171624925770559378}{392886235308725129} & \frac{150536387660814419349}{200311315633112459} & \frac{215251756508891803594}{143855055877022471} \\
\frac{33558038461726421}{302562775998636068} & \frac{6537971266866685}{296703295612952662} & \frac{1618505274891289712}{284508078545877519} & \frac{-19759218705565863024}{756672563173177229} & \frac{9680860675574505043}{227968429951768510} & \frac{4370300225932286561}{13060877346037256} & \frac{2693534846425384193943}{323180459147368667} \\
\frac{-23881855481098385}{598357864539557228} & \frac{147236710102109035}{425123668979012946} & \frac{23658908440486113}{344749918553832 91} & \frac{-850498923789245131}{1016924486353138 84} & \frac{39793490503483141877}{348957106512645789} & \frac{-224536482822016257347}{358440530682514324} & \frac{-1992309331614891976108}{290686439789247343} \\
\frac{17354123417226559}{244318361603075699} & \frac{513149735291268239}{348371818329323043} & \frac{-1262532586396829221}{408867878059755364} & \frac{930875488683736163}{489190274783702 54} & \frac{-15330881243461044783}{304121832997860401} & \frac{-29479348594523216386}{237485092964738541} & \frac{-2092763166951659453265}{467488938623500351} \\
\frac{136280051405393941}{366718930912101223} & \frac{277133229520880429}{190981396460010564} & \frac{-21890681450300165}{354796614330519276} & \frac{3084702531297099302}{384935762061542167} & \frac{-26381889125217306168}{279186153988442479} & \frac{99550352463520936678}{198806368297481299} & \frac{1139459800785539973953}{202467627397058824} \\
\frac{130485945197536079}{287514010333468421} & \frac{166978342237884454}{255070138617545455} & \frac{-72588471678614747}{789387769487745916} & \frac{536520866619510117}{336411626468664911} & \frac{-12015139092106178965}{469516593370880368} & \frac{102111904135095722974}{373222592331408411} & \frac{-1448037879180572861008}{494706091573231671} \\
\frac{101}{200} & \frac{123}{200} & \frac{81}{50} & \frac{-1}{200} & \frac{-1703}{100} & \frac{843}{5} & -1694
\end{bmatrix}
\begin{matrix} S_{81} \\ S_{82} \\ S_{83} \\ S_{84} \\ S_{85} \\ S_{86} \\ S_{87} \\ S_{88} \end{matrix}
$$

$$
\begin{bmatrix}
\frac{-200860359116646742}{253151403719124219} & \frac{-21534371522721286}{40878009238123521} & \frac{-340813158196771963}{429968836779579853} & \frac{-466274391299337739}{586611708738900470} & \frac{-125377071567733689}{179141605210201013} & \frac{16991955661090457}{200629931896421053} & \frac{1012996129643521315}{1022434541085493437} \\
\frac{-177544170830035866}{250061540449156427} & \frac{130673842086534785}{150406175276033226} & \frac{9333563423555816}{334570494098728901} & \frac{135651401626200236}{399647473823787557} & \frac{187774967395179588}{317585522599006487} & \frac{27659955993050071}{406990928757037506} & \frac{114648215864364726}{528748993799675681} \\
\frac{176614650323608357}{294577645804075975} & \frac{-86663528301270023}{337129950972018720} & \frac{-138030532136962691}{1033291823128155258} & \frac{173733535235607929}{309256297288979530} & \frac{-228141927691483541}{364433791940227311} & \frac{73018871834279556}{116459048085152629} & \frac{-40982916722198137}{51355309993774269} \\
\frac{-63002749603656385}{269179307095516178} & \frac{87702797562081707}{137766731079710901} & \frac{-134067160336648358}{163001619404682083} & \frac{93970261574050016}{106682594820325693} & \frac{-296259940105713882}{300898413198554741} & \frac{384954869593398251}{407553997600632838} & \frac{-140822717148057122}{328652816981866077} \\
\frac{-33645045250803752}{293651196718497339} & \frac{46082518106197973}{216999563450625631} & \frac{-211013720654738766}{970278792878765305} & \frac{49475857770798011}{226495434900700289} & \frac{-42817346592697351}{184373463703708950} & \frac{63586165442124949}{292407085658168100} & \frac{-62691919327981859}{873689333012063158} \\
\frac{-7550084425509130}{740846482785205427} & \frac{10293181064830599}{496590995687399558} & \frac{-3079882808141499}{150299368506672779} & \frac{7469084218993334}{352712595020635501} & \frac{-8134174849074867}{358435006703156971} & \frac{16785341473944013}{797073337725233170} & \frac{-895966545871636}{163138636722096437} \\
\frac{315251764905337}{393891122162925696} & \frac{-182780660586829}{213753806187691791} & \frac{2731099381459}{17384732935477340} & \frac{56273601077052}{306067609751989201} & \frac{-145599935652185}{327109345107565816} & \frac{273939609980969}{523451086249023653} & \frac{-1227945631406}{6373219857741103} \\
\frac{-46435091344567}{393967828665462058} & \frac{58481137012982}{416956451347207347} & \frac{-7670381992727}{104892302238012920} & \frac{4029278877697}{134091920658620850} & \frac{-10448722680416}{753170479660575685} & \frac{1443191580751}{215046594190585189} & \frac{-1336215539874}{324079060655481685}
\end{bmatrix}
\begin{matrix} S^{-1}_{81} \\ S^{-1}_{82} \\ S^{-1}_{83} \\ S^{-1}_{84} \\ S^{-1}_{85} \\ S^{-1}_{86} \\ S^{-1}_{87} \\ S^{-1}_{88} \end{matrix}
$$

and $\mathcal{J}$ is created using (2) and $\gamma = \frac{4}{25}$ with

$$
\begin{array}{lllllllll}
a_{81} & = & \frac{6460523713804473}{1609870861788774 62} & & & & & & \\
a_{82} & = & \frac{41216995139588255}{149423520696383126} & S_{81} & = & \frac{-6924033343897697894003}{358169720588708258} & S^{-1}_{81} & = & \frac{410979473430836501}{330727167560904297} \\
a_{83} & = & \frac{89994730623645393}{201483518526225851} & S_{82} & = & \frac{258799848043814044 86984}{704484520193723039} & S^{-1}_{82} & = & \frac{-133939644187788713}{323101146235748098} \\
a_{84} & = & \frac{51188293520736}{148806368065571975} & S_{83} & = & \frac{9517811254060562682323}{143566072252483493} & S^{-1}_{83} & = & \frac{266277536309943957}{568669066141387708} \\
a_{85} & = & \frac{197523672438630791}{511662054305367633} & S_{84} & = & \frac{-3353450719381973612 5767}{394768236630553358} & S^{-1}_{84} & = & \frac{54508424591678656}{386165630232232737} \\
a_{86} & = & \frac{236063906693445793}{358520772900869707} & S_{85} & = & \frac{-10819120644335444557118}{322883782525067479} & S^{-1}_{85} & = & \frac{-10885398289548737}{513968314662463798} \\
a_{87} & = & \frac{32581748939637822}{217360422955891985} & S_{86} & = & \frac{2030265360598743249 3368}{342331260349212683} & S^{-1}_{86} & = & \frac{-884657174401061}{258347586798910835} \\
a_{88} & = & \frac{124915953380470529}{406722054475011836} & S_{87} & = & \frac{-6559286597805249245289}{223946420269894319} & S^{-1}_{87} & = & \frac{-9231173867583}{156806999436140663} \\
b_8 & = & \frac{124915953380470529}{406722054475011836} & S_{88} & = & -8380 & S^{-1}_{88} & = & \frac{604275803587}{357729379349860480} \\
\hat{b}_8 & = & \frac{420923732945085162}{237849283249781227} & & & & & &
\end{array}
\tag{A1}
$$

For the Schur decomposition of the **A**-matrix, we have

$$\mathcal{Q} = \begin{bmatrix} \frac{-32869531059013}{1053648405591425} & \frac{-92957481848378}{735760691262899} & \frac{197623607135423}{852651211052730} & \frac{-400036431682753}{677306836668827} & \frac{62770944981298}{472533302643367} & \frac{445974245785478}{1061993607879743} & \frac{-225544079297913}{1129442774806946} & \mathcal{Q}_{1,8} \\ \frac{58942792612511}{1099211341938285} & \frac{-34583488419091}{758990929698531} & \frac{-151899626846607}{874069047121868} & \frac{-629074246686690}{1047201828452309} & \frac{-154219396808572}{2676539647999273} & \frac{111477827006779}{366430199751952} & \frac{137340738275287}{1046218047228398} & \mathcal{Q}_{2,8} \\ \frac{106561401630645}{756703972887508} & \frac{191547908672553}{1587706255783445} & \frac{-1076770783841229}{1248652719344330} & \frac{-73886345166773}{1035716406289517} & \frac{-87654203759503}{650368945103063} & \frac{29044217034160}{417100795088879} & \frac{254425156967233}{1035375425766231} & \mathcal{Q}_{3,8} \\ \frac{-133328802238441}{2629889461645255} & \frac{-678179264046237}{2645658158419121} & \frac{-336045383587038}{1167929599001603} & \frac{258382803322063}{649737991322415} & \frac{1303182644981397}{2485727603685598} & \frac{858231091625023}{1698775408043329} & \frac{-304360947581437}{818879463435397} & \mathcal{Q}_{4,8} \\ \frac{56129431788556}{622993526608085} & \frac{-624163005581686}{779765496021231} & \frac{70707786548491}{1121657620949998} & \frac{24022430083644}{647677638967351} & \frac{392054376947497}{3108589209453480} & \frac{-98863235154343}{1150171700963636} & \frac{500333192082478}{887670048055327} & \mathcal{Q}_{5,8} \\ \frac{495358898123509}{1050040816602430} & \frac{-412740029055565}{971107305700173} & \frac{-668250630975016}{5394026845492595} & \frac{-55926754716068}{799722661275149} & \frac{-158396339892264}{413497397703307} & \frac{-198882396839771}{816871893314940} & \frac{-311813847137717}{513020475386556} & \mathcal{Q}_{6,8} \\ \frac{964756717906950}{1674350832161713} & \frac{304420551834160}{1989337725404581} & \frac{252779675815367}{963670198844317} & \frac{367694222688761}{1195056981703092} & \frac{-325280441438525}{984101771216868} & \frac{798876061022906}{1418512218872081} & \frac{230360592377734}{988969175350995} & \mathcal{Q}_{7,8} \\ \frac{595002472326163}{928017227767584} & \frac{226008369221188}{947315361862929} & \frac{5478272663312}{140367929793295} & \frac{-100515536593620}{621821591309249} & \frac{746823110378507}{1160531333196531} & \frac{-245203182293974}{830463435545725} & \frac{75205457669720}{1376970636717483} & \mathcal{Q}_{8,8} \end{bmatrix}$$

and

$$\mathcal{U} = \begin{bmatrix} \frac{180244350371637}{1126868276263618} & \frac{-392583468178750}{828881219713327} & \frac{-490045535918397}{875960756546638} & \frac{-190933022178950}{360901038824607} & \frac{1130441123439817}{1001785426529180} & \frac{-411593994924900}{1294802177543183} & \frac{-6349752375614477}{2050000149117882} & \mathcal{U}_{1,8} \\ \frac{0}{1} & \frac{85288341566735}{533166259630668} & \frac{364391849692265}{1281179727879002} & \frac{282427519409327}{847509782376348} & \frac{-316253337224677}{404055296629515} & \frac{305176606279235}{1895646984777073} & \frac{1266878767846480}{681911013172681} & \mathcal{U}_{2,8} \\ \frac{0}{1} & \frac{-3090941}{749706123511361} & \frac{85288341566735}{533166259630668} & \frac{236328209620645}{561859287470453} & \frac{-410966791850897}{695378559556228} & \frac{195652180864971}{704155521594584} & \frac{1746091609096721}{964952745920769} & \mathcal{U}_{3,8} \\ \frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{60860727377309}{380379557091291} & \frac{-200825814647765}{1039950773828948} & \frac{634435057463647}{1562548340843445} & \frac{36110898164319}{719029562510054} & \mathcal{U}_{4,8} \\ \frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{4145023}{341215461830388} & \frac{60860727377309}{380379557091291} & \frac{288457721365118}{663270527454401} & \frac{-1266905243847901}{618980828012415} & \mathcal{U}_{5,8} \\ \frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{250909322856947}{1567847668296140} & \frac{-441585561543613}{2895586895038540} & \mathcal{U}_{6,8} \\ \frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{11689046}{1519374183383503} & \frac{250909322856947}{1567847668296140} & \mathcal{U}_{7,8} \\ \frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{0}{1}\mathcal{U}_{8,8} & \end{bmatrix}$$

where

$$\begin{aligned} \mathcal{Q}_{1,8} &= \tfrac{696056740595916}{1182258379726885} & \mathcal{U}_{1,8} &= \tfrac{-13022786495141}{107570762091310} \\ \mathcal{Q}_{2,8} &= \tfrac{-645066396579240}{920699590860313} & \mathcal{U}_{2,8} &= \tfrac{422188642953562}{1664850210133027} \\ \mathcal{Q}_{3,8} &= \tfrac{283379409722461}{775622404583926} & \mathcal{U}_{3,8} &= \tfrac{705171343261765}{1301705535214028} \\ \mathcal{Q}_{4,8} &= \tfrac{-72176390566629}{480564345191939} & \mathcal{U}_{4,8} &= \tfrac{-1312796603747621}{1015943947240410} \\ \mathcal{Q}_{5,8} &= \tfrac{95010016298042}{1368465647096129} & \mathcal{U}_{5,8} &= \tfrac{-754886232959789}{567349623221281} \\ \mathcal{Q}_{6,8} &= \tfrac{-17184850392129}{510533565156134} & \mathcal{U}_{6,8} &= \tfrac{2224206094287016}{1545385893645085} \\ \mathcal{Q}_{7,8} &= \tfrac{14790098541887}{716263386202895} & \mathcal{U}_{7,8} &= \tfrac{256573320092538}{1181680499411275} \\ \mathcal{Q}_{8,8} &= \tfrac{-15471126938461}{1836063540620563} & \mathcal{U}_{8,8} &= \tfrac{51762958647773}{323420578223002} \end{aligned} \tag{A2}$$

A.3 Stage-Order Five Methods

A.3.1 SIRK5(4)7L[5]SA

The SIRK method, SIRK5(4)7L[5]SA, is given by

$$
\begin{array}{c|ccccccc}
\frac{167}{382} & \frac{-6959398125137693}{487354483412478} & \frac{5248153179816419}{640354388479597} & \frac{12592773310891114}{1048891760614213} & \frac{-17239768565917263}{1236287883631337} & \frac{2872655943827463}{472778874779599} & \frac{9606772816923261}{2125278789546575} & \frac{-660601838655360}{309280394740699} \\
\frac{133}{365} & \frac{-14761751668478125}{997246396607286} & \frac{7676275757941777}{916852583344133} & \frac{1472683394850107}{115853572424231} & \frac{-9314566190072464}{631480020005347} & \frac{7871573132792188}{1256095924147217} & \frac{4788711357540958}{978407155971915} & \frac{-2661810456580252}{1143469406199187} \\
\frac{161}{264} & \frac{-16054194764065017}{1090728268532242} & \frac{6893944587969082}{819808771350593} & \frac{12197847727566805}{934949525304538} & \frac{-16435618374504583}{1111384836730986} & \frac{6225360940409198}{1024038485999581} & \frac{4786178353082867}{971469726773196} & \frac{-1887139050575059}{804866923659600} \\
\frac{257}{359} & \frac{-9114366213032318}{630706184716107} & \frac{6551929918118287}{789945314294067} & \frac{19428967217807226}{1546300075394543} & \frac{-14795222865413813}{1029568148798487} & \frac{3355047403867687}{541837665305397} & \frac{4948178168743275}{1046329190210041} & \frac{-1734362828160869}{773308274999397} \\
\frac{109}{169} & \frac{-3535651769386852}{268591704053503} & \frac{5277703510345904}{682152331119181} & \frac{14250178485408243}{1351137920762893} & \frac{-9493673717761561}{770491866435882} & \frac{6726199773407615}{1151234699644699} & \frac{2240240636528313}{599545298583188} & \frac{-2389925195772603}{1379396553122845} \\
\frac{379}{405} & \frac{-11996783419242664}{904468925812727} & \frac{5968515081802069}{766552517061710} & \frac{9989458692807408}{964849142077123} & \frac{-28985901871493076}{2317577671088965} & \frac{5477117210031022}{856122179552349} & \frac{1649302584514662}{412003443196913} & \frac{-1650162328224991}{899956439942291} \\
\frac{1}{1} & \frac{-8773125108496805}{686426532553586} & \frac{9659664075730697}{1274887517438308} & \frac{12862698552790732}{1339926327792419} & \frac{-12291736478370131}{1048191496206652} & \frac{3776740118599985}{601705552983238} & \frac{4651784258075520}{1267955551167427} & \frac{-4734544907442629}{2932685053214474} \\
\hline
b_i & \frac{-8773125108496805}{686426532553586} & \frac{9659664075730697}{1274887517438308} & \frac{12862698552790732}{1339926327792419} & \frac{-12291736478370131}{1048191496206652} & \frac{3776740118599985}{601705552983238} & \frac{4651784258075520}{1267955551167427} & \frac{-4734544907442629}{2932685053214474} \\
\hline
\hat{b}_i & \frac{-17081550280930987}{1259587583764143} & \frac{5946568925109313}{757415929220436} & \frac{16723840936319911}{1447057440215881} & \frac{-13396131973658136}{976660006793063} & \frac{6465814850763931}{1038507058979580} & \frac{6457508643576915}{1295690406061672} & \frac{-1577759722556877}{674062325691920}
\end{array}
$$

where $\mathbf{S}$ and $\mathbf{S}^{-1}$ are, respectively.

$$
\begin{bmatrix}
\frac{4144219520018}{1146912532528581} & \frac{-26883486012219}{967768487393333} & \frac{542710488948973}{1019154003270205} & \frac{-5902595656269147}{2213477941518368} & \frac{-430970898516728}{2491541393879603} & \frac{149133046072789231}{2533865462943342} & \frac{789181844449995947}{727669696792437} \\
\frac{18738251410588}{3309002732892103} & \frac{-26152669933574}{809872078638311} & \frac{254994534818229}{589838964148669} & \frac{-1887549778528858}{1001552044777977} & \frac{-6893538211485020}{686488139218311} & \frac{15560762069947326}{1390690627732745} & \frac{336201969402543202}{660512645280769} \\
\frac{-19503591937142}{1196193351630431} & \frac{50954114313727}{4001771778216874} & \frac{-1782790479597782}{6958648628024627} & \frac{-1774053568532425}{737488337447617} & \frac{39616069324780373}{1087751489245167} & \frac{745047691382502817}{1257096951715110} & \frac{2676979939614743858}{461447422548071} \\
\frac{-11612326206344}{854797736069977} & \frac{219843405811570}{1903334098313361} & \frac{-315203704765219}{696847542043691} & \frac{-148700241994683}{144157468117301} & \frac{27043208945210421}{764464135276757} & \frac{112760059992317288}{188105678361331} & \frac{4173337909675494657}{754934613740920} \\
\frac{-4189453857279}{736399192698734} & \frac{91864283909078}{1015745330803123} & \frac{334510202017655}{1512310831404273} & \frac{-2090266110262809}{1366950966308080} & \frac{24234807636319331}{1054959135108096} & \frac{228129081741930224}{800148228426541} & \frac{2247529268047174391}{810101560325704} \\
\frac{47246926880747}{1113328300205546} & \frac{349781502538029}{1086560269085483} & \frac{45663327785982}{1870014504494437} & \frac{696799381506356}{2830620241719189} & \frac{-2329226454686751}{1645874748133760} & \frac{27909766065488577}{510568889585876} & \frac{430749539891059781}{1082940623877027} \\
\frac{17}{250} & \frac{159}{500} & \frac{27}{100} & \frac{-9}{100} & \frac{-1}{1000} & \frac{-9947}{1000} & \frac{-146501}{1000}
\end{bmatrix}
$$

$$
\begin{bmatrix}
\frac{-9847742459279645}{830016162627091} & \frac{5201367879625517}{430357485997235} & \frac{6400159911373648}{907513296176687} & \frac{7429510084543013}{1328025663728323} & \frac{-12760646782001888}{764912768251283} & \frac{-48104948861953238}{1423290173020005} & \frac{45883588254232199}{1245627230572259} \\
\frac{11149292578428830}{2384808110049461} & \frac{-2486214014133943}{478242516609424} & \frac{225641356210177}{1036087176597005} & \frac{-1758255228071116}{878494012030867} & \frac{1501166404684916}{1419675479237241} & \frac{4709041470296325}{519774396358774} & \frac{-11726812195800925}{2047027916979674} \\
\frac{-25334850490644379}{988578913892985} & \frac{23899448604393627}{1486206856119308} & \frac{15414421143093957}{872515888791359} & \frac{-25555707206445599}{1169802797915892} & \frac{13920551551992361}{1088436992215049} & \frac{2574397737075577}{494727984867537} & \frac{-3020969816878953}{1323118054885591} \\
\frac{-3077919196999942}{146967371631279} & \frac{17362536984954383}{1466838233924803} & \frac{17271576214408906}{1012907212541233} & \frac{-13395893879711742}{672271734558079} & \frac{5470533408177835}{604950888325636} & \frac{6691720528024903}{1098867308071298} & \frac{-462977907244461}{164816667524150} \\
\frac{-114459613097347}{1303705526393454} & \frac{-7656651378889}{428794898116062} & \frac{364982202443473}{2584497278364937} & \frac{-105691523300961}{628196683325521} & \frac{71860116744972}{993710370450949} & \frac{16896861034141}{506358674601072} & \frac{-7777830285105}{928852906313534} \\
\frac{618211357623167}{1037605157021918} & \frac{-356877719108371}{1120344629024599} & \frac{-472552322540961}{867123048172168} & \frac{1103355125501701}{1748991868442695} & \frac{-289018442753487}{1131089601235619} & \frac{-200778381787116}{930199228745443} & \frac{247517357593699}{2390202368624611} \\
\frac{-72097969774742}{1027366478214531} & \frac{43138861785461}{1125782133349928} & \frac{83903204533547}{1335378363633577} & \frac{-68802372896189}{947683845737802} & \frac{5985925055563}{200089980835096} & \frac{10171992701706}{415491826537063} & \frac{-11776536350129}{1008575161226489}
\end{bmatrix}
$$

and $\mathcal{J}$ is created using (2) and $\gamma = \frac{1}{7}$. For the Schur decomposition of the **A**-matrix, we have

$$\mathcal{Q} = \begin{bmatrix} \frac{43850882924804}{1011921075324525} & \frac{-163268434073943}{994244427425342} & \frac{894060855477621}{1433298789505151} & \frac{207355533917114}{662999525806351} & \frac{-188066290188583}{2071024451165546} & \frac{344088566391067}{788623963337034} & \frac{835153045920250}{1562673512015149} \\ \frac{125832027967880}{1852848937225563} & \frac{-677327881041947}{3133963840499948} & \frac{1839094689167049}{4234159712092298} & \frac{261756376242257}{944717730954432} & \frac{-323092677666281}{745292299237733} & \frac{-317810590586104}{496239987599911} & \frac{-199712246507403}{684368784972148} \\ \frac{-177482215458443}{907658284988712} & \frac{210937414827209}{643096941441385} & \frac{-35875545872899}{877608838203605} & \frac{614073656358057}{848235254635933} & \frac{104076797451537}{889137360305792} & \frac{216010230036421}{737622297636686} & \frac{-31178343241273}{65159635571308} \\ \frac{-104545029727013}{641694443864428} & \frac{250368194024546}{380519740456337} & \frac{-38571841370485}{314432043646897} & \frac{1103648111411547}{5511039446433511} & \frac{-60276988827497}{502259463420659} & \frac{-1052644643449776}{2589112898775089} & \frac{805524584563205}{1456930000926396} \\ \frac{-38906832593785}{570246359115619} & \frac{495143791527617}{1151977533497937} & \frac{480338848148309}{761539643324904} & \frac{-368169854878082}{1007997878534855} & \frac{548371418298147}{1173382404191162} & \frac{-801637802790089}{8432967123963377} & \frac{-123034232976181}{540032453022527} \\ \frac{1292559557330983}{2539691695518473} & \frac{440806785605275}{983153861404126} & \frac{36872719567902}{880403537553125} & \frac{-253344123833133}{1147259638776344} & \frac{-153682819181721}{259320276852464} & \frac{424505875111439}{1319814820927363} & \frac{-241280130490050}{1294129775929477} \\ \frac{623968418781000}{765128622856123} & \frac{-9406843923025}{1337051995722091} & \frac{-102271576369107}{1328322478792838} & \frac{121945922099837}{433734101947028} & \frac{1121647886683343}{2470747877633610} & \frac{-226704989736469}{1196081685891634} & \frac{66901181434653}{752357586074923} \end{bmatrix}$$

and

$$\mathcal{U} = \begin{bmatrix} \frac{1}{7} & \frac{229378301654879}{750123997918710} & \frac{631070149842565}{836325357194854} & \frac{-341632451358124}{304579979169663} & \frac{523005498554017}{988823141162227} & \frac{-1852472618423584}{847658950997753} & \frac{-29919430411686859}{1361870033795279} \\ \frac{0}{1} & \frac{1}{7} & \frac{123049411681103}{318426727549022} & \frac{-492891555788809}{1785710561512040} & \frac{192009874771259}{887122996973415} & \frac{-1162063920902021}{660625863300281} & \frac{-34484033932588283}{937839606962312} \\ \frac{0}{1} & \frac{0}{1} & \frac{1}{7} & \frac{-328910753022265}{1316929652337289} & \frac{161459103626999}{1063107564588481} & \frac{-1384661272280719}{787422173166141} & \frac{-63567824581282015}{1692990742377161} \\ \frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{1}{7} & \frac{-270361706902496}{1527291664198867} & \frac{-198127980452945}{314606142238664} & \frac{-27642996557348524}{831869278312873} \\ \frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{1}{7} & \frac{-188480681907382}{699978390761103} & \frac{3553971565828551}{504851365405175} \\ \frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{1}{7} & \frac{7930883229376013}{1018946034971274} \\ \frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{0}{1} & \frac{1}{7} \end{bmatrix}$$

Appendix B

New ESDIRK Method

An interesting question to ask is whether a stage-order 2 ESDIRK can be made to perform as well as a stage-order 4 SIRK on Kreiss' problem by simply increasing the order of the DAE2_z variable from one to two or three by satisfying (114) and (115)? To do this, we will solve one or three extra order conditions. The method will be an analog to ESDIRK4(3)7[2]SA from [119] but is third-order in the DAE2_z variable following the discussion in §4.4. For a customized ESDIRK4(3)7[2]SA_DAE, we first set

$$\gamma = \frac{9}{50}, \quad c_2 = \frac{9}{25}, \quad c_3 = \frac{9(2-\sqrt{2})}{50}, \quad c_4 = \frac{71}{235}, \quad c_5 = \frac{228}{353}, \quad c_6 = \frac{241}{317}, \quad c_7 = 1, \tag{B1}$$

and then solve for the main and embedded methods with

$$0 = \tau_1^{(1,2,3,4,5)} = q_{2,3,4,5,6}^{(1)} = q_{2,3,4,5,6}^{(2)} = \tau_3^{(4)} = p_6 = R_{\text{int}}^{(3,4,5,6)}(-\infty) = \hat{\tau}_1^{(1,2,3)} = \hat{p}_{6,7}, \tag{B2}$$

$$1 = \frac{1}{3}\tilde{\mathbf{b}}^T\tilde{\mathbf{W}}^2\tilde{\mathbf{c}}^3 = \frac{1}{4}\tilde{\mathbf{b}}^T\tilde{\mathbf{W}}^2\tilde{\mathbf{c}}^4 = \frac{3}{2}\tilde{\mathbf{b}}^T\tilde{\mathbf{W}}^2\tilde{\mathbf{C}}\tilde{\mathbf{A}}^2\tilde{\mathbf{c}}, \tag{B3}$$

along with $\hat{\tau}_1^{(4,5)} = 10^{-6}\{1786, 1062\}$. The properties of this method are given in Table B1 along with ESDIRK4(3)7[2]SA. Method ESDIRK4(3)7[2]SA_DAE has similarities with earlier ESDIRK methods intended for index-2 DAEs [162, 185].

Name	ESDIRK4(3)7L[2]SA_DAE	ESDIRK4(3)7L[2]SA
$(s, p, \hat{p}, \mathfrak{q})$	$(7, 4, 3, 2)$	$(7, 4, 3, 2)$
$\{\gamma, \gamma s\}$	$\{\frac{9}{50}, \frac{63}{50}\}$	$\{\frac{1}{8}, \frac{7}{8}\}$
$\{A^{(p+1)}, A^{(p+2)}\}$	$\{2.99(-3), 5.10(-3)\}$	$\{2.60(-4), 1.18(-4)\}$
$\{\hat{A}^{(\hat{p}+1)}, \hat{A}^{(\hat{p}+2)}\}$	$\{5.66(-3), 8.34(-3)\}$	$\{3.01(-4), 9.77(-4)\}$
$(B, C, E)^{(\hat{p}+2)}$	$(1.52, 1.00, 0.527)$	$(3.24, 3.07, 0.861)$
$\{R(-\infty), \hat{R}(-\infty)\}$	$\{0, 0\}$	$\{0, 0\}$
(Min., Max.) $\{\mathbf{A}, \mathbf{b}, \hat{\mathbf{b}}\}$	$\{(-0.515, 1.01), (-0.234, 0.581), (-0.309, 0.727)\}$	$\{(-0.557, 0.939), (-0.557, 0.939), (-0.571, 0.761)\}$
(Min., Max.) $\{\lambda_{\text{M}}, \lambda_{\hat{\text{M}}}, \lambda_{\text{M}_{(\text{int})}}\}$	$\{(-0.816, 0.509), (-0.613, 0.359), (-1.50, 0.509)\}$	$\{(-1.99, 0.442), (-1.36, 0.534), (-1.99, 0.442)\}$
$\mathcal{C}$	0.466	0.420

Table B1: ESDIRK4(3)7L[2]SA_DAE and ESDIRK4(3)7L[2]SA methods

0	0	0	0	0	0	0	0
$\frac{9}{25}$	a_{21}	$\frac{9}{50}$	0	0	0	0	0
$\frac{9(2-\sqrt{2})}{50}$	a_{31}	$\frac{-37882655889150}{1016186906958877}$	$\frac{9}{50}$	0	0	0	0
$\frac{71}{235}$	a_{41}	$\frac{-73468583640249}{506731441108699}$	$\frac{418580047051346}{1015728999177825}$	$\frac{9}{50}$	0	0	0
$\frac{228}{353}$	a_{51}	$\frac{-133335916217989}{843697985283065}$	$\frac{496091684036408}{1121123730243935}$	$\frac{538386087514823}{1585949949164697}$	$\frac{9}{50}$	0	0
$\frac{241}{317}$	a_{61}	$\frac{-2005852528315818}{3898250075993831}$	$\frac{1470398615489563}{1418916247950218}$	$\frac{257318237488820}{622822153133637}$	$\frac{83044921923448}{519274996222453}$	$\frac{9}{50}$	0
1	a_{71}	$\frac{278044913449129}{1158622709394408}$	$\frac{-188271558442775}{970304042797582}$	$\frac{123113091387085}{659752368881897}$	$\frac{32963424160095}{56706540725936}$	$\frac{-221786804785708}{948505981982203}$	$\frac{9}{50}$
b_i	b_1	$\frac{278044913449129}{1158622709394408}$	$\frac{-188271558442775}{970304042797582}$	$\frac{123113091387085}{659752368881897}$	$\frac{32963424160095}{56706540725936}$	$\frac{-221786804785708}{948505981982203}$	$\frac{9}{50}$
$\hat{b}_i$	$\hat{b}_1$	$\frac{-126733270241222}{18057752056574177}$	$\frac{127639018777231}{699237821800165}$	$\frac{65077903120919}{238793127012202}$	$\frac{376075051514783}{573911111909180}$	$\frac{-142188693942798}{460578779179951}$	$\frac{209989156700087}{988645862306111}$

Table B2: ESDIRK4(3)7L[2]SA_DAE with $a_{i1} = a_{i2}$, $b_1 = b_2$ and $\hat{b}_1 = \hat{b}_2$.

Appendix C

Simplified Order Conditions

Order conditions to Runge–Kutta methods get increasingly messy with increasing order. However, methods with relatively high stage-order, say at least three, can be more easily understood by distinguishing between quadrature, subquadrature, extended subquadrature and nonlinear order conditions [178] as well as casting the order conditions in terms of $\mathbf{q}^{(k)}$ (see §2.1.2). There are several advantages to viewing order conditions in this manner. First and most importantly, when the method is designed with, say, $\mathbf{q}^{(2)} = \mathbf{q}^{(3)} = \mathbf{0}$, it is easily deduced how the original order conditions have been simplified. Beyond this, casting the order conditions in terms of $\mathbf{q}^{(k)}$ demonstrate the assertion that when $C(\eta)$, or $\mathbf{q}^{(k)} = 0,\ k = 1, 2, \ldots, k$, is enforced, any nonlinear order-conditions of order $2k+2$ or less may be ignored because they have been rendered redundant. Up to order seven, the order-conditions for Runge–Kutta methods are given below.

C.1 Quadrature (Q) Conditions

At each order, there is a single quadrature order condition given by

$$\tau_1^{(k)} = \frac{1}{(k-1)!}\mathbf{b}^T\mathbf{c}^{k-1} - \frac{1}{k!},\ k = 1, 2, \cdots .$$

C.2 Subquadrature (SQ) Conditions

At each order p, where the order is greater than two $(p > 2)$, there are $p-2$ subquadrature order conditions. Again, at order p, one subquadrature order condition can be rendered redundant by imposing $\mathbf{q}^{(2)}$ while two can be rendered redundant by imposing $\mathbf{q}^{(3)}$. Ultimately, all subquadrature order conditions can be made redundant by imposing $\mathbf{q}^{(p-1)}$. Alternatively, imposing $\mathbf{q}^{(k)}$ with $k > 1$ renders $k-1$ subquadrature order conditions redundant.

$$\tau_2^{(3)} = \mathbf{b}^T\mathbf{q}^{(2)} + \tau_1^{(3)}$$

$$\tau_3^{(4)} = \frac{1}{2}\mathbf{b}^T\mathbf{q}^{(3)} + \tau_1^{(4)} \qquad \tau_4^{(4)} = \mathbf{b}^T\mathbf{A}\mathbf{q}^{(2)} + \tau_3^{(4)}$$

$$\tau_5^{(5)} = \frac{1}{6}\mathbf{b}^T\mathbf{q}^{(4)} + \tau_1^{(5)} \qquad \tau_8^{(5)} = \frac{1}{2}\mathbf{b}^T\mathbf{A}\mathbf{q}^{(3)} + \tau_5^{(5)} \qquad \tau_9^{(5)} = \mathbf{b}^T\mathbf{A}\mathbf{A}\mathbf{q}^{(2)} + \tau_8^{(5)}$$

$$\tau_7^{(6)} = \frac{1}{24}\mathbf{b}^T\mathbf{q}^{(5)} + \tau_1^{(6)} \qquad \tau_{15}^{(6)} = \frac{1}{6}\mathbf{b}^T\mathbf{A}\mathbf{q}^{(4)} + \tau_7^{(6)} \qquad \tau_{19}^{(6)} = \frac{1}{2}\mathbf{b}^T\mathbf{A}\mathbf{A}\mathbf{q}^{(3)} + \tau_{15}^{(6)}$$
$$\tau_{20}^{(6)} = \mathbf{b}^T\mathbf{A}\mathbf{A}\mathbf{A}\mathbf{q}^{(2)} + \tau_{19}^{(6)}$$

$$\tau_{11}^{(7)} = \frac{1}{120}\mathbf{b}^T\mathbf{q}^{(6)} + \tau_1^{(7)} \qquad \tau_{29}^{(7)} = \frac{1}{24}\mathbf{b}^T\mathbf{A}\mathbf{q}^{(5)} + \tau_{11}^{(7)} \qquad \tau_{42}^{(7)} = \frac{1}{6}\mathbf{b}^T\mathbf{A}\mathbf{A}\mathbf{q}^{(4)} + \tau_{29}^{(7)}$$
$$\tau_{47}^{(7)} = \frac{1}{2}\mathbf{b}^T\mathbf{A}\mathbf{A}\mathbf{A}\mathbf{q}^{(3)} + \tau_{42}^{(7)} \qquad \tau_{48}^{(7)} = \mathbf{b}^T\mathbf{A}\mathbf{A}\mathbf{A}\mathbf{A}\mathbf{q}^{(2)} + \tau_{47}^{(7)}$$

$$\tau_{15}^{(8)} = \frac{1}{720}\mathbf{b}^T\mathbf{q}^{(7)} + \tau_1^{(8)} \qquad \tau_{53}^{(8)} = \frac{1}{120}\mathbf{b}^T\mathbf{A}\mathbf{q}^{(6)} + \tau_{15}^{(8)} \qquad \tau_{89}^{(8)} = \frac{1}{24}\mathbf{b}^T\mathbf{A}\mathbf{A}\mathbf{q}^{(5)} + \tau_{53}^{(8)}$$
$$\tau_{108}^{(8)} = \frac{1}{6}\mathbf{b}^T\mathbf{A}\mathbf{A}\mathbf{A}\mathbf{q}^{(4)} + \tau_{89}^{(8)} \qquad \tau_{114}^{(8)} = \frac{1}{2}\mathbf{b}^T\mathbf{A}\mathbf{A}\mathbf{A}\mathbf{A}\mathbf{q}^{(3)} + \tau_{108}^{(8)} \qquad \tau_{115}^{(8)} = \mathbf{b}^T\mathbf{A}\mathbf{A}\mathbf{A}\mathbf{A}\mathbf{A}\mathbf{q}^{(2)} + \tau_{114}^{(8)}$$

C.3 Extended Subquadrature (ESQ) Conditions

At each order p, where the order is greater than two ($p > 3$), there are $2^{p-2} - p + 1$ ESQ order conditions. At order p, these order conditions may be grouped by the lowest value of k for which the order condition is made redundant, from $\mathbf{q}^{(2)} = \mathbf{0}$ to $\mathbf{q}^{(p-2)} = \mathbf{0}$. The ESQ order conditions reduced by $\mathbf{q}^{(2)} = \mathbf{0}$, number $2^{p-3} - 1$. In general, imposing only $\mathbf{q}^{(k)} = \mathbf{0},\ k > 1$ renders $2^{p-k-1} - 1$ order conditions redundant. If we impose $\mathbf{q}^{(m)} = \mathbf{0},\ m = 2, , 3 \ldots, k$, then $2^{p-2} - 2^{p-k-1} - (k-1)$ ESQ order conditions will have been rendered redundant, leaving $2^{p-k-1} - (p-1)$ unreduced. As an example, imagine we create a seventh-order method which imposes $\mathbf{q}^{(2)} = \mathbf{q}^{(3)} = \mathbf{0}$. At seventh-order ($p = 7$), there are 26 ESQ order conditions. At a stage-order of three ($k = 3$), 22 conditions are redundant and four remain.

$$\tau_2^{(4)} = \mathbf{b}^T\mathbf{C}\mathbf{q}^{(2)} + 3\tau_1^{(4)}$$

$$\tau_2^{(5)} = \frac{1}{2}\mathbf{b}^T\mathbf{C}^2\mathbf{q}^{(2)} + 6\tau_1^{(5)} \qquad \tau_6^{(5)} = \mathbf{b}^T\mathbf{C}\mathbf{A}\mathbf{q}^{(2)} + \tau_4^{(5)} \qquad \tau_7^{(5)} = \mathbf{b}^T\mathbf{A}\mathbf{C}\mathbf{q}^{(2)} + 3\tau_5^{(5)}$$

$$\tau_4^{(5)} = \frac{1}{2}\mathbf{b}^T\mathbf{C}\mathbf{q}^{(3)} + 4\tau_1^{(5)}$$

$$\tau_2^{(6)} = \frac{1}{6}\mathbf{b}^T\mathbf{C}^3\mathbf{q}^{(2)} + 10\tau_1^{(6)} \qquad \tau_8^{(6)} = \frac{1}{2}\mathbf{b}^T\mathbf{C}^2\mathbf{A}\mathbf{q}^{(2)} + \tau_4^{(6)} \qquad \tau_{10}^{(6)} = \mathbf{b}^T\mathbf{C}\mathbf{A}\mathbf{C}\mathbf{q}^{(2)} + 3\tau_6^{(6)}$$
$$\tau_{11}^{(6)} = \frac{1}{2}\mathbf{b}^T\mathbf{A}\mathbf{C}^2\mathbf{q}^{(2)} + 6\tau_7^{(6)} \qquad \tau_{16}^{(6)} = \mathbf{b}^T\mathbf{C}\mathbf{A}\mathbf{A}\mathbf{q}^{(2)} + \tau_{13}^{(6)} \qquad \tau_{17}^{(6)} = \mathbf{b}^T\mathbf{A}\mathbf{C}\mathbf{A}\mathbf{q}^{(2)} + \tau_{14}^{(6)}$$
$$\tau_{18}^{(6)} = \mathbf{b}^T\mathbf{A}\mathbf{A}\mathbf{C}\mathbf{q}^{(2)} + 3\tau_{15}^{(6)}$$

$$\tau_4^{(6)} = \frac{1}{4}\mathbf{b}^T\mathbf{C}^2\mathbf{q}^{(3)} + 10\tau_1^{(6)} \qquad \tau_{13}^{(6)} = \frac{1}{2}\mathbf{b}^T\mathbf{C}\mathbf{A}\mathbf{q}^{(3)} + \tau_6^{(6)} \qquad \tau_{14}^{(6)} = \frac{1}{2}\mathbf{b}^T\mathbf{A}\mathbf{C}\mathbf{q}^{(3)} + 4\tau_7^{(6)}$$

$$\tau_6^{(6)} = \frac{1}{6}\mathbf{b}^T\mathbf{C}\mathbf{q}^{(4)} + 5\tau_1^{(6)}$$

$$\tau_2^{(7)} = \frac{1}{24}\mathbf{b}^T\mathbf{C}^4\mathbf{q}^{(2)} + 15\tau_1^{(7)} \qquad \tau_{12}^{(7)} = \frac{1}{6}\mathbf{b}^T\mathbf{C}^3\mathbf{A}\mathbf{q}^{(2)} + \tau_5^{(7)} \qquad \tau_{16}^{(7)} = \frac{1}{2}\mathbf{b}^T\mathbf{C}^2\mathbf{A}\mathbf{C}\mathbf{q}^{(2)} + 3\tau_8^{(7)}$$
$$\tau_{18}^{(7)} = \frac{1}{2}\mathbf{b}^T\mathbf{C}\mathbf{A}\mathbf{C}^2\mathbf{q}^{(2)} + 6\tau_{10}^{(7)} \qquad \tau_{19}^{(7)} = \frac{1}{6}\mathbf{b}^T\mathbf{A}\mathbf{C}^3\mathbf{q}^{(2)} + 10\tau_{11}^{(7)} \qquad \tau_{30}^{(7)} = \frac{1}{2}\mathbf{b}^T\mathbf{C}^2\mathbf{A}\mathbf{A}\mathbf{q}^{(2)} + \tau_{22}^{(7)}$$
$$\tau_{32}^{(7)} = \mathbf{b}^T\mathbf{C}\mathbf{A}\mathbf{C}\mathbf{A}\mathbf{q}^{(2)} + \tau_{24}^{(7)} \qquad \tau_{33}^{(7)} = \frac{1}{2}\mathbf{b}^T\mathbf{A}\mathbf{C}^2\mathbf{A}\mathbf{q}^{(2)} + \tau_{25}^{(7)} \qquad \tau_{35}^{(7)} = \mathbf{b}^T\mathbf{C}\mathbf{A}\mathbf{A}\mathbf{C}\mathbf{q}^{(2)} + 3\tau_{27}^{(7)}$$
$$\tau_{36}^{(7)} = \mathbf{b}^T\mathbf{A}\mathbf{C}\mathbf{A}\mathbf{C}\mathbf{q}^{(2)} + 3\tau_{28}^{(7)} \qquad \tau_{37}^{(7)} = \frac{1}{2}\mathbf{b}^T\mathbf{A}\mathbf{A}\mathbf{C}^2\mathbf{q}^{(2)} + 6\tau_{29}^{(7)} \qquad \tau_{43}^{(7)} = \mathbf{b}^T\mathbf{C}\mathbf{A}\mathbf{A}\mathbf{A}\mathbf{q}^{(2)} + \tau_{39}^{(7)}$$
$$\tau_{44}^{(7)} = \mathbf{b}^T\mathbf{A}\mathbf{C}\mathbf{A}\mathbf{A}\mathbf{q}^{(2)} + \tau_{40}^{(7)} \qquad \tau_{45}^{(7)} = \mathbf{b}^T\mathbf{A}\mathbf{A}\mathbf{C}\mathbf{A}\mathbf{q}^{(2)} + \tau_{41}^{(7)} \qquad \tau_{46}^{(7)} = \mathbf{b}^T\mathbf{A}\mathbf{A}\mathbf{A}\mathbf{C}\mathbf{q}^{(2)} + 3\tau_{42}^{(7)}$$

$$\tau_5^{(7)} = \frac{1}{12}\mathbf{b}^T\mathbf{C}^3\mathbf{q}^{(3)} + 20\tau_1^{(7)} \qquad \tau_{22}^{(7)} = \frac{1}{4}\mathbf{b}^T\mathbf{C}^2\mathbf{A}\mathbf{q}^{(3)} + \tau_8^{(7)} \qquad \tau_{24}^{(7)} = \frac{1}{2}\mathbf{b}^T\mathbf{C}\mathbf{A}\mathbf{C}\mathbf{q}^{(3)} + 4\tau_{10}^{(7)}$$
$$\tau_{25}^{(7)} = \frac{1}{4}\mathbf{b}^T\mathbf{A}\mathbf{C}^2\mathbf{q}^{(3)} + 10\tau_{11}^{(7)} \qquad \tau_{39}^{(7)} = \frac{1}{2}\mathbf{b}^T\mathbf{C}\mathbf{A}\mathbf{A}\mathbf{q}^{(3)} + \tau_{27}^{(7)} \qquad \tau_{40}^{(7)} = \frac{1}{2}\mathbf{b}^T\mathbf{A}\mathbf{C}\mathbf{A}\mathbf{q}^{(3)} + \tau_{28}^{(7)}$$
$$\tau_{41}^{(7)} = \frac{1}{2}\mathbf{b}^T\mathbf{A}\mathbf{A}\mathbf{C}\mathbf{q}^{(3)} + 4\tau_{29}^{(7)}$$

$$\tau_8^{(7)} = \frac{1}{12}\mathbf{b}^T\mathbf{C}^2\mathbf{q}^{(4)} + 15\tau_1^{(7)} \qquad \tau_{27}^{(7)} = \frac{1}{6}\mathbf{b}^T\mathbf{C}\mathbf{A}\mathbf{q}^{(4)} + \tau_{10}^{(7)} \qquad \tau_{28}^{(7)} = \frac{1}{6}\mathbf{b}^T\mathbf{A}\mathbf{C}\mathbf{q}^{(4)} + 5\tau_{11}^{(7)}$$

$$\tau_{10}^{(7)} = \frac{1}{24}\mathbf{b}^T\mathbf{C}\mathbf{q}^{(5)} + 6\tau_1^{(7)}$$

$$\tau_{2}^{(8)} = \frac{1}{120}\mathbf{b}^T\mathbf{C}^5\mathbf{q}^{(2)} + 21\tau_{1}^{(8)} \qquad \tau_{16}^{(8)} = \frac{1}{24}\mathbf{b}^T\mathbf{C}^4\mathbf{A}\mathbf{q}^{(2)} + \tau_{5}^{(8)} \qquad \tau_{22}^{(8)} = \frac{1}{6}\mathbf{b}^T\mathbf{C}^3\mathbf{A}\mathbf{C}\mathbf{q}^{(2)} + 3\tau_{9}^{(8)}$$

$$\tau_{26}^{(8)} = \frac{1}{4}\mathbf{b}^T\mathbf{C}^2\mathbf{A}\mathbf{C}^2\mathbf{q}^{(2)} + 6\tau_{12}^{(8)} \qquad \tau_{28}^{(8)} = \frac{1}{6}\mathbf{b}^T\mathbf{C}\mathbf{A}\mathbf{C}^3\mathbf{q}^{(2)} + 10\tau_{14}^{(8)} \qquad \tau_{29}^{(8)} = \frac{1}{24}\mathbf{b}^T\mathbf{A}\mathbf{C}^4\mathbf{q}^{(2)} + 15\tau_{15}^{(8)}$$

$$\tau_{54}^{(8)} = \frac{1}{6}\mathbf{b}^T\mathbf{C}^3\mathbf{A}\mathbf{A}\mathbf{q}^{(2)} + \tau_{35}^{(8)} \qquad \tau_{58}^{(8)} = \frac{1}{2}\mathbf{b}^T\mathbf{C}^2\mathbf{A}\mathbf{C}\mathbf{A}\mathbf{q}^{(2)} + \tau_{39}^{(8)} \qquad \tau_{60}^{(8)} = \frac{1}{2}\mathbf{b}^T\mathbf{C}\mathbf{A}\mathbf{C}^2\mathbf{A}\mathbf{q}^{(2)} + \tau_{41}^{(8)}$$

$$\tau_{61}^{(8)} = \frac{1}{6}\mathbf{b}^T\mathbf{A}\mathbf{C}^3\mathbf{A}\mathbf{q}^{(2)} + \tau_{42}^{(8)} \qquad \tau_{66}^{(8)} = \frac{1}{2}\mathbf{b}^T\mathbf{C}^2\mathbf{A}\mathbf{A}\mathbf{C}\mathbf{q}^{(2)} + 3\tau_{46}^{(8)} \qquad \tau_{68}^{(8)} = \frac{1}{2}\mathbf{b}^T\mathbf{C}\mathbf{A}\mathbf{C}\mathbf{A}\mathbf{C}\mathbf{q}^{(2)} + 3\tau_{48}^{(8)}$$

$$\tau_{69}^{(8)} = \frac{1}{2}\mathbf{b}^T\mathbf{A}\mathbf{C}^2\mathbf{A}\mathbf{C}\mathbf{q}^{(2)} + 3\tau_{49}^{(8)} \qquad \tau_{71}^{(8)} = \frac{1}{2}\mathbf{b}^T\mathbf{C}\mathbf{A}\mathbf{A}\mathbf{C}^2\mathbf{q}^{(2)} + 6\tau_{51}^{(8)} \qquad \tau_{72}^{(8)} = \frac{1}{2}\mathbf{b}^T\mathbf{A}\mathbf{C}\mathbf{A}\mathbf{C}^2\mathbf{q}^{(2)} + 6\tau_{52}^{(8)}$$

$$\tau_{73}^{(8)} = \frac{1}{6}\mathbf{b}^T\mathbf{A}\mathbf{A}\mathbf{C}^3\mathbf{q}^{(2)} + 10\tau_{53}^{(8)} \qquad \tau_{90}^{(8)} = \frac{1}{2}\mathbf{b}^T\mathbf{C}^2\mathbf{A}\mathbf{A}\mathbf{A}\mathbf{q}^{(2)} + \tau_{77}^{(8)} \qquad \tau_{92}^{(8)} = \frac{1}{2}\mathbf{b}^T\mathbf{C}\mathbf{A}\mathbf{C}\mathbf{A}\mathbf{A}\mathbf{q}^{(2)} + \tau_{79}^{(8)}$$

$$\tau_{93}^{(8)} = \frac{1}{2}\mathbf{b}^T\mathbf{A}\mathbf{C}^2\mathbf{A}\mathbf{A}\mathbf{q}^{(2)} + \tau_{80}^{(8)} \qquad \tau_{95}^{(8)} = \frac{1}{2}\mathbf{b}^T\mathbf{C}\mathbf{A}\mathbf{A}\mathbf{C}\mathbf{A}\mathbf{q}^{(2)} + \tau_{82}^{(8)} \qquad \tau_{96}^{(8)} = \frac{1}{2}\mathbf{b}^T\mathbf{A}\mathbf{C}\mathbf{A}\mathbf{C}\mathbf{A}\mathbf{q}^{(2)} + \tau_{83}^{(8)}$$

$$\tau_{97}^{(8)} = \frac{1}{2}\mathbf{b}^T\mathbf{A}\mathbf{A}\mathbf{C}^2\mathbf{A}\mathbf{q}^{(2)} + \tau_{84}^{(8)} \qquad \tau_{99}^{(8)} = \frac{1}{2}\mathbf{b}^T\mathbf{C}\mathbf{A}\mathbf{A}\mathbf{A}\mathbf{C}\mathbf{q}^{(2)} + 3\tau_{86}^{(8)} \qquad \tau_{100}^{(8)} = \frac{1}{2}\mathbf{b}^T\mathbf{A}\mathbf{C}\mathbf{A}\mathbf{A}\mathbf{C}\mathbf{q}^{(2)} + 3\tau_{87}^{(8)}$$

$$\tau_{101}^{(8)} = \frac{1}{2}\mathbf{b}^T\mathbf{A}\mathbf{A}\mathbf{C}\mathbf{A}\mathbf{C}\mathbf{q}^{(2)} + 3\tau_{88}^{(8)} \qquad \tau_{102}^{(8)} = \frac{1}{2}\mathbf{b}^T\mathbf{A}\mathbf{A}\mathbf{A}\mathbf{C}^2\mathbf{q}^{(2)} + 6\tau_{89}^{(8)} \qquad \tau_{109}^{(8)} = \frac{1}{2}\mathbf{b}^T\mathbf{C}\mathbf{A}\mathbf{A}\mathbf{A}\mathbf{A}\mathbf{q}^{(2)} + \tau_{104}^{(8)}$$

$$\tau_{110}^{(8)} = \frac{1}{2}\mathbf{b}^T\mathbf{A}\mathbf{C}\mathbf{A}\mathbf{A}\mathbf{A}\mathbf{q}^{(2)} + \tau_{105}^{(8)} \qquad \tau_{111}^{(8)} = \frac{1}{2}\mathbf{b}^T\mathbf{A}\mathbf{A}\mathbf{C}\mathbf{A}\mathbf{A}\mathbf{q}^{(2)} + \tau_{106}^{(8)} \qquad \tau_{112}^{(8)} = \frac{1}{2}\mathbf{b}^T\mathbf{A}\mathbf{A}\mathbf{A}\mathbf{C}\mathbf{A}\mathbf{q}^{(2)} + \tau_{107}^{(8)}$$

$$\tau_{113}^{(8)} = \frac{1}{2}\mathbf{b}^T\mathbf{A}\mathbf{A}\mathbf{A}\mathbf{A}\mathbf{C}\mathbf{q}^{(2)} + 3\tau_{108}^{(8)}$$

$$\tau_{5}^{(8)} = \frac{1}{48}\mathbf{b}^T\mathbf{C}^4\mathbf{q}^{(3)} + 35\tau_{1}^{(8)} \qquad \tau_{35}^{(8)} = \frac{1}{12}\mathbf{b}^T\mathbf{C}^3\mathbf{A}\mathbf{q}^{(3)} + \tau_{9}^{(8)} \qquad \tau_{39}^{(8)} = \frac{1}{4}\mathbf{b}^T\mathbf{C}^2\mathbf{A}\mathbf{C}\mathbf{q}^{(3)} + 4\tau_{12}^{(8)}$$

$$\tau_{41}^{(8)} = \frac{1}{4}\mathbf{b}^T\mathbf{C}\mathbf{A}\mathbf{C}^2\mathbf{q}^{(3)} + 10\tau_{14}^{(8)} \qquad \tau_{42}^{(8)} = \frac{1}{12}\mathbf{b}^T\mathbf{A}\mathbf{C}^3\mathbf{q}^{(3)} + 20\tau_{15}^{(8)} \qquad \tau_{77}^{(8)} = \frac{1}{4}\mathbf{b}^T\mathbf{C}^2\mathbf{A}\mathbf{A}\mathbf{q}^{(3)} + \tau_{46}^{(8)}$$

$$\tau_{79}^{(8)} = \frac{1}{2}\mathbf{b}^T\mathbf{C}\mathbf{A}\mathbf{C}\mathbf{A}\mathbf{q}^{(3)} + \tau_{48}^{(8)} \qquad \tau_{80}^{(8)} = \frac{1}{4}\mathbf{b}^T\mathbf{A}\mathbf{C}^2\mathbf{A}\mathbf{q}^{(3)} + \tau_{49}^{(8)} \qquad \tau_{82}^{(8)} = \frac{1}{2}\mathbf{b}^T\mathbf{C}\mathbf{A}\mathbf{A}\mathbf{C}\mathbf{q}^{(3)} + 4\tau_{51}^{(8)}$$

$$\tau_{83}^{(8)} = \frac{1}{2}\mathbf{b}^T\mathbf{A}\mathbf{C}\mathbf{A}\mathbf{C}\mathbf{q}^{(3)} + 4\tau_{52}^{(8)} \qquad \tau_{84}^{(8)} = \frac{1}{4}\mathbf{b}^T\mathbf{A}\mathbf{A}\mathbf{C}^2\mathbf{q}^{(3)} + 10\tau_{53}^{(8)} \qquad \tau_{104}^{(8)} = \frac{1}{2}\mathbf{b}^T\mathbf{C}\mathbf{A}\mathbf{A}\mathbf{A}\mathbf{q}^{(3)} + \tau_{86}^{(8)}$$

$$\tau_{105}^{(8)} = \frac{1}{2}\mathbf{b}^T\mathbf{A}\mathbf{C}\mathbf{A}\mathbf{A}\mathbf{q}^{(3)} + \tau_{87}^{(8)} \qquad \tau_{106}^{(8)} = \frac{1}{2}\mathbf{b}^T\mathbf{A}\mathbf{A}\mathbf{C}\mathbf{A}\mathbf{q}^{(3)} + \tau_{88}^{(8)} \qquad \tau_{107}^{(8)} = \frac{1}{2}\mathbf{b}^T\mathbf{C}\mathbf{A}\mathbf{A}\mathbf{A}\mathbf{q}^{(3)} + 4\tau_{89}^{(8)}$$

$$\tau_{9}^{(8)} = \frac{1}{36}\mathbf{b}^T\mathbf{C}^3\mathbf{q}^{(4)} + 35\tau_{1}^{(8)} \qquad \tau_{46}^{(8)} = \frac{1}{12}\mathbf{b}^T\mathbf{C}^2\mathbf{A}\mathbf{q}^{(4)} + \tau_{12}^{(8)} \qquad \tau_{48}^{(8)} = \frac{1}{6}\mathbf{b}^T\mathbf{C}\mathbf{A}\mathbf{C}\mathbf{q}^{(4)} + 5\tau_{14}^{(8)}$$

$$\tau_{49}^{(8)} = \frac{1}{12}\mathbf{b}^T\mathbf{A}\mathbf{C}^2\mathbf{q}^{(4)} + 15\tau_{15}^{(8)} \qquad \tau_{86}^{(8)} = \frac{1}{6}\mathbf{b}^T\mathbf{A}\mathbf{A}\mathbf{C}\mathbf{q}^{(4)} + \tau_{51}^{(8)} \qquad \tau_{87}^{(8)} = \frac{1}{6}\mathbf{b}^T\mathbf{A}\mathbf{A}\mathbf{C}\mathbf{q}^{(4)} + \tau_{52}^{(8)}$$

$$\tau_{88}^{(8)} = \frac{1}{6}\mathbf{b}^T\mathbf{A}\mathbf{A}\mathbf{C}\mathbf{q}^{(4)} + 5\tau_{53}^{(8)}$$

$$\tau_{12}^{(8)} = \frac{1}{48}\mathbf{b}^T\mathbf{C}^2\mathbf{q}^{(5)} + 21\tau_{1}^{(8)} \qquad \tau_{51}^{(8)} = \frac{1}{24}\mathbf{b}^T\mathbf{C}\mathbf{A}\mathbf{q}^{(5)} + \tau_{14}^{(8)} \qquad \tau_{52}^{(8)} = \frac{1}{24}\mathbf{b}^T\mathbf{A}\mathbf{C}\mathbf{q}^{(5)} + 6\tau_{15}^{(8)}$$

$$\tau_{14}^{(8)} = \frac{1}{120}\mathbf{b}^T\mathbf{C}\mathbf{q}^{(6)} + 7\tau_{1}^{(8)}$$

C.4 Nonlinear (NL) Conditions

The full topic on nonlinear, Runge–Kutta, order-conditions is beyond the scope of the present discussion. However, some comments can be made. First, imposition of $C(\eta)$ forestalls the first occurrence of a nonlinear order condition to order $p = 2\eta + 3$. When $p = 2\eta + 3$, there will be one nonlinear order condition if p is odd (e.g. $\tau_3^{(5)}$) and four if p is even, (e.g. $\tau_{3,5,9,12}^{(6)}$). In general,

$$\tau_3^{(5)} = \frac{1}{2}\mathbf{b}^T\mathbf{C}^2\mathbf{q}^{(2)} + \frac{1}{2}\mathbf{b}^T\left(\mathbf{q}^{(2)}\right)^2 + 3\tau_1^{(5)}$$

$$\tau_3^{(6)} = \frac{1}{2}\mathbf{b}^T\mathbf{C}^3\mathbf{q}^{(2)} + \frac{1}{2}\mathbf{b}^T\mathbf{C}\left(\mathbf{q}^{(2)}\right)^2 + 15\tau_1^{(6)}$$

$$\tau_5^{(6)} = \frac{1}{6}\mathbf{b}^T\mathbf{C}^3\mathbf{q}^{(2)} + \frac{1}{2}\mathbf{b}^T\mathbf{Q}^{(3)}\mathbf{q}^{(2)} + \tau_4^{(6)}$$

$$\tau_9^{(6)} = \frac{1}{2}\mathbf{b}^T\left(\mathbf{C}^2\mathbf{A} + \mathbf{A}\mathbf{C}^2\right)\mathbf{q}^{(2)} + \mathbf{b}^T\mathbf{Q}^{(2)}\mathbf{A}\mathbf{q}^{(2)} + \tau_4^{(6)}$$

$$\tau_{12}^{(6)} = \frac{1}{2}\mathbf{b}^T\mathbf{A}\mathbf{C}^2\mathbf{q}^{(2)} + \frac{1}{2}\mathbf{b}^T\mathbf{A}\left(\mathbf{q}^{(2)}\right)^2 + 3\tau_7^{(6)}$$

$$\tau_3^{(7)} = \frac{1}{4}\mathbf{b}^T\mathbf{C}^4\mathbf{q}^{(2)} + \frac{1}{4}\mathbf{b}^T\mathbf{C}^2\left(\mathbf{q}^{(2)}\right)^2 + 45\tau_1^{(7)}$$

$$\tau_4^{(7)} = \frac{1}{8}\mathbf{b}^T\mathbf{C}^4\mathbf{q}^{(2)} + \frac{1}{4}\mathbf{b}^T\mathbf{C}^2\left(\mathbf{q}^{(2)}\right)^2 + \frac{1}{6}\mathbf{b}^T\left(\mathbf{q}^{(2)}\right)^3 + 15\tau_1^{(7)}$$

$$\tau_6^{(7)} = \frac{1}{6}\mathbf{b}^T\mathbf{C}^4\mathbf{q}^{(2)} + \frac{1}{2}\mathbf{b}^T\mathbf{C}\mathbf{Q}^{(3)}\mathbf{q}^{(2)} + 3\tau_5^{(7)}$$

$$\tau_9^{(7)} = \frac{1}{24}\mathbf{b}^T\mathbf{C}^4\mathbf{q}^{(2)} + \frac{1}{6}\mathbf{b}^T\mathbf{Q}^{(4)}\mathbf{q}^{(2)} + \tau_8^{(7)}$$

$$\tau_{13}^{(7)} = \frac{1}{6}\mathbf{b}^T\mathbf{C}^4\mathbf{q}^{(2)} + \frac{1}{2}\mathbf{b}^T\mathbf{C}^3\mathbf{A}\mathbf{q}^{(2)} + \mathbf{b}^T\mathbf{C}\mathbf{Q}^{(2)}\mathbf{A}\mathbf{q}^{(2)} + \frac{1}{2}\mathbf{b}^T\mathbf{C}\mathbf{Q}^{(2)}\mathbf{q}^{(3)} + 3\tau_5^{(7)}$$

$$\tau_{14}^{(7)} = \frac{1}{6}\mathbf{b}^T\mathbf{C}^3\mathbf{A}\mathbf{q}^{(2)} + \frac{1}{2}\mathbf{b}^T\mathbf{Q}^{(3)}\mathbf{A}\mathbf{q}^{(2)} + 2\tau_7^{(7)}$$

$$\tau_{15}^{(7)} = \frac{1}{6}\mathbf{b}^T\mathbf{C}^3\mathbf{A}\mathbf{q}^{(2)} + \frac{1}{2}\mathbf{b}^T\mathbf{Q}^{(3)}\mathbf{A}\mathbf{q}^{(2)} + \frac{1}{2}\mathbf{b}^T\left(\mathbf{A}\mathbf{q}^{(2)}\right)^2 + \tau_7^{(7)}$$

$$\tau_{17}^{(7)} = \frac{1}{2}\mathbf{b}^T\mathbf{C}^2\mathbf{A}\mathbf{C}\mathbf{q}^{(2)} + \frac{1}{8}\mathbf{b}^T\mathbf{C}^4\mathbf{q}^{(2)} + \frac{1}{2}\mathbf{b}^T\mathbf{Q}^{(2)}\mathbf{Q}^{(4)} + \mathbf{b}^T\mathbf{Q}^{(2)}\mathbf{A}\mathbf{C}\mathbf{q}^{(2)} + 3\tau_8^{(7)}$$

$$\tau_{20}^{(7)} = \frac{1}{2}\mathbf{b}^T\mathbf{C}\mathbf{A}\mathbf{C}^2\mathbf{q}^{(2)} + \frac{1}{2}\mathbf{b}^T\mathbf{C}\mathbf{A}\left(\mathbf{q}^{(2)}\right)^2 + 3\tau_{10}^{(7)}$$

$$\tau_{21}^{(7)} = \frac{1}{2}\mathbf{b}^T\mathbf{A}\mathbf{C}^3\mathbf{q}^{(2)} + \frac{1}{2}\mathbf{b}^T\mathbf{A}\mathbf{C}\left(\mathbf{q}^{(2)}\right)^2 + 15\tau_{11}^{(7)}$$

$$\tau_{23}^{(7)} = \frac{1}{24}\mathbf{b}^T\mathbf{C}^4\mathbf{q}^{(2)} + \frac{1}{2}\mathbf{b}^T\mathbf{Q}^{(2)}\mathbf{A}\mathbf{q}^{(3)} + \frac{1}{6}\mathbf{b}^T\mathbf{Q}^{(2)}\mathbf{q}^{(4)} + \tau_{22}^{(7)}$$

$$\tau_{26}^{(7)} = \frac{1}{6}\mathbf{b}^T\mathbf{A}\mathbf{C}^3\mathbf{q}^{(2)} + \frac{1}{4}\mathbf{b}^T\mathbf{A}\mathbf{C}^2\mathbf{q}^{(3)} + \frac{1}{6}\mathbf{b}^T\mathbf{A}\mathbf{Q}^{(3)}\mathbf{q}^{(2)} + 10\tau_{11}^{(7)}$$

$$\tau_{31}^{(7)} = \frac{1}{2}\mathbf{b}^T\mathbf{Q}^{(2)}\mathbf{A}\mathbf{A}\mathbf{c}^2 + \frac{1}{2}\mathbf{b}^T\mathbf{C}^2\mathbf{A}\mathbf{A}\mathbf{q}^{(2)} + \mathbf{b}^T\mathbf{Q}^{(2)}\mathbf{A}\mathbf{A}\mathbf{q}^{(2)} + \tau_{22}^{(7)}$$

$$\tau_{34}^{(7)} = \frac{1}{2}\mathbf{b}^T\left(\mathbf{A}\mathbf{A}\mathbf{C}^2 + \mathbf{A}\mathbf{C}^2\mathbf{A}\right)\mathbf{q}^{(2)} + \mathbf{b}^T\left(\mathbf{A}\mathbf{q}^{(2)}\right)^2 + \tau_{25}^{(7)}$$

$$\tau_{38}^{(7)} = \frac{1}{2}\mathbf{b}^T\mathbf{A}\mathbf{A}\mathbf{C}^2\mathbf{q}^{(2)} + \frac{1}{2}\mathbf{b}^T\mathbf{A}\mathbf{A}\left(\mathbf{q}^{(2)}\right)^2 + 3\tau_{29}^{(7)}$$

$$\tau_7^{(7)} = \frac{1}{12}\mathbf{b}^T\mathbf{C}^3\mathbf{q}^{(3)} + \frac{1}{8}\mathbf{b}^T\left(\mathbf{q}^{(3)}\right)^2 + 10\tau_1^{(7)}$$

$$\tau_3^{(8)} = \frac{1}{12}\mathbf{b}^T\mathbf{C}^5\mathbf{Q}^{(2)} + \frac{1}{12}\mathbf{b}^T\mathbf{C}^3\mathbf{Q}^{(2)}\mathbf{q}^{(2)} + 105\tau_1^{(8)}$$
$$\tau_4^{(8)} = \frac{1}{8}\mathbf{b}^T\mathbf{C}^5\mathbf{Q}^{(2)} + \frac{1}{4}\mathbf{b}^T\mathbf{C}^3\mathbf{Q}^{(2)}\mathbf{q}^{(2)} + \frac{1}{6}\mathbf{b}^T\mathbf{C}\mathbf{Q}^{(2)}\mathbf{Q}^{(2)}\mathbf{q}^{(2)} + 105\tau_1^{(8)}$$
$$\tau_6^{(8)} = \frac{1}{12}\mathbf{b}^T\mathbf{C}^5\mathbf{Q}^{(2)} + \frac{1}{8}\mathbf{b}^T\mathbf{C}^4\mathbf{Q}^{(3)} + \frac{1}{4}\mathbf{b}^T\mathbf{C}^2\mathbf{Q}^{(2)}\mathbf{q}^{(3)} + 210\tau_1^{(8)}$$
$$\tau_7^{(8)} = \frac{1}{12}\mathbf{b}^T\mathbf{C}^5\mathbf{Q}^{(2)} + \frac{1}{16}\mathbf{b}^T\mathbf{C}^4\mathbf{Q}^{(3)} + \frac{1}{12}\mathbf{b}^T\mathbf{C}^3\mathbf{Q}^{(2)}\mathbf{q}^{(2)} + \frac{1}{4}\mathbf{b}^T\mathbf{C}^2\mathbf{Q}^{(2)}\mathbf{q}^{(3)} + \frac{1}{4}\mathbf{b}^T\mathbf{Q}^{(2)}\mathbf{Q}^{(2)}\mathbf{q}^{(3)} + 105\tau_1^{(8)}$$
$$\tau_{10}^{(8)} = \frac{1}{24}\mathbf{b}^T\mathbf{C}^5\mathbf{q}^{(2)} + \frac{1}{12}\mathbf{b}^T\mathbf{C}^3\mathbf{q}^{(4)} + \frac{1}{6}\mathbf{b}^T\mathbf{C}\mathbf{Q}^{(2)}\mathbf{q}^{(4)} + 105\tau_1^{(8)}$$
$$\tau_{13}^{(8)} = \frac{1}{120}\mathbf{b}^T\mathbf{C}^5\mathbf{q}^{(2)} + \frac{1}{48}\mathbf{b}^T\mathbf{C}^2\mathbf{q}^{(5)} + \frac{1}{24}\mathbf{b}^T\mathbf{Q}^2\mathbf{q}^{(5)} + 21\tau_1^{(8)}$$
$$\tau_{17}^{(8)} = \frac{1}{12}\mathbf{b}^T\mathbf{C}^5\mathbf{q}^{(2)} + \frac{1}{4}\mathbf{b}^T\mathbf{C}^4\mathbf{A}\mathbf{q}^{(2)} + \frac{1}{2}\mathbf{b}^T\mathbf{C}\mathbf{Q}^{(2)}\mathbf{A}\mathbf{q}^{(2)} + \frac{1}{4}\mathbf{b}^T\mathbf{C}^2\mathbf{Q}^{(2)}\mathbf{q}^{(3)} + 6\tau_5^{(8)}$$
$$\begin{aligned}\tau_{18}^{(8)} = &\frac{1}{8}\mathbf{b}^T\mathbf{C}^4\mathbf{A}\mathbf{q}^{(2)} + \frac{1}{12}\mathbf{b}^T\mathbf{C}^5\mathbf{q}^{(2)} + \frac{1}{2}\mathbf{b}^T\mathbf{C}^2\mathbf{Q}^{(2)}\mathbf{A}\mathbf{q}^{(2)} + \frac{1}{12}\mathbf{b}^T\mathbf{C}^3\mathbf{Q}^{(2)}\mathbf{q}^{(2)} + \frac{1}{4}\mathbf{b}^T\mathbf{C}^2\mathbf{Q}^{(2)}\mathbf{q}^{(3)}\\ &+ \frac{1}{2}\mathbf{b}^T\mathbf{Q}^2\mathbf{Q}^{(2)}\mathbf{A}\mathbf{q}^{(2)} + \frac{1}{4}\mathbf{b}^T\mathbf{Q}^2\mathbf{Q}^{(2)}\mathbf{q}^{(3)} + 3\tau_5^{(8)}\end{aligned}$$
$$\tau_{19}^{(8)} = \frac{1}{6}\mathbf{b}^T\mathbf{C}^4\mathbf{A}\mathbf{q}^{(2)} + \frac{1}{12}\mathbf{b}^T\mathbf{C}^4\mathbf{q}^{(3)} + \frac{1}{2}\mathbf{b}^T\mathbf{C}\mathbf{Q}^{(3)}\mathbf{A}\mathbf{q}^{(2)} + \frac{1}{4}\mathbf{b}^T\mathbf{C}\mathbf{Q}^{(3)}\mathbf{q}^{(3)} + 4\tau_5^{(8)}$$
$$\tau_{20}^{(8)} = \frac{1}{24}\mathbf{b}^T\mathbf{C}^4\mathbf{A}\mathbf{q}^{(2)} + \frac{1}{36}\mathbf{b}^T\mathbf{C}^3\mathbf{q}^{(4)} + \frac{1}{12}\mathbf{b}^T\mathbf{Q}^{(3)}\mathbf{q}^{(4)} + \frac{1}{6}\mathbf{b}^T\mathbf{Q}^{(4)}\mathbf{A}\mathbf{q}^{(2)} + \tau_5^{(8)}$$
$$\tau_{21}^{(8)} = \frac{1}{6}\mathbf{b}^T\mathbf{C}^4\mathbf{A}\mathbf{q}^{(2)} + \frac{1}{12}\mathbf{b}^T\mathbf{C}^4\mathbf{q}^{(3)} + \frac{1}{2}\mathbf{b}^T\mathbf{C}\mathbf{A}\mathbf{Q}^{(2)}\mathbf{q}^{(2)} + \frac{1}{2}\mathbf{b}^T\mathbf{C}\mathbf{Q}^{(3)}\mathbf{A}\mathbf{q}^{(2)} + \frac{1}{8}\mathbf{b}^T\mathbf{C}\mathbf{Q}^{(3)}\mathbf{q}^{(3)} + 70\tau_1^{(8)}$$
$$\tau_{23}^{(8)} = \frac{1}{2}\mathbf{b}^T\mathbf{C}^3\mathbf{A}\mathbf{C}\mathbf{q}^{(2)} + \frac{1}{8}\mathbf{b}^T\mathbf{C}^5\mathbf{q}^{(2)} + \frac{1}{4}\mathbf{b}^T\mathbf{C}^3\mathbf{q}^{(4)} + \frac{1}{1}\mathbf{b}^T\mathbf{C}\mathbf{Q}^{(2)}\mathbf{A}\mathbf{C}\mathbf{q}^{(2)} + \frac{1}{2}\mathbf{b}^T\mathbf{C}\mathbf{Q}^{(2)}\mathbf{q}^{(4)} + 315\tau_1^{(8)}$$
$$\tau_{24}^{(8)} = \frac{1}{6}\mathbf{b}^T\mathbf{C}^3\mathbf{A}\mathbf{C}\mathbf{q}^{(2)} + \frac{1}{12}\mathbf{b}^T\mathbf{C}^3\mathbf{q}^{(4)} + \frac{1}{16}\mathbf{b}^T\mathbf{Q}^{(3)}\mathbf{c}^4 + \frac{1}{2}\mathbf{b}^T\mathbf{Q}^{(3)}\mathbf{A}\mathbf{C}\mathbf{q}^{(2)} + \frac{1}{4}\mathbf{b}^T\mathbf{Q}^{(3)}\mathbf{q}^{(4)} + 105\tau_1^{(8)}$$
$$\begin{aligned}\tau_{25}^{(8)} = &\frac{1}{6}\mathbf{b}^T\mathbf{C}^3\mathbf{A}\mathbf{C}\mathbf{q}^{(2)} + \frac{1}{8}\mathbf{b}^T\mathbf{c}^4\mathbf{A}\mathbf{q}^{(2)} + \frac{1}{16}\mathbf{b}^T\mathbf{C}^4\mathbf{q}^{(3)} + \frac{1}{12}\mathbf{b}^T\mathbf{C}^3\mathbf{q}^{(4)}\\ &+ \frac{1}{2}\mathbf{b}^T i\mathbf{A}\mathbf{C}\mathbf{q}^{(2)}\mathbf{A}\mathbf{q}^{(2)} + \frac{1}{2}\mathbf{b}^T\mathbf{Q}^3\mathbf{A}\mathbf{C}\mathbf{q}^{(2)} + \frac{1}{4}\mathbf{b}^T\mathbf{Q}^3\mathbf{q}^{(4)} + \frac{1}{2}\mathbf{b}^T\mathbf{Q}^4\mathbf{A}\mathbf{q}^{(2)} + 105\tau_1^{(8)}\end{aligned}$$
$$\tau_{27}^{(8)} = \frac{1}{4}\mathbf{b}^T\mathbf{C}^2\mathbf{A}\mathbf{C}^2\mathbf{q}^{(2)} + \frac{1}{2}\mathbf{b}^T\mathbf{Q}^{(2)}\mathbf{A}\mathbf{C}^2\mathbf{q}^{(2)} + \frac{1}{4}\mathbf{b}^T\mathbf{Q}^{(2)}\mathbf{A}\mathbf{C}^4 + 6\tau_{12}^{(8)}$$
$$\tau_{30}^{(8)} = \frac{1}{4}\mathbf{b}^T\mathbf{c}^2\mathbf{A}\mathbf{Q}^{(2)}\mathbf{q}^{(2)} + \frac{1}{4}\mathbf{b}^T\mathbf{C}^2\mathbf{A}\mathbf{C}^2\mathbf{q}^{(2)} + 3\tau_{12}^{(8)}$$
$$\begin{aligned}\tau_{31}^{(8)} = &\frac{1}{4}\mathbf{b}^T\mathbf{C}^2\mathbf{A}\mathbf{C}^2\mathbf{q}^{(2)} + \frac{1}{4}\mathbf{b}^T\mathbf{C}^2\mathbf{A}\mathbf{Q}^{(2)}\mathbf{q}^{(2)} + \frac{1}{40}\mathbf{b}^T\mathbf{Q}^{(2)}\mathbf{c}^5\\ &+ \frac{1}{2}\mathbf{b}^T\mathbf{Q}^{(2)}\mathbf{A}\mathbf{C}^2\mathbf{q}^{(2)} + \frac{1}{2}\mathbf{b}^T\mathbf{Q}^{(2)}\mathbf{A}\mathbf{Q}^{(2)}\mathbf{q}^{(2)} + \frac{1}{8}\mathbf{b}^T\mathbf{Q}^{(2)}\mathbf{q}^{(5)} + 3\tau_{12}^{(8)}\end{aligned}$$
$$\tau_{32}^{(8)} = \frac{1}{2}\mathbf{b}^T\mathbf{C}\mathbf{A}\mathbf{C}^3\mathbf{q}^{(2)} + \frac{1}{2}\mathbf{b}^T\mathbf{C}\mathbf{A}\mathbf{C}\mathbf{Q}^{(2)}\mathbf{q}^{(2)} + 15\tau_{14}^{(8)}$$
$$\tau_{33}^{(8)} = \frac{1}{4}\mathbf{b}^T\mathbf{A}\mathbf{C}^4\mathbf{q}^{(2)} + \frac{1}{4}\mathbf{b}^T\mathbf{A}\mathbf{C}^2\mathbf{Q}^{(2)}\mathbf{q}^{(2)} + 45\tau_{15}^{(8)}$$
$$\tau_{34}^{(8)} = \frac{1}{8}\mathbf{b}^T\mathbf{A}\mathbf{C}^4\mathbf{q}^{(2)} + \frac{1}{4}\mathbf{b}^T\mathbf{A}\mathbf{C}^2\mathbf{Q}^{(2)}\mathbf{q}^{(2)} + \frac{1}{6}\mathbf{b}^T\mathbf{A}\mathbf{Q}^{(2)}\mathbf{Q}^{(2)}\mathbf{q}^{(2)} + 15\tau_{15}^{(8)}$$
$$\tau_{36}^{(8)} = \frac{1}{4}\mathbf{b}^T\mathbf{C}^3\mathbf{A}\mathbf{q}^{(3)} + \frac{1}{6}\mathbf{b}^T\mathbf{C}\mathbf{Q}^{(2)}\mathbf{q}^{(4)} + \frac{1}{24}\mathbf{b}^T\mathbf{C}\mathbf{Q}^{(2)}\mathbf{c}^4 + \frac{1}{2}\mathbf{b}^T\mathbf{C}\mathbf{Q}^{(2)}\mathbf{A}\mathbf{q}^{(3)} + 3\tau_9^{(8)}$$
$$\tau_{38}^{(8)} = \frac{1}{2}\mathbf{b}^T\mathrm{Diag}\left(\mathbf{A}\mathbf{q}^{(2)}\right)\mathrm{Diag}\left(\mathbf{A}\mathbf{q}^{(3)}\right) + \frac{1}{4}\mathbf{b}^T\mathbf{Q}^{(3)}\mathbf{A}\mathbf{q}^{(3)} + \frac{1}{6}\mathbf{b}^T\mathbf{Q}^{(4)}\mathbf{A}\mathbf{q}^{(2)} + \tau_{11}^{(8)}$$
$$\tau_{40}^{(8)} = \frac{1}{30}\mathbf{b}^T\mathbf{Q}^{(2)}\mathbf{c}^5 + \frac{1}{4}\mathbf{b}^T\mathbf{C}^2\mathbf{A}\mathbf{C}\mathbf{q}^{(3)} + \frac{1}{2}\mathbf{b}^T\mathbf{Q}^{(2)}\mathbf{A}\mathbf{C}\mathbf{q}^{(3)} + \frac{1}{6}\mathbf{b}^T\mathbf{Q}^{(2)}\mathbf{q}^{(5)} + 4\tau_{12}^{(8)}$$
$$\tau_{43}^{(8)} = \frac{1}{6}\mathbf{b}^T\mathbf{C}\mathbf{A}\mathbf{C}^3\mathbf{q}^{(2)} + \frac{1}{4}\mathbf{b}^T\mathbf{C}\mathbf{A}\mathbf{C}^2\mathbf{q}^{(3)} + \frac{1}{2}\mathbf{b}^T\mathbf{C}\mathbf{A}\mathbf{Q}^{(2)}\mathbf{q}^{(3)} + 10\tau_{14}^{(8)}$$
$$\tau_{44}^{(8)} = \frac{1}{6}\mathbf{b}^T\mathbf{A}\mathbf{C}^4\mathbf{q}^{(2)} + \frac{1}{4}\mathbf{b}^T\mathbf{A}\mathbf{C}^3\mathbf{q}^{(3)} + \frac{1}{2}\mathbf{b}^T\mathbf{A}\mathbf{C}\mathbf{Q}^{(2)}\mathbf{q}^{(3)} + 60\tau_{15}^{(8)}$$
$$\tau_{47}^{(8)} = \frac{1}{12}\mathbf{b}^T\mathbf{C}^2\mathbf{A}\mathbf{q}^{(4)} + \frac{1}{120}\mathbf{b}^T\mathbf{Q}^{(2)}\mathbf{c}^5 + \frac{1}{24}\mathbf{b}^T\mathbf{Q}^{(2)}\mathbf{q}^{(5)} + \frac{1}{6}\mathbf{b}^T\mathbf{Q}^{(2)}\mathbf{A}\mathbf{q}^{(4)} + \tau_{12}^{(8)}$$
$$\tau_{50}^{(8)} = \frac{1}{24}\mathbf{b}^T\mathbf{A}\mathbf{C}^4\mathbf{q}^{(2)} + \frac{1}{12}\mathbf{b}^T\mathbf{A}\mathbf{C}^2\mathbf{q}^{(4)} + \frac{1}{6}\mathbf{b}^T\mathbf{A}\mathbf{Q}^{(2)}\mathbf{q}^{(4)} + 15\tau_{15}^{(8)}$$

$$\tau_{55}^{(8)} = \frac{1}{2}\mathbf{b}^T\mathbf{C}^3\mathbf{AAq}^{(2)} + \frac{1}{24}\mathbf{b}^T\mathbf{CQ}^{(2)}\mathbf{c}^4 + \mathbf{b}^T\mathbf{CQ}^{(2)}\mathbf{AAq}^{(2)} + \frac{1}{2}\mathbf{b}^T\mathbf{CQ}^{(2)}\mathbf{Aq}^{(3)} + \frac{1}{6}\mathbf{b}^T\mathbf{CQ}^{(2)}\mathbf{q}^{(4)} + 3\tau_{35}^{(8)}$$

$$\tau_{56}^{(8)} = \frac{1}{6}\mathbf{b}^T\mathbf{C}^3\mathbf{AAq}^{(2)} + \frac{1}{48}\mathbf{b}^T\mathbf{Q}^{(3)}\mathbf{c}^4 + \frac{1}{2}\mathbf{b}^T\mathbf{Q}^{(3)}\mathbf{AAq}^{(2)} + \frac{1}{4}\mathbf{b}^T\mathbf{Q}^{(3)}\mathbf{Aq}^{(3)} + \frac{1}{12}\mathbf{b}^T\mathbf{Q}^{(3)}\mathbf{q}^{(4)} + \tau_{35}^{(8)}$$

$$\tau_{57}^{(8)} = \frac{1}{2}\mathbf{b}^T\mathrm{Diag}\left(\mathbf{Aq}^{(2)}\right)\left(\mathbf{Aq}^{(3)}\right) + \mathbf{b}^T\mathrm{Diag}\left(\mathbf{Aq}^{(2)}\right)\mathbf{AAq}^{(3)} + \frac{1}{2}\mathbf{b}^T\mathbf{Q}^{(3)}\mathbf{AAq}^{(2)} + \tau_{37}^{(8)}$$

$$\tau_{59}^{(8)} = \frac{1}{2}\mathbf{b}^T\mathbf{C}^2\mathbf{ACAq}^{(2)} + \frac{1}{30}\mathbf{b}^T\mathbf{Q}^{(2)}\mathbf{c}^5 + \frac{1}{6}\mathbf{b}^T\mathbf{Q}^{(2)}\mathbf{q}^{(5)} + \frac{1}{1}\mathbf{b}^T\mathbf{Q}^{(2)}\mathbf{ACAq}^{(2)} + \frac{1}{2}\mathbf{b}^T\mathbf{Q}^{(2)}\mathbf{ACq}^{(3)} + \tau_{39}^{(8)}$$

$$\tau_{62}^{(8)} = \frac{1}{2}\mathbf{b}^T\mathbf{CAC}^2\mathbf{Aq}^{(2)} + \frac{1}{1}\mathbf{b}^T\mathbf{CAQ}^{(2)}\mathbf{Aq}^{(2)} + \frac{1}{2}\mathbf{b}^T\mathbf{CAQ}^{(2)}\mathbf{q}^{(3)} + \tau_{41}^{(8)}$$

$$\tau_{63}^{(8)} = \frac{1}{2}\mathbf{b}^T\mathbf{AAC}^3\mathbf{q}^{(2)} + \frac{1}{1}\mathbf{b}^T\mathbf{ACQ}^{(2)}\mathbf{Aq}^{(2)} + \frac{1}{2}\mathbf{b}^T\mathbf{ACQ}^{(2)}\mathbf{q}^{(3)} + 3\tau_{42}^{(8)}$$

$$\tau_{64}^{(8)} = \frac{1}{6}\mathbf{b}^T\mathbf{AC}^3\mathbf{Aq}^{(2)} + \frac{1}{12}\mathbf{b}^T\mathbf{AQ}^{(3)}\mathbf{c}^3 + \frac{1}{2}\mathbf{b}^T\mathbf{Aq}^{(3)}\mathbf{Aq}^{(2)} + \frac{1}{4}\mathbf{b}^T\mathbf{AQ}^{(3)}\mathbf{q}^{(3)} + \tau_{42}^{(8)}$$

$$\tau_{65}^{(8)} = \frac{1}{2}\mathbf{b}^T\mathbf{A}\mathrm{Diag}\left(\mathbf{Aq}^{(2)}\right)\left(\mathbf{Aq}^{(2)}\right) + \frac{1}{2}\mathbf{b}^T\mathbf{AQ}^{(3)}\mathbf{Aq}^{(2)} + \tau_{45}^{(8)}$$

$$\tau_{67}^{(8)} = \frac{1}{2}\mathbf{b}^T\mathbf{C}^2\mathbf{AACq}^{(2)} + \frac{1}{40}\mathbf{b}^T\mathbf{Q}^{(2)}\mathbf{c}^5 + \frac{1}{2}\mathbf{b}^T\mathbf{Q}^{(2)}\mathbf{Aq}^{(4)} + \frac{1}{8}\mathbf{b}^T\mathbf{Q}^{(2)}\mathbf{q}^{(5)} + \frac{1}{1}\mathbf{b}^T\mathbf{Q}^{(2)}\mathbf{AACq}^{(2)} + 3\tau_{46}^{(8)}$$

$$\tau_{70}^{(8)} = \frac{1}{2}\mathbf{b}^T\mathbf{AC}^2\mathbf{ACQ}^{(2)} + \frac{1}{8}\mathbf{b}^T\mathbf{AQ}^{(2)}\mathbf{c}^4 + \mathbf{b}^T\mathbf{AQ}^{(2)}\mathbf{ACQ}^{(2)} + \frac{1}{2}\mathbf{b}^T\mathbf{AQ}^{(2)}\mathbf{q}^{(4)} + 3\tau_{49}^{(8)}$$

$$\tau_{74}^{(8)} = \frac{1}{2}\mathbf{b}^T\mathbf{CAAC}^2\mathbf{q}^{(2)} + \frac{1}{2}\mathbf{b}^T\mathbf{CAAQ}^2\mathbf{q}^{(2)} + 3\tau_{51}^{(8)}$$

$$\tau_{75}^{(8)} = \frac{1}{2}\mathbf{b}^T\mathbf{ACAC}^2\mathbf{q}^{(2)} + \frac{1}{2}\mathbf{b}^T\mathbf{ACAQ}^{(2)}\mathbf{q}^{(2)} + 3\tau_{52}^{(8)}$$

$$\tau_{76}^{(8)} = \frac{1}{2}\mathbf{b}^T\mathbf{AAC}^3\mathbf{q}^{(2)} + \frac{1}{2}\mathbf{b}^T\mathbf{AACQ}^{(2)}\mathbf{q}^{(2)} + 15\tau_{53}^{(8)}$$

$$\tau_{78}^{(8)} = \frac{1}{120}\mathbf{b}^T\mathbf{Q}^{(2)}\mathbf{c}^5 + \frac{1}{4}\mathbf{b}^T\mathbf{C}^2\mathbf{AAq}^{(3)} + \frac{1}{2}\mathbf{b}^T\mathbf{Q}^{(2)}\mathbf{AAQ}^{(3)} + \frac{1}{6}\mathbf{b}^T\mathbf{Q}^{(2)}\mathbf{Aq}^{(4)} + \frac{1}{24}\mathbf{b}^T\mathbf{Q}^{(2)}\mathbf{q}^{(5)} + \tau_{46}^{(8)}$$

$$\tau_{81}^{(8)} = \frac{1}{4}\mathbf{b}^T\mathbf{AC}^2\mathbf{AQ}^{(3)} + \frac{1}{24}\mathbf{b}^T\mathbf{AQ}^{(2)}\mathbf{c}^4 + \frac{1}{6}\mathbf{b}^T\mathbf{AQ}^{(2)}\mathbf{q}^{*4)} + \frac{1}{2}\mathbf{b}^T\mathbf{AQ}^{(2)}\mathbf{Aq}^{(3)} + \tau_{49}^{(8)}$$

$$\tau_{85}^{(8)} = \frac{1}{6}\mathbf{b}^T\mathbf{AAC}^3\mathbf{q}^{(2)} + \frac{1}{4}\mathbf{b}^T\mathbf{AAC}^2\mathbf{q}^{(3)} + \frac{1}{2}\mathbf{b}^T\mathbf{AAQ}^{(2)}\mathbf{q}^{(3)} + 10\tau_{53}^{(8)}$$

$$\tau_{91}^{(8)} = \frac{1}{2}\mathbf{b}^T\mathbf{C}^2\mathbf{AAAq}^{(2)} + \frac{1}{120}\mathbf{b}^T\mathbf{q}^{(2)}\mathbf{c}^5 + \frac{1}{24}\mathbf{b}^T\mathbf{Q}^{(2)}\mathbf{q}^{(5)} + \frac{1}{6}\mathbf{b}^T\mathbf{Q}^{(2)}\mathbf{Aq}^{(4)} + \frac{1}{2}\mathbf{b}^T\mathbf{Q}^{(2)}\mathbf{AAq}^{(3)} + \mathbf{b}^T\mathbf{Q}^{(2)}\mathbf{AAAq}^{(2)} + \tau_{77}^{(8)}$$

$$\tau_{94}^{(8)} = \frac{1}{2}\mathbf{b}^T\mathbf{AC}^2\mathbf{AAQ}^{(2)} + \frac{1}{24}\mathbf{b}^T\mathbf{AQ}^{(2)}\mathbf{c}^4 + \frac{1}{2}\mathbf{b}^T\mathbf{AQ}^{(2)}\mathbf{Aq}^{(3)} + \mathbf{b}^T\mathbf{AQ}^{(2)}\mathbf{AAq}^{(2)} + \frac{1}{6}\mathbf{b}^T\mathbf{AQ}^{(2)}\mathbf{q}^{(4)} + \tau_{80}^{(8)}$$

$$\tau_{98}^{(8)} = \frac{1}{2}\mathbf{b}^T\mathbf{AAC}^2\mathbf{AQ}^{(2)} + \frac{1}{6}\mathbf{b}^T\mathbf{AAQ}^{(2)}\mathbf{c}^3 + \mathbf{b}^T\mathbf{AAQ}^{(2)}\mathbf{AQ}^{(2)} + \frac{1}{2}\mathbf{b}^T\mathbf{AAQ}^{(2)}\mathbf{q}^{(3)} + \tau_{84}^{(8)}$$

$$\tau_{103}^{(8)} = \frac{1}{2}\mathbf{b}^T\mathbf{AAAC}^2\mathbf{q}^{(2)} + \frac{1}{2}\mathbf{b}^T\mathbf{AAAQ}^{(2)}\mathbf{q}^{(2)} + 3\tau_{89}^{(8)}$$

$$\tau_{8}^{(8)} = \frac{1}{12}\mathbf{b}^T\mathbf{C}^4\mathbf{Q}^{(3)} + \frac{1}{8}\mathbf{b}^T\mathbf{CQ}^{(3)}\mathbf{q}^{(3)} + 70\tau_{1}^{(8)}$$

$$\tau_{11}^{(8)} = \frac{1}{48}\mathbf{b}^T\mathbf{C}^4\mathbf{q}^{(3)} + \frac{1}{36}\mathbf{b}^T\mathbf{C}^3\mathbf{q}^{(4)} + \frac{1}{12}\mathbf{b}^T\mathbf{Q}^3\mathbf{q}^{(4)} + 35\tau_{1}^{(8)}$$

$$\tau_{37}^{(8)} = \frac{1}{12}\mathbf{b}^T\mathbf{C}^3\mathbf{Aq}^{(3)} + \frac{1}{48}\mathbf{b}^T\mathbf{Q}^{(3)}\mathbf{c}^4 + \frac{1}{4}\mathbf{b}^T\mathbf{Q}^{(3)}\mathbf{Aq}^{(3)} + \frac{1}{12}\mathbf{b}^T\mathbf{Q}^{(3)}\mathbf{q}^{(4)} + \tau_{9}^{(8)}$$

$$\tau_{45}^{(8)} = \frac{1}{12}\mathbf{b}^T\mathbf{AC}^3\mathbf{q}^{(3)} + \frac{1}{8}\mathbf{b}^T\mathbf{AQ}^{(3)}\mathbf{q}^{(3)} + 10\tau_{15}^{(8)}$$

C.5 Row-Simplifying Assumptions: $C(\eta)$

If we have designed a method which satisfies $B(\eta)$ and $C(\eta)$ where $\eta = \mathfrak{q}$, i.e. the stage order, we might ask if there is a reduced set of order conditions required to increase the order of the method. The first matter is the nonlinear order conditions, where the first of which appears at fifth-order. In terms of $\mathfrak{q}$, the first nonlinear order condition appears at $2\mathfrak{q} + 3$.

To take a method satisfying $B(\eta)$ and $C(\eta)$ where $\eta = \mathfrak{q},\ \mathfrak{q} \geq 1$ and increase the order by one to $p = \mathfrak{q}+1$, we simply impose

$$\tau_1^{(\mathfrak{q}+1)} = 0. \tag{C1}$$

To increase the order from $p = \mathfrak{q}+1$ to $p = \mathfrak{q}+2$, one additionally imposes

$$\begin{aligned} \tau_1^{(\mathfrak{q}+2)} &= 0, && \text{(C2)} \\ \tau_{SQ}^{(\mathfrak{q}+2)} &= \frac{1}{\mathfrak{q}!}\mathbf{b}^T\mathbf{q}^{(\mathfrak{q}+1)} + \tau_1^{(\mathfrak{q}+2)} = 0, && \text{(C3)} \end{aligned}$$

where

$$\mathbf{q}^{(k)} = \mathbf{A}\mathbf{C}^{k-1}\mathbf{e} - \frac{1}{k}\mathbf{C}^k\mathbf{e}. \tag{C4}$$

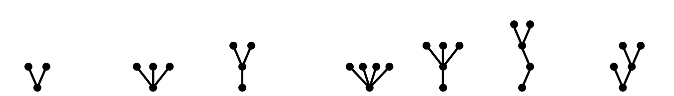
Moving to order $p = \mathfrak{q}+3$, four new order conditions must be imposed

$$\begin{aligned} \tau_1^{(\mathfrak{q}+3)} &= 0, && \text{(C5)} \\ \tau_{SQ,1}^{(\mathfrak{q}+3)} &= \frac{1}{(\mathfrak{q}+1)!}\mathbf{b}^T\mathbf{q}^{(\mathfrak{q}+2)} + \tau_1^{(\mathfrak{q}+3)} = 0, && \text{(C6)} \\ \tau_{SQ,2}^{(\mathfrak{q}+3)} &= \frac{1}{\mathfrak{q}!}\mathbf{b}^T\mathbf{A}\mathbf{q}^{(\mathfrak{q}+1)} + \frac{1}{(\mathfrak{q}+1)!}\mathbf{b}^T\mathbf{q}^{(\mathfrak{q}+2)} + \tau_1^{(\mathfrak{q}+3)} = 0, && \text{(C7)} \\ \tau_{ESQ}^{(\mathfrak{q}+3)} &= \frac{1}{\mathfrak{q}!}\mathbf{b}^T\mathbf{C}\mathbf{q}^{(\mathfrak{q}+1)} + (\mathfrak{q}+2)\tau_1^{(\mathfrak{q}+3)} = 0. && \text{(C8)} \end{aligned}$$

For methods satisfying $\mathfrak{q} \geq 2$, we next consider the additional order conditions needed to take the method from order $\mathfrak{q}+3$ to order $\mathfrak{q}+4$. We must enforce the following eight order conditions

$$\begin{aligned} \tau_1^{(\mathfrak{q}+4)} &= 0, && \text{(C9)} \\ \tau_{SQ,1}^{(\mathfrak{q}+4)} &= \frac{1}{(\mathfrak{q}+2)!}\mathbf{b}^T\mathbf{q}^{(\mathfrak{q}+3)} + \tau_1^{(\mathfrak{q}+4)}, && \text{(C10)} \\ \tau_{SQ,2}^{(\mathfrak{q}+4)} &= \frac{1}{(\mathfrak{q}+1)!}\mathbf{b}^T\mathbf{A}\mathbf{q}^{(\mathfrak{q}+2)} + \frac{1}{(\mathfrak{q}+2)!}\mathbf{b}^T\mathbf{q}^{(\mathfrak{q}+3)} + \tau_1^{(\mathfrak{q}+4)}, && \text{(C11)} \\ \tau_{SQ,3}^{(\mathfrak{q}+4)} &= \frac{1}{\mathfrak{q}!}\mathbf{b}^T\mathbf{A}\mathbf{A}\mathbf{q}^{(\mathfrak{q}+1)} + \frac{1}{(\mathfrak{q}+1)!}\mathbf{b}^T\mathbf{A}\mathbf{q}^{(\mathfrak{q}+2)} + \frac{1}{(\mathfrak{q}+2)!}\mathbf{b}^T\mathbf{q}^{(\mathfrak{q}+3)} + \tau_1^{(\mathfrak{q}+4)}, && \text{(C12)} \\ \tau_{ESQ,1}^{(\mathfrak{q}+4)} &= \frac{1}{(\mathfrak{q}+1)!}\mathbf{b}^T\mathbf{C}\mathbf{q}^{(\mathfrak{q}+2)} + (\mathfrak{q}+3)\tau_1^{(\mathfrak{q}+4)}, && \text{(C13)} \\ \tau_{ESQ,2}^{(\mathfrak{q}+4)} &= \frac{1}{\mathfrak{q}!2!}\mathbf{b}^T\mathbf{C}^2\mathbf{q}^{(\mathfrak{q}+1)} + \frac{1}{2}(\mathfrak{q}+2)(\mathfrak{q}+3)\tau_1^{(\mathfrak{q}+4)}, && \text{(C14)} \\ \tau_{ESQ,3}^{(\mathfrak{q}+4)} &= \frac{1}{\mathfrak{q}!}\mathbf{b}^T\mathbf{C}\mathbf{A}\mathbf{q}^{(\mathfrak{q}+1)} + \frac{1}{(\mathfrak{q}+1)!}\mathbf{b}^T\mathbf{C}\mathbf{q}^{(\mathfrak{q}+2)} + (\mathfrak{q}+3)\tau_1^{(\mathfrak{q}+4)}, && \text{(C15)} \\ \tau_{ESQ,4}^{(\mathfrak{q}+4)} &= \frac{1}{\mathfrak{q}!}\mathbf{b}^T\mathbf{A}\mathbf{C}\mathbf{q}^{(\mathfrak{q}+1)} + \frac{1}{(\mathfrak{q}+1)!}\mathbf{b}^T\mathbf{q}^{(\mathfrak{q}+3)} + (\mathfrak{q}+2)\tau_1^{(\mathfrak{q}+4)}. && \text{(C16)} \end{aligned}$$

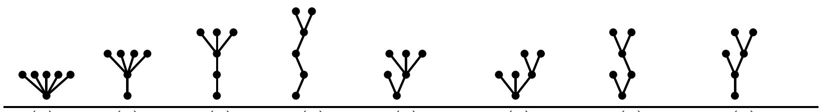
Graphically, the trees involved at $\mathfrak{q} = 2$ are



$t_1^{(3)}$ $t_1^{(4)}$ $t_3^{(4)}$ $t_1^{(5)}$ $t_5^{(5)}$ $t_8^{(5)}$ $t_4^{(5)}$

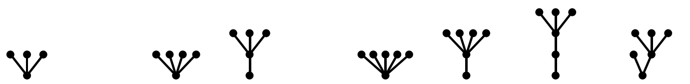
Q   Q   SQ   Q   SQ, 1   SQ, 2   ESQ

(C17)

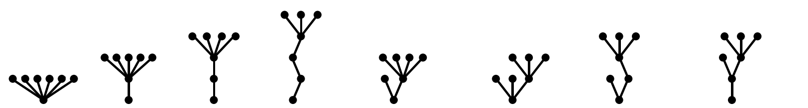


$t_1^{(6)}$	$t_7^{(6)}$	$t_{15}^{(6)}$	$t_{19}^{(6)}$	$t_6^{(6)}$	$t_4^{(6)}$	$t_{13}^{(6)}$	$t_{14}^{(6)}$	(C18)
Q	SQ, 1	SQ, 2	SQ, 3	ESQ, 1	ESQ, 2	ESQ, 3	ESQ, 4	

Moving to methods satisfying $\mathfrak{q} = 3$,

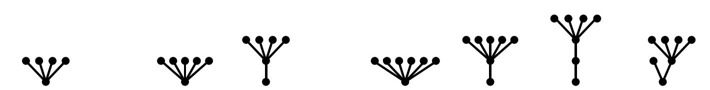


$t_1^{(4)}$	$t_1^{(5)}$	$t_5^{(5)}$	$t_1^{(6)}$	$t_7^{(6)}$	$t_{15}^{(6)}$	$t_6^{(6)}$	(C19)
Q	Q	SQ	Q	SQ, 1	SQ, 2	ESQ	

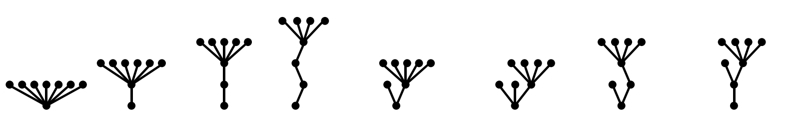


$t_1^{(7)}$	$t_{11}^{(7)}$	$t_{29}^{(7)}$	$t_{42}^{(7)}$	$t_{10}^{(7)}$	$t_8^{(7)}$	$t_{27}^{(7)}$	$t_{28}^{(7)}$	(C20)
Q	SQ, 1	SQ, 2	SQ, 3	ESQ, 1	ESQ, 2	ESQ, 3	ESQ, 4	

Lastly, for methods satisfying $\mathfrak{q} = 4$,



$t_1^{(5)}$	$t_1^{(6)}$	$t_7^{(6)}$	$t_1^{(7)}$	$t_{11}^{(7)}$	$t_{29}^{(7)}$	$t_{10}^{(7)}$	(C21)
Q	Q	SQ	Q	SQ, 1	SQ, 2	ESQ	



$t_1^{(8)}$	$t_{15}^{(8)}$	$t_{53}^{(8)}$	$t_{89}^{(8)}$	$t_{14}^{(8)}$	$t_{12}^{(8)}$	$t_{51}^{(8)}$	$t_{52}^{(8)}$	(C22)
Q	SQ, 1	SQ, 2	SQ, 3	ESQ, 1	ESQ, 2	ESQ, 3	ESQ, 4	

C.6 Leading-Order Error Terms

Using the information from above, one can determine various values of $A^{(\mathfrak{q}+m)}$ for a particular method. If we have a stage-order three method, then

$$A^{(4)} = \sqrt{12\left(t_1^{(4)}\right)^2}, \qquad A^{(5)} = \sqrt{78\left(t_1^{(5)}\right)^2 + 12\left(t_5^{(5)}\right)^2} \tag{C23}$$

$$A^{(6)} = \sqrt{726\left(t_1^{(6)}\right)^2 + 78\left(t_7^{(6)}\right)^2 + 12\left(t_{15}^{(6)}\right)^2 + 12\left(t_6^{(6)}\right)^2} \tag{C24}$$

$$A^{(7)} = \sqrt{\begin{array}{c} 11076\left(t_1^{(7)}\right)^2 + 726\left(t_{11}^{(7)}\right)^2 + 78\left(t_{29}^{(7)}\right)^2 + 12\left(t_{42}^{(7)}\right)^2 \\ +78\left(t_{10}^{(7)}\right)^2 + 24\left(t_8^{(7)}\right)^2 + 12\left(t_{27}^{(7)}\right)^2 + 12\left(t_{28}^{(7)}\right)^2 \end{array}}\,. \tag{C25}$$

If we then impose a stage-order of four on this method, then

$$A^{(4)} = 0, \qquad A^{(5)} = \sqrt{90\left(t_1^{(5)}\right)^2}, \qquad A^{(6)} = \sqrt{1026\left(t_1^{(6)}\right)^2 + 90\left(t_7^{(6)}\right)^2} \tag{C26}$$

$$A^{(7)} = \sqrt{16476\left(t_1^{(7)}\right)^2 + 1026\left(t_{11}^{(7)}\right)^2 + 90\left(t_{29}^{(7)}\right)^2 + 90\left(t_{10}^{(7)}\right)^2}. \tag{C27}$$

Moving to stage-order five,

$$A^{(4)} = A^{(5)} = 0, \qquad A^{(6)} = \sqrt{1116\left(t_1^{(6)}\right)^2}, \qquad A^{(7)} = \sqrt{19716\left(t_1^{(7)}\right)^2 + 1116\left(t_{11}^{(7)}\right)^2}, \tag{C28}$$

and lastly, at stage-order six, we have

$$A^{(4)} = A^{(5)} = A^{(6)} = 0, \qquad A^{(7)} = \sqrt{20832\left(t_1^{(7)}\right)^2}. \tag{C29}$$

Alternatively, as we began with a stage-order two method,

$$A^{(3)} = \sqrt{2\left(t_1^{(3)}\right)^2}, \qquad A^{(4)} = \sqrt{10\left(t_1^{(4)}\right)^2 + 2\left(t_3^{(4)}\right)^2} \tag{C30}$$

$$A^{(5)} = \sqrt{46\left(t_1^{(5)}\right)^2 + 10\left(t_5^{(5)}\right)^2 + 2\left(t_8^{(5)}\right)^2 + 2\left(t_4^{(5)}\right)^2} \tag{C31}$$

$$A^{(6)} = \sqrt{\begin{array}{c} 326\left(t_1^{(6)}\right)^2 + 46\left(t_7^{(6)}\right)^2 + 10\left(t_{15}^{(6)}\right)^2 + 2\left(t_{19}^{(6)}\right)^2 \\ +10\left(t_6^{(6)}\right)^2 + 4\left(t_4^{(6)}\right)^2 + 2\left(t_{13}^{(6)}\right)^2 + 2\left(t_{14}^{(6)}\right)^2 \end{array}}. \tag{C32}$$

Had this been continued to $A^{(7)}$, the first nonlinear order conditions would have appeared. Lastly, at a stage-order of one, we have enforced $t_1^{(1)} = 0$ and the row-sum condition ($\mathbf{q}^{(1)} = 0$), so that we find the unremarkable result that

$$A^{(2)} = \sqrt{\left(t_1^{(2)}\right)^2}, \qquad A^{(3)} = \sqrt{\left(t_1^{(3)}\right)^2 + \left(t_2^{(3)}\right)^2} \tag{C33}$$

$$A^{(4)} = \sqrt{\left(t_1^{(4)}\right)^2 + \left(t_2^{(4)}\right)^2 + \left(t_3^{(4)}\right)^2 + \left(t_4^{(4)}\right)^2}. \tag{C34}$$

In these expressions, for any given value of $\mathsf{q} > 1$, there are four independent parameters, $\psi_1, i = 1, 2, \ldots, 5$. Before giving these, we need to sum the squares of tree cardinality values: α, for a given order, where α appears in the definition of the order conditions as

$$\tau_j^{(p)} = \frac{1}{\sigma_j^{(p)}}\Phi_j^{(p)} - \frac{\alpha_j^{(p)}}{p!}, \quad p = 1, 2, \cdots, \; j = 1, 2, \cdots, \mathsf{a}_p \tag{C35}$$

where, as given earlier, $\mathsf{a}_p = \{1, 1, 2, 4, 9, 20, 48, 115, 286, 719\}$ for $p = \{1, 2, 3, 4, 5, 6, 7, 8, 9, 10\}$. Let us define

$$\phi_{p-1} = \sum_{j=1}^{\mathsf{a}_p} \left(\alpha_j^{(p)}\right)^2, \quad p = 1, 2, \cdots, \tag{C36}$$

Using the functionalities in *Mathematica* [186], `ButcherTrees` and `ButcherAlpha`, it is found that $\phi_i,\ i = 1,2,\ldots,15$= {1, 2,12,90,1116,20832,495888,15019986,572296740,27130410552, 1524170474688,101844008170572,7934076259615824,713284646600406984,73380923894005811664}. Using the various values of ϕ_i, the four parameters of ψ_i can be found for stage-orders from two to ten,

$$
\begin{aligned}
\mathfrak{q} &= 2,\ \psi_i = \{2, 10, 46, 326\},\\
\mathfrak{q} &= 3,\ \psi_i = \{12, 78, 726, 11076\},\\
\mathfrak{q} &= 4,\ \psi_i = \{90, 1026, 16476, 340992\},\\
\mathfrak{q} &= 5,\ \psi_i = \{1116, 19716, 420372, 11440962\},\\
\mathfrak{q} &= 6,\ \psi_i = \{20832, 475056, 13190850, 463113282\},\\
\mathfrak{q} &= 7,\ \psi_i = \{495888, 14524098, 517109826, 23047768812\},\\
\mathfrak{q} &= 8,\ \psi_i = \{15019986, 557276754, 25056115212, 1336921243296\},\\
\mathfrak{q} &= 9,\ \psi_i = \{572296740, 26558113812, 1427792158596, 91427209377516\},\\
\mathfrak{q} &= 10,\ \psi_i = \{27130410552, 1497040064136, 96413058576396, 7244524605626244\},\\
\mathfrak{q} &= 11,\ \psi_i = \{1524170474688, 100319837695884, 7574647441222980,\\
&\qquad 660145833337576392\},\\
\mathfrak{q} &= 12,\ \psi_i = \{101844008170572, 7832232251445252, 685389144739359048,\\
&\qquad 68636811708830731680\},\\
\mathfrak{q} &= 13,\ \psi_i = \{7934076259615824, 705350570340791160, 70882472088991844280,\\
&\qquad 8064807793020966728826\},\\
\mathfrak{q} &= 14,\ \psi_i = \{713284646600406984, 72667639247405404680, 8293309189297902460026,\\
&\qquad 1064861646597632100863466\},\\
\mathfrak{q} &= 15,\ \psi_i = \{73380923894005811664, 8475910058827606647930, 1091247472244674356015594,\\
&\qquad 157030539594982413000150396\}.
\end{aligned}
$$

where

$$
\begin{gathered}
\psi_1 = \phi_{\mathfrak{q}}, \qquad \psi_2 = \phi_{\mathfrak{q}+1} - \phi_{\mathfrak{q}}, \qquad \psi_3 = \phi_{\mathfrak{q}+2} - \phi_{\mathfrak{q}+1} - (\mathfrak{q}+2)^2\phi_{\mathfrak{q}},\\
\psi_4 = \phi_{\mathfrak{q}+3} - \phi_{\mathfrak{q}+2} - (\mathfrak{q}+3)^2\phi_{\mathfrak{q}+1} - \frac{1}{2}(\mathfrak{q}+2)^2(\mathfrak{q}+3)^2\phi_{\mathfrak{q}}.
\end{gathered} \tag{C37}
$$

Together, for a method that has a stage order of $\mathfrak{q} > 1$ and where $p < 2\mathfrak{q}+3$,

$$
A^{(\mathfrak{q}+1)} = \sqrt{\psi_1\left(t_Q^{(\mathfrak{q}+1)}\right)^2}, \qquad A^{(\mathfrak{q}+2)} = \sqrt{\psi_2\left(t_Q^{(\mathfrak{q}+2)}\right)^2 + \psi_1\left(t_{SQ}^{(\mathfrak{q}+2)}\right)^2} \tag{C38}
$$

$$
A^{(\mathfrak{q}+3)} = \sqrt{\psi_3\left(t_Q^{(\mathfrak{q}+3)}\right)^2 + \psi_2\left(t_{SQ,1}^{(\mathfrak{q}+3)}\right)^2 + \psi_1\left(t_{SQ,2}^{(\mathfrak{q}+3)}\right)^2 + \psi_1\left(t_{ESQ}^{(\mathfrak{q}+3)}\right)^2} \tag{C39}
$$

$$
A^{(\mathfrak{q}+4)} = \sqrt{\begin{array}{c}\psi_4\left(t_Q^{(\mathfrak{q}+4)}\right)^2 + \psi_3\left(t_{SQ,1}^{(\mathfrak{q}+4)}\right)^2 + \psi_2\left(t_{SQ,2}^{(\mathfrak{q}+4)}\right)^2 + \psi_1\left(t_{SQ,3}^{(\mathfrak{q}+4)}\right)^2\\ +\psi_2\left(t_{ESQ,1}^{(\mathfrak{q}+4)}\right)^2 + 2\psi_1\left(t_{ESQ,2}^{(\mathfrak{q}+4)}\right)^2 + \psi_1\left(t_{ESQ,3}^{(\mathfrak{q}+4)}\right)^2 + \psi_1\left(t_{ESQ,1}^{(\mathfrak{q}+4)}\right)^2\end{array}}, \tag{C40}
$$

we may evaluate up to the 19^{th}-order error for a stage-order 15 method. Provided that $\mathfrak{q}+m < 2\mathfrak{q}+3$, one could compute the the 2^{m-1} contributing terms to $A^{(\mathfrak{q}+m)}$.

C.7 Truncation Error Terms

A Mathematica routine is included, that computes the truncation error of Runge–Kutta methods from order one to eight.

```
(* ==========================================================================
  The purpose of the Mathematica routine is to compute the truncation error
  of Runge--Kutta methods from orders one to eight. There are no explicit or
  implicit guarantees that the output of this code is correct.
========================================================================== *)

(* ===================================================================== *)
(* Before reading in the Runge--Kutta scheme, set up the needed matrices *)
(*    S = number of stages to the method *)
(* ===================================================================== *)

S  = 4;

a  = Table[0,{i,S},{j,S}];
b  = Table[0,{i,S}];
bh = Table[0,{i,S}];
c  = Table[0,{i,S}];
e  = Table[1,{i,S}];

(* ===================================================================== *)
(* Read in Runge--Kutta scheme  below or from an external text file *)
(* ===================================================================== *)

b[[1]]  = 1/6;
b[[2]]  = 1/3;
b[[3]]  = 1/3;
b[[4]]  = 1/6;

c[[1]]  = 0;
c[[2]]  = 1/2;
c[[3]]  = 1/2;
c[[4]]  = 1;

a[[2,1]] = 1/2;
a[[3,2]] = 1/2;
a[[4,3]] = 1;

(* ===================================================================== *)
(* Set up some useful vectors and matrices *)
(* ===================================================================== *)

q2 = Factor[ a.c^1 - c^2/2 ]; q3 = Factor[ a.c^2 - c^3/3 ];
q4 = Factor[ a.c^3 - c^4/4 ]; q5 = Factor[ a.c^4 - c^5/5 ];
```

```
q6 = Factor[ a.c^5 - c^6/6 ]; q7 = Factor[ a.c^6 - c^7/7 ];

Q2 = DiagonalMatrix[ q2 ]; Q3 = DiagonalMatrix[ q3 ];
Q4 = DiagonalMatrix[ q4 ]; Q5 = DiagonalMatrix[ q5 ];
Q6 = DiagonalMatrix[ q6 ]; Q7 = DiagonalMatrix[ q7 ];

CC = DiagonalMatrix[c];

C2 = DiagonalMatrix[ c^2 ];
C3 = DiagonalMatrix[ c^3 ];
C4 = DiagonalMatrix[ c^4 ];
C5 = DiagonalMatrix[ c^5 ];
C6 = DiagonalMatrix[ c^6 ];

Aq2 = a.q2;
Aq3 = a.q3;
Aq4 = a.q4;

(* ================================================================== *)
(* The number of order conditions at order {1,2,3,4,5,6,7,8} *)
(* ================================================================== *)

len = {1,1,2,4,9,20,48,115};

(* ================================================================== *)
(* Quadrature Trees *)
(* ================================================================== *)

t[1,1]   = b.e           - 1/1!;
t[2,1]   = b.c^1/1!      - 1/2!;
t[3,1]   = b.c^2/2!      - 1/3!;
t[4,1]   = b.c^3/3!      - 1/4!;
t[5,1]   = b.c^4/4!      - 1/5!;
t[6,1]   = b.c^5/5!      - 1/6!;
t[7,1]   = b.c^6/6!      - 1/7!;
t[8,1]   = b.c^7/7!      - 1/8!;

(* ================================================================== *)
(* Subquadrature Trees *)
(* ================================================================== *)

a2       = Factor[ a.a ];
a3       = Factor[ a.a2];
a4       = Factor[ a.a3];
a5       = Factor[ a.a4];

t[3,  2] = b.q2          + t[3,  1];
```

```
t[4,  4] = b.a.q2        + t[4,  3];
t[4,  3] = b.q3/2        + t[4,  1];

t[5,  9] = b.a2.q2       + t[5,  8];
t[5,  8] = b.a.q3/2      + t[5,  5];
t[5,  5] = b.q4/6        + t[5,  1];

t[6, 20] = b.a3.q2       + t[6, 19];
t[6, 19] = b.a2.q3/2     + t[6, 15];
t[6, 15] = b.a.q4/6      + t[6,  7];
t[6,  7] = b.q5/24       + t[6,  1];

t[7, 48] = b.a4.q2       + t[7, 47];
t[7, 47] = b.a3.q3/2     + t[7, 42];
t[7, 42] = b.a2.q4/6     + t[7, 29];
t[7, 29] = b.a.q5/24     + t[7, 11];
t[7, 11] = b.q6/120      + t[7,  1];

t[8,115] = b.a5.q2       + t[8,114];
t[8,114] = b.a4.q3/2     + t[8,108];
t[8,108] = b.a3.q4/6     + t[8, 89];
t[8, 89] = b.a2.q5/24    + t[8, 53];
t[8, 53] = b.a.q6/120    + t[8, 15];
t[8, 15] = b.q7/720      + t[8,  1];

(* ================================================================ *)
(* Extended Subquadrature Trees *)
(* ================================================================ *)

(* ================ Order 4 ================= *)
t[4,  2] = b.CC.q2     +  3*t[4, 1];

(* ================ Order 5 ================= *)
AC       = Factor[ a.CC ]; CA       = Factor[ CC.a ];

t[5,  2] = b.C2.q2/2   +  6*t[5, 1];
t[5,  6] = b.CA.q2     +    t[5, 4];
t[5,  7] = b.AC.q2     +  3*t[5, 5];

t[5,  4] = b.CC.q3/2   +  4*t[5, 1];

(* ================ Order 6 ================= *)
C2A      = Factor[ CC.CA ]; CAC      = Factor[ CA.CC ];
AC2      = Factor[ AC.CC ]; CAA      = Factor[ CA.a  ];
ACA      = Factor[ AC.a  ]; AAC      = Factor[ a.AC  ];

t[6,  2] = b.C3.q2/6   + 10*t[6, 1];
t[6,  8] = b.C2A.q2/2  +    t[6, 4];
```

```
t[6, 10] = b.CAC.q2    +  3*t[6, 6];
t[6, 11] = b.AC2.q2/2  +  6*t[6, 7];
t[6, 16] = b.CAA.q2    +    t[6,13];
t[6, 17] = b.ACA.q2    +    t[6,14];
t[6, 18] = b.AAC.q2    +  3*t[6,15];

t[6,  4] = b.C2.q3/4   + 10*t[6, 1];
t[6, 13] = b.CA.q3/2   +    t[6, 6];
t[6, 14] = b.AC.q3/2   +  4*t[6, 7];

t[6,  6] = b.CC.q4/6   +  5*t[6, 1];

(* ================ Order 7 ================= *)
C3A      = Factor[ CC.C2A ]; C2AC     = Factor[ CC.CAC ];
CAC2     = Factor[ CAC.CC ]; AC3      = Factor[ AC2.CC ];
C2AA     = Factor[ CC.CAA ]; CACA     = Factor[ CC.ACA ];
AC2A     = Factor[ AC2.a  ]; CAAC     = Factor[ CC.AAC ];
ACAC     = Factor[ ACA.CC ]; AAC2     = Factor[ AAC.CC ];
CAAA     = Factor[ CAA.a  ]; ACAA     = Factor[ ACA.a  ];
AAAC     = Factor[ a.AAC  ]; AACA     = Factor[ AAC.a  ];

t[7,  2] = b.C4.q2/24   + 15*t[7, 1];
t[7, 12] = b.C3A.q2/2   +    t[7, 5];
t[7, 16] = b.C2AC.q2    +  3*t[7, 8];
t[7, 18] = b.CAC2.q2/2  +  6*t[7,10];
t[7, 19] = b.AC3.q2     + 10*t[7,11];
t[7, 30] = b.C2AA.q2    +    t[7,22];
t[7, 32] = b.CACA.q2    +    t[7,24];
t[7, 33] = b.AC2A.q2    +    t[7,25];
t[7, 35] = b.CAAC.q2    +  3*t[7,27];
t[7, 36] = b.ACAC.q2    +  3*t[7,28];
t[7, 37] = b.AAC2.q2    +  6*t[7,29];
t[7, 43] = b.CAAA.q2    +    t[7,39];
t[7, 44] = b.ACAA.q2    +    t[7,40];
t[7, 45] = b.AACA.q2    +    t[7,41];
t[7, 46] = b.AAAC.q2    +  3*t[7,42];

t[7,  5] = b.C3.q3/12   + 20*t[7, 1];
t[7, 22] = b.C2A.q3/4   +    t[7, 8];
t[7, 24] = b.CAC.q3/2   +  4*t[7,10];
t[7, 25] = b.AC2.q3/4   + 10*t[7,11];
t[7, 39] = b.CAA.q3/2   +    t[7,27];
t[7, 40] = b.ACA.q3/2   +    t[7,28];
t[7, 41] = b.AAC.q3/2   +  4*t[7,29];

t[7,  8] = b.C2.q4/12   + 15*t[7, 1];
t[7, 27] = b.CA.q4/6    +    t[7,10];
t[7, 28] = b.AC.q4/6    +  5*t[7,11];
```

```
t[7, 10] = b.CC.q5/24   +  6*t[7, 1];

(* ================ Order 8 ================= *)
C4A      = Factor[ CC.C3A  ]; C3AC     = Factor[ CC.C2AC ];
C2AC2    = Factor[ CC.CAC2 ]; CAC3     = Factor[ CAC2.CC ];
AC4      = Factor[ AC3.CC  ]; C3AA     = Factor[ CC.C2AA ];
C2ACA    = Factor[ CC.CACA ]; CAC2A    = Factor[ CC.AC2A ];
AC3A     = Factor[ AC3.a   ]; C2AAC    = Factor[ C2AA.CC ];
CACAC    = Factor[ CACA.CC ]; AC2AC    = Factor[ AC2A.CC ];
CAAC2    = Factor[ CAAC.CC ]; ACAC2    = Factor[ ACAC.CC ];
AAC3     = Factor[ a.AC3   ]; C2AAA    = Factor[ CC.CAAA ];
CACAA    = Factor[ CACA.a  ]; AC2AA    = Factor[ AC2A.a  ];
CAACA    = Factor[ CAAC.a  ]; ACACA    = Factor[ ACAC.a  ];
AAC2A    = Factor[ AAC2.a  ]; CAAAC    = Factor[ CAAA.CC ];
ACAAC    = Factor[ a.CAAC  ]; AACAC    = Factor[ a.ACAC  ];
AAAC2    = Factor[ a.AAC2  ]; CAAAA    = Factor[ CAAA.a  ];
ACAAA    = Factor[ ACAA.a  ]; AACAA    = Factor[ AACA.a  ];
AAACA    = Factor[ AAAC.a  ]; AAAAC    = Factor[ a.AAAC  ];

t[8,  2] = b.C5.q2/120  +  21*t[8,  1];
t[8, 16] = b.C4A.q2/24  +     t[8,  5];
t[8, 22] = b.C3AC.q2/6  +   3*t[8,  9];
t[8, 26] = b.C2AC2.q2/4 +   6*t[8, 12];
t[8, 28] = b.CAC3.q2/6  +  10*t[8, 14];
t[8, 29] = b.AC4.q2/2   +     t[8, 46];
t[8, 54] = b.C3AA.q2/6  +     t[8, 35];
t[8, 58] = b.C2ACA.q2/2 +     t[8, 39];
t[8, 60] = b.CAC2A.q2/2 +     t[8, 41];
t[8, 61] = b.AC3A.q2/2  +     t[8, 42];
t[8, 66] = b.C2AAC.q2/2 +   3*t[8, 46];
t[8, 68] = b.CACAC.q2/2 +   3*t[8, 48];
t[8, 69] = b.AC2AC.q2/2 +   3 t[8, 49];
t[8, 71] = b.CAAC2.q2/2 +   6 t[8, 51];
t[8, 72] = b.ACAC2.q2/2 +   6*t[8, 52];
t[8, 73] = b.AAC3.q2/6  +  10*t[8, 53];
t[8, 90] = b.C2AAA.q2/2 +     t[8, 77];
t[8, 92] = b.CACAA.q2/2 +     t[8, 79];
t[8, 93] = b.AC2AA.q2/2 +     t[8, 80];
t[8, 95] = b.CAACA.q2/2 +     t[8, 82];
t[8, 96] = b.ACACA.q2/2 +     t[8, 83];
t[8, 97] = b.AAC2A.q2/2 +     t[8, 84];
t[8, 99] = b.CAAAC.q2/2 +   3*t[8, 86];
t[8,100] = b.ACAAC.q2/2 +   3*t[8, 87];
t[8,101] = b.AACAC.q2/2  +  3*t[8, 88];
t[8,102] = b.AAAC2.q2/2  +  6*t[8, 89];
t[8,109] = b.CAAAA.q2/2  +    t[8,104];
t[8,110] = b.ACAAA.q2/2  +    t[8,105];
```

```
t[8,111] = b.AACAA.q2/2  +    t[8,106];
t[8,112] = b.AAACA.q2/2  +    t[8,107];
t[8,113] = b.AAAAC.q2/2  +  3*t[8,108];

t[8,  5] = b.C4.q3/48    + 35*t[8,  1];
t[8, 35] = b.C3A.q3/12   +    t[8,  9];
t[8, 39] = b.C2AC.q3/4   +  4*t[8, 12];
t[8, 41] = b.CAC2.q3/2   + 10*t[8, 14];
t[8, 42] = b.AC3.q3      + 20*t[8, 15];
t[8, 77] = b.C2AA.q3     +    t[8, 46];
t[8, 79] = b.CACA.q3     +    t[8, 48];
t[8, 80] = b.AC2A.q3     +    t[8, 49];
t[8, 82] = b.CAAC.q3     +  4*t[8, 51];
t[8, 83] = b.ACAC.q3     +  4*t[8, 52];
t[8, 84] = b.AAC2.q3     + 10*t[8, 53];
t[8,104] = b.CAAA.q3     +    t[8, 86];
t[8,105] = b.ACAA.q3     +    t[8, 87];
t[8,106] = b.AACA.q3     +    t[8, 88];
t[8,107] = b.AAAC.q3     +  4*t[8, 89];

t[8,  9] = b.C3.q4/12    + 35*t[8,  1];
t[8, 46] = b.C2A.q4/4    +    t[8, 12];
t[8, 48] = b.CAC.q4/2    +  5*t[8, 14];
t[8, 49] = b.AC2.q4/4    + 15*t[8, 15];
t[8, 86] = b.CAA.q4/2    +    t[8, 51];
t[8, 87] = b.ACA.q4/2    +    t[8, 52];
t[8, 88] = b.AAC.q4/2    +  5*t[8, 53];

t[8, 12] = b.C2.q5/48    + 21*t[8,  1];
t[8, 51] = b.CA.q5/24    +    t[8, 14];
t[8, 52] = b.AC.q5/24    +  6*t[8, 15];

t[8, 14] = b.CC.q6/120   +  6*t[8,  1];

(* ================================================================== *)
(* Nonlinear  Trees *)
(* ================================================================== *)

(* ================ Order 5 ================= *)
t[5,  3] = b.C2.q2/2 + b.Q2.q2/2
         +  3*t[5, 1];

(* ================ Order 6 ================= *)
t[6,  3] = b.C3.q2/2 + b.CC.Q2.q2/2
         + 15*t[6, 1];
t[6,  5] = b.C3.q2/6 + b.Q3.q2/2
         +    t[6, 4];
t[6,  9] = b.(C2A + AC2).q2/2 + b.Q2.a.q2
```

```
         +    t[6, 4];
t[6, 12] = b.a.C2.q2/2 + b.a.Q2.q2/2
         +  3*t[6, 7];

(* ================ Order 7 ================= *)
t[7,  3] = b.C4.q2/4 + b.C2.Q2.q2/4
         + 45*t[7,  1];
t[7,  4] = b.C4.q2/8 + b.C2.Q2.q2/4 + b.Q2.Q2.q2/6
         + 15*t[7,  1];
t[7,  6] = b.C4.q2/6 + b.C3.q3/4 + b.CC.Q2.q3/2
         + 60*t[7,  1];
t[7,  9] = b.C4.q2/24 + b.C2.q4/12 + b.Q2.q4/6
         + 15*t[7,  1];
t[7, 13] = b.C4.q2/6 + b.AC3.q2/2 + b.CC.Q2.a.q2 + b.CC.Q2.q3/2
         + 3*t[7,  5];
t[7, 14] = b.C3A.q2/6 + b.Q3.a.q2/2
         + 2*t[7,  7];
t[7, 15] = b.a.(q2)^2/2 + b.C3A.q2/6 + b.C3.q3/12 + b.Q3.a.q2/2 + b.(q3)^2/8
         + 10*t[7,  1];
t[7, 17] = b.C4.q2/8 + b.C2AC.q2/2 + b.Q2.a.CC.q2 + b.Q2.q4/2
         + 3*t[7,  8];
t[7, 20] = b.CAC2.q2/2 + b.CA.(q2)^2/2
         + 3*t[7, 10];
t[7, 21] = b.AC3.q2/2 + b.AC.(q2)^2/2
         + 15*t[7, 11];
t[7, 23] = b.C4.q2/24 + b.C2A.q3/4 + b.Q2.a.q3/2 + b.Q2.q4/6
         + t[7,  8];
t[7, 26] = b.AC3.q2/6 + b.AC2.q3/4 + b.a.Q2.q3/2
         + 10*t[7, 11];
t[7, 31] = b.Q2.a2.c^2/2 + b.C2AA.q2/2 + b.Q2.a2.q2
         + t[7, 22];
t[7, 34] = b.a.Q2.a.c^2/2 + b.AC2A.q2/2 + b.a.Q2.a.q2 + b.AC2.q3/4
         + 10*t[7, 11];
t[7, 38] = b.AAC2.q2/2 + b.a2.(q2)^2/2
         + 3*t[7, 29];

t[7,  7] = b.C3.q3/12 + b.Q3.q3/8
         + 10*t[7,  1];

(* ================ Order 8 ================= *)

t[8,  3] = b.C3.Q2.q2/12 + b.C5.q2/12
         + 105*t[8,  1];
t[8,  4] = b.C3.Q2.q2/4 + b.C5.q2/8 + b.CC.Q2.Q2.q2/6
         + 105*t[8,  1];
t[8,  6] = b.C2.Q2.q3/4 + b.C4.q3/8 + b.C5.q2/12
         + 210*t[8,  1];
t[8,  7] = b.C2.Q2.q3/4 + b.C3.Q2.q2/12 + b.C4.q3/16 + b.C5.q2/12 + b.Q2.Q2.q3/4
```

```
         + 105*t[8,  1];
t[8, 10] = b.C3.q4/12 + b.C5.q2/24 + b.CC.Q2.q4/6
         + 105*t[8,  1];
t[8, 13] = b.C2.q5/48 + b.C5.q2/120 + b.Q2.q5/24
         + 21*t[8,  1];
t[8, 17] = b.C2.Q2.q3/4 + b.C4.a.q2/4 + b.C5.q2/12 + b.CC.Q2.a.q2/2
         + 6*t[8,  5];
t[8, 18] = b.C2.Q2.a.q2/2 + b.C2.Q2.q3/4 + b.C3.Q2.q2/12 + b.C4.a.q2/8 + b.C5.q2/12
         + b.Q2.Q2.a.q2/2 + b.Q2.Q2.q3/4 + 3*t[8,  5];
t[8, 19] = b.C4.a.q2/6 + b.C4.q3/12 + b.CC.Q3.a.q2/2 + b.CC.Q3.q3/4
         + 4*t[8,  5];
t[8, 20] = b.C3.q4/36 + b.C4.a.q2/24 + b.Q3.q4/12 + b.Q4.a.q2/6
         + t[8,  5];
t[8, 21] = b.CC.(a.q2)^2/2 + b.C4.a.q2/6 + b.C4.q3/12 + b.CC.Q3.a.q2/2 + b.CC.Q3.q3/8
         + 70*t[8,  1];
t[8, 23] = b.C3.a.CC.q2/2 + b.C3.q4/4 + b.C5.q2/8 + b.CC.Q2.a.CC.q2 + b.CC.Q2.q4/2
         + 315*t[8,  1];
t[8, 24] = b.C3.a.CC.q2/6 + b.C3.q4/12 + b.Q3.a.CC.q2/2 + b.Q3.c^4/16 + b.Q3.q4/4
         + 105*t[8,  1];
t[8, 25] = b.C3.a.CC.q2/6 + b.C3.q4/12 + b.C4.a.q2/8 + b.C4.q3/16 + b.Q3.a.CC.q2/2
         + b.Q3.q4/4 + b.Q4.a.q2/2 + b.(a.CC.Q2).(a.q2) + 105*t[8,  1];
t[8, 27] = b.C2.a.C2.q2/4 + b.Q2.a.C2.q2/2 + b.Q2.a.c^4/4
         + 6*t[8, 12];
t[8, 30] = b.C2A.Q2.q2/4 + (b.C2AC2.q2)/4
         + 3*t[8, 12];
t[8, 31] = b.C2AC2.q2/4 + b.C2A.Q2.q2/4 + b.Q2.AC2.q2/2 + b.Q2.a.Q2.q2/2 + b.Q2.c^5/40
         + b.Q2.q5/8 + 3*t[8, 12];
t[8, 32] = b.CAC3.q2/2 + b.CAC.Q2.q2/2
         + 15*t[8, 14];
t[8, 33] = b.AC2.Q2.q2/4 + b.AC4.q2/4
         + 45*t[8, 15];
t[8, 34] = b.AC2.Q2.q2/4 + b.AC4.q2/8 + b.a.Q2.Q2.q2/6
         + 15*t[8, 15];
t[8, 36] = b.C3A.q3/4 + b.CC.Q2.a.q3/2 + b.CC.Q2.c^4/24 + b.CC.Q2.q4/6
         + 3*t[8,  9];
t[8, 38] = (b*Aq2).Aq3/2 + b.Q3.a.q3/4 + b.Q4.a.q2/6
         + t[8, 11];
t[8, 40] = b.C2AC.q3/4 + b.Q2.AC.q3/2 + b.Q2.c^5/30 + b.Q2.q5/6
         + 4*t[8,  12];
t[8, 43] = b.CAC2.q3/4 + b.CAC3.q2/6 + b.CA.Q2.q3/2
         + 10*t[8,  14];
t[8, 44] = b.AC3.q3/4 + b.AC4.q2/6 + b.AC.Q2.q3/2
         + 60*t[8,  15];
t[8, 47] = b.C2A.q4/12 + b.Q2.a.q4/6 + (b.Q2.c^5)/120 + (b.Q2.q5)/24
         + t[8,  12];
t[8, 50] = b.AC2.q4/12 + b.AC4.q2/24 + b.a.Q2.q4/6
         + 15*t[8,  15];
t[8, 55] = b.C3AA.q2/2 + b.CC.Q2.a2.q2 + b.CC.Q2.a.q3/2 + b.CC.Q2.c^424 + b.CC.Q2.q4/6
```

```
         + 3*t[8,  35];
t[8, 56] = b.C3AA.q2/6 + b.Q3.a.q3/4 + b.Q3.a2.q2/2 + b.Q3.c^4/48 + b.Q3.q4/12
         + t[8,  35];
t[8, 57] = (b*(Aq2)).(Aq3)/2 + (b*(Aq2)).a.(Aq2) + b.Q3.a2.q2/2
         + t[8,  37];
t[8, 59] = b.C2ACA.q2/2 + b.Q2.ACA.q2 + b.Q2.AC.q3/2 + b.Q2.c^5/30 + b.Q2.q5/6
         + t[8,  39];
t[8, 62] = b.CAC2A.q2/2 + b.CA.Q2.a.q2 + b.CA.Q2.q3/2
         + t[8,  41];
t[8, 63] = b.AAC3.q2/2 + b.AC.Q2.a.q2 + b.AC.Q2.q3/2
         + 3*t[8,  42];
t[8, 64] = b.AC3.q3/12 + b.ACA.q2/6 + b.a.Q3.a.q2/2 + b.a.Q3.q3/4
         + t[8,  42];
t[8, 65] = b.a.(Aq2)^2/2 + b.a.Q3.a.q2/2
         + t[8,  45];
t[8, 67] = b.C2AAC.q2/2 + b.Q2.(a.q4)/2 + b.Q2.AAC.q2 + b.Q2.c^5/40 + b.Q2.q5/8
         + 3*t[8,  46];
t[8, 70] = b.AC2AC.q2/2 + b.a.Q2.AC.q2 + b.a.Q2.c^4/8 + b.a.Q2.q4/2
         + 3*t[8,  49];
t[8, 74] = b.CAAC2.q2/2 + b.CAA.Q2.q2/2
         + 3*t[8,  51];
t[8, 75] = b.ACAC2.q2/2 + b.ACA.Q2.q2/2
         + 3*t[8,  52];
t[8, 76] = b.AAC3.q2/2  + b.AAC.Q2.q2/2
         + 15*t[8,  53];
t[8, 78] = b.C2AA.q3/4  + b.Q2.a.q4/6 + b.Q2.a2.q3/2 + b.Q2.c^5/120 + b.Q2.q5/24
         + t[8,  46];
t[8, 81] = b.a.C2.a.q3/4 + b.a.Q2.a.q3/2 + (b.a.Q2.c^4)/24 + b.a.Q2.q4/6
         + t[8, 49];
t[8, 85] = b.a2.C2.q3/4 + b.a2.C3.q2/6 + b.a2.Q2.q3/2
         + 10*t[8, 53];
t[8, 91] = b.C2.a3.q2/2 + b.Q2.a3.q2 + b.Q2.a2.q3/2 + b.Q2.a.q4/6 + b.Q2.c^5/120
         + b.Q2.q5/24 + t[8, 77];
t[8, 94] = b.a.C2.a2.q2/2 + b.a.Q2.a2.q2 + b.a.Q2.a.q3/2 + b.a.Q2.c^4/24 + b.a.Q2.q4/6
         + t[8, 80];
t[8, 98] = b.a2.C2.a.q2/2 + b.a2.Q2.a.q2 + b.a2.Q2.c^3/6 + b.a2.Q2.q3/2
         + t[8, 84];
t[8,103] = b.a3.C2.q2/2 + b.a3.Q2.q2/2
         + 3*t[8, 89];

t[8,  8] = b.C4.q3/12 + b.CC.Q3.q3/8
         + 70*t[8,  1];
t[8, 11] = b.C3.q4/36 + b.C4.q3/48 + b.Q3.q4/12
         + 35*t[8,  1];
t[8, 37] = b.C3A.q3/12 + b.Q3.a.q3/4 + b.Q3.c^4/48 + b.Q3.q4/12
         + t[8,  9];
t[8, 45] = b.AC3.q3/12 + b.a.Q3.q3/8
         + 10*t[8,  15];
```

```
(* ================================================================== *)
(* Compute Truncation Error Vectors *)
(* ================================================================== *)

Do[ tau[i] = {}, {i,1,8}];
Do[ Do[ tau[i] = Append[tau[i], t[i,j]]; ,{j,1,len[[i]]}]; ,{i,1,8}];

(* ================================================================== *)
(* Compute the Principal Error Norms *)
(* ================================================================== *)

Do[ AA[i] = Sqrt[ tau[i].tau[i] ], {i,1,8}];
Do[ Print[" A^{(",i,")} = ", N[ AA[i], 5]], {i,1,8}];

(* ================================================================== *)
(* The End *)
(* ================================================================== *)
```

C.8 Stage Order-Conditions

It is occasionally useful to evaluate the order conditions for the stages rather than the traditional step order-conditions (e.g., constructing stage-value-predictors). There are strong similarities between the step and stage order conditions. Up to order six, the stage order-conditions (vectors) are given by

$$
\begin{array}{|lcl|}
\hline
\mathrm{t}_1^{(1)} & = & \mathbf{q}^{(1)} \\
\hline
\mathrm{t}_1^{(2)} & = & \mathbf{q}^{(2)} \\
\hline
\mathrm{t}_1^{(3)} & = & \frac{1}{2!}\mathbf{q}^{(3)} \\
\mathrm{t}_2^{(3)} & = & \mathbf{A}\mathbf{q}^{(2)} + \frac{1}{2}\mathbf{q}^{(3)} \\
\hline
\mathrm{t}_1^{(4)} & = & \frac{1}{3!}\mathbf{q}^{(4)} \\
\mathrm{t}_2^{(4)} & = & \mathbf{A}\mathbf{C}\mathbf{q}^{(2)} + \frac{1}{2}\mathbf{q}^{(4)} \\
\mathrm{t}_3^{(4)} & = & \frac{1}{2}\mathbf{A}\mathbf{q}^{(3)} + \frac{1}{6}\mathbf{q}^{(4)} \\
\mathrm{t}_4^{(4)} & = & \mathbf{A}\mathbf{A}\mathbf{q}^{(2)} + \frac{1}{2}\mathbf{A}\mathbf{q}^{(3)} + \frac{1}{6}\mathbf{q}^{(4)} \\
\hline
\mathrm{t}_1^{(5)} & = & \frac{1}{4!}\mathbf{q}^{(5)} \\
\mathrm{t}_2^{(5)} & = & \frac{1}{2}\mathbf{A}\mathbf{C}^2\mathbf{q}^{(2)} + \frac{1}{4}\mathbf{q}^{(5)} \\
\mathrm{t}_3^{(5)} & = & \frac{1}{2}\mathbf{A}\mathbf{C}^2\mathbf{q}^{(2)} + \frac{1}{2}\mathbf{A}\left(\mathbf{q}^{(2)}\right)^2 + \frac{1}{8}\mathbf{q}^{(5)} \\
\mathrm{t}_4^{(5)} & = & \frac{1}{2}\mathbf{A}\mathbf{C}\mathbf{q}^{(3)} + \frac{1}{6}\mathbf{q}^{(5)} \\
\mathrm{t}_5^{(5)} & = & \frac{1}{6}\mathbf{A}\mathbf{q}^{(4)} + \frac{1}{24}\mathbf{q}^{(5)} \\
\mathrm{t}_6^{(5)} & = & \mathbf{A}\mathbf{C}\mathbf{A}\mathbf{q}^{(2)} + \frac{1}{2}\mathbf{A}\mathbf{C}\mathbf{q}^{(3)} + \frac{1}{6}\mathbf{q}^{(5)} \\
\mathrm{t}_7^{(5)} & = & \mathbf{A}\mathbf{A}\mathbf{C}\mathbf{q}^{(2)} + \frac{1}{2}\mathbf{A}\mathbf{q}^{(4)} + \frac{1}{8}\mathbf{q}^{(5)}
\end{array}
$$

$$
\begin{array}{|lcl|}
\mathsf{t}_8^{(5)} & = & \frac{1}{2}\mathbf{AAq}^{(3)} + \frac{1}{6}\mathbf{Aq}^{(4)} + \frac{1}{24}\mathbf{q}^{(5)} \\
\mathsf{t}_9^{(5)} & = & \mathbf{AAAq}^{(2)} + \frac{1}{2}\mathbf{AAq}^{(3)} + \frac{1}{6}\mathbf{Aq}^{(4)} + \frac{1}{24}\mathbf{q}^{(5)} \\
\hline
\mathsf{t}_1^{(6)} & = & \frac{1}{5!}\mathbf{q}^{(6)} \\
\mathsf{t}_2^{(6)} & = & \frac{1}{6}\mathbf{AC}^3\mathbf{q}^{(2)} + \frac{1}{12}\mathbf{q}^{(6)} \\
\mathsf{t}_3^{(6)} & = & \frac{1}{2}\mathbf{AC}^3\mathbf{q}^{(2)} + \frac{1}{2}\mathbf{ACQ}^{(2)}\mathbf{q}^{(2)} + \frac{1}{8}\mathbf{q}^{(6)} \\
\mathsf{t}_4^{(6)} & = & \frac{1}{4}\mathbf{AC}^2\mathbf{q}^{(3)} + \frac{1}{12}\mathbf{q}^{(6)} \\
\mathsf{t}_5^{(6)} & = & \frac{1}{6}\mathbf{AC}^3\mathbf{q}^{(2)} + \frac{1}{4}\mathbf{AC}^2\mathbf{q}^{(3)} + \frac{1}{2}\mathbf{AQ}^{(2)}\mathbf{q}^{(3)} + \frac{1}{12}\mathbf{q}^{(6)} \\
\mathsf{t}_6^{(6)} & = & \frac{1}{6}\mathbf{ACq}^{(4)} + 5\frac{1}{}\mathbf{q}^{(6)} \\
\mathsf{t}_7^{(6)} & = & \frac{1}{24}\mathbf{Aq}^{(5)} + \frac{1}{120}\mathbf{q}^{(6)} \\
\mathsf{t}_8^{(6)} & = & \frac{1}{2}\mathbf{AC}^2\mathbf{A}^{(1)}\mathbf{q}^{(2)} + \frac{1}{4}\mathbf{AC}^2\mathbf{q}^{(3)} + \frac{1}{12}\mathbf{q}^{(6)} \\
\mathsf{t}_9^{(6)} & = & \frac{1}{6}\mathbf{AC}^3\mathbf{q}^{(2)} + \frac{1}{2}\mathbf{AAC}^2\mathbf{q}^{(2)} + \frac{1}{4}\mathbf{AC}^2\mathbf{q}^{(3)} + \mathbf{AA}\left(\mathbf{q}^{(2)}\right)^2 \\
 & + & \frac{1}{2}\mathbf{AQ}^{(2)}\mathbf{q}^{(3)} + \frac{1}{12}\mathbf{q}^{(6)} \\
\mathsf{t}_{10}^{(6)} & = & \mathbf{ACACq}^{(2)} + \frac{1}{2}\mathbf{ACq}^{(4)} + \frac{1}{8}\mathbf{q}^{(6)} \\
\mathsf{t}_{11}^{(6)} & = & \frac{1}{2}\mathbf{AAC}^2\mathbf{q}^{(2)}\frac{1}{4}\mathbf{Aq}^{(5)} + 6\,\mathbf{q}_1^{(6)} \\
\mathsf{t}_{12}^{(6)} & = & \frac{1}{2}\mathbf{AA}^{(1)}\mathbf{C}^2\mathbf{q}^{(2)} + \frac{1}{2}\mathbf{AA}\left(\mathbf{q}^{(2)}\right)^2 + \frac{1}{8}\mathbf{Aq}^{(5)} + 3\,\mathbf{q}_1^{(6)} \\
\mathsf{t}_{13}^{(6)} & = & \frac{1}{2}\mathbf{ACA}^{(1)}\mathbf{q}^{(3)} + \frac{1}{6}\mathbf{ACq}^{(4)} + \frac{1}{24}\mathbf{q}_1^{(6)} \\
\mathsf{t}_{14}^{(6)} & = & \frac{1}{2}\mathbf{AA}^{(1)}\mathbf{Cq}^{(3)} + \frac{1}{6}\mathbf{Aq}^{(5)} + \frac{1}{30}\mathbf{q}_1^{(6)} \\
\mathsf{t}_{15}^{(6)} & = & \frac{1}{6}\mathbf{AA}^{(1)}\mathbf{q}^{(4)} + \frac{1}{24}\mathbf{Aq}^{(5)} + \frac{1}{120}\mathbf{q}_1^{(6)} \\
\mathsf{t}_{16}^{(6)} & = & \mathbf{ACA}^{(1)}\mathbf{Aq}^{(2)} + \frac{1}{2}\mathbf{ACAq}^{(3)} + \frac{1}{6}\mathbf{ACq}^{(4)} + \frac{1}{24}\mathbf{q}_1^{(6)} \\
\mathsf{t}_{17}^{(6)} & = & \mathbf{AACAq}^{(2)} + \frac{1}{2}\mathbf{AA}^{(1)}\mathbf{Cq}^{(3)}\frac{1}{6}\mathbf{Aq}^{(5)} + \frac{1}{30}\mathbf{q}_1^{(6)} \\
\mathsf{t}_{18}^{(6)} & = & \mathbf{AAACq}^{(2)} + \frac{1}{2}\mathbf{AAq}^{(4)} + \frac{1}{8}\mathbf{Aq}^{(5)} + \frac{1}{40}\mathbf{q}_1^{(6)} \\
\mathsf{t}_{19}^{(6)} & = & \frac{1}{2}\mathbf{AAAq}^{(3)}\frac{1}{6}\mathbf{AAq}^{(4)} + \frac{1}{24}\mathbf{Aq}^{(5)} + \frac{1}{120}\mathbf{q}_1^{(6)} \\
\mathsf{t}_{20}^{(6)} & = & \mathbf{AAAAq}^{(2)} + \frac{1}{2}\mathbf{AAAq}^{(3)} + \frac{1}{6}\mathbf{AA}^{(1)}\mathbf{q}^{(4)} + \frac{1}{24}\mathbf{Aq}^{(5)} + \frac{1}{120}\mathbf{q}_1^{(6)} \\
\hline
\end{array}
$$

With these terms, the truncation error of the stages within a pth-order Runge–Kutta scheme may be quantified in a general way by taking the L_2 principal error norm,

$$
A_{(\mathrm{int}),i}^{(p+1)} = \sqrt{\sum_{j=1}^{\mathsf{a}_{p+1}} \left(\mathsf{t}_j^{(p+1)}\right)_i^2}, \tag{C41}
$$

where i is the stage index.

Appendix D

Fully-Implicit Runge–Kutta Methods

The most familiar and best studied fully-implicit Runge–Kutta (FIRK) methods are the Gauss, Radau and Lobatto methods. Very good general discussions of these methods may be found in the books by Butcher [51], Dekker and Verwer [74] and Hairer and Wanner [102] while brief reviews [50,104,114] on each may also be found. FIRK methods are important because members of these methods often exhibit exceptional properties. They are, effectively, the *gold standard* for implicit Runge–Kutta methods. It is only through knowing what attributes these methods possess that one can correctly judge whether a SIRK method is competitive with these FIRKs. A brief review of the properties of these methods follows. The FIRK family of methods considered has four subfamilies distinguished by the locations of the abscissae to the methods. These essential methods were all introduced by Butcher [27,28]. For an s-stage method, the abscissae to the Gauss, Radau I, Radau II and Lobatto III methods are the roots to this expression [102]

$$\frac{d^{s-(\alpha+\beta)}}{dx^{s-(\alpha+\beta)}}\left[x^{s-\alpha}\left(x-1\right)^{s-\beta}\right], \tag{D1}$$

where $\{\alpha,\beta\}$ equals $\{0,0\}$ for Gauss methods, $\{0,1\}$ for Radau I methods, $\{1,0\}$ for Radau II methods and $\{1,1\}$ for Lobatto III methods. Extending Table 5.13 in [102], Tables D1 and D6 show the properties of methods from the four FIRK classes. The linear stability function for all of the FIRKs given in this appendix are expressible as a (k,m)-Padé approximation [82,83,109] to e^z, given by

$$\frac{P_{n,m}(z)}{Q_{n,m}(z)}=\frac{\sum_{k=0}^{m}\frac{(m+n-k)!}{(m+n)!}\binom{m}{k}(+z)^k}{\sum_{k=0}^{n}\frac{(m+n-k)!}{(m+n)!}\binom{n}{k}(-z)^k}. \tag{D2}$$

This implies that their respective E-polynomials are

$$E_{s,s}(y)=E_{s-1,s-1}(y)=0, \tag{D3}$$

$$E_{s-1,s}(y)=-E_{s,s-1}(y)=\phi y^{2s},\quad E_{s-2,s}(y)=-E_{s,s-2}(y)=\psi y^{2s}, \tag{D4}$$

$$\phi=\left[2^{s-1}\prod_{i=1}^{s}(2i-1)\right]^{-2},\qquad \psi=\left[\binom{2s-2}{s-2}s!\right]^{-2} \tag{D5}$$

Hence, methods whose (k,m)-Padé approximations are (s,s), $(s-1,s-1)$, $(s-1,s)$ and $(s-2,s)$ are I-stable while methods with $(s,s-1)$ and $(s,s-2)$ are not. For a FIRK method to be symplectic, its algebraic stability matrix must vanish. Partitioned FIRK methods are described by Sun [168] which are symplectic.

D.1 Gauss Methods

Gauss [88,111] methods were introduced by Kuntzmann [124] and Butcher [27]. The single stage method is the implicit midpoint rule and the two-stage method was first given by Hammer and Hollingsworth [106]. Early literature on these methods include that of Ehle [82] and Chipman [68] while they have been reviewed by Butcher [50] and are discussed in the books by Butcher [51], Dekker and Verwer [74], Hairer and Wanner [102] and Hairer, Nørsett and Wanner [100]. The general properties of this class of methods is described in Table D1 while specific properties for the two- through six- stage members of this family

Method	Gauss	Radau I	Radau IA	Radau IB	Radau II	Radau IIA	Radau IIB
order	$2s$	$2s-1$	$2s-1$	$2s-1$	$2s-1$	$2s-1$	$2s-1$
$\mathrm{B(p)}, p =$	$2s$	$2s-1$	$2s-1$	$2s-1$	$2s-1$	$2s-1$	$2s-1$
$\mathrm{C}(\eta), \eta =$	s	s	$s-1$	$s-1$	$s-1$	s	$s-1$
$\mathrm{D}(\zeta), \zeta =$	s	$s-1$	s	$s-1$	s	$s-1$	$s-1$
$\mathrm{I-Stable}$	Yes	No	Yes	Yes	No	Yes	Yes
$\mathrm{A-Stable}$	Yes	No	Yes	Yes	No	Yes	Yes
$\mathrm{L-Stable}$	No	No	Yes	No	No	Yes	No
$\mathrm{R}(-\infty)$	$(-1)^s$	∞	0	$(-1)^{s-1}$	∞	0	$(-1)^{s-1}$
$a_{sj} = b_j$	No	No	No	No	No	Yes	No
$a_{i1} = b_1$	No	No	Yes	No	No	No	No
$a_{1j} = 0$	No	Yes	No	No	No	No	No
$a_{is} = 0$	No	No	No	No	Yes	No	No
Alg.Stable	Yes	No	Yes	Yes	No	Yes	Yes
Symmetric	Yes	No	No	No	No	No	No
Symplectic	Yes	No	No	Yes	No	No	Yes
$\mathrm{Int.I-Stable}$	No	No	No	No	No	No	No
Int.Alg.Stable	No	No	No	No	No	No	No
$\mathrm{Pade}: e^z$	(s,s)	$(s,s-1)$	$(s-1,s)$	$(s-1,s-1)$	$(s,s-1)$	$(s-1,s)$	$(s-1,s-1)$
(α,β)	$(0,0)$	$(0,1)$	$(0,1)$	$(0,1)$	$(1,0)$	$(1,0)$	$(1,0)$

Table D1: Characteristics of Gauss and Radau methods.

are given in Table D2, where $\{s, p, \mathfrak{q}\}$ are the number of stages, the order of the method and the stage-order of the method, respectively. The next four rows provide the minimum and maximum entries in the **A**-matrix and **b**-vector. Minimum, maximum and RMS values of the algebraic matrix and internal algebraic stability matrices are then given. Leading- and next-to-leading- order truncation errors are then given for the step and stages and uniformity of abscissae placement, (96), is quantified with $\mathcal{C}$. Lastly, $\mathrm{C}(\mathbf{A})$ is the condition number of the **A**-matrix. This same format used in describing Radau methods, Tables D3, D4, D5 and, for Lobatto methods, Tables D7, D8, D9 and D10.

Abscissae, **c**, to Gauss methods are symmetrically located about the midpoint of the step. For methods with even and odd stages, the abscissae appear as

$$\mathbf{c}^{(2n)} = \left\{ \frac{1}{2} - \sqrt{\Gamma_1^{(2n)}}, \cdots, \frac{1}{2} - \sqrt{\Gamma_n^{(2n)}}, \frac{1}{2} + \sqrt{\Gamma_n^{(2n)}}, \cdots, \frac{1}{2} + \sqrt{\Gamma_1^{(2n)}} \right\} \tag{D6}$$

$$\mathbf{c}^{(2n+1)} = \left\{ \frac{1}{2} - \sqrt{\Gamma_1^{(2n+1)}}, \cdots, \frac{1}{2} - \sqrt{\Gamma_n^{(2n+1)}}, \frac{1}{2}, \frac{1}{2} + \sqrt{\Gamma_n^{(2n+1)}}, \cdots, \frac{1}{2} + \sqrt{\Gamma_1^{(2n+1)}} \right\}, \tag{D7}$$

{s, p, q}	{2, 4, 2}	{3, 6, 3}	{4, 8, 4}	{5, 10, 5}	{6, 12, 6}
Min.**A**	-0.039	-0.036	-0.028	-0.025	-0.020
Max.**A**	0.539	0.480	0.354	0.309	0.254
Min.**b**	0.500	0.278	0.069	0.118	0.086
Max.**b**	0.500	0.444	0.931	0.284	0.234
$\lambda^{\mathbf{M}}_{\text{Min.}}$	0	0	0	0	0
$\lambda^{\mathbf{M}}_{\text{Max.}}$	0	0	0	0	0
$\lambda^{\mathbf{M}^{(i)}}_{\text{Min.}}$	-0.026	-0.022	-0.013	-0.011	-0.008
$\lambda^{\mathbf{M}^{(i)}}_{\text{Max.}}$	0.067	0.054	0.030	0.024	0.016
$\lambda^{\mathbf{M}^{(i)}}_{\text{RMS}}$	0.102	0.071	0.053	0.041	0.034
$A^{(p+1)}$	$4.33(-3)$	$1.65(-4)$	$5.79(-6)$	$1.93(-7)$	$6.17(-9)$
$A^{(p+2)}$	$5.62(-3)$	$2.92(-4)$	$1.39(-5)$	$5.85(-7)$	$2.26(-8)$
Min.$A^{(q+1)}_{(\text{int})}$	$1.13(-2)$	$1.44(-3)$	$1.72(-4)$	$2.26(-5)$	$3.19(-6)$
Max.$A^{(q+1)}_{(\text{int})}$	$1.13(-2)$	$1.8(-3)$	$2.32(-4)$	$3.45(-5)$	$5.19(-6)$
Min.$A^{(q+2)}_{(\text{int})}$	$1.16(-2)$	$1.64(-3)$	$2.53(-4)$	$4.16(-5)$	$6.76(-6)$
Max.$A^{(q+2)}_{(\text{int})}$	$1.68(-2)$	$2.47(-3)$	$4.37(-4)$	$7.46(-5)$	$1.31(-5)$
$\mathcal{C}$	0.358	0.299	0.270	0.255	0.249
C(**A**)	4.79	10.44	18.20	28.34	40.93

Table D2: Gauss methods.

where

$$\Gamma_1^{(2)} = \frac{1}{12}, \qquad \Gamma_1^{(3)} = \frac{3}{20}, \tag{D8}$$

$$\Gamma_{1,2}^{(4)} = \frac{15 \pm 2\sqrt{30}}{140}, \quad \Gamma_{1,2}^{(5)} = \frac{35 \pm 2\sqrt{70}}{252}, \tag{D9}$$

and

$$\Gamma_1^{(6)} = \frac{\left[15 + 4\sqrt{15}\cos(\phi_6)\right]}{132}, \quad \Gamma_{2,3}^{(6)} = \frac{\left[15 - 2\sqrt{15}\cos(\phi_6) \pm 6\sqrt{5}\sin(\phi_6)\right]}{132} \tag{D10}$$

$$\Gamma_{1,2}^{(7)} = \frac{\left[77 + 2\sqrt{231}\cos(\varphi_7) \pm 6\sqrt{77}\sin(\varphi_7)\right]}{572}, \quad \Gamma_3^{(7)} = \frac{\left[77 - 4\sqrt{231}\cos(\varphi_7)\right]}{572} \tag{D11}$$

$$\varphi_6 = \frac{1}{3}\arctan\left(11\sqrt{\frac{2}{3}}\right) \qquad \varphi_7 = \frac{1}{3}\arctan\left(13\sqrt{\frac{10}{11}}\right). \tag{D12}$$

With these expressions, it is relatively straightforward to generate closed-form expressions for the **A**-matrix and **b**-vector of Gauss methods up to $14th$-order. At orders 16 and 18, closed-form expressions for the scheme are still possible but are very large and messy.

In terms of internal linear stability, all stages of Gauss methods have $R_{\text{int}}^{(i)}(z) = 0$ for $z \to -\infty$. However, inspection of the $E_{\text{int}}^{(i)}(y)$ show that only the $s = 2$ method is I-stable on all stages. Note that $E_{\text{int}}^{(i)}(y) = E_{\text{int}}^{(s-(i-1))}(y)$. For $s > 2$, at least the first and last stages are not I-stable while the center one or two are I-stable.

Gauss methods have an algebraic-stability matrix given by, $\mathbf{M} = \mathbf{O}$. While the internal-algebraic-stability matrices are not zero on any stage,

$$\mathbf{M}_{\text{int}}^{(i)} \cdot \mathcal{S} - \mathcal{S} \cdot \mathbf{M}_{\text{int}}^{(s-(i-1))} = 0, \tag{D13}$$

where $\mathcal{S}$ is the sip, reverse-identity or reversal matrix.

D.2 Radau Methods

At least six distinct Radau [156] methods have been reported in the literature to date. The first two (Radau I and Radau II) were given by Butcher [28]. Because neither was A-stable, Ehle [82] and Axelsson [4] sought to improve these two methods. Ehle [82] introduced Radau IA and IIA. Later, in 1993, Sun [166] introduced Radau IB and IIB methods. The general properties of these six classes of methods are described in Table D1. Specific properties for members of these six families, having 2-, 3-, 4-, 5- and 6-stages, are given in Tables D3, D4 and D5. Generalizations beyond these six methods have been offered by Ding and Tan [80]. Similar to Lobatto methods, (D20), it is possible that several useful methods exist within a general class of Radau I/II, Radau IA/IIA and Radau IB/IIB methods with the **A**-matrix given by

$$\mathbf{A} = \alpha_I \mathbf{A}_I + \alpha_{IA}\mathbf{A}_{IA} + \alpha_B \mathbf{A}_{IB}, \qquad \mathbf{A} = \alpha_{II}\mathbf{A}_{II} + \alpha_{IIA}\mathbf{A}_{IIA} + \alpha_{IIB}\mathbf{A}_{IIB}. \tag{D14}$$

For the solution of stiff ODEs, only Radau IIA is L-stable and stiffly accurate. Hence, Radau IIA [103] is likely to be the best suited to the integration of stiff ODEs amongst the six Radau methods. The specific properties of six Radau method for the 2-, 3-, 4-, 5- and 6-stage members of this family are given in tables D3, D4 and D5.

While is it too cumbersome to present closed-form coefficients for the full four-and five-stage Radau I, IA, IB, II, IIA and IIB methods, the abscissae, $\mathbf{c}_I^{(s)}$ and $\mathbf{c}_{II}^{(s)}$ may be shown for methods of $s = 5$ stages and below as

$$\mathbf{c}_I^{(1)} = \{0\}, \qquad \mathbf{c}_I^{(2)} = \left\{0, \frac{2}{3}\right\}, \qquad \mathbf{c}_I^{(3)} = \left\{0, \frac{6-\sqrt{6}}{10}, \frac{6+\sqrt{6}}{10}\right\}, \tag{D15}$$

$$\mathbf{c}_{II}^{(1)} = \{1\}, \qquad \mathbf{c}_{II}^{(2)} = \left\{\frac{1}{3}, 1\right\}, \qquad \mathbf{c}_{II}^{(3)} = \left\{\frac{4-\sqrt{6}}{10}, \frac{4+\sqrt{6}}{10}, 1\right\}. \tag{D16}$$

Four-stage Radau I, IA, IB and Radau II, IIA, IIB methods have abscissae

$$\begin{aligned}
\mathbf{c}_{I,1}^{(4)} &= 0, \qquad \mathbf{c}_{I,2}^{(4)} = \frac{(20 - 5\sqrt{2}\mathfrak{c}_1 - \mathfrak{c}_2 - 7\mathfrak{s}_2)}{35}, \\
\mathbf{c}_{I,3}^{(4)} &= \frac{(40 + 5\sqrt{2}\mathfrak{c}_1 + (1 - 7\sqrt{3})\mathfrak{c}_2 - 5\sqrt{6}\mathfrak{s}_1 + (7 + \sqrt{3})\mathfrak{s}_2)}{70}, \\
\mathbf{c}_{I,4}^{(4)} &= \frac{(40 + 5\sqrt{2}\mathfrak{c}_1 + (1 + 7\sqrt{3})\mathfrak{c}_2 + 5\sqrt{6}\mathfrak{s}_1 + (7 - \sqrt{3})\mathfrak{s}_2)}{70},
\end{aligned}$$

$$\begin{aligned}
\mathbf{c}_{II,1}^{(4)} &= \frac{(30 - 5\sqrt{2}\mathfrak{c}_1 - (1 + 7\sqrt{3})\mathfrak{c}_2 - 5\sqrt{6}\mathfrak{s}_1 - (7 - \sqrt{3})\mathfrak{s}_2)}{70}, \\
\mathbf{c}_{II,2}^{(4)} &= \frac{(30 - 5\sqrt{2}\mathfrak{c}_1 - (1 - 7\sqrt{3})\mathfrak{c}_2 + 5\sqrt{6}\mathfrak{s}_1 - (7 + \sqrt{3})\mathfrak{s}_2)}{70}, \\
\mathbf{c}_{II,3}^{(4)} &= \frac{(15 + 5\sqrt{2}\mathfrak{c}_1 + \mathfrak{c}_2 + 7\mathfrak{s}_2)}{35}, \qquad \mathbf{c}_{II,4}^{(4)} = 1.
\end{aligned}$$

$$\theta = \frac{1}{3}\arctan(7), \quad \mathfrak{c}_1 = \cos(\theta), \quad \mathfrak{c}_2 = \cos(2\theta), \quad \mathfrak{s}_1 = \sin(\theta), \quad \mathfrak{s}_2 = \sin(2\theta).$$

{s, p, q}	{2, 3, 2}	{3, 5, 3}	{4, 7, 4}	{5, 9, 5}	{6, 11, 6}	{2, 3, 1}	{3, 5, 2}	{4, 7, 3}	{5, 9, 4}	{6, 11, 5}
Min.$\mathbf{A}$	0.000	−0.018	−0.018	−0.018	−0.016	0.000	−0.025	−0.025	−0.020	−0.018
Max.$\mathbf{A}$	0.333	0.578	0.429	0.348	0.288	1.000	0.704	0.456	0.359	0.317
Min.$\mathbf{b}$	0.250	0.111	0.063	0.040	0.028	0.250	0.111	0.063	0.040	0.028
Max.$\mathbf{b}$	0.750	0.512	0.388	0.312	0.260	0.750	0.512	0.388	0.312	0.260
$\lambda^{\mathbf{M}}_{\text{Min.}}$	−0.125	−0.056	−0.031	−0.020	−0.014	−0.125	−0.056	−0.031	−0.020	−0.014
$\lambda^{\mathbf{M}}_{\text{Max.}}$	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
$\lambda^{\mathbf{M}^{(i)}}_{\text{Min.}}$	−0.111	−0.096	−0.049	−0.033	−0.022	−0.333	−0.215	−0.116	−0.067	−0.046
$\lambda^{\mathbf{M}^{(i)}}_{\text{Max.}}$	0.111	0.050	0.035	0.023	0.017	0.111	0.050	0.060	0.043	0.028
$\lambda^{\mathbf{M}^{(i)}}_{\text{RMS}}$	0.157	0.117	0.080	0.059	0.047	0.351	0.231	0.145	0.098	0.073
$A^{(p+1)}$	2.45(−2)	9.90(−4)	3.47(−5)	1.16(−6)	3.74(−8)	2.45(−2)	9.90(−4)	3.47(−5)	1.16(−6)	3.74(−8)
$A^{(p+2)}$	2.47(−2)	1.47(−3)	7.28(−5)	3.16(−6)	1.25(−7)	2.17(−2)	1.42(−3)	6.96(−5)	3.12(−6)	1.25(−7)
Min.$A^{(q+1)}_{\text{(int)}}$	3.49(−2)	2.87(−3)	2.47(−4)	2.53(−5)	2.90(−6)	5.56(−2)	5.04(−3)	6.54(−4)	7.91(−5)	1.05(−5)
Max.$A^{(q+1)}_{\text{(int)}}$	3.49(−2)	3.91(−3)	4.57(−4)	6.60(−5)	9.69(−6)	1.67(−1)	2.36(−2)	4.12(−3)	6.27(−4)	1.00(−4)
Min.$A^{(q+2)}_{\text{(int)}}$	3.49(−2)	3.02(−3)	3.31(−4)	4.25(−5)	5.68(−6)	3.32(−2)	4.09(−3)	6.34(−4)	1.03(−4)	1.76(−5)
Max.$A^{(q+2)}_{\text{(int)}}$	3.49(−2)	5.49(−3)	8.05(−4)	1.40(−4)	2.38(−5)	1.24(−1)	3.30(−2)	6.26(−3)	1.21(−3)	2.35(−4)
$\mathcal{C}$	0.601	0.482	0.423	0.388	0.367	0.167	0.180	0.189	0.199	0.209
C($\mathbf{A}$)	∞	∞	∞	∞	∞	∞	∞	∞	∞	∞

Table D3: Radau I (left) and II (right) methods.

For five-stage Radau I, IA and IB methods,

$$\mathbf{c}_I^{(5)} = \left\{0, \frac{(70-\alpha-\gamma^{(+)})}{126}, \frac{(70-\alpha+\gamma^{(+)})}{126}, \frac{(70+\alpha-\gamma^{(-)})}{126}, \frac{(70+\alpha+\gamma^{(-)})}{126}\right\}, \tag{D17}$$

and, similarly, for five-stage Radau II, IIA and IIB methods,

$$\mathbf{c}_{II}^{(5)} = \left\{\frac{(56-\alpha-\gamma^{(-)})}{126}, \frac{(56-\alpha+\gamma^{(-)})}{126}, \frac{(56+\alpha-\gamma^{(+)})}{126}, \frac{(56+\alpha+\gamma^{(+)})}{126}, 1\right\}, \tag{D18}$$

where $i = \sqrt{-1}$ and

$$\alpha = \sqrt{7}\sqrt{70+x}, \quad \beta = \frac{40\sqrt{7}}{\sqrt{70+x}}, \quad \gamma^{(\pm)} = \sqrt{7}\sqrt{140-x\pm\beta}$$
$$x = \frac{9\sqrt[3]{35}}{\sqrt[3]{y}}\left(\sqrt[3]{35}+\sqrt[3]{y^2}\right), \quad y = 5+i\sqrt{10}. \tag{D19}$$

Using these abscissae, one may generate closed-form expressions for the $\mathbf{A}$-matrix and $\mathbf{b}$-vector of Radau methods up to $9th$-order.

In terms of internal stability, none of the six Radau methods is I-stable on all stages nor are any of them internally algebraically stable. Radau IA, IB and IIA are not internally stable on their first stage while Radau IIB is internally unstable on its last stage. All four of these methods are internally algebraically unstable on all stages except for Radau IIA, which is internally L- and algebraically stable on its last stage since it is stiffly accurate.

{s, p, q}	$\{2,3,1\}$	$\{3,5,2\}$	$\{4,7,3\}$	$\{5,9,4\}$	$\{6,11,5\}$	$\{2,3,2\}$	$\{3,5,3\}$	$\{4,7,4\}$	$\{5,9,5\}$	$\{6,11,6\}$
Min.$\mathbf{A}$	-0.250	-0.192	-0.127	-0.088	-0.063	-0.083	-0.066	-0.048	-0.036	-0.030
Max.$\mathbf{A}$	0.417	0.537	0.413	0.331	0.279	0.750	0.512	0.406	0.326	0.276
Min.$\mathbf{b}$	0.250	0.111	0.063	0.040	0.028	0.250	0.111	0.063	0.040	0.028
Max.$\mathbf{b}$	0.750	0.512	0.388	0.312	0.260	0.750	0.512	0.388	0.312	0.260
$\lambda^{\mathbf{M}}_{\text{Min.}}$	0	0	0	0		0	0	0	0	0
$\lambda^{\mathbf{M}}_{\text{Max.}}$	0.125	0.056	0.031	0.020	0.014	0.125	0.056	0.031	0.020	0.014
$\lambda^{\mathbf{M}^{(i)}}_{\text{Min.}}$	-0.282	-0.175	-0.091	-0.051	-0.037	-0.065	-0.056	-0.029	-0.021	-0.015
$\lambda^{\mathbf{M}^{(i)}}_{\text{Max.}}$	0.202	0.097	0.061	0.045	0.030	0.190	0.097	0.051	0.036	0.024
$\lambda^{\mathbf{M}^{(i)}}_{\text{RMS}}$	0.356	0.219	0.141	0.099	0.075	0.237	0.135	0.090	0.066	0.051
$A^{(p+1)}$	$2.45(-2)$	$9.90(-4)$	$3.47(-5)$	$1.16(-6)$	$3.74(-8)$	$2.45(-2)$	$9.90(-4)$	$3.47(-5)$	$1.16(-6)$	$3.74(-8)$
$A^{(p+2)}$	$3.22(-2)$	$1.48(-3)$	$7.01(-5)$	$3.10(-6)$	$1.24(-7)$	$3.47(-2)$	$1.71(-3)$	$7.77(-5)$	$3.28(-6)$	$1.28(-7)$
Min.$A^{(q+1)}_{(\text{int})}$	$5.56(-2)$	$5.04(-3)$	$6.54(-4)$	$7.91(-5)$	$1.05(-5)$	$3.49(-2)$	$2.87(-3)$	$2.47(-4)$	$2.53(-5)$	$2.90(-6)$
Max.$A^{(q+1)}_{(\text{int})}$	$1.67(-1)$	$2.36(-2)$	$4.12(-3)$	$6.27(-4)$	$1.00(-4)$	$3.49(-2)$	$3.91(-3)$	$4.57(-4)$	$6.60(-5)$	$9.69(-6)$
Min.$A^{(q+2)}_{(\text{int})}$	$4.98(-2)$	$8.46(-3)$	$1.17(-3)$	$1.76(-4)$	$2.79(-5)$	$2.45(-2)$	$4.97(-3)$	$5.44(-4)$	$1.46(-4)$	$8.49(-6)$
Max.$A^{(q+2)}_{(\text{int})}$	$1.24(-1)$	$2.54(-2)$	$5.09(-3)$	$1.00(-3)$	$2.00(-4)$	$4.88(-2)$	$5.38(-3)$	$8.74(-4)$	$6.68(-5)$	$2.35(-5)$
$\mathcal{C}$	0.601	0.482	0.423	0.388	0.367	0.167	0.180	0.189	0.199	0.209
C($\mathbf{A}$)	1.50	5.23	10.11	16.51	24.44	4.62	8.69	13.96	20.43	28.16

Table D4: Radau IA (left) and IIA (right) methods.

{s, p, q}	$\{2,3,1\}$	$\{3,5,2\}$	$\{4,7,3\}$	$\{5,9,4\}$	$\{6,11,5\}$	$\{2,3,1\}$	$\{3,5,2\}$	$\{4,7,3\}$	$\{5,9,4\}$	$\{6,11,5\}$
Min.$\mathbf{A}$	-0.125	-0.096	-0.042	-0.044	-0.032	-0.042	-0.045	-0.032	-0.028	-0.023
Max.$\mathbf{A}$	0.375	0.558	0.875	0.340	0.283	0.875	0.608	0.425	0.343	0.289
Min.$\mathbf{b}$	0.250	0.111	0.250	0.040	0.028	0.250	0.111	0.063	0.040	0.028
Max.$\mathbf{b}$	0.750	0.512	0.750	0.312	0.260	0.750	0.512	0.388	0.312	0.260
$\lambda^{\mathbf{M}}_{\text{Min.}}$	0	0	0	0	0	0	0	0	0	0
$\lambda^{\mathbf{M}}_{\text{Max.}}$	0	0	0	0	0	0	0	0	0	0
$\lambda^{\mathbf{M}^{(i)}}_{\text{Min.}}$	-0.119	-0.071	-0.119	-0.020	-0.016	-0.119	-0.071	-0.037	-0.020	-0.016
$\lambda^{\mathbf{M}^{(i)}}_{\text{Max.}}$	0.149	0.072	0.149	0.029	0.020	0.149	0.072	0.043	0.029	0.020
$\lambda^{\mathbf{M}^{(i)}}_{\text{RMS}}$	0.194	0.118	0.195	0.060	0.047	0.194	0.118	0.081	0.060	0.047
$A^{(p+1)}$	$1.46(-2)$	$8.19(-4)$	$1.46(-2)$	$1.04(-6)$	$3.44(-8)$	$1.46(-2)$	$8.19(-4)$	$2.94(-5)$	$1.04(-6)$	$3.44(-8)$
$A^{(p+2)}$	$2.17(-2)$	$1.29(-3)$	$1.71(-2)$	$2.97(-6)$	$1.19(-7)$	$1.71(-2)$	$1.22(-3)$	$6.42(-5)$	$2.94(-6)$	$1.18(-7)$
Min.$A^{(q+1)}_{(\text{int})}$	$8.33(-2)$	$4.41(-3)$	$2.78(-2)$	$3.96(-5)$	$5.26(-6)$	$2.78(-2)$	$2.52(-3)$	$3.27(-4)$	$3.96(-5)$	$5.26(-6)$
Max.$A^{(q+1)}_{(\text{int})}$	$2.78(-2)$	$1.18(-2)$	$8.33(-2)$	$3.14(-4)$	$5.02(-5)$	$8.33(-2)$	$1.18(-2)$	$2.06(-3)$	$3.14(-4)$	$5.02(-5)$
Min.$A^{(q+2)}_{(\text{int})}$	$5.01(-2)$	$7.06(-3)$	$9.88(-3)$	$1.15(-4)$	$1.76(-5)$	$9.88(-3)$	$7.52(-4)$	$1.26(-4)$	$2.56(-5)$	$5.15(-6)$
Max.$A^{(q+2)}_{(\text{int})}$	$3.94(-2)$	$1.21(-2)$	$6.94(-2)$	$4.96(-4)$	$9.92(-5)$	$6.94(-2)$	$1.69(-2)$	$3.18(-3)$	$6.09(-4)$	$1.18(-4)$
$\mathcal{C}$	0.601	0.482	0.423	0.388	0.367	0.167	0.180	0.189	0.199	0.209
C($\mathbf{A}$)	2.72	6.86	11.53	17.86	25.95	10.99	21.89	36.71	56.56	80.58

Table D5: Radau IB (left) and IIB (right) methods.

D.3 Lobatto Methods

Lobatto [127] methods were introduced by Butcher [28] in 1964. As with his Radau I and Radau II methods, his Lobatto III method was also not A-stable. Soon after the introduction of Lobatto III methods, Ehle [82] introduced the A-stable Lobatto IIIA and IIIB methods. In 1971, Chipman [68] introduced Lobatto IIIC methods. Jay [114] remarks that the **A**-matrices of other Lobatto methods may be constructed as linear combinations of **A**-matrices to the original four methods. He writes the **A**-matrix for a general class of Lobatto methods as

$$\mathbf{A} = \alpha_{III}\mathbf{A}_{III} + \alpha_A\mathbf{A}_A + \alpha_B\mathbf{A}_B + \alpha_C\mathbf{A}_C, \qquad \alpha_{III} + \alpha_A + \alpha_B + \alpha_C = 1, \tag{D20}$$

where, it should be remembered that all Lobatto methods share the same **b** and **c** vectors. Nørsett and Wanner [146] introduced what Jay [114] names Lobatto IIINW with

$$\{\alpha_{III}, \alpha_A, \alpha_B, \alpha_C\} = \{-2, +2, +2, -1\}\,. \tag{D21}$$

In 1990, Chan [63] introduced Lobatto IIIS methods where

$$\mathbf{A}^S(\sigma) = (1-\sigma)\left(\mathbf{A}_A + \mathbf{A}_B\right) + \left(\sigma - \frac{1}{2}\right)\left(\mathbf{A}_{III} + \mathbf{A}_C\right). \tag{D22}$$

Chan offers two cases, $\sigma = 1, \frac{1}{2}$. The last Lobatto method we discuss is the Lobatto IIIF method of Wang and Liao [183] which is equivalent to a generalized Lobatto method with

$$\{\alpha_{III}, \alpha_A, \alpha_B, \alpha_C\} = \left\{\frac{s-1}{4s-2}, \frac{2s}{4s-2}, 0, \frac{s-1}{4s-2}\right\}. \tag{D23}$$

For the solution of stiff ODEs, only Lobatto IIIC is L-stable and stiffly accurate. Hence, Radau IIA and Lobatto IIIC methods are likely to be the best suited to the integration of stiff ODEs amongst the 15 FIRK methods discussed in this appendix. Between these two, Radau IIA has higher stage-order.

Abscissae to many of the lower-order the Lobatto methods may be given in closed form. For methods with two to nine stages, the abscissae are

$$\mathbf{c}^{(2)}_{III} = \{0, 1\}\,, \qquad \mathbf{c}^{(3)}_{III} = \left\{0, \frac{1}{2}, 1\right\} \tag{D24}$$

$$\mathbf{c}^{(4)}_{III} = \left\{0, \frac{1}{2} - \sqrt{\frac{1}{20}}, \frac{1}{2} + \sqrt{\frac{1}{20}}, 1\right\}, \qquad \mathbf{c}^{(5)}_{III} = \left\{0, \frac{1}{2} - \sqrt{\frac{3}{28}}, \frac{1}{2}, \frac{1}{2} + \sqrt{\frac{3}{28}}\right\} \tag{D25}$$

while for the six and seven-stage methods, $\mathbf{c}^{(6)}_{III}$ and $\mathbf{c}^{(7)}_{III}$ are given by

$$\left\{0, \frac{1}{2} - \sqrt{\frac{(7+2\sqrt{7})}{84}}, \frac{1}{2} - \sqrt{\frac{(7-2\sqrt{7})}{84}}, \frac{1}{2} + \sqrt{\frac{(7-2\sqrt{7})}{84}}, \frac{1}{2} + \sqrt{\frac{(7+2\sqrt{7})}{84}}, 1\right\} \tag{D26}$$

$$\left\{0, \frac{1}{2} - \sqrt{\frac{(15+2\sqrt{15})}{132}}, \frac{1}{2} - \sqrt{\frac{(15-2\sqrt{15})}{132}}, \frac{1}{2}, \frac{1}{2} + \sqrt{\frac{(15-2\sqrt{15})}{132}}, \frac{1}{2} + \sqrt{\frac{(15+2\sqrt{15})}{132}}, 1\right\} \tag{D27}$$

$$\tag{D28}$$

At eight and nine -stages, methods which are $14th$- and $16th$-order have abscissae given by

$$\begin{aligned}
\mathbf{c}^{(8)}_{III} &= \left\{0, \frac{1}{2} - \sqrt{\Lambda^{(8)}_1}, \frac{1}{2} - \sqrt{\Lambda^{(8)}_2}, \frac{1}{2} - \sqrt{\Lambda^{(8)}_3}, \frac{1}{2} + \sqrt{\Lambda^{(8)}_3}, \frac{1}{2} + \sqrt{\Lambda^{(8)}_2}, \frac{1}{2} + \sqrt{\Lambda^{(8)}_1}, 1\right\} \\
\mathbf{c}^{(9)}_{III} &= \left\{0, \frac{1}{2} - \sqrt{\Lambda^{(9)}_1}, \frac{1}{2} - \sqrt{\Lambda^{(9)}_2}, \frac{1}{2} - \sqrt{\Lambda^{(9)}_3}, \frac{1}{2}, \frac{1}{2} + \sqrt{\Lambda^{(9)}_3}, \frac{1}{2} + \sqrt{\Lambda^{(9)}_2}, \frac{1}{2} + \sqrt{\Lambda^{(9)}_1}, 1\right\}
\end{aligned}$$

Method	Lobatto III	Lobatto IIIA	Lobatto IIIB	Lobatto IIIC	Lobatto IIINW	Lobatto IIIS	Lobatto IIIS	Lobatto IIIF
σ	$-$	$-$	$-$	$-$	$-$	1	1/2	$-$
order	$2s-2$	$2s-2$	$2s-2$	$2s-2$	$2s-2$	$2s-2$	$2s-2$	$2s-2$
$\mathrm{B(p)}, p =$	$2s-2$	$2s-2$	$2s-2$	$2s-2$	$2s-2$	$2s-2$	$2s-2$	$2s-2$
$\mathrm{C}(\eta), \eta =$	$s-1$	s	$s-2$	$s-1$	$s-2$	$s-1$	$s-2$	$s-1$
$\mathrm{D}(\zeta), \zeta =$	$s-1$	$s-2$	s	$s-1$	$s-2$	$s-1$	$s-2$	$s-2$
$\mathrm{I-Stable}$	No	Yes	Yes	Yes	Yes	Yes	Yes	Yes
$\mathrm{A-Stable}$	No	Yes	Yes	Yes	Yes	Yes	Yes	Yes
$\mathrm{L-Stable}$	No	No	No	Yes	Yes	No	No	No
$\mathrm{R}(-\infty)$	∞	$(-1)^s$	$(-1)^{s-1}$	0	0	$(-1)^s$	$(-1)^{s-1}$	$(-1)^s$
$a_{sj} = b_j$	No	Yes	No	Yes	No	No	No	No
$a_{i1} = b_1$	No	No	Yes	Yes	No	No	No	No
$a_{1j} = 0$	No	Yes	No	No	No	No	No	No
$a_{is} = 0$	Yes	No	Yes	No	No	No	No	No
Alg.Stable	Yes	No	No	Yes	Yes	Yes	Yes	No
Symmetric	No	Yes	Yes	No	No	Yes	Yes	Yes
Symplectic	No	No	No	No	No	Yes	Yes	No
$\mathrm{Int.I-Stable}$	No	Yes	No	No	No	No	No	No
Int.Alg.Stable	No	No	No	No	No	No	No	No
$\mathrm{Pade}: e^z$	$(s, s-2)$	$(s-1, s-1)$	$(s-1, s-1)$	$(s-2, s)$	$(s-2, s)$	$(s-1, s-1)$	$(s-1, s-1)$	(s, s)
(α, β)	$(1,1)$	$(1,1)$	$(1,1)$	$(1,1)$	$(1,1)$	$(1,1)$	$(1,1)$	$(1,1)$

Table D6: Characteristics of Lobatto methods.

$\{s, p, q\}$	$\{2,2,1\}$	$\{3,4,2\}$	$\{4,6,3\}$	$\{5,8,4\}$	$\{6,10,5\}$	$\{2,2,2\}$	$\{3,4,3\}$	$\{4,6,4\}$	$\{5,8,5\}$	$\{6,10,6\}$
Min.$\mathbf{A}$	0.000	0.000	-0.011	-0.012	-0.012	0.000	-0.042	-0.034	-0.031	-0.025
Max.$\mathbf{A}$	1.000	1.000	0.603	0.425	0.374	0.500	0.667	0.451	0.377	0.301
Min.$\mathbf{b}$	0.500	0.167	0.083	0.050	0.033	0.500	0.167	0.083	0.050	0.033
Max.$\mathbf{b}$	0.500	0.667	0.417	0.356	0.277	0.500	0.667	0.417	0.356	0.277
$\lambda^{\mathbf{M}}_{\mathrm{Min.}}$	-1.000	-0.167	-0.083	-0.050	-0.033	-0.250	-0.048	-0.024	-0.014	-0.010
$\lambda^{\mathbf{M}}_{\mathrm{Max.}}$	0.000	0.000	0.000	0.000	0.000	0.250	0.048	0.024	0.014	0.010
$\lambda^{\mathbf{M}^{(i)}}_{\mathrm{Min.}}$	-1.000	-0.604	-0.274	-0.151	-0.106	-0.250	-0.048	-0.043	-0.024	-0.018
$\lambda^{\mathbf{M}^{(i)}}_{\mathrm{Max.}}$	0.000	0.104	0.135	0.084	0.051	0.250	0.117	0.057	0.036	0.024
$\lambda^{\mathbf{M}^{(i)}}_{\mathrm{RMS}}$	1.000	0.619	0.327	0.205	0.147	0.354	0.144	0.092	0.065	0.050
$A^{(p+1)}$	$1.86(-1)$	$6.50(-3)$	$2.20(-4)$	$7.24(-6)$	$2.31(-7)$	$1.18(-1)$	$5.71(-3)$	$2.03(-4)$	$6.93(-6)$	$2.25(-7)$
$A^{(p+2)}$	$1.44(-1)$	$7.83(-3)$	$3.79(-4)$	$1.72(-5)$	$6.99(-7)$	$1.77(-1)$	$8.14(-3)$	$3.98(-4)$	$1.73(-5)$	$6.95(-7)$
Min.$A^{(q+1)}_{(\mathrm{int})}$	$5.00(-1)$	$1.47(-2)$	$1.19(-3)$	$1.04(-4)$	$1.09(-5)$	$1.18(-1)$	$9.02(-3)$	$7.07(-4)$	$6.76(-5)$	$7.42(-6)$
Max.$A^{(q+1)}_{(\mathrm{int})}$	$5.00(-1)$	$5.89(-2)$	$9.62(-3)$	$1.41(-3)$	$2.21(-4)$	$1.18(-1)$	$9.02(-3)$	$7.07(-4)$	$1.04(-4)$	$1.36(-5)$
Min.$A^{(q+2)}_{(\mathrm{int})}$	$2.36(-1)$	$1.10(-2)$	$1.03(-3)$	$1.22(-4)$	$1.65(-5)$	$1.77(-1)$	$5.71(-3)$	$1.11(-3)$	$1.29(-4)$	$1.60(-5)$
Max.$A^{(q+2)}_{(\mathrm{int})}$	$2.36(-1)$	$6.75(-2)$	$1.27(-2)$	$2.44(-3)$	$4.73(-4)$	$1.77(-1)$	$1.21(-2)$	$1.39(-3)$	$2.24(-4)$	$3.46(-5)$
$\mathcal{C}$	0.500	0.373	0.336	0.320	0.313	0.500	0.373	0.336	0.320	0.313
C($\mathbf{A}$)	∞	∞	∞	∞	∞	∞	∞	∞	∞	∞

Table D7: Lobatto III (left) and IIIA (right) methods.

where

$$\Lambda_1^{(8)} = \frac{55 + 8\sqrt{55}\cos(\varpi_8)}{572}, \qquad \Lambda_{2,3}^{(8)} = \frac{55 - 4\sqrt{55}\cos(\varpi_8) \pm 4\sqrt{165}\sin(\varpi_8)}{572}, \tag{D29}$$

$$\Lambda_1^{(9)} = \frac{91 + 8\sqrt{91}\cos(\varpi_9)}{780}, \qquad \Lambda_{2,3}^{(9)} = \frac{91 - 4\sqrt{91}\cos(\varpi_9) \pm 4\sqrt{273}\sin(\varpi_9)}{780}, \tag{D30}$$

$$\varpi_8 = \frac{1}{3}\arctan\left(\frac{13}{\sqrt{11}}\right), \qquad \varpi_9 = \frac{1}{3}\arctan\left(15\sqrt{\frac{15}{13}}\right) \tag{D31}$$

One may generate closed-form expressions for the $\mathbf{A}$-matrix and $\mathbf{b}$-vector of Lobatto methods up to $16th$-order. At orders 18 and 20, closed-form expressions for the scheme are still possible but are large and extremely messy. Detailed properties of the eight types of Lobatto methods, having 2-, 3-, 4-, 5- and 6-stages, are given in tables D7, D8, D9 and D10.

Ding and Tan [80] discuss hybrid Radau-Lobatto methods. Effectively, they propose expressing the abscissae to the hybrid method as

$$\mathbf{c} = \beta_I \mathbf{c}_I + \beta_{II}\mathbf{c}_{II} + \beta_{III}\mathbf{c}_{III} \tag{D32}$$

where $\beta_{I,II,III}$ are constants and $\mathbf{c}_{I,II,III}$ are the abscissae to the Radau I, Radau II and Lobatto III family of methods. Revisiting the Radau IIA method, we enforce a stage-order of s, stiff-accuracy, and $c_s = 1$. Hence, we enforce

$$1 = \beta_I + \beta_{II} + \beta_{III}, \qquad \beta_{II} = 1 - \beta_{III}. \tag{D33}$$

Now, β_{III} is a free parameter. In Radau IIA, it is used to enforce algebraic stability with $\beta_{III} = 0$.

Of all eight Lobatto methods considered here (and all Radau and Gauss methods), only Lobatto IIIA is internally I- and A-stable. However, Lobatto IIIC is probably the best choice, among the Lobatto methods, for the integration of stiff ODEs since it is L-stable and stiffly-accurate.

{s, p, q}	{2, 2, 0}	{3, 4, 1}	{4, 6, 2}	{5, 8, 3}	{6, 10, 4}	{2, 2, 1}	{3, 4, 2}	{4, 6, 3}	{5, 8, 4}	{6, 10, 5}
Min.$\mathbf{A}$	0.000	−0.167	−0.135	−0.097	−0.070	−0.500	−0.333	−0.186	−0.117	−0.096
Max.$\mathbf{A}$	0.500	0.833	0.552	0.396	0.313	0.500	0.667	0.428	0.367	0.290
Min.$\mathbf{b}$	0.500	0.167	0.083	0.050	0.033	0.500	0.167	0.083	0.050	0.033
Max.$\mathbf{b}$	0.500	0.667	0.417	0.356	0.277	0.500	0.667	0.417	0.356	0.277
$\lambda^{\mathbf{M}}_{\text{Min.}}$	−0.250	−0.048	−0.024	−0.014	−0.010	0.000	0.000	0.000	0.000	0.000
$\lambda^{\mathbf{M}}_{\text{Max.}}$	0.250	0.048	0.024	0.014	0.010	0.500	0.167	0.083	0.050	0.033
$\lambda^{\mathbf{M}^{(i)}}_{\text{Min.}}$	0.000	−0.143	−0.104	−0.063	−0.038	−0.809	−0.473	−0.207	−0.114	−0.084
$\lambda^{\mathbf{M}^{(i)}}_{\text{Max.}}$	0.250	0.120	0.058	0.041	0.029	0.500	0.208	0.143	0.092	0.057
$\lambda^{\mathbf{M}^{(i)}}_{\text{RMS}}$	0.354	0.241	0.167	0.114	0.082	1.000	0.557	0.307	0.199	0.145
$A^{(p+1)}$	1.86(−1)	4.97(−3)	2.00(−4)	6.79(−6)	2.23(−7)	1.86(−1)	6.50(−3)	2.20(−4)	7.24(−6)	2.31(−7)
$A^{(p+2)}$	1.44(−1)	5.67(−3)	3.33(−4)	1.53(−5)	6.57(−7)	3.23(−1)	1.02(−2)	4.24(−4)	1.80(−5)	7.13(−7)
Min.$A^{(q+1)}_{(\text{int})}$	5.00(−1)	4.17(−2)	5.27(−3)	7.73(−4)	1.09(−4)	1.86(−1)	5.89(−2)	1.19(−3)	1.04(−4)	1.09(−5)
Max.$A^{(q+1)}_{(\text{int})}$	5.00(−1)	8.33(−2)	1.18(−2)	2.06(−3)	3.14(−4)	5.59(−1)	1.47(−2)	9.62(−3)	1.41(−3)	2.21(−4)
Min.$A^{(q+2)}_{(\text{int})}$	5.00(−1)	2.95(−2)	5.66(−3)	1.04(−3)	1.81(−4)	3.23(−1)	7.93(−2)	2.26(−3)	2.48(−4)	3.07(−5)
Max.$A^{(q+2)}_{(\text{int})}$	5.00(−1)	7.51(−2)	1.85(−2)	3.44(−3)	6.55(−4)	4.41(−1)	2.58(−2)	1.38(−2)	2.54(−3)	6.43(−4)
$\mathcal{C}$	0.500	0.373	0.336	0.320	0.313	0.500	0.373	0.336	0.320	0.313
C($\mathbf{A}$)	∞	∞	∞	∞	∞	1.00	5.66	10.20	16.16	23.32

Table D8: Lobatto IIIB (left) and IIIC (right) methods.

{s, p, q}	{2, 2, 1}	{3, 4, 2}	{4, 6, 3}	{5, 8, 4}	{6, 10, 5}	{2, 2, 0}	{3, 4, 1}	{4, 6, 2}	{5, 8, 3}	{6, 10, 4}
Min.$\mathbf{A}$	−0.250	−0.167	−0.093	−0.058	−0.048	0.000	−0.083	−0.067	−0.048	−0.035
Max.$\mathbf{A}$	0.750	0.833	0.510	0.396	0.326	0.500	0.750	0.484	0.387	0.303
Min.$\mathbf{b}$	0.500	0.167	0.083	0.050	0.033	0.000	0.167	0.083	0.050	0.033
Max.$\mathbf{b}$	0.500	0.667	0.417	0.356	0.277	0.500	0.667	0.417	0.356	0.277
$\lambda^{\mathbf{M}}_{\text{Min.}}$	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
$\lambda^{\mathbf{M}}_{\text{Max.}}$	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
$\lambda^{\mathbf{M}^{(i)}}_{\text{Min.}}$	−0.288	−0.188	−0.080	−0.044	−0.035	0.000	−0.066	−0.039	−0.021	−0.012
$\lambda^{\mathbf{M}^{(i)}}_{\text{Max.}}$	0.163	0.132	0.070	0.046	0.029	0.063	0.115	0.048	0.036	0.023
$\lambda^{\mathbf{M}^{(i)}}_{\text{RMS}}$	0.468	0.308	0.179	0.121	0.090	0.088	0.149	0.095	0.068	0.052
$A^{(p+1)}$	1.86(−1)	6.50(−3)	2.20(−4)	7.24(−6)	2.31(−7)	9.32(−2)	1.87(−3)	1.27(−4)	4.99(−6)	1.81(−7)
$A^{(p+2)}$	1.77(−1)	8.43(−3)	3.90(−4)	1.74(−5)	7.02(−7)	4.77(−2)	2.96(−3)	2.35(−4)	1.26(−5)	5.65(−7)
Min.$A^{(q+1)}_{(\text{int})}$	2.50(−1)	0.00	9.62(−4)	0.00	1.09(−5)	2.50(−1)	2.08(−2)	2.64(−3)	3.87(−4)	5.44(−5)
Max.$A^{(q+1)}_{(\text{int})}$	2.50(−1)	2.95(−2)	4.81(−3)	1.98(−4)	1.10(−4)	2.50(−1)	4.17(−2)	5.89(−3)	1.03(−3)	1.57(−4)
Min.$A^{(q+2)}_{(\text{int})}$	1.77(−1)	9.02(−3)	8.66(−4)	1.00(−4)	1.18(−5)	1.12(−1)	1.47(−2)	2.79(−3)	5.13(−4)	9.05(−5)
Max.$A^{(q+2)}_{(\text{int})}$	2.95(−1)	3.61(−2)	6.59(−3)	1.24(−3)	2.39(−4)	1.12(−1)	4.07(−2)	9.43(−3)	1.74(−3)	3.29(−4)
$\mathcal{C}$	0.042	0.373	0.336	0.320	0.313	0.500	0.373	0.336	0.320	0.313
C($\mathbf{A}$)	2.62	7.97	13.19	21.77	32.06	5.83	20.83	35.56	54.11	76.92

Table D9: Lobatto IIIS methods, $\sigma = 1$ (left) and $\sigma = 1/2$ (right).

$\{s, p, q\}$	$\{2,2,0\}$	$\{3,4,1\}$	$\{4,6,2\}$	$\{5,8,3\}$	$\{6,10,4\}$	$\{2,2,1\}$	$\{3,4,2\}$	$\{4,6,3\}$	$\{5,8,4\}$	$\{6,10,5\}$
Min.$\mathbf{A}$	-0.500	-0.167	-0.083	-0.076	-0.061	-0.083	-0.067	-0.042	-0.031	-0.026
Max.$\mathbf{A}$	0.500	0.500	0.686	0.489	0.346	0.583	0.733	0.459	0.386	0.304
Min.$\mathbf{b}$	0.500	0.167	0.083	0.050	0.033	0.500	0.167	0.083	0.050	0.033
Max.$\mathbf{b}$	0.500	0.667	0.417	0.356	0.277	0.500	0.667	0.417	0.356	0.277
$\lambda^{\mathbf{M}}_{\text{Min.}}$	0.000	0.000	0.000	0.000	0.000	-0.167	-0.029	-0.014	-0.008	-0.005
$\lambda^{\mathbf{M}}_{\text{Max.}}$	0.500	0.167	0.083	0.050	0.033	0.167	0.029	0.014	0.008	0.005
$\lambda^{\mathbf{M}^{(i)}}_{\text{Min.}}$	-0.809	-0.174	-0.257	-0.139	-0.090	-0.249	-0.087	-0.040	-0.024	-0.018
$\lambda^{\mathbf{M}^{(i)}}_{\text{Max.}}$	0.500	0.235	0.121	0.102	0.079	0.179	0.120	0.055	0.037	0.024
$\lambda^{\mathbf{M}^{(i)}}_{\text{RMS}}$	1.000	0.383	0.342	0.220	0.160	0.323	0.171	0.106	0.076	0.059
$A^{(p+1)}$	$3.44(-1)$	$1.33(-2)$	$4.54(-4)$	$1.43(-5)$	$4.19(-7)$	$8.33(-2)$	$4.98(-3)$	$1.78(-4)$	$6.34(-6)$	$2.09(-7)$
$A^{(p+2)}$	$3.23(-1)$	$1.56(-2)$	$6.07(-4)$	$2.33(-5)$	$8.46(-7)$	$1.02(-1)$	$6.71(-3)$	$3.50(-4)$	$1.62(-5)$	$6.60(-7)$
Min.$A^{(q+1)}_{(\text{int})}$	1.00	$8.33(-2)$	$1.05(-2)$	$1.55(-3)$	$2.17(-4)$	$8.33(-2)$	0.00	$4.12(-4)$	0.00	$4.96(-6)$
Max.$A^{(q+1)}_{(\text{int})}$	1.00	$1.67(-1)$	$2.36(-2)$	$4.12(-3)$	$6.27(-4)$	$8.33(-2)$	$1.18(-2)$	$2.06(-3)$	$3.14(-4)$	$5.02(-5)$
Min.$A^{(q+2)}_{(\text{int})}$	$5.00(-1)$	$6.07(-2)$	$1.11(-2)$	$1.93(-3)$	$3.43(-4)$	$5.89(-2)$	$8.27(-3)$	$1.87(-4)$	$9.18(-5)$	$3.08(-6)$
Max.$A^{(q+2)}_{(\text{int})}$	$5.00(-1)$	$1.32(-1)$	$2.89(-2)$	$5.65(-3)$	$1.10(-3)$	$5.89(-2)$	$1.44(-2)$	$2.82(-3)$	$5.52(-4)$	$1.08(-4)$
$\mathcal{C}$	0.500	0.373	0.336	0.320	0.313	0.500	0.373	0.336	0.320	0.313
C($\mathbf{A}$)	1.00	3.46	8.69	14.21	24.27	6.17	13.80	21.12	31.13	42.99

Table D10: Lobatto IIINW (left) and IIIF (right) methods.

No Gauss, Radau or Lobatto method of two-stages or more is internally algebraically stable on all stages.

Appendix E

Other High Stage-Order Implicit Runge–Kutta Methods

Besides the classical fully-implicit Runge–Kutta methods of the Gauss, Radau and Lobatto types, certain other implicit Runge–Kutta methods are available which possess high-stage-orders and good stability properties. The methods considered are not comprehensive with regard to high stage-order Runge–Kutta methods.

Among the methods considered are the SIRK methods implemented in the STRIDE code, Diagonally-Extended Singly Implicit (DESI) methods and Multiply-Implicit Runge–Kutta (MIRK) methods.

E.1 STRIDE: SIRK Methods

The STRIDE code [17, 18, 31] was written by John Butcher and Kevin Burrage in the late 1970's. In spite of great effort, we were unable to find a copy of this code. To resolve precisely which design choices were made, we follow the discussion of these methods given in Hairer and Wanner [102]. First, we compute the zeros to the Laguerre polynomials in order to get the abscissae for an s-stage method using Mathematica [186]

```
lg =  Table[0,{s}];
Do[
  ans = Flatten[ NSolve[LaguerreL[s,x]==0,x,110] ];
  Do[ lg[[j]] = Rationalize[ (x /. Part[ans, j]), 10^(-100)]; , {j,1,s}];
,{i,1,s}];
```

where the abscissae are given by $\mathbf{c} = \gamma \times \mathtt{lg}$. Next, we enforce $C(s)$ to get a stage-order of s and $B(s)$ to get a step-order of s. We forsake the embedded method as we have no intention of actually using the methods. The last design choice is the value of γ. Following Hairer and Wanner, $\gamma = 1/\mathtt{lg}_i$. For schemes with an odd number of stages, $i = (s+1)/2$. However, for even s, we should select either $i = s/2$ or $i = s/2 + 1$. We have chosen $i = s/2 + 1$. Though the code offered methods up to 14 stages, where the condition number of the $\mathbf{A}$-matrix is approximately 5×10^{15}, we only include properties for methods up to eight stages where the same condition number is only 9,761,925. Very crudely, the condition number scales as $\mathrm{C}(\mathbf{A}) \sim \exp(2s)$.

Properties for the SIRK methods from the STRIDE code, from three to eight stages is given in Table E1 where the notation follows that from Tables 6 and 7. Methods with three and four stages possess good properties with the exception of the very large values of the abscissae. At five stages and above, the internal algebraic instability grows rapidly with the number of stages.

E.2 DESI Methods

Many authors have considered DESI [34, 37, 45, 67, 77, 78, 163] methods. Below, we evaluate the properties of the DESI methods generated in the thesis [77] of Michail Diamantakis. The properties are given in Table E2 for methods with six through ten stages. At stage-orders of three and four, the DESI methods have very good properties. As with the SIRK methods in the STRIDE code, the abscissae leave the current step at stage-order of five and higher. From the perspective of the present paper, methods DESI3(4)6L(α)[3]SA and DESI4(5)7L(α)[4]SA are consistent with our goals of finding competitors to Radau IIA.

Name	SIRK 3(−)3L(α)[3]	SIRK 4(−)4L(α)[4]	SIRK 5(−)5L(α)[5]	SIRK 6(−)6L(α)[6]	SIRK 7(−)7L(α)[7]	SIRK 8(−)8L(α)[8]
(s, p, q)	$(3, 3, 3)$	$(4, 4, 4)$	$(5, 5, 5)$	$(6, 6, 6)$	$(7, 7, 7)$	$(8, 8, 8)$
γ	0.4359	0.2204	0.2781	0.1732	0.2041	0.1419
$A^{(p+1)}$	$8.971(-2)$	$1.066(-2)$	$1.771(-2)$	$2.268(-3)$	$4.080(-3)$	$5.052(-4)$
$A^{(p+2)}$	$3.012(-1)$	$3.322(-2)$	$1.003(-1)$	$1.129(-2)$	$3.066(-2)$	$3.467(-3)$
Min., Max. $\mathbf{A}$	$-0.0309, 1.931$	$-0.307, 1.50$	$-1.71, 3.20$	$-5.56, 5.97$	$-26.3, 26.1$	$-73.2, 80.8$
Min., Max. $\mathbf{b}$	$-0.0171, 0.574$	$-0.00582, 0.615$	$-0.0121, 0.580$	$-0.00595, 0.535$	$-0.00919, 0.508$	$-0.00539, 0.461$
Max. $\mathbf{c}$	0.181, 2.74	0.0711, 2.07	0.0733, 3.52	0.0386, 2.77	0.0394, 3.96	0.0242, 3.25
No. I − unstable stages	2	3	4	5	7	7
$R(-\infty)$	0	0	0	0	0	0
Min., Max. λ_{M}	$-0.0921, 0.202$	$-0.174, 0.0724$	$-0.127, 0.0830$	$-0.166, 0.0541$	$-0.127, 0.0452$	$-0.157, 0.0708$
Min., Max. $\lambda_{\mathrm{M}_{(\mathrm{int})}}$	$-2.30, 0.432$	$-2.48, 0.767$	$-20.9, 3.78$	$-84.9, 2.53$	$-181, 12.53$	$-16295, 19.6$
$\mathcal{C}$	1.78	1.12	2.81	2.01	3.59	2.77
C($\mathbf{A}$)	31.1	167	1523	22616	438499	9761925

Table E1: SIRK methods from the STRIDE code

Name	DESI 3(4)6L(α)[3]SA	DESI 4(5)7L(α)[4]SA	DESI 5(6)8L(α)[5]SA	DESI 6(7)9L(α)[6]SA	DESI 7(8)10L(α)[7]SA
$(s, p, \hat{p}, q)$	$(6, 3, 4, 3)$	$(7, 4, 5, 4)$	$(8, 5, 6, 5)$	$(9, 6, 7, 6)$	$(10, 7, 8, 7)$
γ	0.12288	0.100861	0.112847	0.121072	0.103474
$A^{(p+1)}$	$1.60(-5)$	$7.85(-4)$	$8.09(-5)$	$2.32(-4)$	$5.86(-5)$
$A^{(p+2)}$	$1.29(-3)$	$1.06(-3)$	$1.73(-4)$	$8.57(-4)$	$2.20(-4)$
$\hat{A}^{(\hat{p}+1)}$	$1.33(-5)$	$4.40(-4)$	$1.49(-4)$	$1.62(-4)$	$2.57(-5)$
$\hat{A}^{(\hat{p}+2)}$	$2.61(-4)$	$7.80(-4)$	$4.11(-4)$	$6.58(-4)$	$1.04(-4)$
Min., Max. $\mathbf{A}$	$(-0.157, 0.544)$	$(-2.21, 2.26)$	$(-0.692, 1.30)$	$(-3.88, 4.18)$	$(-13.3, 13.2)$
Min., Max. $\mathbf{b}$	$(-0.157, 0.407)$	$(-2.21, 2.26)$	$(-0.164, 0.365)$	$(-0.017, 0.355)$	$(-0.168, 0.392)$
Min., Max. $\hat{\mathbf{b}}$	$(0.061, 0.313)$	$(-1.52, 1.74)$	$(-0.111, 0.302)$	$(-0.754, 0.849)$	$(-0.034, 0.258)$
Max. $\mathbf{c}$	1.00	1.00	1.43	1.94	2.01
I − unstable stages	$\{1, 3\}$	$\{1, 3, 4\}$	$\{1, 4, 5\}$	$\{1, 2, 4, 5, 6\}$	$\{1, 2, 4, 5, 6, 7, 10\}$
$\{R(-\infty), \hat{R}(-\infty)\}$	$\{0, 0\}$	$\{0, 0\}$	$\{0, 0\}$	$\{0, 0\}$	$\{0, 0\}$
Min., Max. λ_{M}	$(-0.188, 0.531)$	$(-10.3, 0.083)$	$(-0.180, 0.058)$	$(-0.098, 0.080)$	$(-0.262, 0.0688)$
Min., Max. $\lambda_{\hat{\mathrm{M}}}$	$(-0.041, 0.072)$	$(-5.34, 0.45)$	$(-0.094, 0.035)$	$(-1.58, 0.126)$	$(-0.492, 0.428)$
Min., Max. $\lambda_{\mathrm{M}_{(\mathrm{int})}}$	$(-0.188, 0.053)$	$(-10.3, 0.161)$	$(-3.45, 0.623)$	$(-41.5, 1.23)$	$(-464.5, 3.22)$
$\mathcal{C}$	0.330	0.512	0.880	1.46	1.55
C($\mathbf{A}$)	74.5	1235	1535	22636	438556

Table E2: DESI methods from Diamantakis

Name	MIRK5 5(4)6L[4]SA	MIRK8 8(7)9L[7]SA	MIRK7 7(4)8L[3]SA	SIRK 6(−)6L[5]SA$_{\text{alg}}$
	MIRK5	*MIRK8*	*MIRK7*	*SIRK*
$(s, p, \hat{p}, q)$	$(6, 5, 4, 4)$	$(9, 8, 7, 7)$	$(8, 7, 4, 3)$	$(6, 6, 0, 5)$
$A^{(p+1)}$	1.59(−2)	4.87(−3)	1.15(−4)	1.14(−2)
$A^{(p+2)}$	4.83(−2)	1.86(−2)	2.16(−4)	3.72(−2)
Min., Max. $\mathbf{A}$	$(-9.22, 4.10)$	$(-275, 238)$	$(-0.505, 0.633)$	$(-26.4, 24.5)$
Min., Max. $\mathbf{b}$	$(0, 0.312)$	$(-0.038, 0.268)$	$(0.039, 0.296)$	$(0.0278, 0.260)$
Max. $\mathbf{c}$	1.00	1.00	1.00	1.00
I − unstable stages	$\{1, 2\}$	$\{1, 2, 3, 4\}$	$\{1, 2, 4, 5, 6, 7\}$	$\{1, 2, 3, 4, 5\}$
$R(-\infty)$	0	0	0	0
Min., Max. λ_{M}	$(-2.40, 4.10)$	$(-122, 115)$	$(0, 0.361)$	$(-14.8, 12.4)$
Min., Max. $\lambda_{\text{M}_{(\text{int})}}$	$(-81.4, 100)$	$(-242354, 90060)$	$(-1.13, 0.486)$	$(-2370, 959)$
$\mathcal{C}$	0.357	0.529	0.353	0.209
C($\mathbf{A}$)	608	46885	79.6	1892

Table E3: MIRK (main) methods from Bendtsen

E.3 MIRK Methods

Multiply-implicit Runge–Kutta (MIRK) methods [6, 9–11, 13, 115, 116, 143–145, 149–151] are a slight variation on the SIRK method. Instead of requiring that all eigenvalues of the **A**-matrix to be identical, MIRKs allow for eigenvalue variation. In a series of papers, Claus Bendtsen [9, 10, 12, 13] produced several MIRK methods with high stage-order. However, two are stage-order two methods: a six-stage method from [9] named *MIRK5* (there is a different *MIRK5* in [13]) and a five-stage, B-stable and stiffly accurate SIRK method (having a negative abscissa) from [10]. The properties of these four methods are given in Table E3, excluding the embedded methods. For the four that had a stage-order of at least three, their properties are given in Table E3. They include *MIRK5* [13], *MIRK8* [13], *MIRK7* [9], and *SIRK* [12], in columns 1-4, respectively. The *MIRK8* and *SIRK* schemes have extremely algebraically unstable stages so they are not considered further. Less unstable but certainly not ideal is *MIRK5*. In spite of not being internally I-stable, the stage-order three *MIRK7* has properties most consistent with a Radau IIA competitor.

Appendix F

SIRK Preconditioning Methods

To solve for the s stage-values, for all m equations, at a given time step, we must iteratively solve

$$\mathbf{U}_{i,m} = U_m^{[n]}\mathbf{e}_{i,m} + (\Delta t)\sum_{j=1}^{s}\mathbf{A}_{ij}\mathbf{F}_{j,m}. \tag{F1}$$

To illuminate the mechanics of this iteration, it is instructive to express F1 in matrix form using Kronecker products. Define the stacked variables

$$\mathbf{U}_{st} = \{\mathbf{U}_1^T, \cdots, \mathbf{U}_s^T\}^T \quad ; \quad \mathbf{F}_{st} = \{\mathbf{F}_1^T, \cdots, \mathbf{F}_s^T\}^T \quad ; \quad \mathbf{U}_{st}^{[n]} = \{\mathbf{e}\otimes\mathbf{U}^{[n]T}\}^T \tag{F2}$$

with $\mathbf{U}_i$ the solutions at the intermediate stages, and $\mathbf{F}_i = \mathbf{F}(\mathbf{U}_i)$ the nonlinear function of equation 5 evaluated with $\mathbf{U}_i$ at the intermediate time $t_i = t^n + c_i(\Delta t)$. The dimension of each stacked vector is $s\,m$. With these definitions an equivalent expression for F1 is the Kronecker form

$$\mathbf{U}_{st} \;=\; \mathbf{U}_{st}^{[n]} + (\Delta t)(\mathbf{A}_s\otimes\mathbf{I}_m)\,\mathbf{F}_{st} \tag{F3}$$

Newton's method is now employed to solve the nonlinear system of equation F3. Define the stacked update and residual vectors

$$d\mathbf{U}_{st}^k \;=\; [(d\mathbf{U}_1^k)^T, \cdots, (d\mathbf{U}_s^k)^T]^T \quad ; \quad \mathbf{R}_{st}^k \;=\; -\mathbf{U}_{st}^k + \mathbf{U}_{st}^{[n]} + (\Delta t)(\mathbf{A}_s\otimes\mathbf{I}_m)\,\mathbf{F}_{st}^k \tag{F4}$$

and the block diagonal Jacobian matrix:

$$\mathbf{J}_{\text{diag}}^k \;=\; \frac{\partial\mathbf{F}_i^k}{\partial\mathbf{U}_j^k} \;=\; \text{Diag}[\frac{\partial\mathbf{F}_1^k}{\partial\mathbf{U}_1^k}\cdots\frac{\partial\mathbf{F}_s^k}{\partial\mathbf{U}_s^k}] \;=\; \text{Diag}[\mathbf{J}_1^k\;\cdots\;\mathbf{J}_s^k] \tag{F5}$$

where the superscript "k" in equations (F4) and (F5) signifies that the variables are evaluated after the k^{th} iteration. With these definitions, the Newton iteration takes the form

$$[(\mathbf{I}_s\otimes\mathbf{I}_m) - (\Delta t)(\mathbf{A}_s\otimes\mathbf{I}_m)\mathbf{J}_{\text{diag}}^k]\,d\mathbf{U}_{st}^k \;=\; [\mathbf{M}_{\text{SIRK}}]\,d\mathbf{U}_{st}^k \;=\; -\mathbf{R}_{st}^k \tag{F6}$$

with $\mathbf{M}_{\text{SIRK}}$ the $(s.m, s.m)$ matrix that must be inverted at every Newton iteration (not to be confused with the algebraic stability matrix). Note that $\mathbf{M}_{\text{SIRK}}$ is not in Kronecker product form, a consequence of the fact that although $\mathbf{J}_{\text{diag}}^k$ is block diagonal, the blocks vary at each stage. Thus the powerful numerical techniques available for Kronecker operators are not available to invert $\mathbf{M}_{\text{SIRK}}$.

Equation F6 is typically approximated using a (right-)preconditioned Krylov subspace method: $\mathbf{K}_n\,(\mathbf{M}_{\text{SIRK}}\,\overline{\mathbf{M}}_{\text{SIRK}}^{-1};\mathbf{R}_{st}^k)$ as follows

$$\begin{aligned}[\mathbf{M}_{\text{SIRK}}\,\overline{\mathbf{M}}_{\text{SIRK}}^{-1}]\,\overline{\mathbf{M}}_{\text{SIRK}}\,d\mathbf{U}_{st}^k \;=\; [\mathbf{M}_{\text{SIRK}}\,\overline{\mathbf{M}}_{\text{SIRK}}^{-1}]\,d\mathbf{V}_{st}^k \;&=\; -\mathbf{R}_{st}^k \\ \overline{\mathbf{M}}_{\text{SIRK}}^{-1}\,d\mathbf{V}_{st}^k \;&=\; d\mathbf{U}_{st}^k\end{aligned} \tag{F7}$$

with $\overline{\mathbf{M}}_{\text{SIRK}}$ an easily invertible preconditioner that is approximately spectrally equivalent to the original matrix $\mathbf{M}_{\text{SIRK}}$. The task now is to simplify $\mathbf{M}_{\text{SIRK}}$ without adversely contaminating its eigen-spectrum.

A common strategy for constructing $\overline{\mathbf{M}}_{\text{SIRK}}$ is to approximate $\mathbf{J}^k_{\text{diag}}$ with a Kronecker approximation of the form

$$\mathbf{J}^k_{\text{diag}} \;=\; (\mathbf{I}_s \otimes \overline{\mathbf{J}}) + (\mathbf{J}^k_{\text{diag}} - (\mathbf{I}_s \otimes \overline{\mathbf{J}})) \;=\; (\mathbf{I}_s \otimes \overline{\mathbf{J}}) + \mathbf{E}^k_{\text{diag}} \;\approx\; (\mathbf{I}_s \otimes \overline{\mathbf{J}}) \quad . \tag{F8}$$

The approximate Jacobian $\overline{\mathbf{J}}$ is typically formed at the beginning of the timestep using $\mathbf{U}^{[n]}$ and is held fixed throughout the timestep or even over several timesteps (provided that Δt remains fixed). A further simplification is achieved by manipulating the Runge-Kutta matrix using either a Jordan-decomposition

$$\mathbf{A}_s \;=\; \mathbf{S}_s\, \mathcal{J}_s\, \mathbf{S}_s^{-1} \quad ; \quad \mathcal{J}_s \;=\; \text{Bidiag}[\gamma, 1] \tag{F9}$$

or a Schur-decomposition

$$\mathbf{A}_s \;=\; \mathcal{Q}_s\, \mathcal{U}_s\, \mathcal{Q}_s^T \quad ; \quad \mathcal{Q}_s\, \mathcal{Q}_s^T \;=\; \mathbf{I}_s \tag{F10}$$

Both these decompositions are guaranteed to exist even if $\mathbf{A}_s$ has degenerate eigenvalues with linearly dependent eigenvectors. The Jordan canonical decomposition matrix $\mathcal{J}_s$ is (upper) bi-diagonal with the eigenvalue of $\mathbf{A}_s$ on the main diagonal and "ones" on the superdiagonal (refer to equation 2 and the discussion therein). The condition number of $\mathbf{S}_s$ can be arbitrarily large, which is problematic since $\mathbf{A}_s$ could already be highly ill-conditioned. The Schur-decomposition is a orthogonal transformation (i.e., $\mathcal{Q}_s$ is orthogonal) and $\mathcal{U}_s$ is upper triangular with the eigenvalue of $\mathbf{A}_s$ on the main diagonal. Since $\mathcal{Q}_s$ is orthogonal, the condition numbers of $\mathcal{U}_s$ and $\mathbf{A}_s$ are equivalent.

Substituting the Kronecker approximation (F8) and the Schur factorization of $\mathbf{A}_s$ (F10) into the equation (F6) yields

$$[(\mathbf{I}_s \otimes \mathbf{I}_m) - (\Delta t)(\mathcal{Q}_s\, \mathcal{U}_s\, \mathcal{Q}_s^T \otimes \overline{\mathbf{J}}^k_{\text{diag}}) - (\Delta t)(\mathbf{A}_s \otimes \mathbf{I}_m)\mathbf{E}^k_{\text{diag}}]\, d\mathbf{U}^k_{st} \;=\; -\mathbf{R}^k_{st} \tag{F11}$$

Further manipulating the first two terms yields

$$\Big\{(\mathcal{Q}_s \otimes \mathbf{I}_m)[(\mathbf{I}_s \otimes \mathbf{I}_m) - (\Delta t)(\mathcal{U}_s \otimes \overline{\mathbf{J}}^k)](\mathcal{Q}_s^T \otimes \mathbf{I}_m) - (\Delta t)(\mathbf{A}_s \otimes \mathbf{I}_m)\mathbf{E}^k_{\text{diag}}\Big\}\; d\mathbf{U}^k_{st} \;=\; -\mathbf{R}^k_{st} \tag{F12}$$

With the definitions

$$\begin{aligned} \overline{\mathbf{M}}_{\text{SIRK}} \;&=\; (\mathcal{Q}_s \otimes \mathbf{I}_m)[(\mathbf{I}_s \otimes \mathbf{I}_m) - (\Delta t)(\mathcal{U}_s \otimes \overline{\mathbf{J}}^k)](\mathcal{Q}_s^T \otimes \mathbf{I}_m) \\ \mathbf{E}_{\text{total}} &= -(\Delta t)(\mathbf{A}_s \otimes \mathbf{I}_m)\mathbf{E}^k_{\text{diag}} \end{aligned} \tag{F13}$$

equation (F12) takes the final form $[\overline{\mathbf{M}}_{\text{SIRK}} + \mathbf{E}_{\text{total}}]\; d\mathbf{U}^k_{st} \;=\; -\mathbf{R}^k_{st}$. It is clearly evident that the efficacy of $\overline{\mathbf{M}}_{\text{SIRK}}$ as a preconditioner depends on the rate of evolution of the Jacobian matrix over the "s" stages of the SIRK.

The three-term preconditioner $\overline{\mathbf{M}}_{\text{SIRK}}$ is advantageous for several reasons. The first and third orthogonal Kronecker product operators (e.g., $(\mathcal{Q}_s \otimes \mathbf{I}_m)$), are trivially inverted by premultiplication by their Kronecker transpose. Both operators have unity condition number and do not amplify numerical errors. The inversion of the interior matrix $[(\mathbf{I}_s \otimes \mathbf{I}_m) - (\Delta t)(\mathcal{U}_s \otimes \overline{\mathbf{J}}^k)]$ is also trivial because it is block upper triangular, with identical diagonal blocks. Thus, only one factorization (exact or approximate) of the block diagonal matrix $\mathcal{B}_m \;=\; (\mathbf{I}_m - \gamma \overline{\mathbf{J}}_m(U^{[n]})) \;=\; (LU)$ is necessary. The (LU) factors are then used "s" times, at a combined cost that is significantly less than building and inverting a preconditioner for the original $(s.m, s.m)$ dimensional block system. Note that the $\mathcal{B}_m$ matrix is identical to those used to precondition diagonally implicit schemes (SDIRKs, ESDIRKs). In the context of SDIRKs, a single high-quality Jacobian formed on the first stage, factorized exactly or approximately, compressed and stored, can be used over the entire timestep. It is common to use the compressed preconditioner factors for approximately $10^2 - 10^3$ search directions before they become stale and must be reformed. There is evidence that this will also be the case with SIRKs, which would make them highly competitive with SDIRKs or Radau IIA schemes.

There are several disadvantages that could make SIRKs less competitive compared to SDIRKs or Radau IIA schemes. Unlike SDIRKs, which sequentially visit each stage (with no stage backtracking), an SIRK iteration must simultaneously converge all stages. It is inevitable that the convergence of the combined iteration of "s" stages will be slower than the sum of the "s" sequential solves of an SDIRK. Another disadvantage is the complexity of providing effective stage-value-predictors (SVPs). SDIRKs are equipped with effective SVPs that can reduce the cost by as much as a factor two. An SIRK, however, must build its SVP from previous timestep information, which requires a lengthy forward extrapolation of a stiff temporal polynomial. This extrapolation is known to be highly ill-conditioned for the stiff solution components and is much less accurate than the local updates available with SDIRKs. Finally, the stage preconditioning operator in an SIRK is sequential in nature. Each of the "s" linear systems must wait until the previous stage is preconditioned before an updated R.H.S. can be constructed (this is equivalent to the sequential nature of SDIRKs). There are iterative strategies, that can expose additional parallelism.