Interpolation and Error Control Schemes for Algebraic Differential Equations Using Continuous Implicit Runge-Kutta Methods

by

Hung Nguyen

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Graduate Department of Computer Science
University of Toronto

Abstract

It is well known in the literature that standard implicit Runge-Kutta methods applied to algebraic differential equations exhibit order reduction in both differential and algebraic components. As a result, interpolation and error control schemes are also affected, especially for higher index problems. This thesis presents alternative interpolation and error control schemes based on the defects and the algebraic residuals of a corresponding perturbed equation for particular classes of semi explicit index 1, index 2 and index 3 problems.

Due to its explicit nature, the proposed scheme can be implemented efficiently and at the same time yields results comparable with those from the literature. At each level of this "bootstrapping" procedure, the differential interpolants and algebraic interpolants can be constructed separately using explicit evaluations of the interpolants constructed from the previous level.

As in the case with any continuous approximation, the perturbed equation corresponding to these interpolation schemes can be converted to an equivalent underlying initial value problem which is independent of the algebraic component. This allows one to apply established results in the literature to a defect-based error control scheme for the differential component. The same idea can be applied to derive an error control scheme for the algebraic component.

Based on the above ideas, we develop the three schemes – namely, Scheme 1, Scheme 2 and Scheme 3 – corresponding to semi explicit algebraic differential equations of index 1, index 2 and index 3 respectively. For each of these schemes, we also derive a corresponding error control scheme based on the defect and algebraic residual of an underlying perturbed initial value problem.

The test problems we use to illustrate our approach are the classical pendulum problem, the seven body problem and the driven cavity problem. While the driven cavity problem is of index 2, the other problems are of index 3 or index 3 reformulated as index 2 problems. These problems arise from two important classes of application: constrained mechanical systems and fluid dynamics.

The three implicit continuous Runge-Kutta formulas used as examples in our investigation are SDIRK(2), Gauss(2) and Gauss(3).

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Chapter 1

Motivation

1.1 Semi explicit form

An algebraic differential equation (ADE) – as its name implies – consists of ordinary differential equations coupled with algebraic constraints of the form,

$$\begin{aligned} y'(t) &= f(y(t), z(t)), \text{ where } f : R^{N_y} \times R^{N_z} \to R^{N_y}, \\ 0 &= g(y(t), z(t)), \text{ where } g : R^{N_y} \times R^{N_z} \to R^{N_z}, \end{aligned} \tag{1.1}$$

where the differential component $y(t)$ and the algebraic component $z(t)$ also satisfy the initial condition, [1]

$$\begin{aligned} (y(t_0), z(t_0))^T &= (y_0, z_0)^T, \\ 0 &= g(y_0, z_0). \end{aligned}$$

The above ADE – cast in autonomous semi explicit form – can also be derived from a fully implicit form $F(y(t), y'(t)) = 0$ with $F_{y'}$ being singular [21]. However, it is the semi explicit form that arises in most applications and will be the focus for this study.

1.2 Index

An ADE is usually classified according to its index, which – for our purpose – is defined as the number of times one needs to differentiate the constraint in order to obtain an explicit expression for $z'(t)$ [22]. This process of differentiation of the original constraint serves various purposes:

[1] Consistent initial values will be described subsequently.

- To convert an ADE to a standard initial value problem (IVP), hence allowing one to utilize extensive results and numerical methods already established in the literature.
- To obtain equivalent lower index formulations of higher index ADEs (higher index problems are generally more difficult to solve).
- To incorporate lower index information in the algorithm for solving higher index problems, which can alleviate some difficulties and improve the order of convergence.

It follows that the standard IVP,

$$y'(t) = f(y(t)),$$

is of index 0, while the semi explicit ADE,

$$\begin{aligned} y'(t) &= f(y(t), z(t)), \\ 0 &= g(y(t), z(t)), \end{aligned} \tag{1.2}$$

with nonsingular g_z is of index 1 and,

$$y'(t) = f(y(t), z(t)), \tag{1.3}$$

$$0 = g(y(t)), \tag{1.4}$$

with nonsingular $g_y f_z$ is an index 2 problem. Finally, the semi explicit ADE,

$$y'(t) = f(y(t), z(t)), \tag{1.5}$$

$$z'(t) = k(y(t), z(t), \lambda(t)), \tag{1.6}$$

$$0 = g(y(t)), \tag{1.7}$$

with nonsingular $g_y f_z k_\lambda$ is of index 3. Here, the differential component is $(y(t), z(t))^T$ and the algebraic component is $\lambda(t)$. Linear ADEs with index higher than 3 are studied in [8, pp. 22–29]. However, we shall restrict our focus to semi explicit systems with index 3 or less and will develop and analyze a class of numerical methods for these problems.

1.3 The local problem and consitent initial values

Mathematically, the initial values of an ADE should satisfy all lower index constraints derived by differentiating the original constraint. Thus the index 1 constraint of the index 2 problem (1.3), (1.4) is,

$$0 = g_y f(y(t), z(t)), \tag{1.8}$$

while the lower index constraints of the index 3 problem (1.5)–(1-7) are,

$$\begin{aligned} 0 &= g3(y(t)) \equiv g(y(t)), \\ 0 &= g2(y(t), z(t)) \equiv (g_y f)(y(t), z(t)), \qquad (1.9) \\ 0 &= g1(y(t), z(t), \lambda(t)) \equiv (g_{yy}(f, f) + g_y f_y f + g_y f_z k)\,(y(t), z(t), \lambda(t)), \qquad (1.10) \end{aligned}$$

which are of index 3, index 2 and index 1 respectively. For numerical schemes, this condition for initial values is required at step n of the associated local problem. This requirement can be enforced by projecting the solution onto the lower index constraint manifolds at each step.

1.4 Lower index formulations

The reformulated ADE (1.3), (1.8) is of index 1, similarly the reformulated ADE (1.5), (1.6), (1.9) is of index 2 while the ADE (1.5), (1.6), (1.10) is of index 1. It is well-known that index 1 and index 2 problems can often be solved effectively. By constrast, numerical schemes for index 3 ADEs are still being under investigation. It is therefore generally desirable to solve an equivalent index 2 or index 1 formulation of an original index 3 problem. A prominent example is the stabilized GGL formulation of constrained mechanical systems (CMSs) which will be discussed in various parts of this document.

1.5 Applications

Two important application areas where ADEs arise are fluid dynamics [25, pp. 27–79] and constrained mechanical systems [15]. The governing equation in fluid dynamics is the Navier-Stokes equation in the velocity (differential) and the pressure (algebraic). In this thesis, we consider a representative problem from fluid dynamics (the driven cavity problem [36]) by discretizing the conservative form of the NS equation using the staggered grid method [31] to obtain an index 2 ADE of the form,

$$\begin{aligned} M\dot{u}(t) + [K + N(u(t))]u(t) - Cp(t) &= f(t), \\ 0 &= C^T u(t), \end{aligned}$$

where M is the mass matrix, K is the viscous stress matrix, $N(u(t))$ is the advection matrix, C is the pressure gradient matrix and C^T the divergence matrix.

CMSs, on the other hand, are index 3 ADEs in the position $q(t)$, the velocity $u(t)$ and the

Lagrange multiplier $\lambda(t)$,

$$\begin{aligned} q'(t) &= u(t), \\ M(q(t))u'(t) &= f(q(t),u(t)) - G^T(q(t))\lambda(t), \\ 0 &= g(q(t)), \end{aligned} \tag{1.11}$$

where $G(q) = \frac{\partial g}{\partial q}$. We choose the classical pendulum problem and the seven body problem [40] as our representative test problems. In addition to the index 2 formulation of the original index 3 ADE, we also study the index 2 stabilized/GGL formulation [23],

$$\begin{aligned} q'(t) &= u(t) + G^T(q(t))\rho(t), \\ M(q(t))u'(t) &= f(q(t),u(t)) - G^T(q(t))\lambda(t), \\ 0 &= g(q(t)), \\ 0 &= G(q(t))u(t), \end{aligned} \tag{1.12}$$

which is derived by introducing another algebraic component $\rho(t)$. However, note that all formulations are linear in the algebraic component, thus allowing one to more easily derive higher order numerical methods than would be the case for the general semi explicit index 3 problems [30].

Among other applications where ADEs arise, we can cite electrical networks [32], trajectory prescribed path control [9] and semiconductor device simulation [3].

1.6 Numerical methods

As with the case for standard ordinary differential equations (ODEs), numerical methods for solving ADEs are usually based on either multistep or one-step methods. Numerical software using the former approach include LSODI [29] and DASSL [38] which employ implicit backward differentiation formulas (BDFs). Numerical software using the latter approach generally are based on implicit Runge-Kutta (RK) formulas. It is this class of methods that we will study in detail in this thesis.

Other methods include extrapolation methods [14], [33], projected implicit RK methods [2], half-explicit RK methods [7], [35] and least squares methods [5].

1.7 Runge-Kutta formulas

Consider the generic ADE (1.1) and let $(y_n(t), z_n(t))^T$ be the local solution of the associated local problem at step n which is also written as,

$$\begin{aligned} y_n'(t) &= f(y_n(t), z_n(t)), \quad t_{n-1} \le t \le t_n, \\ 0 &= g(y_n(t), z_n(t)). \end{aligned}$$

with initial values,

$$\begin{aligned} (y_n(t_{n-1}), z_n(t_{n-1}))^T &= (y_{n-1}, z_{n-1})^T, \\ 0 &= g(y_{n-1}, z_{n-1}). \end{aligned}$$

The standard implicit Runge-Kutta formulas for this local problem [39] determines the stage derivatives $k_i, l_i,\ i = 1, \ldots, s$,

$$\begin{aligned} k_i &= f(Y_i, Z_i), \\ 0 &= g(Y_i, Z_i), \end{aligned}$$

where,

$$\begin{aligned} Y_i &= y_{n-1} + h \sum_{j=1}^{s} a_{ij} k_j, \\ Z_i &= z_{n-1} + h \sum_{j=1}^{s} a_{ij} l_j, \end{aligned}$$

are the internal stage values. As usual, s denotes the number of stages, h the current step size and a_{ij}, b_i, c_i (for non-autonomous systems), $i, j = 1, \ldots, s$, denotes the formula coefficients. Then the solution at t_n is advanced using,

$$\begin{aligned} y_n &= y_{n-1} + h \sum_{i=1}^{s} b_i k_i, \\ z_n &= z_{n-1} + h \sum_{i=1}^{s} b_i l_i. \end{aligned}$$

We will consider in this investigation several popular implicit RK formulas. One formula is the 3 stage 5th order RadauIIA. This formula is used in the RADAU5 package [28, pp. 128–138, 547–555] for solving general ADEs (and stiff problems) of the form $My' = f(t, y(t), z(t))$ with M being a constant matrix (singular or nonsingular). This method will be used as a "benchmark" or "reference" method in our investigation. Its Butcher tableau is given in Table 1.1.

The three implicit RK formulas investigated in detail in this study are SDIRK(2), Gauss(2) and Gauss(3) [34]. They belong to two classes of s-stage formulas: SDIRK(s) and Gauss(s). SDIRK(s), with its lower triangular Butcher tableau (diagonally implicit), is A-stable and of global order $s+1$ for $s \leq 3$ [1]. For diagonally implicit formulas, the associated nonlinear system which must be solved on each step can be decomposed naturally into s uncoupled systems of size N. Table 1.2 displays the corresponding Butcher tableau for $s = 2$.

On the other hand, Gauss(s) is a fully implicit, A-stable formula of global order $2s$. The two members of this class which we will consider have the corresponding Butcher tableaus displayed in Table 1.3. Although Gauss(s) enjoys optimal order, the resulting system of size Ns can not be decomposed into smaller systems in its original form. (Note that the Hessenberg form of the coefficient matrix can be utilized to yield smaller subsystems of size N [12], at the expense of extra overhead and a more complicated code).

1.8 Convergence results

Table 1.4 displays the order of convergence for the above standard implicit RK formulas.

- Index 1: the derivation of these results can be found in [26] (Table 2.3, p. 18, Theorem 3.1, pp. 25, 26). Observe that the order in the $y-$component is also the classical order for standard IVPs.
- Index 2: the results for RadauIIA can be found in [26] (Table 2.3, p. 18, p. 47). The results for SDIRK are derived in [26] (Table 2.3, p. 18, p. 48). The results for Gauss are derived in [26] (Table 2.3, p. 18, p. 47).
- Index 3: the results for RadauIIA can be found in [30] (Theorem 2.2). To our knowledge, there have been no general results established for SDIRK and Gauss formulas.

Note that the order for the algebraic variables is reduced in all cases for SDIRK and Gauss formulas and, while the order for the differential variables is preserved in index 1 ADEs, it is also reduced for higher index ADEs.

Table 1.5 displays the discrete local order for the same standard implicit RK formulas. The derivation of these results can be found in Chapter 5 of this document, in [26] (Lemma 4.3, pp. 34–35), in [28] (Table 7.1, p. 515) and in [30] (Theorem 4.1).

1.9 Interpolants and continuous approximations

A continuous approximation for IVPs with extra (explicit or implicit) stages $\bar{s}$ can be derived based on the underlying discrete formulas and on constructing an interpolant $u_n(t)$ expressed in terms of the basis weight polynomials $b_i(\tau)$,

$$u_n(t) = y_{n-1} + h \sum_{i=1}^{\bar{s}} b_i(\tau) k_i,$$

where $0 \leq \tau \leq 1$ and $t = t_{n-1} + \tau h$. The continuous approximation $u(t)$ is then defined as the piecewise polynomial determined by the $u_n(t)$ associated with each time step n. Examples of interpolants are the collocation polynomial which is used in RADAU5 which is of order 3. In this document, we use the "bootstrapping" procedure [18] to construct higher order interpolants. Other continuous approaches can be found in [42] and [24].

1.10 Error control

Existing codes for solving ADEs use a pair of RK formulas of order $(p, p-1)$ to estimate the size of the discrete local error at the right end point of the current step. In the class of methods we will develop, we employ a defect-based approach [17] which attempts to control the size of the defect $\delta(t)$ which, for the standard IVP,

$$y'(t) = f(y(t)),$$

and a continuous approximation, $u_n(t)$, is defined by,

$$u_n'(t) \quad = \quad f(u_n(t)) + \delta_n(t), \quad t_{n-1} \leq t \leq t_n, \tag{1.13}$$

for an interpolant $u_n(t)$ on the current step. The perturbed equation (1.13) lends itself to the setting of the theory of Gronwall inequalities [6, pp. 36–47] which also gives insight into the global error in $u(t)$. This in turn leads naturally to an analysis for the order of $u(t)$. We will extend this approach to ADEs.

1.11 The underlying ODE

To extend the notion of the defect to the class of ADEs we are considering, we introduce the algebraic residual $\theta(t)$. For the generic ADE (1.1) and the associated continuous approximation $(u(t), v(t))^T$, we define $\delta(t)$ and $\theta(t)$ by,

$$\begin{aligned} u'(t) &= f(u(t), v(t)) + \delta(t), \\ 0 &= g(u(t), v(t)) + \theta(t). \end{aligned} \tag{1.14}$$

In order to analyse the accuracy of $(u(t), v(t))^T$ satisfying (1.14), we convert this perturbed system to an equivalent underlying ODE. Our analysis of the associated perturbed underlying ODE will show that the resulting global error bounds will involve $\delta(t), \theta(t)$ and $\theta'(t)$, and this helps explain the order reduction phenonema in ADEs and provides the basis for our analysis and the development of appropriate error control stategies.

1.12 Contribution

The main contribution of this thesis is the development and analysis of an experimental continuous numerical method for solving semi explicit ADEs (1.3), (1.4) and (1.5)–(1.7) of index 2 and index

3 respectively. By analyzing three implicit RK formulas SDIRK(2), Gauss(2) and Gauss(3) as our starting point, we have incorporated several standard techniques and strategies which have been thoroughly investigated in the ODE as well as the ADE literature.

We extend the bootstrapping procedure introduced by [18] to contruct a continuous approximation to the solution with uniform order of convergence on the whole interval of interest. At the base level, our interpolation scheme employs a Hermite-Birkhoff type interpolant which uses high order values of the computed solution (y-value) and computed derivative values (f-value) available on each integration step. For each higher level of the bootstrapping procedure, explicit extra stages are introduced to determine a higher order interpolant using f-values available from the previous level. It is these explicit extra stages that distinguish our approach from the implicitly defined collocation polynomial for standard implicit RK formulas. Our interpolation scheme is also distinguished by the arbitrary selection of the extra stages and this choice can be independent of the underlying formula. As a result, the scheme can be applied to any numerical method for solving ADEs such as a projected RK method or a BDF method. In addition, the scheme separates the interpolation process for the differential component from the interpolation for the algebraic component.

We also extend the defect-based error control strategy introduced in [16] and [17] to the case of ADEs. The approach attempts to control the size of the defect associated with a continuous approximation on the interval of the current step by sampling the defect at a chosen point. Thus our approach is distinguished from other approaches which control the discrete local error at the right end point only.

While our interpolation scheme and error control scheme are independent of the underlying formula, they are closely related to each other. Gronwall's Lemma applied to the perturbed IVP (1.13) yields,

$$||u(t) - y(t)|| \leq M_1||u(0) - y(0)|| + M_2|| \int_0^t \delta(s)ds||.$$

Therefore the error in an interpolant is also controled indirectly and uniformly on the current interval. This result can be used to derive a similar error analysis for the continuous ADE methods we have developed.

$$
\begin{array}{c|ccc}
\frac{4-\sqrt{6}}{10} & \frac{88-7\sqrt{6}}{360} & \frac{296-169\sqrt{6}}{1800} & \frac{-2+3\sqrt{6}}{225} \\
\frac{4+\sqrt{6}}{10} & \frac{296+169\sqrt{6}}{1800} & \frac{88+7\sqrt{6}}{360} & \frac{-2-3\sqrt{6}}{225} \\
1 & \frac{16-\sqrt{6}}{36} & \frac{16+\sqrt{6}}{36} & \frac{1}{9} \\
\hline
 & \frac{16-\sqrt{6}}{36} & \frac{16+\sqrt{6}}{36} & \frac{1}{9}
\end{array}
$$

Table 1.1: RadauIIA(3)

$$
\begin{array}{c|cc}
\frac{3+\sqrt{3}}{6} & \frac{3+\sqrt{3}}{6} & 0 \\
\frac{3-\sqrt{3}}{6} & -\frac{\sqrt{3}}{3} & \frac{3+\sqrt{3}}{6} \\
\hline
 & \frac{1}{2} & \frac{1}{2}
\end{array}
$$

Table 1.2: SDIRK(2)

$$
\begin{array}{c|cc}
\frac{3-\sqrt{3}}{6} & \frac{1}{4} & \frac{3-2\sqrt{3}}{12} \\
\frac{3+\sqrt{3}}{6} & \frac{3+2\sqrt{3}}{12} & \frac{1}{4} \\
\hline
 & \frac{1}{2} & \frac{1}{2}
\end{array}
\qquad
\begin{array}{c|ccc}
\frac{5-\sqrt{15}}{10} & \frac{5}{36} & \frac{10-3\sqrt{15}}{45} & \frac{25-6\sqrt{15}}{180} \\
\frac{1}{2} & \frac{10+3\sqrt{15}}{72} & \frac{2}{9} & \frac{10-3\sqrt{15}}{72} \\
\frac{5+\sqrt{15}}{10} & \frac{25+6\sqrt{15}}{180} & \frac{10+3\sqrt{15}}{45} & \frac{5}{36} \\
\hline
 & \frac{5}{18} & \frac{4}{9} & \frac{5}{18}
\end{array}
$$

Table 1.3: Gauss(2), Gauss(3)

		Index 1		Index 2		Index 3		
Formula	stage	y	z	y	z	y	z	λ
Radau IIA	s	$2s-1$	$2s-1$	$2s-1$	s	$2s-2$	s	$s-1$
SDIRK	$s=2$	3	2	2	1			
Gauss	s odd	$2s$	$s+1$	$s+1$	$s-1$			
"	s even	$2s$	s	s	$s-2$			

Table 1.4: Order of discrete global error

		Index 1		Index 2		Index 3		
Formula	stage	y	z	y	z	y	z	λ
Radau IIA	s	$2s$	$s+1$	$2s$	s	$s+2$	$s+1$	s
SDIRK	$s=2$	4	3	2	1			
Gauss	s odd	$2s+1$	$s+1$	$s+1$	s	$s+1$	s	$s-1$
"	s even	$2s+1$	$s+1$	$s+1$	s	$s+1$	s	$s-1$

Table 1.5: Order of discrete local error

Chapter 2

Index 1 ADEs

In this chapter, we explore some aspects of the numerical solution of the semi explicit index 1 ADE (1.2) by applying two standard implicit RK formulas with constant step size to a selected problem. For stiffly accurate RK formulas where the right endpoint of a step is also an abscissa (eg., $c_s = 1$), the order of the discrete solution is equal to that associated with standard IVPs [39] since the formulas are equivalent to formulas for IVPs. However, this is not the case for the three specific implicit RK formulas we are considering. For these formulas, the discrete solution $(y_n, z_n)^T$ will not necessarily satisfy the algebraic constraint. In addition, since the formulas are not equivalent to formulas for IVPs, the order for z is reduced although the order for y is still preserved, as illustrated in Table 1.4. To overcome this deficiency, we apply the projected RK method [2] which projects the standard discrete solution onto the constraint manifold. This is achieved by solving $0 = g(y_n, \hat{z}_n)$ to obtain the improved solution $\hat{z}_n$.

For continuous RK methods, we introduce an analysis based on the application of Gronwall inequalities [6, pp. 36–48] by converting the original ADE and its perturbed equation to its natural underlying IVP counterpart. This approach allows us to apply the results established in the IVP literature. In particular, this theory provides an error bound for any continuous approximation which satisfies a perturbed equation.

This approach, together with a version of the bootstrapping procedure for generating interpolants, constitutes Scheme 1 which is used in one implementation of the RK formulas.

In addition, the error bound derived in this way suggests an error control strategy which is based on controlling the size of the defect associated with the underlying IVP.

2.1 Standard RK method applied to a test problem

Consider the index 1 ADE (1.2). Let $(y_n(t), z_n(t))^T$ be the local solution of the associated local problem which is also written as,

$$y_n'(t) = f(y_n(t), z_n(t)), \quad t_{n-1} \leq t \leq t_n, \tag{2.1}$$

$$0 = g(y_n(t), z_n(t)), \tag{2.2}$$

where consistent initial values are prescribed by,

$$\begin{aligned} (y_n(t_{n-1}), z_n(t_{n-1}))^T &= (y_{n-1}, z_{n-1})^T, \\ 0 &= g(y_{n-1}, z_{n-1}). \end{aligned}$$

A numerical solution for this ADE [39] can be determined by applying a standard implicit Runge-Kutta formula which – at step n – determines the stage derivatives $k_i, l_i,\ i = 1, \ldots, s$,

$$k_i = f(Y_i, Z_i), \tag{2.3}$$

$$0 = g(Y_i, Z_i), \tag{2.4}$$

where,

$$\begin{aligned} Y_i &= y_{n-1} + h \sum_{j=1}^{s} a_{ij} k_j, \\ Z_i &= z_{n-1} + h \sum_{j=1}^{s} a_{ij} l_j, \end{aligned}$$

are the internal stage values. As usual, s denotes the number of stages, h the step size, $(y_{n-1}, z_{n-1})^T$ the initial value at t_{n-1} for the associated local problem and $a_{ij}, b_i, c_i,\ (i, j = 1, \ldots, s)$ denote the formula coefficients. The solution at t_n is advanced using,

$$y_n = y_{n-1} + h \sum_{i=1}^{s} b_i k_i, \tag{2.5}$$

$$z_n = z_{n-1} + h \sum_{i=1}^{s} b_i l_i. \tag{2.6}$$

We consider the following index 1 test problem, [37]

$$\begin{pmatrix} y'(t) \\ 0 \end{pmatrix} = \begin{pmatrix} -1 & 1+t \\ 1 & -1 \end{pmatrix} \begin{pmatrix} y(t) \\ z(t) \end{pmatrix} + \begin{pmatrix} t\cos(t) \\ (1-t)\sin(t) - e^{-t} \end{pmatrix},$$

with initial condition,

$$(y(0), z(0))^T = (1, 0)^T,$$

and with known solution,

$$(y(t), z(t))^T = (e^{-t} + t\sin t, \sin t)^T,$$

and apply the two standard implicit RK formulas SDIRK(2) and Gauss(3) formulas as examples with fixed step size. This scheme allows us to measure the discrete global orders using the known exact solution. Specifically, the observed order for the solution is obtained from the error at t_{end} for successive test results with step sizes decreased by a half. [1] The results are summarized in Table 2.1 below.

	y	z
SDIRK(2)	3	2
Gauss(3)	6	4

Table 2.1: Observed order reduction

Note that the order for z has been dropped by one for the SDIRK(2) formula and by two for the Gauss(3) formula, as predicted in Table 1.4.

2.2 The use of the Implicit Function Theorem

One way to compute z to full order is to avoid using the low order stage derivatives l_i. Based on the Implicit Function Theorem (which states that for equation (2.2) with nonsingular g_z, $z(t)$ can be expressed explicitly in term of $y(t)$ for some function $\hat{G}$), we reformulate (2.1), (2.2) as, [14]

$$y'(t) = f(y(t), \hat{G}(y(t))), \tag{2.7}$$

$$z(t) = \hat{G}(y(t)), \tag{2.8}$$

which leads to – instead of (2.3), (2.4) involving both k_i and l_i – an equation in k_i alone,

$$k_i = f(Y_i, \hat{G}(Y_i)). \tag{2.9}$$

Since (2.7) is just an ODE in $y(t)$, one can solve it by applying (2.9) and (2.5) to obtain y_n with the same order, then use (2.8) to solve for z_n with no loss of order.

[1] Let y_n and $\bar{y}_n$ be the values of the solution computed at t_n for the step sizes h and $h/2$ respectively. Let $\epsilon = |y(t_n) - y_n|$ and $\bar{\epsilon} = |y(t_n) - \bar{y}_n|$ be the global errors associated with y_n and $\bar{y}_n$. Then the observed global error order of y is given by $log_2 \frac{\epsilon}{\bar{\epsilon}}$.

The following global orders have been observed in a fixed stepsize implementation applied to the previously mentioned test problem.

	y	z
SDIRK(2)	3	3
Gauss(3)	6	6

Table 2.2: Observed order for an approach based on using the Implicit Function Theorem

Alternatively, one can differentiate the constraint and rearrange terms to obtain, [14]

$$g_z z' = -g_y f. \tag{2.10}$$

Thus (2.1), (2.10) constitute a linear-implicit ODE in which both y and z are differential variables, and hence y_n and z_n will both have the same order (provided that g_z is nonsingular.)

The following global orders have been observed in a fixed stepsize implementation of this approach applied to the problem. As predicted, that the full order for z_n has been preserved.

	y	z
SDIRK(2)	3	3
Gauss(3)	6	6

Table 2.3: Observed order for an approach based on differentiating the constraint

2.3 The underlying ODE and its perturbed equation

Let $(u(t), v(t))^T$ be a continuous approximation to $(y(t), z(t))^T$. Note that in our approach, $(u(t), v(t))^T$ will correspond to piecewise polynomials associated with the sequence of interpolants $(u_n(t), v_n(t))^T$, $(n = 1, \ldots)$. Let $(\delta(t), \theta(t))^T$ be the corresponding defect and algebraic residual defined by,

$$\begin{aligned} u'(t) &= f(u(t), v(t)) + \delta(t), \\ 0 &= g(u(t), v(t)) + \theta(t). \end{aligned} \tag{2.11}$$

By the Implicit Function Theorem and the assumption that g_z is invertible,

$$\begin{aligned} v(t) &= G(u(t), \theta(t)), \\ z(t) &= G(y(t), 0) \\ &\equiv \hat{G}(y(t)), \end{aligned} \tag{2.12}$$

for some function G. The perturbed equation (2.11) becomes,

$$u'(t) = f(u(t), G(u(t), \theta(t))) + \delta(t).$$

Denote $\phi(t, \tau) = f\left(u(t), G(u(t), \tau\theta(t))\right)$, and consider [28, p. 511],

$$\begin{aligned} u'(t) - f(u(t), G(u(t), 0)) &= f\left(u(t), G(u(t), \theta(t))\right) - f\left(u(t), G(u(t), 0)\right) + \delta(t) \\ &= \phi(t, 1) - \phi(t, 0) + \delta(t) \\ &= \int_0^1 \frac{\partial \phi}{\partial \tau}(t, \tau) d\tau + \delta(t) \\ &= \int_0^1 f_z\left(u(t), G(u(t), \tau\theta(t))\right) G_\theta(u(t), \tau\theta(t))\theta(t) d\tau + \delta(t). \end{aligned}$$

We have an IVP and an associated perturbed IVP satisfied by $y(t)$ and $u(t)$ respectively,

$$\begin{aligned} y'(t) &= f(y(t), G(y(t), 0)), \\ u'(t) &= f(u(t), G(u(t), 0)) + \delta(t) + Q(t)\theta(t), \end{aligned} \tag{2.13}$$

with initial condition $y(t_0) = u(t_0) = y_0$ and,

$$Q(t) = \int_0^1 f_z\left(u(t), G(u(t), \tau\theta(t))\right) G_\theta(u(t), \tau\theta(t)) d\tau.$$

As for the algebraic part, denote $\Phi(t, \tau) = G(u(t), \tau\theta(t))$ and consider,

$$\begin{aligned} v(t) - G(u(t), 0) &= G(u(t), \theta(t)) - G(u(t), 0) \\ &= \Phi(t, 1) - \Phi(t, 0) \end{aligned}$$

$$
\begin{aligned}
&= \int_{t_0}^{t} \frac{\partial \Phi}{\partial \tau}(t,\tau)d\tau \\
&= \int_{t_0}^{t} G_\theta(u(t), \tau\theta(t))\theta(t)d\tau,
\end{aligned}
$$

so that,

$$
\begin{aligned}
z(t) &= G(y(t), 0), \\
v(t) &= G(u(t), 0) + P(t)\theta(t),
\end{aligned} \tag{2.14}
$$

where,

$$
P(t) = \int_{t_0}^{t} G_\theta(u(t), \tau\theta(t))d\tau.
$$

2.4 Global error

By the Variation of Constants formula [27, p. 96] and (2.13), we have,

$$
\begin{aligned}
u(t) - y(t) &= \int_{t_0}^{t} \frac{\partial y}{\partial y_0}(t,s)\left(\delta(s) + Q(s)\theta(s)\right) ds \\
&= \int_{t_0}^{t} S_1(t,s)\delta(s) + S_2(t,s)\theta(s)ds,
\end{aligned} \tag{2.15}
$$

where,

$$
\begin{aligned}
S_1(t,s) &= \frac{\partial y}{\partial y_0}(t,s), \\
S_2(t,s) &= \frac{\partial y}{\partial y_0}(t,s)Q(s).
\end{aligned}
$$

Assume that,

$$
\begin{aligned}
||S_1(t,s)|| &\le M_1, \\
||S_2(t,s)|| &\le M_2,
\end{aligned}
$$

then a bound for the global error in $u(t)$ is,

$$
||u(t) - y(t)|| \le M_1 \int_{t_0}^{t} ||\delta(s)||ds + M_2 \int_{t_0}^{t} ||\theta(s)||ds. \tag{2.16}
$$

In addition, we have,

$$
v(t) - z(t) = G(u(t), \theta(t)) - G(y(t), 0).
$$

Assume that G satisfies a Lipschiptz condition in each of its arguments, then a global error bound for $v(t)$ is,

$$\|v(t)-z(t)\| \quad \leq \quad N_1\|u(t)-y(t)\| + N_2\|\theta(t)\|. \tag{2.17}$$

We now extend the bootstrapping idea introduced in [18] to the case of ADEs and construct a polynomial approximation $u_n(t)$ to $y_n(t)$ using Hermite-Birkhoff interpolation and $v_n(t)$ to $z_n(t)$ using Lagrange interpolation. These collection of polynomials will then define the global approximation $(u(t), v(t))^T$ and therefore from (2.11) $(\delta(t), \theta(t))^T$. Also note that an application of the above analysis to the local problem (2.1), (2.2) yields the local error bounds,

$$\begin{array}{rcl} \|u_n(t)-y_n(t)\| & \leq & M_{n,1}\int_{t_{n-1}}^t \|\delta_n(s)\|ds + M_{n,2}\int_{t_{n-1}}^t \|\theta_n(s)\|ds, \\ \|v_n(t)-z_n(t)\| & \leq & N_{n,1}\|u_n(t)-y_n(t)\| + N_{n,2}\|\theta_n(t)\|. \end{array} \tag{2.18}$$

2.5 Scheme 1

- Apply a discrete formula to obtain $(y_n, z_n)^T$.
- Solve for f^1 and $\hat{z}_n$,

$$\begin{array}{rcl} f^1 & = & f(y_n, \hat{z}_n), \\ 0 & = & g(y_n, \hat{z}_n). \end{array}$$

- Level 0:
  - Construct $u_n^{(0)}(t)$ (cubic) which interpolates,

$$y_{n-1}, f_0, \hat{y}_n, f^1.$$

  - Solve for f_{11} and v_{01},

$$\begin{array}{rcl} f_{11} & = & f(u_n^{(0)}(t_{n-1}+\bar{c}_{11}h), v_{01}), \\ 0 & = & g(u_n^{(0)}(t_{n-1}+\bar{c}_{11}h), v_{01}). \end{array}$$

  - Construct $v_n^{(0)}(t)$ (of degree 2) which interpolates,

$$z_{n-1}, v_{01}, \hat{z}_n.$$

- Level i : for $i = 1, 2, \ldots$ until the maximum order is achieved,

– Construct $u_n^{(i)}(t)$ (of degree $i+3$) which interpolates,

$$y_{n-1}, f_0, f_{ij}\ (j = 1, \ldots, i),\ \hat{y}_n, f^1.$$

– Solve for $f_{i+1,j}$ and v_{ij} $(j = 1, \ldots, i+1)$,

$$\begin{aligned} f_{i+1,j} &= f(u_n^{(i)}(t_{n-1} + \bar{c}_{i+1,j}h), v_{ij}), \\ 0 &= g(u_n^{(i)}(t_{n-1} + \bar{c}_{i+1,j}h), v_{ij}). \end{aligned}$$

– Construct $v_n^{(i)}(t)$ (of degree $i+2$) which interpolates,

$$z_{n-1}, v_{ij}\ (j = 1, \ldots, i+1), \hat{z}_n.$$

Note that this approach applies to any RK formula of local order $p \geq 4$. For formulas of order 4 or less (such as SDIRK(2)) the interpolant is simply $(u_n^{(0)}(t), v_n^{(0)}(t))^T$. Also note that this interpolation scheme requires solving an additional algebraic equation for the value of z for each of the interpolation values required for the definition of the interpolant $v_n^{(i)}(t)$.

In the following sections, we derive the bounds on defects and hence the local orders for the interpolants constructed by Scheme 1. We proceed from the base level 0 and show that the orders at level i increase by 1 from level $i-1$.

2.6 Analysis of level 0

Let $(\delta_n^{(i)}(t), \theta_n^{(i)}(t))^T$ be the defect and algebraic residual at level i, that is,

$$\begin{aligned} u_n'^{(i)}(t) &= f(u_n^{(i)}(t), v_n^{(i)}(t)) + \delta_n^{(i)}(t), \\ 0 &= g(u_n^{(i)}(t), v_n^{(i)}(t)) + \theta_n^{(i)}(t). \end{aligned}$$

It follows from Scheme 1 that $\delta_n^{(i)}(t)$ vanishes at the two end-points (for all i),

$$\delta_n^{(i)}(t_{n-1}) = \delta_n^{(i)}(t_n) = 0.$$

In addition, the algebraic residual $\theta_n^{(i)}(t) = -g(u_n^{(i)}(t), v_n^{(i)}(t))$, also vanishes at the points $t = t_{n-1}, t_{n-1} + \bar{c}_{i+1,j}h$ $(j = 1, \ldots, i+1), t_n$. We express $\theta_n^{(i)}(t)$ in terms of the Lagrange basis polymials,

$$\begin{aligned} \theta_n^{(i)}(t) &= \theta_n^{(i)}(t_{n-1})l_0(\tau) + \sum_{j=1}^{i+1} \theta_n^{(i)}(t_{n-1} + \bar{c}_{i+1,j}h)l_j(\tau) + \theta_n^{(i)}(t_n)l_{i+2}(\tau) + O(h^{i+3}) \\ &= O(h^{i+3}). \end{aligned} \tag{2.19}$$

Let $\psi^{(0)}(t)$ interpolate the exact local solution $y_{n-1}, f_0, y_n(t_n), y'_n(t_n)$. We decompose $\delta_n^{(0)}(t)$ into three parts,

$$
\begin{aligned}
\delta_n^{(0)}(t) &= u_n'^{(0)}(t) - f(u_n^{(0)}(t), v_n^{(0)}(t)) \\
&= u_n'^{(0)}(t) - f(u_n^{(0)}(t), G(u_n^{(0)}(t), \delta_n^{(0)}(t))) \\
&= \left[u_n'^{(0)}(t) - \psi'^{(0)}(t)\right] + \left[\psi'^{(0)}(t) - y_n'(t)\right] \\
&\quad + \left[f(y_n(t), G(y_n(t), 0)) - f(u_n^{(0)}(t), G(u_n^{(0)}(t), \theta_n^{(0)}(t))\right] \\
&= (I) + (II) + (III),
\end{aligned}
$$

where,

- (I) is the data error, which can be expressed in terms of the Lagrange basis polynomials as,

$$
\begin{aligned}
u_n'^{(0)}(t) - \psi'^{(0)}(t) &= 0d_0(\tau) + (f^1 - y_n'(t_n))d_1(\tau) \\
&= O(f^1 - y_n'(t_n)).
\end{aligned}
$$

  Here we assume that the discrete error $f^1 - y_n'(t_n)$ is of sufficiently high order.

- (II) is the interpolation error, which is $O(h^3)$.
- (III) is of order $O(e_{n,y}^{(0)}(t)) + O(\theta_n^{(0)}(t))$.

It follows that for $p+1 \geq 3$,

$$\delta_n^{(0)}(t) = 0(h^3),$$

or,

$$
\begin{aligned}
\int_{t_{n-1}}^{t} \|\delta_n^{(0)}(s)\| ds &\leq \int_{t_{n-1}}^{t_n} \|\delta_n^{(0)}(s)\| ds \\
&= O(h^4).
\end{aligned}
$$

Similarly,

$$\int_{t_{n-1}}^{t} \|\theta_n^{(0)}(s)\| ds \leq O(h^4).$$

From (2.18), (2.19) and the above results, the local errors at level 0 are given by,

$$
\begin{aligned}
\|u_n^{(0)}(t) - y_n(t)\| &\leq O(h^4), \\
\|v_n^{(0)}(t) - z_n(t)\| &\leq O(h^3).
\end{aligned}
$$

2.7 Analysis of levels 1 and higher

Let $(e_{n,y}^{(i)}(t), e_{n,z}^{(i)}(t))^T$ be the local error in $(u_n^{(i)}(t), v_n^{(i)}(t))^T$ at level i. Assume that,

$$(e_{n,y}^{(i-1)}(t), e_{n,z}^{(i-1)}(t))^T = (O(h^{i+3}), O(h^{i+2}))^T,$$

we will show that,

$$(e_{n,y}^{(i)}(t), e_{n,z}^{(i)}(t))^T = (O(h^{i+4}), O(h^{(i+3)}))^T.$$

Let $\psi^{(i)}(t)$ interpolate the exact local solution at,

$$y_{n-1}, f_0, y'(t_{n-1} + \bar{c}_{ij}h)\ (j = 1, \ldots, i), y_n(t_n), y_n'(t_n).$$

In addition, assuming that f satisfies the Lipschitz condition, then from the specification of Scheme 1,

$$\begin{aligned}
&\delta_n^{(i)}(t)\\
&= u_n'^{(i)}(t) - f(u_n^{(i)}(t), v_n^{(i)}(t))\\
&= u_n'^{(i)}(t) - f(u_n^{(i)}(t), G(u_n^{(i)}(t), \theta_n^{(i)}(t)))\\
&= \left[u_n'^{(i)}(t) - \psi'^{(i)}(t)\right] + \left[\psi'^{(i)}(t) - y_n'(t)\right] + \left[f(y_n(t), G(y_n(t), 0)) - f(u_n^{(i)}(t), G(u_n^{(i)}(t), \theta_n^{(i)}(t)))\right]\\
&= (I) + (II) + (III),
\end{aligned}$$

where,

- (I) is the data error, which can be expressed in terms of the Lagrange basis polynomials as,

$$\begin{aligned}
&u_n'^{(i)}(t) - \psi'^{(i)}(t)\\
&= 0d_0(\tau) + \sum_{j=1}^{i} \left[f(u_n^{(i-1)}(t), \hat{G}(u_n^{(i-1)}(t))) - f(y_n(t), \hat{G}(y_n(t)))\right]_{t_{n-1}+\bar{c}_{ij}h} d_j(\tau)\\
&\quad +(f^1 - y_n'(t_n))d_{i+1}(\tau)\\
&= O(e_{n,y}^{(i-1)}(t_{n-1} + \bar{c}_{ij}h)) + O(f^1 - y_n'(t_n))\\
&= O(e_{n,y}^{(i-1)}(t)) + O(f^1 - y_n'(t_n))\\
&= O(h^{i+3}) + O(f^1 - y_n'(t_n)).
\end{aligned}$$

- (II) is the interpolation error, which is $O(h^{i+3})$.
- (III) is of order $O(e_{n,y}^{(i)}(t)) + O(\theta_n^{(i)}(t))$, or of order $O(e_{n,y}^{(i)}(t)) + O(h^{i+3})$.

It follows that,

$$\delta_n^{(i)}(t) = O(h^{i+3}).$$

By (2.18) and (2.19), we have,

$$(e_{n,y}^{(i)}(t), e_{n,z}^{(i)}(t))^T = (O(h^{i+4}), O(h^{i+3}))^T.$$

2.8 Error control scheme

Motivated by (2.13) and (2.14), we present a defect-based error control which attempts to control $(D_n(t), E_n(t))^T$ given by,

$$\begin{pmatrix} D_n(t) \\ E_n(t) \end{pmatrix} = \begin{pmatrix} I & Q_n(t) \\ 0 & P_n(t) \end{pmatrix} \begin{pmatrix} \delta_n(t) \\ \theta_n(t) \end{pmatrix},$$

where,

$$\begin{aligned} Q_n(t) &= \int_0^1 f_z\left(u_n(t), G(u_n(t), \tau\theta_n(t))\right) G_\theta(u_n(t), \tau\theta_n(t)) d\tau, \\ P_n(t) &= \int_0^1 G_\theta(u_n(t), \tau\theta_n(t)) d\tau. \end{aligned}$$

Alternatively, we seek $(\hat{D}_n(t), \hat{E}_n(t))^T$ independent of integrations by expanding the differential part of (2.11) about $G(u_n(t), 0)$ and up to $O(\theta_n^2(t))$,

$$\begin{aligned} y_n'(t) &= f(y_n(t), G(y_n(t), 0)), \\ u_n'(t) &= f(u_n(t), G(u_n(t), 0)) + \delta_n(t) + f_z(u_n(t), G(u_n(t), 0)) G_\theta(u_n(t), 0)\theta_n(t) + O(\theta_n^2(t)). \end{aligned}$$

Similarly for the algebraic part, we expand (2.12) about $G(u_n(t), 0)$ and up to $O(\theta_n^2(t))$,

$$\begin{aligned} z_n(t) &= G(y_n(t), 0), \\ v_n(t) &= G(u_n(t), 0) + G_\theta(u_n(t), 0)\theta_n(t) + O(\theta_n^2(t)), \end{aligned}$$

so that,

$$\begin{pmatrix} \hat{D}_n(t) \\ \hat{E}_n(t) \end{pmatrix} = \begin{pmatrix} I & f_z(u_n(t), G(u_n(t), 0)) G_\theta(u_n(t), 0) \\ 0 & G_\theta(u_n(t), 0) \end{pmatrix} \begin{pmatrix} \delta_n(t) \\ \theta_n(t) \end{pmatrix}.$$

Note that by differentiating the constraint,

$$0 = g(u_n(t), v_n(t)) + \theta_n(t),$$

with respect to θ, we find that $G_\theta(u_n(t), 0)$ satisfies,

$$\begin{aligned} 0 &= g_z(u_n(t), G(u_n(t), \theta_n(t)))G_\theta(u_n(t), \theta_n(t)) + I \\ &= g_z(u_n(t), G(u_n(t), 0))G_\theta(u_n(t), 0) + I + O(\theta_n(t)), \end{aligned}$$

or,

$$0 = g_z(u_n(t), G(u_n(t), 0))G_\theta(u_n(t), 0)\theta_n(t) + \theta_n(t) + O(\theta_n^2(t)),$$

or $\hat{E}_n(t)$ satisfies,

$$0 = g_z(u_n(t), G(u_n(t), 0))\hat{E}_n(t) + \theta_n(t) + O(\theta_n^2(t)).$$

We seek $(\hat{D}_n(t), \hat{E}_n(t))^T$ independent of the partials of G and up to $O(\theta_n^2(t))$,

$$\begin{pmatrix} I & -f_z \\ 0 & g_z \end{pmatrix} \begin{pmatrix} \hat{D}_n(t) \\ \hat{E}_n(t) \end{pmatrix} = \begin{pmatrix} \delta_n(t) \\ -\theta_n(t) \end{pmatrix},$$

where the partials take the arguments $(u_n(t), G(u_n(t), 0))$.

In practice, we approximate $G(u_n(t), 0)$ by $v_n(t) = G(u_n(t), \theta_n(t))$ with an error of $O(E_n(t))$ and seek $(\tilde{D}_n(t), \tilde{E}_n(t))^T$ from the equation,

$$\begin{pmatrix} I & -f_z(u_n(t), v_n(t)) \\ 0 & g_z(u_n(t), v_n(t)) \end{pmatrix} \begin{pmatrix} \tilde{D}_n(t) \\ \tilde{E}_n(t) \end{pmatrix} = \begin{pmatrix} \delta_n(t) \\ -\theta_n(t) \end{pmatrix}.$$

This error control scheme also indirectly controls the global error in $(u(t), v(t))^T$, as derived in (2.16) and (2.17). We expect that the error in $(u(t), v(t))^T$ is $(O(h^p), O(h^{p-1})^T$ if $\delta(t) = O(h^{p-1})$.

2.9 Summary

In summary, we have studied the semi explicit index 1 ADE and a simple test problem. In addition to a standard implicit RK method, the scheme requires solving an algebraic equation at the end of each step in order to preserve the order for the computed algebraic solution.

For this class of problems, we have considered an underlying ODE and its perturbed equation and obtained the error bound for the errors in the interpolants. This approach also allowed us to apply the results for generic interpolants to each level of the bootstrapping procedure.

We have presented a proof for the order of convergence by using an analysis based on induction. With the assumptions that certain partial derivatives are bounded, all related functions satisfy a Lipschiptz condition and the discrete formula is of sufficiently high order, we have derived the optimal order for our interpolant, and hence the optimal order for the computed algebraic residual.

In addition to the cost associated with applying the discrete formula (which can be measured in terms of the number of stages multiplied by the number of Newton's iterations), our interpolation scheme requires i extra explicit stages for each level i.

Chapter 3

Semi explicit index 2 ADEs

In this chapter, we extend our analysis of the preceding chapter to the semi explicit index 2 ADE (1.3),(1.4). Our interpolant for the algebraic component is determined by differentiating the constraint once and applying the Implict Function Theorem.

Since the right endpoint of the step is not an abscissa for the three implicit RK formulas we are considering, the discrete solution, y_n, will not necessarily satisfy the algebraic constraint. Accordingly, we apply the projected RK method [2] which projects the discrete solution onto the constraint manifold. This approach, together with a version of the bootstrapping procedure, constitutes Scheme 2 which is used in one implementation of the RK formulas. In addition, we present a proof [2] that the order of the projected RK method for index 2 ADEs is equal to the classical order for ODEs, and hence there should be no order reduction. Finally, we present an error control based on an underlying perturbed ODE and a feasible mechanism to implement it.

3.1 The underlying ODE and its perturbed equation

Consider the index 2 ADE,

$$\begin{aligned} y'(t) &= f(y(t), z(t)), \\ 0 &= g(y(t)), \end{aligned} \tag{3.1}$$

and let $(u(t), v(t))^T$ be any continuous approximation to $(y(t), z(t))^T$. Let $(\delta(t), \theta(t))^T$ be the associated defect and algebraic residual which are defined by the perturbed equation,

$$\begin{aligned} u'(t) &= f(u(t), v(t)) + \delta(t), \\ 0 &= g(u(t)) + \theta(t). \end{aligned} \tag{3.2}$$

To derive an explicit formula for $v(t)$, we differentiate the constraint,

$$0 \quad = \quad g_y(u(t))\,[f(u(t),v(t))+\delta(t)]+\theta'(t), \tag{3.3}$$

to obtain, by the Implicit Function Theorem and the assumption that $g_y f_z$ is invertible,

$$v(t) = G(u(t),\delta(t),\theta'(t)),$$

for some function G whose arguments $(y(t),0,0)$ yield the exact solution $z(t)$, ie.,

$$\begin{aligned} z(t) &= G(y(t),0,0) \\ &= \hat{G}(y(t)). \end{aligned}$$

The underlying perturbed IVP is then,

$$u'(t) = f(u(t),G(u(t),\delta(t),\theta'(t)))+\delta(t).$$

Denote $\phi(t,\tau) = f(u(t),G(u(t),\tau\delta(t),\tau\theta'(t)))$, and consider [28, p. 511],

$$\begin{aligned} u'(t)-f(u(t),G(u(t),0,0)) &= f(u(t),G(u(t),\delta(t),\theta'(t)))-f(u(t),G(u(t),0,0))+\delta(t) \\ &= \phi(t,1)-\phi(t,0)+\delta(t) \\ &= \int_0^1 \frac{\partial\phi}{\partial\tau}(t,\tau)d\tau+\delta(t) \\ &= \int_0^1 f_z(u(t),G(\cdot))\,(G_\delta(\cdot)\delta(t)+G_{\theta'}(\cdot)\theta'(t))\,d\tau+\delta(t), \end{aligned}$$

where $G(\cdot) = G(u(t),\tau\delta(t),\tau\theta'(t))$.

We have an IVP and an associated perturbed IVP satisfied by $y(t)$ and $u(t)$ respectively,

$$\begin{aligned} y'(t) &= f(y(t),G(y(t),0,0)), \\ u'(t) &= f(u(t),G(u(t),0,0))+Q_1(t)\delta(t)+Q_2(t)\theta'(t), \end{aligned} \tag{3.4}$$

with initial condition $y(t_0) = u(t_0) = y_0$ and where,

$$\begin{aligned} Q_1(t) &= \textstyle\int_0^1 f_z(u(t),G(\cdot))G_\delta(\cdot)d\tau+I, \\ Q_2(t) &= \textstyle\int_0^1 f_z(u(t),G(\cdot))G_{\theta'}(\cdot)d\tau. \end{aligned} \tag{3.5}$$

As for the algebraic part, denote $\Phi(t,\tau) = G(u(t),\tau\delta(t),\tau\theta'(t))$, and consider,

$$v(t)-G(u(t),0,0) \quad = \quad G(u(t),\delta(t),\theta'(t))-G(u(t),0,0)$$

$$
\begin{aligned}
&= \Phi(t,1) - \Phi(t,0) \\
&= \int_{t_0}^{t} \frac{\partial \Phi}{\partial \tau}(t,\tau)d\tau \\
&= \int_{t_0}^{t} G_\delta(u(t),\tau\delta(t),\tau\theta'(t))\delta'(t) + G_{\theta'}(u(t),\tau\delta(t),\tau\theta'(t))\theta'(t)d\tau,
\end{aligned}
$$

so that,

$$
\begin{aligned}
z(t) &= G(y(t),0,0), \\
v(t) &= G(u(t),0,0) + P_1(t)\delta(t) + P_2(t)\theta'(t),
\end{aligned}
$$

where,

$$
\begin{aligned}
P_1(t) &= \textstyle\int_{t_0}^{t} G_\delta(u(t),\tau\delta(t),\tau\theta'(t))d\tau, \\
P_2(t) &= \textstyle\int_{t_0}^{t} G_{\theta'}(u(t),\tau\delta(t),\tau\theta'(t))d\tau.
\end{aligned}
\tag{3.6}
$$

3.2 Global error

By the Variation of Constants formula, [27, p. 96] [1] we have,

$$
u(t) - y(t) = \int_{t_0}^{t} \frac{\partial y}{\partial y_0}(t,s)\left(Q_1(s)\delta(s) + Q_2(s)\theta'(s)\right)ds \tag{3.7}
$$

$$
= \int_{t_0}^{t} S_1(t,s)\delta(s) + S_2(t,s)\theta'(s)ds, \tag{3.8}
$$

where,

$$
\begin{aligned}
S_1(t,s) &= \frac{\partial y}{\partial y_0}(t,s)Q_1(s), \\
S_2(t,s) &= \frac{\partial y}{\partial y_0}(t,s)Q_2(s).
\end{aligned}
$$

Assume that,

$$
\begin{aligned}
\|S_1(t,s)\| &\le M_1, \\
\|S_2(t,s)\| &\le M_2,
\end{aligned}
$$

[1] **Theorem:** *Denote by y and z the solutions of*

$$
\begin{aligned}
y' &= f(t,y), \quad y(t_0) = y_0, \\
z' &= f(t,z) + g(t,z), \quad z(t_0) = y_0,
\end{aligned}
$$

respectively and suppose that $\frac{\partial f}{\partial y}$ exists and is continuous. Then the solutions of the IVP and the "perturbed" equation are connected by

$$
z(t) = y(t) + \int_{t_0}^{t} \frac{\partial y}{\partial y_0}(t,s,z(s))g(s,z(s))ds.
$$

then a bound for the global error in $u(t)$ is given by,

$$\|u(t)-y(t)\| \leq M_1 \int_{t_0}^{t} \|\delta(s)\|ds + M_2 \int_{t_0}^{t} \|\theta'(s)\|ds. \tag{3.9}$$

In addition, the error in $v(t)$ is given by,

$$\begin{aligned} v(t)-z(t) &= G(u(t),\delta(t),\theta'(t)) - G(y(t),0,0) \\ &= [G(u(t),0,0)-G(y(t),0,0)] + [G(u(t),\delta(t),\theta'(t)) - G(u(t),0,\theta'(t))], \\ &\quad + [G(u(t),0,\theta'(t)) - G(u(t),0,0)]. \end{aligned}$$

Assume that G satisfies the Lipschizt condition in each of its arguments, then a bound for the global error in $v(t)$ is given by,

$$\|v(t)-z(t)\| \leq N_1\|u(t)-y(t)\| + N_2\|\delta(t)\| + N_3\|\theta'(t)\|, \tag{3.10}$$

for some constants N_1, N_2 and N_3. As in the previous chapter, observe that a local error bound can be derived in a similar way,

$$\begin{array}{lll} \|u_n(t)-y_n(t)\| & \leq & M_{n,1}\int_{t_{n-1}}^{t} \|\delta_n(s)\|ds + M_{n,2}\int_{t_{n-1}}^{t} \|\theta_n'(s)\|ds, \\ \|v_n(t)-z(t)\| & \leq & N_{n,1}\|u_n(t)-y_n(t)\| + N_{n,2}\|\delta_n(t)\| + N_{n,3}\|\theta_n'(t)\|. \end{array} \tag{3.11}$$

3.3 Scheme 2

We consider the associated local problem and present Scheme 2 which is based on applying the projected RK method to the standard discrete RK value and determining a Hermite-Birkhoff type interpolant iteratively by introducing extra explicit stages corresponding to the nodes $\bar{c}_{i0}=0, \bar{c}_{i1}, \bar{c}_{i2}, \ldots$

- Apply a discrete formula to obtain $(y_n, z_n)^T$.
- Solve for the projected value $\hat{y}_n$,

$$\begin{aligned} \hat{y}_n &= y_n + f_z(\hat{y}_n, z_n)\nu, \\ 0 &= g(\hat{y}_n). \end{aligned}$$

- Solve [2] for f^1 and $\hat{z}_n$,

$$\begin{aligned} f^1 &= f(\hat{y}_n, \hat{z}_n), \\ 0 &= g_y(\hat{y}_n) f^1. \end{aligned}$$

[2] ie., $\hat{z}_n$ satisfies $\hat{z}_n = G(\hat{y}_n, 0, 0)$.

- Level 0:
  - Construct $u_n^{(0)}(t)$ (cubic) which interpolates,

$$y_{n-1}, f_0, \hat{y}_n, f^1.$$

  - Solve for f_{11} and v_{01},

$$\begin{aligned} f_{11} &= f(u_n^{(0)}(t_{n-1} + \bar{c}_{11}h), v_{01}), \\ 0 &= g_y(u_n^{(0)}(t_{n-1} + \bar{c}_{11}h))f_{11}. \end{aligned}$$

  - Construct $v_n^{(0)}(t)$ (of degree 2) which interpolates,

$$z_{n-1}, v_{01}, \hat{z}_n.$$

- Level i : for $i = 1, \ldots,$ until the maximum order is reached:
  - Construct $u_n^{(i)}(t)$ (of degree $i+3$) which interpolates,

$$y_{n-1}, f_0, f_{ij} \ (j = 1, \ldots, i), \hat{y}_n, f^1.$$

  - Solve for $f_{i+1,j}$ and v_{ij} $(j = 1, \ldots, i+1)$,

$$\begin{aligned} f_{i+1,j} &= f(u_n^{(i)}(t_{n-1} + \bar{c}_{i+1,j}h), v_{ij}), \\ 0 &= g_y(u_n^{(i)}(t_{n-1} + \bar{c}_{i+1,j}h))f_{i+1,j}. \end{aligned}$$

  - Construct $v_n^{(i)}(t)$ (of degree $i+2$) which interpolates, [3]

$$z_{n-1}, v_{ij} \ (j = 1, \ldots, i+1), \hat{z}_n.$$

3.4 Analysis of level 0

Since at level i,

$$0 = g_y(u_n^{(i)}(t))f(u_n^{(i)}(t), v_n^{(i)}(t))_{t=t_{n-1}, t_{n-1}+\bar{c}_j h \ (j=1,\ldots,i+1), t_n},$$

[3] ie., $v_n^{(i)}(t_{n-1} + \bar{c}_{i+1,j}h)$ satisfies,

$$0 = (g_y(u_n^{(i)}(t))f(u_n^{(i)}(t), v_n^{(i)}(t)))_{t_{n-1}+\bar{c}_{i+1,j}h}.$$

we have,

$$\begin{aligned} -\theta_n'^{(i)}(t) &= g_y(u_n^{(i)}(t))(f(u_n^{(i)}(t), v_n^{(i)}(t)) + \delta_n^{(i)}(t)) \\ &= O(\delta_n^{(i)}(t)) + O(g_y(u_n^{(i)}(t))f(u_n^{(i)}(t), v_n^{(i)}(t))) \\ &= O(\delta_n^{(i)}(t)) + O(h^{i+3}). \end{aligned} \tag{3.12}$$

Let $\psi^{(0)}(t)$ interpolate the exact local solution $y_{n-1}, f_0, y(t_n), y'(t_n)$. We have,

$$\begin{aligned} \delta_n^{(0)}(t) &= u_n'^{(0)}(t) - f(u_n^{(0)}(t), v_n^{(0)}(t)) \\ &= u_n'^{(0)}(t) - f(u_n^{(0)}(t), G(u_n^{(0)}(t), \delta_n^{(0)}(t), \theta_n'^{(0)}(t))) \\ &= \left[u_n'^{(0)} - \psi'^{(0)}(t)\right] + \left[\psi'^{(0)}(t) - y_n'(t)\right] \\ &\quad + \left[f(y_n(t), G(y_n(t), 0, 0)) - f(u_n^{(0)}(t), G(u_n^{(0)}(t), \delta_n^{(0)}(t), \theta_n'^{(0)}(t)))\right] \\ &= (I) + (II) + (III), \end{aligned}$$

where,

- (I) is the data error, which can be expressed in terms of the Lagrange basis polynomials as,

$$u_n'^{(0)}(t) - \psi'^{(0)}(t) = 0d_0(\tau) + (f^1 - y_n'(t_n))d_1(\tau),$$

  which is assumed to be of sufficiently high order.

- (II) is the interpolation error, which is $O(h^3)$.

- (III) is $O(e_{n,y}^{(0)}(t)) + O(\delta_n^{(0)}(t)) + O(\theta_n'^{(0)}(t))$.

It follows that for $p + 1 \geq 4$,

$$\delta_n^{(0)}(t) = 0(h^3).$$

We have,

$$\begin{aligned} \int_{t_{n-1}}^{t} \|\delta_n^{(0)}(s)\| ds &\leq \int_{t_{n-1}}^{t_n} \|\delta_n^{(0)}(s)\| ds \\ &= O(h^4). \end{aligned}$$

Hence by (3.12),

$$\int_{t_{n-1}}^{t} \theta_n'^{(0)}(s) ds = O(h^4).$$

Combining (3.11) with the above results, we obtain the local error at level 0 as,

$$\begin{aligned} u_n^{(0)}(t) - y_n(t) &= O(h^4), \\ v_n^{(0)}(t) - z_n(t) &= O(h^3). \end{aligned}$$

3.5 Analysis of levels 1 and higher

Denote $(e_{n,y}^{(i)}(t), e_{n,y}^{(i)}(t))^T$ to be the local error in $(u_n^{(i)}(t), v_n^{(i)}(t))^T$ at level i. Assume that,

$$(e_{n,y}^{(i-1)}(t), e_{n,z}^{(i-1)}(t))^T = (O(h^{i+3}), O(h^{i+2}))^T,$$

we will show that,

$$(e_{n,y}^{(i)}(t), e_{n,z}^{(i)}(t))^T = (O(h^{i+4}), O(h^{(i+3)}))^T.$$

Let $\psi^{(i)}(t)$ interpolate the exact local solution at,

$$y_{n-1}, f_0, y'(t_{n-1} + \bar{c}_{ij} h) \ (j = 1, \ldots, i), y(t_n), y'_n(t_n).$$

We have,

$$\begin{aligned}
\delta_n^{(i)}(t) &= u_n'^{(i)}(t) - f(u_n^{(i)}(t), v_n^{(i)}(t)) \\
&= u_n'^{(i)}(t) - f(u_n^{(i)}(t), G(u_n^{(i)}(t), \delta_n^{(i)}(t), \theta_n'^{(i)}(t))) \\
&= \left[u_n'^{(i)}(t) - \psi'^{(i)}(t)\right] + \left[\psi'^{(i)}(t) - y'_n(t)\right] \\
&\quad + \left[f(y_n(t), G(y_n(t)), 0, 0) - f(u_n^{(i)}(t), G(u_n^{(i)}(t), \delta_n^{(i)}(t), \theta_n'^{(i)}(t)))\right] \\
&= (I) + (II) + (III),
\end{aligned}$$

where,

- (I) is the data error, which can be expressed in terms of the Lagrange basis polynomials as,

$$\begin{aligned}
u_n'^{(i)}(t) - \psi'^{(i)}(t) &= 0 d_0(\tau) + \sum_{j=1}^{i} f(u_n^{(i-1)}(t), \hat{G}(u_n^{(i-1)}(t))) - f(y_n(t), \hat{G}(y_n(t)))_{t_{n-1}+\bar{c}_{ij}h} d_j(\tau) \\
&\quad + (f^1 - y'_n(t_n)) d_{i+1}(\tau) \\
&= O(e_{n,y}^{(i-1)}(t_{n-1} + \bar{c}_{ij} h)) + O(f^1 - y'_n(t_n)) \\
&= O(e_{n,y}^{(i-1)}(t)) + O(f^1 - y'_n(t_n)) \\
&= O(h^{(i+3)}) + O(f^1 - y'_n(t_n)).
\end{aligned}$$

- (II) is the interpolation error, which is $O(h^{i+3})$.

- (III) is $O(e_n^{(i)}(t)) + O(\delta_n^{(i)}(t)) + O(\theta_n'^{(i)}(t))$.

It follows that,

$$\delta_n^{(i)}(t) = O(h^{i+3}).$$

By (3.11) and (3.12), the local error is,

$$\begin{aligned} e_{n,y}^{(i)}(t) &= O(h^{i+4}) + hO(\theta_n'^{(i)}(t)), \\ &= O(h^{i+4}), \\ e_{n,z}^{(i)}(t) &= O(h^{i+3}). \end{aligned}$$

3.6 Error control

We describe an error control scheme which attempts to control the underlying defect and residual given by,

$$\begin{pmatrix} D_n(t) \\ E_n(t) \end{pmatrix} = \begin{pmatrix} Q_{n,1}(t) & Q_{n,2}(t) \\ P_{n,1}(t) & P_{n,2}(t) \end{pmatrix} \begin{pmatrix} \delta_n(t) \\ \theta_n'(t) \end{pmatrix},$$

where $Q_{n,1}(t), Q_{n,2}(t), P_{n,1}(t)$ and $P_{n,2}(t)$ possess analogous expressions as those in (3.5) and (3.6). This error control yields,

$$\begin{aligned} u_n(t) - y_n(t) &= O\left(\int_{t_{n-1}}^{t} \frac{\partial y_n}{\partial y_{n-1}}(t,s) D_n(s) ds\right), \\ v_n(t) - z_n(t) &= O(u_n(t) - y_n(t)) + O(E_n(t)), \end{aligned}$$

for the local errors in $(u_n(t), v_n(t))^T$.

Alternatively, we seek $(\hat{D}_n(t), \hat{E}_n(t))^T$ independent of integrations by expanding the differential part about $G(u_n(t), 0, 0)$ and up to $O(\delta_n^2(t)) + O(\delta_n(t)\theta_n'(t)) + O(\theta_n'^2(t))$,

$$\begin{aligned} y_n'(t) &= f(y_n(t), G(y_n(t), 0, 0)), \\ u_n'(t) &= f(u_n(t), G(u_n(t), 0, 0)) + (I + f_z G_\delta)\delta_n(t) + f_z G_{\theta'} \theta_n'(t) \\ &\quad + O(\theta_n^2(t)) + O(\delta_n(t)\theta_n'(t)) + O(\theta_n'^2(t)). \end{aligned}$$

where $f_z = f_z(u_n(t), G(u_n(t), 0, 0))$ and $\frac{\partial G}{\partial \cdot} = \frac{\partial G}{\partial \cdot}(u_n(t), 0, 0)$.

Similarly for the algebraic part,

$$\begin{aligned} z_n(t) &= G(y_n(t), 0, 0), \\ v_n(t) &= G(u_n(t), 0, 0) + G_\delta(u_n(t), 0, 0)\delta_n(t) + G_{\theta'}(u_n(t), 0, 0)\theta_n'(t) \\ &\quad + O(\theta_n^2(t)) + O(\delta_n(t)\theta_n'(t)) + O(\theta_n'^2(t)). \end{aligned}$$

We choose to compute $(\hat{D}_n(t), \hat{E}_n(t))^T$ given by,

$$\begin{pmatrix} \hat{D}_n(t) \\ \hat{E}_n(t) \end{pmatrix} = \begin{pmatrix} I + f_z G_\delta & f_z G_{\theta'} \\ G_\delta & G_{\theta'} \end{pmatrix} \begin{pmatrix} \delta_n(t) \\ \theta'_n(t) \end{pmatrix}.$$

We seek another representation for $(\hat{D}_n(t), \hat{E}_n(t))^T$ which is independent of the partials of G and up to $O(\theta_n^2(t)) + O(\delta_n(t)\theta'_n(t)) + O(\theta_n'^2(t))$. By differentiating the constraint,

$$0 = g_y(u_n(t))\left(f(u_n(t), v_n(t)) + \delta_n(t)\right) + \theta'_n(t),$$

with respect to δ and to θ', we find that $G_\delta(u_n, \delta_n, \theta'_n)$ and $G_{\theta'}(u_n, \delta_n, \theta'_n)$ satisfy,

$$\begin{aligned} 0 &= g_y(u_n)\left[f_z(u_n, v_n)G_\delta(u_n, \delta_n, \theta'_n) + I\right], \\ 0 &= g_y(u_n)f_z(u_n, v_n)G_{\theta'}(u_n, \delta_n, \theta'_n) + I, \end{aligned}$$

and hence,

$$\begin{aligned} 0 &= g_y(u_n)f_z(u_n, v_n)\left[G_\delta(u_n, \delta_n, \theta'_n)\delta_n + G_{\theta'}(u_n, \delta_n, \theta'_n)\theta'_n\right] + g_y(u_n)\delta_n + \theta'_n \\ &= g_y(u_n)f_z(u_n, G(u_n, \delta_n, \theta'_n))\left[G_\delta(u_n, \delta_n, \theta'_n)\delta_n + G_{\theta'}(u_n, \delta_n, \theta'_n)\theta'_n\right] + g_y(u_n)\delta_n + \theta'_n \\ &= g_y(u_n)f_z(u_n, G(u_n, 0, 0))\left[G_\delta(u_n, 0, 0)\delta_n + G_{\theta'}(u_n, 0, 0)\theta'\right] + g_y(u_n)\delta_n + \theta'_n \\ &\quad + O(\delta_n^2) + O(\delta_n\theta'_n) + O(\theta_n'^2) \\ &= g_y(u_n)f_z(u_n, G(u_n, 0, 0))\hat{E}_n(t) + g_y(u_n)\delta_n + \theta'_n + O(\delta_n^2) + O(\delta_n\theta'_n) + O(\theta_n'^2). \end{aligned}$$

It follows that,

$$\begin{aligned} \hat{D}_n(t) &= \delta_n(t) + f_z(u_n(t), G(u_n(t), 0, 0))\hat{E}_n(t), \\ g_y(u_n(t))\hat{D}_n(t) &= g_y(u_n(t))\delta_n(t) + g_y(u_n(t))f_z(u_n(t), G(u_n(t), 0, 0))\hat{E}_n(t) \\ &= -\theta'_n(t) + O(\delta_n^2(t)) + O(\delta_n(t)\theta'_n(t)) + O(\theta_n'^2(t)). \end{aligned}$$

Thus an implicit expression for $(\hat{D}_n(t), \hat{E}_n(t))^T$ is given by,

$$\begin{pmatrix} I & -f_z \\ g_y(u_n(t)) & 0 \end{pmatrix} \begin{pmatrix} \hat{D}_n(t) \\ \hat{E}_n(t) \end{pmatrix} = \begin{pmatrix} \delta_n(t) \\ -\theta'_n(t) \end{pmatrix},$$

where $f_z = f_z(u_n(t), G(u_n(t), 0, 0))$. In practice, we shall approximate $G(u_n(t), 0, 0)$ by $v_n(t)$ with an error of $E_n(t)$ since generally there is no explicit expressions for G. Thus,

$$\begin{pmatrix} I & -f_z(u_n(t), v_n(t)) \\ g_y(u_n(t)) & 0 \end{pmatrix} \begin{pmatrix} \tilde{D}_n(t) \\ \tilde{E}_n(t) \end{pmatrix} = \begin{pmatrix} \delta_n(t) \\ -\theta_n'(t) \end{pmatrix},$$

is the final implicit formula for our error control.

Also note that the above matrix is nonsingular since $g_y f_z$ is nonsingular by the initial assumption.

3.7 Summary

In summary, we have studied the semi index 2 ADE and presented Scheme 2 which is identical to Scheme 1 for index 1 ADEs except for the use of projected discrete RK values. Accordingly, both schemes share the same cost in terms of the number of function evaluations and additional algebraic equations.

We have shown that while $u_n^{(i)}(t)$ retains the full order, the order for $v_n^{(i)}(t)$ may be reduced by one.

For Scheme 2, we expect the optimal order in $u_n^{(i)}(t)$ and one order less in $v_n^{(i)}(t)$. Specifically, we expect that, at level i, the local errors in $(u_n^{(i)}(t), v_n^{(i)}(t))^T$ is

$$\begin{aligned} u_n^{(i)}(t) - y_n(t) &= O(h^{i+4}), \\ v_n^{(i)}(t) - z_n(t) &= O(h^{i+3}). \end{aligned}$$

Chapter 4

Semi explicit index 3 ADEs

In this chapter, we extend the analysis in the preceding two chapters to the semi explicit index 3 ADE (1.5)–(1.7). First, we derive the perturbed equation associated with a continous approximation $(u(t), v(t), w(t))^T$ for the solution $(y(t), z(t), \lambda(t))^T$. Next, we present Scheme 3 and derive a local error bound for the constructed interpolants. Finally, we prescribe an error control scheme for any continuous approximation.

4.1 The perturbed equation

Consider the semi explicit index 3 ADE,

$$\begin{aligned} y'(t) &= f(y(t), z(t)), \\ z'(t) &= k(y(t), z(t), \lambda(t)), \\ 0 &= g(y(t)). \end{aligned} \tag{4.1}$$

where $g_y f_z k_\lambda$ is invertible.

Let $(u(t), v(t), w(t))^T$ be a continuous approximation to $(y(t), z(t), \lambda(t))^T$, and let the associated defects and algebraic residuals $(\delta(t), \mu(t), \theta(t))^T$ be defined by,

$$\begin{aligned} u'(t) &= f(u(t), v(t)) + \delta(t), \\ v'(t) &= k(u(t), v(t), w(t)) + \mu(t), \\ 0 &= g(u(t)) + \theta(t). \end{aligned} \tag{4.2}$$

We differentiate the original constraint to obtain an index 2 contraint,

$$\begin{aligned} 0 &= g_y(u(t))(f(u(t), v(t)) + \delta(t)) + \theta'(t) \\ &= g2(u(t), v(t)) + g_y(u(t))\delta(t) + \theta'(t). \end{aligned} \tag{4.3}$$

We determine an expression for $w(t)$ explicitly by differentiating (4.3) one more time,

$$
\begin{aligned}
0 &= g_{yy}(u(t))(f(u(t),v(t))+\delta(t), f(u(t),v(t))+\delta(t)) \\
&\quad + g_y(u(t))\left[f_y(u(t),v(t))(f(u(t),v(t))+\delta(t)) + f_z(u(t),v(t))(k(u(t),v(t),w(t))+\mu(t)) + \delta'(t)\right] + \theta''(t) \\
&= g1(u(t),v(t),w(t)) + g_{yy}(u(t))(u'(t),u'(t)) - g_{yy}(u(t))(f(u(t),v(t)), f(u(t),v(t))) \\
&\quad + g_y(u(t))\left[f_y(u(t),v(t))\delta(t) + f_z(u(t),v(t))\mu(t) + \delta'(t)\right] + \theta''(t)
\end{aligned} \tag{4.4}
$$

which, by the Implicit Function Theorem and the assumption that $g_y f_z k_\lambda$ is invertible, yields,

$$
\begin{aligned}
w(t) &= G(u(t),v(t),\delta(t),\delta'(t),\mu(t),\theta''(t)), \\
\lambda(t) &= G(y(t),z(t),0,0,0,0) \\
&\equiv \hat{G}(y(t),z(t)),
\end{aligned} \tag{4.5}
$$

for some function G. Denote $\phi(t,\tau) = k(u,v,G(u,v,\tau\delta,\tau\delta',\tau\mu,\tau\theta''))$ and consider the term,

$$
\begin{aligned}
& v'(t) - k(u(t),v(t),G(u(t),v(t),0,0,0,0)) \\
&= k(u(t),v(t),G(u(t),v(t),\delta(t),\delta'(t),\mu(t),\theta''(t))) - k(u(t),v(t),G(u(t),v(t),0,0,0,0)) + \mu(t) \\
&= \phi(t,1) - \phi(t,0) + \mu(t) \\
&= \int_0^1 \frac{\partial \phi}{\partial \tau}(t,\tau)\,d\tau + \mu(t) \\
&= \int_0^1 k_\lambda(u(t),v(t),G(\cdot))\left(G_\delta(\cdot)\delta(t) + G_{\delta'}(\cdot)\delta'(t) + G_\mu(\cdot)\mu(t) + G_{\theta''}(\cdot)\theta''(t)\right)d\tau + \mu(t),
\end{aligned}
$$

where $G(\cdot)$ and its partials are evaluated at $(u(t),v(t),\tau\delta(t),\tau\delta'(t),\tau\mu(t),\tau\theta''(t))$. Thus we obtain an IVP and an associated perturbed IVP satisfied by $(y(t),z(t))^T$ and $(u(t),v(t))^T$ respectively,

$$
\begin{aligned}
\begin{pmatrix} y'(t) \\ z'(t) \end{pmatrix} &= \begin{pmatrix} f(y(t),z(t)) \\ k(y(t),z(t),G(y(t),z(t),0,0,0,0)) \end{pmatrix}, \\
\begin{pmatrix} u'(t) \\ v'(t) \end{pmatrix} &= \begin{pmatrix} f(u(t),v(t)) + \delta(t) \\ k(u(t),v(t),G(u,v,0,0,0,0)) + Q_1(t)\delta(t) + Q_2(t)\delta'(t) + Q_3(t)\mu(t) + Q_4(t)\theta''(t) \end{pmatrix},
\end{aligned} \tag{4.6}
$$

with initial condition $(y(t_0),z(t_0))^T = (u(t_0),v(t_0))^T = (y_0,z_0)^T$ and where,

$$
\begin{aligned}
Q_1(t) &= \textstyle\int_0^1 k_\lambda(u(t),v(t),G(\cdot))G_\delta(\cdot)d\tau, \\
Q_2(t) &= \textstyle\int_0^1 k_\lambda(u(t),v(t),G(\cdot))G_{\delta'}(\cdot)d\tau, \\
Q_3(t) &= \textstyle\int_0^1 k_\lambda(u(t),v(t),G(\cdot))G_\mu d\tau(\cdot) + I, \\
Q_4(t) &= \textstyle\int_0^1 k_\lambda(u(t),v(t),G(\cdot))G_{\theta''}(\cdot)d\tau,
\end{aligned} \tag{4.7}
$$

where $G(\cdot)$ and its partials are evaluated at $(u(t),v(t),\tau\delta(t),\tau\delta'(t),\tau\mu(t),\tau\theta''(t))$.

As for the algebraic part, denote $\Phi(t,\tau) = G(u(t), v(t), \tau\delta(t), \tau\delta'(t), \tau\mu(t), \tau\theta''(t))$, and consider,

$$\begin{aligned}
& w(t) - G(u(t), v(t), 0, 0, 0, 0) \\
&= G(u(t), v(t), \delta(t), \delta'(t), \mu(t), \theta''(t)) - G(u(t), v(t), 0, 0, 0, 0) \\
&= \Phi(t, 1) - \Phi(t, 0) \\
&= \int_{t_0}^{t} \frac{\partial \Phi}{\partial \tau}(t, \tau) d\tau \\
&= \int_{t_0}^{t} G_\delta(\cdot)\delta(t) + G_{\delta'}(\cdot)\delta'(t) + G_\mu(\cdot)\mu(t) + G_{\theta''}(\cdot)\theta''(t) d\tau,
\end{aligned}$$

where the arguments of the partials of G are $(u(t), v(t), \tau\delta(t), \tau\delta'(t), \tau\mu(t), \tau\theta''(t))$. It follows that,

$$\begin{aligned}
\lambda(t) &= G(y(t), z(t), 0, 0, 0, 0), \\
w(t) &= G(u(t), v(t), 0, 0, 0, 0) + P1(t)\delta(t) + P2(t)\delta'(t) + P_3(t)\mu(t) + P4(t)\theta''(t),
\end{aligned}$$

where,

$$\begin{aligned}
P_1(t) &= \textstyle\int_0^1 G_\delta(u(t), v(t), \tau\delta(t), \tau\delta'(t), \tau\mu(t), \tau\theta''(t)) d\tau, \\
P_2(t) &= \textstyle\int_0^1 G_{\delta'}(u(t), v(t), \tau\delta(t), \tau\delta'(t), \tau\mu(t), \tau\theta''(t)) d\tau, \\
P_3(t) &= \textstyle\int_0^1 G_\mu(u(t), v(t), \tau\delta(t), \tau\delta'(t), \tau\mu(t), \tau\theta''(t)) d\tau, \\
P_4(t) &= \textstyle\int_0^1 G_{\theta''}(u(t), v(t), \tau\delta(t), \tau\delta'(t), \tau\mu(t), \tau\theta''(t)) d\tau.
\end{aligned} \tag{4.8}$$

4.2 Global error

Let $(u, v)(t, s, y_0, z_0)$ be the solution at t of the perturbed equation passing through (y_0, z_0) at $s = t_0$. Then the resolvent,

$$R(t, s) \equiv \frac{\partial(u, v)}{\partial(y_0, z_0)}(t, s, y_0, z_0),$$

is the solution of an associated variational equation. By the Variation of Constants formula applied to (4.4), the global error can be expressed as,

$$\begin{aligned}
\begin{pmatrix} u(t) - y(t) \\ v(t) - z(t) \end{pmatrix} &= \textstyle\int_{t_0}^{t} R(t, s) \begin{pmatrix} \delta(s) \\ Q_1(s)\delta(s) + Q_2(s)\delta'(s) + Q_3(s)\mu(s) + Q_4(s)\theta''(s) \end{pmatrix} ds \\
&= \textstyle\int_{t_0}^{t} (S_1(t, s)\delta(s) + S_2(t, s)\delta'(s) + S_3(t, s)\mu(s) + S_4(t, s)\theta''(s)) ds,
\end{aligned} \tag{4.9}$$

where,

$$S_1(t, s) = R(t, s) \begin{pmatrix} I \\ Q_1(s) \end{pmatrix},$$

$$
\begin{aligned}
S_2(t,s) &= R(t,s)\begin{pmatrix} 0 \\ Q_2(s) \end{pmatrix}, \\
S_3(t,s) &= R(t,s)\begin{pmatrix} 0 \\ I+Q_3(s) \end{pmatrix}, \\
S_4(t,s) &= R(t,s)\begin{pmatrix} 0 \\ Q_4(s) \end{pmatrix},
\end{aligned}
$$

Integrations by parts yield [30],

$$
\begin{aligned}
\begin{pmatrix} u(t)-y(t) \\ v(t)-z(t) \end{pmatrix} &= \left[S_2(t,s)\delta(s) - \tfrac{\partial S_4}{\partial s}(t,s)\theta(s) + S_4(t,s)\theta'(s)\right]_{s=t_0}^{s=t} + \textstyle\int_{t_0}^{t}\sigma(t,s)ds \\
&= S_2(t,t)\delta(t) - \tfrac{\partial S_4}{\partial s}(t,t)\theta(t) + S_4(t,t)\theta'(t) + \textstyle\int_{t_0}^{t}\sigma(t,s)ds
\end{aligned}
\tag{4.10}
$$

where,

$$
\begin{aligned}
\sigma(t,s) &= \left(S_1(t,s) - \frac{\partial S_2}{\partial s}(t,s)\right)\delta(s) + S_3(t,s)\mu(s) + \frac{\partial^2 S_4}{\partial s^2}(t,s)\theta(s), \\
\frac{\partial S_4}{\partial s}(t,s) &= \frac{\partial R}{\partial s}(t,s)\begin{pmatrix} 0 \\ Q_4(s) \end{pmatrix} + R(t,s)\begin{pmatrix} 0 \\ Q_4'(s) \end{pmatrix}.
\end{aligned}
$$

Assume that all related functionals are bounded, then the bound for the error in $(u(t),v(t))^T$ are given by,

$$
\begin{aligned}
\|u(t)-y(t)\| &\leq M_1 \textstyle\int_{t_0}^{t}\|\delta(s)\|ds, \\
\|v(t)-z(t)\| &\leq M_2 \textstyle\int_{t_0}^{t}\left(\|\delta(s)\| + \|\delta'(s)\| + \|\mu(s)\| + \|\theta''(s)\|\right)ds.
\end{aligned}
\tag{4.11}
$$

In addition, the error in $w(t)$ is given by,

$$
w(t) - \lambda(t) = G(u(t),v(t),\delta(t),\delta'(t),\mu(t),\theta''(t)) - G(y(t),z(t),0,0,0,0). \tag{4.12}
$$

We also assume that G satisfies the Lipschipz condition in each of its arguments, hence the global error in $w(t)$ is bounded by a sum of multiples of $u(t)-y(t), v(t)-z(t), \delta(t), \delta'(t), \mu(t)$ and $\theta''(t)$. We now extend the bootstrapping idea to the case of ADEs and construct a polynomial approximation $(u_n(t),v_n(t))^T$ to $(y_n(t),z_n(t))^T$ using Hermite-Birkhoff interpolation and $w_n(t)$ to $\lambda_n(t)$ using Lagrange interpolation. These collection of polynomials will then define the global approximation $(u(t),v(t),w(t))^T$ and therefore - by (4.2) - $(\delta(t),\mu(t),\theta(t))^T$. Note that an application of the above analysis to the local problem yields the local error bound corresponding to (4.7) and (4.8),

$$
\begin{aligned}
\|u_n(t) - y_n(t)\| &\leq M_1 \int_{t_{n-1}}^{t} \|\delta_n(s)\| ds, \\
\|v_n(t) - z_n(t)\| &\leq M_2 \int_{t_{n-1}}^{t} \left(\|\delta_n(s)\| + \|\delta_n'(s)\| + \|\mu_n(s)\| + \|\theta''(s)\|\right) ds, \\
\|w_n(t) - \lambda_n(t)\| &\leq N \left(\|u_n(t) - y_n(t)\| + \|v_n(t) - z_n(t)\| + \|\delta_n(t)\| + \|\delta_n'(t)\| + \|\mu_n(t)\| + \|\theta_n''(t)\|\right).
\end{aligned}
\tag{4.13}
$$

4.3 Scheme 3

We consider the associated local problem and present Scheme 3 which is based on applying the projected RK method to the standard RK formula and determining a Hermite-Birkhoff type interpolant iteratively by introducing extra explicit stages $\bar{c}_{ij}$ ($\bar{c}_{0j} = 0$). In the following, $g1$ and $g2$ refer to the index 1 and index 2 constraints as defined in (1.9) and (1.10).

- Apply a discrete formula to obtain $(y_n, z_n, \lambda_n)^T$.
- Solve for the projected value $\hat{y}_n$,

$$
\begin{aligned}
\hat{y}_n &= y_n + k_\lambda(\hat{y}_n, \hat{z}_n, \lambda_n)\nu, \\
0 &= g(\hat{y}_n).
\end{aligned}
$$

- Solve for the projected value $\hat{z}_n$,

$$
\begin{aligned}
\hat{z}_n &= z_n + k_\lambda(\hat{y}_n, \hat{z}_n, \lambda_n)\nu, \\
0 &= g_y(\hat{y}_n) f(\hat{y}_n, \hat{z}_n).
\end{aligned}
$$

- Compute $f^1 = f(\hat{y}_n, \hat{z}_n)$.
- Solve for k^1 anf $\hat{\lambda}_n$,

$$
\begin{aligned}
k^1 &= k(\hat{y}_n, \hat{z}_n, \hat{\lambda}_n), \\
0 &= g_{yy}(\hat{y}_n)(f^1, f^1) + g_y(\hat{y}_n)\left[f_y(\hat{y}_n, \hat{z}_n) f^1 + f_z(\hat{y}_n, \hat{z}_n) k^1\right],
\end{aligned}
$$

  which can be written as,

$$
\begin{aligned}
k^1 &= k(\hat{y}_n, \hat{z}_n, \hat{\lambda}_n), \\
0 &= g1(\hat{y}_n, \hat{z}_n, \hat{\lambda}_n).
\end{aligned}
$$

- Level 0:

– Construct $u_n^{(0)}(t)$ (cubic) which interpolates $y_{n-1}, f_0, \hat{y}_n, f^1$.

– Construct $v_n^{(0)}(t)$ (cubic) which interpolates $z_{n-1}, k_0, \hat{z}_n, k^1$.

– Solve for k_{11} and w_{01},

$$\begin{aligned} k_{11} &= k(u_n^{(0)}(t), v_n^{(0)}(t), w_{01})_{t=t_{n-1}+\bar{c}_{11}h}, \\ 0 &= g1(u_n^{(0)}(t), v_n^{(0)}(t), w_{01})_{t=t_{n-1}+\bar{c}_{11}h}. \end{aligned}$$

– Construct $w_n^{(0)}(t)$ (of degree 2) which interpolates $\lambda_{n-1}, w_{01}, \hat{\lambda}_n$.

- Level i : For $i = 1, \ldots$ until the maximum order is reached,

– Construct $u_n^{(i)}(t)$ (of degree $i+3$) which interpolates,

$$y_{n-1}, f_0, f_{ij} = f(u_n^{(i-1)}(t), v_n^{(i-1)}(t))_{t_{n-1}+\bar{c}_{ij}h}\ (j = 1, \ldots, i), \hat{y}_n, f^1.$$

– Construct $v_n^{(i)}(t)$ (of degree $i+3$) which interpolates,

$$z_{n-1}, k_0, k_{ij}\ (j = 1, \ldots, i), \hat{z}_n, k^1.$$

– Solve for $k_{i+1,j}$ and w_{ij} $(j = 1, \ldots, i+1)$,

$$\begin{aligned} k_{i+1,j} &= k(u_n^{(i)}(t), v_n^{(i)}(t), w_{ij})_{t=t_{n-1}+\bar{c}_{i+1,j}h}, \\ 0 &= g1(u_n^{(i)}(t), v_n^{(i)}(t), w_{ij})_{t=t_{n-1}+\bar{c}_{i+1,j}h}. \end{aligned}$$

– Construct $w_n^{(i)}(t)$ (of degree $i+2$) which interpolates,

$$\lambda_{n-1}, w_{ij}\ (j = 1, \ldots, i+1), \hat{\lambda}_n.$$

4.4 Analysis of level 0

From (4.4), we have,

$$\theta_n''^{(i)}(t) = O(\delta_n^{(i)}(t)) + O(\mu_n^{(i)}(t)) + O(\delta_n'^{(i)}(t)) + O(h^{i+3}).$$

Let $\psi_y^{(0)}(t)$ interpolate the exact local solution $y_{n-1}, f_0, y(t_n), y'(t_n)$, and consider,

$$\begin{aligned} \delta_n^{(0)}(t) &= u_n'^{(0)}(t) - f(u_n^{(0)}(t), v_n^{(0)}(t)) \\ &= \left[u_n'^{(0)}(t) - \psi_y'^{(0)}(t)\right] + \left[\psi_y'^{(0)}(t) - y_n'(t)\right] \end{aligned}$$

$$
\begin{aligned}
& + \left[f(y_n(t), z_n(t)) - f(u_n^{(0)}(t), v_n^{(0)}(t)) \right] \\
= \; & O(h^3) + O(e_{n,y}^{(0)}(t)) + O(e_{n,z}^{(0)}(t)).
\end{aligned}
$$

Let $\psi_z^{(0)}(t)$ interpolate the exact local solution $z_{n-1}, k_0, z(t_n), z'(t_n)$, and consider,

$$
\begin{aligned}
& \mu_n^{(0)}(t) \\
= \; & v_n'^{(0)}(t) - k(u_n^{(0)}(t), v_n^{(0)}(t), w^{(0)}(t)) \\
= \; & \left[v_n'^{(0)}(t) - \psi_z'^{(0)}(t) \right] + \left[\psi_z'^{(0)}(t) - z_n'(t) \right] + k(y_n(t), z_n(t), G(y_n(t), z_n(t), 0, 0, 0, 0)) \\
& - k(u_n^{(0)}(t), v_n^{(0)}(t), G(u_n^{(0)}(t), v_n^{(0)}(t), \delta_n^{(0)}(t), \delta_n'^{(0)}(t), \mu_n^{(0)}(t), \theta_n''^{(0)}(t))) \\
= \; & O(h^3) + O(e_{n,y}^{(0)}(t)) + O(e_{n,z}^{(0)}(t)) + O(\delta_n^{(0)}(t)) + O(\delta_n'^{(0)}(t)) + O(\mu_n^{(0)}(t)) + O(\theta_n''^{(0)}(t)).
\end{aligned}
$$

By (4.), it follows that,

$$
\begin{aligned}
e_{n,z}^{(0)}(t) &= O(h^4) + hO(e_{n,z}^{(0)}(t)), \\
e_{n,z}^{(0)}(t) &= O(h^4) + h\left(O(e_{n,y}^{(0)}(t)) + O(\delta_n'^{(0)}(t)) + O(\mu_n^{(0)}(t)) \right).
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
e_{n,y}^{(0)}(t) &= O(h^4), \\
e_{n,z}^{(0)}(t) &= O(h^3), \\
e_{n,\lambda}^{(0)}(t) &= O(h^2).
\end{aligned}
$$

4.5 Analysis of levels 1 and higher

Assume that,

$$
\begin{aligned}
e_n^{(i-1)}(t)_{n,y} &= O(h^{i+2}), \\
e_n^{(i-1)}(t)_{n,z} &= O(h^{i+2}), \\
e_n^{(i-1)}(t)_{n,\lambda} &= O(h^{i+1}),
\end{aligned}
$$

we will show that,

$$
\begin{aligned}
e_n^{(i)}(t)_{n,y} &= O(h^{i+3}), \\
e_n^{(i)}(t)_{n,z} &= O(h^{i+3}), \\
e_n^{(i)}(t)_{n,\lambda} &= O(h^{i+2}),
\end{aligned}
$$

Let $\psi_y^{(i)}(t)$ interpolate the exact local solution at $y_{n-1}, f_0, y_n(t_{n-1}+\bar{c}_{ij}h)$ $(j=1,\ldots,i), y_n, y_n'(t_n)$. We have,

$$\begin{aligned}
\delta_n^{(i)}(t) &= u_n'^{(i)}(t) - f(u_n^{(i)}(t), v_n^{(i)}(t)) \\
&= \left[u_n'^{(i)}(t) - \psi_y'^{(i)}(t)\right] + \left[\psi_y'^{(i)}(t) - y_n'(t)\right] + \left[f(y_n(t), z_n(t)) - f(u_n^{(i)}(t), v_n^{(i)}(t))\right] \\
&= (I) + (II) + (III),
\end{aligned}$$

where,

- (I) is the data error, which can be expressed in terms of the Lagrange basis polynomials as,

$$\begin{aligned}
u_n'^{(i)}(t) - \psi_y'^{(i)}(t) &= 0d_0(\tau) + \sum_{j=1}^{i}\Big(f(u_n^{(i-1)}(t), v_n^{(i-1)}(t)) - f(y_n(t), z_n(t))\Big)_{t_{n-1}+\bar{c}_{ij}h} d_j(\tau) \\
&\quad + (f^1 - y_n'(t_n))d_{i+1}(\tau) \\
&= O(e_{n,y}^{(i-1)}(t)) + O(e_{n,z}^{(i-1)}(t)) + O(f^1 - y_n'(t_n)) \\
&= O(h^{i+2}) + O(f^1 - y_n'(t_n)).
\end{aligned}$$

- (II) is the interpolation error, which is $O(h^{i+3})$.
- (III) is $O(e_{n,y}^{(i)}(t)) + O(e_{n,z}^{(i)}(t))$.

Let $\psi_z^{(i)}(t)$ interpolate the exact local solution $z_{n-1}, k_0, z_n'(t_{n-1}+\bar{c}_{ij}h)$ $(j=1,\ldots,i), z(t_n), z'(t_n)$, and consider,

$$\begin{aligned}
&\mu_n^{(i)}(t) \\
&= v_n'^{(i)}(t) - k(u_n^{(i)}(t), v_n^{(i)}(t), w^{(i)}(t)) \\
&= \left[v_n'^{(i)}(t) - \psi_z'^{(i)}(t)\right] + \left[\psi_z'^{(i)}(t) - z_n'(t)\right] + k(y_n(t), z_n(t), G(y_n(t), z_n(t), 0, 0, 0, 0)) \\
&\quad - k(u_n^{(i)}(t), v_n^{(i)}(t), G(u_n^{(i)}(t), v_n^{(i)}(t), \delta_n^{(i)}(t), \delta_n'^{(i)}(t), \mu_n^{(i)}(t), \theta_n''^{(i)}(t))) \\
&= (I) + (II) + (III),
\end{aligned}$$

where,

- (I) is the data error, which can be expressed in terms of the Lagrange basis polynomials as,

$$\begin{aligned}
&v_n'^{(i)}(t) - \psi_z'^{(i)}(t) \\
&= 0d_0(\tau) \\
&\quad + \sum_{j=1}^{i}\Big(k(u_n^{(i)}(t), v_n^{(i)}(t), \hat{G}(u_n^{(i-1)}(t), v_n^{(i-1)}(t))) - k(y_n(t), z_n(t), \hat{G}(y_n(t), z_n(t)))\Big)_{t_{n-1}+\bar{c}_{ij}h} d_j(\tau) \\
&\quad + (k^1 - z_n'(t_n))d_{i+1}(\tau)
\end{aligned}$$

$$
\begin{aligned}
&= O(e_{n,y}^{(i-1)}(t)) + O(e_{n,z}^{(i-1)}(t)) + O(k^1 - z_n'(t_n)) \\
&= O(h^{i+2}) + O(k^1 - z_n'(t_n)).
\end{aligned}
$$

- (II) is the interpolation error, which is $O(h^{i+3})$.
- (III) is $O(e_{n,y}^{(i)}(t)) + O(e_{n,z}^{(i)}(t)) + O(\delta_n^{(i)}(t)) + O(\delta_n'^{(i)}(t)) + O(\mu_n^{(i)}(t)) + O(\theta_n''^{(i)}(t))$.

By (4.), it follows that,

$$
\begin{aligned}
e_{n,z}^{(i)}(t) &= O(h^{i+3}) + hO(e_{n,z}^{(i)}(t)), \\
e_{n,z}^{(i)}(t) &= O(h^{i+3}) + h\left(O(e_{n,y}^{(i)}(t)) + O(\delta_n'^{(i)}(t)) + O(\mu_n^{(i)}(t))\right).
\end{aligned}
$$

It follows from (4.6) that the local error at level i is,

$$
\begin{aligned}
\begin{pmatrix} u_n^{(i)}(t) - y_n(t) \\ v_n^{(i)}(t) - z_n(t) \end{pmatrix} &= \begin{pmatrix} O(h^{i+4}) \\ h(O(\delta_n^{(i)}(t)) + O(\delta_n'^{(i)}(t)) + O(\mu_n^{(i)}(t)) + O(\theta_n''^{(i)}(t))) \end{pmatrix} \\
&= \begin{pmatrix} O(h^{i+4}) \\ hO(\theta_n''^{(i)}(t)) \end{pmatrix} \\
&= \begin{pmatrix} O(h^{i+3}) \\ O(h^{i+3}) \end{pmatrix},
\end{aligned}
$$

and,

$$
w_n^{(i)}(t) - \lambda_n^{(i)}(t) = O(h^{i+2}),
$$

which completes the induction step.

4.6 Error control

We describe an error control scheme which attempts to control the underlying defect and residual given by,

$$
\begin{pmatrix} D_n(t) \\ E_n(t) \end{pmatrix} = \begin{pmatrix} Q_{n,1}(t) & Q_{n,2}(t) & Q_{n,3}(t) & Q_{n,4}(t) \\ P_{n,1}(t) & P_{n,2}(t) & P_{n,3}(t) & P_{n,4}(t) \end{pmatrix} \begin{pmatrix} \delta_n(t) \\ \delta_n'(t) \\ \mu_n(t) \\ \theta_n''(t) \end{pmatrix},
$$

where $Q_{n,i}(t)$ and $P_{n,i}(t)$, $i = 1, \ldots, 4$ possess expressions analogue to those given in (4.5) and (4.6).

This error control yields,

$$\begin{aligned}\begin{pmatrix} u_n(t)-y_n(t) \\ v_n(t)-z_n(t)\end{pmatrix} &= \int_{t_{n-1}}^{t} R_n(t,s)\begin{pmatrix}\delta_n(s) \\ D_n(s)\end{pmatrix} ds, \\ w_n(t)-\lambda_n(t) &= O(u_n(t)-y_n(t)) + O(v_n(t)-z_n(t)) + O(E_n(t)),\end{aligned}$$

for the local errors in $(u_n(t), v_n(t), w_n(t))^T$.

Alternatively, we seek $(\hat{D}_n(t), \hat{E}_n(t))^T$ independent of integrations by expanding the differential part about $G(u_n(t),0,0,0,0)$ and up to quadratic order in $\delta_n(t), \delta_n'(t), \mu_n(t)$ and $\theta_n''(t)$.

$$\begin{aligned} z_n'(t) &= k(y_n(t), z_n(t), G(\cdot)), \\ v_n'(t) &= k(u_n(t), v_n(t), G(\cdot)) + \mu(t) k_\lambda\left(G_\delta \delta(t) + G_{\delta'}\delta'(t) + G_\mu \mu(t) + G_{\theta''}\theta''(t)\right) + O(\Psi(t)),\end{aligned}$$

where,

$$\begin{aligned} G(\cdot) &= G(y_n(t), z_n(t), 0,0,0,0)), \\ k_\lambda &= k_\lambda(u_n(t), v_n(t), G(\cdot)), \\ \frac{\partial G}{\partial \cdot} &= \frac{\partial G}{\partial \cdot}(y_n(t), z_n(t), 0,0,0,0)), \\ \Psi(t) &= \delta_n^2(t) + \cdots + \theta_n''^2(t).\end{aligned}$$

Similarly for the algebraic part,

$$\begin{aligned} \lambda_n(t) &= G(y_n(t), z_n(t), 0,0,0,0), \\ w_n(t) &= G(u_n(t), v_n(t), 0,0,0,0) + G_\delta\delta_n(t) + G_{\delta'}\delta_n'(t) + G_\mu\mu_n(t) G_{\theta''}\theta_n''(t) + O(\Psi(t)).\end{aligned}$$

We choose to compute $(\hat{D}_n(t), \hat{E}_n(t))^T$ given by,

$$\begin{pmatrix}\hat{D}_n(t) \\ \hat{E}_n(t)\end{pmatrix} = \begin{pmatrix} k_\lambda G_\delta & k_\lambda G_{\delta'} & k_\lambda G_\mu + I & k_\lambda G_{\theta''} \\ G_\delta & G_{\delta'} & G_\mu & G_{\theta''}\end{pmatrix}\begin{pmatrix}\delta_n(t) \\ \delta_n'(t) \\ \mu_n(t) \\ \theta_n''(t)\end{pmatrix}. \tag{4.14}$$

By differentiating the constraint,

$$\begin{aligned} 0 &= g_{yy}(u_n)(f(u_n,v_n)+\delta_n, f(u_n,v_n)+\delta_n) \\ &\quad + g_y(u_n)\left[f_y(u_n,v_n)(f(u_n,v_n)+\delta_n) + f_z(u_n,v_n)(k(u_n,v_n,w_n)+\mu_n) + \delta_n'\right] + \theta_n'',\end{aligned}$$

with respect to $\delta_n, \delta'_n, \mu_n, \theta''_n$,

$$
\begin{aligned}
0 &= g_y f_z k_\lambda G_\delta + \frac{\partial}{\partial \delta_n} g_{yy}(u'_n, u'_n) + g_y f_y, \\
0 &= g_y f_z k_\lambda G_{\delta'} + g_y, \\
0 &= g_y f_z k_\lambda G_\mu + g_y f_z, \\
0 &= g_y f_z k_\lambda G_{\theta''} + I,
\end{aligned}
$$

we find that,

$$
\begin{aligned}
0 = {} & (g_y f_z k_\lambda)\left(G_\delta \delta_n + G_{\delta'}\delta'_n + G_\mu \mu_n + G_{\theta''}\theta''_n\right) \\
& + g_y f_z \mu_n + \left(\frac{\partial}{\partial \delta_n} g_{yy}(u'_n, u'_n) + g_y f_y\right)\delta_n + g_y \delta'_n + \theta''_n.
\end{aligned} \tag{4.15}
$$

It follows from (4.11) and (4.12) that,

$$
\begin{aligned}
\hat{D}_n(t) &= \mu_n(t) + k_\lambda \hat{E}_n(t), \\
g_y f_z \hat{D}_n(t) &= g_y f_z \mu_n + g_y f_z k_\lambda \hat{E}_n(t) \\
&= -\left[\left(\frac{\partial}{\partial \delta} g_{yy}(u', u') + g_y f_y\right)\delta + g_y \delta' + \theta''\right] + O(\delta^2) + \cdots + O(\theta''^2).
\end{aligned}
$$

As a result, we estimate $\tilde{D}(t)$ and $\tilde{E}(t)$ from the equation,

$$
\begin{pmatrix} I & -k_\lambda \\ g_y f_z & 0 \end{pmatrix}
\begin{pmatrix} \tilde{D}(t) \\ \tilde{E}(t) \end{pmatrix}
=
\begin{pmatrix} \mu(t) \\ -\left[\left(\frac{\partial}{\partial \delta} g_{yy}(u', u') + g_y f_y\right)\delta + g_y \delta' + \theta''\right] \end{pmatrix},
$$

where,

$$
\begin{aligned}
g_y &= g_y(u(t)), \\
f_z &= f_z(u(t), v(t)), \\
k_\lambda &= k_\lambda(u(t), v(t), w(t)), \\
f_y &= f_y(u(t), v(t)).
\end{aligned}
$$

4.7 Summary

In summary, we have studied the semi index 3 ADE and presented Scheme 3 which is similar to Scheme 1 and Scheme 2 except for the use of projected RK values

We have shown that while $u(t)$ retains the full order, the order for $v(t)$ is reduced by one and the order for $w(t)$ reduced by two. This agree with the optimal order for the discrete local solution reported in the literature.

For Scheme 3, we expect the optimal order in $u_n^{(i)}(t), g3(u_n^{(i)}(t))$, one order less in $v_n^{(i)}(t)$, and in $g2(u_n^{(i)}(t))f(u_n^{(i)}(t), v_n^{(i)}(t))$, and two orders less in $w_n^{(i)}(t), g1(u_n^{(i)}(t))f(u_n^{(i)}(t), v_n^{(i)}(t))$. Specifically, at level i, we expect that the local errors in $(u_n^{(i)}(t), v_n^{(i)}(t), w_n^{(i)}(t))$ and the original index 3 and the index 2 and index 1 constraints satisfy,

$$\begin{aligned}
u_n^{(i)}(t) - y_n(t) &= O(h^{i+4}), \\
v_n^{(i)}(t) - z_n(t) &= O(h^{i+3}), \\
w_n^{(i)}(t) - \lambda_n(t) &= O(h^{i+2}), \\
g3(u_n^{(i)}(t)) &= O(h^{i+4}), \\
g2(u_n^{(i)}(t), v_n^{(i)}(t)) &= O(h^{i+3}), \\
g1(u_n^{(i)}(t), v_n^{(i)}(t), w_i(t)) &= O(h^{i+2}).
\end{aligned}$$

Chapter 5

Implicit Runge-Kutta formulas

In this chapter, we consider some standard implicit Runge-Kutta formulas and the associated projected discrete values applied to ADEs and derive the optimal order for these methods. As justified in earlier chapters, the local order of our constructed interpolants (or, in general, of any continuous approximation) depends on the discrete order of the original Runge-Kutta formula (which may depend on the index of the problem). This can be determined by applying the Variation of Constants analysis to the local problem to derive an expression for the discrete local order. This can be achieved by considering the collocation polynomial, which is associated with the underlying standard RK formula.

Although this approach is straightforward for IVPs and index 1 problems, one needs to analyze the accuracy of some intermediate stages in the cases of higher index problems. In the latter cases, we begin with a rough local bound on the order for the discrete solution, then use this bound to derive a sharp higher order bound.

Throughout this chapter, we will be refering to the local ADE only.

5.1 ODEs

Consider the local IVP $y_n'(t) = f(y_n(t))$, $y_n(t_{n-1}) = y_{n-1}$, and let $\tilde{u}_n(t)$ be the collocation polynomial which is defined by,

$$\begin{aligned}
\tilde{u}_n(t_{n-1}) &= y_{n-1}, \\
\tilde{u}_n'(t_{n-1} + c_i h) &= f(\tilde{u}_n(t_{n-1} + c_i h)), \quad i = 1, \ldots, s.
\end{aligned}$$

It follows that the corresponding defect $\tilde{\delta}_n(t) = \tilde{u}_n'(t) - f(\tilde{u}_n(t))$ vanishes at the integration abscissas,

$$\tilde{\delta}_n(t_{n-1} + c_i h) = 0, \quad i = 1, \ldots, s,$$

and hence, by the Variation of Constants formula, the discrete local error is given by,

$$\begin{aligned} y_n - y_n(t_n) &= \int_{t_{n-1}}^{t_n} \frac{\partial y_n}{\partial y_{n-1}}(t_n,\tau)\tilde{\delta}_n(\tau)d\tau \\ &= h\sum_{i=1}^{s} b_i \left[\frac{\partial y_n}{\partial y_{n-1}}(t_n,\tau)\delta(\tau)\right]_{\tau=t_{n-1}+c_ih} + O(h^{p+1}) \\ &= 0 + O(h^{p+1}), \end{aligned}$$

where p is the order of the RK formula.

5.2 Index 1

Consider the local problem (2.1), (2.2) and the associated perturbed equation,

$$\begin{aligned} \tilde{u}_n'(t) &= f(\tilde{u}_n(t),\tilde{v}_n(t)) + \tilde{\delta}_n(t), \\ 0 &= g(\tilde{u}_n(t),\tilde{v}_n(t)) + \tilde{\theta}_n(t), \end{aligned}$$

where $(\tilde{u}_n(t),\tilde{v}_n(t))^T$ are the collocation polynomials defined by,

$$\begin{aligned} (\tilde{u}_n(t_{n-1}),\tilde{v}_n(t_{n-1}))^T &= (y_{n-1},z_{n-1})^T, \\ \tilde{u}_n'(t_{n-1}+c_ih) &= f(\tilde{u}_n(t_{n-1}+c_ih),\tilde{v}_n(t_{n-1}+c_ih)), \quad i=1,\ldots,s, \\ 0 &= g(\tilde{u}_n(t_{n-1}+c_ih),\tilde{v}_n(t_{n-1}+c_ih)), \quad i=1,\ldots,s. \end{aligned}$$

It follows that $(\tilde{\delta}_n(t),\tilde{\theta}_n(t))^T$ satisfies,

$$\begin{aligned} \tilde{\delta}_n(t_{n-1}+c_ih) &= 0, \quad i=1,\ldots,s, \\ \tilde{\theta}_n(t_{n-1}+c_ih) &= 0, \quad i=1,\ldots,s, \\ \tilde{\theta}_n(t_{n-1}) &= 0, \end{aligned}$$

by the consistent initial value assumption which is enforced since we use projected values. Hence $\tilde{\theta}_n(t) = O(h^{s+1})$. By (2.15), the discrete local error for y_n is given by,

$$\begin{aligned} y_n - y_n(t_n) &= \int_{t_{n-1}}^{t_n} S_1(t_n,\tau)\tilde{\delta}_n(\tau) + S_2(t_n,\tau)\tilde{\theta}_n(\tau)d\tau \\ &= h\sum_{i=1}^{s} b_i \left[S_1(t_n,\tau)\tilde{\delta}_n(\tau) + S_2(t_n,\tau)\tilde{\theta}_n(\tau)\right]_{\tau=t_{n-1}+c_ih} + O(h^{p+1}) \\ &= O(h^{p+1}). \end{aligned}$$

By (2.17), the discrete local error for the unprojected value z_n is given by,

$$\begin{aligned} z_n - z_n(t_n) &= O(y_n - y_n(t_n)) + O(\tilde{\theta}_n(t_n)) \\ &= O(h^{s+1}). \end{aligned}$$

By constrast, the discrete local error for the projected value $\hat{z}_n$ is,

$$\begin{aligned} \hat{z}_n - z(t_n) &= \hat{G}(y_n) - \hat{G}(y_n(t_n)) \\ &= O(y_n - y_n(t_n)) \\ &= O(h^{p+1}). \end{aligned}$$

Thus both y_n and $\hat{z}_n$ have full order.

5.3 Index 2

Consider the local index 2 ADE,

$$\begin{aligned} y_n'(t) &= f(y_n(t), z_n(t)), \\ 0 &= g(y_n(t)), \end{aligned}$$

and the associated perturbed equation,

$$\begin{aligned} \tilde{u}_n'(t) &= f(\tilde{u}_n(t), \tilde{v}_n(t)) + \tilde{\delta}_n(t), \\ 0 &= g(\tilde{u}_n(t)) + \tilde{\theta}_n(t), \end{aligned}$$

where $(\tilde{u}_n(t), \tilde{v}_n(t))^T$ are the collocation polynomials defined by,

$$\begin{aligned} (\tilde{u}_n(t_{n-1}), \tilde{v}_n(t_{n-1}))^T &= (y_{n-1}, z_{n-1})^T, \\ \tilde{u}_n'(t_{n-1} + c_i h) &= f(\tilde{u}_n(t_{n-1} + c_i h), \tilde{v}_n(t_{n-1} + c_i h)), \quad i = 1, \ldots, s, \\ 0 &= g(\tilde{u}_n(t_{n-1} + c_i h)), \quad i = 1, \ldots, s. \end{aligned}$$

It follows that the corresponding defect and the algebraic residual satisfy,

$$\begin{aligned} \tilde{\delta}_n(t_{n-1} + c_i h) &= 0, \quad i = 1, \ldots, s, \\ \tilde{\theta}_n(t_{n-1} + c_i h) &= 0, \quad i = 1, \ldots, s, \\ \tilde{\theta}_n(t_{n-1}) &= 0, \text{ since projected values are used,} \end{aligned}$$

and hence, from interpolation theory,

$$\begin{aligned}\tilde{\delta}_n(t) &= O(h^s),\\ \tilde{\theta}_n(t) &= O(h^{s+1}),\\ \tilde{\theta}'_n(t) &= O(h^s).\end{aligned}$$

The discrete local error in y_n is given by (3.8),

$$\begin{aligned}e_{n,y} &= y_n - y_n(t_n)\\ &= \int_{t_{n-1}}^{t_n} \left(S_1(t_n,\tau)\tilde{\delta}_n(\tau) + S_2(t_n,\tau)\tilde{\theta}'_n(\tau)\right) d\tau\\ &\leq O(h^{s+1}).\end{aligned}$$

This rough lower bound on the order of $e_{n,y}$ in turn yields a rough lower bound on the order of the algebraic component $e_{n,z} = z_n - z_n(t_n) = O(h^s)$, which will be utilized later. In order to derive the full order, we integrate by parts the formula (3.7) and apply the quadrature rule with weights b_i and nodes $c_i, i = 1, \ldots, s$,

$$\begin{aligned}e_{n,y} &= \int_{t_{n-1}}^{t_n} \frac{\partial y_n}{\partial y_{n-1}}(t_n,\tau)(Q_1(\tau)\tilde{\delta}_n(\tau) + Q_2(\tau)\tilde{\theta}'_n(\tau))d\tau\\ &= \int_{t_{n-1}}^{t_n} \left(S_1(t_n,\tau)\tilde{\delta}_n(\tau) - \frac{\partial S_2}{\partial \tau}(t_n,\tau)\tilde{\theta}_n(\tau)\right) d\tau + S_2(t_n,t_n)\tilde{\theta}_n(t_n)\\ &= \int_{t_{n-1}}^{t_n} \sigma(t_n,\tau)d\tau + S_2(t_n,t_n)\tilde{\theta}_n(t_n)\\ &= 0 + S_2(t_n,t_n)\tilde{\theta}_n(t_n) + O(h^{p+1}).\end{aligned}$$

Now from the definition of $S_2(t_n,s)$ and $Q_2(s)$, and from the fact that $e_{n,y} \leq O(h^{s+1})$, $\tilde{\delta}_n(t_n) \leq O(h^s)$, $\tilde{\theta}'_n(t_n) \leq O(h^s)$, we have, [1]

$$\begin{aligned}S_2(t_n,t_n) &= -\int_0^1 \left(f_z(g_y f_z)^{-1}\right)(y_n, G(y_n, \tau\tilde{\delta}_n(t_n), \tau\tilde{\theta}'_n(t_n)))d\tau\\ &= -\int_0^1 \left(f_z(g_y f_z)^{-1}\right)(y_n, G(y_n,0,0) + \tau O(h^s))d\tau\\ &= -\left(f_z(g_y f_z)^{-1}\right)(y_n, G(y_n,0,0)) + O(h^s)\\ &= -\left(f_z(g_y f_z)^{-1}\right)(y_n(t_n) + e_{n,y}, G(y_n(t_n) + e_{n,y},0,0)) + O(h^s)\\ &= -\left(f_z(g_y f_z)^{-1}\right)(y_n(t_n), G(y_n(t_n),0,0)) + O(e_{n,y}) + O(h^s)\end{aligned}$$

[1] Upon differentiating (3.3) with respect to θ', we find that,

$$G_{\theta'} = -(g_y f_z)^{-1}(u(t), v(t)).$$

$$= \quad -\left(f_z(g_y f_z)^{-1}\right)(y_n(t_n), z_n(t_n)) + O(h^s).$$

In addition, since $\tilde{\theta}_n(t_n) \le O(h^{s+1})$ and since $p+1 \le 2s+1$, we have,

$$e_{n,y} \quad \le \quad -\left(f_z(g_y f_z)^{-1}\right)(y_n(t_n), z_n(t_n))\tilde{\theta}_n(t_n) + O(h^{p+1}).$$

In order to annihilate the first term of the above bound, we apply the projected RK method for $\hat{y}_n$ as prescribed in Scheme 2. Consider the projections [28, p. 514],

$$\begin{aligned} Q(\hat{y}_n, z) &= \left(f_z(g_y f_z)^{-1} g_y\right)(\hat{y}_n, z_n), \\ P(\hat{y}_n, z_n) &= I - Q(\hat{y}_n, z_n). \end{aligned}$$

According to Scheme 2, we have,

$$\hat{y}_n = y_n + f_z(\hat{y}_n, z_n)\nu.$$

With $\hat{e}_{n,y} = \hat{y}_n - y_n(t_n)$, we have (since $P f_z \nu \equiv 0$),

$$\begin{aligned} P\hat{e}_{n,y} &= P(y_n + f_z(\hat{y}_n, z_n)\nu - y_n(t_n)), \\ &= P e_{n,y}. \end{aligned}$$

Using the following results,

$$\begin{aligned} 0 &= g(y_n(t_n)) \\ &= g(\hat{y}_n - \hat{e}_{n,y}) \\ &= g(\hat{y}_n) - g_y(\hat{y}_n)\hat{e}_{n,y} + O(\hat{e}_{n,y}^2) \\ &= 0 - g_y(\hat{y}_n)\hat{e}_{n,y} + O(\hat{e}_n^2), \end{aligned}$$

we have,

$$\begin{aligned} Q\hat{e}_{n,y} &= \left(f_z(g_y f_z)^{-1} g_y\right)(\hat{y}_n, z_n)\hat{e}_{n,y} \\ &= \left(f_z(g_y f_z)^{-1}\right)(\hat{y}_n, z_n) g_y(\hat{y}_n)\hat{e}_{n,y} \\ &= \left(f_z(g_y f_z)^{-1}\right)(\hat{y}_n, z_n) O(\hat{e}_{n,y}^2) \\ &= O(\hat{e}_{n,y}^2). \end{aligned}$$

Finally,

$$P e_{n,y} \quad = \quad -(I-Q)(\hat{y}_n, z_n)\left(f_z(g_y f_z)^{-1}\right)(y_n(t_n), z_n(t_n))\tilde{\theta}_n(t_n) + O(h^{p+1})$$

$$
\begin{aligned}
&= -(I-Q)(\hat{y}_n, z_n)\left(f_z(g_y f_z)^{-1}\right)(\hat{y}_n + O(\hat{e}_{n,y}), z_n + O(h^s))\tilde{\theta}_n(t_n) + O(h^{p+1}) \\
&= -(I-Q)\left(f_z(g_y f_z)^{-1}\right)(\hat{y}_n, z_n)\tilde{\theta}_n(t_n) + O(\hat{e}_{n,y}\tilde{\theta}_n(t_n)) + O(h^{p+1}) \\
&= 0 + O(\hat{e}_{n,y}\tilde{\theta}_n(t_n)) + O(h^{p+1}) \\
&= O(h^{p+1}),
\end{aligned}
$$

or,

$$
\begin{aligned}
\hat{y}_n - y_n(t_n) &= O(h^{p+1}), \\
\hat{z}_n - z_n(t_n) &= G(\hat{y}_n, 0, 0) - G(y_n(t_n), 0, 0) \\
&= O(h^{p+1}).
\end{aligned}
$$

Thus the discrete values $\hat{y}_n$ and $\hat{z}_n$ retain this full order.

5.4 Index 3

Consider the local semi explicit index 3 ADE,

$$
\begin{aligned}
y_n'(t) &= f(y_n(t), z_n(t)), \\
z_n'(t) &= k(y_n(t), z_n(t), \lambda_n(t)), \\
0 &= g(y_n(t)),
\end{aligned}
$$

and the associated perturbed equation,

$$
\begin{aligned}
\tilde{u}_n'(t) &= f(\tilde{u}_n(t), \tilde{v}_n(t)) + \tilde{\delta}_n(t), \\
\tilde{v}_n'(t) &= k(\tilde{u}_n(t), \tilde{v}_n(t), \tilde{w}_n(t)) + \tilde{\mu}_n(t), \\
0 &= g(\tilde{u}_n(t)) + \tilde{\theta}_n(t),
\end{aligned}
$$

where, $(\tilde{u}_n(t), \tilde{v}_n(t), \tilde{w}_n(t))^T$ are the collocation polynomials of degree s defined by,

$$
\begin{aligned}
(\tilde{u}_n(t_{n-1}), \tilde{v}_n(t_{n-1}), \tilde{w}_n(t_{n-1}))^T &= (y_{n-1}, z_{n-1}, \lambda_{n-1})^T, \\
\tilde{u}_n'(t_{n-1} + c_i h) &= k(\tilde{u}_n(t_{n-1} + c_i h), \tilde{v}_n(t_{n-1} + c_i h)), \quad i = 1, \ldots, s, \\
\tilde{v}_n'(t_{n-1} + c_i h) &= f(\tilde{u}_n(t_{n-1} + c_i h), \tilde{v}_n(t_{n-1} + c_i h), \tilde{w}_n(t_{n-1} + c_i h)), \quad i = 1, \ldots, s, \\
0 &= g(\tilde{u}_n(t_{n-1} + c_i h)), \quad i = 1, \ldots, s.
\end{aligned}
$$

It follows that the corresponding defects and algebraic residual satisfy,

$$
\begin{aligned}
\tilde{\delta}_n(t_{n-1}+c_ih) &= 0, \quad i=1,\ldots,s, \\
\tilde{\mu}_n(t_{n-1}+c_ih) &= 0, \quad i=1,\ldots,s, \\
\tilde{\theta}_n(t_{n-1}+c_ih) &= 0, \quad i=1,\ldots,s.
\end{aligned}
$$

According to Scheme 3, we also have,

$$
\begin{aligned}
\tilde{\theta}_n(t_{n-1}) &= 0, \\
\tilde{\theta}_n'(t_{n-1}) &= 0,
\end{aligned}
$$

and hence the following rough bounds on the orders can be justified (from interpolation theory alone),

$$
\begin{aligned}
\tilde{\delta}_n(t) &\leq O(h^s), \\
\tilde{\delta}_n'(t) &\leq O(h^{s-1}), \\
\tilde{\mu}_n(t) &\leq O(h^s), \\
\tilde{\theta}_n(t) &\leq O(h^{s+1}), \\
\tilde{\theta}_n'(t) &\leq O(h^s), \\
\tilde{\theta}_n''(t) &\leq O(h^{s-1}),
\end{aligned}
\tag{5.1}
$$

By (4.9), the discrete local error in y_n is given by,

$$
\begin{aligned}
y_n - y_n(t_n) &= O\left(\int_{t_{n-1}}^{t_n} \tilde{\delta}_n(s)ds\right), \\
&= O(h^{p+1}).
\end{aligned}
$$

By (4.10) and the fact that,

$$
\int_{t_{n-1}}^{t_n} \sigma(t,\tau)d\tau = O(h^{p+1}),
$$

the discrete local error in z_n is given by,

$$
\begin{aligned}
& z_n - z_n(t_n) \\
&= O\left(Q_2(t_n)\tilde{\delta}_n(t_n) - \left[\frac{\partial R}{\partial t}(t_n,t_n)\begin{pmatrix} 0 \\ Q_4(t_n)\end{pmatrix} + \begin{pmatrix} 0 \\ Q_4'(t_n)\end{pmatrix}\right]_z \tilde{\theta}_n(t_n) + Q_4(t_n)\tilde{\theta}_n'(t_n)\right) + O(h^{p+1}) \\
&= O(h^s),
\end{aligned}
$$

where $[\cdots]_z\tilde{\theta}_n(t_n)$ denotes the projection of $[\cdots]\tilde{\theta}_n(t_n)$ onto the z component.

In addition, we have

$$\lambda_n - \lambda_n(t_n) = O(h^{s-1}).$$

While y_n achieves full order already, we only obtain a lower bound for the local errors in z_n and λ_n. In order to annihilate the low order terms involving $\tilde{\delta}_n(t_n)$ and $\tilde{\theta}'_n(t_n)$, we consider the terms $Q_2(t)$ and $Q_4(t)$ as defined by (4.7), or $Q_4(t)$ only. [2] We have,

$$\begin{aligned}
Q_4(t_n) = & -\int_0^1 \left(k_\lambda(g_y f_z k_\lambda)^{-1}\right)(y_n, z_n, G(y_n, z_n, \tau\tilde{\delta}_n(t_n), \tau\tilde{\delta}'_n(t_n), \tau\tilde{\mu}_n(t_n), \tau\tilde{\theta}''_n(t_n)))d\tau \\
= & -\int_0^1 \left(k_\lambda(g_y f_z k_\lambda)^{-1}\right)(y_n, z_n, G(y_n, z_n, 0,0,0,0) + \tau(O(h^{s-1}))d\tau \\
= & -\left(k_\lambda(g_y f_z k_\lambda)^{-1}\right)(y_n(t_n) + e_{n,y}, z_n(t_n) + e_{n,z}, G(y_n(t_n) + e_{n,y}, z_n(t_n) + e_{n,z}, 0,0,0,0)) + O(h^{s-1}) \\
= & -\left(k_\lambda(g_y f_z k_\lambda)^{-1}\right)(y_n(t_n), z_n(t_n), \lambda_n(t_n)) + O(e_{n,y}) + O(e_{n,z}) + O(h^{s-1}) \\
= & -\left(k_\lambda(g_y f_z k_\lambda)^{-1}\right)(y_n(t_n), z_n(t_n), \lambda_n(t_n)) + O(h^{s-1}),
\end{aligned}$$

where we have used $O(h^s)$ as a lower bound for $e_{n,z}$. Therefore,

$$\begin{aligned}
e_{n,y} &= O(h^{p+1}), \\
e_{n,z} &= -\left(k_\lambda(g_y f_z k_\lambda)^{-1}\right)(y_n(t_n), z_n(t_n), \lambda_n(t_n))\tilde{\theta}'_n(t_n) + O(h^{\min(2s-1, p+1)}).
\end{aligned}$$

Consider the projections [26, p. 77], [30],

$$\begin{aligned}
S(\hat{y}_n, \hat{z}_n, \lambda_n) &= \left(k_\lambda(g_y f_z k_\lambda)^{-1} g_y\right)(\hat{y}_n, \hat{z}_n, \lambda_n), \\
Q(y_n, \hat{z}_n, \lambda_n) &= (S f_z)(\hat{y}_n, \hat{z}_n, \lambda_n), \\
P(\hat{y}_n, \hat{z}_n, \lambda_n) &= (I - Q)(\hat{y}_n, \hat{z}_n, \lambda_n).
\end{aligned}$$

and the discrete unprojected and projected local error in z,

$$\begin{aligned}
e_{n,z} &= z_n - z_n(t_n), \\
\hat{e}_{n,z} &= \hat{z}_n - z_n(t_n).
\end{aligned}$$

We have (since $P k_\lambda \nu \equiv 0$),

$$P\hat{e}_{n,z} = P(\hat{z}_n - z_n(t_n))$$

[2] Upon differentiating (4.4) with respect to δ', θ'', we find that,

$$\begin{aligned}
G_{\delta'} &= -(g_y f_z k_\lambda)^{-1} g_y, \\
G_{\theta''} &= -(g_y f_z k_\lambda)^{-1}.
\end{aligned}$$

$$
\begin{aligned}
&= P(z_n + k_\lambda(\hat{y}_n, \hat{z}_n, \lambda_n)\nu - z_n(t_n)) \\
&= Pe_{n,z}.
\end{aligned}
$$

Using the following result,

$$
\begin{aligned}
0 &= (g_y f)(y_n(t_n), z_n(t_n)) \\
&= (g_y f)(\hat{y}_n + O(h^{p+1}), \hat{z}_n - \hat{e}_{n,z}) \\
&= (g_y f)(\hat{y}_n, \hat{z}_n) - (g_y f_z)(\hat{y}_n, \hat{z}_n)\hat{e}_{n,z} + O(h^{p+1}) + O(\hat{e}_{n,z}^2) \\
&= 0 - (g_y f_z)(\hat{y}_n, \hat{z}_n)\hat{e}_{n,z} + O(h^{p+1}) + O(\hat{e}_{n,z}^2),
\end{aligned}
$$

we have,

$$
\begin{aligned}
Q\hat{e}_{n,z} &= \left(k_\lambda(g_y f_z k_\lambda)^{-1}\right)(g_y f_z)(\hat{y}_n, \hat{z}_n, \lambda_n)\hat{e}_{n,z} \\
&= \left(k_\lambda(g_y f_z k_\lambda)^{-1}\right)(\hat{y}_n, \hat{z}_n, \lambda_n)(g_y f_z)(\hat{y}_n, \hat{z}_n)\hat{e}_{n,z} \\
&= \left(k_\lambda(g_y f_z k_\lambda)^{-1}\right)(\hat{y}_n, \hat{z}_n, \lambda_n)O(\hat{e}_{n,z}^2) \\
&= O(\hat{e}_{n,z}^2).
\end{aligned}
$$

Finally,

$$
\begin{aligned}
Pe_{n,z} &= -(I-Q)(\hat{y}_n, \hat{z}_n, \lambda_n)\left(k_\lambda\,(g_y f_z k_\lambda)^{-1}\right)(y_n(t_n), z_n(t_n), \lambda_n(t_n))\tilde{\theta}_n'(t_n) + O(h^{\min\,(2s-1,p+1)}) \\
&= -(I-Q)(\hat{y}_n, \hat{z}_n, \lambda_n)\left(k_\lambda\,(g_y f_z k_\lambda)^{-1}\right)(\hat{y}_n + O(h^{p+1}), \hat{z}_n + O(\hat{e}_{n,z}), \lambda_n + O(h^{s-1}))\tilde{\theta}_n'(t_n) \\
&\quad + O(h^{\min\,(2s-1,p+1)}) \\
&= -(I-Q)\left(k_\lambda\,(g_y f_z k_\lambda)^{-1}\right)(\hat{y}_n, \hat{z}_n, \lambda_n)\tilde{\theta}_n'(t_n) + O(\hat{e}_{n,z}\tilde{\theta}_n'(t_n)) + O(h^{\min\,(2s-1,p+1)}) \\
&= 0 + O(\hat{e}_{n,z}\tilde{\theta}_n'(t_n)) + O(h^{\min(p+1,2s-1)}) \\
&= O(h^{\min\,(2s-1,p+1)}),
\end{aligned}
$$

or, assuming that, $2s-1 \le p+1$,

$$
\begin{aligned}
\hat{z}_n - z_n(t_n) &= O(h^{2s-1}), \\
\hat{\lambda}_n - \lambda_n(t_n) &= G(\hat{y}_n, \hat{z}_n, 0,0,0,0) - G(y_n(t_n), z_n(t_n), 0,0,0,0) \\
&= O(h^{2s-1}).
\end{aligned}
$$

5.5 Summary

In summary, we have applied the Variation of Constants formula to the local problem to derive the discrete local error for projected RK formulas. The obtained results are summarized in Table 5.1. We note that in most cases the classical order is achieved except for the index 3 case, whose discrete

	Differential	Algebraic	Assumption
ODE	$p+1$		
Index 1	$p+1$	$p+1$	
Index 2	$p+1$	$p+1$	
Index 3	$(p+1, 2s-1)$	$2s-1$	$2s-1 \leq p+1$

Table 5.1: Optimal discrete local order

local error in $\hat{y}_n$ is $p+1$ but $\hat{z}_n$ and $\hat{\lambda}_n$ are reduced to $2s-1$. The local error bound we have derived in this chapter can be directly adopted to the theory developed in Chapters 2–4 to derive sharp bounds for the global error associated with level i interpolants.

Chapter 6

Implementation

For implementation, we modified the code of RADAU5 to adopt our approach. While we kept intact the basic program structure, we have used the three methods DIRK2, GAUSS2 and GAUSS3 which are based on the three formulas SDIRK(2), Gauss(2) and Gauss(3) respectively.

Reference [28] describes major implementation issues of the code. These issues include standard implicit RK methods with Hessenberg transformations, direct linear solvers, a simplified newton iterative method, the projected RK technique, initial step size selection strategy and a continuing step size selection strategy.

6.1 DIRK2, GAUSS2, GAUSS3

For the IVP $y'(t) = f(y(t))$, consider the standard implicit RK formula,

$$y_n = y_{n-1} + h\sum_{i=1}^{s} b_i f(Y_i), \quad i = 1, \ldots, s,$$

where the stage values Y_i are defined implicitly by,

$$Y_i = y_{n-1} + h\sum_{j=1}^{s} a_{ij} f(Y_j), \quad i = 1, \ldots, s.$$

Denote,

$$\begin{aligned} Z_i &= Y_i - y_{n-1}, \quad i = 1, \ldots, s, \\ F(Z_j) &= f(y_{n-1} + Z_j), \quad j = 1, \ldots, s, \end{aligned}$$

then alternatively one seeks the stage values Z_i defined implicitly by,

$$Z_i = h\sum_{j=1}^{s} a_{ij}F(Z_j), \quad i = 1,\ldots,s, \tag{6.1}$$

which can be solved iteratively by the simplified Newton technique, where the Newton Jacobian is approximated on each step by assuming that $\frac{\partial F}{\partial Z}$ is fixed across each step (rather than re-evaluating $\frac{\partial F}{\partial Z}$ at each stage).

- DIRK2: since SDIRK(2) is diagonally implicit, we decoupled (6.1) of size $2N$ into 2 systems of size N,

$$\begin{aligned} Z_1 &= ha_{11}F(Z_1), \\ Z_2 &= h\left(a_{21}F(Z_1) + a_{22}F(Z_2)\right). \end{aligned}$$

  As a result, the corresponding simplified Newton iteration is reduced to 2 linear systems of size N,

$$\begin{aligned} \left(\frac{1}{ha_{11}}I - J\right)\Delta Z_1^k &= \frac{-1}{ha_{11}}Z_1^k + F(Z_1^k), \\ \left(\frac{1}{ha_{22}}I - J\right)\Delta Z_2^k &= \frac{-1}{ha_{22}}Z_2^k + \frac{a_{21}}{a_{22}}F(Z_1^k) + F(Z_2^k), \end{aligned}$$

  where $J = f_y|_{t=t_{n-1}}$ and $\Delta Z_i^k = Z_i^{k+1} - Z_i^k, \quad k = 0,1,\ldots; \quad i = 1,2.$

- GAUSS2, GAUSS3: in order to reduce the cost for large N, we transformed the coefficient matrix A of Gauss(3) to block diagonal form such that,

$$T^{-1}A^{-1}T = \Lambda = \begin{pmatrix} \hat{\gamma} & 0 & 0 \\ 0 & \hat{\alpha} & -\hat{\beta} \\ 0 & \hat{\beta} & \hat{\alpha} \end{pmatrix},$$

  where $\hat{\gamma}$ is the real eigenvalue of A^{-1} and $\hat{\alpha} \pm i\hat{\beta}$ are the complex conjugate pair of eigenvalues of A^{-1}. The matrix T contains the corresponding eigenvectors of A^{-1}.

  The resulting simplified Newton iteration correponds to linear system of sizes N associated with the real eigenvalue whose coefficient matrix is,

$$E_1 = \frac{\hat{\gamma}}{h}I - J,$$

  and a linear system of size $2N$ associated with the pair of complex conjugate eigenvalues. In additiona, this coefficient matrix has a special structure which can be exploited to yield two systems of size N whose coefficient matrices are,

$$\begin{aligned} E_2^R &= \frac{\hat{\alpha}}{h} I - J, \\ E_2^I &= \frac{\hat{\beta}}{h} I. \end{aligned}$$

- Initial iteration values: For the first step, we expanded Z_i^0, $i = 1, \ldots, s$, about the left end point to obtain,

$$\begin{aligned} Z_i^0 &= h \sum_{j=1}^{s} a_{ij} f(y_{n-1} + Z_j^0) \\ &= h \sum_{j=1}^{s} a_{ij} \left(f_0 + O(h) \right) \\ &= h \sum_{j=1}^{s} a_{ij} f_0 + O(h^2) \\ &= h c_i f_0 + O(h^2), \end{aligned}$$

  where f_0 is available for the first step and we have used the standard condition C(1) for implicit Runge-Kutta formulas, ie., $\sum_{j=1}^{s} a_{ij} = c_i$, $i = 1, \ldots, s$.

  For subsequent steps, we extrapolated the interpolant $u_{n-1}(t)$ from the previous step,

$$Z_i^0 = u_{n-1}(t_{n-2} + \tau h) - y_{n-1},$$

  where $\tau = 1 + \frac{c_i h}{h_{old}}$, and h_{old} is the stepsize used in the previous step.

In addition, we implemented the following,

- Interpolants: we constructed the differential and algebraic interpolants as specified by Scheme 2 and Scheme 3.

- Algebraic residuals: we computed all relevant constraints of the concerned ADE as prescribed in (1.9) and (1.10). For CMSs, we computed,

$$\begin{aligned} & g3(Q(t)) \ (\equiv g(Q(t))), \\ & g2(Q(t), U(t)), \\ & g1(Q(t), U(t), \Lambda(t)), \end{aligned}$$

  where $g3$ is the original position level constraint (index 3), $g2$ the velocity level constraint (index 2) and $g1$ the acceleration level constraint (index 1). For the cavity problem with velocity $(u_{ij}(t), v_{ij}(t))$ and pressure $p_{ij}(t)$, we computed the discretized divergence term (index

2) (cf. subsection 6.2.7),

$$\begin{aligned} g2(i,j) &= \frac{1}{Dx}(u_{ij} - u_{i-1j} + v_{ij} - v_{ij-1}), \quad (i,j) \neq (5,5), \\ g2(K,K) &= \sum_{i,j=1}^{K} p_{ij}, \end{aligned}$$

and its derivative (index 1),

$$\begin{aligned} g1(i,j) &= \frac{1}{Dx}(u'_{ij} - u'_{i-1j} + v'_{ij} - v'_{ij-1}), \quad (i,j) \neq (K,K) \\ &= \frac{1}{Dx}(f_{ij} - f_{i-1j} + f_{ij} - f_{ij-1}), \\ g1(5,5) &= 0, \end{aligned}$$

- Defect: we computed the sampled underlying defect $D(t)$ whose expressions will be derived in Subsections 6.2.1–6.2.7.
- Error control scheme: we sampled the underlying defect and algebraic residual at a chosen point,

  $$ERR = \max(\|D(\tau^\star)\|, \|E(\tau^\star)\|),$$

  where $g(t)$ is the original constraint presented in the formulation. There is one exception concerning the first step of the cavity problem where there is a discontinuity which results in inconsistent initial values. For this step only, we ignored $g1$ for our error control scheme.
- Step-size selection: we selected $h_{new} = h_{old}(fac\ \frac{TOL}{ERR})^{\frac{1}{\nu}}$, where ν is some integer which we arbitrarily set to 4 for our testing.

6.2 Test problems

Although we have developed a rigorous estimation of $\tilde{D}(t)$ and $\tilde{E}(t)$ for general semi explicit ADEs, some of the following test problems exhibits special structures so that the exact $D(t)$ and $E(t)$ can be easily computed.

6.2.1 Index 3 pendulum problem

Consider the index 3 pendulum problem, [26, pp. 8–9],

$$\begin{aligned} q'(t) &= u(t), \quad 0 \leq t \leq 10, \\ u'(t) &= f - \lambda(t) q(t), \\ 0 &= \frac{1}{2}(q^T(t) q(t) - 1), \end{aligned}$$

where $f = (0, -1)^T$, and,

$$\begin{aligned} q : R &\to R^2, \quad q(0) = (1,0)^T, \\ u : R &\to R^2, \quad u(0) = (0,0)^T, \\ \lambda : R &\to R, \quad \lambda(0) = 0. \end{aligned}$$

Denote $L(q(t)) = q^T(t)q(t)$, then by differentiating the constraint twice we have,

$$\lambda(t) = \frac{1}{L(q(t))}\left(q^T(t)f + u^T(t)u(t)\right),$$

and $u(t)$ satisfies the associated underlying ODE,

$$u'(t) = f - \frac{1}{L(q(t))}(q^T(t)f + u^T(t)u(t))q(t). \tag{6.2}$$

Let $(Q(t), U(t), \Lambda(t))^T$ be a continuous approximation to $(q(t), u(t), \lambda(t))^T$ satisfying the perturbed equation,

$$\begin{aligned} Q'(t) &= U(t) + \delta(t), \\ U'(t) &= f - \Lambda(t)Q(t) + \mu(t), \\ 0 &= \frac{1}{2}(Q^T(t)Q(t) - 1) + \theta(t). \end{aligned}$$

By differentiating the constraint twice we find that,

$$\begin{aligned} 0 &= Q^T(U + \delta) + \theta', \\ 0 &= Q^T(U' + \delta') + (U+\delta)^T(U+\delta) + \theta'' \\ &= Q^T(f - \Lambda Q + \mu + \delta') + (U+\delta)^T(U+\delta) + \theta'', \\ L(Q)\Lambda &= Q^T(f + \mu + \delta') + (U+\delta)^T(U+\delta) + \theta'', \\ \Lambda &= \frac{1}{L(Q)}\left(Q^T(f + \mu + \delta') + (U+\delta)^T(U+\delta) + \theta''\right), \end{aligned}$$

and,

$$\begin{aligned} U' &= f - \frac{1}{L(Q)}\left(Q^T(f + \mu + \delta') + (U+\delta)^T(U+\delta) + \theta''\right)Q + \mu \\ &= f - \frac{1}{L(Q)}(Q^T f + U^T U)Q - \frac{1}{L(Q)}\left(Q^T(\mu + \delta') + 2U^T\delta + \delta^T\delta + \theta''\right)Q + \mu. \end{aligned}$$

Therefore the exact defect $D(t)$ actually used in the error control for this problem is,

$$
\begin{aligned}
D &= \frac{1}{L(Q)}\left(-Q^T(\mu+\delta') - 2U^T\delta - \delta^T\delta + Q^T(U'+\delta') + (U+\delta)^T(U+\delta)\right)Q + \mu \\
&= \frac{1}{L(Q)}\left(Q^T(U'-\mu) + U^TU\right)Q + \mu \\
&= \frac{1}{L(Q)}\left(Q^T(f-\Lambda Q) + U^TU\right)Q + \mu,
\end{aligned}
$$

which can be computed for any t.

As for the algebraic part, the exact formula for $E(t)$ is,

$$
\begin{aligned}
E &= \frac{1}{L(Q)}\left(Q^T(\mu+\delta') + Q'^TQ' + \theta'' - U^TU\right) \\
&= \frac{1}{L(Q)}\left(Q^T(\mu+\delta') - Q^T(U'+\delta') - U^TU\right) \\
&= \frac{1}{L(Q)}\left(Q^T(\mu-U') - U^TU\right) \\
&= \frac{1}{L(Q)}\left(Q^T(-f+\Lambda Q) - U^TU\right).
\end{aligned}
$$

Note that $(D(t), E(t))^T$ as given above is independent of the derivatives of the interpolants as well as of the derivatives of the defects and residuals.

The exact formulas of $(D_n(t), E_n(t))^T$ for the local problem is,

$$
\begin{aligned}
D_n(t) &= \frac{1}{L(Q_n(t))}\left(Q_n^T(t)(f-\Lambda_n(t)Q_n(t)) + U_n^T(t)U_n(t)\right)Q_n(t) + \mu_n(t), \\
E_n(t) &= \frac{1}{L(Q_n(t))}\left(Q_n^T(t)(-f+\Lambda_n(t)Q_n(t)) - U_n^T(t)U_n(t)\right).
\end{aligned}
$$

In addition, we used exact formulas for the projected values $(\hat{y}_n, \hat{z}_n, \hat{\lambda}_n)^T$.

6.2.2 Index 2 pendulum problem

The index 2 formulation of the pendulum problem is,

$$
\begin{aligned}
q'(t) &= u(t), \\
u'(t) &= f - \lambda(t)q(t), \\
0 &= q^T(t)u(t).
\end{aligned}
$$

The underlying ODE is (6.2). Let $(Q(t), U(t), \Lambda(t))^T$ be a continuous approximation to $(q(t), u(t), \lambda(t))^T$ satisfying the perturbed equation,

$$
Q'(t) = U(t) + \delta(t),
$$

$$\begin{aligned} U'(t) &= f - \Lambda(t)Q(t) + \mu(t), \\ 0 &= Q^T(t)U(t) + \theta(t). \end{aligned}$$

We have, after differentiating the constraint,

$$\begin{aligned} 0 &= Q^T U' + Q'^T U + \theta' \\ &= Q^T(f - \Lambda Q + \mu) + Q'^T U + \theta', \\ L(Q)\Lambda &= Q^T(f+\mu) + Q'^T U + \theta', \\ \Lambda &= \frac{1}{L(Q)}\left(Q^T(f+\mu) + Q'^T U + \theta'\right), \\ U' &= f - \frac{1}{L(Q)}\left(Q^T(f+\mu) + (U+\delta)^T U + \theta'\right) Q + \mu \\ &= f - \frac{1}{L(Q)}\left(Q^T f + U^T U\right) Q - \frac{1}{L(Q)}\left(Q^T \mu + \delta^T U + \theta'\right) Q + \mu. \end{aligned}$$

Therefore the underlying exact defect is,

$$\begin{aligned} D(t) &= -\frac{1}{L(Q)}\left(Q^T \mu + \delta^T U + \theta'\right) Q + \mu \\ &= \frac{1}{L(Q)}\left(Q^T(U' - \mu) + (Q' - \delta)^T U\right) Q + \mu \\ &= \frac{1}{L(Q)}\left(Q^T(f - \Lambda Q) + U^T U\right) Q + \mu. \end{aligned}$$

The underlying residual is given by,

$$\begin{aligned} E(t) &= \frac{1}{L(Q)}\left(Q^T \mu + \delta^T U + \theta'\right) \\ &= \frac{1}{L(Q)}\left(Q^T(-f + \Lambda Q - U^T U\right), \end{aligned}$$

which is independent of the derivatives of the interpolants as well as of the derivatives of the defects and residuals.

The exact formulas of $(D_n(t), E_n(t))^T$ for the local problem is,

$$\begin{aligned} D_n(t) &= \frac{1}{L(Q_n(t))}\left(Q_n^T(t)(f - \Lambda_n(t)Q_n(t)) + U_n^T(t)U_n(t)\right) Q_n(t) + \mu_n(t), \\ E_n(t) &= \frac{1}{L(Q_n(t))}\left(Q_n^T(t)(-f + \Lambda_n(t)Q_n(t)) - U_n^T(t)U_n(t)\right). \end{aligned}$$

In addition, we used exact formulas for the projected values $(\hat{y}_n, \hat{z}_n)^T$.

6.2.3 Stabilized index 2 pendulum problem

The stabilized index 2 pendulum problem is given by [23],

$$\begin{aligned}
q'(t) &= u(t) - \rho(t)q(t), \\
u'(t) &= f - \lambda(t)q(t), \\
0 &= q(t)^T q(t) - 1, \\
0 &= q(t)^T u(t),
\end{aligned}$$

where in addition, $\rho(0) = 0$. We use the same underlying defect and residual as developed in the two preceding subsections. In addition, we used exact formulas for the projected values $(\hat{y}_n, \hat{z}_n)^T$.

6.2.4 Index 3 seven body problem

Consider the index 3 seven body problem [28, pp. 531–544],

$$\begin{aligned}
q'(t) &= u(t), \\
u'(t) &= M(q(t))^{-1}(f(q(t), u(t)) - G^T(q(t))\lambda(t)), \\
0 &= g(q(t)),
\end{aligned}$$

where the mass matrix $M(q(t))$ of size 7×7 is nonsingular and $G(q(t)) = g_q(q(t))$. The system consists of 7 rigid bodies connected by joints without friction in plane motion (Figure 6.1). The system is driven by a motor with constant drive torque mom. The position coordinates (measured in angles) $q(t) = (q_1(t), \ldots, q_7(t))^T$ are denoted by,

$$(\beta(t), \Theta(t), \gamma(t), \Phi(t), \rho(t), \Omega(t), \epsilon(t))^T.$$

The data are,

- c_0 : the spring coefficient.
- l_0 : the unstretched spring length.
- mom : the drive torque.
- m_i : the mass of the ith body.
- I_i : the inertia of the ith body.

The ADEs consists 14 first order ODEs and 6 constraints,

$$rr\cos\beta - d\cos(\beta + \Theta) - ss\sin\gamma = xb,$$

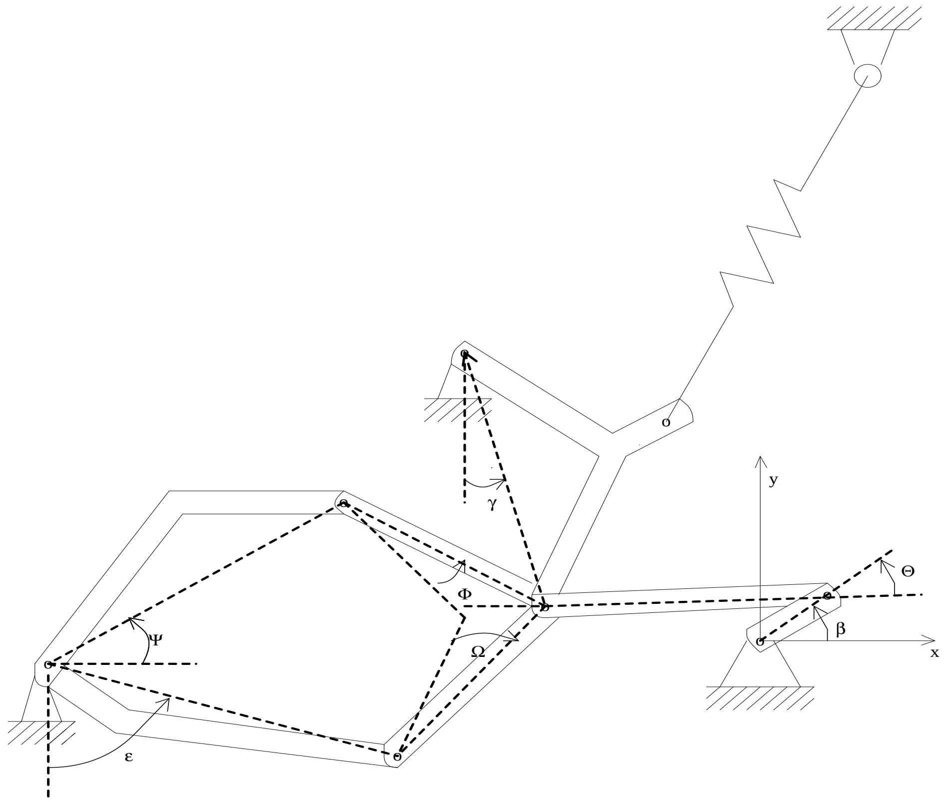

Figure 6.1: The seven body problem

$$\begin{aligned}
rr\sin\beta - d\sin(\beta+\Theta) + ss\cos\gamma &= yb, \\
rr\cos\beta - d\cos(\beta+\Theta) - e\sin(\Phi+\Psi) - zt\cos\Psi &= xa, \\
rr\sin\beta - d\sin(\beta+\Theta) + e\cos(\Phi+\Psi) - zt\sin\Psi &= ya, \\
rr\cos\beta - d\cos(\beta+\Theta) - zf\cos(\Omega+\epsilon) - u\sin\epsilon &= xa, \\
rr\sin\beta - d\sin(\beta+\Theta) - zf\sin(\Omega+\epsilon) + u\cos\epsilon &= ya,
\end{aligned}$$

where,

$$rr, ss, d, e, zf, zt, u, xa, xb, ya, yb,$$

are the geometry parameters of the system. Let $L(q) = G(q)M(q)^{-1}G^T(q)$ and denote $G_q(q)(u,u) =$

$g_{qq}(q)(u,u)$ (a bilinear form). We derive the underlying ODE by differentiating the constraint,

$$
\begin{aligned}
0 &= G(q)u, \\
0 &= G(q)u' + G_q(q)(u,u) \\
&= G(q)M(q)^{-1}\left(f(q,u) - G^T(q)\lambda\right) + G_q(q)(u,u), \\
L(q)\lambda &= G(q)M(q)^{-1}f(q,u) + G_q(q)(u,u), \\
\lambda &= L(q)^{-1}\left(G(q)M(q)^{(-1)}f(q,u) + G_q(q)(u,u)\right).
\end{aligned}
$$

The underlying ODE is,

$$
u' = M(q)^{-1}\left(f(q,u) - G^T(q)L(q)^{-1}\left[G(q)M(q)^{-1}f(q,u) + G_q(q)(u,u)\right]\right). \tag{6.3}
$$

Now consider the perturbed equation,

$$
\begin{aligned}
Q'(t) &= U(t) + \delta(t), \\
U'(t) &= M(Q(t))^{-1}\left(f(Q(t),U(t)) - G^T(Q(t))\Lambda(t)\right) + \mu(t), \\
0 &= g(Q(t)) + \theta(t).
\end{aligned}
$$

By differentiating the constraint twice, we have,

$$
\begin{aligned}
0 &= G(Q)(U+\delta) + \theta', \ \text{(index 2)}, \\
0 &= G(Q)(U'+\delta') + G_q(Q)(U+\delta,U+\delta) + \theta'', \ \text{(index 1)}, \\
&= G(Q)\left(M(Q)^{-1}(f(Q,U) - G^T\Lambda) + \mu + \delta'\right) + G_q(Q)(U+\delta,U+\delta) + \theta'', \\
L(Q)\Lambda &= G(Q)\left(M(Q)^{-1}f(Q,U) + \mu + \delta'\right) + G_q(Q)(U+\delta,U+\delta) + \theta'', \\
\Lambda &= L(Q)^{-1}\left(G(Q)\left(M(Q)^{-1}f(Q,U) + \mu + \delta'\right) + G_q(Q)(U+\delta,U+\delta) + \theta''\right).
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
&U' \\
&= M(Q)^{-1}\left(f - G^T(Q)L(Q)^{-1}[G(Q)(M(Q)^{-1}f + \mu + \delta') + G_q(Q)(U+\delta,U+\delta) + \theta'']\right) + \mu \\
&= M(Q)^{-1}\left(f - G^T(Q)L(Q)^{-1}[G(Q)M^{-1}f + G_q(Q)(U,U)]\right) \\
&\quad - M(Q)^{-1}G^T(Q)L(Q)^{-1}\left(G(Q)(\mu+\delta') + G_q(Q)(U+\delta,U+\delta) - G_q(Q)(U,U) + \theta''\right) + \mu,
\end{aligned}
$$

so that the defect associated with the underlying ODE is given by,

$$
D - M(Q)^{-1}G^T(Q)L(Q)^{-1}\left(G(Q)(\mu+\delta') + G_q(Q)(U+\delta,U+\delta) - G_q(Q)(U,U) + \theta''\right) + \mu,
$$

or,

$$\begin{aligned} -G(Q)D &= G(Q)(\mu+\delta') + G_q(Q)(U+\delta, U+\delta) - G_q(Q)(U,U) + \theta'' - G(Q)\mu \\ &= -G(Q)U' - G_q(Q)(U,U). \end{aligned}$$

In addition, the residual $E(t)$ can be derived to be,

$$E(t) = L(Q)^{-1}\left(G(Q)(\mu+\delta') + G_q(Q)(U+\delta, U+\delta) - G_q(Q)(U,U) + \theta''\right).$$

Therefore, $(D(t), E(t))^T$ satisfies the equation,

$$\begin{pmatrix} M(Q(t)) & G^T(Q(t)) \\ G(Q(t)) & 0 \end{pmatrix} \begin{pmatrix} D(t) \\ E(t) \end{pmatrix} = \begin{pmatrix} M(Q(t))\mu(t) \\ G(Q(t))U'(t) + G_q(Q(t))(U(t), U(t)) \end{pmatrix}, \quad (6.4)$$

Since $(D(t), E(t))^T$ as writen in (6.4) involves the computation of the inverse $L(Q)^{-1}$, it is preferable to seek their values by solving the above system. Also, note that the second component of the RHS can be computed by differentiating (with respect to t) the term $G(Q(t))U(t)$.

The exact formulas of $(D_n(t), E_n(t))^T$ for the local problem is,

$$\begin{pmatrix} M(Q_n(t)) & G^T(Q_n(t)) \\ G(Q_n(t)) & 0 \end{pmatrix} \begin{pmatrix} D_n(t) \\ E_n(t) \end{pmatrix} = \begin{pmatrix} M(Q_n(t))\mu_n(t) \\ G(Q_n(t))U_n'(t) + G_q(Q_n(t))(U_n(t), U_n(t)) \end{pmatrix},$$

However, we used simplified Newton iterations for the projected value $\hat{q}_n$, and a linearized formula for the projected value $\hat{u}_n$,

$$\begin{pmatrix} M(q_n) & G^T(q_n) \\ G(q_n) & 0 \end{pmatrix} \begin{pmatrix} \hat{u}_n \\ \nu \end{pmatrix} = \begin{pmatrix} M(q_n)u_n \\ 0 \end{pmatrix}.$$

6.2.5 Index 2 seven body problem

Consider the index 2 seven body problem,

$$\begin{aligned} q'(t) &= u(t), \\ u'(t) &= M(q(t))^{-1}(f(q(t), u(t)) - G^T(q(t))\lambda(t)), \\ 0 &= G(q(t))u(t). \end{aligned}$$

The underlying ODE is (6.3). Consider the perturbed equation,

$$Q'(t) = U(t) + \delta(t),$$

$$
\begin{aligned}
U'(t) &= M(Q(t))^{-1}(f(Q(t),U(t)) - G^T(Q(t))\Lambda(t)) + \mu(t), \\
0 &= G(Q(t))U(t) + \theta(t).
\end{aligned}
$$

To derive the underlying perturbed equation, we differentiate the constraint,

$$
\begin{aligned}
0 &= G(Q)U' + G_q(Q)(U,U) + \theta' \\
&= G(Q)\left(M(Q)^{-1}\left(f(Q,U) - G^T(Q)\Lambda\right) + \mu\right) + G_q(Q)(U,U) + \theta', \\
L(Q)\Lambda &= G(Q)M(Q)^{-1}f(Q,U) + G(Q)\mu + G_q(Q)(U,U) + \theta', \\
\Lambda &= L(Q)^{-1}(G(Q)M(Q)^{-1}f(Q,U) + G(Q)\mu + G_q(Q)(U,U) + \theta'), \\
U' &= M^{-1}[f - G^T L^{-1}(GM^{-1}f + G\mu + G_q(Q)(U,U) + \theta')] + \mu \\
&= M^{-1}[f - G^T L^{-1}(GM^{-1}f + G_q(Q)(U,U)] - M^{-1}G^T L^{-1}(G\mu + \theta') + \mu.
\end{aligned}
$$

So that the corresponding defect of the underlying ODE is given by,

$$
\begin{aligned}
D &= M(Q)^{-1}G(Q)^T L(Q)^{-1}(-G(Q)\mu + G(Q)U' + G_q(Q)(U,U)) + \mu, \\
G(Q)D &= G(Q)U' + G_q(Q)(U,U) \\
&= -\theta'.
\end{aligned}
$$

The residual is given by,

$$
E(t) = L(Q)^{-1}(-G(Q)\mu + G(Q)U' + G_q(Q)(U,U).
$$

Note that $(D(t),E(t))^T$ satifies the equation,

$$
\begin{pmatrix} M(Q(t)) & G^T(Q(t)) \\ G(Q(t)) & 0 \end{pmatrix} \begin{pmatrix} D(t) \\ E(t) \end{pmatrix} = \begin{pmatrix} M(Q(t))\mu(t) \\ -\theta'(t) \end{pmatrix}.
$$

However, we used a linearized formula for the projected value $\hat{u}_n$,

$$
\begin{pmatrix} M(q_n) & G^T(q_n) \\ G(q_n) & 0 \end{pmatrix} \begin{pmatrix} \hat{u}_n \\ \nu \end{pmatrix} = \begin{pmatrix} M(q_n)u_n \\ 0 \end{pmatrix}.
$$

6.2.6 GGL index 2 seven body problem

The formulation is given by [28, p. 540],

$$
\begin{aligned}
q'(t) &= u(t) + G^T(q)\rho(t), \\
u'(t) &= M(q(t))^{-1}(f(q(t),u(t)) + G^T(q(t))\lambda(t)),
\end{aligned}
$$

$$
\begin{aligned}
0 &= g(q(t)), \\
0 &= G(q(t))u(t),
\end{aligned}
$$

where $\rho : R \to R^6$. We used the same defect, residual and projected values as prescribed in the preceding subsection. as developed in the preceding subsection.

6.2.7 Index 2 cavity problem

Consider the (conservative) Navier-Stokes equation [13], [25], [43], [31],

$$
\begin{aligned}
\mathbf{u}' &= \frac{1}{Re}\nabla^2\mathbf{u} - \nabla \cdot (\mathbf{u}\mathbf{u}) - \nabla p, \quad 0 \le t \le 50, \\
0 &= div\, \mathbf{u},
\end{aligned}
$$

on the unit square. Here Re is the Reynolds number and $\mathbf{u} = (u(t), v(t))^T$ is the velocity. The initial condition is $(u(0), v(0)) = (0, 0)$, $p(t) = 0$. The boundary condition is $(u(x, y), v(x, y)) = (1, 0)$ on the top and $(u(x, y), v(x, y)) = 0$ elsewhere. We will discretize this PDE into an ADE by discretizing

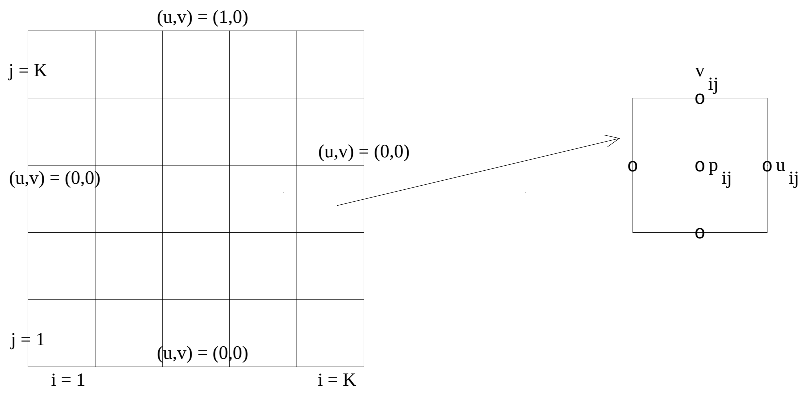

Figure 6.2: A staggered grid

in space to yield a system of ODEs (with constraints) in time. This system of ADEs will then be our test problem. Note that there are several spatial discretizations that could be used. We have chosen one the staggered grid method that has been recommended in the literature (Figure 6.2). For one test, we chose $t_end = 50, Re = 100, Dx = Dy = \frac{1}{5}$ and this results in 65 unknowns for our direct linear solver. We denote $K = 5$ the number of cells in each direction. For another test, we chose $t_end = 3, Re = 105, Dx = Dy = \frac{1}{10}$ (or $K = 10$.) The discretized unknowns are,

$$
u_{ij}(t), v_{ij}(t), p_{ij}(t), \quad i, j = 1, \ldots, K.
$$

Denote:

- ∇^2: the 5-point operator.
- ∇_ν : forward difference in the ν direction.
- $\triangle_\nu$: backward difference in the ν direction.
- D_ν : centered difference in the ν direction.

and denote,

$$\begin{aligned}\bar{u}^y_{ij} &= \frac{1}{2}(u_{i,j} + u_{i,j+1}),\\ \bar{v}^x_{ij} &= \frac{1}{2}(v_{i,j} + v_{i+1,j}),\end{aligned}$$

to be the mean values. Then the discretized $ij-$th differential equation, $(i,j = 1,\ldots,K)$ is,

$$\begin{aligned}u'_{ij} &= \tfrac{1}{Re}\nabla^2 u_{ij} - \nabla_x p_{ij} - D_x u^2_{ij} - \tfrac{1}{Dx}(\bar{u}^y_{ij}\bar{v}^x_{ij} - \bar{u}^y_{i,j-1}\bar{v}^x_{i,j-1}), \quad i = 1,\ldots,K-1,\ j = 1,\ldots,K,\\ v'_{ij} &= \tfrac{1}{Re}\nabla^2 v_{ij} - \nabla_y p_{ij} - D_y v^2_{ij} - \tfrac{1}{Dx}(\bar{u}^y_{ij}\bar{v}^x_{ij} - \bar{u}^y_{i-1,j}\bar{v}^x_{i-1,j}), \quad i = 1,\ldots,K,\ j = 1,\ldots,K-1,\end{aligned} \tag{6.5}$$

where the values of the boundary points u_{0j}, u_{Kj} and the "imaginary" points u_{i0}, u_{iK+1} (determined by the boundary conditions) are,

$$\begin{aligned}u_{0j} &= 0, \quad j = 1,\ldots,K,\\ u_{Kj} &= 0, \quad j = 1,\ldots,K,\\ u_{i0} &= -u_{i1}, \quad j = 1,\ldots,K-1,\\ u_{iK+1} &= 2 - u_{iK-1}, \quad j = 1,\ldots,K-1.\end{aligned}$$

Similarly, the values of the boundary points v_{i0}, v_{iK} and the "imaginary" points v_{0j}, u_{K+1j} (determined by the boundary conditions) are,

$$\begin{aligned}v_{i0} &= 0, \quad i = 1,\ldots,K,\\ v_{iK} &= 0, \quad i = 1,\ldots,K,\\ v_{0j} &= -v_{1j}, \quad j = 1,\ldots,K-1,\\ v_{K+1j} &= -v_{Kj}, \quad j = 1,\ldots,K-1.\end{aligned}$$

The discretized $ij-$th constraint $(i,j = 1,\ldots,K)$ is,

$$0 = g_{ij} \equiv \triangle_x u_{ij} + \triangle_y v_{ij}. \tag{6.6}$$

Thus (6.5) and (6.6) constitute a system of ADEs of the form,

$$\begin{aligned} y'(t) &= f(y(t)) - Cp(t), \\ 0 &= C^T y(t), \end{aligned} \tag{6.7}$$

where C^T is a constant matrix representing the discretized divergence term. The resulting ADE (6.7) is of index 2 since in order to obtain the (unique) expression for the algebraic variables $p(t)$ in terms of the differential variable $y(t)$, one must use $y'(t)$, or one must differentiate the constraint once.

We derive the underlying IPV by differentiating the constraint,

$$\begin{aligned} 0 &= C^T y'(t) \\ &= C^T (f(y(t)) - Cp(t)) \\ &= C^T f(y(t)) - C^T C p(t), \\ p(t) &= (C^T C)^{-1} C^T f(y(t)), \\ y'(t) &= f(y(t)) - C(C^T C)^{-1} C^T f(y(t)). \end{aligned}$$

On the other hand, consider an approximation $(U(t), P(t))$ for $(y(t), p(t))$ and the corresponding perturbed equation,

$$\begin{aligned} U'(t) &= f(U(t)) - CP(t) + \delta(t), \\ 0 &= C^T U(t) + \theta(t). \end{aligned}$$

It follows that,

$$\begin{aligned} 0 &= C^T U'(t) + \theta'(t) \\ &= C^T (f(U(t)) - CP(t) + \delta(t)) + \theta'(t), \\ P(t) &= (C^T C)^{-1} \left[C^T (f(U(t)) + \delta(t)) + \theta'(t) \right], \\ U'(t) &= f(U(t)) - C(C^T C)^{-1} \left[C^T (f(U(t)) + \delta(t)) + \theta'(t) \right] + \delta(t) \\ &= f(U(t)) - C(C^T C)^{-1} C^T f(U(t)) - C(C^T C)^{-1} (C^T \delta(t) + \theta'(t)) + \delta(t). \end{aligned}$$

Therefore the exact defect is,

$$\begin{aligned} D(t) &= -C(C^T C)^{-1} (C^T \delta(t) + \theta'(t)) + \delta(t), \\ C^T D(t) &= -\theta'(t). \end{aligned}$$

To compute $D(t)$, note that it satifies the equation,

$$\begin{pmatrix} I & -C \\ C^T & 0 \end{pmatrix} \begin{pmatrix} D(t) \\ E(t) \end{pmatrix} = \begin{pmatrix} \delta(t) \\ -\theta'(t) \end{pmatrix},$$

where,

$$-\theta'(t) = C^T U'(t),$$

and where $E(t)$ can be used to control the computed algebraic residual.

However, note that one must discard one constraint equation as this results in an overdetermined linear system otherwise. The substituted constraint can be any linear combination of p_{ij} provided that the resulting matrix is nonsingular. This can also be explained by the fact that the pressure is unique up to a constant as there is no boundary condition for the pressure. Thus an alternative choice for the constraints (6.6) is,

$$\begin{aligned} 0 &= g_{ij} \equiv \triangle_x u_{ij} + \triangle_y v_{ij}, \quad (i,j) \neq (K,K), \\ 0 &= g_{K,K} \equiv \sum_{i,j=1}^{K} p_{ij}, \end{aligned}$$

Here the additional condition,

$$0 = \sum_{i,j=1}^{K} p_{ij},$$

or,

$$0 = \int p,$$

fixes the choice of the arbitrary constant in the pressure [43].

In practice, we used the original defect and residual $(\delta_n(t), \theta_n(t))^T$ in our error control.

Chapter 7

Numerical Results

We applied Scheme 2 and Scheme 3 to the test problems described in Chapter 6. We are mainly concerned with the following measurements, [1]

- ACC, REJ: the number of accepted and rejected steps.
- NFCN, NSOL: the number of function evaluations and the number of Newton iterations.
- G1, G2, G3: the index 1, index2 and index 3 constraints satisfied by the contructed interpolants. For each accepted step, we sampled $\max(g1(Q(t), U(t), \Lambda(t)))$, $\max(g2(Q(t), U_n(t)))$ and $\max(g3(Q_n(t)))$ at 20 equally-spaced points.
- Q, U, LAM: the global errors in $Q(t), U(t)$ and $\Lambda(t)$ respectively, where we used the computed values from RADAU5 at a strict tolerance (TOL $= 10^{-10}$) as the "true" values. We sampled $\max(Q(t) - q(t))$, $\max(U(t) - u(t))$ and $\max(\Lambda(t) - \lambda(t))$ at the middle and at the right end points for each accepted step.
- DEL: the defect $\delta(t)$ associated with the interpolants. We sampled $\max(\delta(t))$ on 20 equally-spaced points for each accepted step.

We tabulated these results with the rows of each table corresponding to tolerance values TOL in the default range $10^{-2}, 10^{-3}, \ldots$ (except where indicated otherwise.) The associated average values or the observed orders of convergence are presented in the last row of each table.

[1] Note that these apply to CMS problems, similar discussions can be applied to the driven cavity problem.

7.1 Index 2 pendulum problem

RADAU5									
ACC	REJ	NFCN	NSOL	G1	G2	G3	Q	U	LAM
40	6	642	200	.13D-01	.34D-03	.38D-03	.41D-03	.84D-03	.41D-02
53	7	683	209	.39D-02	.68D-04	.52D-04	.52D-04	.98D-04	.11D-02
86	7	854	256	.59D-03	.57D-05	.81D-05	.55D-05	.11D-04	.16D-03
146	3	1274	376	.63D-04	.41D-06	.14D-05	.99D-06	.20D-05	.21D-04
257	1	2021	588	.99D-05	.23D-07	.14D-06	.15D-06	.26D-06	.28D-05
456	1	3168	904	.17D-05	.21D-08	.14D-07	.19D-07	.32D-07	.71D-06
		8.1	2.4	3.7	4.9	4.2	4.1	4.2	3.6

GAUSS2, (TOL = $10^{-3}, \ldots$), levels 0, 1										
ACC	REJ	NFCN	NSOL	G1	G2	G3	Q	U	LAM	DEL
94	0	661	236	.26D-04	.93D-05	.21D-04	.17D-04	.25D-04	.41D-04	.12D-03
192	0	1195	405	.12D-05	.36D-06	.53D-06	.25D-05	.35D-05	.48D-05	.94D-05
408	0	2445	814	.55D-07	.16D-07	.27D-07	.36D-07	.52D-07	.67D-06	.83D-06
870	0	5209	1734	.25D-08	.69D-09	.13D-08	.31D-08	.44D-08	.20D-06	.76D-07
1868	0	11189	3726	.11D-09	.32D-10	.61D-10	.13D-09	.36D-09	.75D-07	.71D-08
		6.0	2.0	4.1	4.2	4.3	3.9	3.7	2.1	3.3
46	6	567	179	.28D-04	.37D-04	.30D-04	.28D-03	.43D-03	.37D-03	.17D-03
77	4	819	247	.11D-05	.20D-05	.24D-05	.35D-04	.50D-04	.58D-04	.17D-04
129	2	1289	382	.61D-07	.10D-06	.20D-06	.39D-05	.56D-05	.87D-05	.16D-05
221	1	2163	637	.35D-08	.56D-08	.10D-07	.40D-06	.57D-06	.20D-05	.15D-06
395	7	3893	1142	.17D-09	.30D-09	.58D-09	.40D-07	.57D-07	.68D-06	.14D-07
707	12	6967	2045	.11D-10	.16D-10	.30D-10	.38D-08	.66D-08	.28D-06	.14D-08
		9.8	2.9	5.4	5.4	5.1	4.1	4.1	2.6	4.3

GAUSS3, levels 0, 1, 2, 3										
ACC	REJ	NFCN	NSOL	G1	G2	G3	Q	U	LAM	DEL
74	0	740	197	.52D-03	.11D-03	.31D-03	.25D-03	.34D-03	.43D-03	.10D-02
145	0	1296	335	.26D-04	.43D-05	.13D-04	.67D-05	.92D-05	.13D-04	.81D-04
282	0	2287	574	.11D-05	.24D-06	.64D-06	.87D-06	.12D-05	.15D-05	.77D-05
537	0	4051	992	.52D-07	.14D-07	.36D-07	.60D-07	.84D-07	.50D-06	.79D-06
1044	0	7381	1764	.25D-08	.70D-09	.16D-08	.16D-08	.28D-08	.19D-06	.74D-07
2070	0	14233	3364	.11D-09	.32D-10	.64D-10	.14D-09	.37D-09	.74D-07	.71D-08
		7.2	1.7	4.6	4.5	4.6	4.3	4.1	2.6	3.6
42	1	644	157	.30D-03	.39D-03	.30D-03	.40D-03	.93D-03	.68D-03	.12D-02
57	4	842	199	.26D-04	.17D-04	.35D-04	.48D-04	.13D-03	.15D-03	.13D-03
85	6	1124	253	.17D-05	.89D-06	.18D-05	.83D-05	.15D-04	.25D-04	.13D-04
135	3	1573	340	.98D-07	.54D-07	.17D-06	.17D-05	.18D-05	.57D-05	.14D-05
230	5	2537	532	.71D-08	.27D-08	.72D-08	.22D-06	.21D-06	.19D-05	.13D-06
399	5	4176	853	.53D-09	.15D-09	.46D-09	.36D-07	.28D-07	.70D-06	.14D-07
		11.2	2.4	5.9	6.6	5.9	4.1	4.6	3.1	5.1
40	0	731	150	.39D-03	.96D-04	.32D-03	.12D-02	.37D-02	.43D-02	.49D-03
44	5	947	201	.93D-04	.20D-04	.31D-04	.36D-03	.11D-02	.12D-02	.84D-04
52	5	1081	227	.71D-05	.23D-05	.50D-05	.67D-04	.22D-03	.24D-03	.18D-04
76	5	1372	268	.92D-06	.20D-06	.41D-06	.14D-04	.37D-04	.56D-04	.19D-05
104	9	1923	377	.59D-07	.13D-07	.30D-07	.25D-05	.68D-05	.14D-04	.22D-06
150	5	2580	498	.10D-07	.76D-09	.28D-08	.69D-06	.11D-05	.44D-05	.21D-07
		17.4	3.5	8.0	8.9	8.8	5.6	6.2	5.2	7.6
36	0	850	151	.12D-02	.17D-03	.25D-03	.32D-02	.86D-02	.76D-02	.95D-03
41	1	1147	228	.28D-04	.44D-04	.17D-04	.10D-02	.32D-02	.38D-02	.17D-03
44	2	1218	237	.40D-05	.51D-05	.19D-05	.31D-03	.84D-03	.96D-03	.22D-04
58	4	1616	311	.98D-06	.32D-06	.54D-06	.15D-03	.25D-03	.22D-03	.24D-05
73	7	2066	395	.15D-06	.36D-07	.42D-07	.36D-04	.74D-04	.10D-03	.33D-06
86	7	2455	477	.14D-07	.29D-08	.28D-08	.85D-05	.19D-04	.33D-04	.35D-07
		26.1	5.0	13.0	12.6	13.1	6.8	7.0	6.3	11.7

7.2 Stabilized index 2 pendulum problem

RADAU5									
ACC	REJ	NFCN	NSOL	G1	G2	G3	Q	U	LAM
38	4	637	199	.16D-01	.38D-03	.23D-03	.24D-03	.74D-03	.49D-02
57	7	703	214	.28D-02	.37D-04	.40D-04	.66D-04	.89D-04	.88D-03
94	1	881	262	.13D-02	.35D-05	.57D-05	.82D-05	.11D-04	.30D-03
161	4	1410	416	.63D-04	.26D-06	.58D-06	.39D-05	.55D-05	.17D-04
285	2	2095	603	.87D-05	.19D-07	.38D-07	.19D-06	.28D-06	.28D-05
505	1	3503	999	.15D-05	.18D-08	.52D-08	.84D-08	.16D-07	.70D-06
		8.0	2.3	3.6	4.7	4.1	4.0	4.2	3.4

DIRK2										
ACC	REJ	NFCN	NSOL	G1	G2	G3	Q	U	LAM	DEL
68	14	516	351	.14D-03	.50D-04	.27D-03	.16D-01	.23D-01	.21D-01	.14D-02
136	6	837	552	.47D-05	.18D-05	.17D-04	.18D-02	.26D-02	.24D-02	.14D-03
289	0	1647	1068	.25D-06	.61D-07	.67D-06	.19D-03	.26D-03	.24D-03	.13D-04
616	0	3492	2259	.80D-08	.23D-08	.36D-07	.18D-04	.26D-04	.23D-04	.12D-05
1315	0	7570	4939	.31D-09	.10D-09	.16D-08	.18D-05	.26D-05	.23D-05	.12D-06
2829	6	16897	11226	.12D-10	.46D-11	.74D-10	.18D-06	.26D-06	.24D-06	.13D-07
		5.9	3.9	4.3	4.3	4.1	3.1	3.1	3.1	3.1

GAUSS2, levels 0, 1										
ACC	REJ	NFCN	NSOL	G1	G2	G3	Q	U	LAM	DEL
49	7	439	163	.49D-03	.24D-03	.26D-03	.15D-02	.20D-02	.18D-02	.15D-02
90	0	655	237	.25D-04	.11D-04	.15D-04	.67D-04	.94D-04	.94D-04	.13D-03
186	0	1177	402	.11D-05	.41D-06	.73D-06	.41D-05	.58D-05	.72D-05	.10D-04
393	0	2345	779	.50D-07	.18D-07	.32D-07	.16D-06	.23D-06	.83D-06	.91D-06
844	0	5051	1681	.22D-08	.79D-09	.15D-08	.72D-08	.10D-07	.21D-06	.81D-07
1812	0	10857	3616	.10D-09	.36D-10	.69D-10	.43D-09	.61D-09	.83D-07	.77D-08
		6.1	2.0	4.3	4.4	4.2	4.2	4.2	2.8	3.4
37	2	485	164	.50D-03	.58D-03	.29D-03	.26D-02	.39D-02	.31D-02	.18D-02
48	4	603	197	.27D-04	.44D-04	.27D-04	.46D-03	.70D-03	.52D-03	.19D-03
78	4	881	276	.17D-05	.28D-05	.18D-05	.61D-04	.90D-04	.78D-04	.21D-04
131	3	1401	432	.95D-07	.16D-06	.99D-07	.66D-05	.96D-05	.10D-04	.21D-05
226	2	2365	726	.51D-08	.92D-08	.54D-08	.66D-06	.95D-06	.21D-05	.22D-06
395	0	4037	1228	.27D-09	.52D-09	.30D-09	.66D-07	.95D-07	.58D-06	.22D-07
		10.5	3.3	6.1	5.9	5.8	4.5	4.5	3.6	4.8

GAUSS3, levels 0, 1, 2, 3 (TOL = $10^{-3}, \ldots$)										
ACC	REJ	NFCN	NSOL	G1	G2	G3	Q	U	LAM	DEL
74	0	821	224	.47D-03	.81D-04	.16D-03	.19D-03	.25D-03	.30D-03	.12D-02
130	0	1320	353	.24D-04	.51D-05	.12D-04	.24D-05	.53D-05	.28D-04	.11D-03
242	0	2105	540	.11D-05	.26D-06	.70D-06	.11D-05	.16D-05	.42D-05	.10D-04
447	0	3478	861	.49D-07	.13D-07	.35D-07	.47D-07	.66D-07	.66D-06	.84D-06
853	0	5922	1405	.22D-08	.79D-09	.17D-08	.28D-08	.39D-08	.21D-06	.81D-07
1809	0	13072	3151	.10D-09	.36D-10	.80D-10	.17D-09	.40D-09	.81D-07	.77D-08
		7.5	1.8	4.8	4.6	4.5	4.4	4.2	2.6	3.7
43	2	916	245	.25D-03	.29D-03	.28D-03	.36D-03	.11D-02	.11D-02	.13D-02
48	7	938	239	.18D-04	.23D-04	.31D-04	.48D-04	.16D-03	.19D-03	.16D-03
77	6	1086	251	.14D-05	.10D-05	.21D-05	.94D-05	.17D-04	.33D-04	.15D-04
126	5	1674	383	.11D-06	.57D-07	.12D-06	.17D-05	.20D-05	.20D-04	.15D-05
217	4	2748	621	.87D-08	.30D-08	.76D-08	.40D-06	.24D-06	.37D-05	.15D-06
381	4	3983	814	.52D-09	.17D-09	.42D-09	.40D-07	.30D-07	.97D-06	.14D-07
		12.3	2.8	6.0	6.6	6.1	4.2	4.8	3.2	5.2
38	0	900	211	.11D-02	.32D-03	.55D-03	.29D-02	.90D-02	.11D-01	.12D-02
38	6	1050	247	.11D-03	.19D-04	.46D-04	.46D-03	.14D-02	.17D-02	.16D-03
46	7	1122	250	.13D-04	.29D-05	.64D-05	.82D-04	.25D-03	.27D-03	.21D-04
65	6	1401	301	.11D-05	.19D-06	.47D-06	.17D-04	.45D-04	.11D-03	.23D-05
94	5	1864	390	.11D-06	.14D-07	.28D-07	.35D-05	.78D-05	.36D-04	.23D-06
147	3	2731	560	.59D-08	.80D-09	.14D-08	.56D-06	.12D-05	.53D-05	.23D-07
		19.9	4.3	9.0	9.5	9.5	6.3	6.6	5.6	8.0
38	1	1114	228	.51D-04	.94D-05	.12D-04	.11D-02	.27D-02	.29D-02	.52D-04
42	2	1292	269	.18D-04	.25D-05	.23D-05	.42D-03	.10D-02	.11D-02	.16D-04
53	2	1662	352	.18D-05	.25D-06	.82D-06	.19D-03	.38D-03	.30D-03	.29D-05
62	9	1994	404	.14D-06	.29D-07	.40D-07	.37D-04	.62D-04	.23D-03	.25D-06
82	5	2329	457	.16D-07	.26D-08	.28D-08	.11D-04	.19D-04	.92D-04	.31D-07
112	4	3002	575	.10D-08	.15D-09	.51D-09	.24D-05	.57D-05	.26D-04	.46D-08
		27.7	5.5	10.0	10.2	9.3	5.6	5.7	4.4	8.6

7.3 Index 3 pendulum problem

RADAU5									
ACC	REJ	NFCN	NSOL	G1	G2	G3	Q	U	LAM
50	23	815	248	.21D+01	.42D-02	.22D-03	.11D-02	.25D-02	.77D+00
129	17	1136	331	.26D+00	.12D-02	.26D-04	.14D-03	.76D-03	.69D-01
169	30	1454	421	.42D-01	.16D-03	.22D-05	.28D-04	.84D-04	.11D-01
232	20	1843	532	.19D-02	.13D-04	.19D-06	.21D-04	.33D-04	.15D-02
404	17	2952	845	.53D-03	.17D-05	.10D-07	.26D-05	.41D-05	.36D-03
709	13	4947	1410	.20D-03	.40D-06	.11D-08	.22D-06	.41D-06	.16D-03
		7.3	2.1	3.5	3.5	4.6	3.2	3.3	3.2

GAUSS2, (TOL = $10^{-1}, \ldots$) levels 0, 1										
ACC	REJ	NFCN	NSOL	G1	G2	G3	Q	U	LAM	DEL
32	4	595	261	.13D-01	.21D-02	.24D-02	.21D-01	.29D-01	.34D-01	.15D-01
58	7	1339	604	.66D-03	.10D-03	.18D-03	.61D-02	.86D-02	.73D-02	.24D-02
148	7	3193	1441	.16D-04	.19D-05	.11D-04	.10D-02	.15D-02	.11D-02	.24D-03
445	6	8187	3642	.77D-06	.37D-07	.56D-06	.10D-03	.14D-03	.11D-03	.27D-04
1384	3	22029	9627	.35D-07	.75D-09	.26D-07	.10D-04	.14D-04	.11D-04	.30D-05
		16.9	7.4	3.4	3.9	3.0	2.0	2.0	2.1	2.3
37	3	599	219	.39D-02	.12D-02	.36D-03	.21D-01	.29D-01	.28D-01	.97D-02
73	11	1081	372	.26D-03	.17D-04	.11D-05	.44D-02	.62D-02	.48D-02	.11D-02
201	12	2275	711	.87D-05	.50D-06	.48D-07	.49D-03	.70D-03	.54D-03	.11D-03
608	16	5811	1657	.26D-06	.48D-08	.22D-09	.50D-04	.71D-04	.55D-04	.11D-04
1910	17	16517	4404	.12D-07	.10D-09	.31D-11	.51D-05	.73D-05	.57D-05	.11D-05
		9.1	2.5	3.2	4.1	4.7	2.1	2.1	2.2	2.3

GAUSS3, levels 0, 1, 2, 3										
ACC	REJ	NFCN	NSOL	G1	G2	G3	Q	U	LAM	DEL
48	1	1659	520	.47D-03	.24D-03	.20D-03	.10D-02	.15D-02	.14D-02	.13D-02
95	0	3680	1163	.21D-04	.79D-05	.11D-04	.89D-04	.13D-03	.13D-03	.12D-03
197	0	8456	2687	.91D-06	.31D-06	.55D-06	.83D-05	.12D-04	.13D-04	.93D-05
420	0	19618	6259	.40D-07	.13D-07	.26D-07	.81D-06	.12D-05	.15D-05	.80D-06
903	0	45262	14485	.18D-08	.59D-09	.12D-08	.79D-07	.11D-06	.26D-06	.74D-07
1947	0	*****	33608	.79D-10	.26D-10	.54D-10	.77D-08	.11D-07	.80D-07	.71D-08
		50.8	16.3	4.2	4.3	4.1	3.2	3.2	2.6	3.3
37	5	1318	383	.51D-03	.25D-03	.35D-03	.43D-02	.64D-02	.59D-02	.10D-02
58	7	2421	720	.24D-04	.11D-04	.18D-04	.45D-03	.65D-03	.64D-03	.11D-03
107	5	4154	1235	.10D-05	.53D-06	.11D-05	.40D-04	.58D-04	.65D-04	.11D-04
210	5	7989	2376	.41D-07	.20D-07	.58D-07	.42D-05	.59D-05	.90D-05	.11D-05
431	7	16369	4872	.26D-08	.11D-08	.29D-08	.38D-06	.54D-06	.19D-05	.11D-06
904	3	33176	9849	.16D-09	.61D-10	.16D-09	.38D-07	.54D-07	.53D-06	.12D-07
		36.8	10.9	4.7	4.8	4.6	3.6	3.7	2.9	3.6
33	5	1347	360	.40D-03	.11D-03	.25D-03	.36D-02	.54D-02	.65D-02	.11D-02
57	12	2569	695	.36D-04	.46D-05	.13D-04	.34D-03	.66D-03	.52D-03	.12D-03
105	8	3441	883	.11D-05	.41D-07	.13D-06	.34D-04	.49D-04	.58D-04	.12D-04
209	10	4945	1137	.69D-07	.10D-08	.25D-08	.38D-05	.55D-05	.90D-05	.12D-05
429	10	8048	1658	.35D-08	.38D-10	.79D-10	.38D-06	.54D-06	.20D-05	.12D-06
915	11	14847	2788	.19D-09	.72D-12	.17D-11	.37D-07	.52D-07	.69D-06	.11D-07
		19.5	4.2	4.4	5.7	5.7	3.5	3.5	2.8	3.5
31	4	1151	255	.41D-03	.28D-04	.35D-04	.45D-02	.65D-02	.70D-02	.13D-02
59	9	2030	427	.23D-04	.49D-06	.16D-06	.36D-03	.52D-03	.49D-03	.13D-03
107	7	2953	566	.13D-05	.26D-07	.70D-08	.29D-04	.42D-04	.50D-04	.13D-04
215	8	5151	899	.69D-07	.69D-09	.84D-10	.32D-05	.46D-05	.69D-05	.14D-05
448	9	9651	1541	.31D-08	.16D-10	.97D-12	.32D-06	.46D-06	.22D-05	.13D-06
952	8	18793	2744	.18D-09	.47D-12	.14D-13	.32D-07	.46D-07	.65D-06	.13D-07
		21.4	3.5	4.3	5.2	6.3	3.5	3.5	2.7	3.4

7.4 Index 2 seven body problem

RADAU5									
ACC	REJ	NFCN	NSOL	G1	G2	G3	Q	U	LAM
45	14	955	302	.18D+01	.59D-03	.13D-05	.25D-03	.36D-01	.66D-01
72	28	1207	377	.18D+01	.33D-03	.36D-06	.38D-04	.58D-01	.30D-01
115	43	1575	486	.14D+01	.90D-04	.55D-07	.77D-05	.60D-02	.69D-02
194	56	2262	689	.53D+00	.97D-05	.77D-08	.48D-06	.31D-03	.14D-02
328	24	3038	903	.16D+00	.12D-05	.96D-09	.78D-07	.49D-04	.46D-03
577	11	4595	1339	.39D-01	.11D-06	.92D-10	.71D-08	.15D-05	.12D-03
		9.0	2.7	1.5	3.4	3.7	4.1	4.0	2.5

DIRK2, (TOL= $10^{-1}, \ldots$)										
ACC	REJ	NFCN	NSOL	G1	G2	G3	Q	U	LAM	DEL
84	20	607	398	.15D+01	.32D-03	.63D-04	.23D-01	.11D+02	.64D+01	.14D-01
155	35	1112	731	.55D+00	.65D-04	.10D-04	.38D-02	.71D+01	.89D+00	.21D-02
300	42	2008	1323	.86D-01	.54D-05	.15D-05	.54D-03	.47D+00	.13D+00	.36D-03
		5.9	3.9	2.3	3.2	2.9	3.0	2.5	3.1	2.9

GAUSS2, levels 1, 2										
ACC	REJ	NFCN	NSOL	G1	G2	G3	Q	U	LAM	DEL
85	26	1083	319	.91D+00	.19D-04	.18D-06	.85D-04	.28D-01	.12D-01	.73D-02
129	29	1539	453	.11D+00	.26D-05	.33D-07	.11D-04	.51D-02	.43D-02	.69D-03
205	33	2311	679	.16D-01	.25D-06	.57D-08	.14D-05	.93D-03	.11D-02	.42D-04
329	25	3409	996	.11D-02	.18D-07	.81D-09	.17D-06	.80D-04	.23D-03	.38D-05
550	54	5985	1784	.13D-03	.12D-08	.11D-09	.19D-07	.22D-04	.18D-03	.59D-06
934	63	9613	2812	.88D-05	.79D-10	.13D-10	.22D-08	.15D-05	.39D-04	.52D-07
		9.7	2.9	4.8	5.2	4.0	4.4	4.1	2.4	4.9
63	17	1073	256	.86D+00	.52D-05	.48D-06	.23D-03	.21D+00	.27D-01	.76D-03
91	28	1636	401	.90D-01	.92D-06	.12D-06	.31D-04	.17D-01	.68D-02	.27D-03
132	33	2284	564	.93D-02	.89D-07	.27D-07	.43D-05	.51D-02	.28D-02	.28D-04
211	27	3185	759	.11D-02	.36D-08	.44D-08	.61D-06	.37D-03	.53D-03	.14D-05
340	28	4875	1149	.12D-03	.11D-09	.60D-09	.98D-07	.91D-04	.42D-03	.17D-06
559	38	7890	1855	.66D-05	.47D-11	.68D-10	.12D-07	.18D-04	.10D-03	.13D-06
		13.4	3.2	5.4	6.4	4.1	4.5	4.3	2.6	4.0

GAUSS3, levels 1, 2, 3										
ACC	REJ	NFCN	NSOL	G1	G2	G3	Q	U	LAM	DEL
91	37	1773	420	.83D+00	.20D-04	.12D-06	.12D-04	.29D-02	.40D-02	.17D-02
131	31	1975	442	.18D+00	.24D-05	.15D-07	.24D-05	.17D-03	.95D-03	.36D-03
203	27	2628	569	.18D-01	.21D-06	.16D-08	.33D-06	.30D-04	.64D-03	.98D-04
327	31	3905	824	.13D-02	.16D-07	.12D-09	.61D-07	.12D-04	.26D-03	.74D-05
546	41	6177	1276	.13D-03	.11D-08	.83D-11	.92D-08	.11D-05	.70D-04	.39D-06
		11.2	2.4	4.9	5.5	5.4	4.0	4.4	2.2	4.7
67	32	1714	340	.97D+00	.67D-05	.29D-07	.70D-04	.93D-02	.14D-01	.13D-02
88	30	1955	376	.89D-01	.61D-06	.27D-08	.15D-04	.20D-02	.21D-02	.16D-03
125	38	2708	522	.10D-01	.40D-07	.35D-09	.51D-05	.70D-03	.89D-03	.28D-04
178	38	3541	676	.19D-02	.69D-08	.37D-10	.93D-06	.14D-03	.50D-03	.56D-05
259	29	4630	871	.17D-03	.76D-09	.37D-11	.20D-06	.26D-04	.20D-03	.87D-06
379	27	6482	1213	.19D-04	.72D-10	.35D-12	.37D-07	.61D-05	.12D-03	.67D-07
		16.3	3.1	6.3	6.6	6.5	4.4	4.2	2.7	5.7
50	19	1549	263	.11D+01	.25D-05	.11D-07	.10D-03	.15D-01	.63D-01	.66D-02
68	26	2106	357	.20D+00	.73D-06	.22D-08	.57D-04	.85D-02	.49D-02	.28D-02
90	29	2675	455	.14D-01	.42D-07	.10D-09	.17D-04	.20D-02	.40D-02	.28D-04
123	33	3523	602	.13D-02	.78D-08	.20D-10	.44D-05	.57D-03	.17D-02	.59D-05
169	29	4408	743	.19D-03	.44D-09	.30D-11	.17D-05	.24D-03	.56D-03	.51D-06
231	24	5662	952	.19D-04	.37D-10	.41D-12	.37D-06	.54D-04	.26D-03	.88D-06
		22.4	3.8	7.2	7.3	6.6	3.7	3.7	3.6	5.8

7.5 GGL seven body problem

RADAU5									
ACC	REJ	NFCN	NSOL	G1	G2	G3	Q	U	LAM
46	9	851	267	.20D+01	.62D-03	.70D-06	.44D-03	.95D-01	.18D+00
64	22	1118	350	.19D+01	.36D-03	.32D-06	.58D-04	.21D-01	.67D-01
103	34	1491	462	.14D+01	.13D-03	.74D-07	.67D-05	.56D-02	.78D-02
169	37	1987	605	.61D+00	.20D-04	.16D-07	.10D-05	.16D-03	.31D-02
289	26	2831	847	.11D+00	.22D-05	.27D-08	.16D-06	.16D-04	.78D-03
506	16	4431	1308	.18D-01	.21D-06	.27D-09	.17D-07	.59D-05	.15D-03
		9.6	2.9	2.0	3.3	3.3	4.2	4.0	3.0

DIRK2, (TOL $= 10^{-1}, \ldots$)										
ACC	REJ	NFCN	NSOL	G1	G2	G3	Q	U	LAM	DEL
80	24	618	409	.17D+01	.36D-03	.48D-06	.18D-01	.49D+01	.24D+01	.27D-01
139	33	1050	705	.61D+00	.81D-04	.82D-07	.29D-02	.12D+01	.42D+00	.35D-02
269	43	1928	1303	.55D-01	.75D-05	.91D-08	.42D-03	.53D+00	.94D-01	.46D-03
		6.1	4.1	2.8	3.2	3.3	3.1	1.8	2.7	3.4

GAUSS2, (TOL = $10^{-1}, \ldots$), levels 0, 1											
ACC	REJ	NFCN	NSOL	G1	G2	G3	Q	U	LAM	DEL	
78	24	761	278	.18D+01	.41D-03	.48D-06	.35D-03	.16D+00	.65D-01	.11D-01	
139	36	1217	433	.73D+00	.76D-04	.12D-06	.11D-04	.92D-02	.21D-02	.17D-02	
265	50	2035	702	.81D-01	.75D-05	.12D-07	.27D-06	.20D-03	.27D-03	.14D-03	
521	85	3701	1244	.60D-02	.51D-06	.79D-09	.26D-07	.23D-04	.48D-04	.56D-04	
1109	141	7511	2505	.40D-03	.29D-07	.42D-10	.23D-07	.56D-04	.20D-04	.48D-05	
		6.2	2.1	3.2	3.6	3.5	3.6	3.0	3.0	2.9	
54	17	693	204	.19D+01	.93D-04	.64D-06	.80D-03	.46D+00	.43D-01	.13D-01	
84	29	1125	336	.80D+00	.20D-04	.11D-06	.94D-04	.30D-01	.82D-02	.15D-02	
127	30	1561	466	.13D+00	.18D-05	.12D-07	.12D-04	.59D-02	.39D-02	.24D-03	
200	35	2335	697	.14D-01	.22D-06	.13D-08	.16D-05	.12D-02	.61D-03	.13D-03	
326	35	3591	1073	.13D-02	.18D-07	.86D-10	.19D-06	.16D-03	.32D-03	.21D-04	
543	50	6125	1876	.93D-04	.12D-08	.53D-11	.23D-07	.24D-04	.84D-04	.45D-06	
		10.1	3.0	4.3	4.9	5.1	4.5	4.3	2.7	4.5	

GAUSS3, levels 0 (TOL = $10^{-1}, \ldots$), 1, 2, 3											
ACC	REJ	NFCN	NSOL	G1	G2	G3	Q	U	LAM	DEL	
97	13	1121	300	.18D+01	.57D-03	.60D-06	.12D-03	.17D+00	.18D-01	.14D-01	
174	17	1802	473	.74D+00	.79D-04	.12D-06	.88D-05	.41D-02	.15D-02	.19D-02	
320	39	3140	807	.77D-01	.75D-05	.13D-07	.23D-06	.34D-03	.13D-03	.13D-03	
599	61	5491	1390	.57D-02	.50D-06	.78D-09	.33D-07	.64D-04	.41D-04	.15D-04	
1183	112	10142	2517	.40D-03	.28D-07	.42D-10	.31D-08	.47D-05	.15D-04	.31D-05	
		8.3	2.1	3.4	4.0	3.8	4.2	4.2	2.8	3.4	
84	23	1449	340	.10D+01	.23D-04	.12D-06	.16D-04	.61D-02	.64D-02	.29D-02	
129	36	2119	486	.11D+00	.18D-05	.14D-07	.25D-05	.92D-03	.15D-02	.51D-03	
199	32	2737	604	.17D-01	.25D-06	.16D-08	.49D-06	.74D-04	.65D-03	.10D-03	
322	31	3879	822	.14D-02	.18D-07	.14D-09	.81D-07	.52D-05	.23D-03	.16D-04	
537	47	6216	1293	.13D-03	.12D-08	.97D-11	.15D-07	.57D-06	.12D-03	.16D-04	
908	83	10574	2203	.11D-04	.86D-10	.65D-12	.40D-08	.33D-06	.46D-04	.79D-07	
		11.1	2.4	4.8	5.3	5.1	3.5	4.1	2.1	4.4	
61	19	1314	251	.90D+00	.82D-05	.34D-07	.68D-04	.56D-02	.82D-02	.14D-02	
86	29	1925	373	.69D-01	.33D-06	.34D-08	.16D-04	.28D-02	.24D-02	.13D-03	
123	36	2674	520	.10D-01	.81D-07	.46D-09	.53D-05	.72D-03	.12D-02	.48D-04	
176	38	3530	677	.21D-02	.83D-08	.45D-10	.11D-05	.15D-03	.33D-03	.32D-05	
253	31	4617	876	.17D-03	.87D-09	.44D-11	.22D-06	.30D-04	.27D-03	.53D-06	
374	26	6440	1213	.18D-04	.83D-10	.53D-12	.50D-07	.94D-05	.12D-03	.20D-06	
		16.4	3.1	6.0	6.3	6.1	4.0	3.5	2.3	4.9	
50	19	1558	266	.12D+01	.24D-05	.16D-08	.12D-03	.15D+00	.58D-01	.19D-02	
66	24	2020	343	.14D+00	.59D-06	.88D-09	.89D-04	.96D-02	.83D-02	.28D-02	
89	26	2559	431	.12D-01	.52D-07	.84D-10	.20D-04	.19D-02	.43D-02	.27D-04	
120	30	3379	576	.11D-02	.26D-08	.51D-11	.45D-05	.62D-03	.11D-02	.29D-05	
167	31	4483	768	.17D-03	.60D-09	.80D-12	.16D-05	.23D-03	.53D-03	.78D-06	
237	26	5957	1021	.17D-04	.85D-10	.12D-12	.45D-06	.69D-04	.32D-03	.10D-05	
		22.5	3.8	7.2	6.6	6.1	3.6	4.9	3.3	4.8	

7.6 Index 3 seven body problem

RADAU5									
ACC	REJ	NFCN	NSOL	G1	G2	G3	Q	U	LAM
26	3	539	171	.18D+01	.28D-02	.21D-06	.30D-01	.28D+01	.28D+01
37	9	706	223	.18D+01	.16D-02	.97D-07	.31D-02	.17D+01	.93D+00
54	17	873	273	.18D+01	.93D-03	.51D-07	.92D-03	.40D+00	.22D+00
87	22	1159	356	.18D+01	.51D-03	.11D-07	.54D-03	.11D+00	.84D-01
149	21	1518	455	.18D+01	.18D-03	.31D-08	.98D-04	.11D+00	.68D-01
258	19	2229	655	.16D+01	.49D-04	.50D-09	.76D-05	.35D-02	.13D-01
		10.0	3.0	0.0	1.8	2.6	3.6	2.9	2.4

GAUSS2, (TOL = $10^{-1}, \ldots$), level 1										
ACC	REJ	NFCN	NSOL	G1	G2	G3	Q	U	LAM	DEL
60	8	677	202	.18D+01	.20D-03	.55D-06	.21D-01	.31D+01	.12D+01	.70D-01
153	39	1683	457	.11D+01	.25D-04	.25D-07	.23D-02	.73D+00	.40D+00	.67D-02
476	147	4545	1026	.18D+00	.28D-05	.10D-08	.25D-03	.21D+00	.81D-01	.12D-01
1529	417	13607	2911	.11D-01	.11D-06	.30D-10	.26D-04	.20D-01	.66D-02	.40D-01
		7.3	1.6	1.6	2.3	3.0	2.1	1.6	1.6	0.2

GAUSS3, (TOL = $10^{-1}, \ldots$), levels 1, 2, 3										
ACC	REJ	NFCN	NSOL	G1	G2	G3	Q	U	LAM	DEL
92	3	1416	345	.18D+01	.23D-03	.47D-06	.24D-02	.33D+00	.16D+00	.10D+00
148	18	2393	576	.17D+01	.52D-04	.20D-06	.62D-03	.38D+00	.10D+00	.28D+01
332	30	3882	811	.68D+00	.39D-05	.22D-07	.14D-03	.13D+00	.25D-01	.23D-02
252	28	3545	808	.92D-01	.44D-06	.12D-08	.15D-04	.11D-01	.58D-02	.78D-03
490	59	6523	1442	.48D-02	.25D-07	.90D-10	.19D-05	.16D-02	.63D-03	.32D-03
		12.2	2.7	3.6	5.5	5.1	4.3	3.2	3.3	3.5
71	3	1509	330	.18D+01	.46D-04	.11D-06	.83D-02	.34D+01	.14D+01	.19D+00
107	12	2280	482	.18D+01	.35D-04	.60D-07	.10D-02	.25D+00	.18D+00	.17D-01
129	14	2625	541	.16D+01	.44D-05	.58D-08	.31D-03	.12D+00	.30D-01	.92D-02
					...					
414	49	7076	1278	.62D-02	.13D-07	.21D-10	.72D-05	.40D-02	.76D-03	.17D-03
		17.0	3.3	3.2	4.6	4.9	4.0	3.8	4.3	4.0
100	5	2389	411	.18D+01	.56D-04	.42D-07	.32D-02	.95D+00	.27D+00	.61D+00
103	10	2534	430	.18D+01	.23D-04	.14D-07	.60D-03	.67D-01	.89D-01	.36D-01
109	14	2776	474	.17D+01	.54D-05	.13D-08	.48D-03	.10D+00	.96D-01	.30D-02
296	30	6674	1029	.21D-01	.24D-06	.44D-10	.48D-04	.16D-01	.65D-02	.17D-02
		21.5	3.5	4.1	5.0	6.3	3.9	3.8	3.4	5.4

7.7 Cavity problem $(t_{end} = 50, Re = 100, K = 5)$

RADAU5							
ACC	REJ	NFCN	NSOL	G1	G2	U	P
15	0	90	25	.92D-03	.13D-10	.51D-03	.20D-03
19	0	112	31	.16D-03	.14D-11	.49D-04	.22D-04
26	0	155	43	.22D-04	.92D-11	.61D-05	.28D-05
38	0	233	65	.53D-04	.10D-11	.66D-06	.13D-05
61	0	367	102	.12D-04	.72D-13	.76D-07	.31D-06
101	0	570	156	.16D-06	.17D-13	.10D-07	.85D-08
		5.9	1.6	4.6	3.5	5.7	5.3

DIRK2								
ACC	REJ	NFCN	NSOL	G1	G2	U	P	DEL
19	0	79	40	.79D-02	.18D-09	.80D-02	.22D-02	.12D-01
25	0	105	54	.11D-03	.29D-10	.54D-03	.10D-03	.18D-02
39	1	170	89	.80D-05	.63D-11	.79D-04	.17D-04	.92D-03
79	13	356	171	.53D-06	.11D-09	.55D-05	.18D-05	.18D-04
190	69	925	406	.31D-07	.12D-07	.10D-05	.20D-06	.18D-05
		3.8	1.7	5.4	? (4.7)	3.9	4.0	3.8

GAUSS2, levels 0, 1								
ACC	REJ	NFCN	NSOL	G1	G2	U	P	DEL
17	0	87	26	.86D-03	.16D-09	.14D-03	.46D-04	.21D-03
24	0	121	36	.12D-03	.55D-10	.15D-04	.45D-05	.75D-04
38	0	185	54	.11D-04	.76D-11	.11D-05	.41D-06	.48D-05
66	0	315	91	.71D-06	.12D-11	.11D-06	.26D-07	.55D-06
123	0	575	164	.42D-07	.20D-12	.13D-07	.59D-08	.58D-07
248	0	1151	326	.22D-08	.19D-13	.24D-08	.26D-08	.59D-08
		4.7	1.4	4.8	3.4	4.1	3.7	3.9
16	0	117	26	.38D-03	.44D-10	.31D-03	.98D-04	.19D-03
20	0	143	31	.61D-04	.19D-09	.53D-04	.17D-04	.11D-03
27	0	197	44	.47D-05	.70D-11	.69D-05	.19D-05	.62D-05
40	0	293	66	.45D-06	.26D-11	.94D-06	.23D-06	.56D-06
61	0	455	105	.35D-07	.24D-12	.14D-06	.37D-07	.64D-07
99	0	759	179	.24D-08	.77D-13	.20D-07	.78D-08	.73D-08
		7.5	1.7	6.6	3.5	5.3	5.2	5.6

GAUSS3, levels 0, 1, 2, 3								
ACC	REJ	NFCN	NSOL	G1	G2	U	P	DEL
19	0	123	28	.83D-03	.11D-09	.59D-04	.36D-04	.20D-03
25	0	162	37	.12D-03	.22D-10	.74D-05	.46D-05	.36D-04
38	0	242	55	.11D-04	.86D-11	.66D-06	.42D-06	.44D-05
67	0	399	88	.63D-06	.10D-11	.90D-07	.22D-07	.51D-06
128	0	728	157	.35D-07	.79D-13	.11D-07	.59D-08	.54D-07
256	0	1418	301	.19D-08	.12D-13	.25D-08	.26D-08	.57D-08
		5.8	1.2	5.0	3.5	3.9	3.7	4.0
17	0	147	26	.62D-03	.57D-10	.24D-03	.71D-04	.78D-03
20	0	180	33	.14D-03	.13D-11	.31D-04	.17D-04	.35D-04
27	0	238	43	.17D-04	.17D-10	.57D-05	.34D-05	.49D-05
38	0	336	61	.14D-05	.29D-11	.78D-06	.48D-06	.59D-06
57	0	481	84	.92D-07	.47D-12	.12D-06	.58D-07	.65D-07
93	0	770	131	.59D-08	.46D-13	.15D-07	.11D-07	.28D-07
		8.5	1.5	6.8	4.2	5.7	5.1	6.0
15	0	187	27	.19D-02	.56D-10	.19D-02	.73D-03	.37D-03
18	0	217	30	.26D-03	.24D-11	.37D-03	.13D-03	.10D-03
22	0	269	38	.32D-04	.16D-12	.75D-04	.28D-04	.55D-05
28	0	341	48	.30D-05	.12D-11	.12D-04	.47D-05	.70D-06
38	0	465	66	.19D-06	.19D-12	.19D-05	.76D-06	.83D-07
54	0	665	93	.17D-07	.19D-12	.32D-06	.14D-06	.93D-08
		12.3	1.7	9.1	4.5	6.8	6.7	8.3
20	1	331	33	.57D-03	.41D-10	.43D-03	.12D-03	.48D-03
20	0	317	32	.97D-04	.54D-11	.17D-03	.80D-04	.39D-04
23	0	365	37	.18D-04	.32D-11	.49D-04	.19D-04	.50D-05
29	3	506	51	.28D-05	.12D-09	.31D-04	.13D-04	.30D-05
33	0	532	56	.28D-06	.95D-12	.11D-04	.46D-05	.21D-06
45	0	744	79	.52D-07	.65D-12	.14D-05	.63D-06	.97D-08
		16.1	1.7	11.5	5.1	7.0	6.4	13.3

7.8 Cavity problem $(t_{end} = 3, Re = 105, K = 10)$

RADAU5							
ACC	REJ	NFCN	NSOL	G1	G2	U	P
10	0	65	18	.41D-01	.57D-09	.22D-02	.16D-02
11	0	69	19	.41D-01	.24D-09	.39D-03	.34D-03
14	0	84	23	.10D-01	.17D-10	.56D-04	.89D-04
19	0	122	34	.77D-03	.51D-12	.75D-05	.64D-05
28	0	179	50	.48D-04	.61D-12	.13D-05	.13D-05
		6.3	1.8	6.6	6.7	7.2	6.9

GAUSS2, level 0							
ACC	REJ	NFCN	NSOL	G1	G2	U	DEL
12	0	59	17	.63D-02	.71D-10	.43D-03	.13D-02
16	0	81	24	.11D-02	.56D-10	.77D-04	.60D-03
22	0	115	35	.14D-03	.38D-11	.84D-05	.48D-04
37	0	209	67	.96D-05	.18D-14	.92D-06	.18D-04
71	0	417	137	.54D-06	.28D-14	.81D-07	.39D-05
		5.6	1.8	5.3	5.7	4.8	3.3

GAUSS3, level 0							
ACC	REJ	NFCN	NSOL	G1	G2	U	DEL
12	0	79	18	.76D-02	.56D-10	.30D-03	.15D-02
16	0	102	23	.11D-02	.75D-11	.75D-04	.58D-03
23	0	164	39	.13D-03	.17D-14	.10D-04	.49D-04
38	0	290	71	.93D-05	.24D-14	.99D-06	.44D-05
71	0	554	137	.53D-06	.29D-14	.60D-07	.49D-06
		7.4	1.8	5.4	5.5	4.8	4.5

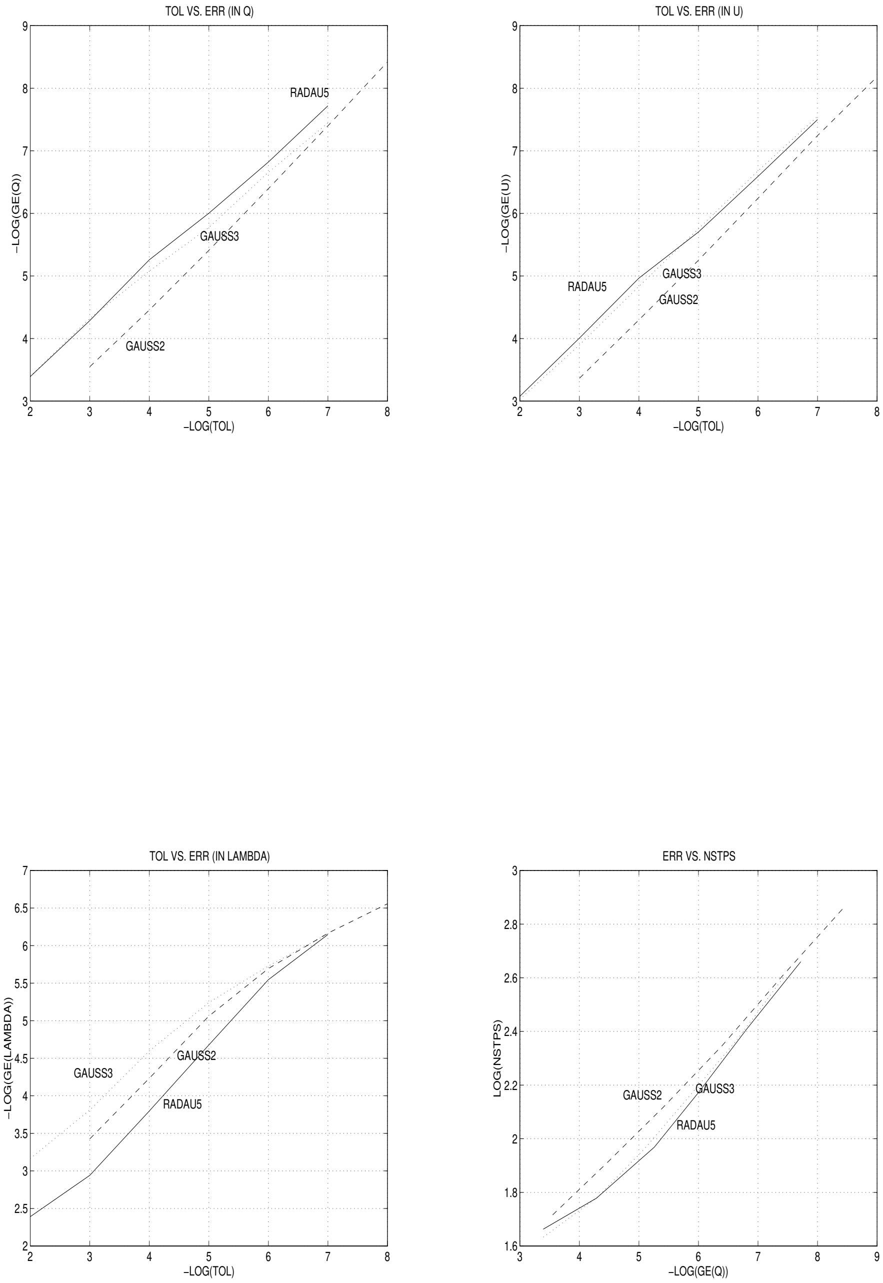

Figure 7.1: Index 2 pendulum problem

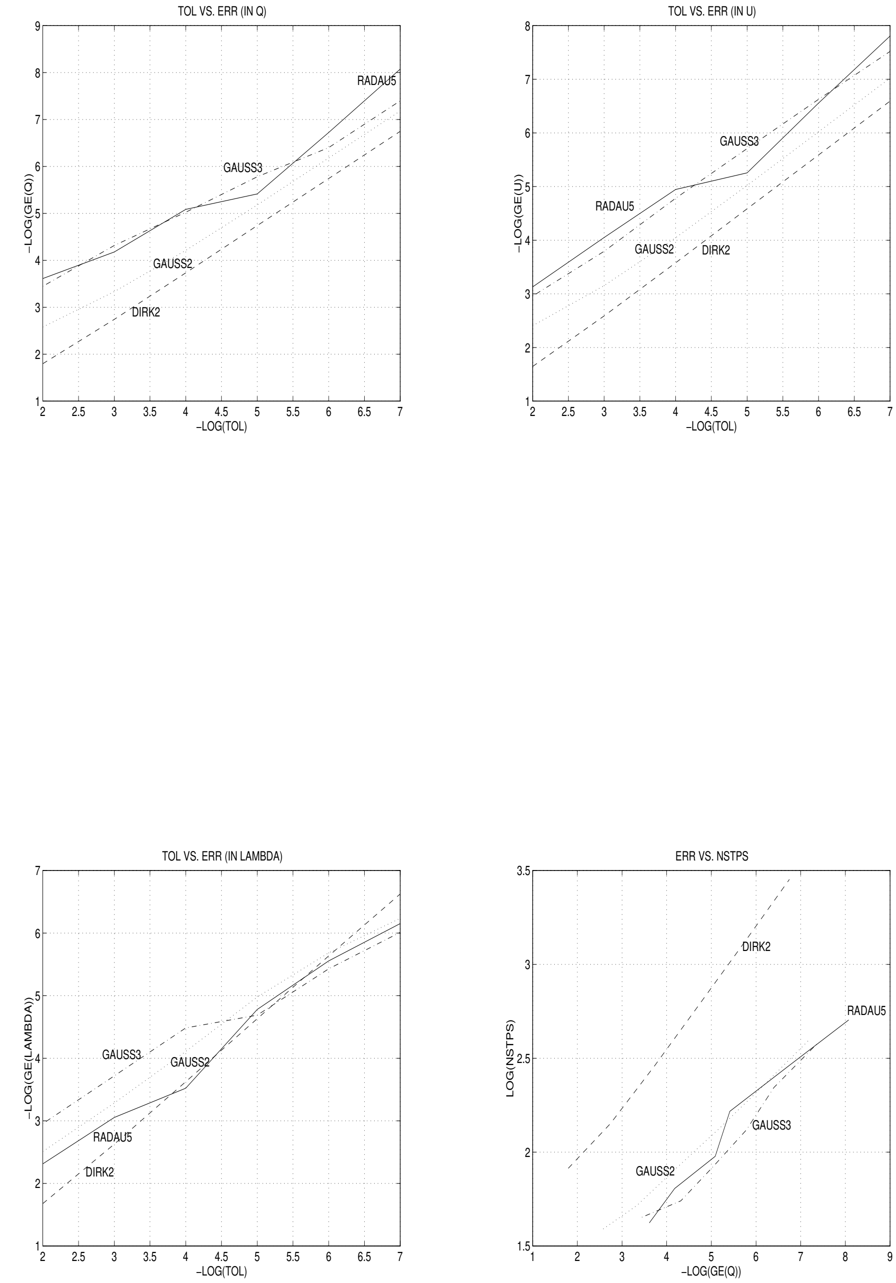

Figure 7.2: Stabilized index 2 pendulum problem

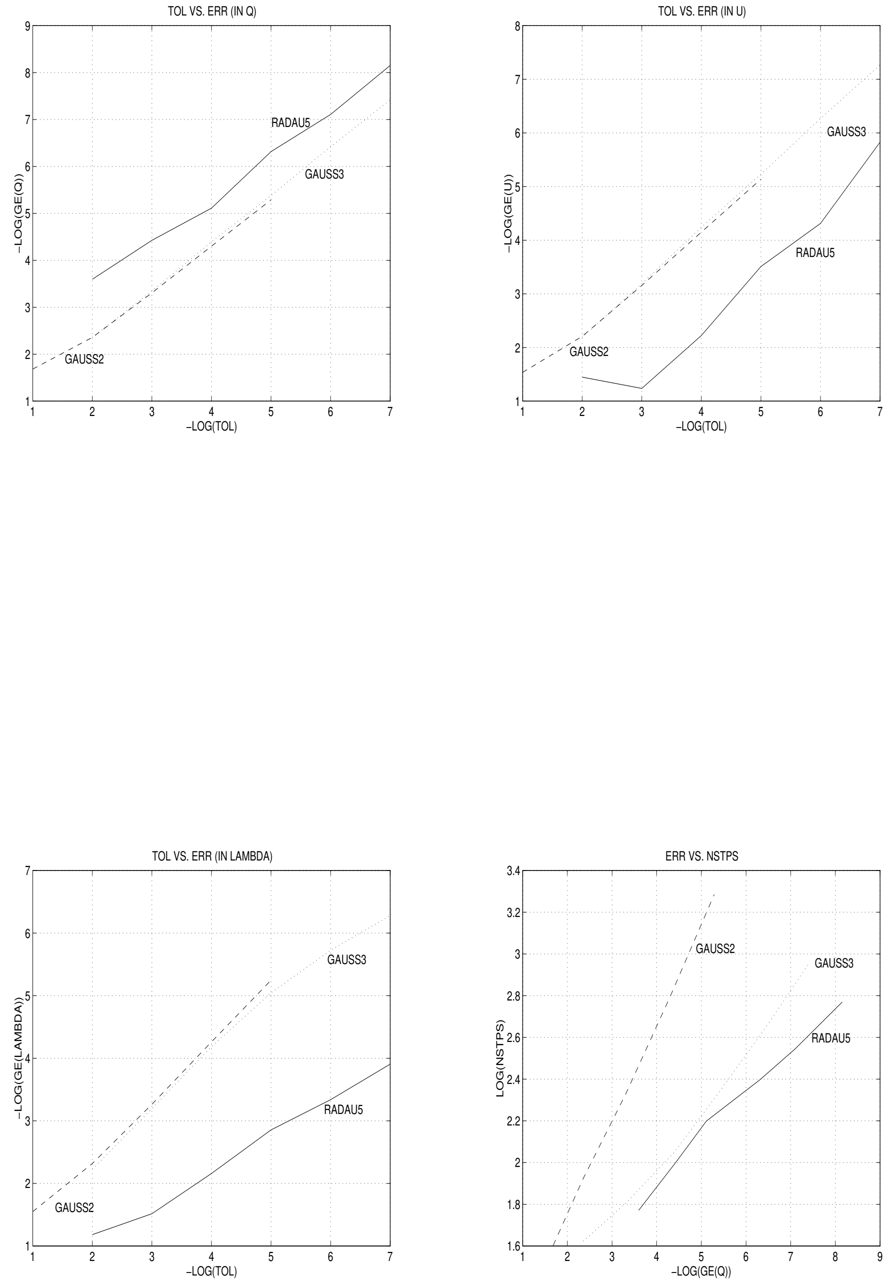

Figure 7.3: Index 3 pendulum problem

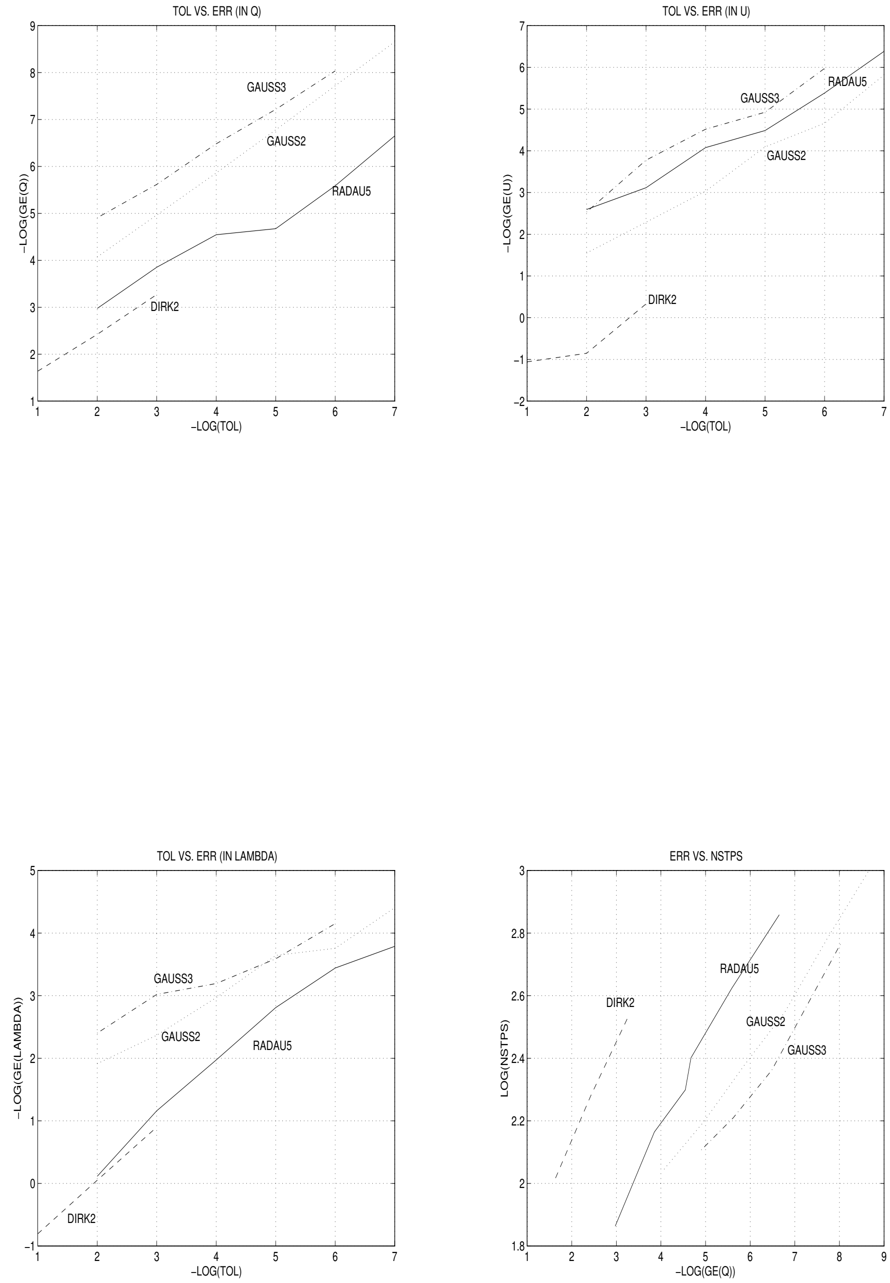

Figure 7.4: Index 2 seven body problem

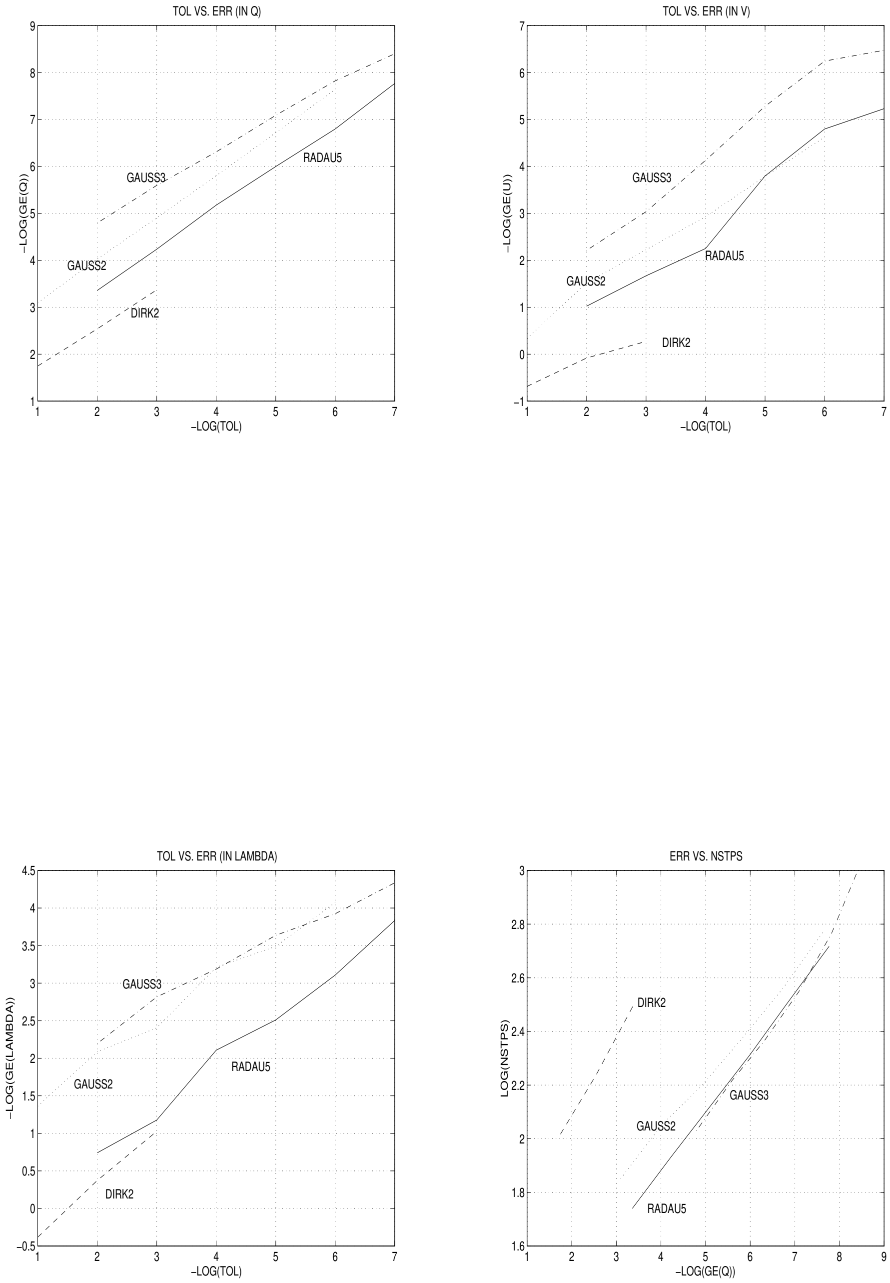

Figure 7.5: GGL index 2 seven body problem

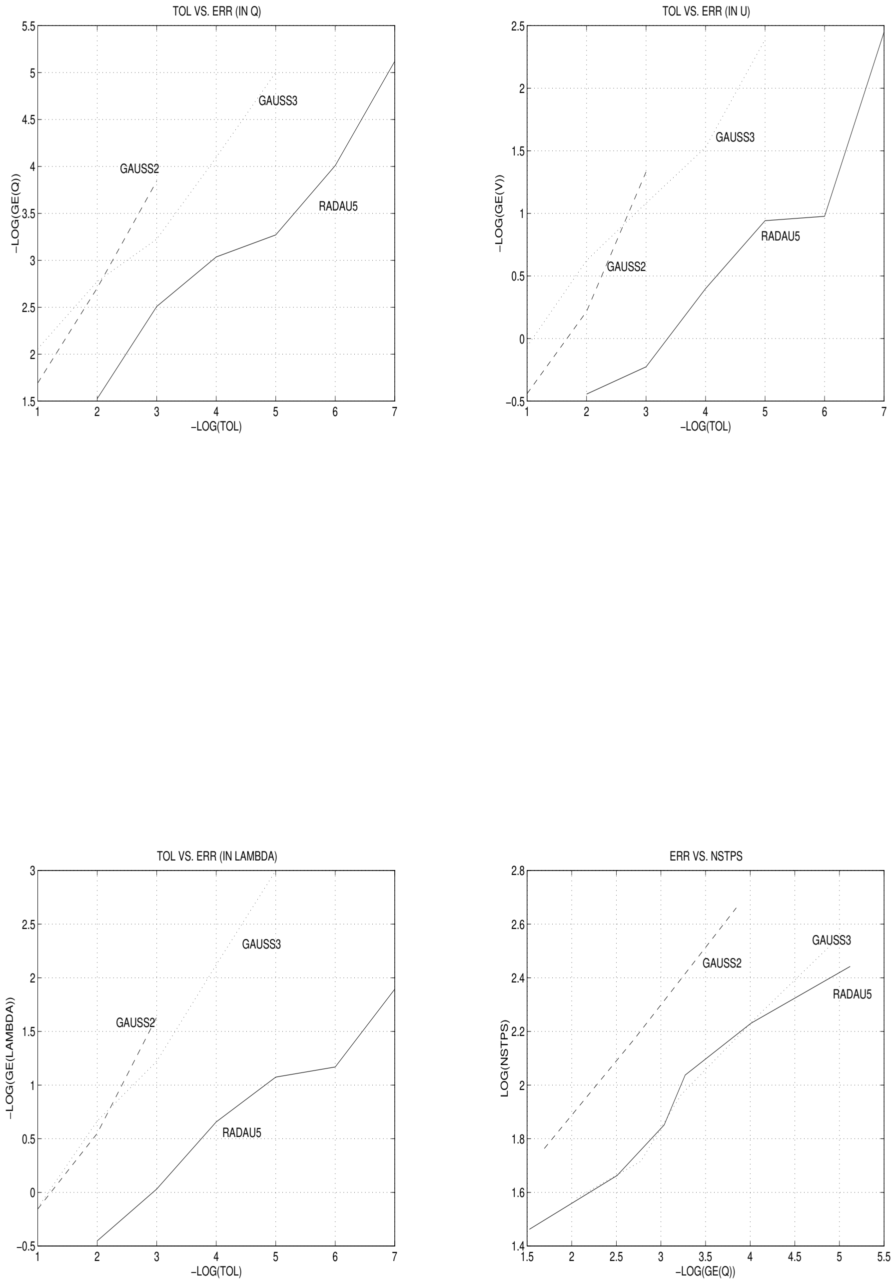

Figure 7.6: Index 3 seven body problem

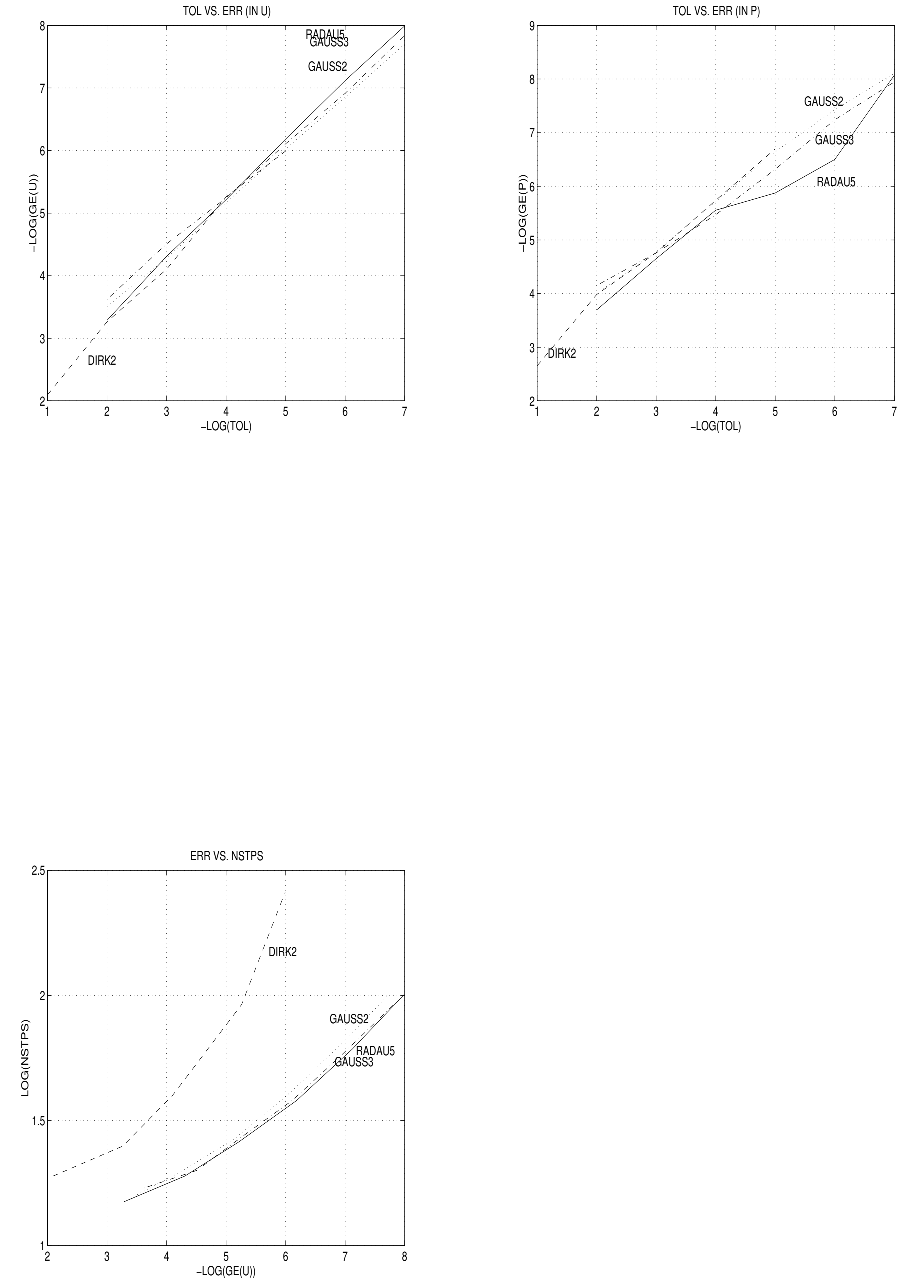

Figure 7.7: Cavity problem

Chapter 8

Conclusion

In this final chapter, we review our approach as applied to semi explicit ADEs of index 1, index 2 and index 3. We also discuss what we have accomplished, the advantages as well as the limitations of our approach.

In general, this thesis is on the numerical solution of (initial value) semi explicit ADEs using implicit Runge-Kutta methods. We are interested in interpolation and error control schemes which will extend the computed solution obtained from a discrete implicit RK formula to a continuous approximating solution. In particular, we extend the bootstrapping procedure and the defect-based error control strategy as introduced in [16], [17], [18] to semi explicit ADEs of index 1, index 2 and index 3 and apply the results to the three projected RK formulas SDIRK(2), Gauss(2) and Gauss(3).

Our analysis is based on an underlying perturbed equation corresponding to any continuous approximation and hence it is independent of particular interpolants. This allows us to apply the same formalism to derive order results for collocation polynomials, for continuous global errors, for continuous local errors and for discrete local errors of standard and as well as projected RK methods.

Our analysis reveals the close relationship between the interpolation and error control schemes. The error in an interpolant can be expressed in terms of an associated defect or algebraic residual and the underlying defect used in our error control scheme in turn imposes constraints on the interpolation scheme. In particular, Schemes 1, 2 and 3 were devised with the intention that the associated defect of each level is of sufficiently high order.

Thus our interpolation and error control schemes are justified. In addition, the schemes as devised can be viewed as being independent of the index of the concerned problem. Specifically, Scheme 1, Scheme 2 and Scheme 3 differ only by their use of discrete projected RK values. Similarly, the approach as devised can be viewed as being independent of the underlying discrete formula. Specifically, Scheme 1, Scheme 2 and Scheme 3 only depend on the order of the discrete RK formulas.

In the case of ADEs, the perturbed equation associated with an ADE can also be converted to

	Q	U	LAM
Index 2 pendulum	4.1	4.2	3.6
Stabilized index 2 pendulum	4.0	4.2	3.4
Index 3 pendulum	3.2	3.3	3.2
Index 2 seven body	4.1	4.0	2.5
GGL index 2 seven body	4.2	4.0	3.0
Index 3 seven body	3.6	2.9	2.4
	U	P	
Driven cavity	5.7	5.3	

Table 8.1: Observed order for RADAU5

	Q	U	LAM
Index 2 pendulum			
Stabilized index 2 pendulum	3.1	3.1	3.1
Index 3 pendulum			
Index 2 seven body	3.0	2.5	3.1
GGL index 2 seven body	3.1	1.8	2.7
Index 3 seven body			
	U	P	
Driven cavity	3.9	4.0	

Table 8.2: Observed order for DIRK2

the equivalent IVP counterpart, which involves differential variables only. However, the derived perturbed equation involves both the defect and the algebraic residual, as well as subsequent derivatives of these defects and algebraic residuals.

However, there are some limitations to our approach. Our qualitative analysis is mainly concerned with the asymptotic order of convergence. The magnitude of the principal error term in the error bound can be significant in complicated problems.

As mentioned earlier, we found it is necessary to use the projected RK values for each of the three considered implicit RK formulas. Therefore a knowledge of all lower index formulations is required. In particular, our approach requires the knowledge of the associated index 1 constraint which can be impractical for complicated problems.

Formally, our error control schemes are dependent on the index of a particular problem. Therefore different error control schemes for different problems of different indices are also required.

In the preceding chapter, we have presented the numerical results of seven problems representing the two important classes of ADEs: constrained mechanical systems and fluid dynamics.

Tables 8.1–8.4 present the observed orders of each method. We note that the observed orders for the pendulum problems are higher than those for the seven body problems, even though they are formally of the same indices and of the same class of CMSs. This observation is also reflected in their relative performances in terms of the number accepted and rejected steps, the number of

	Q	U	LAM	Level
Index 2 pendulum	4.1	4.1	2.6	1
Stabilized index 2 pendulum	4.5	4.5	3.6	1
Index 3 pendulum	2.1	2.1	2.1	1
Index 2 seven body	4.4	4.1	2.4	1
GGL index 2 seven body	4.5	4.3	2.7	1
Index 3 seven body	2.1	1.6	1.6	1
	U	P		Level
Driven cavity	5.3	5.2		1

Table 8.3: Observed order for GAUSS2

	Q	U	LAM	Level
Index 2 pendulum	6.8	7.0	6.3	3
Stabilized index 2 pendulum	6.3	6.6	5.6	2
Index 3 pendulum	3.6	3.7	2.9	1
Index 2 seven body	3.7	3.7	3.6	3
GGL index 2 seven body	3.6	4.9	3.3	3
Index 3 seven body	4.0	3.8	4.3	2
	U	P		Level
Driven cavity	6.8	6.7		2

Table 8.4: Observed order for GAUSS3

Newton iterations, the magnitudes of the algebraic residuals and the global errors.

For each of the pendulum and seven body problems, we observe that for all methods, the observed orders for index 2 and GGL formulations are higher than those of index 3 formulation; and the observed orders for the differential variable are higher than those of the algebraic variable.

As for the cavity problem, we find that there is little to choose among all methods (Section 7.7 and Figure 7.7).

We find that DIRK2 does not perform robustly: it often failed and could not satisfy the requested tolerances tolerances. On the other hand, we observe that GAUSS2, GAUSS3 were robust and able to generate an acceptable continuous approximation at a cost that was comparable to that required by RADAU5 to generate only a discrete approximation.

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