REGULAR SOLUTIONS OF NONLINEAR DIFFERENTIAL-ALGEBRAIC EQUATIONS AND THEIR NUMERICAL DETERMINATION

PETER KUNKEL* AND VOLKER MEHRMANN†

Abstract. For a general class of nonlinear (possibly higher index) differential-algebraic equations we show existence and uniqueness of solutions. These solutions are regular in the sense that Newton's method will converge locally and quadratically. On the basis of the presented theoretical results, numerical methods for the determination of consistent initial values and for the computation of regular solutions are developed. Several numerical examples are included.

Key words. Nonlinear differential-algebraic equations, regular solutions, strangeness index, existence and uniqueness, consistent initial values, numerical methods.

AMS subject classifications. 65L99, 34A09.

1. Introduction. If physical systems contain constraints such as links in mechanical systems or if they are governed by some conservation laws as Kirchhoff's laws for electric circuits, their modelling usually leads to nonlinear equations of the form

$$F(t, x, \dot{x}) = 0, \tag{1}$$

so-called differential-algebraic equations (DAEs), with $F \in C(\mathbb{I} \times \mathbb{D}_x \times \mathbb{D}_{\dot{x}}, \mathbb{R}^n)$, $\mathbb{I} \subseteq \mathbb{R}$ (compact) interval, $\mathbb{D}_x, \mathbb{D}_{\dot{x}} \subseteq \mathbb{R}^n$ open. Obviously, ordinary differential equations form a special case of (1). Although the theory and numerical methods are well developed for the latter class, similar results for (1) are still rare. In the last years, great effort was made in understanding the properties of (1) and finding existence and uniqueness results that are as general as possible and, from a numerical analysis point of view, suitable for building a base for numerical methods. Remarkably, this not only concerned the nonlinear case. Already the linear case

$$E(t)\dot{x} = A(t)x + f(t), \tag{2}$$

where $E, A \in C(\mathbb{I}, \mathbb{R}^{n,n})$, $f \in C(\mathbb{I}, \mathbb{R}^n)$, required some hard analysis.

In the last decade, several more or less different approaches were taken to understand special or general nonlinear DAEs. Most of them require that some step-by-step index reduction process is possible, see, e. g., [7, 15, 17, 18, 19, 20]. The assumptions needed for this process mainly consist of constant rank conditions for each level of the reduction process in the neighborhood of the solution under investigation. Although these approaches give a good insight into a large class of nonlinear problems, in general they do not lead to practical numerical procedures. Only very recently, a rather general theory together with a method for the numerical treatment of nonlinear DAEs was developed in [3, 4, 5]. This approach is theoretically based on the concept of the differentiation index which played a central role in the understanding of linear DAEs.

* Fachbereich Mathematik, Carl von Ossietzky Universität, Postfach 2503, D–26111 Oldenburg, Fed. Rep. Germany

† Fakultät für Mathematik, Technische Universität Chemnitz-Zwickau, D–09107 Chemnitz, Fed. Rep. Germany.

This work has been supported by *Deutsche Forschungsgemeinschaft, Research grant Me 790/5-2 Differentiell-algebraische Gleichungen.*

The aim of this paper is to present a local existence and uniqueness theory for a class of nonlinear DAEs that is more general than in the above approaches and that also leads to suitable numerical procedures for the computation of the solution.

The paper is organized as follows. In Section 2 we briefly discuss the linear case as far as it is relevant for the nonlinear case which is treated in Section 3. On the basis of the obtained results we then develop appropriate numerical methods in Section 4 and discuss some numerical tests in Section 5. Finally we give some conclusions in Section 6.

2. The linear case. The standard method to solve nonlinear problems is by means of Newton's method. In principle, it consists of linearizing around some given initial guess, solving the so obtained linear problem and then correcting the initial guess. The main problem therefore is to be able to treat the arizing linear subproblems. Moreover, for a local existence theorem for solutions these subproblems must be regular in some sense, see, e. g., [6].

Following an idea of Campbell [2], we can differentiate (2) for sufficiently smooth coefficient functions to obtain *inflated* DAEs

$$M_\ell(t)\dot{z}_\ell = N_\ell(t)z_\ell + g_\ell(t) \tag{3}$$

with

$$\begin{aligned} (M_\ell)_{i,j} &= \tbinom{i}{j}E^{(i-j)} - \tbinom{i}{j+1}A^{(i-j-1)},\ i,j = 0,\dots,\ell,\\ (N_\ell)_{i,j} &= \begin{cases} A^{(i)} & \text{for } i = 0,\dots,\ell,\ j = 0,\\ 0 & \text{else,}\end{cases}\\ (z_\ell)_i &= x^{(i)},\ i = 0,\dots,\ell,\\ (g_\ell)_i &= f^{(i)},\ i = 0,\dots,\ell, \end{aligned} \tag{4}$$

where we use the convention that $\binom{i}{j} = 0$ for $i < 0$, $j < 0$ or $j > i$. The most general class of linear problems that possess the desired properties seems to be characterized by the following hypothesis.

HYPOTHESIS 2.1. *There exist integers μ, a, and d such that the inflated pair (M_μ, N_μ) associated with (E, A) has the following properties.*

1. For all $t \in \mathbb{I}$ we have $\operatorname{rank} M_\mu(t) = (\mu+1)n - a$. *This implies the existence of a smooth matrix function Z_2 of size $((\mu+1)n, a)$ with orthonormal columns satisfying $Z_2^T M_\mu = 0$.*

2. For all $t \in \mathbb{I}$ we have $\operatorname{rank} \hat{A}_2(t) = a$, *where $\hat{A}_2 = Z_2^T N_\mu [I_n\ 0\ \cdots\ 0]^T$. This implies the existence of a smooth matrix function T_2 of size (n, d), $d = n - a$, with orthonormal columns satisfying $\hat{A}_2 T_2 = 0$.*

3. For all $t \in \mathbb{I}$ we have $\operatorname{rank} E(t)T_2(t) = d$. *This implies the existence of a smooth matrix function Z_1 of size (n, d) with orthonormal columns satisfying* $\operatorname{rank} \hat{E}_1 = \operatorname{rank} Z_1^T E = d$.

When the coefficient functions of a linear DAE (2) satisfy Hypothesis 2.1, we call the least possible μ the *(global) strangeness index* (or abbreviated as s-index in the following) of (2).

In [12] it has been shown that requiring Hypothesis 2.1 is equivalent to requiring that the *differentiation index* (see, e. g., [1]) is well-defined, but it needs less smoothness of the coefficient functions. In addition, Hypothesis 2.1 seems to be extendable to underdetermined systems (e. g., control problems), for which the differentiation index is not defined. Compared with so-called index reduction methods (see, e. g.,

[2, 7, 10, 18]) which represent recursive procedures that iteratively lower the index by one until one arrives at a DAE with vanishing s-index, systems that satisfy Hypothesis 2.1 allow for an index reduction to a DAE with vanishing s-index in a single step (such that no assumptions on ranks are needed for intermediate steps).

Defining

$$\hat{E} = \begin{bmatrix} \hat{E}_1(t) \\ 0 \end{bmatrix}, \quad \hat{A} = \begin{bmatrix} \hat{A}_1(t) \\ \hat{A}_2(t) \end{bmatrix}, \quad \hat{f} = \begin{bmatrix} \hat{f}_1(t) \\ \hat{f}_2(t) \end{bmatrix} \tag{5}$$

with $\hat{A}_1 = Z_1^T A$ and $\hat{f}_1 = Z_1^T f$, $\hat{f}_2 = Z_2^T g_\mu$ for sufficiently smooth f, Hypothesis 2.1 obviously yields that all solutions of (2) are also solutions of the DAE

$$\hat{E}(t)\dot{x} = \hat{A}(t)x + \hat{f}(t). \tag{6}$$

But one can also show that even the reverse is true, see [12].

THEOREM 2.2. *Consider the linear DAE*

$$E(t)\dot{x} = A(t)x + f(t), \tag{7}$$

together with the initial condition

$$x(t_0) = x_0. \tag{8}$$

Let (E, A) satisfy Hypothesis 2.1 with μ and a. In particular, let $E, A \in C^{\mu+1}(\mathbb{I}, \mathbb{R}^{n,n})$ and $f \in C^{\mu+1}(\mathbb{I}, \mathbb{R}^n)$. Then the following holds.

1. An initial condition (8) is consistent (i. e., the corresponding initial value problem has at least one solution) if and only if (8) implies the a conditions

$$\hat{A}_2(t_0)x_0 + \hat{f}_2(t_0) = 0. \tag{9}$$

2. Every initial value problem with consistent initial condition has a unique solution.

According to [8, 11], the so obtained strangeness-free DAE (i. e., with vanishing s-index) can be formulated as an operator equation with an underlying regular operator.

THEOREM 2.3. *Let $D: \mathbb{X} \to \mathbb{Y}$ be defined by*

$$(Dx)(t) = \hat{E}(t)\dot{x}(t) - \hat{A}(t)x(t), \quad t \in \mathbb{I}, \tag{10}$$

where the Banach spaces

$$\mathbb{X} = \{x \in C(\mathbb{I}, \mathbb{R}^n) \mid \hat{E}^+\hat{E}x \in C^1(\mathbb{I}, \mathbb{R}^n),\ \hat{E}^+\hat{E}x(t_0) = 0\}, \quad \mathbb{Y} = C(\mathbb{I}, \mathbb{R}^n) \tag{11}$$

are equipped with the norms

$$\|x\|_{\mathbb{X}} = \|x\|_{\mathbb{Y}} + \|\frac{d}{dt}(\hat{E}^+\hat{E}x)\|_{\mathbb{Y}}, \quad \|f\|_{\mathbb{Y}} = \max_{t\in\mathbb{I}} \|f(t)\|_\infty. \tag{12}$$

Then D is continuous and invertible with continuous inverse.

Note that homogeneous initial conditions can be obtained without loss of generality by replacing $x(t)$ with $x(t) - x_0$. The operator $\hat{E}^+\hat{E}$ is defined pointwise by $(\hat{E}^+\hat{E}x)(t) = \hat{E}(t)^+\hat{E}(t)x(t)$ where $\hat{E}(t)^+$ denotes the Moore-Penrose pseudoinverse of $\hat{E}(t)$.

3. The nonlinear case. Turning to the general nonlinear problem (1), we assume that a solution x^* is given. To guarantee local uniqueness of x^* and the applicability of Newton's method for the determination of x^*, we need some regularity property of x^* which can be extended to a whole neighborhood of x^*. The results of the previous section propose that the linearization of (1) along x^* should satisfy Hypothesis 2.1. But requiring Hypothesis 2.1 for all linearizations along x in a neighborhood of x^* may be too restrictive.

EXAMPLE 3.1. The DAE

$$\begin{bmatrix} 1 & 0 \\ \dot{x}_1 & 1 \end{bmatrix} \begin{bmatrix} \dot{x}_2 - x_1 \\ x_2 \end{bmatrix} = 0$$

may be seen as a regularly transformed linear DAE satisfying Hypothesis 2.1 with $\mu = 1$, $a = 2$, and $d = 0$. Its linearization is given by

$$\begin{bmatrix} 0 & 1 \\ \dot{x}_2 - x_1 & \dot{x}_1 \end{bmatrix} \begin{bmatrix} \Delta\dot{x}_1 \\ \Delta\dot{x}_2 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ \dot{x}_1 & -1 \end{bmatrix} \begin{bmatrix} \Delta x_1 \\ \Delta x_2 \end{bmatrix} + \begin{bmatrix} x_1 - \dot{x}_2 \\ -\dot{x}_1\dot{x}_2 + x_1\dot{x}_1 - x_2 \end{bmatrix}.$$

For $(x_1, x_2) = (0, 0)$ we find that M_ℓ is always rank deficient whereas for $(x_1, x_2) = (\varepsilon, 0)$ with $\varepsilon \neq 0$ it always has full rank. Thus Hypothesis 2.1 does not hold uniformly for all linearizations in a neighborhood of the solution $(x_1^*, x_2^*) = (0, 0)$.

In general, we must therefore expect that away from the solution the constant rank assumptions as required in Hypothesis 2.1 for the linear case do not hold for the linearization. This suggests that for higher index problems the linearization of the original equation alone makes no sense. We must include derivatives of the equation. Moreover, the common constant rank assumptions must be restricted to a subset of a neighborhood. For these reasons, we generalize Hypothesis 2.1 to nonlinear problems (1) in the following way denoting by

$$F_\ell(t, x, \dot{x}, \ldots, x^{(\ell+1)}) = 0 \tag{13}$$

the *inflated* nonlinear DAEs obtained by successive differentiation and by

$$\begin{aligned} M_\ell(t, x, \dot{x}, \ldots, x^{(\ell+1)}) &= F_{\ell;\dot{x},\ldots,x^{(\ell+1)}}(t, x, \dot{x}, \ldots, x^{(\ell+1)}), \\ N_\ell(t, x, \dot{x}, \ldots, x^{(\ell+1)}) &= -(F_{\ell;x}(t, x, \dot{x}, \ldots, x^{(\ell+1)}), 0, \ldots, 0) \end{aligned} \tag{14}$$

its Jacobians.

HYPOTHESIS 3.2. *There exist integers μ, a, and d such that for all values $(t, x, \dot{x}, \ldots, x^{(\mu+1)}) \in \mathbb{L}$, where $\mathbb{L}$ associated with F is given by*

$$\mathbb{L} = \{(t, x, \dot{x}, \ldots, x^{(\mu+1)}) \in \mathbb{I} \times \mathbb{R}^n \times \mathbb{R}^n \times \ldots \times \mathbb{R}^n \mid F_\mu(t, x, \dot{x}, \ldots, x^{(\mu+1)}) = 0\}, \tag{15}$$

the following properties hold.

1. We have $\operatorname{rank} M_\mu(t, x, \dot{x}, \ldots, x^{(\mu+1)}) = (\mu+1)n - a$. *This implies the existence of a matrix function Z_2 of size $((\mu+1)n, a)$ with orthonormal columns which is smooth on $\mathbb{L}$ and satisfies there $Z_2^T M_\mu = 0$.*

2. We have $\operatorname{rank} \hat{A}_2(t, x, \dot{x}, \ldots, x^{(\mu+1)}) = a$, *where $\hat{A}_2 = Z_2^T N_\mu [I_n\ 0\ \cdots\ 0]^T$. This implies the existence of a matrix function T_2 of size (n, d), $d = n - a$, with orthonormal columns which is smooth on $\mathbb{L}$ and satisfies there $\hat{A}_2 T_2 = 0$.*

3. We have $\operatorname{rank} F_{\dot{x}}(t, x, \dot{x}) T_2(t, x, \dot{x}, \ldots, x^{(\mu+1)}) = d$. *This implies the existence of a matrix function Z_1 of size (n, d) with orthonormal columns which is smooth on $\mathbb{L}$ and satisfies there* $\operatorname{rank} \hat{E}_1 = \operatorname{rank} Z_1^T E = d$.

It is clear that Hypothesis 3.2 reduces to Hypothesis 2.1 for linear problems. The main differences between Hypothesis 3.2 and the assumptions in [4, 5] are that we do not require constant rank in a neighborhood of the solution in the whole space but only on a submanifold, and that we need less smoothness of the function F. The latter observation is described in detail in [12].

REMARK 3.3. Note that due to Taylor's theorem we obtain the same matrix functions when we first differentiate F and then linearize along some x or when we first linearize along x and then differentiate.

The first immediate consequences of Hypothesis 3.2 are the following.

LEMMA 3.4. *We have*

$$\operatorname{rank} F_{\mu;x,\dot{x},\ldots,x^{(\mu+1)}}(t,x,\dot{x},\ldots,x^{(\mu+1)}) = (\mu+1)n \tag{16}$$

for all $(t,x,\dot{x},\ldots,x^{(\mu+1)}) \in \mathbb{L}$.

Proof. The claim follows directly from

$$F_{\mu;x,\dot{x},\ldots,x^{(\mu+1)}} = (-N_\mu [I_n\, 0\, \cdots\, 0]^T, M_\mu).$$

□

COROLLARY 3.5. *The set* $\mathbb{L} \subseteq \mathbb{R}^{1+n+(\mu+1)n}$ *forms a (smooth) manifold of dimension* $n+1$.

EXAMPLE 3.6. For the nonlinear problem from Example 3.1 written in the form

$$\dot{x}_2 - x_1 = 0, \quad \dot{x}_1\dot{x}_2 - \dot{x}_1 x_1 + x_2 = 0,$$

differentiation yields

$$\ddot{x}_2 - \dot{x}_1 = 0, \quad \ddot{x}_1\dot{x}_2 + \dot{x}_1\ddot{x}_2 - \ddot{x}_1 x_1 - \dot{x}_1^2 + \dot{x}_2 = 0.$$

Thus for $\mu = 1$ we find

$$(-N_1[I\ 0]^T, M_1)(t,x,\dot{x},\ddot{x}) = \left[\begin{array}{cc|cc|cc} -1 & 0 & 0 & 1 & & \\ -\dot{x}_1 & 1 & \dot{x}_2 & \dot{x}_1 & & \\ \hline 0 & 0 & -1 & 0 & 0 & 1 \\ -\ddot{x}_1 & 0 & \ddot{x}_2 - 2\dot{x}_1 & \ddot{x}_1 + 1 & \dot{x}_2 - x_1 & \dot{x}_1 \end{array}\right]$$

and

$$\begin{aligned}\mathbb{L} &= \{(t,x_1,x_2,\dot{x}_1,\dot{x}_2,\ddot{x}_1,\ddot{x}_2) \mid x_1 = \dot{x}_2,\ x_2 = \dot{x}_1 x_1 - \dot{x}_1\dot{x}_2, \\ &\qquad\qquad \dot{x}_1 = \ddot{x}_2,\ \dot{x}_2 = \ddot{x}_1 x_1 + \dot{x}_1^2 - \ddot{x}_1\dot{x}_2 - \dot{x}_1\ddot{x}_2\} \\ &= \{(t,x_1,x_2,\dot{x}_1,\dot{x}_2,\ddot{x}_1,\ddot{x}_2) \mid x_1 = 0,\ x_2 = 0,\ \dot{x}_1 = \ddot{x}_2,\ \dot{x}_2 = 0\}.\end{aligned}$$

Hence, we have $\operatorname{rank} M_1 = 2$ and $\operatorname{rank}(-N_1[I\ 0]^T, M_1) = 4$ on $\mathbb{L}$ and the above problem satisfies Hypothesis 3.2 with $\mu = 1$, $a = 2$, and $d = 0$. Note that $\mathbb{L}$ forms a manifold of dimension three which can be parametrized by $(t, \ddot{x}_1, \ddot{x}_2)$.

Following Section 2, the idea now is to transform the original problem to a new one such that x^* remains a solution but such that the new problem has s-index zero (differentiation index at most one).

According to Corollary 3.5, the set $\mathbb{L}$ can be locally parametrized by $n+1$ variables. These can be chosen from $(t,x,\dot{x},\ldots,x^{(\mu+1)})$ by checking which columns of $F_{\mu;t,x,\dot{x},\ldots,x^{(\mu+1)}}$ can be discarded without rank drop. Following Hypothesis 3.2, the

variable t can always be taken as parameter. Let now $y_0 = (t_0, x_0, \dot{x}_0, \ldots, x_0^{(\mu+1)}) \in \mathbb{L}$ be fixed. Because of

$$\operatorname{corank} M_\mu(y_0) = a, \quad \operatorname{rank} Z_2(y_0)^T N_\mu(y_0) = a,$$

$(N_\mu(y_0), M_\mu(y_0))$ is of full rank and there are a variables from x, say (without loss of generality) x_2 from $x = (x_1, x_2)$, such that discarding the $d = n - a$ columns of $F_{\mu;t,x,\dot{x},\ldots,x^{(\mu+1)}}$ that belong to x_1 indeed does not lead to a rank drop. The remaining a variables, say v, can therefore be chosen from $(\dot{x}, \ldots, x^{(\mu+1)})$.

Let (t_0, x_{10}, v_0) be that part of y_0 that corresponds to the variables (t, x_1, v). The above considerations imply that there is a neighborhood $\mathbb{U} \subseteq \mathbb{R}^{n+1}$ of (t_0, x_{10}, v_0), without loss of generality an open ball with radius $\varepsilon > 0$ and center (t_0, x_{10}, v_0), and a neighborhood $\mathbb{V}$ of y_0 such that

$$\mathbb{L} \cap \mathbb{V} = \{\varphi(t, x_1, v) \mid (t, x_1, v) \in \mathbb{U}\}$$

where $\varphi\colon \mathbb{U} \to \mathbb{L} \cap \mathbb{V}$ is a diffeomorphism. In other words, the relation

$$F_\mu(t, x, \dot{x}, \ldots, x^{(\mu+1)}) = 0$$

can locally be solved according to

$$(t, x, \dot{x}, \ldots, x^{(\mu+1)}) = \varphi(t, x_1, v).$$

In particular, there are locally defined functions G_2 and G_3 such that

$$F_\mu(t, x_1, G_2(t, x_1, v), G_3(t, x_1, v)) \equiv 0. \tag{17}$$

Let us now consider

$$\hat{F}_2 = Z_2^T F_\mu \tag{18}$$

with Z_2 as defined by Hypothesis 3.2. From

$$\hat{F}_2(t, x_1, G_2(t, x_1, v), G_3(t, x_1, v)) \equiv 0$$

it follows by differentiation with respect to v that (omitting arguments)

$$\begin{aligned} \frac{d}{dv}\hat{F}_2 &= (Z_{2;x_2}^T F_\mu + Z_2^T F_{\mu;x_2}) G_{2;v} + (Z_{2;\dot{x},\ldots,x^{(\mu+1)}}^T F_\mu + Z_2^T F_{\mu;\dot{x},\ldots,x^{(\mu+1)}}) G_{3;v} \\ &= Z_2^T F_{\mu;x_2} G_{2;v} \equiv 0 \end{aligned}$$

on $\mathbb{U}$. By construction, x_2 was selected such that $Z_2^T F_{\mu;x_2}$ is nonsingular, hence

$$G_{2;v}(t, x_1, v) = 0$$

for all $(t, x_1, v) \in \mathbb{U}$. Therefore,

$$x_2 = \hat{G}_2(t, x_1) = G_2(t, x_1, v_0).$$

Differentiating now $\hat{F}_2$ with respect to x_1, we get (without arguments)

$$\begin{aligned} \frac{d}{dx_1}\hat{F}_2 &= (Z_{2;x_1}^T F_\mu + Z_2^T F_{\mu;x_1}) + (Z_{2;x_2}^T F_\mu + Z_2^T F_{\mu;x_2}) G_{2;x_1} \\ &\qquad + (Z_{2;\dot{x},\ldots,x^{(\mu+1)}}^T F_\mu + Z_2^T F_{\mu;\dot{x},\ldots,x^{(\mu+1)}}) G_{3;x_1} \\ &= Z_2^T F_{\mu;x_1} + Z_2^T F_{\mu;x_2} G_{2;x_1} = -Z_2^T N_\mu [I_n\ 0\ \cdots\ 0]^T \begin{bmatrix} I \\ G_{2;x_1} \end{bmatrix} \equiv 0 \end{aligned}$$

on $\mathbb{U}$. Following Hypothesis 3.2, we therefore can choose

$$T_2(t,x_1) = \begin{bmatrix} I \\ \hat{G}_{2;x_1}(t,x_1) \end{bmatrix} \tag{19}$$

and hence Z_1 as a function in $(t,x,\dot{x})$.

Finally setting

$$\hat{F}_1 = Z_1^T F, \tag{20}$$

we now know that $(t_0, x_{10}, x_{20}, \dot{x}_{10}, \dot{x}_{20})$ as part of y_0 solves the system

$$\hat{F}_1(t,x_1,x_2,\dot{x}_1,\dot{x}_2) = 0, \quad x_2 = \hat{G}_2(t,x_1). \tag{21}$$

Writing this in short form as

$$\hat{F}(t,x,\dot{x}) = 0, \tag{22}$$

we have for all $(t,x,\dot{x})$ satisfying $F(t,x,\dot{x}) = 0$ that

$$\hat{F}_{\dot{x}}(t,x,\dot{x}) = \begin{bmatrix} Z_1^T F_{\dot{x}_1}(t,x_1,x_2,\dot{x}_1,\dot{x}_2) & Z_1^T F_{\dot{x}_2}(t,x_1,x_2,\dot{x}_1,\dot{x}_2) \\ 0 & 0 \end{bmatrix}$$

and

$$\hat{F}_x(t,x,\dot{x}) = \begin{bmatrix} * & * \\ \hat{G}_{2;x_1}(t,x_1) & -I \end{bmatrix}.$$

Because of

$$\operatorname{rank} \begin{bmatrix} Z_1^T F_{\dot{x}_1} & Z_1^T F_{\dot{x}_2} \\ \hat{G}_{2;x_1}(t,x_1) & -I \end{bmatrix} = \operatorname{rank} \begin{bmatrix} Z_1^T F_{\dot{x}} T_2 & 0 \\ \hat{G}_{2;x_1}(t,x_1) & -I \end{bmatrix} = n$$

by Hypothesis 3.2, the DAE (22) has vanishing s-index (or differentiation index at most one).

Differentiating the second equation in (21) and inserting into the first equation, we can then locally solve for $\dot{x}_1$. Finally eliminating x_2 from this new equation, we obtain a system of the form

$$\dot{x}_1 = \hat{G}_1(t,x_1), \quad x_2 = \hat{G}_2(t,x_1). \tag{23}$$

In summary, we have shown that the first part of each $y_0 \in \mathbb{L}$ solves an equation of the form (23). Therefore, given a sufficiently smooth solution x^* of a DAE (1) satisfying Hypothesis 3.2, x^* locally also solves a DAE of the form (23). But the latter DAE now has the desired regularity property. In particular, (23) is a well-posed problem in the following sense (we again assume without loss of generality that we have a homogeneous initial condition).

THEOREM 3.7. *Let a sufficiently smooth solution $x^* \in \mathbb{D}$ of*

$$F(t,x,\dot{x}) = 0, \quad x(t_0) = 0, \tag{24}$$

be given, where F satisfies Hypothesis 3.2, and let $\bar{F}\colon \mathbb{D} \to \mathbb{Y}$, $\mathbb{D} \subseteq \mathbb{X}$ open, be defined by

$$\bar{F}(x)(t) = \begin{bmatrix} \dot{x}_1(t) - \hat{G}_1(t,x_1(t)) \\ x_2(t) - \hat{G}_2(t,x_1(t)) \end{bmatrix} \tag{25}$$

with

$$\mathbb{X} = \{x \in C(\mathbb{I}, \mathbb{R}^n) \mid x_1 \in C^1(\mathbb{I}, \mathbb{R}^d),\ x_1(t_0) = 0\}, \quad \mathbb{Y} = C(\mathbb{I}, \mathbb{R}^n), \tag{26}$$

according to the construction given above. Then there is a neighborhood of $0 \in \mathbb{Y}$ *such that the (strangeness-free) problem*

$$\bar{F}(x) = \delta \tag{27}$$

has a unique solution $x \in \mathbb{D}$ *for every* δ *in this neighborhood. The solution* x *depends continuously on* δ *and* x^* *is the unique solution belonging to* $\delta = 0$.

Proof. The Fréchet derivative $\bar{F}_x(x)\colon \mathbb{X} \to \mathbb{Y}$ of $\bar{F}$ at some $x \in \mathbb{D}$ given by

$$\begin{aligned} \bar{F}_x(x)(\Delta x)(t) &= \begin{bmatrix} \Delta\dot{x}_1(t) - \hat{G}_{1;x_1}(t, x_1(t))\Delta x_1(t) \\ \Delta x_2(t) - \hat{G}_{2;x_1}(t, x_1(t))\Delta x_1(t) \end{bmatrix} \\ &= \begin{bmatrix} I_d & 0 \\ 0 & 0 \end{bmatrix} \Delta\dot{x}(t) - \begin{bmatrix} \hat{G}_{1;x_1}(t, x_1(t)) & 0 \\ \hat{G}_{2;x_1}(t, x_1(t)) & -I_a \end{bmatrix} \Delta x(t) \end{aligned} \tag{28}$$

is a linear homeomorphism according to Section 2. The claim then follows by the implicit function theorem in Banach space or, more constructive, by means of Newton's method in Banach space, see, e. g., [6, Theorems 15.2 and 15.6]. □

4. Numerical methods. The numerical treatment of initial value problems for DAEs mainly consists of two parts. First, the consistency of the given initial value must be checked. If consistency does not hold, a consistent initial value must be computed. Second, starting from a consistent initial value we must stepwise integrate the DAE.

In Section 3, it has been shown that each $y_0 \in \mathbb{L}$ can be locally extended to a solution of (1). Thus, consistency of an initial value x_0 at t_0 means that (t_0, x_0) is part of some $y_0 \in \mathbb{L}$. To determine a consistent initial value or to check it for consistency, we must therefore solve

$$F_\mu(t_0, x, \dot{x}, \ldots, x^{(\mu+1)}) = 0. \tag{29}$$

for $(x, \dot{x}, \ldots, x^{(\mu+1)})$. By Hypothesis 3.2, the Jacobian of this underdetermined system of nonlinear equations has full row rank at every solution. Thus, the Gauß-Newton method will converge locally and quadratically (see, e. g., [16]). This remains valid when we do not allow t_0 to change during the iteration. Following Section 3, there are d additional values from x_0 that can be kept fixed. For ODEs $\dot{x} = f(t, x)$, this corresponds to the procedure to choose $y_0 = (t_0, x_0, \dot{x}_0) \in \mathbb{L}$ by taking (t_0, x_0) from the initial condition and computing $\dot{x}_0$ by $\dot{x}_0 = f(t_0, x_0)$. Of course, this approach is preferable to that of simply solving the underdetermined problem $\dot{x} - f(t, x) = 0$ which may also alter x_0.

Denoting by $\tilde{T}_2$ some fixed approximation (with orthonormal columns) to T_2 at the desired solution, the method of choice here is to solve

$$F_\mu(t_0, \tilde{T}_2\tilde{T}_2^T x_0 + (I - \tilde{T}_2\tilde{T}_2^T)x, \dot{x}, \ldots, x^{(\mu+1)}) = 0 \tag{30}$$

for $(x, \dot{x}, \ldots, x^{(\mu+1)})$. Since $\tilde{T}_2\tilde{T}_2^T$ is an orthogonal projector of rank d, (30) applied to ODEs becomes $\dot{x} - f(t_0, x_0) = 0$ which does not depend on x. Hence, the Gauß-Newton method will never change the corresponding starting value and we indeed obtain the preferred value $y_0 = (t_0, x_0, f(t_0, x_0)) \in \mathbb{L}$. For a bad initial guess of a

consistent initial value, it may not be possible to choose a good estimate for $\tilde{T}_2$ of T_2. In this case, it makes no sense to replace (29) by (30) for the determination of a consistent initial value.

THEOREM 4.1. *Let F of (1) satisfy Hypothesis 3.2. Then the Jacobian J of (30) at a solution $(x, \dot{x}, \ldots, x^{(\mu+1)})$ has full row rank provided $\tilde{T}_2$ is a sufficiently good approximation to T_2 corresponding to this solution.*

Proof. We have (without arguments)

$$J = [-N_\mu [I_n \; 0 \; \cdots \; 0]^T (I - \tilde{T}_2 \tilde{T}_2^T) \mid M_\mu].$$

By Hypothesis 3.2, it follows

$$\operatorname{rank} J = (\mu+1)n - a + \operatorname{rank}[\hat{A}_2 (I - \tilde{T}_2 \tilde{T}_2^T)].$$

For $\tilde{T}_2 = T_2$, this reduces to

$$\operatorname{rank} J = (\mu+1)n - a + \operatorname{rank} \hat{A}_2 = (\mu+1)n,$$

such that $\tilde{T}_2$ must approximate T_2 in such a way that $\hat{A}_2 (I - \tilde{T}_2 \tilde{T}_2^T)$ keeps full rank. □

To integrate the DAE (1) numerically, we must discretize it. For simplicity, we concentrate here on BDF methods. It is well-known that these are suited for the numerical solution of general nonlinear DAEs with differentiation index at most one, see, e. g., [1]. For DAEs with higher index, BDF directly applied to (1) may give wrong results or may not define a numerical solution at all. In the following, let D_h denote the backward difference operator which is of the form

$$D_h x_i = \frac{1}{h} \sum_{l=0}^{k} \alpha_l x_{i-l} \tag{31}$$

where h is the stepsize, x_i denote numerical approximations to $x(t_i)$ with $t_i = t_0 + ih$, and α_l are the coefficients of the k-step BDF method. The only property of D_h we need is that it is linear with respect to the actual approximation x_i with nonzero derivative α_0/h.

Our method of choice to proceed from t_0 to $t_0 + h$ then is to solve

$$\begin{array}{ll} \text{(a)} & F_\mu(t_0 + h, x, \dot{x}, \ldots, x^{(\mu+1)}) = 0, \\ \text{(b)} & \tilde{Z}_1^T F(t_0 + h, x, D_h x) = 0 \end{array} \tag{32}$$

for $(x, \dot{x}, \ldots, x^{(\mu+1)})$ and to take the part x as approximation x_1 to $x(t_1)$. Here $\tilde{Z}_1$ denotes some fixed approximation (with orthonormal columns) to Z_1 at the desired solution.

According to the considerations of Section 3, system (32) can be interpreted as follows. The first part (32.a) yields a solution for which $x_2 = \hat{G}_2(t_0 + h, x_1)$ holds. For a sufficiently good approximation $\tilde{Z}_1$, the same arguments (see also the proof of the following theorem) as for (21) show that

$$\tilde{Z}_1^T F(t, x_1, x_2, \dot{x}_1, \dot{x}_2) = 0, \quad x_2 = \hat{G}_2(t, x_1) \tag{33}$$

has differentiation index at most one and therefore has a unique solution $x = (x_1, x_2)$ at $t_0 + h$ not depending on the specific choice of $\tilde{Z}_1$. In particular, we can apply BDF

to solve it numerically. But discretizing (33) by BDF is nothing else than imposing (32) which together with $x_2 = \hat{G}_2(t_0 + h, x_1)$ implies

$$\tilde{Z}_1^T F(t, x_1, x_2, D_h x_1, D_h x_2) = 0, \quad x_2 = \hat{G}_2(t, x_1).$$

In contrast to $\tilde{T}_2$ above, the choice of $\tilde{Z}_1$ is not problematic because we can here reduce the stepsize in critical situations. Due to the smoothness of the problem, Z_1 at the last accepted solution point for example will become a better and better guess for Z_1 at the new point which is to be computed.

To solve (32) numerically, an important property is again full row rank of the associate Jacobian. Recall that we keep $\tilde{Z}_1$ fixed during an integration step.

THEOREM 4.2. *Let F of (1) satisfy Hypothesis 3.2. Then the Jacobian J of (32) at a solution $(x, \dot{x}, \ldots, x^{(\mu+1)})$ has full row rank for sufficiently small h provided $\tilde{Z}_1$ is a sufficiently good approximation to Z_1 corresponding to this solution.*

Proof. We have (without arguments)

$$J = \left[\begin{array}{c|c} -N_\mu [I_n\ 0\ \cdots\ 0]^T & M_\mu \\ \hline \tilde{Z}_1^T (\frac{\alpha_0}{h} F_{\dot{x}} + F_x) & 0 \end{array}\right].$$

By Hypothesis 3.2, it follows

$$\operatorname{rank} J = (\mu+1)n - a + \operatorname{rank} \left[\begin{array}{c} \hat{A}_2 \\ \hline \tilde{Z}_1^T (\frac{\alpha_0}{h} F_{\dot{x}} + F_x) \end{array}\right] = (\mu+1)n + \operatorname{rank}[\tilde{Z}_1^T (\tfrac{\alpha_0}{h} F_{\dot{x}} + F_x) T_2].$$

For sufficiently small h, we then obtain

$$\operatorname{rank} J = (\mu + 1)n + \operatorname{rank}[\tilde{Z}_1^T F_{\dot{x}} T_2].$$

For $\tilde{Z}_1 = Z_1$, this reduces to

$$\operatorname{rank} J = (\mu + 1)n + d$$

such that $\tilde{Z}_1$ must approximate Z_1 in such a way that $\tilde{Z}_1^T F_{\dot{x}} T_2$ keeps full rank. □

REMARK 4.3. The approach developed here consists of first discretizing the nonlinear DAE and then solving the nonlinear discrete problem by linearization (Newton's method). For the BDF discretization, however, one can show that linearization and discretization commute, i. e., that we obtain the same method when we first linearize (linearization in function spaces is sometimes called quasi-linearization) and then discretize by BDF.

REMARK 4.4. Solving underdetermined nonlinear systems of equations by the Gauß-Newton method, the most important property one has to look for, is full row rank at the desired solutions. This property then not only extends to a neighborhood of the solution set and guarantees local and quadratic convergence to some solution but also allows for some techniques known from Newton's method to improve the efficiency of the method such as simplified Gauß-Newton method (fixing the Jacobian) or Quasi-Gauß-Newton method (Broyden rank one updates of the Jacobian), see, e. g., [16].

REMARK 4.5. If it is known that Z_2 of Hypothesis 3.2 only depends on t, then one can choose $\tilde{Z}_2 = Z_2$ and system (32) can be reduced to

$$\begin{array}{ll} \text{(a)} & Z_2^T F_\mu(t_0 + h, x, \dot{x}, \ldots, x^{(\mu+1)}) = 0, \\ \text{(b)} & \tilde{Z}_1^T F(t_0 + h, x, D_h x) = 0. \end{array} \tag{34}$$

Due to Hypothesis 3.2, the dependence of (34.a) on $(\dot{x}, \ldots, x^{(\mu+1)})$ can be neglected such that (34) represents a system which only depends on x. In particular, this simplification applies to ODEs where Z_2 is an empty matrix and $\tilde{Z}_1 = I_n$ such that (34) becomes the standard BDF method applied to the ODE. Moreover, it applies to linear DAEs where (34) becomes nothing else than (6) such that we have rediscovered the techniques of [13, 14] for linear problems with unique solution.

Note that already for the determination of consistent initial values, we must know at least the value of μ. In the linear case, it can be computed even when we have no consistent value because the linearization here does not depend on the trajectory along which we linearize. But in the nonlinear case we must take into consideration that we can compute μ (as well as a and d) only when we already have a consistent value due to possibly different ranks of the quantities in Hypothesis 3.2 away from the manifold $\mathbb{L}$. In case the values of μ, a, and d are not known in advance the only possibility is to try to fix them during the determination of a consistent initial value. One may proceed as follows. Set $\mu = 0$, $a = 0$, and $d = n - a$. In each iteration step for solving (29) or (30), perform the numerical rank checks

$$\begin{array}{ll} \text{(a)} & \operatorname{corank} M_\mu \leq a\,, \\ \text{(b)} & \operatorname{rank} \tilde{Z}_2^T N_\mu = a\,, \\ \text{(c)} & \operatorname{rank} F_{\dot{x}} \tilde{T}_2 = d\,, \end{array} \tag{35}$$

say by singular value decompositions. Here $\tilde{Z}_2$ denotes a matrix whose orthonormal columns span the corange of M_μ perturbed to a matrix of corank a and $\tilde{T}_2$ denotes a matrix whose orthonormal columns span the kernel of $\tilde{Z}_2^T N_\mu$ perturbed to a matrix of rank a. These perturbations can easily be obtained from the singular value decompositions by neglecting the superfluous nonzero singular values, i. e., expecting a certain rank r proposed by the current setting of a and d according to (35), we simply set the $(r+1)$-st and all following singular values to zero. This corresponds to replacing the given matrix by the in some sense nearest matrix of the required (lower) rank. A violation of the numerical rank check in (35.a) then indicates that there may be additional constraints and a should be increased by one (and d decreased by one), a violation of the numerical rank check in (35.b) indicates that local uniqueness may not hold for the given problem and one should terminate, and a violation of the numerical rank check in (35.c) indicates that one is near a higher index problem and μ should be increased by one. The determination of the characteristic values μ, a, and d is successful if the iteration methods ends with accepting a consistent initial value under the rank checks (35). Note, however, that this procedure may not work if the given problem is not well scaled or the initial guess is too poor. But this seems to be a common observation in dealing with challenging nonlinear problems.

5. Numerical examples. We have implemented the techniques introduced in Section 4 in a `FORTRAN` subroutine on a fixed stepsize fixed order basis. Additionally to the subroutine evaluating F and its derivatives with respect to t together with their Jacobians, the program uses the input parameters given in Table 5.1. The matrices $\tilde{T}_2$ and $\tilde{Z}_1$ are determined according to the definition of T_2 and Z_1 in Hypothesis 3.2 at which all matrix functions are evaluated at the current guess for the unknowns and all intermediate matrices are perturbed to the nearest (with respect to the spectral norm) matrix of the rank we expect at the solution.

Note that this code is on the level of a research implementation. We therefore give no comparisons even when the specific problem is of a form that can be treated by a

TABLE 5.1
Input parameters

t_0	initial time
$\tilde{z}_0$	initial guess for $(x_0, \dot{x}_0, \ldots, x^{(\mu+1)})$
μ, d, a	characteristic values due to Hypothesis 3.2
h	stepsize
N	number of steps to be performed
$k_{\max}$	maximal order of BDF to be used
m	mode parameter $m = 0$: linear problem (use system (34) and perform only one Gauß-Newton step) $m = 1$: special nonlinear problem (use system (34) according to Remark 4.5) $m = 2$: general nonlinear problem (use system (32))

TABLE 5.2
Rank checks during the determination of the characteristic values for Example 5.1

trial	characteristic values	violated rank check
1	$\mu = 0$, $d = 2$, $a = 0$	(35.a)
2	$\mu = 0$, $d = 1$, $a = 1$	(35.c)
3	$\mu = 1$, $d = 1$, $a = 1$	(35.a)
4	$\mu = 1$, $d = 0$, $a = 2$	none

different code. We should emphasize that currently there are no production codes for general nonlinear DAEs with arbitrary index available to compare with. A production code on the basis of the research code discussed here is under development. Because we get back the techniques of [13] for linear problems (i. e., for mode parameter $m = 0$) and those for the well-known code `DASSL` (see, e. g., [1]) for strangeness-free problems (i. e., for s-index $\mu = 0$), we concentrate here on results for nonlinear problems with $\mu \geq 1$. All computations were performed on an HP715/33 workstation in `FORTRAN` double precision.

EXAMPLE 5.1. We first consider the problem of Example 3.1 with inhomogeneity in the form

$$\begin{bmatrix} 1 & 0 \\ \dot{x}_1 & 1 \end{bmatrix} \begin{bmatrix} \dot{x}_2 - x_1 - e^{t-1} \\ x_2 - t \end{bmatrix} = 0.$$

Working in mode $m = 2$, we took the initial guess $\tilde{z}_0 = (1, 0, 0, 1, 0, 0)$ for $t_0 = 0$. The determination of the correct characteristic values μ, d, and a by the procedure described at the end of Section 4 brought a sequence of rank checks given in Table 5.2.

For $N = 100$, $h = 0.01$, and $k_{\max} = 1$, the solution $x(1) = (0, 1)$ was reproduced without difficulty. The computing time was 0.53 seconds.

EXAMPLE 5.2. A model of a ring modulator is described in [9]. It consists of $n = 15$ differential-algebraic equations. The characteristic values are given by $\mu = 1$, $d = 10$, and $a = 5$. Starting with the initial guess $\tilde{z}_0 = 0$, we obtained after $N = 2000$ steps with $h = 5 \cdot 10^{-7}$ and $k_{\max} = 1$ in mode $m = 1$ a numerical solution whose first component is shown in Figure 5.1 consuming 352 seconds computing time. The

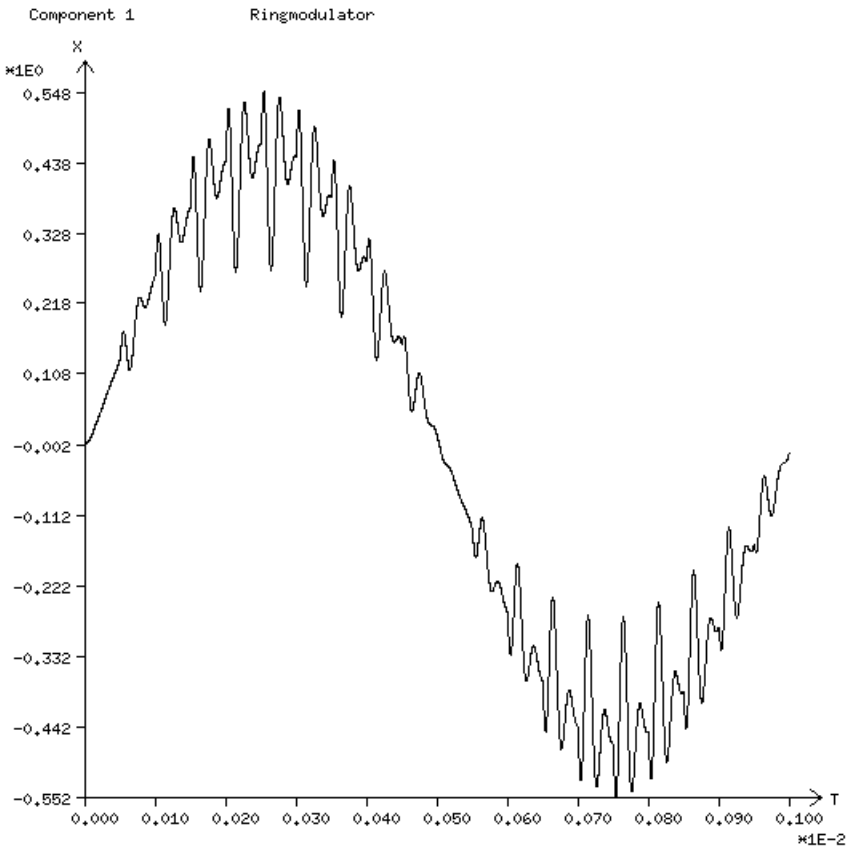

FIG. 5.1. *First solution component of Example 5.2*

computed solution is similar to that given in [9] for a nearby system of differential equations. One easily recognizes in Figure 5.1 the superposition of two oscillations with different amplitudes and frequencies.

It should be mentioned that in this example the arising Jacobians are badly scaled. For the rank decisions, we had to scale first the independent variables to about the same size and then to equilibrate the corresponding Jacobians with respect to the rows.

EXAMPLE 5.3. A planar model of a truck is given in [21]. It is of the standard Euler-Lagrangian form of multibody systems with characteristic values $\mu = 2$, $d = 20$, and $a = 3$. As initial guess for $t_0 = 0$, we took $\tilde{z}_0 = (x_0, 0, 0, 0)$ where x_0 is the consistent initial value given in [21]. The solution given there was reproduced using the parameters $N = 500$, $h = 0.04$, $k_{\max} = 1$, and $m = 2$ within 776 seconds of computing time. Figure 5.2 shows the vertical motion of the driver seat with respect to its equilibrium position when the truck moves along a street which is not completely plain.

EXAMPLE 5.4. The last example is a path prescribed control problem for a two-link planar robot arm taken from [4]. The characteristic values here are $\mu = 4$, $d = 0$,

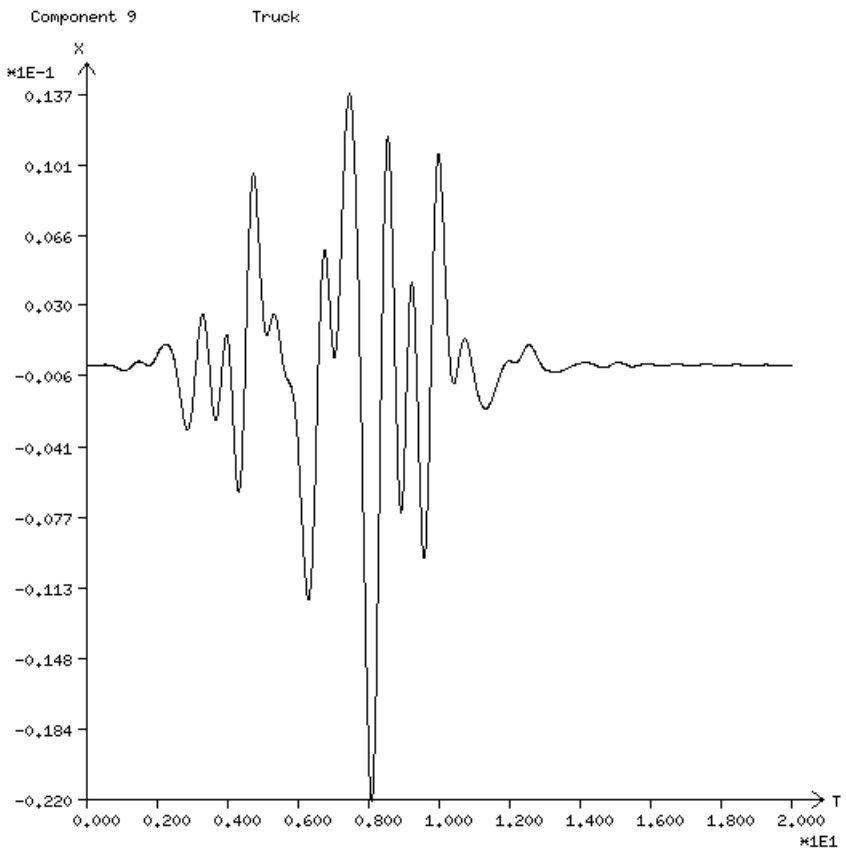

FIG. 5.2. *Vertical motion of the driver seat in the truck model of Example 5.3*

and $a = 8$. Table 5.3 gives a possible sequence of characteristic values tried for $\tilde{z}_0 = 0$ while performing the procedure described at the end of Section 4 to find the correct ones. Note that some of the rank checks indicated a rank deficiency of two which was used to reduce the number of necessary steps.

The computations for $N = 100$, $h = 0.01$, $k_{\max} = 6$, and $m = 2$ needed 103 seconds computing time. Although the given problem has a high strangeness index $\mu = 4$, there were no problems in the necessary rank checks due to well scaled Jacobians.

6. Conclusions. We defined a class of nonlinear DAEs for which we showed existence and uniqueness of solutions. In particular, the definition of this class also included the definition of an index. For this class it is also obvious what should be understood by consistency of initial values. The used techniques were similar to those used for nonlinear problems in finite dimensional spaces, namely to show regularity of the solution in the sense of Newton's method which implies existence and (local) uniqueness. The results obtained in this way were used to design numerical methods for the determination of consistent initial values and the integration of the DAE so that we obtained a procedure for the numerical treatment of nonlinear DAEs with arbitrary index. The numerical examples show that these methods indeed work. A

TABLE 5.3
Rank checks during the determination of the characteristic values for Example 5.4

trial	characteristic values	violated rank check
1	$\mu = 0,\ d = 8,\ a = 0$	(35.a)
2	$\mu = 0,\ d = 6,\ a = 2$	(35.c)
3	$\mu = 1,\ d = 6,\ a = 2$	(35.a)
4	$\mu = 1,\ d = 4,\ a = 4$	(35.c)
5	$\mu = 2,\ d = 4,\ a = 4$	(35.a)
6	$\mu = 2,\ d = 2,\ a = 6$	(35.c)
7	$\mu = 3,\ d = 2,\ a = 6$	(35.a)
8	$\mu = 3,\ d = 1,\ a = 7$	(35.c)
9	$\mu = 4,\ d = 1,\ a = 7$	(35.a)
10	$\mu = 4,\ d = 0,\ a = 8$	none

generalization to DAEs with undetermined solution components as treated in [13, 10] for linear problems seems to be possible and is currently under investigation.

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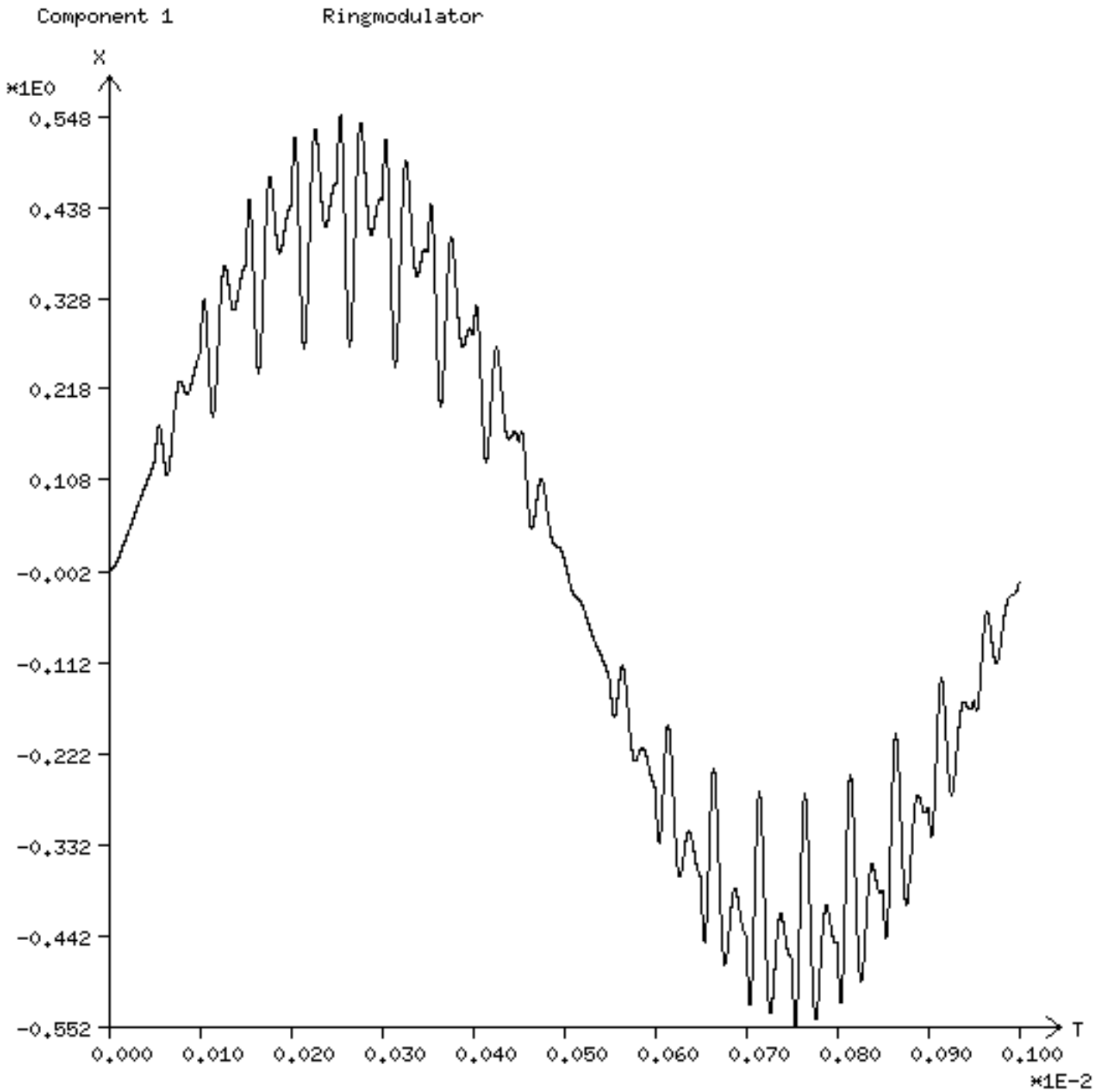
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-0.552
0.000
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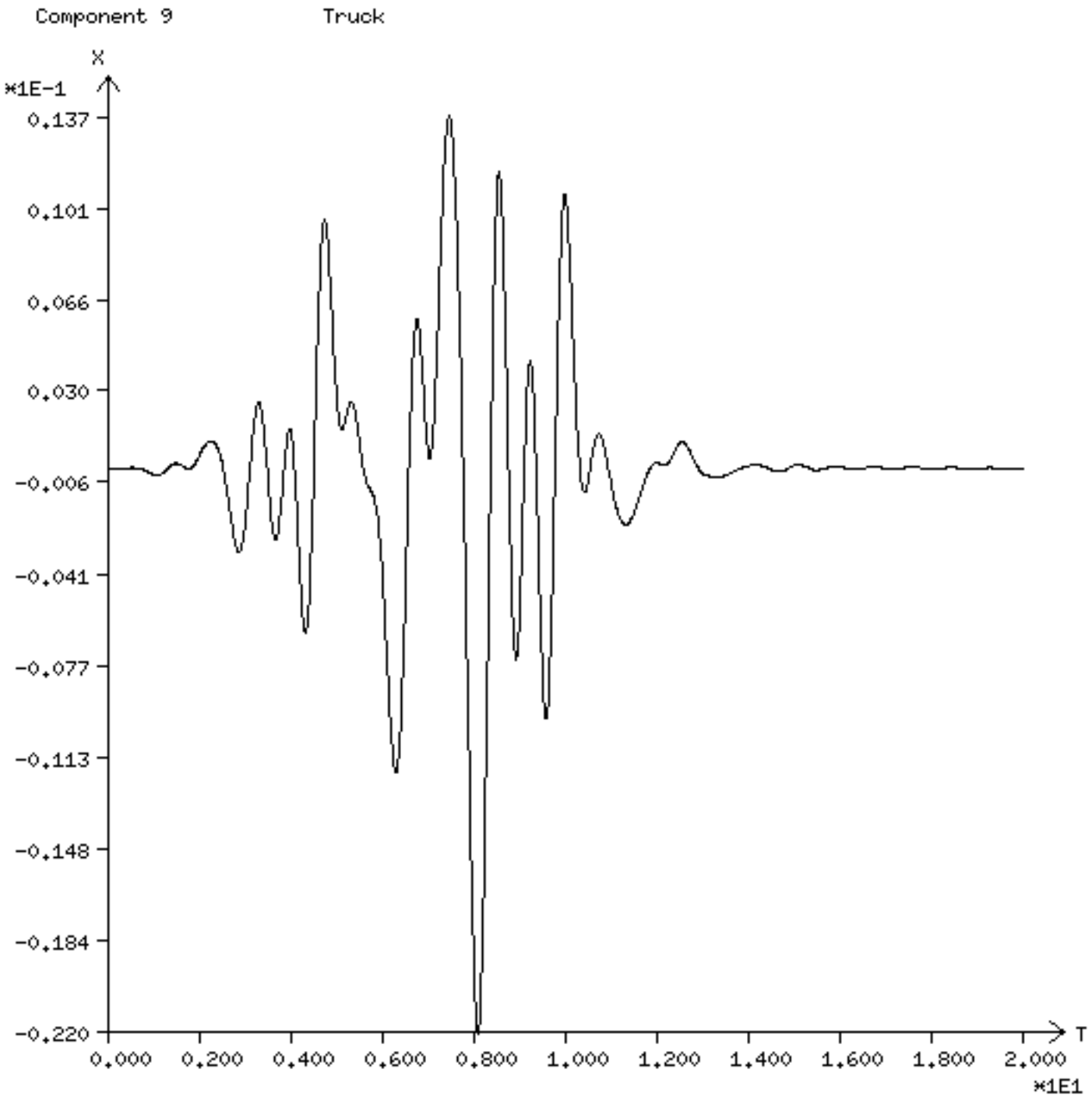
T
*1E-2


Component 9
Truck
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0.000
0.200
0.400
0.600
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1.000
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