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Efficient integration of strangeness-free non-stiff differential-algebraic equations by half-explicit methods

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ABSTRACT

Numerical integration methods for nonlinear differential-algebraic equations (DAEs) in strangeness-free form are studied. In particular, half-explicit methods based on popular explicit methods like one-leg methods, linear multistep methods, and Runge–Kutta methods are proposed and analyzed. Compared with well-known implicit methods for DAEs, these half-explicit methods demonstrate their efficiency particularly for a special class of semi-linear matrix-valued DAEs which arise in the numerical computation of spectral intervals for DAEs. Numerical experiments illustrate the theoretical results.

1. Introduction

Differential-algebraic equations are an important and convenient modeling concept in many different application areas such as multibody mechanics, circuit design, optimal control, chemical reactions, and fluid dynamics, see [1–7] and the references therein. In this work, we discuss efficient numerical integration methods for initial value problems associated with differential-algebraic equations (DAEs) of the form

$$\begin{aligned} f(t, x(t), \dot{x}(t)) &= 0 \\ g(t, x(t)) &= 0, \end{aligned} \tag{1}$$

on an interval $\mathbb{I} = [t_0, t_f]$, together with an initial condition $x(t_0) = x_0$. Here we assume that $f = f(\cdot,\cdot,\cdot) : \mathbb{I} \times \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}^d$ and $g = g(\cdot,\cdot) : \mathbb{I} \times \mathbb{R}^n \to \mathbb{R}^a$, where $n = d + a$, are sufficiently smooth functions with bounded partial derivatives. Furthermore, we assume that (1) is strangeness-free, see [5, Definition 4.4], which means that the combined Jacobian

$$\begin{bmatrix} f_{\dot{x}}(t, x(t), \dot{x}(t)) \\ g_x(t, x(t)) \end{bmatrix} \tag{2}$$

is nonsingular along the solution $x(t)$.

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Throughout this paper, for the analysis of the numerical method we assume that the initial value problem for (1) has a unique solution $x^*(t)$ which is sufficiently smooth and that the derivatives of x^* are bounded on $\mathbb{I}$. Furthermore, f and g are assumed to be sufficiently smooth with bounded partial derivatives in a neighborhood of $(t, x^*(t))$, $t \in \mathbb{I}$. For the purpose of analysis, due to the assumption (1), the state x in (1) can be reordered and partitioned as $x = [x_1^T, x_2^T]^T$, where $x_1 : \mathbb{I} \to \mathbb{R}^d$, $x_2 : \mathbb{I} \to \mathbb{R}^a$, so that the Jacobian g_{x_2} of g with respect to the variables x_2 (or $f_{\dot{x}_1}$ of f with respect to $\dot{x}_1$) is invertible in the neighborhood of the solution. If g_{x_2} is nonsingular, then it has been shown in [5, Theorem 4.11] that (1) can be locally transformed to a system of the form

$$\dot{x}_1 = \mathcal{L}(t, x_1), \qquad x_2 = \mathcal{R}(t, x_1). \tag{3}$$

Strangeness-free DAEs of the form (1) have differentiation index 1 (see e.g. [1]) and they typically arise from the reduction process described in [5, Section 4.1] applied to general implicit nonlinear DAEs

$$G(t, x, \dot{x}) = 0, \quad t \in \mathbb{I}. \tag{4}$$

Linearizing (1) along x^* yields a linear DAE with coefficient functions

$$E(t) = \begin{bmatrix} E_1(t) \\ 0 \end{bmatrix} = \begin{bmatrix} f_{\dot{x}}(t, x^*, \dot{x}^*) \\ 0 \end{bmatrix}, \qquad A(t) = \begin{bmatrix} A_1(t) \\ A_2(t) \end{bmatrix} = \begin{bmatrix} f_x(t, x^*, \dot{x}^*) \\ g_x(t, x^*) \end{bmatrix}. \tag{5}$$

We will frequently use this linearization in the analysis of the numerical methods presented in this paper, for consistency, stability and convergence, see [8] or [5, Section 5.1] in the DAE framework.

The DAE (1) is more general than DAEs of differentiation index 1 in semi-explicit form, which is the special case that $f_{\dot{x}_1} = I_d$ and $f_{\dot{x}_2} = 0$, since here $\dot{x}_2$ is involved in the differential part, too. However, the algebraic constraint is explicitly given and this fact can be exploited when constructing numerical methods for solving (1). Furthermore, there is an interesting relationship of (1) to semi-explicit DAEs of differentiation index 2, [3]. If x is reordered and partitioned so that $f_{\dot{x}_1}$ is nonsingular, then we may introduce new variables $y_1 = x_1$, $y_2 = x_2$, $z = \dot{x}_2$ and (1) is equivalent to

$$\begin{aligned} 0 &= \phi(t, y(t), z(t), \dot{y}(t)), \\ 0 &= \gamma(t, y(t)), \end{aligned} \tag{6}$$

where

$$\phi(t, y(t), z(t), \dot{y}(t)) = \begin{bmatrix} f(t, y_1(t), y_2(t), \dot{y}_1(t), z(t)) \\ \dot{y}_2(t) - z(t) \end{bmatrix}, \qquad \gamma(t, y(t)) = g(t, y(t)).$$

Condition (2) together with the nonsingularity of $f_{\dot{x}_1}$ implies that $\gamma_y(\phi_y)^{-1}\phi_z(t, y(t), z(t), \dot{y}(t))$ is nonsingular along the solution. Invoking the Implicit Function Theorem, there exists a function φ such that (6) can be rewritten as

$$\begin{aligned} \dot{y}(t) &= \varphi(t, y(t), z(t)), \\ 0 &= \gamma(t, y(t)), \end{aligned} \tag{7}$$

with nonsingular Jacobian $[\gamma_y\varphi_z](t, y(t), z(t))$. In the literature, (7) is called an index-2 DAE in semi-explicit form.

Numerical methods for DAEs of index at most two, including those in semi-explicit form, are analyzed in [1,9,3,4] and several software packages for DAEs are available, see [5, Chapter 8]. In particular, it has been shown, see [5, Chapter 5], that for regular strangeness-free DAEs of the form (1), well-known implicit methods like Runge–Kutta collocation methods and BDF methods are convergent of the same order as for ordinary differential equations (ODEs).

In this paper we study half-explicit methods (HEMs) for strangeness-free DAEs of the form (1). Such methods based on explicit Runge–Kutta methods have been suggested in [10–12,4,13] for the efficient integration of semi-explicit DAEs $\dot{x} = f(t, x, y)$, $0 = g(t, x, y)$ of differentiation index less than or equal to two. One applies an explicit integration scheme to the differential part and an implicit scheme (even simply the implicit Euler scheme) to the algebraic part. In every integration step this combination yields an algebraic system which uniquely determines the numerical solution. In general, the complexity of such methods is smaller than that of fully implicit schemes and the implementation is less complicated as well.

Here we propose and analyze half-explicit methods for the systems of the form (1) for which the convergence analysis has not been discussed yet in the literature.

Our main motivation to study half-explicit methods for problems of the form (1) arises from a special class of semi-linear matrix-valued DAEs of the form

$$\begin{aligned} E_1(t)\dot{X}(t) &= F(t, X(t)), \\ 0 &= A_2(t)X(t), \end{aligned} \tag{8}$$

where $E_1 : \mathbb{I} \to \mathbb{R}^{d\times n}$, $A_2 : \mathbb{I} \to \mathbb{R}^{a\times n}$ are continuous matrix valued functions, and $X : \mathbb{I} \to \mathbb{R}^{n\times \ell}$ $(1 \le \ell \le d)$ and $F : \mathbb{I} \times \mathbb{R}^{n\times\ell} \to \mathbb{R}^{d\times\ell}$ are (nonlinear) matrix-valued functions as well.

Matrix-valued DAEs of the form (8) arise in the stability analysis of DAEs via the numerical approximation of Lyapunov or Sacker–Sell spectral intervals by methods as developed recently in [14,15]. In this application one has to solve strangeness-free DAEs of the form (8), i.e., with nonsingular $\bar{E}(t) = \begin{bmatrix} E_1(t)^T & A_2(t)^T \end{bmatrix}^T$, on a very long interval $[0, t_f]$ with $t_f = O(10^3) - O(10^6)$. Furthermore, the exact solution has to satisfy some orthogonality condition in addition to the algebraic constraint explicitly given in (8), i.e., it is a DAE operating on the set of $n \times \ell$ isometries. In order to approximate the spectral quantities accurately, the numerical solution must satisfy both conditions within machine precision [15].