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Constraint preserving integrators for general nonlinear higher index DAEs

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Summary. In the last few years there has been considerable research on numerical methods for differential algebraic equations (DAEs) $f(x', x, t) = 0$ where $f_{x'}$ is identically singular. The index provides one measure of the singularity of a DAE. Most of the numerical analysis literature on DAEs to date has dealt with DAEs with indices no larger than three. Even in this case, the systems were often assumed to have a special structure. Recently a numerical method was proposed that could, in principle, be used to integrate general unstructured higher index solvable DAEs. However, that method did not preserve constraints. This paper will discuss a modification of that approach which can be used to design constraint preserving integrators for general nonlinear higher index DAEs.

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1 Introduction

Many physical problems are most easily initially modeled as a nonlinear implicit system of differential and algebraic equations (DAEs),

$$f(x', x, t) = 0 \tag{1}$$

with $f_{x'} = \partial f / \partial x'$ identically singular Brenan et al. (1989). The index ν, which will be defined shortly, is one measure of how singular a DAE is. An ordinary differential equation is index zero, and increasing index implies more complex behavior. Initially most of the numerical work on DAEs assumed that the DAE was index one. Many of the problems in constrained mechanics are initially formulated as index two and three DAEs. However, DAEs of index up to six naturally occur in mechanics if actuator dynamics, joint flexibility, and other effects are included Campbell (1994). Higher index DAEs ($\nu \geq 2$) also occur in several other areas Brenan et al. (1989), Campbell (1994).

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Most of the numerical methods for DAEs require that the systems have special structure, such as being a mechanical system with holonomic constraints Lubich et al. (1993), or have indices of only one or two. A more general approach is introduced in Campbell (1989). However, that approach is explicit and does not preserve constraints. Constraint preservation is important in many applications. In this paper we begin the development of the first approach for the constraint preserving numerical integration of general unstructured higher index DAEs. An alternative approach could probably be developed based on the ideas in Rabier and Rheinboldt (1992). The method developed will preserve both explicit and hidden constraints. In fact, it works equally well if all constraints are implicit. The approach is geared toward the integration of moderate sized nonlinear DAEs with indices of approximately six or less such as typically arise in control and mechanics problems.

We see this approach as being especially useful in the early stages of design and simulation when various computer generated models are being used to investigate system behavior. It will also be useful as a truth model for investigating other integration methods and the validity of various simplified models.

This paper will develop the basic mathematical results needed for the development of our approach. One numerical example will be given. A multistep integrator is being developed within this framework. A description of this algorithm, and the many computational details involved in its implementation are discussed in Moore (1994a), Moore (1994b).

Section 2 will present a few basic ideas about DAEs. This is followed by some comments on constraint preservation in Sect. 3. The general explicit numerical approach is outlined in Sect. 4. In Sect. 4 we also we explain why the obvious approach of projecting back on the manifold does not work in the general nonlinear case. The mathematical justification for an alternative which we call implicit coordinate partitioning is in Sect. 5. A test example is in Sect. 6.

2 Higher index DAEs

Suppose that the DAE (1) is a system of n equations in the $(2n + 1)$-dimensional variable (x', x, t) and that $f_{x'}$ is always singular. We also assume that f is sufficiently differentiable in the variables (x', x, t) so that all needed differentiations can be carried out.

Intuitively the DAE (1) is *solvable* in an open set $\Omega \subseteq \mathbb{R}^{2n+1}$ if the graphs $(x'(t), x(t), t)$ of the solutions x form a smooth $2m + 1$ dimensional manifold in Ω and solutions are uniquely determined by their value x_0 at any t_0 such that $(v_0, x_0, t_0) \in \Omega$. More precise definitions appear in Campbell (1993), Campbell and Gear (1993), Campbell and Griepentrog (1994), Rabier and Rheinboldt (1991), Rabier and Rheinboldt (1992) and their references. Solvable DAEs are also sometimes called regular Reich (1990), Reich (1991).

In general, the solution x of (1) is known to depend on derivatives of f. If (1) is differentiated k times with respect to t, we get the $(k+1)n$ *derivative array equations*, Campbell (1993)

$$(2) \qquad F_k(x', w, x, t) = \begin{bmatrix} f(x', x, t) \\ f_t(x', x, t) + f_x(x', x, t)x' + f_{x'}(x', x, t)x'' \\ \vdots \\ \dfrac{d^k}{dt^k}[f(x', x, t)] \end{bmatrix} = 0$$

where $w = [x^{(2)}, \ldots, x^{(k+1)}]$. The *index* ν of the DAE (1) is often taken to be the least integer k for which (2) uniquely determines x' for consistent (x, t). If such a k exists, then x' is a function of just (x, t) (for consistent (x, t)) so that $v = g(x, t)$. For general unstructured DAEs, the index is actually a somewhat more subtle concept than this definition suggests Campbell and Gear (1993). The index given here is often called the *differentiation index* and denoted ν_{d} when more than one index is being considered.

3 Constraint preservation

BDF methods preserve explicit constraints but are only appropriate for a restricted class of problems. Another way to preserve a constraint is to modify the differential equations so that the constraint is still an invariant but that the dynamics now work to prevent deviation from the constraint. In the context of DAEs the first approach was that of Baumgarte (1972). This approach is often useful, although a general implementation can be difficult Ascher and Petzold (1993), Ascher et al. (1992). However, Baumgarte stabilization requires that the constraint be explicit and that there be a differentiable expression for the constraint. These are not reasonable assumptions in our setting.

Several approaches have been followed with DAEs in order to preserve constraints besides constraint stabilization Gear (1986). One approach, if one knows the solution manifold, is to project back onto the solution manifold during the integration. Shampine discusses one step methods for ODEs and suggests that after each step the numerical solution can be perturbed by the minimum amount needed to satisfy the known constraints, Shampine (1984). The last step is repeated whenever this perturbation is too large. This maintains adequate error control. The projection may be included in the integration method Ascher and Petzold (1991). Alternatively, one can replace the DAE with some type of ODE on a manifold. This can be done either by picking subsets of the current variables Haug and Deyo (1991), Wehage and Haug (1982), or by using some other parameterization Potra (1993), Potra and Yen (1991), Potra and Rheinboldt (1991). For Hamiltonian systems one can define numerical methods, call symplectic integrators, which preserve constraints Reich (1993). In any case most of these approaches have been developed for particular classes of systems and often require the user to be able to determine the index of individual variables. The approach of Rabier and Rheinboldt (1992) could, in principle, also be applied to high index DAEs. A different approach is developed in Barrlund (1989), Barrlund (1991), where one treats the equations (2) as constraints to be imposed and then minimizes the error in the numerical method. This approach requires that there be no undetermined higher derivatives in (2) so that the systems are similar to Hessenberg systems.

4 The general explicit approach

The widespread occurrence of DAEs has lead to an intensive examination of the numerical solution of DAE initial value problems. Several numerical methods have been developed. These methods are discussed in Brenan et al. (1989), Byrne and Schiesser (1991), Hairer et al. (1989), and some of the cited literature. Here we briefly describe a more general approach and explain why the traditional projection approach as described previously does not work. We shall assume that the DAE is in a moderate number of variables and that formulas are known for the equations making up the DAE. The following assumptions on F_k permit a robust numerical least squares solution of the derivative array equations and will be the basis of the methods discussed in this paper.

(A1) Sufficient smoothness of F_k.
(A2) Consistency of $G = F_k = 0$ as an algebraic equation.
(A3) $\bar{J}_k = [\ G_{x'} \quad G_w\ ]$ is 1-full with respect to x' and has constant rank independent of (x', w, x, t).
(A4) $J_k = [\ G_{x'} \quad G_w \quad G_x\ ]$ has full row rank independent of (x', w, x, t).

Here the matrix C of the equation $Cx = b$ is said to be *1-full* with respect to x_1 if there is a nonsingular matrix Q such that

$$QC = \begin{bmatrix} I & 0 \\ 0 & M \end{bmatrix}, \quad x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

Note that (A1)–(A4) are directly in terms of the original equations and their derivatives and do not require any sort of coordinate changes. Also (A3) and (A4) hold in a full neighborhood since $\{x', x, w\}$ are considered to be independent variables. Conditions (A1)–(A4) frequently hold in practice and are numerically verifiable using a combination of symbolic and numeric software Campbell and Griepentrog (1994). They are almost equivalent to a type of uniform solvability Campbell and Gear (1993).

In some of our later developments it will be more convenient to work with the following weaker version of (A3)

(A3') $\bar{J}_k = [\ G_{x'} \quad G_w\ ]$ is 1-full with respect to x' on $G = 0$ and has constant rank independent of (x', w, x, t).

Suppose then that we have the DAE (1) and that Assumptions (A1)–(A4) hold. When solving an equation $G(z) = 0$ we shall use a Gauss-Newton iteration

$$z_{n+1} = z_n - G'(z_n)^{\dagger} G(z_n) \tag{3}$$

Here $B^{\dagger}b$ is the minimum norm least squares solution of $Bq = b$, Campbell and Meyer (1991). In the intialization procedure we fix t and take $z = (x, v, w)$, $G = F_k$ for the DAE (1). Then the Jacobian $G' = J = \left[\ G_{x'} \quad G_w \quad G_x\ \right]$. In the integration procedure we fix (t, x) and take $z = (v, w)$. Then the Jacobian $G' = \bar{J} = \left[\ G_{x'} \quad G_w\ \right]$. Under our assumptions (3) converges to a limit. For the integration procedure this limit satisfies the *least squares equation (LSE)*

$$G'(v^*, w^*)^{\mathrm{T}} G(v^*, w^*) = 0 \tag{4}$$

The LSE is not equivalent to $F_k = 0$ but has additional nonunique solutions. However, v^* depends only on (x, t). Thus $v^* = \bar{h}(x, t)$ defines a smooth *completion*

$$x' = \overline{h}(x, t) \tag{5}$$

This ODE can be integrated by standard ODE integrators provided $\overline{h}$ is smooth enough. A detailed discussion of some of the technical issues with this approach can be found in Campbell (1989), Campbell (1993), Campbell and Moore (1994), Campbell et al. (1994), Campbell and Zhong (1994). The computational effort in carrying out this approach centers on evaluating G, evaluating the Jacobians, and carrying out the linear algebra in the least squares solves.

Since Jacobians similar to J and $\overline{J}$ will be used in the method of Sect. 5, we note that two approaches for computing G and these Jacobians have been investigated Campbell and Moore (1994), Campbell et al. (1994). Even for moderate sized nonlinear DAEs, the use of automatic differentiation reduces the cost of Jacobian evaluation so much that the least squares solution is now the dominate cost.

In attempting to develop a general constraint preserving integrator the obvious first approach, based on the literature cited earlier, would go something as follows. Given a current value of the solution, one predicts by integrating (5). Then one takes the predicted value and projects it back onto the manifold by using some variant of the initilization procedure. This can work for some specific problems Moore (1994b), but there are fundamental problems in the general case. The difficulty is that in solving the least squares equation (4) there are w variables which are less accurate, and in some cases, even arbitrary. In the projection process this lower accuracy in the higher derivative variables is transmitted down to the x variables. This can drastically reduce the accuracy and stability. The difficulty occurs not because the system is a DAE, but rather because of the need to use the least squares projection. We illustrate with a simple example which one should think of as buried inside the solution of some bigger DAE.

Consider the ordinary differential equation $x' + x = 0$. The derivative array equations (2) with $k = 2$ are thus

$$\mathscr{A}\begin{bmatrix} x' \\ x'' \\ x''' \\ x \end{bmatrix} = 0, \quad \mathscr{A} = \begin{bmatrix} 1 & 0 & 0 & 1 \\ 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 \end{bmatrix}$$

Suppose that we have computed values $\widehat{x}^{(i)}$ for $x^{(i)}$ which are $O(h^{k-i})$ accurate. If the projected values are denoted by $\overline{x}^{(i)}$, we get that projecting the vector of $\widehat{x}^{(i)}$ onto the consistent set $\mathscr{A}z = 0$ is given by

$$\begin{bmatrix} \overline{x}' \\ \overline{x}'' \\ \overline{x}''' \\ \overline{x} \end{bmatrix} = \left(I - \mathscr{A}^{\dagger}\mathscr{A}\right)\begin{bmatrix} \widehat{x}' \\ \widehat{x}'' \\ \widehat{x}''' \\ \widehat{x} \end{bmatrix} = \frac{1}{4}\begin{bmatrix} 1 & -1 & 1 & -1 \\ -1 & 1 & -1 & 1 \\ 1 & -1 & 1 & -1 \\ -1 & 1 & -1 & 1 \end{bmatrix}\begin{bmatrix} \widehat{x}' \\ \widehat{x}'' \\ \widehat{x}''' \\ \widehat{x} \end{bmatrix}$$

Then we would have that *all* of the $\overline{x}^{(i)}$ including the new $\overline{x}$ value are only $O(h^{k-3})$ accurate.

5 Implicit coordinate partitioning

This paper emphasizes the theoretical basis for the design of constraint preserving integrators for general nonlinear higher index DAEs. In Moore (1994a) a specific

multistep integrator is developed in detail and extensively tested. In this section we develop the theoretical basis for this method. The next section briefly discusses one test problem from Moore (1994b) to show the viability of the method as presented in this paper.

In order to get around the projection problem described in the previous section we shall use subsets of the state variables to set up a local set of coordinates for the solution manifold. Within this local set of coordinates we will be able to use an explicit integrator in order to stay on the manifold and avoid drift. This is similar in principle to the generalized coordinate partitioning used in mechanics Wehage and Haug (1982). However, a fundamental difference is that in our setting, we do not assume that any of the constraints are known explicitly. Thus the coordinates must be picked in an implicit manner. Also we do not assume that the equations have any specific structure such as being Euler-Lagrange equations.

Our working assumption throughout this section is that (A1)–(A4) hold on a neighborhood of the solution that we are interested in and the DAE is solvable with index ν. Here ν is that value of k for which (A1)–(A4) hold. That is, ν is the *uniform differentiation index* ν_{UD}, Campbell and Gear (1993). For Hessenberg systems, $\nu_{\text{d}} = \nu_{\text{UD}}$, but in general ν_{UD} is the maximum of ν_{d} over a set of perturbations.

We begin by discussing the properties of the partitions that we shall need. The first three results do not directly concern DAEs. $\mathcal{O}$ denotes an open set. If $\mathcal{V}$ is an open set that includes a point v_0 we write $\mathcal{V}(v_0)$. We omit the proofs of special cases such as $k = m_1$ in Lemma 2.

Lemma 1. *Let $f : \mathcal{O} \subset \mathbb{R}^{m_1} \to \mathbb{R}^{m_2}$ be n-times differentiable. Let f' have constant rank $k > 0$ on an open neighborhood $\mathcal{V}(x_0)$. Then there is an open neighborhood $\widehat{\mathcal{V}}(x_0) \subset \mathcal{V}$ and a nonsingular $n-1$ times differentiable function R defined on $\widehat{\mathcal{V}}$ such that*

$$Rf' = \begin{bmatrix} X \\ 0 \end{bmatrix} \tag{6}$$

where X has full row rank k.

Proof. There exist permutation matrices P, Q and a neighborhood $\widehat{\mathcal{V}}$ such that on $\widehat{\mathcal{V}}$ we have

$$Pf'Q = \begin{bmatrix} X_1 & X_2 \\ X_3 & X_4 \end{bmatrix} \tag{7}$$

with X_1 nonsingular and rank $(X_1) = k$. Then

$$R = \begin{bmatrix} I & 0 \\ -X_3X_1^{-1} & I \end{bmatrix} P$$

gives (6) since rank (Rf') = rank $(f') = k$. □

Lemma 2. *Let $f : \mathcal{O}(x_0, y_0) \subset \mathbb{R}^{m_1} \times \mathbb{R}^{m_2} \to \mathbb{R}^{m_3}$ be n-times differentiable. Let f' have constant rank k on an open neighborhood $\mathcal{V}(x_0, y_0) \subset \mathcal{O}$ and assume that $k \geq m_1$. Let $f(x_0, y_0) = b$. Also assume that f' is 1-full with respect to x on $\mathcal{V} \cap f^{-1}(\{b\})$. Then there is an open neighborhood $\widehat{\mathcal{V}}(x_0, y_0) \subset \mathcal{V}$ and a nonsingular $n-1$ times differentiable function R defined on $\widehat{\mathcal{V}}$ and a permutation Q which only permutes y variables such that*

$$Rf'Q = \begin{bmatrix} I & 0 & Z \\ 0 & I & X \\ 0 & 0 & 0 \end{bmatrix} \tag{8}$$

where the first identity matrix is $m_1 \times m_1$ and the second identity matrix is $(k-m_1)\times(k-m_1)$. Furthermore $Z = 0$ on $\widehat{\mathscr{V}} \cap f^{-1}(\{b\})$.

Proof. Assume that $k > m_1$. From Lemma 1 we get that

$$R_1 f'Q = \left[\begin{array}{cc|c} X_1 & X_2 & X_3 \\ X_4 & X_5 & X_6 \\ \hline 0 & 0 & 0 \end{array}\right] \tag{9}$$

where the $(1,1)$ block matrix is nonsingular. The 1-fullness of f' with respect to x means Q does not need to permute the first m_1 columns of f'. Multiplying (9) by the inverse of the (1,1) block we get that

$$R_2R_1f'Q = \begin{bmatrix} I & 0 & \overline{X}_3 \\ 0 & I & \overline{X}_6 \\ 0 & 0 & 0 \end{bmatrix} \tag{10}$$

on $\widehat{\mathscr{V}}$. The 1-fullness of (10) on $\mathscr{V} \cap f^{-1}(\{b\})$ implies that $\overline{X}_3$ is zero on $\widehat{\mathscr{V}} \cap f^{-1}(\{b\})$ and (8) follows. □

Finally we have

Theorem 1. *Let $f : \mathscr{O} \subset \mathbb{R}^{m_1} \times \mathbb{R}^{m_2} \times \mathbb{R}^{m_3} \to \mathbb{R}^{m_4}$ be n-times differentiable with $n \geq 2$ and $m_4 \leq m_1 + m_2 + m_3$. Let $w_0 = (x_0, y_0, z_0) \in \mathscr{O}$ and suppose that*

(i) $f(w_0) = 0$
(ii) $f'(w_0)$ has full row rank.

Furthermore suppose that there is a neighborhood $\mathscr{V}(w_0) \subset \mathscr{O}$ such that

(iii) $\begin{bmatrix} f_x & f_y \end{bmatrix}$ has constant rank k on $\mathscr{V}$
(iv) $\begin{bmatrix} f_x & f_y \end{bmatrix}$ is 1-full with respect to x on $\mathscr{V} \cap f^{-1}(\{0\})$.

Then there are coordinate partitions $y = (\xi, \eta)$ and $z = (u, v)$, and open $\mathscr{N}(w_0) \subset \mathscr{V}$, open $\widehat{\mathscr{N}}(\eta_0, v_0)$, and n-times differentiable functions ϕ_i, $i = 1, 2, 3$, such that

$$\begin{aligned} \mathscr{N} \cap f^{-1}(\{0\}) &= \{(x, y, z)\} = \{(x, [\xi, \eta], [u, v])\} \\ &= \left\{(\phi_1(v), [\phi_2(\eta, v), \eta], [\phi_3(v), v]) : (\eta, v) \in \widehat{\mathscr{N}}\right\} \end{aligned} \tag{11}$$

The partitions may involve permuting components of y and z.

Proof. From (iv) we have that $k \geq m_1$. We shall give the proof for $k > m_1$. The special case $k = m_1$ is similar but (11) is simpler. On the basis of the above assumptions and Lemmas 1 and 2 there is a $n-1$ times differentiable R and appropriate neighborhoods so that on $\widehat{\mathscr{V}} \cap f^{-1}(0)$ we have

$$Rf' = \begin{bmatrix} R_1 \\ R_2 \\ R_3 \end{bmatrix} f' = \begin{bmatrix} I & 0 & X_1 \\ 0 & C & X_2 \\ 0 & 0 & X_3 \end{bmatrix} \tag{12}$$

where the right hand matrix in (12) is partitioned compatible with (x, y, z) and C has full row rank.

Now we can partition $y = (\xi, \eta)$, $z = (u, v)$ so that $\begin{bmatrix} f_x(w_0) & f_\xi(w_0) & f_u(w_0) \end{bmatrix}$ is nonsingular on a neighborhood $\widetilde{\mathscr{T}}(w_0) \subset \mathscr{T}$. Thus by the implicit function theorem there is open $\mathscr{N}(w_0) \subset \mathscr{T}$, open $\widehat{\mathscr{N}}(\eta_0, v_0)$, and n-times differentiable functions ϕ_i such that

$$\begin{aligned} \mathscr{N} \cap f^{-1}(\{0\}) &= \{(x, y, z)\} = \{(x, [\xi, \eta], [u, v])\} \\ &= \left\{(\phi_1(\eta, v), [\phi_2(\eta, v), \eta], [\phi_3(\eta, v), v]) : (\eta, v) \in \widehat{\mathscr{N}}\right\} \end{aligned} \tag{13}$$

That is, we can solve for (x, ξ, u) in terms of (η, v). To prove the theorem we need to show that ϕ_1 and ϕ_3 are independent of η. By definition we have that

$$f(\phi_1, [\phi_2, \eta], [\phi_3, v]) = 0 \tag{14}$$

for η, v in an open set. Differentiating (14) with respect to η, v we get that

$$\begin{bmatrix} f_x & f_\xi & f_\eta & f_u & f_v \end{bmatrix} \begin{bmatrix} (\phi_1)_\eta & (\phi_1)_v \\ (\phi_2)_\eta & (\phi_2)_v \\ I & 0 \\ (\phi_3)_\eta & (\phi_3)_v \\ 0 & I \end{bmatrix} = 0 \tag{15}$$

Note that in (15) that the partials on the left are all evaluated at points where $f = 0$. Thus we can multiply (15) by R and get

$$\begin{bmatrix} I & 0 & 0 & Y_1 & Z_1 \\ 0 & C_1 & C_2 & Y_2 & Z_2 \\ 0 & 0 & 0 & Y_3 & Z_3 \end{bmatrix} \begin{bmatrix} (\phi_1)_\eta & (\phi_1)_v \\ (\phi_2)_\eta & (\phi_2)_v \\ I & 0 \\ (\phi_3)_\eta & (\phi_3)_v \\ 0 & I \end{bmatrix} = 0 \tag{16}$$

where

$$\begin{bmatrix} I & 0 & Y_1 \\ 0 & C_1 & Y_2 \\ 0 & 0 & Y_3 \end{bmatrix} \tag{17}$$

is nonsingular. Multiplying (16) by the inverse of (17) we get that

$$\begin{bmatrix} I & 0 & 0 & 0 & Z_1 \\ 0 & I & \overline{C}_2 & 0 & \overline{Z}_2 \\ 0 & 0 & 0 & I & \overline{Z}_3 \end{bmatrix} \begin{bmatrix} (\phi_1)_\eta & (\phi_1)_v \\ (\phi_2)_\eta & (\phi_2)_v \\ I & 0 \\ (\phi_3)_\eta & (\phi_3)_v \\ 0 & I \end{bmatrix} = 0 \tag{18}$$

from which it follows immediately that $\dfrac{\partial \phi_1}{\partial \eta} = 0$, $\dfrac{\partial \phi_3}{\partial \eta} = 0$, and the proof of Theorem 1 is complete. □

We shall now outline a general strategy for integration. There are numerous algorithmic details and decisions which must be made. These are discussed in Moore (1994a). We shall break our discussion into three parts.

5.1 Basic integration

Let $G = 0$ be the derivative array equations (2). We assume that $[G_{x'}\ G_w\ G_x]$ satisfies (A1)–(A4). Suppose that we have chosen a partition consistent with Theorem 1 where the (x, y, z) of Theorem 1 are now (x', w, x) and $z = [u, v]$ becomes

$$x = (x_1, x_2) \tag{19}$$

For notational convenience we are suppressing the permutation. The variables x_2 of (19) are the v variables of Theorem 1 and will be used to paramaterize the solution manifold locally.

Define the variables $\widetilde{z}, \omega$ by

$$\widetilde{z} = ([x', w], x_1) = (\omega, x_1) \tag{20}$$

Thus $\widetilde{z}$ is everything but x_2 and ω is everything but x. Then $G_{\widetilde{z}}$ is not only 1-full with respect to x' but it is also full row rank by the choice of x_1. Thus $G_{\widetilde{z}}(\widetilde{z}, x_2, t)^{\mathrm{T}} G(\widetilde{z}, x_2, t) = 0$ is equivalent to $G(\widetilde{z}, x_2, t) = 0$. Accordingly, unlike with the explicit integration discussed earlier, we may now use any method of finding $\widetilde{z}$ given (x_2, t) which minimizes $C(\widetilde{z}) = \frac{1}{2} G(\widetilde{z}, x_2, t)^{\mathrm{T}} G(\widetilde{z}, x_2, t)$. We have chosen to use a Gauss-Newton iteration

$$\widetilde{z}^{[m+1]} = \widetilde{z}^{[m]} - \rho_m G_{\widetilde{z}}(\widetilde{z}^{[m]}, x_2, t)^{\dagger} G(\widetilde{z}^{[m]}, x_2, t) \tag{21}$$

Suppose then that we have a point $(\widetilde{z}_0, x_{20}, t_0)$ where $G(\widetilde{z}_0, x_{20}, t_0) = 0$ and our assumptions hold. Then by Theorem 1 there is a partitioning such that $z = (x', [\xi, \eta], [x_1, x_2])$ and open neighborhoods $\widetilde{\mathscr{N}}(\widetilde{z}_0, x_{20}, t_0)$ and $\overline{\mathscr{N}}(\eta_0, x_{20}, t_0)$ such that

$$\widetilde{\mathscr{N}} \cap G^{-1}(\{0\}) = \left\{ \left(\widehat{f}(x_2, t), [g(\eta, x_2, t), \eta], [h(x_2, t), x_2], t \right) : (\eta, x_2, t) \in \overline{\mathscr{N}} \right\} \tag{22}$$

where $\phi_1 = \widehat{f}, \phi_2 = g, \phi_3 = h$. That is,

$$x' = \widehat{f}(x_2, t) \tag{23a}$$

$$\xi = g(\eta, x_2, t) \tag{23b}$$

$$x_1 = h(x_2, t) \tag{23c}$$

Upon partitioning (23a) the same way that x is partitioned and retaining (23c), we get the fundamental equations

$$x_1' = f_1(x_2, t) \tag{24a}$$

$$x_2' = f_2(x_2, t) \tag{24b}$$

$$x_1 = h(x_2, t) \tag{24c}$$

Note that given (x_2, t), the least squares iteration (21) returns the values of f_1, f_2 and h in (24) simultaneously. Also, except for conditioning or round off effects, the

value of f_1, f_2 for a given consistent (x, t) is independent of the choice of acceptable partition since x' is unique. Thus the value of x' varies in a smooth manner. This is not true for h in (24c). It is dependent on the partition.

One step of the integration of the DAE now goes as follows. Given $x_{n-1} = (x_{1,n-1}, x_{2,n-1})$ we apply our multistep integrator to (24a)–(24b) to get $\widehat{x}_n = (\widehat{x}_{1,n}, \widehat{x}_{2,n})$. A final function evaluation gives $x'_n = (x'_{1,n}, x'_{2,n})$ and $\overline{x}_{1,n} = h(\widehat{x}_{2,n}, t_n)$. Then the value for x_n is taken to be $(\overline{x}_{1,n}, \widehat{x}_{2,n})$. Thus x_n lies on the solution manifold and satisfies all constraints.

5.2 The partition

The partition of x can be monitored as the iterations and function evaluations are performed. Suppose that we have $[G_{x'}\ G_w\ G_x]$. Performing a QR only considering the x' and w columns and not permuting between these two sets of columns, but applying Q to the x columns, we get

$$\left[\begin{array}{c|cc|cc} B_1 & C_1 & C_2 & D_1 & D_2 \\ 0 & C_3 & C_4 & D_1 & D_4 \\ 0 & 0 & 0 & D_5 & D_6 \end{array}\right] \tag{25}$$

where B_1, C_3 are nonsingular and $[D_5\ D_6]$ is full row rank. The columns of D_5 correspond to x_1. If D_5 is well conditioned, the current partition of x is kept. But how do we know when to change the partition? Specific strategies and their justification are given in Moore (1994a). Here we discuss some general concerns.

It is important to keep in mind that $[D_5\ D_6]$ is a much smaller matrix than the other matrices that we are working with so that extra computation with it is not very expensive.

Let $\overline{\sigma}(X)$ denote the maximum singular value of a $m \times n$ matrix X with $m < n$. Let $\underline{\sigma}(X)$ be the mth singular value of X in decreasing order. If X is full rank, then this is just the smallest nonzero singular value of X. We would like $\underline{\sigma}(D_5) >> 0$. But in regulating $\underline{\sigma}(D_5)$ we need to know what it is possible to achieve. The following theorem describes what can happen. We have not seen this result elsewhere in the literature so we include a proof.

Theorem 2. *Suppose that B is an $m \times n$ matrix with $m < n$ and rank m.*

(i) Then $\overline{\sigma}(\widehat{B}) \le \overline{\sigma}(B)$ for any $m \times m$ submatrix $\widehat{B}$ of B.
(ii) There exists a $m \times m$ submatrix $\widehat{B}$ of B such that

$$\underline{\sigma}(\widehat{B}) \ge \frac{1}{\sqrt{\binom{n}{m}}}\, \underline{\sigma}(B) \tag{26}$$

Proof. Suppose that B is a $m \times n$ matrix with rank m. Let $\sigma_i(X), \lambda_i(X)$ denote the singular values and the eigenvalues of a matrix X in decreasing and increasing order respectively. To see (i) note that $B = [\widehat{B}\ \overline{B}]P$ were P is a permutation. Then since $\widehat{B}\widehat{B}^{\mathrm{T}}, \overline{B}\,\overline{B}^{\mathrm{T}}$ are both positive semidefinite we have $\overline{\sigma}(B)^2 = \lambda_m(BB^{\mathrm{T}}) = \lambda_m(\widehat{B}\widehat{B}^{\mathrm{T}} + \overline{B}\,\overline{B}^{\mathrm{T}}) \ge \lambda_m(\widehat{B}\widehat{B}^{\mathrm{T}}) = \overline{\sigma}(\widehat{B})^2$.

Proving (ii) is more difficult. If $m < n$, then $\sigma_i(B)^2 = \lambda_{n+1-i}(B^{\mathrm{T}}B)$ for $i = 1, \ldots, m$. In this case, since rank(B) = rank$(B^{\mathrm{T}}B)$, we have $\lambda_1(B^{\mathrm{T}}B) = \cdots = \lambda_{n-m}(B^{\mathrm{T}}B) = 0$.

Let A be an $n \times n$ Hermitian matrix. Let $A_1, \ldots, A_n$ denote the n principle submatrices of A, each obtained by deleting one row and the corresponding column from A. Then from Johnson and Robinson (1981) we have for $1 \leq i \leq n-1$

$$\max_{1 \leq j \leq n} \lambda_i(A_j) \quad \geq \quad \frac{n-i}{n}\lambda_1(A) + \frac{i}{n}\lambda_{i+1}(A). \tag{27}$$

Let B be an $m \times n$ matrix, $m < n$, and let $\widetilde{B}_1, \ldots, \widetilde{B}_n$ denote the n matrices obtained from B by deleting one of its columns. The principle submatrices of $B^{\mathrm{T}}B$ are given by $\widetilde{B}_1^{\mathrm{T}}\widetilde{B}_1, \ldots, \widetilde{B}_n^{\mathrm{T}}\widetilde{B}_n$. In this setting, the inequality (27) becomes for each j

$$\max_{1 \leq j \leq n} \lambda_i(\widetilde{B}_j^{\mathrm{T}}\widetilde{B}_j) \quad \geq \quad \frac{n-i}{n}\lambda_1(B^{\mathrm{T}}B) + \frac{i}{n}\lambda_{i+1}(B^{\mathrm{T}}B) \tag{28}$$

Taking $i = n - m$ in (28), we have that there is a j such that $\widetilde{B}_j$ satisfies (27) without the maximum. Let B_1 be this $\widetilde{B}_j$. Thus

$$\lambda_{n-m}(B_1^{\mathrm{T}}B_1) \quad \geq \quad \frac{m}{n}\lambda_1(B^{\mathrm{T}}B) + \frac{n-m}{n}\lambda_{n-m+1}(B^{\mathrm{T}}B) \tag{29}$$

Since rank$(B^{\mathrm{T}}B) \leq m$ and $B^{\mathrm{T}}B$ is $n \times n$, we have $\lambda_1(B^{\mathrm{T}}B) = \cdots = \lambda_{n-m}(B^{\mathrm{T}}B) = 0$. Therefore, (29) says that

$$\lambda_{n-m}(B_1^{\mathrm{T}}B_1) \quad \geq \quad \frac{n-m}{n}\lambda_{n-m+1}(B^{\mathrm{T}}B). \tag{30}$$

Repeating this process on B_1, let B_2 be the $m \times (n-2)$ matrix formed by discarding one column of B_1 which satisfies

$$\lambda_{n-m-1}(B_2^{\mathrm{T}}B_2) \geq \frac{m}{n-1}\lambda_1(B_1^{\mathrm{T}}B_1) + \frac{n-m-1}{n-1}\lambda_{n-m}(B_1^{\mathrm{T}}B_1). \tag{31}$$

Since rank$(B_1^{\mathrm{T}}B_1) \leq m$ and $B_1^{\mathrm{T}}B_1$ is $(n-1) \times (n-1)$, we have $\lambda_1(B_1^{\mathrm{T}}B_1) = \cdots = \lambda_{n-m-1}(B_1^{\mathrm{T}}B_1) = 0$. Therefore, (31) becomes

$$\lambda_{n-m-1}(B_2^{\mathrm{T}}B_2) \geq \frac{n-m-1}{n-1}\lambda_{n-m}(B_1^{\mathrm{T}}B_1). \tag{32}$$

If we continue in this fashion, at the $(i+1)st$ step we obtain

$$\begin{aligned} \lambda_{n-m-i}(B_{i+1}^{\mathrm{T}}B_{i+1}) \quad &\geq \quad \frac{m}{n-i}\lambda_1(B_i^{\mathrm{T}}B_i) \\ &\quad + \frac{n-m-i}{n-i}\lambda_{n-m-i+1}(B_i^{\mathrm{T}}B_i). \end{aligned} \tag{33}$$

Since rank$(B_i^{\mathrm{T}}B_i) \leq m$ and $B_i^{\mathrm{T}}B_i$ is $(n-i) \times (n-i)$, we have $\lambda_1(B_i^{\mathrm{T}}B_i) = \cdots = \lambda_{n-m-i}(B_i^{\mathrm{T}}B_i) = 0$. Therefore, (33) is

$$\lambda_{n-m-i}(B_{i+1}^{\mathrm{T}}B_{i+1}) \quad \geq \quad \frac{n-m-i}{n-i}\lambda_{n-m-i+1}(B_i^{\mathrm{T}}B_i), \quad 0 \leq i \leq n-m-1 \tag{34}$$

At the $(n-m)th$ step we obtain the inequality

$$\lambda_1(B_{n-m}^{\mathrm{T}} B_{n-m}) \geq \frac{1}{m+1}\lambda_2(B_{n-m-1}^{\mathrm{T}} B_{n-m-1}). \tag{35}$$

Combining the above inequalities (30)–(35), we obtain

$$\begin{aligned}\lambda_1(B_{n-m}^{\mathrm{T}} B_{n-m}) &\geq \frac{1}{m+1}\frac{2}{m+2}\cdots\frac{n-m}{n}\lambda_{n-m+1}(B^{\mathrm{T}}B)\\ &= \frac{1}{\binom{n}{m}}\lambda_{n-m+1}(B^{\mathrm{T}}B).\end{aligned}$$

where B_{n-m} is $m \times m$. Observe that

$$\begin{aligned}\underline{\sigma}(B_{n-m})^2 = \sigma_m(B_{n-m})^2 &= \lambda_1(B_{n-m}^{\mathrm{T}} B_{n-m})\\ &\geq \frac{1}{\binom{n}{m}}\lambda_{n-m+1}(B^{\mathrm{T}}B)\\ &= \frac{1}{\binom{n}{m}}\sigma_m(B)^2 = \frac{1}{\binom{n}{m}}\underline{\sigma}(B)^2\end{aligned}$$

and (26) follows with $\widehat{B} = B_{n-m}$. □

Since $\underline{\sigma}([D_5\ D_6])$ is relatively easy to compute, Theorem 2 gives us an idea of what improvement in $\underline{\sigma}(D_5)$ is possible by changing the partition. In general, we do not change the partition unless D_5 is becoming ill conditioned and a significant improvement in $\underline{\sigma}(D_5)$ is possible.

5.3 The least squares solver

The higher derivative variables w do not explicitly appear in the theoretical formulas (24) for (x, x'). However, the convergence proofs for the iterative solver (21) require that $\widetilde{z}^{[0]}$ be in an appropriate neighborhood of a point $\widetilde{z}_0$ such that $G(\widetilde{z}_0, x_2, t) = 0$. The simplest way to insure convergence of the method is to have at least first order estimates of all derivatives that appear in the derivative array. Provided that our multistep method has order equal to the highest derivative that appears in the derivative array, first order estimates will be readily available, say from the Nordiesk vector.

In the simplified implementation from Moore (1994a) that we shall use in the next section, the basic integrator was a fifth order Adams-Bashford-Moulton method. Thus it provides estimates for up to fifth derivatives and would be suitable for general DAEs of index up to 4. The full implementation in Moore (1994a) is variable order and will accept even higher index problems.

6 A test example

Our test example is designed so that all constraints are implicit. We begin with the DAE

$$x_1' = u_1 \tag{36a}$$

(36b) $$x_2' = u_2$$

(36c) $$x_3' = u_3$$

(36d) $$u_1' = u_3\cos(t) - x_3\sin(t) - u_2 + 2x_1[1 - r(x_1^2 + x_2^2)^{-1/2}]\lambda$$

(36e) $$u_2' = u_3\sin(t) + x_3\cos(t) + u_1 + 2x_2[1 - r(x_1^2 + x_2^2)^{-1/2}]\lambda$$

(36f) $$u_3' = -x_3 + 2x_3\lambda$$

(36g) $$0 = x_1^2 + x_2^2 + x_3^2 - 2r(x_1^2 + x_2^2)^{1/2} + r^2 - \rho^2$$

Here $r > \rho$ are positive parameters. This is an index 3 DAE in the seven state variables $\{x_1, x_2, x_3, u_1, u_2, u_3, \lambda\}$. The solution manifold is four dimensional. In our tests we take $\rho = 5,\ r = 10$. The solution we will be computing is given by

(37a) $$x_1 = [\rho\cos(2\pi - t) + r]\cos t$$

(37b) $$x_2 = [\rho\cos(2\pi - t) + r]\sin t$$

(37c) $$x_3 = \rho\sin(2\pi - t)$$

which lies on a torus.

Given the DAE $f(x', x, t) = 0$ defined by (36) we shall take a function Φ from $\mathbb{R}^7$ into $\mathbb{R}^7$ such that $\Phi(0) = 0$, and consider the DAE

(38) $$\Phi(f(x', x, t)) = 0$$

With suitably chosen Φ this will create a DAE with all of its constraints fully implicit and without any of the recognized structures. Intuitively this corresponds to choosing a different nonlinear coordinate system for the range of f. Such a transformation will not alter our working assumptions as shown by the next Lemma. It's proof is straightforward and is ommited.

Lemma 3. *Suppose that the DAE* $f(x', x, t) = 0$ *satisfies* (A1)–(A4) *for* $k = \nu$ *and is uniformly solvable. Let* Φ *be a function such that* $\Phi(0) = 0$, Φ *is a least* n *times differentiable, and* $\Phi'(0)$ *is nonsingular. Then the DAE* $\Phi(f(x', x, t)) = 0$ *also satisfies* (A1)–(A4).

The Φ we shall use is defined by $\Phi = [\Phi_1, \ldots, \Phi_s]^{\mathrm{T}}$ where for a vector $y = [y_1, \ldots, y_n]^{\mathrm{T}}$,

(39) $$\Phi_i(y) = \left(\sum_{j=1}^{i}(y_j - \alpha)^2\right) - i\alpha^2$$

6.1 Numerical results

We solved the DAE (38) with Φ from (39) and f from (36) on the interval $[0, 5]$ with fixed stepsizes of h = .1, .05, and .01. Three different error criteria ϵ for termination of the Gauss-Newton iteration were used. While the value of ϵ effected the residual in G and the number of iterations performed, it did not, for the values we used, affect the error in the solution. The basic multistep method was a fifth order fixed step Adams-Bashforth-Moulton. Exact initial conditions were used. In general initial conditions can be found by modifications of the initialization procedure. Jacobians were automatically generated as in Campbell and Moore (1994).

Define the local error functions by

$$e_{i,n} = \begin{cases} x_{i,n} - x_i(t_n) & \text{for} \quad i = 1, 2, 3 \\ u_{i-3,n} - u_{i-3}(t_n) & \text{for} \quad i = 4, 5, 6 \\ \lambda_n - \lambda(t_n) & \text{for} \quad i = 7 \end{cases}$$

Table 1 gives the maximum absolute error in all of the state variables. The numbers are consistent with the expected fifth order convergence in all variables.

Table 1. Global errors

	h = .1	h = .05	h = .01
$\max_n \lvert e_{1n}\rvert$	$0.83566D-01$	$0.29705D-03$	$0.17743D-07$
$\max_n \lvert e_{2n}\rvert$	$0.24277D+00$	$0.84379D-03$	$0.51185D-07$
$\max_n \lvert e_{3n}\rvert$	$0.66823D-01$	$0.24762D-03$	$0.15315D-07$
$\max_n \lvert e_{4n}\rvert$	$0.10225D+00$	$0.35684D-03$	$0.21250D-07$
$\max_n \lvert e_{5n}\rvert$	$0.23177D+00$	$0.79445D-03$	$0.47475D-07$
$\max_n \lvert e_{6n}\rvert$	$0.23452D+00$	$0.82335D-03$	$0.49834D-07$
$\max_n \lvert e_{7n}\rvert$	$0.29790D-01$	$0.10072D-03$	$0.60497D-08$

The maximum residuals over the interval are given in Table 2.

Table 2. Residual for different stepsizes and stopping criteria

	$\max_n \lVert G_n\rVert$		
ϵ	h = .1	h = .05	h = .01
$0.10000D-07$	$0.23370D-05$	$0.12732D-05$	$0.10146D-05$
$0.10000D-09$	$0.15205D-07$	$0.12004D-07$	$0.40104D-11$
$0.10000D-11$	$0.13550D-09$	$0.38454D-09$	$0.40104D-11$

As a check on our theory which says that we have no order reduction, we estimated the order of the method by forming the ratio

$$\frac{|x_{N_1} - x(b)|}{|x_{N_2} - x(b)|} \tag{40}$$

where x_{N_1} is an estimate for $x(b)$ and x_{N_2} is another estimate for $x(b)$ computed with half the stepsize. If $|x_n - x(b)|$ satisfies an h^γ error estimate, then one expects (40) to converge to 2^γ. The natural log of the ratio (40) divided by $\ln 2$ was computed for several stepsizes using b = 5. The results are reported in Tables 3 and 4 and are consistent with the method being fifth order in all variables. The last row in Tables 3 and 4 is probably showing the effect of roundoff error.

Table 3. Order estimate for the computed solution of the DAE

h	x_1	x_2	x_3
0.1000000	$0.822D+01$	$0.817D+01$	$0.804D+01$
0.0500000	$0.617D+01$	$0.616D+01$	$0.616D+01$
0.0250000	$0.597D+01$	$0.597D+01$	$0.597D+01$
0.0125000	$0.576D+01$	$0.576D+01$	$0.576D+01$
0.0062500	$0.553D+01$	$0.537D+01$	$0.536D+01$
0.0031250	$0.240D+01$	$0.389D+01$	$0.361D+01$

Table 4. Order estimate for the computed solution of the DAE

h	u_4	u_5	u_6	λ_n
0.1000000	$0.814D+01$	$0.842D+01$	$0.815D+01$	$0.847D+01$
0.0500000	$0.617D+01$	$0.618D+01$	$0.617D+01$	$0.619D+01$
0.0250000	$0.598D+01$	$0.598D+01$	$0.597D+01$	$0.601D+01$
0.0125000	$0.577D+01$	$0.578D+01$	$0.576D+01$	$0.582D+01$
0.0062500	$0.535D+01$	$0.549D+01$	$0.536D+01$	$0.541D+01$
0.0031250	$0.315D+01$	$0.414D+01$	$0.356D+01$	$0.247D+01$

All of these calculations were done on a SUN 470 sparcserver. The CPU times are reported in Table 5. It should be noted that these times are longer than would be expected for a finished code since in this feasibility study we used fixed stepsizes, a modified SVD, and the best choices of some of the stopping criteria is still under investigation. Jacobians were only evaluated and factored once per time step. Table 5 also illustrates the effect that one decision variable, ϵ, can have on CPU time with no change in the accuracy of the solution. Initial studies suggest that the linear algebra in the iteration, especially the least squares solve, can be greatly reduced. This is under investigation. We expect that CPU time can be reduced by a factor of at least three for complex problems Campbell and Zhong (1994). Even so, Table 5 shows that we can integrate a highly nonlinear fully implicit index three DAE in seven state variables for 500 time steps in under 1.5 minutes.

Table 5. CPU times in seconds

ϵ	$h = .1$	$h = .05$	$h = .01$
$0.10000D-07$	12.5	20.7	91.3
$0.10000D-09$	13.3	22.0	98.2
$0.10000D-11$	14.0	22.2	98.5

While we leave a careful discussion to Moore (1994a), it should be noted that in integrating this DAE that the partitioning was changed 4 times during the interval of integration. There was an at least two orders of magnitude improvement in $\underline{\sigma}(D_5)$ each time the partition was reselected.

7 Conclusion

A numerical approach has been described for integrating higher index nonlinear differential algebraic equations. The method preserves all of the constraints defining the solution manifold. The DAEs do not have to have any of the usually assumed

structure, may have all constraints implicit, and can have index greater than three. The only objects that need to be differentiated are the original equations defining the DAE and this may be done either symbolically and converted to FORTRAN code or computed using automatic differentiation.

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