

Differential algebraic equations

Citation for published version (APA):

Wijckmans, P. M. E. J. (1992). *Differential algebraic equations*. (RANA : reports on applied and numerical analysis; Vol. 9302). Eindhoven University of Technology.

Document status and date:

Published: 01/01/1992

Document Version:

Publisher's PDF, also known as Version of Record (includes final page, issue and volume numbers)

Please check the document version of this publication:

- A submitted manuscript is the version of the article upon submission and before peer-review. There can be important differences between the submitted version and the official published version of record. People interested in the research are advised to contact the author for the final version of the publication, or visit the DOI to the publisher's website.
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RANA 93-02
January 1993
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Reports on Applied and Numerical Analysis
Department of Mathematics and Computing Science
Eindhoven University of Technology
P.O. Box 513
5600 MB Eindhoven
The Netherlands
ISSN: 0926-4507

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A.M.S. Classifications : 65L05

Keywords : differential algebraic equations, multistep methods,
Runge-Kutta methods, numerical methods.

Differential Algebraic Equations

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January 18, 1993

Abstract

Differential Algebraic Equations (DAE's) arise in many applications, such as mechanical systems with constraints, the modeling of electrical networks, flow of incompressible fluids. This class of problems presents numerical and analytical difficulties which are quite different from Ordinary Differential Equations (ODE's). In this paper the theory and the numerical solution of DAE's are examined.

1 Theory of Differential Algebraic Equations

1.1 Introduction

We shall focus on problems which are of the general form of an *implicit* differential equation

$$f(t, x(t), x'(t)) = 0, \quad (1.1)$$

where the function $f : \mathbb{R}^{2n+1} \rightarrow \mathbb{R}^n$ is assumed to be sufficiently often differentiable, and $x \in \mathbb{R}^n$. The partial derivative $\partial f / \partial x'$ may be singular. This class of differential equations includes ordinary differential equations (ODE's) as a special case. If the Jacobian $\partial f / \partial x'$ is nonsingular, equation (1.1) is a system of ordinary differential equations. However, if the Jacobian is singular, equation (1.1) is in fact a system of *differential algebraic equations* (DAE's). ODE's. In a system of DAE's there are algebraic constraints on the variables. Consider the following example

Example 1.1

$$\frac{dx}{dt} = Ax + By + q \quad (E.1.2a)$$

$$0 = Cx + Dy + r \quad (E.1.2b)$$

In this system the algebraic constraints appear explicitly in equation (E.1.2b). Note, that this system can easily be rewritten as an ODE if the matrix D is nonsingular.

1.2 Linear DAE's with Constant Coefficients

The simplest and best understood problems of the form (1.1) are linear differential algebraic equations with constant coefficients

$$Ax'(t) + Bx(t) = g(t), \quad (1.3)$$

where $A, B \in \mathbb{R}^{n \times n}$, and $g \in \mathbb{R}^n$. We study these systems to give insight in the behaviour of solutions of DAE's.

Consider equation (1.3) with a nonsingular matrix A . This system can be rewritten as

$$x'(t) = -A^{-1}Bx(t) + A^{-1}g(t), \quad (1.4)$$

which is just a (familiar) explicit ordinary differential equation. Hence, we concentrate on the case of singular matrices A . For homogeneous equations (1.3) solutions of the form

$$x(t) = \exp(\lambda t)x_0, \quad (1.5)$$

lead to the relation

$$\det(\lambda A + B) = 0. \quad (1.6)$$

It is therefore useful to consider the *matrix pencil* $\lambda A + B$. This matrix pencil is called *singular* if $\lambda A + B$ is singular for all values of λ , otherwise it is called *regular*.

Definition 1.2 *The vector $x_0 \in \mathbb{R}^n$ is said to be a consistent initial vector associated with $t_0 \in \mathbb{R}$ if problem (1.3) with initial value $x(t_0) = x_0$ possesses at least one solution. If the initial value problem possesses a unique solution for all consistent initial vectors associated with t_0 , then the problem is called solvable.¹*

Solvability of a linear DAE with constant coefficients can be characterized by the following theorem.

Theorem 1.3 *For $A, B \in \mathbb{R}^{n \times n}$ the DAE*

$$Ax'(t) + Bx(t) = g(t)$$

is solvable if and only if the matrix pencil $\lambda A + B$ is regular.

Proof. Suppose the matrix pencil $\lambda A + B$ is singular. Choose an arbitrary set of $n + 1$ distinct λ_i and $v_i \neq 0$, $i = 1, 2, \dots, n + 1$ such that $(\lambda_i A + B)v_i = 0$. There is a nontrivial combination $\sum_{i=1}^{n+1} \alpha_i v_i = 0$, but $\sum_{i=1}^{n+1} \alpha_i \exp(\lambda_i t) v_i \neq 0$. For that reason, the problem $Ax' + Bx = 0$ with $x(0) = 0$ has two different solutions, namely $\sum_{i=1}^{n+1} \alpha_i \exp(\lambda_i t) v_i$ and 0. Therefore the DAE (1.3) is not solvable for a singular matrix pencil $\lambda A + B$.

Assume the matrix pencil is regular. The polynomial $p(z) = \det(zA + B)$ has degree $k \leq n$ and the unicity of the solution is obvious. \square

In the following we assume that the matrix pencil $\lambda A + B$ is regular. Problems of the form (1.3) can be solved using the *Weierstraß-Kronecker canonical form*.

Theorem 1.4 *Suppose the matrix pencil $\lambda A + B$ is regular. Then there exist nonsingular matrices P and Q such that*

$$PAQ = \begin{bmatrix} I & O \\ O & N \end{bmatrix}, \quad PBQ = \begin{bmatrix} C & O \\ O & I \end{bmatrix},$$

¹Campbell [8], and, Griepentrog and März [21] use the term *tractable* instead of solvable.

where $N = \text{diag}(N_1, \dots, N_k)$. Each matrix N_i is a Jordan block of the form

$$N_i = \begin{bmatrix} 0 & 1 & & \\ & 0 & \ddots & \\ & & \ddots & 1 \\ & & & 0 \end{bmatrix}, \quad \text{of dimension } m_i,$$

and C can be assumed to be in Jordan canonical form.

This theorem is proved by Gantmacher [15] in 1954. Historically, the work of Gantmacher [15] has been an inspiration for the use of matrix pencils in studying DAE's. It induced the concept of the so called *index* of DAE's. This is the most important concept in classifying DAE systems. The notion of index of nilpotency of a matrix pencil can be defined as follows.

Definition 1.5 *The matrix pencil $\lambda A + B$ has index of nilpotency $n_i = m$, where $m = \max_{1 \leq i \leq k} m_i$, i.e. m is the smallest integer for which $N^m = 0$. The DAE (1.3) has index of nilpotency n_i .*

In the special case that matrix A is nonsingular, system (1.3) has index of nilpotency 0. The DAE (1.3) can be solved, using the Weierstraß-Kronecker canonical form of Theorem 1.4, as follows: premultiply (1.3) by P and define the coordinate change

$$x = Q \begin{bmatrix} u \\ v \end{bmatrix},$$

and the transformation

$$Pg(t) = \begin{bmatrix} r(t) \\ s(t) \end{bmatrix}.$$

System (1.3) can be written in decoupled form as

$$u'(t) + Cu(t) = r(t), \quad (1.7a)$$

$$Nv'(t) + v(t) = s(t), \quad (1.7b)$$

with initial value $\begin{bmatrix} u_0 \\ v_0 \end{bmatrix} = Q^{-1}x_0$. Equation (1.7a) is an ODE. For any initial value u_0 and any continuous function $r(t)$ it has a unique solution. However, equation (1.7b) is **not** an ODE. Suppose that DAE (1.3) has index of nilpotency m (such that $N^{m-1} \neq 0$ and $N^m = 0$), then we find from (1.7b) by differentiation

$$\begin{aligned} v(t) &= s(t) - Nv'(t) \\ &= s(t) - Ns'(t) + N^2v''(t) \\ &\vdots \\ &= s(t) - Ns'(t) + \dots + (-1)^{m-1}N^{m-1}s^{(m-1)}(t) + (-1)^mN^mv^{(m)}(t). \end{aligned}$$

Since $N^m = 0$, the solution $v(t)$ of (1.7b) can be written as

$$v(t) = \sum_{i=0}^{m-1} (-1)^i N^i s^{(i)}(t). \quad (1.8)$$

Thereby, the initial value v_0 must satisfy

$$v_0 = \sum_{i=0}^{m-1} (-1)^i N^i s^{(i)}(t_0). \quad (1.9)$$

This means that equation (1.7b) with initial value $v(t_0) = v_0$ only has a solution if the initial values are consistent, i.e. if v_0 satisfies (1.9). From the derivation process of the solution $v(t)$ (1.8) of equation (1.7b) it is obvious that not all components of v are necessarily differentiable.

There are some properties, in which DAE's behave differently compared with ODE's, viz.:

- the initial value x_0 has to be consistent,
- the solution can involve derivatives of order $m-1$ of the forcing function g (or at least s) if the DAE is of higher index (i.e. $m \geq 2$),
- the solution x may be only continuous in some components,
- higher index DAE's can have hidden algebraic constraints.

This last point can be seen from the following example.

Example 1.6 Consider the linear constant coefficient DAE

$$x_2' + x_1 = g_1, \quad (E.1.10a)$$

$$x_3' + x_2 = g_2, \quad (E.1.10b)$$

$$x_3 = g_3. \quad (E.1.10c)$$

There is one explicit algebraic constraint, namely equation (E.1.10c). However, the DAE has only the solution

$$x_1 = g_1 - g_2' + g_3'',$$

$$x_2 = g_2 - g_3',$$

$$x_3 = g_3.$$

Apparently there are two hidden algebraic constraints.

From the solution v of problem (1.7b) one can conclude that the solution depends on derivatives of order $m-1$ of function s .

For linear DAE's of the form (1.3) where A and B are time dependent the *local index* of the pencil $\lambda A + B$ is defined as the index of nilpotency of this pencil at any time t . However, this local index doesn't necessarily determine the structure of these DAE problems as in the case of linear DAE's with constant coefficients. This local index, on the other hand, will play an important role in solving DAE's numerically (as we shall see).

For DAE's of the form (1.3) Campbell [8] derived an explicit expression for the solution x in terms of the Drazin inverse of A and B . This expression doesn't give further insight than the results already noted above. The case of rectangular matrices A and B has also been studied by Campbell [8].

1.3 Nonlinear Systems

Next, we consider general DAE's of the form (1.1). It is obvious that the definition of the index of nilpotency (cf. Definition 1.5) has to be extended for these systems. This can be done in various ways. The first and probably most important extension is the so called *differential index* (first defined by Gear [16]).

Definition 1.7 Consider the general DAE $f(t, x(t), x'(t)) = 0$. This DAE has differential index $di = m$ if m is the smallest number of differentiations such that the system of equations

$$\begin{aligned} f(t, x(t), x'(t)) &= 0, \\ \frac{df(t, x, x')}{dt} &= 0, \\ &\vdots \\ \frac{d^m f(t, x, x')}{dt^m} &= 0, \end{aligned} \tag{1.11}$$

uniquely determines the explicit ODE $x' = g(t, x)$. This explicit ODE is called the underlying ODE (UODE).

It is obvious that an ODE has index 0. The index is a measure of the degree of singularity in the system. In general, the higher the index the more complex the problem and the more difficulties we are likely to encounter in solving the DAE by a numerical method (as we shall see). For linear DAE's with constant coefficients the index of nilpotency and the differential index are equal, i.e. $ni = di$. Consider system (1.7b). After $m - 1$ differentiations the solution v of (1.7b) is obtained. So, after one more differentiation the UODE for v is obtained. This means that $di = m = ni$. Further, the initial value $x(t_0) = x_0$ at t_0 is consistent for equation (1.1) if system (1.11) in the separate variables $x', x^{(2)}, \dots, x^{(m+1)}$ at $t = t_0$ and $x = x_0$ has a solution $x' = x'(t_0, x_0)$. System (1.11) shows that every differentiation of the original DAE reduces the index of the new system by one. So, equation $\frac{d^m f}{dt^m} = 0$ has index $m - n$.

Hairer, Lubich and Roche [23] introduced the so called *perturbation index* as a measure of the sensitivity of the solutions with respect to perturbations of a given equation (1.1).

Definition 1.8 Equation (1.1) has perturbation index $pi = m$, along a solution x on $[0, T]$, if m is the smallest integer such that for all functions y having a defect

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

the difference on $[0, T]$ is bounded by an estimate

$$\|x(t) - y(t)\| \leq K(\|x(0) - y(0)\| + \max_{0 \leq \xi \leq t} \|\delta(\xi)\| + \dots + \max_{0 \leq \xi \leq t} \|\delta^{(m-1)}(\xi)\|),$$

whenever the expression on the right-hand side is sufficiently small. The constant K depends only on f and the length of the interval. Further we say that equation (1.1) has perturbation index zero, if

$$\|x(t) - y(t)\| \leq K(\|x(0) - y(0)\| + \max_{0 \leq \xi \leq t} \|\delta(\xi)\| + \max_{0 \leq \xi \leq t} \|\int_0^\xi \delta(t) dt\|).$$

For system (1.7b) $v(t)$ depends on the $(m - 1)$ th derivative of $s(t)$. Therefore, for a linear constant coefficient DAE the perturbation index and the index of nilpotency are equal, i.e. $pi = mi$.

Gear [17] showed that for general DAE's the following relation holds between the perturbation index and the differential index,

$$di \leq pi \leq di + 1,$$

for problems (1.1) for which both the differential index and the perturbation index exist. For DAE's that have *integral form*, i.e.

$$f(t, x(t), x'(t)) = a_x(t, x)x' + b(t, x) = 0,$$

the perturbation index and the differential index coincide, i.e. $pi = di$.

1.4 Semi-Explicit Systems

DAE's of the form (1.1) are called *fully-implicit* DAE's.

There are several special classes of implicit DAE's. These subclasses can easily be recognized and they often appear in applications. Their structure is relatively simple, whereas fully-implicit DAE's are very complicated. *Semi-explicit* DAE's of the form

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

illustrate that DAE's can be considered as systems of differential equations combined with algebraic equations. These algebraic equations define a manifold to which the solution is constrained. Therefore, DAE's can be interpreted as differential equations on manifolds (cf. [30]). For semi-explicit DAE's the variables can be divided into *differential variables* and *algebraic variables*. In the equation above, for example, x is the differential variable and y is the algebraic variable.

The simplest form of a nonlinear DAE is a semi-explicit index one DAE of the form

$$x' = f(x, y), \tag{1.12a}$$

$$0 = g(x, y), \tag{1.12b}$$

with $\frac{\partial g}{\partial y}$ nonsingular. The solution of this system lies on the manifold defined by (1.12b). Differentiation of the algebraic equation (1.12b) gives

$$0 = \frac{\partial g}{\partial x} x' + \frac{\partial g}{\partial y} y'. \tag{1.13}$$

After substitution of (1.12a) for x' , equation (1.13) yields

$$y' = -\left(\frac{\partial g}{\partial y}\right)^{-1} \frac{\partial g}{\partial x} f, \tag{1.14}$$

because the Jacobian $\frac{\partial g}{\partial y}$ is nonsingular. Together, equation (1.12a) and equation (1.14) form the UODE (cf. Section 1.3) for x and y . By Definition 1.7 the differential index di is one in

this case. Consistent initial values must satisfy $0 = g(x_0, y_0)$. Hairer, Lubich and Roche [23] showed that DAE (1.12) has perturbation index ν one.

Consider the semi-explicit system

$$x' = f(x, y), \quad (1.15a)$$

$$0 = g(x), \quad (1.15b)$$

where $\frac{\partial g}{\partial x} \frac{\partial f}{\partial y}$ is nonsingular. Differentiation of equation (1.15b) and substitution of equation (1.15a) for x' yields

$$0 = \frac{\partial g}{\partial x} f. \quad (1.16)$$

As in the case of DAE (1.12) we see that system (1.15) has differential index one if $\frac{\partial g}{\partial x} \frac{\partial f}{\partial y}$ is nonsingular. Because of this, equation (1.15) has differential index two. The solution of DAE (1.15) is not only constrained to lie on the manifold (1.15b), but also on the manifold (1.16). Now, initial conditions are consistent if they satisfy both equation (1.15b) and equation (1.16). Again, for this system the perturbation index coincides with the differential index as shown in [23].

Under the assumption that $\frac{\partial g}{\partial x} \frac{\partial f}{\partial y} \frac{\partial k}{\partial z}$ is nonsingular, the problem

$$x' = f(x, y), \quad (1.17a)$$

$$y' = k(x, y, z), \quad (1.17b)$$

$$0 = g(x), \quad (1.17c)$$

has differential index (and perturbation index) three. After differentiation of equation (1.17c) one gets

$$0 = \frac{\partial g}{\partial x} f. \quad (1.18)$$

Compare system (1.17a), (1.17b), (1.18) with DAE (1.15). Clearly, system (1.17a), (1.17b), (1.18) is an index two system, so DAE (1.17) has index three.

In general, the differential index is the most important and most often used definition of the index of a DAE. Therefore, in the following index stands for differential index, and, the index shall be denoted as ν .

1.5 Applications

DAE's arise in many applications. They occur in connection with the dynamical analysis of mechanical systems. They also arise in the study of nonlinear circuits and in the study of optimal control problems. Further, DAE's are important in investigating the structure of the solutions of singular perturbation problems. In this subsection some of these applications are briefly described.

Multibody Systems

The motion of a system of rigid bodies can be described using concepts of classical mechanics. Let $q \in \mathbb{R}^n$ be a vector of generalized coordinates and $v \in \mathbb{R}^n$ a vector of generalized

velocities. Assume that the rigid bodies are connected by m holonomic constraints which can be expressed as $\Phi(q, t) = 0$. The equations of motion for this multibody system can be written as

$$\dot{q} = v, \quad (1.19a)$$

$$M(q, t)\dot{v} = g(q, v, t) + \Phi_q^T \lambda, \quad (1.19b)$$

$$0 = \Phi(q, t), \quad (1.19c)$$

where $M(q, t) \in \mathbb{R}^{n \times n}$ denotes the positive definite mass matrix and the vector $g(q, v, t) \in \mathbb{R}^n$ the applied forces. Further, the unknown Lagrange multipliers $\lambda \in \mathbb{R}^m$ account for the unknown constraint forces. Moreover, assume that the Jacobian matrix $\Phi_q = \frac{\partial \Phi}{\partial q}$ has constant rank m . This system of equations forms a DAE of index three, as will be explained. Differentiating the constraint (1.19c) twice with respect to time one obtains the velocity constraint

$$\Phi_q \dot{q} = -\Phi_t \equiv \nu, \quad (1.20)$$

and the acceleration constraint

$$\Phi_q \ddot{q} = -(\Phi_q \dot{q})_q \dot{q} - 2\Phi_{qt} \dot{q} - \Phi_{tt} \equiv \gamma, \quad (1.21)$$

respectively. Combining equations (1.19b) and (1.21) results in

$$\begin{bmatrix} M & \Phi_q^T \\ \Phi_q & O \end{bmatrix} \begin{bmatrix} \dot{v} \\ \lambda \end{bmatrix} = \begin{bmatrix} g \\ \gamma \end{bmatrix}. \quad (1.22)$$

This system has a unique solution for the accelerations \dot{v} and the Lagrange multipliers λ , viz.

$$\dot{v} = M^{-1}(g - \Phi_q^T \lambda), \quad (1.23)$$

$$\lambda = (\Phi_q M^{-1} \Phi_q^T)^{-1}(\Phi_q M^{-1} g - \gamma). \quad (1.24)$$

Substitution of the expression (1.24) for λ into equation (1.23) yields the *UODE*. Hence,

- DAE (1.19) with position constraint has index three,
- DAE (1.19a),(1.19b),(1.20) with velocity constraint has index two,
- DAE (1.19a),(1.19b),(1.21) with acceleration constraint has index one,

and the equations of motion can be formulated as a DAE of index three, index two, or index one. All these formulations are mathematically equivalent if the initial values are consistent. The initial values q_0 , v_0 and λ_0 are consistent if the position constraint (1.19c) and the velocity constraint (1.20) are satisfied and if λ_0 is determined by (1.24).

Singular Perturbations

There is a close relationship between singular perturbations and DAE systems. Consider for example the problem

$$x' = f(x, y), \quad (1.25a)$$

$$\varepsilon y' = g(x, y), \quad (1.25b)$$

where $x(t) \in \mathbb{R}^n$, $y(t) \in \mathbb{R}^m$ and f and g are sufficiently smooth vector functions of the same dimensions as x and y , respectively. Setting $\varepsilon = 0$ in (1.25b) one obtains the *reduced* DAE

$$x' = f(x, y), \quad (1.26a)$$

$$0 = g(x, y). \quad (1.26b)$$

Suppose that the Jacobian $\frac{\partial g}{\partial y}$ is invertible in a neighbourhood of the solution. Then system (1.26) has index one (as explained in Subsection 1.4). By the Implicit Function Theorem, equation (1.26b) possesses a locally unique solution $y = G(x)$. Substitution of this solution into equation (1.26a) results in the ODE

$$x' = f(x, G(x)). \quad (1.27)$$

This is the so called *state space form*.

It is well known that system (1.25) possesses a power expansion in ε [26] with smooth ε -independent coefficients x_k and y_k

$$x(t) = x_0(t) + \varepsilon x_1(t) + \varepsilon^2 x_2(t) + \dots + \varepsilon^N x_N(t) + \mathcal{O}(\varepsilon^{N+1}), \quad (1.28a)$$

$$y(t) = y_0(t) + \varepsilon y_1(t) + \varepsilon^2 y_2(t) + \dots + \varepsilon^N y_N(t) + \mathcal{O}(\varepsilon^{N+1}). \quad (1.28b)$$

Substitution of equations (1.28a) and (1.28b) into system (1.25) leads to the following system of equations

$$\begin{aligned} x'_0 &= f(x_0, y_0), \\ 0 &= g(x_0, y_0), \end{aligned} \quad (1.29a)$$

$$\begin{aligned} x'_1 &= f_x(x_0, y_0)x_1 + f_y(x_0, y_0)y_1, \\ y'_0 &= g_x(x_0, y_0)x_1 + g_y(x_0, y_0)y_1, \end{aligned} \quad (1.29b)$$

$$\begin{aligned} &\vdots \\ x'_l &= f_x(x_0, y_0)x_l + f_y(x_0, y_0)y_l + \varphi_l(x_0, y_0, \dots, x_{l-1}, y_{l-1}), \\ y'_{l-1} &= g_x(x_0, y_0)x_l + g_y(x_0, y_0)y_l + \psi_l(x_0, y_0, \dots, x_{l-1}, y_{l-1}). \end{aligned} \quad (1.29l)$$

System (1.29a) is an index one DAE, system (1.29a), (1.29b) is a DAE of index two, and, DAE (1.29) has index $l + 1$.

2 Multistep Methods

Consider the index 1 DAE

$$Ax' + Bx = q, \quad t \geq 0, \quad (2.1)$$

where $A = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$, and $B = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$.

Applying Euler forward to problem (2.1) yields the equation

$$A(x_n - x_{n-1}) + hBx_{n-1} = hq_{n-1}, \quad (2.2)$$

where $h = t_n - t_{n-1}$, and because A is singular this equation is not solvable. However, application of the implicit Euler method to the above problem results in

$$A(x_n - x_{n-1}) + hBx_n = hq_n. \quad (2.3)$$

The matrix pencil $\lambda A + B$ is nonsingular for all $\lambda \neq 0$. Therefore, equation (2.3) is solvable for $h \neq 0$.

The method above can easily be extended to k -step backward difference formulae (BDF) by replacing the derivatives by a backward difference $\rho x_n = \sum_{i=0}^k \alpha_i x_{n-i}$. This yields equation

$$A\rho x_n + hBx_n = hq_n. \quad (2.4)$$

2.1 Constant Coefficient DAE's

For linear DAE's with constant coefficients it is easy to prove the following theorem (cf. [6]).

Theorem 2.1 *The k -step BDF method ($k \leq 6$) with constant stepsize applied to linear DAE's with constant coefficients of index ν ($\nu \geq 1$) is convergent of order $\mathcal{O}(h^k)$ after $(\nu - 1)k + 1$ steps.*

So, the numerical solution converges in an interval bounded away from the initial time. This convergence result is not easily extendable to variable stepsizes, because the error estimates used in BDF codes are not realistic for DAE's of higher index; moreover the solution is not accurate at the first two steps after a change in the stepsize as can be seen from the following example. In particular, the backward Euler method fails to converge at the end of the first step following a change in the stepsize, as can be seen from the following example [6].

Example 2.2 Consider the index three problem

$$\begin{aligned} x_1' &= x_2, \\ x_2' &= x_3, \\ 0 &= x_1 - f(t). \end{aligned}$$

Applying Euler backward results in

$$\begin{aligned} x_{1,n} &= f(t_n), \\ x_{2,n} &= \frac{1}{h_n}(f(t_n) - f(t_{n-1})), \\ x_{3,n} &= \frac{1}{h_n} \left(\frac{f(t_n) - f(t_{n-1})}{h_n} - \frac{f(t_{n-1}) - f(t_{n-2})}{h_{n-1}} \right), \end{aligned}$$

where $h_n = t_n - t_{n-1}$. Notice that $x_{3,n}$ is a wrong approximation of $f''(t_{n-1})$, because of the division by h_n instead of $(1/2)(h_n + h_{n-1})$. This results in an error given by

$$\frac{1}{2} \left(\frac{h_{n-1}}{h_n} - 1 \right) f''(t_{n-1}).$$

This means that $x_{3,n}$ converges to $f''(t_n)$ with accuracy $\mathcal{O}(h_n^2)$ if the stepsize is effectively constant, i.e. $h_n = h_{n-1}(1 + \mathcal{O}(h_{n-1}))$. However, if $h_n = \mathcal{O}(h_{n-1})$ with $h_n \neq h_{n-1}$ then this results in an error $\mathcal{O}(1)$ and Euler backward does not converge.

However, Gear et al. [18] showed for variable stepsize BDF methods that if the ratio of the adjacent steps is kept bounded, then the global error in the numerical solution for the k -step BDF method applied to linear DAE's with constant coefficients of index ν is $\mathcal{O}(h_{max}^q)$, where $q = \min(k, k - \nu + 2)$. Therefore, Euler backward will fail integrating even a simple linear constant coefficient DAE of index 3, because of a global error of $\mathcal{O}(1)$.

The foregoing can be generalized to general problems of the form (1.1). Application of the k -step BDF method leads to the following difference equation

$$f(t_n, x_n, (1/h)\rho x_n) = 0. \quad (2.5)$$

This equation is solvable if the *local matrix pencil* $\lambda f_x + f_{x'}$ is nonsingular for most $\lambda \neq 0$. In this case, the *local index at t_l* , denoted as ν_l , is the index of the local pencil $\lambda f_x + f_{x'}$ at t_l .

2.2 Index One Systems

Due to the close relationship between singular perturbations and DAE's (cf. Subsection 1.5) a multistep method (i.e. the so called *direct approach*) for semi-explicit DAE's of index 1 can be obtained from applying a multistep method to the singular perturbation (1.25), and afterwards letting $\varepsilon \rightarrow 0$ (cf. [22]). This results in the difference equations

$$\sum_{i=0}^k \alpha_i x_{n-i} = h \sum_{i=0}^k \beta f(x_{n-i}, y_{n-i}) \quad (2.6a)$$

$$0 = h \sum_{i=0}^k \beta g(x_{n-i}, y_{n-i}) \quad (2.6b)$$

and the following theorem (cf. [22]) holds.

Theorem 2.3 *Suppose that system (1.12), has a nonsingular Jacobian $\frac{\partial g}{\partial y}$. Consider a multistep method of order k which is stable at the origin and at infinity and suppose that the error of the starting values x_i, y_i for $j = 0, 1, \dots, k-1$ is $\mathcal{O}(h^k)$. Then the global error of (2.6), satisfies*

$$x_n - x(t_n) = \mathcal{O}(h^k), \quad y_n - y(t_n) = \mathcal{O}(h^k),$$

for $t_n - t_0 = nh \leq \text{Const.}$

In this direct approach x_n, y_n will usually not lie on the constraint $g(x, y) = 0$, because of equation (2.6b). However, in the *indirect approach* (2.6b) is replaced by

$$g(x_n, y_n) = 0. \quad (2.7)$$

It follows from the Implicit Function Theorem that for the indirect approach Theorem 2.3 holds and the condition that infinity is in the stability region of the multistep method may be dropped. Therefore, even explicit methods can be applied.

Another important class of index one systems is the class of *uniform index one* systems, i.e. fully-implicit index one systems (1.1) with constant rank $\partial f / \partial x'$ and whose index is identically equal to one in a neighbourhood of the solution. Gear and Petzold [20] proved the following result for these uniform index one DAE's.

Theorem 2.4 *Let (1.1) be a uniform index one DAE, and assume that f is differentiable with respect to x and x' . Then the solution of (1.1) by the k -step BDF method with fixed stepsize for $k \leq 6$ converges to $\mathcal{O}(h^k)$ if all initial values are correct of order $\mathcal{O}(h^k)$.*

It can be shown [19] that if variable stepsize BDF methods are implemented in such a way that the method is stable for ODE's, then the k -step BDF method ($k \leq 6$) is convergent for fully-implicit index one DAE's. Griepentrog and März [21] studied the application of general linear multistep and one-leg methods to index one DAE's. They obtained convergence results for several different formulations of the multistep methods applied to fully implicit index one DAE's.

The codes DASSL [27] and LSODI [25] are developed to solve DAE's of index zero and index one numerically.

2.3 Semi-Explicit Index Two Systems

For higher index systems it is impossible to obtain convergence in general, even for backward Euler. Therefore, attention has been focused on higher index systems of a special structure, such as semi-explicit index two DAE's and index three systems of Hessenberg form (cf. Subsection 2.4). In this subsection the behaviour of multistep methods applied to semi-explicit index two problems is studied. Let

$$x' = f(x, y), \quad (2.8a)$$

$$0 = g(x), \quad (2.8b)$$

where f and g are assumed to be sufficiently differentiable, and where $g_x f_y$ is assumed to be invertible in a neighbourhood of the solution. Hence, the DAE (2.8) has index 2. Again, a linear multistep method for this DAE system can be applied in two different ways, viz.

$$\sum_{i=0}^k \alpha_i x_{n-i} = h \sum_{i=0}^k \beta_i f(x_{n-i}, y_{n-i}), \quad (2.9a)$$

$$0 = g(x_n), \quad (2.9b)$$

or replacing (2.9b) by

$$0 = \sum_{i=0}^k \beta_i g(x_{n-i}). \quad (2.10)$$

This last equation is the analogue of equation (2.6b).

Hairer and Wanner [22] showed that a multistep method (2.9) of order p applied to DAE (2.8), yields a local error $\mathcal{O}(h^{p+1})$ for the x component and a local error $\mathcal{O}(h^p)$ for the y component.

For BDF methods the study of convergence is simpler than for general multistep methods because the x - and y - component can be treated separately (due to $\beta_0 = \dots = \beta_{k-1} = 0$). For BDF methods the following convergence result holds (cf. [6]).

Theorem 2.5 *Suppose the nonlinear semi-explicit index two DAE (2.8), is to be solved by the k -step BDF method ($k \leq 6$). Then the k -step BDF method is convergent of order k , i.e., $x_n - x(t_n) = \mathcal{O}(h^k)$, $y_n - y(t_n) = \mathcal{O}(h^k)$, after $k + 1$ steps, whenever the initial values satisfy $x_i - x(t_i) = \mathcal{O}(h^{k+1})$, for $i = 0, \dots, k - 1$.*

If variable stepsize BDF methods are implemented in such a way that they are stable for ODE's, then the k -step BDF method ($k \leq 6$) converges for semi-explicit index 2 DAE's (cf. [19]).

The main result for general multistep methods of the form (2.9), is the following result [22].

Theorem 2.6 *Consider the index 2 system (2.8), where $g_x f_y$ is assumed to be invertible in a neighbourhood of the solution. Assume that the k -step multistep method is stable and strictly stable at infinity. If the k -step multistep method has order $p \geq 2$, then the global error satisfies*

$$x_n - x(t_n) = \mathcal{O}(h^k), \quad y_n - y(t_n) = \mathcal{O}(h^k), \quad (2.11)$$

whenever the initial values satisfy

$$x_i - x(t_i) = \mathcal{O}(h^{k+1}), \quad \text{for } i = 0, \dots, k-1.$$

The previous results can easily be extended to the second approach, with equation (2.9b) replaced by (2.10)

2.4 Index Three Systems of Hessenberg Form

In previous subsections it was noted that BDF methods converge for fully implicit index one systems, semi-explicit index two systems and for linear constant coefficient DAE's of arbitrary index with the same accuracy as for standard ODE's. In the following, convergence results for Hessenberg systems of size three are discussed.

In general, DAE (1.1) is in *Hessenberg form of size m* if it can be written as

$$\begin{aligned} x_1' &= f_1(x_1, x_2, \dots, x_m, t), \\ x_2' &= f_2(x_1, x_2, \dots, x_{m-1}, t), \\ &\vdots \\ x_i' &= f_i(x_{i-1}, x_i, \dots, x_{m-1}, t), \\ &\vdots \\ 0 &= f_m(x_{m-1}, t), \end{aligned} \quad (2.12)$$

where the matrix $\partial f_m / \partial x_{m-1} \partial f_{m-1} / \partial x_{m-2} \cdots \partial f_1 / \partial x_m$ is nonsingular in a neighbourhood of the solution. Assume that the f_i are sufficiently smooth. Then the Hessenberg system of size m has index m and is solvable. Apparently, Hessenberg index 3 systems can be expressed as

$$\begin{aligned} x_1' &= f_1(x_1, x_2, x_3, t), \\ x_2' &= f_2(x_1, x_2, t), \\ 0 &= f_3(x_2, t), \end{aligned} \quad (2.13)$$

where the matrix $\partial f_3 / \partial x_2 \partial f_2 / \partial x_1 \partial f_1 / \partial x_3$ is invertible in a neighbourhood of the solution. Multibody systems are Hessenberg index 3 systems, since they can be written as

$$\begin{aligned} M(p, t)q' &= f(p, q, t) + G^T \lambda \\ p' &= q \\ 0 &= g(p, t), \end{aligned} \quad (2.14)$$

where $G = \partial g / \partial p$.

Brenan and Engquist [7] showed that BDF methods converge of order $\mathcal{O}(h^k)$ for sufficiently accurate initial values.

Theorem 2.7 *Suppose the Hessenberg index three system (2.13) is solved by a k -step BDF method ($k \leq 6$) with constant stepsize. Let the initial values be consistent of order $k + 1$, i.e.*

$$\begin{aligned}\|x_{1,j} - x_1(t_j)\| &= \mathcal{O}(h^{k+1}), \\ \|x_{2,j} - x_2(t_j)\| &= \mathcal{O}(h^{k+1}), \\ \|f_3(x_{2,j}, t_j)\| &= \mathcal{O}(h^{k+2}),\end{aligned}$$

for $i = 0, 1, \dots, k-1$, and the algebraic equations be solved with accuracy $\mathcal{O}(h^{k+2})$ for $k \geq 2$, and $\mathcal{O}(h^{k+3})$ for $k = 1$. Then the k -step BDF method is convergent of order $k + 1$ after $k + 1$ steps.

For semi-explicit index two systems the convergence results could be extended to variable stepsizes (cf. the previous subsection). However, for Hessenberg index three systems the above convergence result cannot be extended to hold for variable stepsizes, because a new boundary layer of reduced convergence rates is initiated each time the stepsize is changed. In particular, the backward Euler method fails to converge at the end of the first step following a change in the stepsize, as can be seen from Example 2.2.

In the previous it is shown that BDF methods with constant stepsize applied to several classes of DAE systems converge of order $\mathcal{O}(h^k)$, provided the initial values are consistent and the functions are sufficiently smooth. BDF codes with variable stepsize can be used to solve these DAE's. However, there occur some difficulties. For systems of index m the iteration matrix used by the code has a condition number of $\mathcal{O}(h^{-m})$. By scaling the variables and the equations this problem can be remedied. The convergence test and error test must also be modified to allow a BDF code to solve this type of problems. For a detailed discussion we refer to [4] and [5].

3 Runge-Kutta Methods

In this section the numerical solution of DAE's by Runge-Kutta methods (RK) is studied. A class of problems where RK methods because of their one step nature are potentially advantageous over multistep methods, such as BDF methods, is the class of DAE systems with frequent discontinuities. Also, RK methods can be used to generate starting values for higher order BDF methods. Therefore, problems as in Example 2.2 where the first order BDF method (i.e. backward Euler) fails to integrate a DAE of index three (or higher) can be avoided. Further, it is important that it is possible to construct high order A -stable RK methods, whereas there are no A -stable multistep methods of order higher than two. A disadvantage of RK methods is that, in general, the amount of work per time step is much more than for multistep methods. Therefore, it is important to consider RK methods that are efficiently implementable (such as diagonally-implicit (DIRK's) or singly-implicit RK methods (SIRK's)).

Application of an m -stage implicit RK method (IRK) to DAE system (1.1) results in the following system of equations

$$x_n = x_{n-1} + h \sum_{i=1}^m b_i k_{ni}, \quad (3.1a)$$

where

$$f(t_{ni}, X_{ni}, k_{ni}) = 0, \quad i = 1, \dots, m, \quad (3.1b)$$

and the internal stages are given by

$$X_{ni} = x_{n-1} + h \sum_{j=1}^m a_{ij} k_{nj}. \quad (3.1c)$$

Further h and t_{ni} are given by

$$\begin{aligned} t_n &= t_{n-1} + h, \text{ and,} \\ t_{ni} &= t_{n-1} + \rho_i h, \quad 0 \leq \rho_1 \leq \dots \leq \rho_m \leq 1. \end{aligned}$$

This method can be displayed by the Butcher diagram

$$\frac{\rho \mid \mathcal{A}}{\mid b^T} = \begin{array}{c|cccc} \rho_1 & a_{11} & a_{12} & \dots & a_{1m} \\ \rho_2 & a_{21} & a_{22} & \dots & a_{2m} \\ \vdots & \vdots & \vdots & & \vdots \\ \rho_m & a_{m1} & a_{m2} & \dots & a_{mm} \\ \hline & b_1 & b_2 & \dots & b_m \end{array}$$

In the following, \mathcal{A} is assumed to be nonsingular. For the understanding of RK methods it is important to consider the simplifying assumptions

$$\begin{aligned} B(p) &: \sum_{i=1}^m b_i \rho_i^{q-1} = \frac{1}{q}, \quad q = 1, \dots, p; \\ C(\eta) &: \sum_{j=1}^m a_{ij} \rho_j^{q-1} = \frac{\rho_i^q}{q}, \quad i = 1, \dots, m, \quad q = 1, \dots, \eta; \\ D(\zeta) &: \sum_{i=1}^m b_i \rho_i^{q-1} a_{ij} = \frac{b_j}{q} (1 - \rho_j^q), \quad j = 1, \dots, m, \quad q = 1, \dots, \zeta; \end{aligned} \quad (3.2)$$

Condition $B(p)$ means that the quadrature formula with weights b_1, \dots, b_m and nodes ρ_1, \dots, ρ_m is of order p , and therefore, it integrates polynomials up to degree $p - 1$ exactly on the interval $[0, 1]$. Condition $C(\eta)$ means that the quadrature formula with weights a_{i1}, \dots, a_{im} integrates polynomials up to degree at least $\eta - 1$ exactly on the interval $[0, \rho_i]$, for each i .

Another important subject is the *stability function* $R(z)$ of the RK method. It is defined by the concept of A -stability: application of the RK method to equation $x' = \lambda x$ yields $x_{n+1} = R(h\lambda)x_n$, where the stability function $R(z)$ is given by $R(z) = 1 + zb^T(I - z\mathcal{A})^{-1}\mathbb{1}$, where $\mathbb{1} = (1, \dots, 1)^T$. The RK method is called A -stable if

$$|R(z)| \leq 1, \quad \text{for } Re(z) \leq 0.$$

The limit of the stability function at ∞ plays an important role for DAE's. For nonsingular matrices \mathcal{A} it is given by

$$R(\infty) = \lim_{z \rightarrow \infty} R(z) = 1 - b^T \mathcal{A}^{-1} \mathbb{1}. \quad (3.3)$$

For linear constant coefficient DAE's the following theorem [6] can easily be obtained.

Theorem 3.1 Suppose the IRK method (3.1) satisfies the strict stability condition $|R(\infty)| < 1$ and has a nonsingular matrix A . Then the IRK method applied to a linear constant coefficient index ν DAE (1.3) converges of order k_ν , i.e.

$$x_n - x(t_n) = \mathcal{O}(h^{k_\nu}), \quad \text{with } k_\nu = \min_{1 \leq i \leq \nu} (k_d, k_{a,i} - \nu + 2), \quad (3.4)$$

where k_d is the order of the method for nonstiff ODE's and $k_{a,\nu}$ is the largest integer such that

$$b^T A^{-i} \mathbb{1} = \frac{b^T A^{-\nu} \rho^{\nu-i}}{(\nu-i)!}, \quad i = 1, 2, \dots, \nu-1, \quad \text{and} \quad (3.5a)$$

$$b^T A^{-\nu} \rho^i = i(i-1) \cdots (i-\nu+1), \quad i = \nu, \nu+1, \dots, k_{a,\nu}, \quad (3.5b)$$

hold, where ρ^j is defined as $\rho^j = (\rho_1^j, \dots, \rho_m^j)^T$. The above means that $k_{a,\nu}$ is the algebraic order of the IRK method applied to index ν constant coefficient canonical algebraic systems of the form (1.7b)

And therefore, for higher index DAE's it is more difficult to find implicit Runge-Kutta methods that are convergent in all variables.

3.1 Index One Systems

As in Subsection 2.2 an IRK method can be applied in two different ways to a semi explicit index one DAE (1.12). Here, the direct approach leads to the system of equations

$$x_n = x_{n-1} + h \sum_{i=1}^m b_i k_{ni}, \quad X_{ni} = x_{n-1} + h \sum_{j=1}^m a_{ij} k_{nj}, \quad (3.6a)$$

$$y_n = y_{n-1} + h \sum_{i=1}^m b_i l_{ni}, \quad Y_{ni} = y_{n-1} + h \sum_{j=1}^m a_{ij} l_{nj}, \quad (3.6b)$$

where

$$k_{ni} = f(X_{ni}, Y_{ni}), \quad (3.6c)$$

$$0 = g(X_{ni}, Y_{ni}). \quad (3.6d)$$

(Notice that the second equation of (3.6b) determines l_{ni} uniquely if the RK matrix A is nonsingular.) In this direct approach (x_n, y_n) usually will not lie on the algebraic constraint $g(x, y) = 0$. However, if (3.6d) is replaced by

$$0 = g(x_n, y_n), \quad (\text{indirect approach}) \quad (3.7)$$

then the constraint is fulfilled not only at t_{ni} but also on t_n . If the RK method is *stiffly accurate* (i.e. $b_i = a_{mi}$, $i = 1, \dots, m$) then $y_n = Y_{nm}$ and the direct and the indirect approach are equivalent. These stiffly accurate methods are L -stable, i.e. $R(\infty) = 0$.

For both approaches IRK methods applied to semi-explicit index one DAE systems achieve the same order of accuracy in the x variable for DAE's as for nonstiff ODE's, i.e. $x_n - x(t_n) = \mathcal{O}(h^p)$, where p is the classical order of the RK method. In the indirect approach the same convergence result is obtained for the y variable, i.e. $y_n - y(t_n) = \mathcal{O}(h^p)$ (because of the Implicit Function Theorem, cf. (1.27)).

For the direct approach the following convergence result [23] holds.

Theorem 3.2 Suppose that system (1.12) has a nonsingular Jacobian $\frac{\partial g}{\partial y}$ in a neighbourhood of the solution, and that the initial values are consistent. Consider a Runge-Kutta method of order p , stage order q and with invertible matrix \mathcal{A} . If $|R(\infty)| \leq 1$, then the numerical solution of (3.6a)-(3.6d) converges globally with an error

$$y_n - y(t_n) = \mathcal{O}(h^r), \quad \text{for } t_n - t_0 = nh \leq \text{Const}, \quad (3.8)$$

where

- a. $r = p$ for stiffly accurate methods,
- b. $r = \min(p, q + 1)$ if the stability function satisfies $-1 \leq R(\infty) < 1$,
- c. $r = \min(p - 1, q)$ if $R(\infty) = 1$.

Otherwise if $|R(\infty)| > 1$ then the numerical solution diverges.

Hence, IRK methods whose solution does not satisfy the constraint can generally suffer an order reduction in the algebraic variable y . For fully implicit index one DAE's there is an extra loss of accuracy which can occur because of mixing between the errors in the differential and the algebraic parts of the DAE system. Therefore, IRK methods are, in general, less accurate for fully implicit index one DAE's than for semi-explicit index one DAE systems [6].

Theorem 3.3 Suppose DAE (1.1) is a uniform index one DAE and suppose the Runge-Kutta method satisfies the stability condition $|R(\infty)| \leq 1$. Assume the starting values are $\mathcal{O}(h^r)$ ($r > 1$), and the errors in terminating the Newton iterations are $\mathcal{O}(h^{r+\delta})$, where $\delta = 1$ if $|R(\infty)| = 1$ and $\delta = 0$ otherwise. Then the global error satisfies

$$x_n - x(t_n) = \mathcal{O}(h^r), \quad (3.9)$$

where

$$r = \begin{cases} q, & \text{if } C(q) \text{ and } B(q), \\ q + 1, & \text{if } C(q), B(q + 1) \text{ and } -1 \leq R(\infty) < 1, \\ q + 1, & \text{if } C(q), B(q + 1), A_1(q + 1) \text{ and } R(\infty) = 1, \end{cases}$$

Here,

$$A_1(q): \quad b^T \mathcal{A}^{-1} c^i = 1, \quad i = 1, \dots, q, \quad (3.10)$$

corresponds to the order conditions for IRK methods applied to linear constant coefficient index one DAE systems (i.e. $k_{a,1} = q$ iff $A_1(q)$ cf. (3.5b)).

This result gives a lower bound for the order of an IRK method applied to nonlinear index one DAE's. There exist methods which achieve a higher order of accuracy than the lower bounds predict (cf. [6] for some numerical experiments which confirm this statement). The strict stability condition $|R(\infty)| < 1$ is very important. Symmetric methods such as the implicit midpoint rule (which satisfies $R(\infty) = -1$) can be unstable for this class of problems (cf. [6]).

3.2 Semi Explicit Index Two Systems

In this subsection a study is given of the behaviour of Runge-Kutta methods applied to semi-explicit index two problems of the form

$$x' = f(x, y), \quad (3.11a)$$

$$0 = g(x), \quad (3.11b)$$

where $g_x f_y$ is assumed to be invertible in a neighbourhood of the solution. For this class of problems the direct approach of Subsection 3.1 yields the difference equations

$$x_n = x_{n-1} + h \sum_{i=1}^m b_i k_{ni}, \quad y_n = y_{n-1} + h \sum_{i=1}^m b_i l_{ni}, \quad (3.12a)$$

where

$$k_{ni} = f(X_{ni}, Y_{ni}), \quad 0 = g(X_{ni}) \quad (3.12b)$$

and the internal stages are given by

$$X_{ni} = x_{n-1} + h \sum_{j=1}^m a_{ij} k_{nj}, \quad Y_{ni} = y_{n-1} + h \sum_{j=1}^m a_{ij} l_{nj}. \quad (3.12c)$$

The first convergence results for RK-methods applied to index two systems are obtained by Petzold [28]. Replacing y in (3.11a) by z' transforms the index two system (3.11), in an index one system. Because of this close relationship between semi-explicit index two systems and uniform index one systems the global error in the differential variable x is given by Theorem 3.3.

For methods satisfying the strict stability condition $|R(\infty)| < 1$, a lower bound for the global error in the y component is given (cf. [6]) by

$$y_n - y(t_n) = \mathcal{O}(h^r), \quad (3.13)$$

where

$$r = \begin{cases} q, & \text{if } C(q), B(q), A_1(q), \\ q+1, & \text{if } C(q), B(q+1), A_1(q+1), A_2(q+1), \end{cases}$$

where A_2 are the order conditions for IRK methods applied to linear constant coefficient index two systems and are given by

$$A_2(q) : \begin{cases} b^T \mathcal{A}^{-1} \mathbb{1} = b^T \mathcal{A}^{-2} c, \\ b^T \mathcal{A}^{-2} c^i = i, \quad i = 2, 3, \dots, q, \end{cases} \quad (3.14)$$

cf. (3.5a) and (3.5b).

Hairer, Lubich and Roche [23] improved this result. They showed that, if the RK method (3.12) with invertible RK-matrix \mathcal{A} satisfies $B(p)$ and $C(q)$ ($p \geq q$), then the local error satisfies

$$\begin{aligned} \delta x_h(t) &= \mathcal{O}(h^{q+1}), \quad P(t) \delta x_h(t) = \mathcal{O}(h^{\min(p+1, q+2)}), \\ \delta y_h(t) &= \mathcal{O}(h^q), \end{aligned} \quad (3.15)$$

where $P(t)$ is a projector given by

$$P(t) = I - Q(t), \quad Q(t) = (f_y(g_x f_y)^{-1} g_x)(x(t), y(t)). \quad (3.16)$$

However, if the RK-method is stiffly accurate then

$$\delta x_h(t) = \mathcal{O}(h^{\min(p+1, q+2)}). \quad (3.17)$$

The main results are the following two theorems (cf. [23]) for the global error of the x and the y component, respectively.

Theorem 3.4 Suppose that $g_x f_y$ is invertible in a neighbourhood of the solution $(x(t), y(t))$ of (3.11) and that the initial values are consistent. Suppose further that the RK-matrix A is invertible, that $|R(\infty)| < 1$ and that the local error satisfies

$$\delta x_h(t) = \mathcal{O}(h^r), \quad P(t)\delta x_h(t) = \mathcal{O}(h^{r+1}), \quad (3.18)$$

with $P(t)$ as in (3.16). Then the method (3.12) is convergent of order r , i.e.,

$$x_n - x(t_n) = \mathcal{O}(h^r) \quad \text{for } t_n = nh \leq \text{Const.} \quad (3.19)$$

If in addition $\delta x_h(t) = \mathcal{O}(h^{r+1})$, then $g(x_n) = \mathcal{O}(h^{r+1})$.

This shows that for methods, which satisfy in addition to the invertibility of A and $|R(\infty)| < 1$, the conditions $B(p)$ and $C(q)$ ($p \geq q$), the order of convergence of the x component is at least $r = q + 1$.

The order of convergence for the y component is given by the following theorem.

Theorem 3.5 Consider the index two DAE (3.11) with consistent initial values and assume that the RK-matrix A is invertible and $|R(\infty)| < 1$. If the global error of the x component is $\mathcal{O}(h^r)$, $g(x_n) = \mathcal{O}(h^{r+1})$ and the local error of the y component is $\mathcal{O}(h^r)$, then the global error satisfies

$$y_n - y(t_n) = \mathcal{O}(h^r) \quad \text{for } t_n = nh \leq \text{Const.} \quad (3.20)$$

If the conditions $B(p)$ and $C(q)$ ($p \geq q$) are satisfied, then the order of convergence for the y component is at least $r = q$.

The results summarized here give only a lower bound for the order of convergence. Hairer and Wanner [22] give a complete set of order results based on a nontrivial extension of Butcher's theory of rooted trees. In [22] order results are given for the case of a singular RK-matrix, for Rosenbrock methods and for extrapolation methods.

Here, convergence results are not presented for methods which satisfy $|R(\infty)| = 1$. The order of convergence for the y component is generally quite poor for these methods (cf. [23]). A more serious problem is that these methods can suffer from oscillations and instabilities [1]. This problem of instability, oscillation and order reduction can be solved by applying so called *Projected Implicit Runge-Kutta methods* [2] to semi explicit index two systems:

Let x_n be the numerical solutions of IRK method (3.12), and \hat{x}_n and λ be defined by

$$\hat{x}_n = x_n + f_y(\hat{x}_n, y_n)\lambda, \quad (3.21a)$$

$$0 = g(\hat{x}_n), \quad (3.21b)$$

then \hat{x}_n is the projection of x_n onto the constraint. For stiffly accurate RK-methods the projected and unprojected RK-methods coincide. Now, stability and order are recovered by means of this extra projection onto the constraint, and for projected collocation methods superconvergence can be proved.

3.3 Hessenberg Index Three Systems

Hairer, Lubich and Roche [23] studied convergence of RK-methods applied to Hessenberg Index Three Systems (cf. Subsection 2.4). Let

$$\begin{aligned} x' &= f(x, y), \\ y' &= k(x, y, z), \\ 0 &= g(x), \end{aligned} \quad (3.22)$$

where $g_x f_y k_z$ is assumed to be invertible in a neighbourhood of the solution. Application of a RK-method to Hessenberg system (3.22) yields

$$x_n = x_{n-1} + h \sum_{i=1}^m b_i k_{ni}, \quad y_n = y_{n-1} + h \sum_{i=1}^m b_i l_{ni}, \quad z_n = z_{n-1} + h \sum_{i=1}^m b_i u_{ni}, \quad (3.23a)$$

where

$$k_{ni} = f(X_{ni}, Y_{ni}), \quad l_{ni} = k(X_{ni}, Y_{ni}, Z_{ni}), \quad 0 = g(X_{ni}), \quad (3.23b)$$

and the internal stages are given by

$$X_{ni} = x_{n-1} + h \sum_{j=1}^m a_{ij} k_{nj}, \quad Y_{ni} = y_{n-1} + h \sum_{j=1}^m a_{ij} l_{nj}, \quad Z_{ni} = z_{n-1} + h \sum_{j=1}^m a_{ij} u_{nj}. \quad (3.23c)$$

For this class of problems the local error of the RK-method (3.23), which satisfies $B(p)$ and $C(q)$ ($p \geq q + 1$, $q \geq 2$), is given by

$$\begin{aligned} \delta x_h(t) &= \mathcal{O}(h^{q+1}), & (I - (f_y S)(t)) \delta x_h(t) &= \mathcal{O}(h^{q+2}), \\ \delta y_h(t) &= \mathcal{O}(h^q), & (I - (S f_y)(t)) \delta y_h(t) &= \mathcal{O}(h^{q+1}), \\ \delta z_h(t) &= \mathcal{O}(h^{q-1}), \end{aligned} \quad (3.24)$$

with

$$S = k_z (g_x f_y k_z)^{-1} g_x. \quad (3.25)$$

Convergence of this RK-method applied to DAE (3.22) is given by the following Theorem (cf. [23]).

Theorem 3.6 *Consider the Hessenberg index three system (3.22) with consistent initial values and assume that the RK-matrix \mathcal{A} is invertible, that $|R(\infty)| < 1$, and that the conditions $B(p)$, $C(q)$ hold with $p \geq q + 1$ and $q \geq 2$. Then the global error satisfies*

$$x_n - x(t_n) = \mathcal{O}(h^q), \quad y_n - y(t_n) = \mathcal{O}(h^q), \quad z_n - z(t_n) = \mathcal{O}(h^{q-1}), \quad (3.26)$$

for $t_n = nh \leq \text{Const.}$

It is important to note that for all reasonable methods, i.e. the methods of Gaußlike type, estimates for the x component can be improved by at least one power of h .

In this section convergence results are discussed for implicit Runge-Kutta methods with constant stepsize applied to several classes of DAE's. It is shown that these methods can suffer from order reduction and therefore care must be taken in choosing a RK method appropriate for DAE's. Implementation of RK methods in a code for solving DAE systems gives the same problems [23], with respect to poor conditioning and error estimation, as for BDF methods (cf. 2.4).

4 Solution Techniques For Higher Index DAE's

In this section integration schemes for the equations of motion generated by multibody systems are discussed. In Sections 2 and 3 the numerical solution of DAE's by multistep and Runge-Kutta methods is studied. These methods can generally not be applied to higher index ($\nu \geq 2$) DAE's, since most of them are convergent for index one problems only. Another problem is the loss of the approximation order of the algebraic variables. This causes standard techniques of error estimation and stepsize selection to fail. These problems can be avoided by differentiating the DAE $\nu - 1$ times with respect to time. Afterwards this index-reduced system can be solved numerically by multistep or Runge-Kutta methods, for example. This approach gives rise to two problems. Firstly, the numerical solution of the index-reduced system does not fulfill the original constraints on every step, and because of error propagation the numerical solution tends to drift away from the algebraic constraints (cf. [12]). Secondly, the stability of the DAE with respect to perturbations in the solution may change due to the index transformation (cf. [13]).

In the following, several methods especially designed for solving the equations of motion for multibody systems are discussed.

4.1 Regularization Methods

The regularization of a DAE can be interpreted as the introduction of a small parameter into the DAE such that the solution of the perturbed system approaches the solution of the original DAE as the parameter tends to zero. In this subsection several approaches which can be interpreted as regularization methods are described.

The oldest regularization method for circumventing the problem of drifting off the constraints $\Phi = 0$ (1.19c) was introduced by Baumgarte [3]. He introduced stabilizing control terms into the index one DAE (1.19a),(1.19b),(1.21). Now, instead of the acceleration constraints $\ddot{\Phi} = 0$ (1.21) a linear combination of $\ddot{\Phi}$ (1.21), $\dot{\Phi}$ (1.20), and Φ (1.19c)

$$\ddot{\Phi} + 2\alpha\dot{\Phi} + \beta^2\Phi = 0, \quad (4.1)$$

with parameters α and β is used. Here, DAE (1.19a),(1.19b),(4.1) has index one. The Baumgarte parameters α and β in (4.1) are chosen such that the resulting system damps errors in satisfying the constraint equation, i.e. $\Phi \equiv 0$ is a stable solution of equation (4.1). This yields $\alpha > 0$. Often one chooses $\alpha = \beta$, which corresponds with the aperiodic limit case (or the critical damping condition).

Baumgarte's approach results in the following DAE

$$\begin{aligned} \dot{q} &= v, \\ M(q, t)\dot{v} &= g(q, v, t) + \Phi_q^T \lambda, \\ 0 &= \ddot{\Phi} + 2\alpha\dot{\Phi} + \beta^2\Phi. \end{aligned} \quad (4.2)$$

This index one DAE can be solved by integration techniques which are convergent for index one DAE's. Numerical evidence shows that the drift-off from the algebraic constraint becomes essentially weaker than in the original case. However, a problem is the choice of the Baumgarte parameters α and β . Choosing them too large results in a stiff system, because extraneous eigenvalues are introduced into the system. Choosing the parameters too small

minimizes the stabilization effect. The question of the choice of α and β has never been cleared sufficiently. But, this approach is quite general and has proven to be useful in several applications.

Other regularization techniques were proposed by Lötstedt, Knorrenschild and Hanke and have been compared by Eich and Hanke [10], who showed that these methods are very similar. Lötstedt introduced penalty functions which lead to the equation

$$M\ddot{q} = g - \varepsilon^{-1}\kappa. \quad (4.3)$$

Applying Knorrenschild's approach yields

$$\begin{aligned} M\ddot{q} &= g + \Phi_q^T \lambda, \\ 0 &= \Phi(q + (\varepsilon + \mu)\dot{q} + \mu\varepsilon M^{-1}(g + \Phi^T \lambda)), \end{aligned} \quad (4.4)$$

while Hanke's regularization technique results into

$$\begin{aligned} \dot{q} &= v + \mu\dot{v}, \\ M\dot{v} &= g(q, v, t) + \Phi_q^T \lambda, \\ 0 &= \Phi(q + \varepsilon\dot{q} + \mu\varepsilon M^{-1}(g + \Phi^T \lambda)). \end{aligned} \quad (4.5)$$

Eich and Hanke showed that the methods of Baumgarte, Knorrenschild and Hanke differ only in higher order terms in ε , μ .

4.2 Generalized Coordinate Partitioning

Using a differential geometric approach [30] DAE's can be interpreted as differential equations on manifolds. Therefore, DAE's can be parametrized, at least locally, as differential equations on manifolds. The constraints can be used to define this local parametrization, which defines a local bijective correspondence between the state variable and the variable on the parameter space. Wehage and Haug [32] and Rheinboldt [30] developed differential geometric techniques to determine this local coordinate system, where the ODE is integrated by standard methods. It is illustrative to describe the generalized coordinate partitioning method developed by Wehage and Haug [32]. Consider the equations of motion (cf. also Subsection 1.5)

$$\dot{q} = v, \quad (4.6a)$$

$$M(q, t)\dot{v} = g(q, v, t) + \Phi_q^T \lambda, \quad (4.6b)$$

$$0 = \Phi(q, t), \quad (4.6c)$$

together with the velocity and acceleration constraints

$$\Phi_q \dot{q} = \nu, \quad (4.7)$$

and,

$$\Phi_q \ddot{q} = \gamma, \quad (4.8)$$

respectively. The Jacobian matrix $\Phi_q = \frac{\partial \Phi}{\partial q}$ has full row rank m . So, there is at least one nonsingular submatrix of Φ_q of rank m . Vector q can be partitioned as

$$q = \begin{bmatrix} u \\ v \end{bmatrix}, \quad (4.9)$$

such that Φ_u is the submatrix of Φ_q corresponding to u . Here, u denotes the dependent generalized coordinates, and, v denotes the independent generalized coordinates. The implicit function Theorem assures that there exists a twice differentiable function $h = h(v, t)$ such that

$$u = h(v, t), \quad (4.10)$$

is the solution of (4.6c) for u as function of v and t . By relation (4.10) the equations of motion can be rewritten in terms of the independent generalized coordinates v . After elimination of the Lagrange multipliers, the equations of motion can be expressed as an ODE for the coordinates v , i.e.

$$\widehat{M}(v, t)\dot{v} = \widehat{g}(v, \dot{v}, t). \quad (4.11)$$

This ODE can be solved numerically by standard methods. Given the complexity of matrix \widehat{M} and vector \widehat{g} of (4.11) as functions of v and s , direct discretization of (4.11) would be very complicated and impracticable. Therefore, consider DAE (4.6a),(4.6b),(4.7). From this system $\vec{q} = [\ddot{u}^T, \ddot{v}^T]^T$ can be solved. Now, \ddot{v} can be integrated, by any explicit ODE solver, to find \dot{v} and v . Afterwards u and \dot{u} can be obtained by solving (4.6c) and (4.7), respectively. This can be continued to the final time, as long as partitioning (4.9) does not need to be changed. However, if Φ_u becomes ill conditioned, then the generalized coordinates q should be repartitioned. The partitioning of q can be carried out by e.g. Gauß-Jordan reduction with complete pivoting or by SVD or QU factorization. Haug and Yen [24] also developed an implicit DAE solver based on generalized coordinate partitioning.

4.3 Projection Methods

Drift-off from the constraints can be avoided by numerically solving a DAE with lower index and afterwards projecting the solution back on the original constraints. Eich et al. [11] showed that these projections can be divided into two classes depending on whether they rely on stabilizing projections of position and velocity variables (*coordinate projection methods*) or on projections of residuals (*derivative projection methods*).

Gear et al. [19] introduced *stabilizing Lagrange multipliers* μ to simultaneously reduce the index and satisfy the position constraint and the velocity constraint

$$\begin{aligned} \dot{q} &= v + \Phi_q^T \mu, \\ M(q, t)\dot{v} &= g(q, v, t) + \Phi_q^T \lambda, \\ 0 &= \Phi(q, t), \\ 0 &= \Phi_q(q, t)v. \end{aligned} \quad (4.12)$$

A solution of (4.12) exists only if the additional stabilizing multipliers μ satisfy $\mu = 0$. Hence, (4.12) and the original system have the same solution. DAE (4.12) has index two and can be integrated numerically. Führer and Leimkuhler [14] extended this idea to the index one system. Therefore, two additional multipliers μ and ν have to be introduced to satisfy the position constraint, the velocity constraint and the acceleration constraint

$$\begin{aligned} \dot{q} &= v + \Phi_q^T \mu + [v^T \Phi_q]^T \eta, \\ M(q, t)\dot{v} &= g(q, v, t) + \Phi_q^T \lambda + \Phi_q^T \eta, \\ 0 &= \Phi_q(q, t)\ddot{q} - \gamma, \\ 0 &= \Phi_q(q, t)\dot{q} - \nu, \\ 0 &= \Phi(q, t). \end{aligned} \quad (4.13)$$

This DAE has index two and the index two variables μ and ν have to be equal to zero to assure existence of a solution. These two approaches can be interpreted as derivative projections onto state space forms, since they project the derivative f onto the constraint manifolds. One can show that the coordinate projection methods [32] (cf. Subsection 4.2), the differential geometric approach [29] and methods using overdetermined DAE's (discussed in the next subsection) can be seen as derivative projection methods.

Coordinate projection methods do not project the derivative f onto the constraints, but they project the computed solution of the state space form or the index one DAE onto the constraint manifold. Shampine [31] first described this technique for one step methods and Eich [9] gave a convergence proof of this method in the context of multistep methods.

4.4 Overdetermined Differential Algebraic Equations

Another approach is taken by Führer [12]. To circumvent the problem of drift-off from the constraints, not only the position constraints (1.19c), but also the velocity (1.20) and the acceleration constraints (1.21) are used. Together with equations (1.19a) and (1.19b) this yields an overdetermined system of DAE's (ODAE)

$$\dot{q} = v, \quad (4.14a)$$

$$M(q, t)\dot{v} = g(q, v, t) + \Phi_q^T \lambda, \quad (4.14b)$$

$$0 = \Phi_q(q, t)\ddot{q} - \gamma, \quad (4.14c)$$

$$0 = \Phi_q(q, t)\dot{q} - \nu, \quad (4.14d)$$

$$0 = \Phi(q, t). \quad (4.14e)$$

This ODAE has index one. For consistent initial values this ODAE has a unique solution. This solution is identical to the solution of the original DAE (4.14a),(4.14b),(4.14e). Discretizing this ODAE by e.g. BDF results in

$$0 = \begin{bmatrix} \rho q_n - v_n \\ M(q_n, t_n)\rho v_n - g(q_n, v_n, t_n) - \Phi_q(q_n, t_n)^T \lambda_n \\ \Phi_q(q_n, t_n)\rho v_n - \gamma_n \\ \Phi_q(q_n, t_n)\rho q_n - \nu_n \\ \Phi(q_n, t_n) \end{bmatrix}. \quad (4.15)$$

However, the discretized version (4.15) of this ODAE does not have a unique numerical solution. Therefore, this system has to be solved in a least squares sense. In other words, the numerical solution must satisfy equations (4.14) in a generalized inverse sense. Führer and Leimkuhler [14] showed that there exists a generalized solution, the so called *ssf-solution*, which is (in the linearized case) numerically equivalent to the reduction to state space form of the linearized equations of motion. Moreover, using the *ssf-solution* of (4.15) within a BDF method is equivalent to solving the following stabilized problem with the same BDF-method, i.e.

$$\begin{aligned} \dot{q} &= v + \Phi_q^T \mu + [v^T \Phi_q]^T \eta, \\ M(q, t)\dot{v} &= g(q, v, t) + \Phi_q^T \lambda + \Phi_q^T \eta, \\ 0 &= \Phi_q(q, t)\ddot{q} - \gamma, \\ 0 &= \Phi_q(q, t)\dot{q} - \nu, \\ 0 &= \Phi(q, t). \end{aligned} \quad (4.16)$$

Gear et al. [19] introduced the additional Lagrange multipliers $\eta(t)$ and $\mu(t) \in \mathbb{R}^m$ and in order to stabilize the equations of motion. They showed that the algebraic variable λ in equation (4.16) is an index one variable, while η and μ are negligible for the numerical integration.

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